What is a gauge field?

Part 2: Adding matter

Santiago Quintero de los Ríos
for homotopico.com

December 16, 2020

A long time ago, we showed that a "quicker" way to solve Maxwell's equations (at least in the vacuum)

$$\nabla \times \mathbf{E} + \frac{1}{c}\frac{\partial \mathbf{B}}{\partial t} = 0 \qquad \nabla \cdot \mathbf{E} = 4\pi\rho$$
$$\nabla \cdot \mathbf{B} = 0 \qquad \nabla \times \mathbf{B} - \frac{1}{c}\frac{\partial \mathbf{E}}{\partial t} = \frac{4\pi}{c}\mathbf{J},$$

is by writing the fields $\mathbf{E}$ and $\mathbf{B}$ in terms of electromagnetic potentials φ and $\mathbf{A}$ which satisfy

$$\mathbf{B} = \nabla \times \mathbf{A};$$
$$\mathbf{E} = -\nabla\varphi - \frac{1}{c}\frac{\partial \mathbf{A}}{\partial t}.$$

These potentials are not uniquely determined: given a smooth function Λ, we can define new potentials as

$$\mathbf{A}' = \mathbf{A} + \nabla\Lambda,$$
$$\varphi' = \varphi - \frac{1}{c}\frac{\partial \Lambda}{\partial t},$$

and these give rise to the *same* electric and magnetic fields $\mathbf{E}$, $\mathbf{B}$.

We want to see what happens if we add a test particle, and our end goal is seeing at how it looks in the *quantum case*.

A particle of charge e moving in an electric field $\mathbf{E}$ and a magnetic field $\mathbf{B}$ feels a force given by

$$\mathbf{F}_{\text{Lor}} = e\left(\mathbf{E} + \frac{1}{c}\mathbf{v} \times \mathbf{B}\right),$$

where $\mathbf{v}$ is the velocity of the particle. This force, called the **Lorentz force**, is a vector function that depends on the position $\mathbf{x}$ and velocity $\mathbf{v}$ of the particle, and possibly on time (if the fields $\mathbf{B}$, $\mathbf{E}$ do).

If we wanted to introduce the Lorentz force to a quantum-mechanical system, we would need a Hamiltonian H such that the Hamilton equations of motions

$$\dot{q}^i = \frac{\partial H}{\partial p_i}$$
$$\dot{p}_i = -\frac{\partial H}{\partial q^i}$$

are equivalent to the usual Newtonian equations of motion

$$m\ddot{\mathbf{x}} = \mathbf{F}_{\text{Lor}}.$$

With this Hamiltonian, we would apply our favorite quantization rules.

But how do we find such a Hamiltonian? The best way to do so is to write the Lorentz force in terms of a Lagrangian, and then do the Legendre transform to obtain a Hamiltonian.

1 The classical case

Here's where the *gauge fun* begins. Choose a pair of potentials $\varphi, \mathbf{A}$ for $\mathbf{E}, \mathbf{B}$. These satisfy

$$\mathbf{B} = \nabla \times \mathbf{A};$$
$$\mathbf{E} = -\nabla\varphi - \frac{1}{c}\frac{\partial \mathbf{A}}{\partial t}.$$

It can be shown (and we do so below in the last section) that a Lagrangian for the Lorentz force is given by

$$L(\mathbf{x}, \mathbf{v}, t) = \frac{1}{2}m\|\mathbf{v}\|^2 - e\varphi(\mathbf{x}, t) + \frac{e}{c}\mathbf{v} \cdot \mathbf{A}(\mathbf{x}, t).$$

Of course, one way to "prove" that this is a Lagrangian for the Lorentz force is simply showing that the Euler-Lagrange equations are precisely the equations of the Lorentz force. But that's really *ad hoc*, and below we show a more "natural" derivation.

From the Lagrangian, we see that the canonical momenta conjugate to the positions $\mathbf{x}$ are

$$p_i = \frac{\partial L}{\partial \dot{x}^i} = m\dot{x}^i + \frac{e}{c}A^i,$$

so

$$\mathbf{p} = m\dot{\mathbf{x}} + \frac{e}{c}\mathbf{A}.$$

Note that $\mathbf{p}$ depends *explicitly* on the vector potential $\mathbf{A}$, which is a sign that it is *not* a physical quantity, since we can change the potential $\mathbf{A}$ to another physically equivalent one. This means that we shouldn't be able to measure $\mathbf{p}$, since $\mathbf{A}$ is not uniquely determined. We will return to this issue of *physical quantities* later.

