Lecture 12

Relevant sections in text: §2.1

The Hamiltonian and the Schrödinger equation

Consider time evolution from t to $t+\epsilon$. As before, we expand in powers of ϵ; we have

$$U(t+\epsilon,t) = I + \epsilon\left(-\frac{i}{\hbar}H(t)\right) + \mathcal{O}(\epsilon^2).$$

As usual, the unitarity of U implies that $H(t)$ is Hermitian, *i.e.,* it represents an observable – the Hamiltonian.

There is one significant difference between the spatial momentum and the Hamiltonian, however. The spatial momentum is defined once and for all by its geometrical nature as generator of translations. The Hamiltonian depends on the details of the interactions within the system and with its environment and different interactions demand different Hamiltonian operators. Thus there can be many useful Hamiltonians for, say, a particle moving in 3-d, but we always use the same momentum operator (in the Schrödinger picture).

There is an alternative characterization of the time evolution operator which is very important. We have that

$$U(t+\epsilon,t_0) = U(t+\epsilon,t)U(t,t_0) = U(t,t_0) + \epsilon H(t)U(t,t_0) + \mathcal{O}(\epsilon^2).$$

We can rewrite this as

$$U(t+\epsilon,t_0) - U(t,t_0) = \epsilon H(t)U(t,t_0) + \mathcal{O}(\epsilon^2).$$

Divide both sides by ϵ and take the limit as $\epsilon \to 0$. We thus get the following differential relationship between U and H (exercise)

$$i\hbar\frac{dU(t,t_0)}{dt} = H(t)U(t,t_0).$$

Let us turn the logic of this around. Given a self-adjoint Hamiltonian, $H(t)$, we can *define* $U(t,t_0)$ as the solution of the above differential equation.* When solving the differential equation an initial condition will have to specified in order to get a unique solution. The initial condition we need is that

$$U(t_0,t_0) = I.$$

* That this strategy works as advertised can be proved rigorously when the Hamiltonian doesn't depend upon time. One will have to make additional hypotheses in the more general case, but we won't worry with those technical details.

Thus we can say that, given a Hamiltonian, the time evolution of the system is determined according to solution of a differential equation. By focusing attention on H rather than U we get a considerable advantage in our ability to describe physical systems. Indeed, we shall always define the dynamics of a system by specifying its Hamiltonian. Note that it is much easier to give a formula for the energy of a dynamical system than to explicitly display its dynamical behavior. Indeed, rarely will we be able to explicitly compute the time evolution operator.†

The relationship we just derived between the time evolution operator and the Hamiltonian is an abstract version of the Schrödinger equation. To see this, simply apply both sides of this operator relation to an arbitrary state vector, representing the initial state of a system at time t_0. We have

$$i\hbar\frac{d}{dt}\Big\{U(t,t_0)|\psi,t_0\rangle\Big\} = H(t)U(t,t_0)|\psi,t_0\rangle.$$

Using

$$|\psi,t\rangle = U(t,t_0)|\psi,t_0\rangle,$$

this is

$$i\hbar\frac{d}{dt}|\psi,t\rangle = H(t)|\psi,t\rangle,$$

which is the traditional form of the Schrödinger equation in terms of abstract vectors. You are probably more familiar with its coordinate wave function version in the case where the Hamiltonian is of the kinetic+potential form for a particle:

$$H = \frac{P^2}{2m} + V(\vec{X}).$$

We then get

$$H\psi(\vec{x}) = \langle\vec{x}|\frac{P^2}{2m} + V(\vec{X})|\psi\rangle = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{x})\right)\psi(\vec{x}).$$

To see this, you should verify that

$$\langle\vec{x}|P_i|\psi\rangle = \frac{\hbar}{i}\frac{\partial}{\partial x^i}\psi(\vec{x}), \quad \langle\vec{x}|(P_i)^2|\psi\rangle = -\hbar^2\frac{\partial^2}{\partial x^{i2}}\psi(\vec{x}),$$

and, using the definition,

$$V(\vec{X}) = \int d^3x\, V(\vec{x})|\vec{x}\rangle\langle\vec{x}|,$$

that

$$\langle\vec{x}|V(\vec{X})|\psi\rangle = V(\vec{x})\psi(\vec{x}).$$

† This does not mean U does not exist, of course, but rather it means the dynamical evolution of the system is sufficiently complicated that no simple formula will suffice to describe it.

