

Lecture 12

Relevant sections in text: §2.1

The Hamiltonian and the Schrödinger equation

Consider time evolution from t to $t + \epsilon$. 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 (in the Schrödinger picture). The Hamiltonian depends on the details of the interactions within the system and with its environment. 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).

Let us extract the Hamiltonian in a different way. We have that

$$U(t + \epsilon, t_0) = U(t + \epsilon, t)U(t, t_0).$$

Substitute our result above for $U(t + \epsilon, t)$, divide both sides by ϵ and take the limit as $\epsilon \rightarrow 0$, thereby defining the derivative of U . We get (exercise)

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

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

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

Thus we can say that, given a Hamiltonian, the time evolution of the system is determined. 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

* This supposition 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.

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

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

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. Perhaps you would be more familiar with its coordinate wave function form 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

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

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)

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

† 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.

Solving the Schrödinger equation for the state vector at time t given any initial state vector is equivalent to determining the time evolution operator. You see that the Schrödinger equation simply captures the fact 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 can be viewed as a transformation 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.
- (2) Expand the initial state vector in the energy basis.
- (3) The components of the state vector at time t in the energy basis are the original components times the phase $e^{-\frac{i}{\hbar}(t-t_0)E_j}$.

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

Stationary states

Suppose the Hamiltonian does not depend upon time. If the initial state vector for a system is an energy eigenvector,

$$H|E_k\rangle = E_k|E_k\rangle,$$

(so that the energy is known with certainty at $t = t_0$) then the this state vector changes in a trivial fashion as time progresses. This can be seen in 2 ways. Firstly, simply apply the time evolution operator:

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

You can also check this result by using the 3 step process described above (exercise). The energy eigenvectors change only by a phase factor, hence *all physical predictions (probability distributions) will not change in time*. Thus energy eigenvectors are states in which the system exhibits “stationary” behavior. Such states are naturally called *stationary states*. Nothing ever happens in a stationary state.

Often times we prepare the initial state by a filtering process based upon measurement of one (or more commuting) observables. If these observables commute with the Hamiltonian, then one can arrange that the prepared/filtered states are energy eigenvectors, thus stationary states.

Let me point out a paradox here. Surely you have heard of the process called “spontaneous emission”. You know, where you put an atomic electron in an excited state and even if you do nothing to the atom it will decay to a lower energy state? And I know you have learned about energy levels of atoms in a previous course in quantum mechanics. The energy levels are eigenvectors of the Hamiltonian for the atom, *i.e.*, stationary states. Now the paradox appears: how can an excited state of the atom — a stationary state — decay into anything if nothing ever happens in a stationary state? Think about it!

Conservation of energy

The components of a state vector along the energy eigenvector basis determine the probability distribution for the energy in that state. Time evolution amounts to multiplying these coefficients by phase factors. In general, this changes the vector in a non-trivial way; this causes probability distributions for various observables to change in time. However, since the probabilities for energy arise via the absolute values of the components, you can easily see that the probability distribution for energy does *not* change in time (still assuming that the Hamiltonian is time independent). This is how energy is conserved in quantum mechanics.

Of course, in classical mechanics we usually consider conservation of energy to be characterized by (i) measure the energy initially, (ii) measure the energy at some later time, (iii) energy is conserved if these results are the same. One can do that here as well, but if you measure the energy initially you will then have prepared/filtered your system state to be an energy eigenvector. Then, of course, the probability distribution is quite simple! As we have seen, if the system is in an energy eigenvector at one time, it remains

there for all time. Thus you will always get the same result for any subsequent measurement of energy. That is certainly much like the classical way of viewing conservation of energy. However, as we have seen, in a stationary state *all* probability distributions are time independent. In non-stationary states, where the dynamical evolution is non-trivial, one cannot say with statistical certainty what the initial energy is – one has a non-trivial probability distribution. What one *can* say is that, while other probability distributions will, in general, change in time (energy-compatible observables being the exceptions), the energy probability distribution will not. This is what conservation of energy means in quantum mechanics.