With the Legendre transform, we can find the Hamiltonian (this is just a computation, no tricks involved):

$$H(\mathbf{x}, \mathbf{p}, t) = \dot{\mathbf{x}} \cdot \mathbf{p} - L = \frac{1}{2m}\left\|\mathbf{p} - \frac{e}{c}\mathbf{A}(\mathbf{x}, t)\right\|^2 + e\varphi(\mathbf{x}, t).$$

The Hamiltonian (and the Lagrangian too) has an explicit dependence on the potentials $\varphi, \mathbf{A}$, whereas the Lorentz force is only dependent on the fields $\mathbf{E}$ and $\mathbf{B}$. If we change the potentials via a gauge transformation, the Lorentz force doesn't change, but the Lagrangian does! So there's something funky going on here. How do we reconcile this?

Well, the Lagrangian changes, but the equations of motion don't. Let's see this explicitly: let Λ be a smooth (time-dependent) function and let's do the gauge transformation

$$\mathbf{A}' = \mathbf{A} + \nabla\Lambda$$
$$\varphi' = \varphi - \frac{1}{c}\frac{\partial \Lambda}{\partial t}.$$

Substituting in the Lagrangian and doing a little reordering, we obtain

$$L'(\mathbf{x}, \mathbf{v}, t) = \frac{1}{2}m\|\mathbf{v}\|^2 - e\varphi(\mathbf{x}, t) + \frac{e}{c}\mathbf{v} \cdot \mathbf{A}(\mathbf{x}, t) + \frac{e}{c}\left(\mathbf{v} \cdot \nabla\Lambda + \frac{\partial \Lambda}{\partial t}\right) := L(\mathbf{x}, \mathbf{v}, t) + \frac{e}{c}\frac{\mathrm{d}\Lambda}{\mathrm{d}t}.$$

Here, we have defined L' as L but with φ' and $\mathbf{A}'$ instead of $\varphi, \mathbf{A}$, and we have defined the total derivative of Λ as

$$\left(\frac{\mathrm{d}\Lambda}{\mathrm{d}t}\right)(\mathbf{x}, \mathbf{v}, t) := \mathbf{v} \cdot \boldsymbol{\nabla}\Lambda + \frac{\partial \Lambda}{\partial t}.$$

This total derivative coincides with the derivative obtained from the chain rule, if we evaluate it on $\mathbf{x}(t), \dot{\mathbf{x}}(t), t$ for a curve $\mathbf{x} : \mathbb{R} \to \mathbb{R}^3$. That is,

$$\left(\frac{\mathrm{d}\Lambda}{\mathrm{d}t}\right)(\mathbf{x}(t), \dot{\mathbf{x}}(t), t) = \frac{\mathrm{d}}{\mathrm{d}t}(\Lambda(\mathbf{x}(t), t)).$$

Therefore, our transformed Lagrangian has the form

$$L' = L + \frac{\mathrm{d}F}{\mathrm{d}t}$$

with $F = (e/c)\Lambda$. This tells us that the Lagrangian itself is not gauge-invariant; however, since it transforms up to a *total derivative*, the equations of motion are invariant. We show this below in the gory details (section 5.2).

What about the Hamiltonian picture? First, let's see what happens to the canonical momenta. Under a gauge transformation, they transform as

$$p_i' = \frac{\partial L'}{\partial \dot{x}^i} = \frac{\partial L}{\partial \dot{x}^i} + \frac{\partial}{\partial \dot{x}^i}\left(\frac{\mathrm{d}F}{\mathrm{d}t}\right) = p_i + \frac{\partial F}{\partial x^i}.$$

Therefore, the canonical momentum changes under a change of gauge as $\mathbf{p}' = \mathbf{p} + \boldsymbol{\nabla}F$. If we perform the Legendre transform of L', we obtain a Hamiltonian in terms of this new canonical momentum $\mathbf{p}'$

$$H'(\mathbf{x}, \mathbf{p}', t) = \dot{\mathbf{x}}(\mathbf{p}') \cdot \mathbf{p}' - L'(\mathbf{x}, \dot{\mathbf{x}}(\mathbf{p}'), t);$$

where we have made it explicit that we must write $\dot{\mathbf{x}}$ in terms of $\mathbf{p}'$ and not $\mathbf{p}$. Carrying out the computation we obtain

$$H'(\mathbf{x}, \mathbf{p}', t) = \frac{1}{2m}\left\|\mathbf{p}' - \frac{e}{c}\mathbf{A}'(\mathbf{x}, t)\right\|^2 + e\varphi'(\mathbf{x}, t).$$

Does this mean that the Hamiltonian is gauge invariant? *No, it does not.* This Hamiltonian is written in terms of the new momentum $\mathbf{p}'$, and we need to see how it relates to the Hamiltonian with the old momentum $\mathbf{p}$. So we substitute all the new momenta and potentials in terms of the old:

$$\begin{aligned} H'(\mathbf{x}, \mathbf{p}', t) &= \frac{1}{2m}\left\|\mathbf{p} + \frac{e}{c}\boldsymbol{\nabla}\Lambda - \frac{e}{c}\mathbf{A} - \frac{e}{c}\boldsymbol{\nabla}\Lambda\right\|^2 + e\varphi(\mathbf{x}, t) - \frac{e}{c}\frac{\partial \Lambda}{\partial t} \\ &= \frac{1}{2m}\left\|\mathbf{p} - \frac{e}{c}\mathbf{A}\right\|^2 + e\varphi(\mathbf{x}, t) - \frac{e}{c}\frac{\partial \Lambda}{\partial t} \\ &= H(\mathbf{x}, \mathbf{p}, t) - \frac{e}{c}\frac{\partial \Lambda}{\partial t}. \end{aligned}$$

Thus, the Hamiltonian is in general *not* gauge-invariant! But once again, the day is saved since Hamilton's *equations of motion* are. Again, we leave this to the gory details below (section 5.2).

