Lecture 19

Relevant sections in text: §2.6

Charged particle in an electromagnetic field

We now turn to another extremely important example of quantum dynamics. Let us describe a non-relativistic particle with mass m and electric charge q moving in a given electromagnetic field. This system has obvious physical significance.

We use the same position and momentum operators (in the Schrödinger picture) $\vec{X}$ and $\vec{P}$ (although there is a subtlety concerning the meaning of momentum, to be mentioned later). To describe the electromagnetic field we need to use the electromagnetic scalar and vector potentials $\phi(\vec{x}, t), \vec{A}(\vec{x}, t)$. They are related to the familiar electric and magnetic fields $(\vec{E}, \vec{B})$ by

$$\vec{E} = -\nabla\phi - \frac{1}{c}\frac{\partial \vec{A}}{\partial t}, \quad \vec{B} = \nabla \times \vec{A}.$$

The dynamics of a particle with mass m and charge q is determined by the Hamiltonian

$$H = \frac{1}{2m}\left(\vec{P} - \frac{q}{c}\vec{A}(\vec{X}, t)\right)^2 + q\phi(\vec{X}, t).$$

This Hamiltonian takes the same form as the classical expression in Hamiltonian mechanics. We can see that this is a reasonable form for H by computing the Heisenberg equations of motion, and seeing that they are equivalent to the Lorentz force law, which we shall now demonstrate.

For simplicity we assume that the potentials are time independent, so that the Heisenberg and Schrödinger picture Hamiltonians are the same, taking the form

$$H = \frac{1}{2m}\left(\vec{P} - \frac{q}{c}\vec{A}(\vec{X})\right)^2 + q\phi(\vec{X}).$$

For the positions we get (exercise)

$$\frac{d}{dt}\vec{X}(t) = \frac{1}{i\hbar}[\vec{X}(t), H] = \frac{1}{m}\{\vec{P}(t) - \frac{q}{c}\vec{A}(\vec{X}(t))\}.$$

We see that (just as in classical mechanics) the momentum – defined as the generator of translations – is not necessarily given by the mass times the velocity, but rather

$$\vec{P}(t) = m\frac{d\vec{X}(t)}{dt} + \frac{q}{c}\vec{A}(\vec{X}(t)).$$

As in classical mechanics we sometimes call $\vec{P}$ the *canonical momentum*, to distinguish it from the *mechanical momentum*

$$\vec{\Pi} = m\frac{d\vec{X}(t)}{dt} = \vec{P} - \frac{q}{c}\vec{A}(\vec{X}(t))$$

Note that the mechanical momentum has a direct physical meaning, while the canonical momentum depends upon the non-unique form of the potentials. We will discuss this in detail soon.

While the components of the canonical momenta are compatible,

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

the mechanical momenta are not (!):

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

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.

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

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

Some typical electromagnetic potentials that are considered are the following.

(i) The Coulomb field, with

$$\phi = \frac{k}{|\vec{x}|}, \quad \vec{A} = 0,$$

which features in a simple model of the hydrogen atom; the spectrum and stationary states should be familiar to you. We will soon study it a bit in the context of angular momentum issues.

(ii) A uniform magnetic field $\vec{B}$, where

$$\phi = 0, \quad \vec{A} = \frac{1}{2}B\times\vec{x}.$$

The vector potential is not unique, of course. This potential is in the Coulomb gauge. You will explore this system in your homework. The results for the stationary states are interesting. One has a continuous spectrum coming from the motion along the magnetic field; but for a given momentum value there is a discrete spectrum of "Landau levels" coming from motion in the plane orthogonal to $\vec{B}$. To see this one massages the Hamiltonian into the mathematical form of a free particle in one dimension added to a harmonic oscillator; this is the gist of your homework problem.

(iii) An electromagnetic plane wave, in which

$$\phi = 0, \quad \vec{A} = \vec{A}_0\cos(\vec{k}\cdot\vec{x} - kct), \quad \vec{k}\cdot\vec{A}_0 = 0.$$

Of course, this latter example involves a time dependent potential. This potential is used to study the very important issue of interaction of atoms with a radiation field; maybe we will have time to study this toward the end of the semester.

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.

To be continued...