We also have

$$\langle \vec{x}|i\hbar\frac{d}{dt}|\psi,t\rangle = i\hbar\frac{\partial}{\partial t}\psi(\vec{x},t).$$

So, the Schrödinger equation is (after taking components in the position basis)

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{x})\right)\psi(\vec{x},t) = i\hbar\frac{\partial}{\partial t}\psi(\vec{x},t).$$

Solving the Schrödinger equation for the state vector at time t for all possible initial state vectors, *i.e.,* finding the general solution of the Schrödinger equation, is equivalent to determining the time evolution operator. You see that the Schrödinger equation is just the statement that the Hamiltonian is the generator of time evolution. To see what that time evolution actually is, one needs to get information about the solutions to the Schrödinger equation. But a key observation here is that the solutions are, ultimately, determined by the choice of Hamiltonian. Determining the Hamiltonian is the key step in making a model of a physical system.

Formal solutions to the Schrödinger equation

It is possible to give formulas for the time evolution operator analogous to the exponential form of the spatial translation operator. There are 3 cases to consider. First suppose that H doesn't depend upon time. Then we are in an identical setting, mathematically speaking, as with the spatial translations. We have

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

You can easily check that this operator satisfies the operator version of the Schrödinger equation including the initial condition.

Second, suppose that $H = H(t)$, but that for any times t, t' we have that

$$[H(t), H(t')] = 0.$$

Then it is not hard to check that

$$U(t,t_0) = e^{-\frac{i}{\hbar}\int_{t_0}^{t} dt'\, H(t')}.$$

Note that this formula includes the previous result as a special case. To check this result just note that one can manipulate the operators as if they were ordinary functions since all the different operators $H(t)$ commute.

Finally, suppose that $H = H(t)$, but that the operators at different times do not commute. This case is somewhat harder and we shall take a crack at it much later. For

completeness, let me just say that the resulting evolution operator is given in terms of the "time ordered exponential",

$$U(t,t_0) = \mathbf{T} e^{-\frac{i}{\hbar}\int_{t_0}^{t} dt'\, H(t')}.$$

For a formula, see your text. We won't be using this last case for a while so we defer its discussion.

State vector evolution when $\frac{\partial H}{\partial t} = 0$

From now on, let us focus on the common case where $\frac{\partial H}{\partial t} = 0$.* We have seen how to build $U(t,t_0)$ in this case. Let us have a look at how state vectors evolve in time (in the Schrödinger picture). Given H, let us denote its orthonormal basis of energy eigenvectors by $|E_i\rangle$. Any state can be expanded in this basis, particularly the initial state:

$$|\psi, t_0\rangle = \sum_j \langle E_j|\psi, t_0\rangle |E_j\rangle.$$

The state at time t is given by

$$\begin{aligned} |\psi, t\rangle &= e^{-\frac{i}{\hbar}(t-t_0)H} \sum_j \langle E_j|\psi, t_0\rangle |E_j\rangle \\ &= \sum_j \langle E_j|\psi, t_0\rangle e^{-\frac{i}{\hbar}(t-t_0)E_j} |E_j\rangle. \end{aligned}$$

As a good exercise you should check directly that this formula gives the solution to the Schrödinger equation matching the initial state $|\psi, t_0\rangle$.

So, the effect of time evolution on a state vector (in the Schrödinger picture) can be viewed as a change of phase of the components in the energy basis:

$$\langle E_j|\psi, t_0\rangle \longrightarrow \langle E_j|\psi, t_0\rangle e^{-\frac{i}{\hbar}(t-t_0)E_j}.$$

This is a very important result. If you want to find the state vector at time t (in the Schrödinger picture) given the initial state vector, you must perform the following computations.

(1) Find the energy eigenvectors and eigenvalues, $|E_j\rangle$ E_j.

(2) Expand the initial state vector in the energy basis, $|\psi, t_0\rangle = \sum_k c_k |E_k\rangle$.

* This case includes many familiar examples: oscillators, atomic electrons, *etc.* Generally speaking, time independent Hamiltonians will occur whenever we are dealing with a closed system.

(3) The j^{th} component of the state vector at time t in the energy basis is the component at the initial time multiplied by the phase $e^{-\frac{i}{\hbar}(t-t_0)E_j}$, *i.e.,* time evolution means

$$c_j \rightarrow c_j e^{-\frac{i}{\hbar}(t-t_0)E_j}.$$

You can now see why the energy eigenvectors are so important. Finding them is the key to understanding time evolution.