In conclusion, even though the Lagrangian and Hamiltonian are explicitly dependent on the potentials, and therefore *not* gauge-invariant, the equations of motions *are* gauge-invariant, so the dynamics of the system are well-defined. This is to be expected, since both the Lagrangian and the Hamiltonian picture are equivalent to Newton's equations of motion, which do not even include the potentials explicitly.

2 The quantum case

Now that we have a Hamiltonian, we can write the Schrödinger equation

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi = \frac{1}{2m}\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)^2 \psi + e\varphi\psi.$$

Here comes another problem: The Hamiltonian is dependent on the choice of potential! But this time we can't shield ourselves under the "don't worry, the equations of motion are safe" that we used in the last section, since the Schrödinger equation *is* the equation of motion! So there's nothing stopping the evolution of the wavefunction ψ from depending on the choice of potential!

But we *do* have one more trick under our sleeve. The wavefunction is not the measurable object, but rather its square norm $|\psi|^2$, and in general the *expectation values*[1] of Hermitian operators $\hat{O}$

$$\langle\psi|\hat{O}|\psi\rangle .$$

This means that we can save this Hamiltonian if we guarantee that whenever we change the potentials to some new ones $\mathbf{A}', \varphi'$ (via some gauge transformation), then every solution ψ of the Schrödinger equation and every observable $\hat{O}$ have *physically equivalent* solutions ψ' (to the Schrödinger equation with the new potentials) and observables $\hat{O}'$ such that

$$\langle\psi'|\hat{O}'|\psi'\rangle = \langle\psi|\hat{O}|\psi\rangle .$$

One way to guarantee this is with unitary transformations. Suppose that ψ is a solution to the Schrödinger equation with potentials $\varphi, \mathbf{A}$. Now let Λ be a smooth function and let $\varphi', \mathbf{A}'$ be the gauge-transformed potentials

$$\begin{aligned} \mathbf{A}' &= \mathbf{A} + \nabla\Lambda \\ \varphi' &= \varphi - \frac{1}{c}\frac{\partial\Lambda}{\partial t}. \end{aligned}$$

Suppose that there exists a unitary transformation $U(\Lambda)$ associated to Λ such that the new "gauge-transformed" wavefuntion

$$\psi' = U\psi$$

is a solution of the Schrödinger equation with the potentials $\varphi', \mathbf{A}'$. If for every observable $\hat{O}$ we define

$$\hat{O}' = U\hat{O}U^{-1},$$

then necessarily

$$\langle\psi'|\hat{O}'|\psi'\rangle = \langle U\psi|U\hat{O}U^{-1}|U\psi\rangle = \langle\psi|U^\dagger U\hat{O}|\psi\rangle = \langle\psi|\hat{O}|\psi\rangle .$$

This follows from the fact that $U^\dagger U = I$, since U is unitary.

Now we have a problem. The rule $\hat{O} \mapsto U\hat{O}U^{-1}$ gives us a way to transform observables between different gauges. However, we may already have a definition of the observable in a different gauge! For example, if we write the momentum operator $\mathbf{p}$ in the position representation, it becomes $-i\hbar\nabla$. This definition *should* be the same for *all* gauges, since changing gauges does not alter the coordinates. That means that we define

$$\mathbf{p}_{\mathbf{A},\varphi} = \mathbf{p}_{\mathbf{A}',\varphi'} \overset{\text{position rep.}}{:=} -i\hbar\nabla$$

[1] We can obtain $|\langle\phi|\psi\rangle|^2$ as the expectation value of the projection operator $\mathrm{pr}_\psi = |\psi\rangle\langle\psi|$ in the ϕ state.

for all potentials[2]. However, we also have a gauge transformation rule that tells us how operators transform between gauges. Do these prescriptions agree with one another? That is, do we have

$$U\mathbf{p}_{A,\varphi}U^{-1} \stackrel{?}{=} \mathbf{p}_{\mathbf{A}',\varphi'}$$

As we will see below, the answer is **no**, since, assuming that U depends only on positions and not momenta,

$$U\mathbf{p}_{A,\varphi}U^{-1} = \mathbf{p}_{A,\varphi} + i\hbar(\nabla U)U^{-1} \neq \mathbf{p}_{A',\varphi'}.$$

There is a conflict between the transformation law and our *definition* of the momentum operator between different gauges. This tells us that the observable $\mathbf{p}$ is *not physical*, because the results of observations cannot be defined consistently between gauges (and remember, up to this point, the gauges are just mathematical tools).

