Lecture 5

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1 Quantum dynamics and time evolution

1.1 Time evolution operator

Over the past two weeks, we have discussed the formalism for the quantum theory in terms of states and observables. However, we have not discussed how such states or observables change with time. Note that unlike position which is promoted in the quantum theory to an operator, time remains a parameter. Nevertheless, we will see that there are several similarities between the way we introduced translation operator which translates states in space and time-evolution operator which translates them in time. We define the time evolution operator $\mathcal{U}(t, t_0)$ as the operator which takes an initial state $|\alpha, t_0\rangle$ at time t_0 to a final state $|\alpha, t_0; t\rangle$ at time t:

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

Similar to our discussion of spatial translation operator, we can deduce some general properties of the time evolution operator that are system- and basis-independent.

First, the time evolution should conserve the probability, which means that it should map normalized states to normalized states. As we have seen before, operators which preserve norm are unitary. Thus, time-evolution needs to be unitary

$$\mathcal{U}(t, t_0)\mathcal{U}^\dagger(t, t_0) = \mathbb{1} \tag{2}$$

The second important property of time-evolution is that we can build time evolution over a long interval by combining time-evolution over shorter intervals. That is, the time evolution operator from t_0 to t is equal to the product of the time evolution operator from t_0 to t_1 and the evolution from t_1 to t. Since the operator on the **right** acts first on the state, this is written as

$$\mathcal{U}(t, t_0) = \mathcal{U}(t, t_1)\mathcal{U}(t_1, t_0), \qquad t_0 < t_1 < t \tag{3}$$

The final property is that time evolution should approach the identity as t approaches t_0

$$\lim_{t \to t_0} \mathcal{U}(t, t_0) = \mathbb{1} \tag{4}$$

Similar to our previous discussion for the translation operator, we can consider infitesmal time evolution $t = t_0 + dt$ and expand $\mathcal{U}$ to first order in dt:

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

The unitarity of $\mathcal{U}$ implies that the generator of time-translation Ω is a Hermitian operator $\Omega^\dagger = \Omega$. The operator Ω has units of frequency or inverse time. Now, recall that one of the very first steps in the development of the quantum theory by Planck and Einstein was to assign to vibrational modes with frequency ω an energy $E = \hbar\omega$. This is similar to the identification of the momentum with the wavevector we discussed in the previous lecture. This means that we can identify the operator $\hbar\Omega$ with the energy operator. Such operator is called the Hamiltonian after the classical Hamiltonian which gives the energy as a functional on configuration space. Substituting in (5), we get

$$\mathcal{U}(t_0+dt,t_0)=\mathbb{1}-i\frac{\mathcal{H}}{\hbar}dt \tag{6}$$

We can now derive one of the most fundamental relations in the quantum theory, which relates the Hamiltonian to the time-evolution operator *for arbitrary time separations* $t-t_0$. Use the relation (3), we write

$$\mathcal{U}(t+dt,t_0)=\mathcal{U}(t+dt,t)\mathcal{U}(t,t_0)=\mathcal{U}(t,t_0)-i\frac{dt}{\hbar}\mathcal{H}\mathcal{U}(t,t_0) \tag{7}$$

which yields

$$i\hbar\frac{\partial}{\partial t}\mathcal{U}(t,t_0)=\mathcal{H}\mathcal{U}(t,t_0) \tag{8}$$

If we act with both sides on an initial state ket $|\alpha,t_0\rangle$ (which is time-independent), we get the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\alpha,t_0;t\rangle=\mathcal{H}\,|\alpha,t_0;t\rangle \tag{9}$$

Note that the Hamiltonian operator itself can depend on time.

We would now like to solve Eq. 8 to write the time evolution operator as a function of the Hamiltonian. It turns out that the solution depends on whether the Hamiltonian depends on time or not. To see this, recall the solution to first order differential equations. For the DE

$$\frac{d}{dt}f(t)=\alpha f(t) \tag{10}$$

the solution is given simply by $f(t)=Ce^{\alpha t}$ where C is determined by the initial conditions $f(0)=f_0$. On the other hand, if α is time-dependent, we write $\frac{df}{f}=\alpha(t)dt$ which is solved by

$$f(t)=Ce^{\int_0^t dt' f(t')} \tag{11}$$

To solve for the time-evolution operator, we do something very similar. To make our notation as simple as possible, we will assume $t_0=0$ and write $\mathcal{U}(t,t_0)=\mathcal{U}(t)$. If $\mathcal{H}$ is time-independent, the solution have exactly the same form as in the scalar case

$$\mathcal{U}(t)=e^{-\frac{i}{\hbar}\mathcal{H}t} \tag{12}$$

We can verify that this is indeed a solution to Eq. 8, by direct substitution and using the series expansion.

