Lecture 8 (Oct. 2, 2017)

8.1 General Time Dependent Hamiltonians

The Schrödinger equation dictates that quantum states evolve in time according to

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = H(t)|\psi(t)\rangle\,. \tag{8.1}$$

In the last class, we saw that if the Hamiltonian is independent of time, $H(t) = H$, then we can solve this differential equation as

$$|\psi(t)\rangle = e^{-iHt/\hbar}|\psi(0)\rangle\,. \tag{8.2}$$

We are now interested in what happens if H has explicit time dependence.

We can always expand an infinitesimal time-evolution operator as

$$U(t+\mathrm{d}t, t) = 1 - \frac{i}{\hbar}H(t)\,\mathrm{d}t + \big((\mathrm{d}t)^2\big)\,. \tag{8.3}$$

From the composition rule for time evolution, we then have

$$\begin{aligned} U(t+\mathrm{d}t, t_0) &= U(t+\mathrm{d}t, t)U(t, t_0) \\ &= \left(1 - \frac{i}{\hbar}H(t)\,\mathrm{d}t\right)U(t, t_0)\,. \end{aligned} \tag{8.4}$$

We can rearrange this to give

$$U(t+\mathrm{d}t, t_0) - U(t, t_0) = -\frac{i}{\hbar}H(t)\,\mathrm{d}tU(t, t_0)\,. \tag{8.5}$$

Dividing both sides by $\mathrm{d}t/i\hbar$ and taking the limit $\mathrm{d}t \to 0$, this becomes

$$i\hbar\frac{\mathrm{d}U(t, t_0)}{\mathrm{d}t} = H(t)U(t, t_0)\,. \tag{8.6}$$

We now discuss solutions to Eq. (8.6) in several cases:

1. If $H(t) = H$, this result reduces to our previous result,

$$U(t, t_0) = e^{-iH(t-t_0)/\hbar}\,. \tag{8.7}$$

2. If $[H(t), H(t')] = 0$ for all t, t', then we can simultaneously diagonalize the Hamiltonian at all times, meaning we can choose a basis of states that are eigenstates of $H(t)$ for all time (the associated eigenvalues may change as a function of time). We then have

$$U(t, t_0) = \exp\left(-\frac{i}{\hbar}\int_{t_0}^{t}\mathrm{d}t'\;H(t')\right). \tag{8.8}$$

We can check that this is the correct expression by going to the diagonal basis of $H(t)$ and considering the action of $U(t, t_0)$ in this basis, or by differentiating the right-hand side to see that it satisfies Eq. (8.6).

3. In the most general case, $[H(t), H(t')] \neq 0$. An example is a spin-$\frac{1}{2}$ particle in a magnetic field that changes orientation as a function of time. What can we say in this case?

   We know that the Hamiltonian completely defines the time evolution for an infinitesimal time step, and we know that we can build up finite time evolution from infinitesimal time evolution using the composition law. We discretize time into N steps,

$$t_0 < t_1 < t_2 < \cdots < t_{N-1} < t\,, \tag{8.9}$$

   with

$$\Delta t = t_{i+1} - t_i = \frac{t - t_0}{N}\,. \tag{8.10}$$

   We could choose each time interval to have a different length, but the ultimate result will not be affected by our choice.

   We take N large, so that Δt is small. Then,

$$U(t_{i+1}, t_i) = 1 - \frac{i}{\hbar} H(t_i)\Delta t + O\big((\Delta t)^2\big)\,. \tag{8.11}$$

   If we are ignoring terms of order $(\Delta t)^2$, then we can write

$$U(t_{i+1}, t_i) \approx e^{-iH(t_i)\Delta t/\hbar}\,. \tag{8.12}$$

   We then build up the finite time-evolution operator as

$$U(t, t_0) = U(t, t_{N-1})U(t_{N-1}, t_{N-2}) \cdots U(t_{i+1}, t_i) \cdots U(t_1, t_0) = \prod_{i=0}^{N-1} U(t_{i+1}, t_i)\,. \tag{8.13}$$

   Note that the ordering of these operators is crucial, because these operators do not commute. We must ensure that the operators are ordered so that later times are to the left. This prescription for ordering of the operators is called *time ordering*, and the right-hand side of Eq. (8.13) is called a *time-ordered product*.