In general, we say that an observable $\hat{O}$ is **physical** if its definition in different gauges is consistent with the transformation law. That is, if

$$U\hat{O}_{\mathbf{A},\varphi}U^{-1} = \hat{O}_{\mathbf{A}',\varphi'}.$$

Another example of an *un*physical observable is the potential $\mathbf{A}$. If we assume that the unitary transformation U depends only on the position, then it commutes with $\mathbf{A}$, so

$$U\mathbf{A}U^{-1} = \mathbf{A} \stackrel{!}{\neq} \mathbf{A}'.$$

So how do we find $U(\Lambda)$? Does it even exist? In the gory details below, we show that the correct unitary transformation is

$$U(\Lambda) = \exp\left(\frac{ie}{\hbar c}\Lambda\right),$$

so that the wavefunction ψ transforms as

$$\psi' = \exp\left(\frac{ie}{\hbar c}\Lambda\right)\psi.$$

Let's check that ψ' does indeed satisfy the Schrödinger equation with the Hamiltonian with respect to the new gauge. We have

$$\begin{aligned} i\hbar\frac{\partial\psi'}{\partial t} &= i\hbar\frac{\partial U(\Lambda)}{\partial t}\psi + i\hbar U(\Lambda)\frac{\partial\psi}{\partial t} \\ &= -\frac{e}{c}\frac{\partial\Lambda}{\partial t}\exp\left(\frac{ie}{\hbar c}\Lambda\right)\psi + U(\Lambda)\left(i\hbar\frac{\partial\psi}{\partial t}\right). \end{aligned}$$

By hypothesis ψ satisfies the Schrödinger equation with the potentials $\mathbf{A}, \varphi$, so

$$i\hbar\frac{\partial\psi'}{\partial t} = -\frac{e}{c}\frac{\partial\Lambda}{\partial t}\psi' + U(\Lambda)\left(\frac{1}{2m}\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)^2 + e\varphi\right)\psi.$$

Now we note that

$$U(\Lambda)\mathbf{p} = \mathbf{p}U(\Lambda) + [U(\Lambda), \mathbf{p}] = \mathbf{p}U(\Lambda) + i\hbar\nabla U(\Lambda) = \mathbf{p}U(\Lambda) - \frac{e}{c}\nabla\Lambda U(\Lambda) = \left(\mathbf{p} - \frac{e}{c}\nabla\Lambda\right)U(\Lambda).$$

Therefore,

$$U(\Lambda)\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)^2 = \left(\mathbf{p} - \frac{e}{c}\mathbf{A} - \frac{e}{c}\nabla\Lambda\right)^2 U(\Lambda)$$

[2] This is in stark contrast from the Lagrangian case, where canonical momentum changes as the potentials change.

Since $U(\Lambda)$ depends only on position, then it commutes with φ. Therefore, we obtain (after a little rearrangement)

$$\begin{aligned} i\hbar\frac{\partial\psi'}{\partial t} &= \frac{1}{2m}\left(\mathbf{p} - \frac{e}{c}\left(\mathbf{A} + \nabla\Lambda\right)\right)^2\psi' + e\left(\varphi - \frac{1}{c}\frac{\partial\Lambda}{\partial t}\right)\psi' \\ &= \frac{1}{2m}\left(\mathbf{p} - \frac{e}{c}\mathbf{A}'\right)^2\psi' + e\varphi'\psi'. \end{aligned}$$

Finally, we note that the definition of $\mathbf{p}$ is the same for all gauges, so we write $\mathbf{p}' = \mathbf{p}$, and thus obtain

$$i\hbar\frac{\partial\psi'}{\partial t} = H_{\mathbf{A}',\varphi'}\psi'.$$

Therefore, the wavefunction $\psi' = \exp\left(\frac{ie}{\hbar c}\Lambda\right)\psi$ satisfies the Schrödinger equation with the gauge-transformed potentials φ', $\mathbf{A}'$. In the context of gauge theories, we call ψ a **matter field**.

3 Minimal coupling and covariant derivatives

The Schrödinger equation for the particle coupled to an electromagnetic field is not very different from the free equation. If we start with the free equation

$$i\hbar\frac{\partial\psi}{\partial t} = \frac{1}{2m}\mathbf{p}^2\psi,$$

and make the changes

$$\begin{aligned} \frac{\partial}{\partial t} &\mapsto \frac{\partial}{\partial t} + \frac{ie}{\hbar}\varphi, \\ \mathbf{p} &\mapsto \mathbf{p} - \frac{e}{c}\mathbf{A}, \end{aligned}$$

then we obtain the coupled equation

$$i\hbar\frac{\partial\psi}{\partial t} = \frac{1}{2m}\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)^2\psi + e\varphi\psi.$$

This is called the *minimal coupling* prescription.

