

## Lecture 6 (Sep. 25, 2017)

### 6.1 Solving Problems in Convenient Bases

Last time we talked about the momentum and position bases. From a practical point of view, it often pays off to not solve a particular problem in the position basis, and instead choose a more convenient basis, such as the momentum basis. Suppose we have a Hamiltonian

$$H = -\frac{1}{2m} \frac{d^2}{dx^2} + ax. \quad (6.1)$$

We could solve this in the position basis; it is a second-order differential equation, with solutions called Airy functions. However, this is easy to solve in the momentum basis. In the momentum basis, the Hamiltonian becomes

$$H = \frac{p^2}{2m} + ia\hbar \frac{d}{dp}, \quad (6.2)$$

which is only a first-order differential equation.

For other problems, the most convenient basis may not be the position or the momentum basis, but rather some mixed basis. It is worth becoming comfortable with change of basis in order to simplify problems.

### 6.2 Quantum Dynamics

Recall the fourth postulate: time evolution is a map

$$|\psi(t)\rangle \mapsto |\psi(t')\rangle = U(t', t)|\psi(t)\rangle, \quad (6.3)$$

where  $U(t', t)$  is the time-evolution operator, which is unitary. In the case where  $t'$  and  $t$  differ by an infinitesimal amount, we can rewrite time evolution as a differential equation,

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H(t)|\psi(t)\rangle, \quad (6.4)$$

where  $H(t)$  is the Hamiltonian, which is a Hermitian operator.

In general, we can always write

$$|\psi(t')\rangle = U(t', t)|\psi(t)\rangle \quad (6.5)$$

for *some* operator  $U(t', t)$ . What statements can we make about the operator  $U(t', t)$ ? We can say the following:

1. The probability must be conserved. We start with a state for which the total probability of all outcomes of a measurement is 1, and so we expect that after evolving in time, we should arrive at a state that also has total probability 1. This implies that  $U$  must be unitary, which we will now prove.

*Proof.* Let us expand the state  $|\psi(t)\rangle$  as

$$|\psi(t)\rangle = \sum_n c_n(t) |a_n\rangle, \quad (6.6)$$

with  $\{|a_n\rangle\}$  a basis of eigenstates of any observable  $A$ . The probability of a measurement of  $A$  yielding the result  $a_n$  at time  $t$  is given by

$$\text{Prob}(A = a_n \text{ at time } t) := p(a_n; t) = |c_n(t)|^2, \quad (6.7)$$

where we have introduced the shorthand notation  $p(a_n; t)$  for this probability. The total probability must be 1,

$$\sum_n p(a_n; t) = 1, \quad (6.8)$$

which is simply the statement that the state  $|\psi(t)\rangle$  must be normalized,

$$\sum_n |c_n(t)|^2 = 1. \quad (6.9)$$

At a later time  $t'$ , we have

$$p(a_n; t') = |c_n(t')|^2, \quad (6.10)$$

and once again, requiring that the total probability be 1 requires that  $|\psi(t')\rangle$  be normalized,

$$\sum_n |c_n(t')|^2 = 1. \quad (6.11)$$

Thus, we must have

$$\langle \psi(t') | \psi(t') \rangle = \langle \psi(t) | U^\dagger(t', t) U(t', t) | \psi(t) \rangle = 1 \quad (6.12)$$

for arbitrary normalized  $|\psi(t)\rangle$ . This is satisfied if and only if  $U^\dagger(t', t)U(t', t) = \mathbb{1}$ , i.e., if  $U$  is unitary.  $\square$

2. We demand that the time-evolution operator satisfy composition, i.e.,

$$U(t_f, t_i) = U(t_f, t)U(t, t_i) \quad (6.13)$$

for all  $t_i < t < t_f$ .

3. We require that

$$U(t, t) = \mathbb{1}. \quad (6.14)$$

We will now build up an arbitrary time-evolution operator as a sequence of infinitesimal time-evolution operators. Consider a time evolution  $U(t + dt, t)$ ; we can expand this as a power series in the infinitesimal  $dt$ , yielding

$$U(t + dt, t) = \mathbb{1} - \frac{i}{\hbar} H dt + O((dt)^2) \quad (6.15)$$

for some operator  $H$  (which we do not yet know anything about). The factors of  $i$  and  $\hbar$  are put in for historical reasons, but note that we can always expand  $U(t + dt, t)$  in this way. We will neglect higher-order terms because  $dt$  is infinitesimal. We then have

$$U^\dagger(t + dt, t) = \mathbb{1} + \frac{i}{\hbar} H^\dagger dt + O((dt)^2). \quad (6.16)$$

Requiring unitarity,  $U^\dagger U = \mathbb{1}$ , then gives us

$$U^\dagger U = \left( \mathbb{1} - \frac{i}{\hbar} H dt + \dots \right) \left( \mathbb{1} + \frac{i}{\hbar} H^\dagger dt + \dots \right) = \mathbb{1} + \frac{i}{\hbar} (H^\dagger - H) dt + O((dt)^2) = \mathbb{1}. \quad (6.17)$$

We conclude that we must have  $H^\dagger = H$ , i.e.,  $H$  must be Hermitian. The statement that  $U$  is a unitary operator is equivalent to the statement that  $H$  is Hermitian. We will call  $H$  the *Hamiltonian*. Shortly, we will make the connection between this operator and the Hamiltonian we know from classical physics.