   We want to take the limit $N \to \infty, \Delta t \to 0$ with $N\Delta t$ held fixed. Note that every term in the product Eq. (8.13) is an exponential, and so we may be tempted to write the product as the exponential of a sum of operators. We cannot do this, strictly speaking, because the operators do not commute. However, we can invent notation, and formally write

$$U(t, t_0) = \mathrm{T}\left[\exp\left(-\frac{i}{\hbar}\int_{t_0}^{t} \mathrm{d}t'\; H(t')\right)\right]. \tag{8.14}$$

   This is called a *time-ordered exponential*, and is defined to be the product in Eq. (8.13) in the limit $N \to \infty, \Delta t \to 0$ with $N\Delta t$ held constant. The operator T is called the *time-ordering operator*; it reorders the operators in its argument so that they are time-ordered (disregarding commutation rules when moving the operators around). What guarantees that this limit is well-defined and exists? This is guaranteed because the operator $U(t, t_0)$ is well-defined, and can be written as a composition of infinitesimal time evolution operators for any partition of the time interval $[t_0, t]$.

   An alternate approach is to solve Eq. (8.6) as a formal power series. We can integrate Eq. (8.6) to reach

$$\int_{t_0}^{t} \mathrm{d}t'\; \frac{\mathrm{d}}{\mathrm{d}t}\big(U(t', t_0)\big) = -\frac{i}{\hbar}\int_{t_0}^{t} \mathrm{d}t'\; H(t')U(t', t_0)\,. \tag{8.15}$$

If we carry out the integration on the left-hand side, we find

$$\int_{t_0}^{t} \mathrm{d}t' \, \frac{\mathrm{d}}{\mathrm{d}t}\big(U\big(t',t_0\big)\big) = U(t,t_0) - U(t_0,t_0) = U(t,t_0) - 1\,. \tag{8.16}$$

Subtracting the 1 to the right-hand side of Eq. (8.15), we have

$$U(t,t_0) = 1 - \frac{i}{\hbar}\int_{t_0}^{t} \mathrm{d}t' \, H\big(t'\big)U\big(t',t_0\big)\,. \tag{8.17}$$

This is an expression in terms of the Hamiltonian and time-evolution operator at times t' with $t' \leq t$. We can similarly write

$$U\big(t',t_0\big) = 1 - \frac{i}{\hbar}\int_{t_0}^{t'} \mathrm{d}t'' \, H\big(t''\big)U\big(t'',t_0\big)\,, \tag{8.18}$$

where the integrand is evaluated at values $t'' \leq t'$. We can carry this process out an infinite number of times and compose the results to give

$$\begin{aligned} U(t,t_0) = 1 &- \frac{i}{\hbar}\int_{t_0}^{t} \mathrm{d}t' \, H\big(t'\big) + \left(-\frac{i}{\hbar}\right)^2 \int_{t_0}^{t}\mathrm{d}t' \int_{t_0}^{t'} H\big(t'\big)H\big(t''\big) + \cdots \\ &+ \left(-\frac{i}{\hbar}\right)^n \int_{t_0}^{t}\mathrm{d}t_1 \int_{t_0}^{t_1}\mathrm{d}t_2 \cdots \int_{t_0}^{t_{n-1}} \mathrm{d}t_n \, H(t_1)\cdots H(t_n) + \cdots\,. \end{aligned} \tag{8.19}$$

Note that the operators in each integrand are time-ordered. This observation allows us to write Eq. (8.19) in such a way that the limits of integration are not so complicated, using

$$\int_{t_0}^{t} \mathrm{d}t' \int_{t_0}^{t'} \mathrm{d}t'' \, H\big(t'\big)H\big(t''\big) = \frac{1}{2}\int_{t_0}^{t}\int_{t_0}^{t} \mathrm{T}\big[H\big(t'\big)H\big(t''\big)\big]\,. \tag{8.20}$$

The factor of $\frac{1}{2}$ here deals with overcounting. If we rewrite each term in Eq. (8.19) in a similar way, there will be a factor of $\frac{1}{n!}$ on the nth term to deal with overcounting. We then have

$$\begin{aligned} U(t,t_0) = 1 &- \frac{i}{\hbar}\int_{t_0}^{t} \mathrm{d}t_1 \, H(t_1) + \cdots \\ &+ \frac{1}{n!}\left(-\frac{i}{\hbar}\right)^n \int_{t_0}^{t}\mathrm{d}t_1 \int_{t_0}^{t}\mathrm{d}t_2 \cdots \int_{t_0}^{t} \mathrm{d}t_n \, \mathrm{T}[H(t_1)\cdots H(t_n)] + \cdots\,. \end{aligned} \tag{8.21}$$