These seem like arbitrary changes. However, if we write everything in the unified four-dimensional framework we talked about last time, we'll see that they are similar. Our four-dimensional coordinates are $x^0 = ct$, $x^1 = x$, $x^2 = y$, $x^3 = z$. We condense the fields and potentials into four-dimensional differential forms: The potentials become a one-form $A = A_\mu \mathrm{d}x^\mu$ with components

$$A_0 = \varphi \qquad\qquad A_i = -\mathbf{A}^i,$$

and the fields become a two-form $F = \frac{1}{2}F_{\mu\nu}\mathrm{d}x^\mu \wedge \mathrm{d}x^\nu$ with components

$$F_{0i} = \mathbf{E}^i \qquad\qquad F_{ij} = -\varepsilon_{ijk}\mathbf{B}^k,$$

satisfying

$$F = \mathrm{d}A.$$

Under a gauge transformation, the electromagnetic potential A transforms as

$$A \mapsto A' = A - \mathrm{d}\Lambda,$$

and of course the field strength F remains invariant.

The minimal coupling prescription is now obtained by making the change

$$\partial_\mu \mapsto \mathcal{D}_\mu := \partial_\mu + \frac{ie}{\hbar c} A_\mu.$$

The symbol $\mathcal{D}_\mu$ is called the *covariant derivative*. Indeed, we can check that the compontents $\mathcal{D}_0$ and $\mathcal{D}_i$ correspond to the operators $\partial_t + \frac{ie}{\hbar}\varphi$ and $\mathbf{p} - \frac{e}{c}\mathbf{A}$ that we discussed above.

Why do we care about this covariant derivative? If transform to a new gauge $A' = A - \mathrm{d}\Lambda$, then the covariant derivative changes as

$$\mathcal{D}_\mu \mapsto \mathcal{D}'_\mu = \mathcal{D}_\mu - \frac{ie}{\hbar c}\partial_\mu \Lambda.$$

So it's not quite gauge-invariant on its own. However, when we let $\mathcal{D}_\mu$ act on the wavefunction ψ, and apply a gauge transformation to *both* at the same time, we get

$$\begin{aligned}
\mathcal{D}'_\mu \psi' &= \left(\mathcal{D}_\mu - \frac{ie}{\hbar c}\partial_\mu \Lambda\right) \exp\left(\frac{ie}{\hbar c}\Lambda\right)\psi \\
&= \partial_\mu \left(\exp\left(\frac{ie}{\hbar c}\Lambda\right)\psi\right) - \exp\left(\frac{ie}{\hbar c}\Lambda\right)\left(\frac{ie}{\hbar c}A_\mu \psi + \frac{ie}{\hbar c}\partial_\mu \Lambda \psi\right) \\
&= \exp\left(\frac{ie}{\hbar c}\Lambda\right)\left(\frac{ie}{\hbar c}\partial_\mu \Lambda \psi + \partial_\mu \psi - \frac{ie}{\hbar c}A_\mu \psi - \frac{ie}{\hbar c}\partial_\mu \Lambda \psi\right) \\
&= \exp\left(\frac{ie}{\hbar c}\Lambda\right)\mathcal{D}_\mu \psi \\
&= (\mathcal{D}_\mu \psi)'.
\end{aligned}$$

Thus, after applying the covariant derivative to the wavefunction ψ, we get another wavefunction which transforms properly under gauge transformations. We call this gauge *covariance*: If apply the gauge-transformed covariant derivative to the gauge-transformed matter field, we get the same result as applying the un-transformed derivative to the un-transformed field and *then* transforming the result.

4 The takeaway

We started with some *fields* **E** and **B** which could be written in terms of some *potentials* **A**, φ. The potentials are *not* uniquely determined, since we can change them by a *gauge transformation*, and the fields remain the same. The quantities that are invariant under these gauge transformations are *physical*.

In quantum mechanics, the wavefunction ψ and *physical* observables $\hat{O}$ might be gauge-dependent, but under a gauge transformation, they transform by a unitary transformation in a way that the expectation values of physical observables are all invariant.

In summary, we have the following objects and how they transform under a gauge transformation:

$$\begin{array}{lcl}
\mathbf{A} & \mapsto & \mathbf{A}' = \mathbf{A} + \nabla \Lambda \\
\varphi & \mapsto & \varphi' = \varphi - \dfrac{1}{c}\dfrac{\partial \Lambda}{\partial t} \\
\mathbf{E} & \mapsto & \mathbf{E} \\
\mathbf{B} & \mapsto & \mathbf{B} \\
\psi & \mapsto & \psi' = \exp\left(\dfrac{ie}{\hbar c}\Lambda\right)\psi \\
\hat{O} & \mapsto & \hat{O}' = \exp\left(\dfrac{ie}{\hbar c}\Lambda\right)\hat{O}\exp\left(-\dfrac{ie}{\hbar c}\Lambda\right).
\end{array}$$

Finally, we saw that an "easy" way to go from the free theory to the minimally coupled theory is substituting ordinary derivatives with covariant derivatives:

$$\partial_\mu \mapsto \mathcal{D}_\mu = \partial_\mu + \frac{ie}{\hbar c}A_\mu.$$

This is how it is often done for more complicated gauge theories (which we will explore later).