Applying the infinitesimal time-evolution operator to a state, we find

$$|\psi(t + dt, t)\rangle = \left( \mathbb{1} - \frac{i}{\hbar} H dt + O((dt)^2) \right) |\psi(t)\rangle. \quad (6.18)$$

We can write this statement as

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H |\psi(t)\rangle, \quad (6.19)$$

which we recognize as the Schrödinger equation.

Now let's connect this to the discussion of unitary spatial translations. We can think of time evolution as translation in time. At the end of the last lecture, we alluded to the fact that an infinitesimal spatial translation is generated by the Hermitian momentum operator. This is exactly analogous to the statement that infinitesimal time evolutions are generated by the Hamiltonian, which is Hermitian. (Note that momentum is the conserved Noether charge associated to spatial translations, and energy is the conserved Noether charge associated to time translations.)

### 6.2.1 Brief Aside on Classical Mechanics

In classical mechanics, time evolution is dictated by Newton's laws. Over the centuries, Newton's laws have been massaged into various forms. Classically, the state of a particle is specified by its position  $q(t)$  and momentum  $p(t)$ . Given such a state, how do  $q(t), p(t)$  change as a function of time? This is described by the equations of motion for the particle, which are known as Hamilton's equations:

$$\frac{dq}{dt} = \frac{\partial H}{\partial p}, \quad \frac{dp}{dt} = -\frac{\partial H}{\partial q}, \quad (6.20)$$

where  $H = H(q, p)$  is the classical Hamiltonian.

As an example, consider

$$H(q, p) = \frac{p^2}{2m} + V(q). \quad (6.21)$$

Hamilton's equations then give

$$\dot{q} = \frac{p}{m}, \quad \dot{p} = -\nabla_q V, \quad (6.22)$$

which are simply Newton's equations of motion.

The space of  $(q, p)$  is known as *phase space*. The classical time evolution given by Hamilton's equation is such that the area of a region of phase space is preserved by the time evolution (Liouville's theorem). Suppose we have a collection of particles, each with different values of  $q, p$ . This collection fills out a region in phase space. If we evolve each particle in time, the shape of the region in phase space will change, but its area will be conserved.

We can state Liouville's theorem formally in terms of the Poisson bracket, defined as

$$\{f, g\} = \frac{\partial f}{\partial q} \frac{\partial g}{\partial p} - \frac{\partial g}{\partial q} \frac{\partial f}{\partial p}. \quad (6.23)$$

Any observable  $A$  (that only depends on time through  $q$  and  $p$ ) evolves in time according to

$$\frac{dA}{dt} = \{A, H\}. \quad (6.24)$$

In particular, taking  $A = q$  yields

$$\frac{dq}{dt} = \{q, H\} = \frac{\partial H}{\partial p} \quad (6.25)$$

and taking  $A = p$  yields

$$\frac{dp}{dt} = \{p, H\} = -\frac{\partial H}{\partial q}. \quad (6.26)$$

Classically, the Hamiltonian is (usually) the total energy of the system. In quantum mechanics, we refer to  $H$  as the Hamiltonian because it is the operator that returns the energy of the system. In quantum mechanics, the Hamiltonian (energy) operator and the time operator are more deeply related because of the time-energy uncertainty relation.

### 6.2.2 The Heisenberg Picture

Let's start with the Schrödinger equation

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H |\psi(t)\rangle. \quad (6.27)$$

For a closed system,  $H$  is independent of time, and we can solve this equation exactly, in some formal sense, as

$$|\psi(t)\rangle = e^{-iHt/\hbar} |\psi(0)\rangle. \quad (6.28)$$

Thus, the time-evolution operator is given by

$$U(t, 0) = e^{-iHt/\hbar}. \quad (6.29)$$

The physically significant quantities are matrix elements of operators,

$$\langle \psi'(t) | A | \psi(t) \rangle = \langle \psi'(0) | U^\dagger(t, 0) A U(t, 0) | \psi(0) \rangle. \quad (6.30)$$

Here, we have assumed that  $A$  does not have explicit time dependence. Thus, the time dependence of the matrix element comes only from the fact that the states change in time. However, we can look at the expression on the right-hand side and define a time-dependent operator

$$A_H(t) := U^\dagger(t, 0) A_H(0) U(t, 0), \quad A_H(0) = A, \quad (6.31)$$

that acts on states  $|\psi_H\rangle := |\psi(0)\rangle$  that do not evolve in time. Viewing time evolution in this way is referred to as working in the *Heisenberg picture*. Up until now, we have been working in the *Schrödinger picture*, in which the time dependence of matrix elements comes from the time dependence of states  $|\psi(t)\rangle$ , and operators without explicit time dependence do not evolve in time. By design, we have

$$\langle \psi'_H | A_H(t) | \psi_H \rangle = \langle \psi'(0) | U^\dagger(t, 0) A U(t, 0) | \psi(0) \rangle. \quad (6.32)$$

