Putting the Magnetic Field into the Lagrangian and QM

1 Fixing up the Lagrangian

We will consider a particle of mass m and charge q moving in *static* electric and magnetic fields; we will work in the non-relativistic regime.

With the possibility of both electric *and* magnetic forces, we want to set up the Lagrangian L for the problem so that the equations of motion will follow from the Euler–Lagrange equations. How do we do this?

The electric potential energy is $U_{\rm elec} = qV$, where $\mathbf{E} = -\nabla V$. In elementary discussions of the Lagrangian, we are told to form

$$L(\mathbf{r}, \dot{\mathbf{r}}) = T - U = \tfrac{1}{2}mv^2 + U(\mathbf{r}) \tag{1}$$

where $v = |\dot{\mathbf{r}}|$.

Obviously the electric potential energy $U_{\rm elec}$ just adds on to the other kinds of potential energy in 1 that might be in the problem; if there is *only* electric potential energy, then the Lagrangian is

$$L(\mathbf{r}, \dot{\mathbf{r}}) = \tfrac{1}{2}mv^2 - qV(\mathbf{r}) \tag{2}$$

But there is no potential energy associated with the magnetic field (it does no work!) so how can it possibly be included in the Lagrangian? The answer is that for a force like that of magnetism which arises from a vector potential $\mathbf{A}$, the thing we write down (instead of 2) is

$$L(\mathbf{r}, \dot{\mathbf{r}}) = \tfrac{1}{2}mv^2 - qV(\mathbf{r}) + q\mathbf{v}\cdot\mathbf{A} \tag{3}$$

Note the functional dependence of of the parts of L: v contains the components of $\dot{\mathbf{r}}$; V depends only on the components of $\mathbf{r}$; $\mathbf{A}$ depends only on the components of $\mathbf{r}$ but it appears dotted with $\mathbf{v} = \dot{\mathbf{r}}$. The latter fact will give some interesting results.

With 3 as the Lagrangian, we *do* get the correct equation of motion, but showing this takes some care and that's what we'll do now.

2 Getting the Equations of Motion from L

We want to show that when we apply the Euler–Lagrange equations,

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}_i}\right) = \frac{\partial L}{\partial x_i} \qquad \text{where} \quad x_i = x, y, z \tag{4}$$

we get the Lorentz force equation, $\mathbf{F} = q(\mathbf{E} + \mathbf{v}\times\mathbf{B})$. At first glance it may seem impossible, because the latter contains a cross product which mixes up the components, while the Euler–Lagrange equations are written out for *each* degree of freedom separately. But we will get it!

We'll work on the left side of 4 first. We'll form the E–L equation for the degree of freedom x (of course y and z will be similar). First, find $\partial L/\partial \dot{x}$. Eq. 3 gives

$$\frac{\partial L}{\partial \dot{x}} = m\dot{x} + qA_x \tag{5}$$

Now take $\frac{d}{dt}(\partial L/\partial \dot{x})$. The first term in 5 gives $m\ddot{x}$, but the second term requires some care. A_x has an explicit dependence on (x, y, z) and (by our assumption) no *explicit* dependence on t, but each of the three coordinates has a dependence on time; in fact the total time derivative of A_x is

$$\frac{d}{dt}A_x = \frac{\partial A_x}{\partial x}\frac{dx}{dt} + \frac{\partial A_x}{\partial y}\frac{dy}{dt} + \frac{\partial A_x}{\partial z}\frac{dz}{dt} = \frac{\partial A_x}{\partial x}\dot{x} + \frac{\partial A_x}{\partial y}\dot{y} + \frac{\partial A_x}{\partial z}\dot{z} \tag{6}$$

This can be written as $\mathbf{v} \cdot \nabla$ operating on A_x:

$$\frac{d}{dt}A_x = (\mathbf{v} \cdot \nabla)A_x = [(\mathbf{v} \cdot \nabla)\mathbf{A}] \cdot \hat{\mathbf{x}} \tag{7}$$

Using these results in 5, we get:

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}}\right) = m\ddot{x} + q[(\mathbf{v} \cdot \nabla)\mathbf{A}] \cdot \hat{\mathbf{x}} \tag{8}$$