The next step is interpreting all these objects as *local* representations of global objects in the theory of *principal bundles*.

5 The gory details

5.1 Finding the Lagrangian

Substituting the expressions for $\mathbf{E}$ and $\mathbf{B}$ in terms of the potentials φ and $\mathbf{A}$ in the Lorentz force, we obtain

$$\mathbf{F} = e\left(-\nabla\varphi - \frac{1}{c}\frac{\partial \mathbf{A}}{\partial t} + \frac{1}{c}\mathbf{v}\times(\nabla\times\mathbf{A})\right).$$

Now we use one of those super fun vector product identities,

$$\mathbf{a}\times(\mathbf{b}\times\mathbf{c}) = (\mathbf{a}\cdot\mathbf{c})\mathbf{b} - (\mathbf{a}\cdot\mathbf{b})\mathbf{c},$$

which becomes in our case

$$\mathbf{v}\times(\nabla\times\mathbf{A}) = \nabla(\mathbf{v}\cdot\mathbf{A}) - (\mathbf{v}\cdot\nabla)\mathbf{A}.$$

Therefore,

$$\mathbf{F} = e\left(-\nabla\left(\varphi - \frac{1}{c}\mathbf{v}\cdot\mathbf{A}\right) - \frac{1}{c}\left(\frac{\partial \mathbf{A}}{\partial t} + (\mathbf{v}\cdot\nabla)\mathbf{A}\right)\right).$$

Let's plug this into Newton's equation of motion. Let $\mathbf{x} : \mathbb{R} \to \mathbb{R}^3$ be the trajectory of a particle of mass m, and let $\dot{\mathbf{x}}$ be its velocity. Newton's second law reads

$$m\ddot{\mathbf{x}}(t) = \mathbf{F}(\mathbf{x}(t), \dot{\mathbf{x}}(t), t) = e\left(-\nabla\left(\varphi - \frac{1}{c}\dot{\mathbf{x}}\cdot\mathbf{A}\right) - \frac{1}{c}\left(\frac{\partial \mathbf{A}}{\partial t} + (\dot{\mathbf{x}}\cdot\nabla)\mathbf{A}\right)\right).$$

It is important to note that here we are implicitly evaluating the time-dependent fields $\varphi, \mathbf{A}$ at $(\mathbf{x}(t), t)$. In particular, the rightmost term becomes, applying the chain rule,

$$\frac{\partial \mathbf{A}}{\partial t}(\mathbf{x}(t), t) + ((\dot{\mathbf{x}}\cdot\nabla)\mathbf{A})(\mathbf{x}(t), t) = \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{A}(\mathbf{x}(t), t).$$

Then Newton's second law becomes, in components,

$$m\ddot{\mathbf{x}}^i(t) = e\left(-\frac{\partial}{\partial x^i}\left(\varphi - \frac{1}{c}\sum_k \dot{\mathbf{x}}^k\mathbf{A}^k\right) - \frac{1}{c}\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{A}^i(\mathbf{x}(t), t)\right).$$

Now comes the *dirty trick*. We can write $\mathbf{A}^i$ as

$$-\frac{1}{c}\mathbf{A}^i = -\frac{1}{c}\frac{\partial}{\partial \dot{x}^i}\left(\sum_k \dot{x}^k\mathbf{A}^k\right) = \frac{\partial}{\partial \dot{x}^i}\left(\varphi - \frac{1}{c}\sum_k \dot{x}^k\mathbf{A}^k\right).$$

Similarly, we can write $\ddot{\mathbf{x}}^i$ as

$$\ddot{\mathbf{x}}^i = \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial}{\partial \dot{x}^i}\frac{1}{2}\sum_k \dot{x}^k\dot{x}^k\right).$$

With these replacements, Newton's equation takes the form of an Euler-Lagrange equation:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial}{\partial \dot{x}^i}\frac{m}{2}\sum_k \dot{x}^k\dot{x}^k\right) = \frac{\partial}{\partial x^i}\left(-e\varphi + \frac{e}{c}\sum_k \dot{x}^k\mathbf{A}^k\right) + \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial}{\partial \dot{x}^i}\left(e\varphi - \frac{e}{c}\sum_k \dot{x}^k\mathbf{A}^k\right).$$

Or, well, after a few rearrangements:

