Notes for Lecture 19

Adiabatic theorem, Berry phase, Gauge symmetry, Aharanov-Bohm effect

As our last topic, we shall consider the adiabatic theorem, Berry's phase, and related topics.

First off, let us note that the word "adiabatic" is used in a different way here than in thermal physics or statistical mechanics. If you say "quantum adiabatic," then physicists will understand what you mean. The difference between these two usages will be explained below.

Closely connected with the adiabatic theorem is the geometrical effect, called **Berry's phase**. This is relatively speaking a very recently discovered effect (1984). The geometrical effect or the topological effect is a very important part of modern physics!

As we end this course, you may be pleasantly surprised that this adiabatic theorem is derived from a perturbation expansion, albeit a bit tricky one!

19.1 Adiabatic theorem

In statistical mechanics, we learn about an "adiabatic process." In that case, it means no heat exchange between the system of concern and the environment. Here, we are concerned with another type of "adiabatic process." In quantum mechanics, an adiabatic process means a *slow* process. Note that the word "adiabatic" does not necessary mean slow! It comes from the Greek word, that means "no passing" or "no crossing." In statistical mechanics, an adiabatic process is a process during which no heat is passed between systems of interest. **In quantum mechanics, an adiabatic process is a process by which no energy eigenstates cross each other**. In contrast, a "sudden process" would be a such process in which a potential is turned on abruptly, so that "all energy eigenstates mix." The book describes well the difference between these two types of processes in Figure T10.2 and its discussions.

Note that this means, right off the bat, **energy eigenvalues must be distinct** in an adiabatic process! This is so, since if at some point of the process, the two eigenvalues become identical, there will be a great mixing[1] between them, and the identities of the two eigenstates involved will be lost!

So, here are some of the assumptions that we make for an adiabatic process.

$$\hat{H}(t)\,|n;t\rangle \;=\; E_n(t)\,|n;t\rangle \qquad \hat{H} \text{ is slowly changing in time (see below)} \tag{19.1}$$

$$E_n(t) \;\neq\; E_m(t) \qquad m \neq n, \text{ at any } t \tag{19.2}$$

$$\frac{\partial \hat{H}}{\partial t} \;\propto\; \frac{1}{T_e} \ll \frac{1}{T_i} \sim \frac{\omega_i}{2\pi} \tag{19.3}$$

The ket $|n;t\rangle$ means the n-th eigenstate of $\hat{H}$ at time t. $\hbar\omega_i$ is the typical level spacing of the system. T_e is the time scale that characterizes the slow tuning of the Hamiltonian (by an external "knob": the subscript e means external). T_i is the period of the system (with the subscript i meaning internal), given by $T_i \sim 2\pi/\omega_i$.

The third condition is summarized as

$$\omega_e \ll \omega_i, \quad T_e \gg T_i, \quad \omega_e \equiv 2\pi/T_e \tag{19.4}$$

For brevity, we shall write

$$|n\rangle \;\equiv\; |n;t\rangle \tag{19.5}$$

That is, even without the explicit use of t, let us know that $|n\rangle$ is time dependent in general, in this lecture. Regardless of its time dependence, $\hat{H}(t)$ remains an observable operator at any fixed time, and so it is possible to expand any state in terms of its eigenstates $|n\rangle$.

$$|\Psi(t)\rangle \;=\; \sum_n C_n(t) e^{i\theta_n(t)}\,|n\rangle \tag{19.6}$$

$$\theta_n(t) \;\equiv\; -\frac{1}{\hbar}\int_0^t dt'\,E_n(t') \tag{19.7}$$

[1]Unless forbidden by symmetry.

Note that $\theta_n(t)$ is the phase factor that will exist even when $\hat{H}$ is time-independent. Now, we apply Schrödinger equation to $|\Psi(t)\rangle$, and we get

$$i\hbar \frac{d}{dt} |\Psi\rangle = \hat{H} |\Psi\rangle \tag{19.8}$$

To avoid any possible mistake, we will re-write $d/dt \to \partial/\partial t$, since as soon as any ket is represented, the total time derivative becomes the partial time derivative. In any case, we get, after canceling out the time derivative on the θ_n term with the right hand side,

$$\sum_n \left(\dot{C}_n(t) e^{i\theta_n(t)} |n\rangle + C_n(t) e^{i\theta_n(t)} \frac{\partial}{\partial t} |n\rangle \right) = 0 \tag{19.9}$$

Multiplying $\langle m|$ from the left, and using the orthonormality

$$\langle m | n \rangle = \delta_{m,n} \tag{1.9}$$

we get

$$\dot{C}_m(t) e^{i\theta_m(t)} = -\sum_n C_n(t) e^{i\theta_n(t)} \left\langle m \left| \frac{\partial}{\partial t} \right| n \right\rangle \tag{19.10}$$

$$= -C_m(t) e^{i\theta_m(t)} \left\langle m \left| \frac{\partial}{\partial t} \right| m \right\rangle + \sum_{n \neq m} C_n(t) e^{i\theta_n(t)} \left\langle m \left| \frac{\partial}{\partial t} \right| n \right\rangle \tag{19.11}$$

