Lecture 20

Relevant sections in text: §2.6

More on the mechanical momentum

Here is an interesting observation: while the components of the canonical momenta are compatible,

$$[P_i, P_j] = 0,$$

the mechanical momenta are not when there is a magnetic field:

$$[\Pi_i, \Pi_j] = i\hbar\frac{q}{c}(\frac{\partial A_i}{\partial x^j} - \frac{\partial A_j}{\partial x^i}) = i\hbar\frac{q}{c}\epsilon_{ijk}B^k.$$

Thus, in the presence of a magnetic field, the mechanical momenta obey an uncertainty relation! This is a surprising, non-trivial and quite robust prediction of quantum mechanics. In particular, if the field is uniform, then two components of mechanical momentum will obey a state independent uncertainty relation rather like ordinary position and momentum. Can this prediction be verified? As you will see in your homework problems, this incompatibility of the mechanical momentum components in the presence of a magnetic field is responsible for the "Landau levels" for the energy of a charged particle in a uniform magnetic field. These levels are well-known in condensed matter physics.

Heisenberg equations for a charged particle in an electromagnetic field

The remaining set of Heisenberg equations are most simply expressed using the mechanical momentum. Starting with

$$H = \frac{\Pi^2}{2m} + q\phi(\vec{X}),$$

using the commutation relations between components of the mechanical momentum (above), and using

$$[X^i, \Pi_j] = i\hbar\delta^i_j I,$$

we have (exercise)

$$\frac{d}{dt}\vec{\Pi}(t) = \frac{1}{i\hbar}[\vec{\Pi}(t), H] = q\left\{\vec{E}(\vec{X}(t)) + \frac{1}{2mc}\left(\vec{\Pi}(t)\times\vec{B}(\vec{X}(t)) - \vec{B}(\vec{X}(t))\times\vec{\Pi}(t)\right)\right\}.$$

Except for the possible non-commutativity of $\vec{\Pi}$ and $\vec{B}$, this is the usual Lorentz force law for the operator observables.

The Schrödinger equation

Dynamics in the Schrödinger picture is controlled by the Schrödinger equation. If we compute it for position wave functions then we get (exercise)

$$\frac{1}{2m}\left(\frac{\hbar}{i}\nabla - \frac{q}{c}\vec{A}(\vec{x})\right)^2\psi(\vec{x},t) + q\phi(\vec{x},t)\psi(\vec{x},t) = i\hbar\frac{\partial}{\partial t}\psi(\vec{x},t).$$

The left hand side represents the action of the Hamiltonian as a linear operator on position wave functions. We have in detail

$$H\psi = -\frac{\hbar^2}{2m}\nabla^2\psi - \frac{q\hbar}{imc}\left[\vec{A}\cdot\nabla\psi + \frac{1}{2}(\nabla\cdot\vec{A})\psi\right] + [\left(\frac{q}{c}\right)^2 A^2 + q\phi]\psi.$$

As you may know, one can always arrange (by making a gauge transformation if necessary) to use a vector potential that satisfies the "Coulomb gauge":

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

In this case the Hamiltonian on position wave functions takes the form

$$H\psi = -\frac{\hbar^2}{2m}\nabla^2\psi - \frac{q\hbar}{imc}\vec{A}\cdot\nabla\psi + [\left(\frac{q}{c}\right)^2 A^2 + q\phi]\psi.$$

Gauge transformations

There is a subtle issue lurking behind the scenes of our model of a charged particle in a prescribed EM field. It has to do with the explicit appearance of the potentials in the operators representing various observables. For example, the Hamiltonian – which should represent the energy of the particle – depends quite strongly on the form of the potentials. The issue is that there is a lot of mathematical ambiguity in the form of the potentials and hence operators like the Hamiltonian are not uniquely defined. Let me spell out the source of this ambiguity.

You may recall from your studies of electrodynamics that, if $(\phi, \vec{A})$ define a given EM field $(\vec{E}, \vec{B})$, then the potentials $(\phi', \vec{A}')$, given by

$$\phi' = \phi - \frac{1}{c}\frac{\partial f}{\partial t}, \quad \vec{A}' = \vec{A} + \nabla f,$$

define the same $(\vec{E}, \vec{B})$ *for any choice of* $f = f(t, \vec{x})$. Because all the physics in classical electrodynamics is determined by $\vec{E}$ and $\vec{B}$, we declare that all potentials related by such *gauge transformations* are physically equivalent in the classical setting. In the quantum setting, we must likewise insist that this gauge ambiguity of the potentials does not affect physically measurable quantities. Both the Hamiltonian and the mechanical momentum are represented by operators which change their mathematical form when gauge-equivalent potentials are used. The issue is how to guarantee the physical predictions are nonetheless gauge invariant.

Let us focus on the Hamiltonian for the moment. The eigenvalues of H define the allowed energies; the expansion of a state vector in the eigenvectors of H defines the probability distribution for energy; and the Hamiltonian defines the time evolution of the system. The question arises whether or not these physical aspects of the Hamiltonian operator are in fact influenced by a gauge transformation of the potentials. If so, this would be a Very Bad Thing. Fortunately, as we shall now show our model for a particle in an EM field can be completed so that the physical output of quantum mechanics (spectra, probabilities) are unaffected by gauge transformations.

For simplicity (only) we still assume that H is time-independent and we only consider gauge transformations for which $\frac{\partial f}{\partial t} = 0$. The key observation is the following. Consider two charged particle Hamiltonians H and H' differing only by a gauge transformation of the potentials, so that they should be physically equivalent. Our notation is that if H is defined by $(\phi, \vec{A})$ then H' is defined by the gauge transformed potentials

$$\phi' = \phi, \quad \vec{A}' = \vec{A} + \nabla f(\vec{x}),$$

It is now straightforward to verify (see below) that if $|E\rangle$ satisfies

$$H|E\rangle = E|E\rangle,$$

then

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

satisfies

$$H'|E\rangle' = E|E\rangle'.$$

Note that the eigenvalue is the same in each case. The operator $e^{\frac{iq}{\hbar c} f(\vec{X})}$ is unitary, and this implies the spectra of H and H' are identical. Thus one can say that the spectrum of the Hamiltonian is unaffected by a gauge transformation, that is, the spectrum is *gauge invariant.* Thus one can use whatever potentials one wishes to compute the energy spectrum and the prediction is always the same.

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,

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

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)

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

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.