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial}{\partial \dot{x}^i}\left(\frac{m}{2}\sum_k \dot{x}^k\dot{x}^k - e\varphi + \frac{e}{c}\sum_k \dot{x}^k\mathbf{A}^k\right) - \frac{\partial}{\partial x^i}\left(\frac{m}{2}\sum_k \dot{x}^k\dot{x}^k - e\varphi + \frac{e}{c}\sum_k \dot{x}^k\mathbf{A}^k\right) = 0.$$

Therefore, we can use the Lagrangian

$$L(\mathbf{x}, \mathbf{v}, t) = \frac{1}{2}m\|\mathbf{v}\|^2 - e\varphi(\mathbf{x}, t) + \frac{e}{c}\mathbf{v}\cdot\mathbf{A}(\mathbf{x}, t).$$

5.2 Gauge-invariance of the equations of motion

Under a gauge transformation, the Lagrangian changes as

$$L' = L + \frac{\mathrm{d}F}{\mathrm{d}t}$$

with $F = (e/c)\Lambda$. Although the Lagrangian itself is not gauge-invariant, since it transforms up to a *total derivative*, then the equations of motion are invariant:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L'}{\partial \dot{x}^i}\right) - \frac{\partial L'}{\partial x^i} &= \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{x}^i}\right) - \frac{\partial L}{\partial x^i} + \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial}{\partial \dot{x}^i}\frac{\mathrm{d}F}{\mathrm{d}t}\right) - \frac{\partial}{\partial x^i}\left(\frac{\mathrm{d}F}{\mathrm{d}t}\right)\\ &= \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{x}^i}\right) - \frac{\partial L}{\partial x^i} + \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial F}{\partial x^i}\right) - \frac{\partial}{\partial x^i}\left(\frac{\mathrm{d}F}{\mathrm{d}t}\right)\\ &= \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{x}^i}\right) - \frac{\partial L}{\partial x^i}.\end{aligned}$$

Here we used the fact that

$$\frac{\partial}{\partial \dot{x}^i}\left(\frac{\mathrm{d}F}{\mathrm{d}t}\right) = \frac{\partial}{\partial \dot{x}^i}\left(\frac{\partial F}{\partial t} + \sum_k \dot{x}^k\frac{\partial F}{\partial x^k}\right) = \frac{\partial F}{\partial x^i}.$$

In the Hamiltonian picture, the canonical momenta transform as

$$\mathbf{p}' = \mathbf{p} + \boldsymbol{\nabla}F,$$

and the Hamiltonian transforms like

$$H'(\mathbf{x}, \mathbf{p}', t) = H(\mathbf{x}, \mathbf{p}, t) - \frac{\partial F}{\partial t}.$$

Although the Hamiltonian is *not* gauge-invariant, the *equations of motion* are. If we have a trajectory $\mathbf{x}(t)$, $\mathbf{p}(t)$ which satisfies

$$\begin{aligned}\dot{\mathbf{x}}^i &= \frac{\partial H}{\partial p_i}\\ \dot{\mathbf{p}}_i &= -\frac{\partial H}{\partial x^i},\end{aligned}$$

then it also satisfies

$$\begin{aligned}\dot{\mathbf{x}}^i = \frac{\partial H}{\partial p_i} &= -\frac{\partial}{\partial p_i}\left(H'(\mathbf{x}, \mathbf{p}', t) + \frac{\partial F}{\partial t}\right)\\ &= \sum_j \frac{\partial H'}{\partial p'_j}\frac{\partial p'_j}{\partial p_i}\\ &= \frac{\partial H'}{\partial p'_i}.\end{aligned}$$

The equations of motion for the momenta are more subtle. We have to note that when we write $\mathbf{p}' = \mathbf{p} + \nabla F$, we are introducing an *explicit* dependence of $\mathbf{p}'$ on the position variables x^i. And so, we must be careful when applying the chain rule:

$$\begin{aligned}
\dot{\mathbf{p}}_i' &= \dot{\mathbf{p}}_i + \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial F}{\partial x^i} \\
&= -\frac{\partial H}{\partial x^i} + \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial F}{\partial x^i} \\
&= -\frac{\partial}{\partial x^i}\left(H'(\mathbf{x}, \mathbf{p}', t) + \frac{\partial F}{\partial t}\right) + \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial F}{\partial x^i} \\
&= -\frac{\partial H'}{\partial x^i} - \sum_j \frac{\partial H'}{\partial p_j'}\frac{\partial p_j'}{\partial x^i} - \frac{\partial}{\partial x^i}\frac{\partial F}{\partial t} + \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial F}{\partial x^i} \\
&= -\frac{\partial H'}{\partial x^i} - \sum_j \dot{\mathbf{x}}_j \frac{\partial}{\partial x^i}\frac{\partial F}{\partial x^j} - \frac{\partial}{\partial x^i}\frac{\partial F}{\partial t} + \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial F}{\partial x^i} \\
&= -\frac{\partial H'}{\partial x^i} - \frac{\partial}{\partial x^i}\left(\sum_j \dot{\mathbf{x}}^j \frac{\partial F}{\partial x^j} + \frac{\partial F}{\partial t}\right) + \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial F}{\partial x^i} \\
&= -\frac{\partial H'}{\partial x^i} - \frac{\partial}{\partial x^i}\frac{\mathrm{d}F}{\mathrm{d}t} + \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial F}{\partial x^i} \\
&= -\frac{\partial H'}{\partial x^i}.
\end{aligned}$$

Then Hamilton's equations are preserved under the gauge transformation, and so the dynamics of the system is the same independent of the chosen gauge.