Now, by taking the time derivative on Eq. 19.1, it is possible to show that

$$\left\langle m \left| \frac{\partial}{\partial t} \right| n \right\rangle = \frac{\left\langle m \left| \frac{\partial \hat{H}}{\partial t} \right| n \right\rangle}{E_n(t) - E_m(t)} \qquad m \neq n \tag{19.12}$$

Note that the right hand side is proportional to $1/(T_e \omega_i)$, which is a very small number by assumption. So, it is reasonable to take the $\sum_{n \neq m}$ term as the perturbation. Then, in the zeroth order, we get

$$\dot{C}_m(t) = -C_m(t) \left\langle m \left| \frac{\partial}{\partial t} \right| m \right\rangle \tag{19.13}$$

This zeroth order solution is all we need here. Solving this differential equation, we get

$$C_m(t) = C_m(t) e^{-\int_0^t dt' \langle m | \frac{\partial}{\partial t'} | m \rangle}$$

Now, what kind of operator is $\frac{\partial}{\partial t}$ any way? Since $i\hbar \frac{\partial}{\partial t}$ is the "Hamiltonian operator" by Schrödinger equation, we see that $i \frac{\partial}{\partial t}$ is a "frequency operator" of sort. So, we define

$$\gamma_m(t) \equiv i \int_0^t dt' \left\langle m \left| \frac{\partial}{\partial t'} \right| m \right\rangle \tag{19.14}$$

as "phase." From the normalized nature of $|m\rangle$, we get $\frac{\partial}{\partial t}\langle m|m\rangle = 0 = 2\,\mathrm{Re}\left(\left\langle m\left|\frac{\partial}{\partial t}\right|m\right\rangle\right) = 0$, and so $\gamma_m(t)$ is real, as expected. Therefore, what we have is that

$$|\Psi(t)\rangle = \sum_n C_n(0)e^{i\gamma_n(t)}e^{i\theta_n(t)}|n;t\rangle \qquad \gamma_n \text{ (Eq. 19.14) and } \theta_n \text{ (Eq. 19.7) are real.} \tag{19.15}$$

which amounts to the **adiabatic theorem**, which states that if the initial state is the m-th energy eigenstate, then it will remain so as the system is slowly tuned with a time scale T_e that is much longer than the internal time scale. It is easy to see that this is the case, if we assign $C_n(0) = \delta_{m,n}$ as our initial condition.

19.2 Berry phase

Suppose the system is changing by a time-dependent parameter $R(t)$, then (after recovering the total time derivative, since the following expression is representation independent)

$$\begin{aligned}\gamma_m(t) &\equiv i\int_0^t dt'\left\langle m\left|\frac{d}{dt'}\right|m\right\rangle = i\int_0^t dt'\frac{dR}{dt'}\left\langle m\left|\frac{d}{dR}\right|m\right\rangle \\ &= i\int_{R_0}^R dR\left\langle m\left|\frac{d}{dR}\right|m\right\rangle\end{aligned}$$

If there are multiple parameters, then we have a vector calculus, and get

$$\gamma_m(t) = i\int_{\vec{R}_0}^{\vec{R}} d\vec{R}\cdot\langle m|\nabla_R|m\rangle \tag{19.16}$$

Now, consider making a closed path

$$\gamma_m(T) \equiv i\oint d\vec{R}\cdot\langle m|\nabla_R|m\rangle \qquad \textbf{Berry phase} \tag{19.17}$$

where T means the (long) time in which the state is brought back to the original state. Note that the Berry phase is non-zero in general!

If $\vec{R}$ is a three dimensional vector, then by Stoke's theorem we get

$$\gamma_m(T) = \int d\vec{\sigma}\cdot\vec{\mathcal{B}} \tag{19.18}$$

where

$$\vec{\mathcal{B}} \equiv i\nabla_R\times\langle m|\nabla_R|m\rangle \tag{19.19}$$

and so, in this case, **the Berry phase is the Berry "flux"** for some fictitious field $\vec{\mathcal{B}}$.