$$i\hbar\frac{\partial}{\partial t}\mathcal{U}=i\hbar\frac{\partial}{\partial t}\sum_n\frac{t^n}{n!}\left(\frac{\mathcal{H}}{i\hbar}\right)^n=\mathcal{H}\sum_n\frac{nt^{n-1}}{n!}\left(\frac{\mathcal{H}}{i\hbar}\right)^{n-1}=\mathcal{H}\sum_n\frac{t^{n-1}}{(n-1)!}\left(\frac{\mathcal{H}}{i\hbar}\right)^{n-1}=\mathcal{H}\mathcal{U} \tag{13}$$

Now if $\mathcal{H}$ is time-dependent, we can write an equation similar to (11):

$$\mathcal{U}(t)=e^{-\frac{i}{\hbar}\int_0^t dt'\mathcal{H}(t')} \tag{14}$$

Let us see if this satisfies Eq. 8. We can again use the series expansion of the exponential

$$i\hbar\frac{\partial}{\partial t}\mathcal{U}=i\hbar\frac{\partial}{\partial t}\sum_n\frac{1}{n!}\left(-\frac{i}{\hbar}\right)^n\left(\int_0^t dt'\mathcal{H}(t')\right)^n \tag{15}$$

However, we now encounter a problem. The action of the derivative on an operator to the n-th power $\frac{\partial}{\partial t}A^n$ is *not* equal to $n(\frac{\partial}{\partial t}A)A^{n-1}$ in general. The reason is that the operators A and $(\frac{\partial}{\partial t}A)$ do not necessarily commute. This means that, in general, Eq. 14 does not provide a solution to the time evolution equation.

However, it will be a solution provided that the operators $\int_0^t dt'\mathcal{H}(t')$ and $\frac{\partial}{\partial t}\int_0^t dt'\mathcal{H}(t') = \mathcal{H}(t)$ commute. This is only possible if $\mathcal{H}(t)$ commute at different times, i.e. $[\mathcal{H}(t), \mathcal{H}(t')] = 0$ for all t and t'.

So what happens if $\mathcal{H}(t)$'s at different times do not commute. In this case, the general solution is given by the so-called Dyson series

$$\mathcal{U}(t) = \mathbb{1} + \sum_{n=1}^{\infty}\left(-\frac{i}{\hbar}\right)^n A_n(t,\mathcal{H}), \quad A_n(t,\mathcal{H}) = \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n \mathcal{H}(t_1)\mathcal{H}(t_2)\ldots\mathcal{H}(t_n) \tag{16}$$

Notice that t only enters in the integration limit for the first integral, so that action of the t derivative only pulls out the first $\mathcal{H}$:

$$\frac{\partial}{\partial t}A_n(t) = \mathcal{H}(t)\int_0^t dt_2 \cdots \int_0^{t_{n-1}} dt_n \mathcal{H}(t_2)\ldots\mathcal{H}(t_n) = \mathcal{H}(t)A_{n-1}(t) \tag{17}$$

This is also the reason there is no $n!$ in the denominator. To convince yourself that this expression reduces to Eq. 14 when $\mathcal{H}(t)$'s commute with each other, consider $A_2(t)$ and recall the heaviside theta function

