

## Lecture 22

- Tunneling in the two-state system
- Feynman, chapter 7, 8.6, 9.1

### Tunneling in the two-state system

Let's now look in more depth at an interesting two-state system: the maser or laser. The physics behind the two is the same: the difference is that the radiation emitted is microwaves (maser = “microwave amplification (by) stimulated emission of radiation”); for a laser it's visible light. For a laser, the two states are two energy levels; for a maser it's two states of an atom, like  $NH_3$ .  $NH_3$  has three hydrogen atoms in a triangle. The hydrogen then outside the plane of the atoms to form (roughly) a tetrahedron. The triangle has a spin around an axis through its center, so one can distinguish between the hydrogen being on one side or the other. Denote these states by  $|1\rangle$  and  $|2\rangle$ .

To understand the maser, we need to understand what happens when this atom is put in an electric field. But before this, we need to understand the system without a field! For the spin-1/2 atom in a magnetic field, we knew which states were stationary states. Here we don't, however, because in quantum mechanics, particles can go through regions which are classically forbidden. This is called “tunneling”, and later in the class we will discuss this in more detail. Here, all we need to know is that in  $NH_3$ , even if we start the nitrogen on one side, there is some probability it will eventually end up on the other. Thus the stationary state will involve the atom on both sides, just as a  $|+X\rangle$  state involved both  $|+Z\rangle$  and  $|-Z\rangle$ .

To see how this goes, we need to introduce a differential equation. Earlier, I stated that by definition, a stationary state has probabilities unchanging in time. This means it can have a phase  $e^{-iEt/\hbar}$ , because when you take the magnitude squared, it goes away. This fact is expressed in a differential equation for the amplitude  $\psi(t)$  by

$$i\hbar \frac{\partial \psi(t)}{\partial t} = E\psi(t)$$

You can check that  $\psi(t) = e^{-iEt}$  is a solution by directly plugging this in. Note that this equation has only one derivative, unlike the wave equation.

The reason that I introduced the differential equation is that it makes it possible to include tunneling in the situation. Let's consider our two-state system. Since there are two states, there are two possible stationary states, which we call  $|I\rangle$  and  $|II\rangle$ . However, since there is tunneling, we don't know how to relate the stationary states  $|I\rangle$  and  $|II\rangle$  to the states  $|1\rangle$  and  $|2\rangle$ , which are the states with the nitrogen atom and the top and the bottom. Because the states  $|1\rangle$  and  $|2\rangle$  form a basis, at any time, any state can be written as

$$|state(t)\rangle = C_1(t)|1\rangle + C_2(t)|2\rangle$$

for some amplitudes  $C_1(t)$  and  $C_2(t)$ . If we neglect tunneling, then this means that both states  $|1\rangle$  and  $|2\rangle$  are stationary states. We denote their energies in the absence of tunneling as  $E_0$ ; this is the same for both because of the symmetry. In differential equations, we have

$$\begin{aligned} i\hbar \frac{\partial C_1(t)}{\partial t} &= E_0 C_1(t) \\ i\hbar \frac{\partial C_2(t)}{\partial t} &= E_0 C_2(t) \end{aligned}$$

when there is no tunneling.

Now let's include tunneling, and introduce a new parameter  $A$  to indicate the "amount" of tunneling from state 1 to state 2. The tunneling from 2 to 1 is the same, by symmetry. What this means precisely is that the differential equations that describe the system are now

$$\begin{aligned} i\hbar \frac{\partial C_1(t)}{\partial t} &= E_0 C_1(t) - A C_2(t) \\ i\hbar \frac{\partial C_2(t)}{\partial t} &= -A C_1(t) + E_0 C_2(t) \end{aligned}$$

I haven't proved this. Basically, it follows if you demand that quantum mechanics be "linear" (the sum of solutions to a differential equation is also a solution). Feynman explains the origin of these differential equations of results in much more detail in chapter 8: he introduces what is called the "Hamiltonian" matrix on general grounds like this. Here, I hope you agree that this is a natural way of allowing tunneling, and trust me that it is the only way of consistently doing so. Physically, the key point is that when  $A \neq 0$ , the equations say that the amplitude  $C_1$  changes in time when there is a non-zero  $C_2$ . That corresponds to tunneling from  $|2\rangle$  to  $|1\rangle$ . Likewise, the extra term in the second equation is a result of tunneling from  $|1\rangle$  to  $|2\rangle$ . Note that when  $A = 0$ , the equations simplify, and we get  $C_1(t) \propto e^{-iE_0 t/\hbar}$  and  $C_2(t) \propto e^{-iE_0 t/\hbar}$ .

