Lecture 20

Relevant sections in text: §2.6, 3.1

Gauge transformations (cont.)

Our proof that the spectrum of the Hamiltonian does not change when the potentials are redefined by a gauge transformation also indicates how we are to use our model so that all probabilities are unaffected by gauge transformations. We decree that if $|\psi\rangle$ is the state vector of a particle in an EM field described by the potentials $(\phi, \vec{A})$, then

$$|\psi\rangle' = e^{\frac{iq}{\hbar c}f(\vec{X})}|\psi\rangle$$

is the state vector of the particle when using the gauge transformed potentials $(\phi', \vec{A}')$. Note that this is a unitary transformation.

Let us now see why this prescription works. For a particle, all observables are functions of the position and momentum operators. Here "momentum" means either canonical or mechanical. The position observable is represented (in the Schrödinger picture) by the usual operator $\vec{X}$, no matter the gauge. Any observable function G of the position has an expectation value which does not change under a gauge transformation:

$${}'\langle\psi|G(\vec{X})|\psi\rangle' = \langle\psi|e^{-\frac{iq}{\hbar c}f(\vec{X})}G(\vec{X})e^{\frac{iq}{\hbar c}f(\vec{X})}|\psi\rangle = \langle\psi|G(\vec{X})|\psi\rangle.$$

The momentum operator is where things get more interesting. The mechanical momentum is a gauge-invariant observable. But it is represented by an operator which changes under a gauge transformation! Indeed, we have

$$\vec{\Pi} = \vec{p} - \frac{q}{c}\vec{A}, \quad \vec{\Pi}' = \vec{p} - \frac{q}{c}(\vec{A} + \nabla f).$$

However, it is straightforward to check that (exercise)

$$\vec{\Pi}' e^{\frac{iq}{\hbar c}f(\vec{X})}|\psi\rangle = e^{\frac{iq}{\hbar c}f(\vec{X})}\vec{\Pi}|\psi\rangle.$$

Put differently, we have the operator representing the mechanical momentum – which is a gauge-invariant observable – transforming under a gauge transformation as a unitary transformation:

$$\vec{\Pi}' = e^{\frac{iq}{\hbar c}f(\vec{X})}\vec{\Pi}e^{-\frac{iq}{\hbar c}f(\vec{X})}.$$

Any function of the position and (mechanical) momentum will have a similar transformation law. In particular, the Hamiltonian can be expressed as (exercise)

$$H = \frac{1}{2m}\Pi^2 + q\phi,$$

so it follows that (exercise)

$$H' e^{\frac{iq}{\hbar c} f(\vec{X})} |\psi\rangle = e^{\frac{iq}{\hbar c} f(\vec{X})} H|\psi\rangle,$$

that is,

$$H' = e^{\frac{iq}{\hbar c} f(\vec{X})} H e^{-\frac{iq}{\hbar c} f(\vec{X})}.$$

The physical output of quantum mechanics is not changed by a unitary transformation of the state vectors and a unitary (similarity transformation) of the observables. This is because the expectation values will not change in this case:

$$\langle\psi|C|\psi\rangle = \langle\psi'|C'|\psi'\rangle,$$

where

$$|\psi'\rangle = U|\psi\rangle, \quad C' = UCU^\dagger.$$

It is now easy to see that if you compute the expectation value of (any function of the) mechanical momentum you can use the state $|\psi\rangle$ and operator $\vec{\Pi}$, or you can use the vector $|\psi\rangle'$ and operator $\vec{\Pi}'$, and get the same answer. In this way one says that the physical output of quantum mechanics is suitably gauge invariant. Different choices of potentials lead to unitarily equivalent mathematical representations of the same physics.

It is not hard to generalize all this to time dependent gauge transformations$f = f(t, \vec{x})$. Here we simply observe that if $|\psi, t\rangle$ is a solution to the Schrödinger equation for one set of potentials then (exercise)

$$|\psi, t\rangle' = e^{\frac{iq}{\hbar c} f(t,\vec{X})} |\psi, t\rangle$$

is the solution for potentials obtained by a gauge transformation defined by f. Thus one gets gauge invariant results for the probability distributions as functions of time. This result also shows that position wave function solutions to the Schrödinger equation transform as

$$\psi(\vec{x}, t) \to e^{\frac{iq}{\hbar c} f(t,\vec{x})} \psi(\vec{x}, t)$$

under a gauge transformation.

Aharonov-Bohm effect

The Aharonov-Bohm effect involves the effect of a magnetic field on the behavior of a particle even when the particle has vanishing probability for being found where the magnetic field is non-vanishing. Of course, classically the Lorentz force law would never lead to such behavior. Nevertheless, the AB effect has been seen experimentally. You will explore one version of this effect in a homework problem. Here let me just show you how, technically, such a result can occur.

The key to the AB effect is to cook up a physical situation where the magnetic field is non-vanishing in a region (from which the charged particle will be excluded) and vanishing in a non-simply connected region where the particle is allowed to be. Since the magnetic field vanishes in that region we have that

$$\nabla \times \vec{A} = 0.$$

In a simply connected, "contractible" region of space such vector fields must be the gradient of a function. In this case the potential can be gauge transformed to zero, and there will be no physically observable influence of the magnetic field in this region. However, if the region is not simply connected it need not be true that $\vec{A}$ is a gradient, *i.e.,* "pure gauge". As an example (relevant to your homework), we study the following scenario.

Consider a cylindrical region with uniform magnetic field (magnitude B) along the axis of the cylinder. You an imagine this being set up via an (idealized) solenoid. Outside of the cylinder the magnetic field vanishes, but the vector potential outside the cylinder must be non-trivial. In particular $\vec{A}$ cannot be the gradient of a function everyhwere outside the cylinder. To see this, we have from Stokes theorem:

$$\int_C \vec{A} \cdot d\vec{l} = \int_S \vec{B} \cdot d\vec{s},$$

where C is a closed contour enclosing the cylinder and S is a surface with boundary C, so that the right-hand side is never zero if the flux of $\vec{B}$ through S is non-zero (which it isn't in our example). But if $\vec{A}$ is a gradient then the left-hand side vanishes (exercise) – contradiction. In fact, the vector potential can be taken to be (exercise)

$$\vec{A} = \frac{1}{2}\frac{BR^2}{2r}\hat{e}_\theta, \quad r > R$$

where R is the radius of the cylinder, $r > R$ is the cylindrical radial coordinate and $\hat{e}_\theta$ is a unit vector in the direction of increasing cylindrical angle. Since $\vec{A}$ is necessarily not (gauge-equivalent to) zero, it can affect the energy spectrum – and it does.

Angular momentum - introductory remarks

The theory of angular momentum in quantum mechanics is important in many ways. The myriad of results of this theory, which follow from a few simple principles, are used extensively in applications of quantum mechanics to atomic, molecular, nuclear and other subatomic systems. The mathematical strategies involved have a number of important generalizations to other types of symmetries and conservation laws in quantum mechanics. The quantum mechanical theory of angular momentum leads naturally to the concept of "intrinsic spin". Just as we saw for spin 1/2, a general feature of angular momentum in quantum mechanics is the incompatibility of the observables corresponding to any two components of spin. The nature of this incompatibility is at the heart of virtually all features of angular momentum.

Just as linear momentum is intimately connected with the notion of translation of the physical system, so angular momentum is deeply tied to the theory of rotations of the physical system being considered. We shall use this geometric interpretation of angular momentum as the starting point for our discussion.