A well-known example of a Berry's phase is when an angular momentum state (with the maximum angular momentum quantum number, $m = j$; Here, m is the quantum number for $\hat{J}_z$, and happens to be the same alphabet letter for the state index that we have been using in this section, so far!) is rotated around and then brought back to the original state. In this case, the Berry's phase is given by $-j\Omega$ (cf., homework), where Ω is the total solid angle swept by the rotational motion.

$$\gamma_{m=j}(T) = -j\Omega \tag{19.20}$$

Note that this is consistent with what we already know as an odd property of spin 1/2. If we take a z spin up state and then rotate it around the, say, x axis, then the total solid angle swept is given by 2π (because the solid angle swept by the motion corresponds to a hemisphere in this case). So, the Berry's phase is given by $-\pi$! Considering the geometric phase alone (γ_m, but not θ_m), we get the strange result that the spin 1/2 wave function acquires a negative sign when it is rotated 360 degrees—however, we already knew it from HW 1.5! Here we have a much more general result for a general angular momentum value in the above equation.

When expressed in terms of its spatial integral, γ_m is recognized clearly as a **geometrical phase** as opposed to the **dynamic phase** θ_n. It does not depend on how it occurs in the time domain, as long as it is the result of a slow motion. The value of γ_m is dependent only on the geometrical parameters $\vec{R}$.

19.3 Gauge invariance

If the vector potential problem is somewhat strange (HW 7.1, 7.2), it is an interesting one! One can work the same problem in different "gauges," with interesting results, some of which are gauge-dependent (no measurable consequence) while all measurable quantities are gauge-independent. This is the notion of the gauge symmetry, or the gauge invariance. In modern physics, this symmetry plays an important role.

Let us recall that the gauge transformation of classical E&M. The transformation

$$\vec{A} \to \vec{A} + \nabla f \tag{14.4}$$

$$\phi \to \phi - \frac{\partial f}{\partial t} \tag{14.5}$$

leaves the classical E&M unchanged, since neither the $\vec{E}$ field, nor the $\vec{B}$ field is affected by f (cf. Eqs. 14.2,14.3).

How might this affect quantum mechanics?

Consider two Hamiltonians

$$H_1(\vec{r},\vec{p},t) = \frac{(\vec{p}-q\vec{A})^2}{2m} + q\phi \tag{14.1}$$

$$H_2(\vec{r},\vec{p},t) = \frac{(\vec{p}-q\vec{A}-q\nabla f)^2}{2m} + q\phi - q\frac{\partial f}{\partial t} \tag{19.21}$$

These two Hamiltonians *must be* equivalent in quantum mechanics! But, in what sense?

Suppose that

$$\hat{H}_1 |\Psi_1\rangle = i\hbar\frac{d}{dt}|\Psi_1\rangle \tag{19.22}$$

Define

$$\Psi_2(\vec{r},t) = e^{i\frac{q}{\hbar}f}\Psi_1(\vec{r},t) \tag{19.23}$$

It is easy to verify that if

$$H_1(\vec{r},-i\hbar\nabla,t)\Psi_1 = i\hbar\frac{\partial}{\partial t}\Psi_1 \tag{19.24}$$

then

$$H_2(\vec{r},-i\hbar\nabla,t)\Psi_2 = i\hbar\frac{\partial}{\partial t}\Psi_2 \tag{19.25}$$

holds.

Namely, the gauge transformation corresponds to the phase shift of the wave function, while the phase is position and time dependent. Physically measurable quantities are invariant upon the gauge transformation.

19.4 Aharanov-Bohm effect

The topology of space in which particles exist can have a dramatic consequence. The Aharanov-Bohm effect is a famous example.

Here, the infinitely long cylinder such as we considered in page 3 of LN 14 is re-considered. Outside the solenoid, the vector potential is given by

$$\vec{A} = B_0\frac{R^2}{2r}\vec{e}_\theta, \quad r > R \tag{14.10}$$

where B_0 is the field inside the solenoid. By line-integrating this vector potential along a circle, we get

$$\int^{\theta} d\vec{l} \cdot \vec{A} = B_0 \frac{R^2}{2} \theta + \text{ const} \tag{19.26}$$

Taking note of this, one might try a gauge transformation such as

$$\vec{A} \to \vec{A} + \nabla f \quad \text{with } f = -B_0 \frac{R^2}{2} \theta \qquad (\textit{not} \text{ a valid gauge transformation})$$

to claim that one can simply get rid of the vector potential of the problem! But such a claim is clearly false. This is because the magnetic flux enclosed $\oint d\vec{l} \cdot \vec{A}$ must be clearly invariant upon a gauge transformation, but this transformation that we just considered make that flux vanish. What is wrong with this f? The answer is that it is not a good function at all. First of all, it is multi-valued! One might say—so what? It is not like it represents a physically observable quantity. This is a reasonable argument. However, here is a more serious problem. It is not analytic at the origin!

While the above gauge transformation is not allowed, it does give us the solution to the problem, if we simply take into account the mathematical consequence for outside the solenoid[2]! From Eq. 19.23

$$\Psi(\vec{r}) = \exp\left(i \frac{q B_0 R^2}{2\hbar} \theta \right) \Psi_2(\vec{r}) = \exp\left(i \frac{q\Phi}{h} \theta \right) \Psi_2(\vec{r}) \tag{19.27}$$

where

$$\Phi = B_0 \pi R^2 \tag{19.28}$$

is the total flux enclosed inside the solenoid.