We have two unknown functions  $C_1(t)$  and  $C_2(t)$ , and two differential equations relating them. So how do we solve them? Just think how you would solve two coupled linear algebraic equations: you eliminate one of the variables by adding the equations together, solve for the one variable, and then plug it back in to get the other. It's a little trickier here, but not much. In particular, here just try adding the two equations together. Then you get

$$i\hbar \frac{\partial C_1(t)}{\partial t} + i\hbar \frac{\partial C_2(t)}{\partial t} = (E_0 - A)C_1(t) + (E_0 - A)C_2(t)$$

Regrouping the terms, you have

$$i\hbar \frac{\partial}{\partial t} (C_1(t) + C_2(t)) = (E_0 - A)(C_1(t) + C_2(t))$$

Note that we've got a single equation for  $C_1 + C_2$ , and in fact, it's the same as our earlier differential equation. Thus we get

$$C_1(t) + C_2(t) = F e^{-i(E_0 - A)t}$$

for some constant  $F$  independent of time. Likewise, if we take the difference of equations, we get

$$i\hbar \frac{\partial}{\partial t} (C_1(t) - C_2(t)) = (E_0 + A)(C_1(t) - C_2(t))$$

The solution of this is

$$C_1(t) - C_2(t) = G e^{-i(E_0 + A)t}$$

for some constant  $G$  independent of time. Disentangling this, we have for the answer

$$\begin{aligned} C_1(t) &= \frac{1}{2} (F e^{-i(E_0 - A)t} + G e^{-i(E_0 + A)t}) \\ C_2(t) &= \frac{1}{2} (F e^{-i(E_0 - A)t} - G e^{-i(E_0 + A)t}) \end{aligned}$$

The constants  $F$  and  $G$  don't depend on time: the only time dependence on the right-hand-side of these equations is the explicit one. Thus  $F$  and  $G$  can be determined by the initial conditions. Once we set those, then we know the state of the system for all time.

Let's start with a system where at  $t = 0$ , we know the nitrogen is on one side of the hydrogens. This means that at  $t = 0$ , the state is say  $|1\rangle$ . This is not a stationary state, because it can tunnel to the other side. This is reflected in the solutions to these differential equations. For starting in the state  $|1\rangle$  at  $t = 0$ ,  $C_1(0) = 1$ , and  $C_2(0) = 0$ . This is our initial condition, which fixes  $F = G = 1$ . Then solving our two equations for  $C_1$  and  $C_2$  gives

$$\begin{aligned} C_1(t) &= \frac{1}{2} (e^{-i(E_0 - A)t/\hbar} + e^{-i(E_0 + A)t/\hbar}) = e^{-iE_0 t} \cos(At/\hbar) \\ C_2(t) &= \frac{1}{2} (e^{-i(E_0 - A)t/\hbar} - e^{-i(E_0 + A)t/\hbar}) = i e^{-iE_0 t} \sin(At/\hbar) \end{aligned}$$

Thus the nitrogen atom oscillates back and forth between the two sides, just like the spins. The probability it is on side 1 is

$$|\langle 1 | state(t) \rangle|^2 = |C_1(t)|^2 = |e^{iE_0 t} \cos(At/\hbar)|^2 = \cos^2(At/\hbar)$$

Similarly, the probability it is on the other side is  $\sin^2(At/\hbar)$ .

So here's an important thing: the states  $|1\rangle$  (where the nitrogen is definitely on one side) and  $|2\rangle$  (where the nitrogen is on the other) are *not* stationary states. They are akin to the states  $|+X\rangle$  and  $|-X\rangle$  in a  $z$  magnetic field.

So what are the stationary states? Let's change the initial condition and say that at time  $t = 0$ , it is in the state

$$|II(t = 0)\rangle = \frac{1}{\sqrt{2}}|1\rangle + \frac{1}{\sqrt{2}}|2\rangle$$

(This is called  $II$  instead of  $I$  to conform with Feynman.) The state  $|II\rangle$  evolves in time as

$$|II(t)\rangle = C_1(t)|1\rangle + C_2(t)|2\rangle$$

The equations we derived for  $C_1(t)$  and  $C_2(t)$  above apply for any initial condition. The only effect of the initial conditions is to fix the time-independent constants  $F$  and  $G$ . Here, we have  $C_1(0) = C_2(0) = 1/\sqrt{2}$ . This means that  $F = \sqrt{2}$  and  $G = 0$ . Since  $G = 0$ , this means that  $C_1(t) = C_2(t)$  for all times  $t$ . Thus

$$|II(t)\rangle = C_1(t)(|1\rangle + |2\rangle)$$

where we can plug in  $F = \sqrt{2}$  to get

$$C_1(t) = \frac{1}{\sqrt{2}}e^{-i(E_0 - A)t/\hbar}$$

The state  $|II\rangle$  is a stationary state! Note that it does not have energy  $E_0$ , but rather energy  $E_0 - A$ . The tunneling has not only changed what the stationary states are, but it has changed their energy!

The other stationary state is

$$|I\rangle = \frac{1}{\sqrt{2}}|1\rangle - \frac{1}{\sqrt{2}}|2\rangle$$

Here we have  $C_1(0) = -C_2(0) = 1/\sqrt{2}$ , so that  $F = 0$  and  $G = \sqrt{2}$ . Because  $F$  vanishes here, the state  $|I\rangle$  has  $C_1(t) = -C_2(t)$  for all times. Plugging this in gives

$$|I(t)\rangle = \frac{1}{\sqrt{2}}e^{-i(E_0 + A)t/\hbar}(|1\rangle - |2\rangle)$$

The state  $|I(t)\rangle$  is therefore a stationary state with energy  $E_0 + A$ .

So we've solved our problem! We've seen that in the absence of tunneling ( $A = 0$ ), we have two stationary states, the nitrogen atom on each side of the hydrogens. Both of these states have energy  $E_0$ . When we allow tunneling ( $A \neq 0$ ), the stationary states both include some of both  $|1\rangle$  and  $|2\rangle$ .