5.3 Finding the unitary transformation

Suppose that ψ is a solution to the Schrödinger equation

$$i\hbar\frac{\partial\psi}{\partial t} = \frac{1}{2m}\left(\mathbf{p} - \frac{e}{c}\mathbf{A}(\mathbf{x}, t)\right)^2 \psi + e\varphi(\mathbf{x}, t)\psi,$$

and suppose that there is a unitary transformation $U(\Lambda)$ such that $\psi' = U(\Lambda)\psi$ satisfies the Schrödinger equation with the transformed potentials:

$$i\hbar\frac{\partial\psi'}{\partial t} = \frac{1}{2m}\left(\mathbf{p}' - \frac{e}{c}\mathbf{A}'(\mathbf{x}, t)\right)^2 \psi' + e\varphi'(\mathbf{x}, t)\psi'.$$

Since $U(\Lambda)$ is unitary, it is a general fact[3] that it can be written as

$$U(\Lambda) = \exp(iG(\Lambda))$$

for some Hermitian $G(\Lambda)$. In general, G is going to be a function only of $\mathbf{x}$ and t, since it depends only on Λ. We want to find G.

Let's split the Schrödinger equation with transformed potentials into little bits. On the left-hand side, we have

$$i\hbar\frac{\partial\psi'}{\partial t} = i\hbar\frac{\partial}{\partial t}(\exp(iG)\psi) = -\hbar\frac{\partial G}{\partial t}\exp(iG)\psi + i\hbar\exp(iG)\frac{\partial\psi}{\partial t}.$$

On the right-hand side, we use the fact that

$$\mathbf{p}U = U\mathbf{p} - i\hbar\nabla U = \exp(iG)\mathbf{p} + \hbar\nabla G\exp(iG),$$

[3] See references. This is relatively easy to show in the finite-dimensional case, but quite non-trivial for general Hilbert spaces!

so

$$\left(\mathbf{p}' - \frac{e}{c}\mathbf{A}'\right)^2 \psi' = \left(\mathbf{p}' - \frac{e}{c}\mathbf{A}'\right)^2 \exp(iG)\psi = \exp(iG)\left(\mathbf{p}' - \frac{e}{c}\mathbf{A}' + \hbar\nabla G\right)^2 \psi.$$

If we write $\mathbf{A}' = \mathbf{A} + \nabla\Lambda$, $\varphi' = \varphi - \frac{1}{c}\partial_t\Lambda$, and $\mathbf{p}' = \mathbf{p}$, plug everything back in and reorder a little bit, we obtain

$$\exp(iG)\left(i\hbar\frac{\partial\psi}{\partial t}\right) = \exp(iG)\left(\mathbf{p} - \frac{e}{c}\mathbf{A} - \frac{e}{c}\nabla\Lambda + \hbar\nabla G\right)^2 \psi + \exp(iG)\varphi\psi + \exp(iG)\left(\hbar\frac{\partial G}{\partial t} - \frac{e}{c}\frac{\partial\Lambda}{\partial t}\right)\psi.$$

This equation looks like the Schrödinger equation for ψ, but with an $\exp(iG)$ in front and a bunch of other things that we want to get rid of. We would easily get rid of them if

$$\hbar\nabla G = \frac{e}{c}\nabla\Lambda$$
$$\hbar\frac{\partial G}{\partial t} = \frac{e}{c}\frac{\partial\Lambda}{\partial t}.$$

This is a differential equation for G, which has an easy solution[4]:

$$G = \frac{e}{\hbar c}\Lambda.$$

Therefore, if we choose the unitary transformation to be

$$U(\Lambda) = \exp\left(\frac{ie}{\hbar c}\right),$$

then $\psi' = U(\Lambda)\psi$ is a solution to the Schrödinger equation with the potentials $\mathbf{A}'$, φ' whenever ψ is a solution to the equation with potentials $\mathbf{A}$, φ.

6 References

- Landau, L. D. and Lifschitz, E. M. (1977). *Quantum Mechanics: Non-relativistic theory*. Chapter XV.
- Sakurai, J.J. and Napolitano, J. (2011). *Modern Quantum Mechanics, Second Edition*, Section 2.7.

[4]Which is not unique, but that doesn't matter.