Now work on the right side of 4. We find:

$$\begin{aligned} \frac{\partial L}{\partial x} &= -q\frac{\partial V}{\partial x} + q\left[v_x\frac{\partial A_x}{\partial x} + v_y\frac{\partial A_y}{\partial x} + v_z\frac{\partial A_z}{\partial x}\right] \\ &= -q\frac{\partial V}{\partial x} + q\left[\nabla(\mathbf{v} \cdot \mathbf{A})\right] \cdot \hat{\mathbf{x}} \end{aligned} \tag{9}$$

Replace both sides of Eq. 4 (and use $-\partial V/\partial x = E_x$) and get

$$m\ddot{x} + q[(\mathbf{v} \cdot \nabla)\mathbf{A}] \cdot \hat{\mathbf{x}} = qE_x + q\left[\nabla(\mathbf{v} \cdot \mathbf{A})\right] \cdot \hat{\mathbf{x}} \tag{10}$$

Combine the two terms with the $\hat{\mathbf{x}}$ and get:

$$m\ddot{x} = qE_x + q\left[\nabla(\mathbf{v} \cdot \mathbf{A}) - (\mathbf{v} \cdot \nabla)\mathbf{A}\right] \cdot \hat{\mathbf{x}} \tag{11}$$

Now, using that fact that $\mathbf{v}$ has no dependence on $\mathbf{r}$, one of the vector product rules from the inside front cover of the book gives:

$$\nabla(\mathbf{v} \cdot \mathbf{A}) = \mathbf{v} \times (\nabla \times \mathbf{A}) + (\mathbf{v} \cdot \nabla)\mathbf{A} \tag{12}$$

Using this in 11 gives

$$m\ddot{x} = qE_x + q\left[\mathbf{v} \times (\nabla \times \mathbf{A})\right] \cdot \hat{\mathbf{x}} \tag{13}$$

Use $\nabla \times \mathbf{A} = \mathbf{B}$ and get:

$$m\ddot{x} = qE_x + q\left[\mathbf{v} \times \mathbf{B}\right] \cdot \hat{\mathbf{x}} \tag{14}$$

for which we notice that each term is the x–component of a vector. Making a full vector equation out of 14, and using $\mathbf{F} = m\ddot{\mathbf{r}} = m\mathbf{a}$, we get

$$\mathbf{F} = m\mathbf{a} = q\mathbf{E} + q\mathbf{v} \times \mathbf{B} \tag{15}$$

The Lorentz force equation does follow from our Lagrangian in 3…when we do all the steps carefully!

3 Two Kinds of Momentum

In first year physics we learn that the (non-relativistic) momentum of a particle is $m\mathbf{v}$. Later when we first encounter the Lagrangian we get a more general definition of momentum: The momentum corresponding to the coordinate q_i is

$$p_i \equiv \frac{\partial L}{\partial \dot{q}_i}$$

(often called the "generalized momentum"!).

But with our complete Lagrangian in Eq. 3 this definition would seem to give us a problem. Because for p_x it gives:

$$p_x = \frac{\partial L}{\partial \dot{x}} = \frac{\partial L}{\partial v_x} = mv_x + qA_x$$

or, written as a vector,

$$\mathbf{p} = m\mathbf{v} + q\mathbf{A} \tag{16}$$

So which one *is* the momentum... $m\mathbf{v}$ or $m\mathbf{v} + q\mathbf{A}$? Both, actually; we just have *two kinds* of momentum. The momentum given in 16 is the **canonical momentum**, and we will use the symbol $\mathbf{p}$ for this. The quantity $m\mathbf{v}$ is known as the **mechanical** or **kinetic** momentum, so that

$$\mathbf{p}_{\mathrm{mech}} = m\mathbf{v} = \mathbf{p} - q\mathbf{A} \tag{17}$$

Note, one can get very confused about the signs in Eqs. 16 and 17 if we are not careful about the notation for the charge. In these equations, q *is* the charge; substitute what you want! But in some books, the charge of the particle is represented by e which can get confusing if we are applying it to the electron (as we so often do) whose charge we normally want to write as $-e$. It can be quite aggravating to decide if some equation really means "e" or "$-e$" for our application.