This series is known as the *Dyson series*. This looks like the series expansion of an exponential, with each term time-ordered. Thus, we have reproduced Eq. (8.14) with a different approach,

$$U(t,t_0) = \mathrm{T}\left[\exp\left(-\frac{i}{\hbar}\int_{t_0}^{t}\mathrm{d}t' \, H\big(t'\big)\right)\right]. \tag{8.22}$$

8.2 Interaction Picture

We have seen the Schrödinger picture and the Heisenberg picture; now we will discuss a third picture, due to Dirac, called the *interaction picture*. This is a mixed picture that is useful when we can write the Hamiltonian in the form

$$H(t) = H_0(t) + V(t)\,, \tag{8.23}$$

where we have a very good understanding of the dynamics under the Hamiltonian $H_0(t)$, and we think of $V(t)$ as a small perturbation to the system described by $H_0(t)$.

In the interaction picture, we remove the evolution due to H_0 from the state by writing

$$|\psi_{\mathrm{I}}(t)\rangle = U_0^{-1}(t)|\psi_{\mathrm{S}}(t)\rangle\,, \tag{8.24}$$

with $U_0(t)$ the time-evolution operator generated by H_0. Contrast this with the expression in the Heisenberg picture, where the states were defined as

$$|\psi_{\mathrm{H}}(t)\rangle = U^{-1}(t)|\psi_{\mathrm{S}}(t)\rangle\,, \tag{8.25}$$

The state $|\psi_{\mathrm{I}}(t)\rangle$ evolves in time according to

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi_{\mathrm{I}}(t)\rangle = V_{\mathrm{I}}(t)|\psi_{\mathrm{I}}(t)\rangle\,, \tag{8.26}$$

where

$$V_{\mathrm{I}}(t) = U_0^{-1}(t)V(t)U_0(t)\,. \tag{8.27}$$

Operators in the interaction picture evolve according to

$$A_{\mathrm{I}}(t) = U_0^{-1}(t)AU_0(t)\,. \tag{8.28}$$

The interaction picture is useful when we fully understand the dynamics of H_0, and V is a weak probe. We can then use this approach to determine how quickly our system absorbs energy from the weak probe. In the interaction picture, we are hiding the time evolution due to the system we understand, so that we only see the time evolution coming from the unknown part of the system.

We can now derive the equation of motion for the time-evolution operator in the interaction picture. We define

$$U(t) := U_0(t)U_{\mathrm{I}}(t)\,, \tag{8.29}$$

where $U_{\mathrm{I}}(t)$ captures the time-evolution due to the perturbation. We know that the time-evolution operator must satisfy

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}U(t) = (H_0 + V)U(t)\,. \tag{8.30}$$

By definition, $U_0(t)$ is the time-evolution operator in the system with Hamiltonian $H_0(t)$, so it satisfies

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}U_0(t) = H_0U_0(t)\,. \tag{8.31}$$

We compute

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}U(t) = i\hbar\frac{\mathrm{d}}{\mathrm{d}t}(U_0U_{\mathrm{I}}) = i\hbar\left(\frac{\mathrm{d}U_0}{\mathrm{d}t}U_{\mathrm{I}} + U_0\frac{\mathrm{d}U_{\mathrm{I}}}{\mathrm{d}t}\right). \tag{8.32}$$

Using Eq. (8.31) on the first term of the right-hand side yields

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}U(t) = H_0U_0U_{\mathrm{I}} + i\hbar U_0\frac{\mathrm{d}U_{\mathrm{I}}}{\mathrm{d}t} = H_0U + i\hbar U_0\frac{\mathrm{d}U_{\mathrm{I}}}{\mathrm{d}t}\,. \tag{8.33}$$

On the other hand, from Eq. (8.30), we have

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}U(t) = H_0U + VU\,. \tag{8.34}$$

Thus,

$$i\hbar U_0\frac{\mathrm{d}U_{\mathrm{I}}}{\mathrm{d}t} = VU = VU_0U_{\mathrm{I}}\,, \tag{8.35}$$

which gives us

$$i\hbar\frac{\mathrm{d}U_{\mathrm{I}}}{\mathrm{d}t} = U_0^{-1}VU_0U_{\mathrm{I}} = V_{\mathrm{I}}(t)U_{\mathrm{I}}(t)\,. \tag{8.36}$$