

**PROFESSOR:** Let's do a case that this mostly solvable and illustrates all these things. It's a very entertaining case. It's called Landau-Zener transitions. For these two people, Lev Landau, who you've probably heard from Landau and Lifshitz. He's the first person that tried to do this. And Zener did it more carefully. In fact, apparently found that Landau made a factor of two error.

And the paper of Zener, it's actually quite nice, and it's a very nice example that illustrates the physics of this transition. So we'll devote the rest of the lecture to that Landau-Zener thing. OK. So it will give us a little bit into the spirit of the adiabatic approximation in the language that Berry used.

So Landau-Zener transitions. OK, Zener and Landau were interested in molecules, and some way of thinking of molecules is to think of nuclei as fixed, separated by some distance  $R$ , and then you assume they are fixed, and they're separated by some distance  $R$ . And then you calculate what is the electronic configuration.

So Zener imagined that you would have  $\psi_1$ , one electronic configuration. It's a wave function that depends on some  $x$ 's for the electrons, but it represents the situation where the two protons, say, for a simple molecule, maybe they're more distances, but in particular, they are separated by a distance,  $R$ . So that's an electronic configuration. Electronic configuration, protons a distance  $R$  away.

And suppose there's another configuration  $\psi_2$  of  $R$ . It's another configuration, so two configurations. Two different states. Maybe in the first state, the electrons are in some ground state. In the second state, they're in some kind of excited state, two different configurations.

Now, we could plot. So we'll have [INAUDIBLE] here, distance  $R$ , and here's the cloud of electrons. We could plot a graph as a function of the separation, what are the values of the energies. And here is one possibility for the states. And here's another one. And that's the plot of the style that Zener drew in his paper.

And this represents  $E_1$  of  $R$  and this  $E_2$  of  $R$ . That is the energy of the first state, the energy of the second state as a function of  $R$ . So we are having here-- oops-- two energy eigenstates. So we have  $H$  of  $R$ . The Hamiltonian depends on the  $R$ . And basically you're putting the two protons, the distance  $R$ , and calculating the electrons, how they move.  $\psi_i$  of  $x$   $R$  equals  $E_i$  of  $R$   $\psi_i$  of  $x$ .

This is for  $i$  equal 1 and 2. The case that the people were interested in was the case where this molecule here, for example, in the state 2, for this value of  $R$ , there is a critical  $R_0$ , where things, the levels get very close. For some value of  $R$ , this molecule, for example, could be a polar molecule. A polar molecule is a permanent dipole moment. It has plus charges and minus charges, not evenly distributed. So you get a dipole.

And maybe here, the molecule is non-polar. And here, it's non-polar. Here polar. So if you would follow one of the energy eigenstates, there's a critical value of  $R$ , where the electronic configuration is such that it goes from non-polar to polar and in the other energy eigenstate, it goes from polar to non-polar.

So the question is well, OK, what-- first of all, what does all this have to do with instantaneous energy eigenstates and time dependence? Why are we thinking about this? The issue is that sometimes, you can think of these molecules as forming or being subjected to extra interactions in which you will have a process or a reaction in which the radius changes in time.

So it's possible under some configuration that  $R$  becomes  $R$  of  $t$ . And then, this Hamiltonian is a Hamiltonian that depends on  $R$  of  $t$ . This wave functions  $\psi_i$  are  $R$  of  $t$   $E_i$ 's become  $R$  of  $t$ ,  $\psi_i$ 's become  $\chi$  of  $R$  of  $t$ .

This is an important point. It's simple, but important. The most important points in physics are simple. But you have to stop and recognize that something slightly new is happening here. If you have solved this equation for all values of  $R$ , if you know those energy eigenstates for all separations of the molecule, you now have found instantaneous energy eigenstates if it so happens that  $R$  is a function of  $t$ , because if this is true for any value of this [INAUDIBLE]  $R$ , well, then this is true for all times.

Because for any specific time, this is the  $R$ , the same  $R$  is here, the same  $R$  is here, and the same  $R$  is here. And that equation holds for all  $R$ . So if this can be solved for all  $R$ , this holds for all times. And you have your instantaneous energy eigenstates. You have found those instantaneous energy eigenstates. And therefore, the instantaneous energy eigenstates are these ones. And the instantaneous energies are these ones.

So many times in quantum mechanics, you do that. You solve for the energy eigenstates for a whole range of some parameters. And then it so happens that those parameters may change in time. But then you have found the instantaneous energy eigenstates for all times.

So in that picture, we have the following situation, in which the energies now could be thought if  $R$  is some function alpha of  $t$ , then the same picture would basically hold true for time here and the energies as a function of time, because as time changes,  $R$  changes, and as  $R$  changes, you already know how the figure looks. So this is a figure of the energy levels as a function of time.