4 The Magnetic Field and Quantum Mechanics

In quantum mechanics, some of the familiar quantities from mechanics become *operators* which work on wave functions. The time-independent Schrödinger equation features the total energy operator H_{op} (the sum of the kinetic and potential energy operators) acting on the wavefunction $\Psi(\mathbf{r})$:

$$H_{\mathrm{op}}\Psi = \left(\frac{\mathbf{p}_{\mathrm{op}}^2}{2m} + U(\mathbf{r})\right)\Psi(\mathbf{r}) = E\Psi(\mathbf{r}) \tag{18}$$

Now we can appreciate the subtleties: *Which* $\mathbf{p}$ are we talking about here, and what operator is it replaced by? The answer is that the momentum operator in 18 should be the one for the *kinetic* momentum, since that's what gives the kinetic energy. But it the *canonical* momentum $\mathbf{p}$ which goes with the famous "momentum" operator $\frac{\hbar}{i}\nabla$. So the Hamiltonian operator in 18 needs to be written in terms of the canonical momentum. Including an electric potential energy for U, it is:

$$\begin{aligned} H &= \frac{1}{2m}(\mathbf{p} - q\mathbf{A})^2 + qV \\ &= \frac{\mathbf{p}^2}{2m} - \frac{q}{2m}(\mathbf{p}\cdot\mathbf{A} + \mathbf{A}\cdot\mathbf{p}) + \frac{q^2}{2m}\mathbf{A}^2 + qV \end{aligned} \tag{19}$$

where we have been very careful to preserve the order of the operators.

Now we can replace the operator $\mathbf{p}$ by $\frac{\hbar}{i}\nabla$; for most of the terms in 19 it is clear how to do this:

$$\frac{\mathbf{p}^2}{2m} \;\Rightarrow\; -\frac{\hbar^2}{2m}\nabla^2 \qquad\qquad -\frac{q}{2m}\mathbf{A}\cdot\mathbf{p} \;\Rightarrow\; \frac{iq\hbar}{2m}\mathbf{A}\cdot\nabla$$

with the functions of $\mathbf{r}$ becoming multiplicative factors, but the term we need to be careful about is the second one, $-\frac{q}{2m}\mathbf{p}\cdot\mathbf{A}$. In this term, the meaning of the $\mathbf{p}$ operator is to operate on *everything* that lies to the right of it, so that when it is applied to the wavefunction Ψ, it works as:

$$\frac{i\hbar q}{2m}(\nabla\cdot\mathbf{A})\Psi = \frac{i\hbar q}{2m}\left(\frac{\partial}{\partial x}[A_x\Psi] + \frac{\partial}{\partial y}[A_y\Psi] + \frac{\partial}{\partial z}[A_z\Psi]\right)$$

The product rule and a little simplifying then gives this as:

$$\frac{i\hbar q}{2m}[(\nabla\cdot\mathbf{A})\Psi + \mathbf{A}\cdot\nabla\Psi] = \frac{i\hbar q}{2m}[(\nabla\cdot\mathbf{A}) + \mathbf{A}\cdot\nabla]\Psi \tag{20}$$

where here $(\nabla\cdot\mathbf{A})$ means to just hit the $\mathbf{A}$ with the ∇. We can now remove the Ψ from the right hand side to get the *operator* that we want to put back into 19.

Now substitute for all the terms in 19 and get:

$$\begin{aligned} H &= -\frac{\hbar^2}{2m}\nabla^2 + \frac{i\hbar q}{2m}[(\nabla\cdot\mathbf{A}) + \mathbf{A}\cdot\nabla] + \frac{iq\hbar}{2m}\mathbf{A}\cdot\nabla + \frac{q^2}{2m}\mathbf{A}^2 + qV \\ &= -\frac{\hbar^2}{2m}\nabla^2 + \frac{i\hbar q}{2m}(\nabla\cdot\mathbf{A}) + \frac{iq\hbar}{m}\mathbf{A}\cdot\nabla + \frac{q^2}{2m}\mathbf{A}^2 + qV \end{aligned} \tag{21}$$

The meaning of the operators is clearer in this form; if the ∇ is out in front, then clearly it works on the Ψ; if it is dotted with the $\mathbf{A}$, it works *only* on the $\mathbf{A}$.

So we now have a Hamiltonian operator which can handle magnetic fields. We note that it is the *potentials* (both scalar and vector) of the fields that enter into H. In general, the really cool equations of advanced physics deal with the potentials and *not* with the fields.

But we have reason to be bothered by this: Didn't we show that there is some ambiguity in the choice of potentials that go with particular $\mathbf{E}$ and $\mathbf{B}$ fields (called *gauge* choices)? Won't this ambiguity give *different solutions* to the equations for different gauge choices? But the fields (and initial conditions) *determine* the phyiscal solutions, don't they?

The issue of gauge choices is an important one and beyond the scope of this blurb.