Here, Ψ_2 is the wave function that one would get, if one assumes that $\vec{A}$ is simply absent, i.e., it would be the wave function that would be written down by someone who did not know at all that there is a solenoid somewhere at the center of space. That someone would not know about the extra phase factor $\exp\left(i \frac{q\Phi}{h} \theta\right)$ at all. Would this be bad? For the most time, or more precisely speaking for local physics, the answer is no. From that person's local point of view, the "kinematical momentum" (the part that corresponds to $m\vec{v}$ of classical mechanics, i.e., $\vec{p} - q\vec{A}$) is equal to the canonical momentum. However, there is a situation when this naive picture breaks down. Such is an experiment that Aharanov-Bohm originally proposed.

[2]Put another way, if the space that we are concerned with excludes the solenoid, then it is as though we do not know the existence of the magnetic flux! So, it would *seem* to us that the above gauge transformation is valid! As we accept this viewpoint, the topological nature of this problem becomes clear, since we are defining the space as excluding the region at the center, where the solenoid resides.

In this experiment a beam of quantum particles is sent through a "beam splitter" so that half the beam is sent to the left and then made to circle around the solenoid clockwise (from top view) and half the beam is sent to the right and then made to circle around the solenoid counter-clockwise. We shall assume that the two paths are completely symmetrical and so that the two beams take exactly the same time to arrive at the other side. When the two beams arrive at the other side of the solenoid and meet, the two wave functions differ in phase by

$$\frac{q\Phi}{h}2\pi \tag{19.29}$$

since the Ψ_2 part would be completely identical (the time evolution phase factor would be identical due to the symmetric nature of the paths). So there *would be an interference effect* when the two beams meet on the other side of the solenoid, if the magnetic flux Φ is changed!

This is a topological effect, in the following sense. As already mentioned, if the person who is living in this field free region outside the solenoid is only concerned with local affairs, there will be nothing to note. However, if this person is, say, carrying a quantum particle from point A, around the solenoid, and then back to A, there will be a **geometric phase accumulation** exactly by $q\Phi 2\pi/h$ due to the transport. If this person does the same transport again, then there will be an additional phase accumulation of the same amount. If this person is very far away from the solenoid, then the person may not see the solenoid and may not know about it. However, if the person measures the phase accumulation by an interference experiment, then it may be concluded that there is a **winding number** associated with the space itself! That person may send a team of explorers to figure out the topology of space, and if that team is successful, they will know that at the center of space, there is a mysterious column (of solenoid)! Topologically speaking, it is like the world the person is living in is a donut/bagel (let us assume that the living space is the volume of the donut, so that there is only one kind of winding number)!

Such donut like space is actually created routinely in a laboratory, in the form of a superconducting ring. In such a setup, there is actually no solenoid at the center, but there is a magnetic flux trapped inside the donut hole. So, in terms of the existence of a magnetic flux, the effect is the same having a solenoid. The wave function of superconducting electrons is *spread throughout the entire ring*. This is due to the macroscopic condensation nature of the superconducting state. In any case, if the wave function is extended throughout the ring, then one would have to say that for the wave function, Eq. 19.27, to be single valued

$$\frac{q\Phi}{h} = n \qquad n = 0, \pm 1, \pm 2, \ldots \tag{19.30}$$

This is the so-called **flux quantization** condition.

$$\Phi = n\frac{h}{|q|} \qquad n = 0, \pm 1, \pm 2, \ldots \tag{19.31}$$

Note the similarity with what we found in HW 7.2, if $q = -e$ is taken! Well, for a superconducting ring, it turns out that the flux is quantized with $q = -2e$ instead of $-e$, which is the proof that the so-called "Cooper pair" of two electrons are indeed responsible for the superconductivity.

It is clear that the Aharanov-Bohm effect is a geometric effect, as from Eq. 19.27, the dynamic phase is completely included in the time evolution of Ψ_2, and the phase $q\Phi\theta/h$ corresponds to an additional phase "γ_m" described in Section 19.2. It is also possible to demonstrate this explicitly, as done in the textbook.

Lastly, notice that the physically observable effect is dependent only on the gauge independent quantity Φ, the magnetic flux, in this problem. So, the Aharanov-Bohm phenomenon *is* gauge-invariant, and there is no reason to think that $\vec{A}$ itself is playing an important role—it is not.

Having said this, and as we conclude this course of quantum mechanics, let us note (as you might already know) that in a superconductor, the gauge symmetry *is* broken, and the system chooses a certain value of $\vec{A}$, which is directly related to the super-current. So, a *very* interesting phenomenon like that happens in fascinating materials that we can hold in our hands!