And now the physical question is do we get a transition or not? So the adiabatic theorem would say, OK, you should stay in your instantaneous energy eigenstate, but we're going to get precisely to this situation where these things could be so small, so little, that there is a possibility of a non adiabatic transition, in which you jump to the other one, because the gap is small.

So this goes to the real physics of the adiabatic theorem, can we get an estimate or a calculation that tells us how much probability you have of jumping the gap and going to the other branch? That's what we're going to try to do. So for that, we'll do a particular example.

So let's do that. It's an easy one to begin with. I'll erase this. So baby example, toy example. So take a Hamiltonian,  $H$  of  $t$ , which is going to be of this form, time dependent one, but relatively simple. Elements just along the diagonal. OK, that's your Hamiltonian, two by two matrix, elements on the diagonal, but just simple things, the same thing.

So let's calculate the instantaneous energy eigenstates. OK, sounds like a task. It's actually pretty simple. The instantaneous energy eigenstates are  $|1, 0\rangle$  and  $|0, 1\rangle$ . They don't depend on time, because essentially this Hamiltonian is just  $\alpha t$  over 2,  $|1, 0\rangle$  is-- it's a constant matrix times an overall factor.

The eigenstates of this matrix are  $|1, 0\rangle$  and  $|0, 1\rangle$ . And they are the eigenstates of this matrix for any time, because the time goes in front. The matrix doesn't quite change shape. So these are the instantaneous energy eigenstates. They are good forever.

To plot this, I will assume from now on that  $\alpha$  is positive. The energy of the first state is-- well, what do you get when you add with the Hamiltonian on this state? The matrix [INAUDIBLE] and this is just  $\alpha t$  over 2. And the energy of the second state is going to be minus  $\alpha t$  over 2.

We can plot those energies, and here is the energy of the first state is  $\alpha t$  over 2 with  $\alpha$  positive. This is like this, thick output of here. This is the state  $|1, 0\rangle$  is here,  $|1, 0\rangle$  is here,

$\alpha t$  over  $[\dots]$  Here is the energy  $E_1$  of  $t$ . The energy time dependent. Here is time. And here are energies. This is  $E_1$ . And then we have the  $E_2$  is the other one that goes like this. It's state 0, 1. That's the state 2, 0, 1. And the energy is  $E_2$  of  $t$ , which is minus  $\alpha t$  over 2.

So it's negative for large positive time and positive for the other one. So these are your instantaneous energy eigenstates. OK, and this is not quite what we wanted here. We wanted things to avoid themselves. But this is going to illustrate an important effect. I claim, actually, that the true solutions of the Schrodinger equation are in this case dressed up versions of the instantaneous energy eigenstates.

So what I claim is the kind of-- you do the adiabatic state corresponding to this, the adiabatic state corresponding to that, and those are exact solutions. So there is no coupling between the states, 1 and 2. So this is plausible. So let's write those solutions. I claim here is  $\psi_1$  of  $t$  I claim is the exponential of minus  $i$  over  $\hbar$  integral up to  $t$  of  $E_1$  of  $t'$  prime  $dt'$  prime times the state 1.

I claim this solves the Schrodinger equation.  $i \hbar \frac{d}{dt}$  of this  $\psi$  should be equal to  $H \psi$ . Is it clear? Yes, I think it's clear. It solves it, because if you take the time derivative of this thing, it multiplies by  $E_1$ . The  $i \hbar$  cancels that factor of minus  $i$  over  $\hbar$ . The time derivatives brings out an  $E_1$  of  $t$ .

But this state, despite the phase when  $\hbar$  [INAUDIBLE], it goes through the phase, hits the state 1, and produces the  $E_1$  energy. So this is solved by that equation, and you can do the integral. It looks OK. It's exponential of minus  $i \alpha t^2$  over  $4 \hbar$ , and the state  $\psi_2$  of  $t$  is the same exponential with  $E_2$  with 2 here, and it's the exponential of plus  $i \alpha t^2$  over  $4 \hbar$ .

OK. Let's appreciate the lesson again. We got a very simple system, two levels, crossing-- they cross. The energy levels cross. That generally doesn't happen. You have to have a very special Hamiltonian for the energy levels to cross. We found the instantaneous energy eigenstate, and we found two exact solutions of this Schrodinger equation, two perfect complete exact solutions of the Schrodinger equation that represent the system doing just zoom, like that, or doing like that. Totally oblivious that there's a state they're crossing, the Schrodinger equation doesn't couple them in this case.