We can write an infinitesimal version of Eq. (6.31) as

$$\begin{aligned} \frac{dA_H}{dt} &= \frac{d}{dt} \left( e^{iHt/\hbar} A_H(0) e^{-iHt/\hbar} \right) \\ &= \frac{i}{\hbar} e^{iHt/\hbar} (H A_H(0) - A_H(0) H) e^{-iHt/\hbar} \\ &= \frac{1}{i\hbar} [A_H(t), H]. \end{aligned} \quad (6.33)$$

Comparing this with the classical time-evolution expression

$$\frac{dA}{dt} = \{A, H\}, \quad (6.34)$$

we see that the commutator in quantum mechanics plays a similar role as the Poisson bracket in classical mechanics.

### 6.3 Energy Eigenstates

We will now assume that the Hamiltonian  $H$  corresponds to the energy of the system. Because  $H$  is Hermitian, we can diagonalize it with a unitary transformation. Let  $|j\rangle$  be its eigenstates,

$$H|j\rangle = E_j|j\rangle, \quad (6.35)$$

which form an orthonormal basis. We call the  $|j\rangle$  *energy eigenstates*, and the  $E_j$  the corresponding *energy eigenvalues*. An arbitrary state  $|\psi\rangle$  can be decomposed as

$$|\psi\rangle = \sum_j c_j |j\rangle \quad (6.36)$$

with

$$c_j = \langle j|\psi\rangle. \quad (6.37)$$

Similarly, an arbitrary operator  $A$  can be decomposed as

$$A = \sum_{j,j'} A_{jj'} |j\rangle\langle j'|. \quad (6.38)$$

In the Schrödinger picture,  $A_{jj'}$  is time-independent, and the states evolve as

$$\begin{aligned} |\psi(0)\rangle &\mapsto |\psi(t)\rangle = e^{-iHt/\hbar} |\psi(0)\rangle \\ &= e^{-iHt/\hbar} \sum_j c_j |j\rangle \\ &= \sum_j c_j e^{-iE_j t/\hbar} |j\rangle. \end{aligned} \quad (6.39)$$

Thus, we can write

$$|\psi(t)\rangle = \sum_j c_j(t) |j\rangle, \quad (6.40)$$

where the coefficients  $c_j(t)$  evolve in time as

$$c_j(t) = c_j e^{-iE_j t/\hbar}. \quad (6.41)$$

The matrix element of  $A$  is then

$$\begin{aligned} \langle\psi(t)|A|\psi(t)\rangle &= \sum_{j,j'} c_j^*(t) c_{j'}(t) \langle j|A|j'\rangle \\ &= \sum_{j,j'} c_j^*(0) c_{j'}(0) e^{i(E_j - E_{j'})t/\hbar} A_{jj'}. \end{aligned} \quad (6.42)$$

In the Heisenberg picture, the states are time-independent, so the  $c_j$  are fixed, while  $A$  evolves as

$$\begin{aligned} A \mapsto A(t) &= e^{iHt/\hbar} A e^{-iHt/\hbar} \\ &= \sum_{j,j'} A_{jj'} \left( e^{iHt/\hbar} |j\rangle \langle j'| e^{-iHt/\hbar} \right) \\ &= \sum_{j,j'} \left( A_{jj'} e^{i(E_j - E_{j'})t/\hbar} \right) |j\rangle \langle j'|. \end{aligned} \quad (6.43)$$

The matrix element is then

$$\langle \psi | A(t) | \psi \rangle = \sum_{j,j'} c_j^* c_{j'} e^{i(E_j - E_{j'})t/\hbar} A_{jj'}, \quad (6.44)$$

which agrees with the result in the Schrödinger picture.

## 6.4 Example: Spin Precession In a Magnetic Field

Consider a spin- $\frac{1}{2}$  moment in a magnetic field, with Hamiltonian

$$H = -\frac{ge}{2m} \mathbf{S} \cdot \mathbf{B}. \quad (6.45)$$

Here,  $e$  is the electric charge,  $m$  is the mass of the particle, and  $g$  is the g-factor, which has  $g \approx 2$  for the electron. Assuming that  $\mathbf{B} = B\hat{z}$ , we can write the Hamiltonian as

$$H = -\frac{ge}{2m} S^z B. \quad (6.46)$$

With this assumption, the  $S^z$  eigenstates are also energy eigenstates,

$$H |S_{\pm}^z\rangle = \mp \frac{ge\hbar B}{4m} |S_{\pm}^z\rangle \quad (6.47)$$

with energy eigenvalues

$$E_{\pm} = \mp \frac{ge\hbar B}{4m}. \quad (6.48)$$

The energy separation is

$$\hbar\omega = |E_+ - E_-| = \left| \frac{ge\hbar B}{2m} \right|. \quad (6.49)$$

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