

## Lecture 4

# Adiabatic Theorem

So far we have considered time independent semiclassical problems. What makes these "semiclassical" is that the gradient term (which is multiplied by  $\hbar^2$ ) was small. In other words, the potential was varying slowly in space. There is a completely different context for semiclassics – namely when a Hamiltonian varies slowly in time. These can be looked at as what happens to the *time dependent* Schrodinger equation when the  $\hbar$  in front of the time derivative goes to zero.

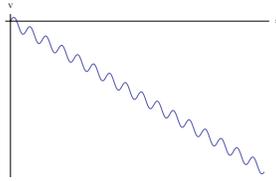
We will see three important results here. First we will see the Adiabatic theorem (which I assume you are all familiar with). Next we will see the breakdown of the adiabatic theorem near an avoided crossing: the physics will be analogous to tunneling between two wells. Finally we will explore phases on matrix elements which appear in adiabatic processes. These will be important in subsequent lectures.

### A. Time dependence from separation of timescales

One thing worth emphasizing is that one does not need an explicitly time dependent Hamiltonian for this logic to be relevant. The classic example is electrical breakdown of a semiconductor – where we will see yet another version of semiclassics.

**Group Activity:** Imagine you have a semiconductor with a single electron in the conduction band. Imagine you put this material in a constant electric field. Describe what happens.

Such an electron experiences a potential which qualitatively looks like



The standard semiclassical description of electron motion in a semiconductor is to start with Newton's laws:

$$\partial_t p = F \quad (4.1)$$

with  $F = -qE$  constant. To relate the momentum to the velocity, however, one uses the dispersion relationship

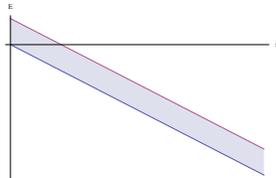
$$\partial_t x = \frac{\partial \epsilon}{\partial p}. \quad (4.2)$$

These equations are called semiclassical as they are in the same spirit as the WKB approximation. One imagines having a wave packet which is much larger than the lattice spacing. If it has momentum centered around  $p$ , then its group velocity will be given by Eq. (4.2). The momentum of this packet will evolve in time via Eq. (4.1),

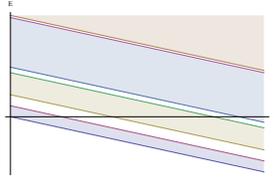
It turns out that these rather innocuous looking equations lead to pretty strange behavior. For example, in a lattice  $\epsilon$  is a periodic function of  $p$ . Thus  $v$  will oscillate. This means that the center of mass of the wave packet will oscillate! These are known as Bloch oscillations, and they have been seen for atoms trapped in optical lattices.

**Group Activity:** What is the period of Bloch oscillations?  
What is their amplitude in real space?

One way of understanding this result is that the allowed energies of the electron as a function of space form a tilted band. All states of a given energy are localized:

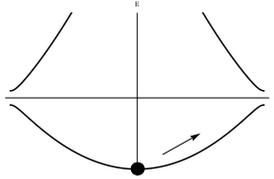


If you have a given energy, then there is only a limited range of motion. You should contrast this to the continuum, where an electron will accelerate without band. How does the lattice result connect with the continuum? The answer is that there are multiple bands:



As the electron accelerates it can tunnel from one band to another. This is known as Zener tunneling. We want to know the rate of this process.

A nice picture of this is in momentum space:



The role of the electric field is just to uniformly move  $k$ . When one comes to the band edge there is some probability that you stay in the first band, and some that you jump to the second band. Since all the action happens near the band edge, we will use a simple 2-level model, where the two levels represents the states in the first and second band,

$$H(t) = \begin{pmatrix} \alpha t & \Delta \\ \Delta & -\alpha t \end{pmatrix}. \quad (4.3)$$

Here  $\Delta$  is the band gap, and  $\alpha$  is related to how strong the electric fields is. Hence the time independent Hamiltonian, leads to an effective time dependent problem.

Similar physics also occurs if you have something like a Born-Openheimer approximation. The motion of the nucleus looks like a slow time dependent Hamiltonian to the electron.