$$\theta(x) = \begin{cases} 1 & : x \geq 0 \\ 0 & : x < 0 \end{cases} \tag{18}$$

Then we can write

$$\begin{aligned} A_2(t) &= \int_0^t dt_1 \int_0^{t_1} dt_2 \mathcal{H}(t_1)\mathcal{H}(t_2) = \int_0^t dt_1 \int_0^t dt_2 \theta(t_1 - t_2)\mathcal{H}(t_1)\mathcal{H}(t_2) \\ &= \frac{1}{2}\int_0^t dt_1 \int_0^t dt_2 \left\{\theta(t_1 - t_2)\mathcal{H}(t_1)\mathcal{H}(t_2) + \theta(t_2 - t_1)\mathcal{H}(t_2)\mathcal{H}(t_1)\right\} \\ &= \frac{1}{2}\int_0^t dt_1 \int_0^t dt_2 \mathcal{H}(t_1)\mathcal{H}(t_2)\left\{\theta(t_1 - t_2) + \theta(t_2 - t_1)\right\} \\ &= \frac{1}{2}\int_0^t dt_1 \int_0^t dt_2 \mathcal{H}(t_1)\mathcal{H}(t_2) = \frac{1}{2}\left(\int_0^t dt_1 \mathcal{H}(t_1)\right)^2 \end{aligned} \tag{19}$$

In the second line, we have added to the integral an identical term by exchanging the dummy variables $t_1 \leftrightarrow t_2$. In the third line, we used the assumption that $[\mathcal{H}(t_1), \mathcal{H}(t_2)] = 0$ and in the fourth lines, we used $\theta(x) + \theta(-x) = 1$. The same analysis can be done for $A_n(t)$ leading to $A_n(t) = \frac{1}{n!}\left(\int_0^t dt_1 \mathcal{H}(t_1)\right)^n$ if $[\mathcal{H}(t), \mathcal{H}(t')] = 0$ for all t, t'.

1.2 Energy eigenkets

While the Dyson series represents the most general case for time-evolution, for most of our applications, we will consider time-independent Hamiltonians where the time-evolution operator has the significantly simpler form (12). For a time-independent Hamiltonian $\mathcal{H}$, we can introduce the energy eigenkets

$$\mathcal{H}|a\rangle = E_a|a\rangle \tag{20}$$

If the eigenvalues are non-degenerate, we have a one-to-one corresponence between the label a and the energy eigenvalues. For the degenerate case, we can follow the same procedure described last lecture where we find a set of operators which commute with the Hamiltonian and use their eigenvalues to label the eigenstates. In the following, I will assume the label a already combines all these eigenvalue labels such that different a's could correspond to the same energy eigenvalue. Energy eigenkets are stationary states for the time evolution since they only change by a phase

$$e^{-\frac{i}{\hbar}\mathcal{H}t}|a\rangle = e^{-\frac{i}{\hbar}E_a t}|a\rangle \tag{21}$$

For a more general state $|u\rangle = \sum_a c_a|a\rangle$, with $c_a = \langle a|u\rangle$, we have

$$e^{-\frac{i}{\hbar}\mathcal{H}t}|u\rangle = \sum_a e^{-\frac{i}{\hbar}\mathcal{H}t}|a\rangle\langle a|u\rangle = \sum_a e^{-\frac{i}{\hbar}E_a t}|a\rangle\langle a|u\rangle = \sum_a c_a(t)|a\rangle, \qquad c_a(t) = c_a e^{-\frac{i}{\hbar}E_a t} \tag{22}$$

Thus, the change of a general state is not just by an overall phase but by the relative phase between the different basis vectors. Changing the relative phase produces physically distinct states. For example, the difference between $|+x\rangle$ and $|+y\rangle$ was in the relative phase between the basis vectors: $|x+\rangle = \frac{1}{\sqrt{2}}(|z+\rangle + |z-\rangle)$ whereas $|x+\rangle = \frac{1}{\sqrt{2}}(|z+\rangle + i|z-\rangle)$. The time-evolution operator can be written in the energy eigenbasis as

$$e^{-\frac{i}{\hbar}\mathcal{H}t} = \sum_a e^{-\frac{i}{\hbar}E_a t}|a\rangle\langle a| \tag{23}$$

A simple example which illustrates the different aspects of the formalism above is that of spin precession. Consider a spin $1/2$ electron under the effect of magnetic field $\boldsymbol{B}$. The Hamiltonian is given by

$$\mathcal{H} = -\gamma \boldsymbol{S}\cdot\boldsymbol{B} \tag{24}$$

where $\gamma = \frac{e}{m}$. If we take $\boldsymbol{B}$ to be in the z-direction, the Hamiltonian takes the form

$$\mathcal{H} = \omega S_z, \qquad \omega = \gamma B = \frac{|e|B}{m} \tag{25}$$

Since $\mathcal{H}$ is proportional to S_z, they commute and the eigenkets of the Hamiltonian are given by $|\pm z\rangle$ which we will denote for simplicity by

$$|+z\rangle := |\uparrow\rangle, \qquad |-z\rangle := |\downarrow\rangle \tag{26}$$