## B. Conditions for adiabaticity

I always find it easier to go from the specific to the general, so lets think about the Hamiltonian we already introduced

$$H(t) = \begin{pmatrix} \alpha t & \Delta \\ \Delta & -\alpha t \end{pmatrix}. \quad (4.4)$$

While this can describe Zener tunneling, it is probably more concrete to think of Eq. (4.4) as the Hamiltonian for a spin-1/2 particle in a time dependent magnetic field. You get this sort of Hamiltonian all the time when you have time dependence in your Hamiltonian which takes you through an avoided crossing.

The time dependent Schrodinger equation is

$$i\hbar\partial_t\psi = H\psi. \quad (4.5)$$

We want to solve this equation in the semiclassical limit.

**Group Activity:** What is the semiclassical parameter?

In the limit  $\hbar\alpha/\Delta^2 \ll 1$  the time dependence of  $H$  is slow. This is analogous to our semiclassics in space, where in the limit  $\epsilon \ll 1$  the spatial variance of  $H$  was slow. In this limit it is natural to transform to the "adiabatic basis". That is, we diagonalize  $H(t)$  to find  $H(t)|+(t)\rangle = \epsilon(t)|+(t)\rangle$  and  $H(t)|-(t)\rangle = -\epsilon(t)|-(t)\rangle$ . Explicitly,

$$\epsilon(t)^2 = \Delta^2 + \alpha^2 t^2 \quad (4.6)$$

$$|+(t)\rangle = \begin{pmatrix} \cos(\xi/2) \\ \sin(\xi/2) \end{pmatrix} \quad (4.7)$$

$$|-(t)\rangle = \begin{pmatrix} -\sin(\xi/2) \\ \cos(\xi/2) \end{pmatrix} \quad (4.8)$$

where  $\tan \xi = \alpha t/\Delta$ . Note that in general  $|e\rangle$  and  $|g\rangle$  are ambiguous. We could always add an arbitrary phase to them. In the present case the ambiguity is trivial, and it has no effect. The general case, which we will treat later, gives additional phase factors: Berry's phase.

We want to know if you start at time  $-\infty$  in state  $|-\rangle$ , what is the probability that you end up in the state  $|+\rangle$ . To lowest order the probability is zero, and

$$|\psi(t)\rangle = e^{i \int^t \epsilon(t) dt/\hbar} |-(t)\rangle. \quad (4.9)$$

One gets this result by looking at the equations of motion for  $|\psi\rangle = a|+\rangle + b|-\rangle$ . Schrodinger's equation reads

$$\langle -|i\hbar\partial_t|\psi\rangle = i\hbar\partial_t b + a\langle -|i\hbar\partial_t|+\rangle + b\langle -|i\hbar\partial_t|-\rangle \quad (4.10)$$

$$= \langle -|H|\psi\rangle = -b\epsilon, \quad (4.11)$$

and a similar expression of  $a$ . Rewriting, this becomes

$$(i\hbar\partial_t + \epsilon)b = -a\langle -|i\hbar\partial_t|+\rangle - b\langle -|i\hbar\partial_t|-\rangle. \quad (4.12)$$

The right hand side is small in the semiclassical limit, leading to Eq. (4.13). The first term on the right hand side is responsible for the tunneling between branches, while the second term is a phase factor. If we neglect the first term, but include the second, we can improve Eq. (4.13) to become

$$|\psi(t)\rangle = e^{i \int^t \epsilon(t) dt/\hbar - i \int^t \langle -|i\partial_t|-\rangle} |-(t)\rangle. \quad (4.13)$$

The term  $\langle -|i\partial_t|-\rangle$  has to be real. This is because the operator  $i\partial_t$  is Hermitian. Interestingly, this phase factor does not depend on how fast  $\xi$  changes – it just depends on the path. Thus this is a "geometric" phase. It has had a profound impact on modern condensed matter physics.

In this particular example, it turns out that  $\langle -|i\partial_t|-\rangle = 0$ , so this whole discussion is moot, but soon we will repeat the argument with a more complicated Hamiltonian.

**Group Activity:** What is  $\langle -|i\hbar\partial_t|+\rangle, \langle -|i\hbar\partial_t|-\rangle$  and  $\langle +|i\hbar\partial_t|+\rangle$ ?

### C. Classic Approach to the Landau-Zener problem

Explicitly, the equations of motion for  $a$  and  $b$  are

$$(i\hbar\partial_t - \epsilon)a = \frac{i}{2}\partial_t\xi b \quad (4.14)$$

$$(i\hbar\partial_t + \epsilon)b = -\frac{i}{2}\partial_t\xi a \quad (4.15)$$

with

$$\partial_t\xi = \frac{\alpha/\Delta}{1 + \alpha^2 t^2/\Delta^2}. \quad (4.16)$$

Solving these is a real pain. The classic approach is to avoid this adiabatic basis altogether, and instead work in the original basis:

$$|\psi\rangle = \begin{pmatrix} C_1 e^{-\frac{i}{\hbar} \int^t \epsilon_1 dt} \\ C_2 e^{-\frac{i}{\hbar} \int^t \epsilon_2 dt} \end{pmatrix} \quad (4.17)$$

where  $\epsilon_1 = \alpha t$ , and  $\epsilon_2 = -\alpha t$  are the energies of the two basis states in the absence of coupling between the levels. This leads to equations of motion

$$i\hbar\partial_t C_1 = \Delta e^{\frac{i}{\hbar} \int (\epsilon_1 - \epsilon_2) dt} C_2 \quad (4.18)$$

$$i\hbar\partial_t C_2 = \Delta e^{\frac{i}{\hbar} \int (\epsilon_2 - \epsilon_1) dt} C_1 \quad (4.19)$$

with boundary conditions that at large negative time  $C_1 = 0$  and  $C_2 = 1$ . The two equations can be recast into a single second order differential equation, for

$$U_1 = e^{-\frac{i}{2\hbar} \int (\epsilon_1 - \epsilon_2) dt} C_1, \quad (4.20)$$

that reads

$$\partial_z^2 U_1 + (n + 1/2 - z^2/4)U_1 = 0 \quad (4.21)$$

where  $z = \alpha^{1/2} e^{-i\pi/4} t$ ,  $n = i\Delta^2/\alpha$ , and I lost my hbar's somewhere. Regardless, equation (4.21) is nothing but the equation of motion for a quantum mechanical

harmonic oscillator – except that we have a funny boundary condition. The solution is a "parabolic cylinder function" whose asymptotics can be used to calculate the probability of a transition:

$$P = \exp\left(-\frac{\pi}{2} \frac{\Delta^2}{\alpha}\right). \quad (4.22)$$

Ugh – I would hardly wish this on my worst enemy.

#### D. Analytic Continuation approach to the Landau-Zener Problem

There is a trick, similar to the one we used to find our connection formulas, which spares us much of that 18th century mathematics. Again it is not rigorous, but is a heck of a lot easier. What we do is assume that adiabaticity holds, and write

$$|\psi(t)\rangle = |\xi(t)\rangle_- e^{\frac{i}{\hbar} \int^t \epsilon(t) dt}, \quad (4.23)$$

where we have written  $|\xi(t)\rangle_-$  as a slightly more explicit notation for  $|-\rangle$ .

Now we do a bit of profound "out of the box" thinking. Equation (4.23) defines  $|\psi(t)\rangle$  on the entire complex  $t$  plane. There are two branch points in the complex plane at  $t = \pm i\Delta/\alpha$ . If one moves around one of them,  $|-\rangle$  turns into  $|+\rangle$ . Just as we were able to reproduce the asymptotics of the Airy function by analytically continuing around a branch point, perhaps we can reproduce the asymptotics of the parabolic cylinder functions by a similar procedure. If one goes on the path around the upper branch point

$$|\psi(t)\rangle = e^{i\Phi} e^{2i \int_0^{\Delta/\alpha} \epsilon(t) dt / \hbar} |\xi(t)\rangle_+ \quad (4.24)$$

$$= e^{i\Phi} e^{-2 \int_0^{\Delta/\alpha} \sqrt{\Delta^2 - \alpha^2 \tau^2} d\tau / \hbar} |\xi(t)\rangle_+, \quad (4.25)$$

where  $\Phi$  is an unimportant phase factor.

**Group Activity:** What is  $2 \int_0^{\Delta/\alpha} \sqrt{\Delta^2 - \alpha^2 \tau^2} d\tau / \hbar$ ?

Thus the probability of tunneling is

$$P = e^{-\frac{\pi}{2} \Delta^2 / \hbar \alpha}. \quad (4.26)$$