Both $|\uparrow\rangle$ and $|\downarrow\rangle$ are stationary states since

$$e^{-\frac{i}{\hbar}\mathcal{H}t}|\uparrow\rangle = e^{-\frac{i}{2}\omega t}|\uparrow\rangle, \qquad e^{-\frac{i}{\hbar}\mathcal{H}t}|\downarrow\rangle = e^{\frac{i}{2}\omega t}|\downarrow\rangle \tag{27}$$

On the other hand, let us consider the state $|+x\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$. Under time evolution, this state evolves as

$$|+x;t\rangle = e^{-\frac{i}{\hbar}\mathcal{H}t}|+x\rangle = \frac{1}{\sqrt{2}}(e^{-\frac{i}{2}\omega t}|\uparrow\rangle + e^{\frac{i}{2}\omega t}|\downarrow\rangle) \tag{28}$$

This state rotates in the x-y place as can be seen from the fact that the relative phase of the two terms takes arbitrary values. We can see this more directly by computing the expectation values

$$\langle S_x\rangle = \frac{\hbar}{4}((e^{\frac{i}{2}\omega t}\langle\uparrow| + e^{-\frac{i}{2}\omega t}\langle\downarrow|))(|\downarrow\rangle\langle\uparrow| + |\uparrow\rangle\langle\downarrow|)(e^{-\frac{i}{2}\omega t}|\uparrow\rangle + e^{\frac{i}{2}\omega t}|\downarrow\rangle) = \frac{\hbar}{2}\cos\omega t \tag{29}$$

$$\langle S_y\rangle = \frac{i\hbar}{4}((e^{\frac{i}{2}\omega t}\langle\uparrow| + e^{-\frac{i}{2}\omega t}\langle\downarrow|))(|\downarrow\rangle\langle\uparrow| - |\uparrow\rangle\langle\downarrow|)(e^{-\frac{i}{2}\omega t}|\uparrow\rangle + e^{\frac{i}{2}\omega t}|\downarrow\rangle) = \frac{\hbar}{2}\sin\omega t \tag{30}$$

Thus, the spin does precess in the x-y plane with frequency ω.

An important property of time-evolution is that non-stationary states lose their memory of the initial state after a certain characteristic time. This can be seen by considering the overlap between a non-stationary state and its time-evolved version

$$C(t) = \langle u|e^{-\frac{i}{\hbar}\mathcal{H}t}|u\rangle = \sum_a |c_a|^2 e^{-\frac{i}{\hbar}E_a t} \tag{31}$$

Now let us say that the dominant contribution to the sum above comes from a set of eigenkets within a certain energy interval $(E_0 - \Delta E, E_0 + \Delta E)$ such that $|c_a|^2$ is neglegible for E_a outside this range. We can then write

$$C(t) = e^{-\frac{i}{\hbar}E_0 t}\sum_a |c_a|^2 e^{-\frac{i}{\hbar}\Delta E_a t}, \qquad \Delta E_a = E_a - E_0 \tag{32}$$

We notice that for $t \ll \hbar/\Delta E$, the phase factors are all close to one so the sum over a is close to 1 which means that the time-evolved state is close to the initial state. However, once t is comparable to $\hbar/\Delta E$, then the sum above contains many oscillating terms that cancel out leading to a very small value. Thus, after a characteristic time $t \sim \frac{\hbar}{\Delta E}$, a non-stationary state loses its memory about where it started [1]. This is sometimes called energy-time uncertainty principle. However, we should bear in mind that, due to the asymmetry between position (which is an operator) and time (which is a parameter), the energy-time uncertainty does not have the same meaning as the position momentum uncertainty relation which is a precise statement about operator expectation values.

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[1] Note that if the sum over a contains only finitely many terms and the ratio of the oscillating frequencies are all rational, there will be a time where the initial state is recovered. If the ratios are irrational, there will be times where $C(t)$ get very close to 1, corresponding to rational approximants for the different oscillating terms. As the number of terms increase, the recurrence time goes to infinity and the system loses its memory of the initial state