Classical and Quantum Mechanics of a Charged Particle Moving in Electric and Magnetic Fields

In these notes I consider a charged particle moving through given electromagnetic fields $\mathbf{E}(\mathbf{x}, t)$ and $\mathbf{B}(\mathbf{x}, t)$. I am allowing for completely general time-dependent electric and magnetic fields (as long as they obey the Maxwell equations), but I am treating these fields as generated by some sources external to the particle in question. The back-reaction of the moving charged particle on the EM fields will be studied in the second EMT class 387 L.

Classical Mechanics

In a purely electrostatic field $\mathbf{E}(\mathbf{x})$, the net force $\mathbf{F} = q\mathbf{E}(\mathbf{x})$ acting on a charged particle is a potential force. Consequently, the Lagrangian and the Hamiltonian of the particle's dynamics involve the scalar potential $\Phi(\mathbf{x})$ rather then the electric field $\mathbf{E}$ itself, thus

$$L(\mathbf{x}, \mathbf{v}) \;=\; \frac{m}{2}\mathbf{v}^2 \;-\; q\Phi(\mathbf{x}), \tag{1}$$

$$H(\mathbf{x}, \mathbf{p}) \;=\; \frac{\mathbf{p}^2}{2m} \;+\; q\Phi(\mathbf{x}). \tag{2}$$

Likewise, when we turn on a magnetic field $\mathbf{B}(\mathbf{x})$, the Lagrangian and the Hamiltonian involve the vector potential $\mathbf{A}(\mathbf{x})$ rather than the magnetic field $\mathbf{B}$ itself. Specifically, the Lagrangian becomes

$$L(\mathbf{x}, \mathbf{v}) \;=\; \frac{m}{2}\mathbf{v}^2 \;-\; q\Phi(\mathbf{x}) \;+\; q\mathbf{v}\cdot\mathbf{A}(\mathbf{x}) \tag{3}$$

in MKSA units, or

$$L(\mathbf{x}, \mathbf{v}) \;=\; \frac{m}{2}\mathbf{v}^2 \;-\; q\Phi(\mathbf{x}) \;+\; \frac{q}{c}\mathbf{v}\cdot\mathbf{A}(\mathbf{x}) \tag{4}$$

in Gauss units. Arguably, the vector-potential term in this Lagrangian is a relativistic correction to the scalar-potential term, but I don't want to get into relativity at this time. Instead, I am going to justify the Lagrangian (3) by showing that it leads to the Euler–Lagrange equation of motion which agrees with the Newton's Second Law for the usual electric+magnetic force,

$$m\mathbf{a} \;=\; \mathbf{F}_{\rm net} \;=\; q\mathbf{E}(\mathbf{x}) \;+\; q\mathbf{v}\times\mathbf{B}(\mathbf{x}). \tag{5}$$

Physically, we know this equation of motion is correct, and that's what justifies the Lagrangian (3).

For simplicity, in these notes I assume all fields and all potentials to be time-independent, but there is a version of these notes written for my graduate class in which I show how the Lagrangian (3) leads to the Newton eq. (5) even for the time-dependent fields.

Let's start with the Euler-Lagrange equations of motion

$$\begin{aligned} \mathbf{p} \;&=\; \frac{\partial L(\mathbf{x},\mathbf{v})}{\partial\mathbf{v}}\,, \\ \frac{d\mathbf{p}}{dt} \;&=\; \frac{\partial L(\mathbf{x},\mathbf{v})}{\partial\mathbf{x}} \end{aligned} \tag{6}$$

for the Lagrangian (3). The first step is the *canonical momentum*

$$\mathbf{p} \;\stackrel{\rm def}{=}\; \frac{\partial L}{\partial\mathbf{v}} \;=\; m\mathbf{v} \;+\; q\mathbf{A}(\mathbf{x}), \tag{7}$$

which turn out to be different from the usual kinematical momentum $\vec{\pi}=m\mathbf{v}$. This difference will be very important for the Hamiltonian of the charged particle.

Note: in the Lagrangian (3) — and hence in the canonical momentum (7) — $\mathbf{A}(\mathbf{x})$ is the vector potential evaluated at the particle's location $\mathbf{x}$ rather than some fixed location in space. Consequently, when the particle moves, the $\mathbf{A}(\mathbf{x})$ changes with time as

$$\frac{d}{dt}\mathbf{A}(\mathbf{x}(t)) \;=\; \sum_j \frac{\partial\mathbf{A}}{\partial x_j}\,\frac{dx_j}{dt} \;=\; (\mathbf{v}\cdot\nabla)\mathbf{A}(\mathbf{x}(t)), \tag{8}$$

hence on the LHS of the Euler–Lagrange eq. (6)

$$\frac{d\mathbf{p}}{dt} \;=\; m\frac{d\mathbf{v}}{dt} \;+\; q(\mathbf{v}\cdot\nabla)\mathbf{A}(\mathbf{x}). \tag{9}$$

At the same time, on the RHS of the Euler–Lagrange eq. (6), we have

$$\frac{\partial L(\mathbf{x},\mathbf{v})}{\partial\mathbf{x}} \;=\; -q\nabla\Phi \;+\; q\nabla(\mathbf{v}\cdot\mathbf{A}) \tag{10}$$

where in the second term the space derivative ∇ acts on $\mathbf{A}(\mathbf{x})$ while treating $\mathbf{v}$ as constant (*i.e.*, $\mathbf{x}$-independent) vector. Altogether, the Euler–Lagrange equation of motion for the Lagrangian (3) becomes

$$m\frac{d\mathbf{v}}{dt} \;+\; q(\mathbf{v}\cdot\nabla)\mathbf{A} \;=\; -q\nabla\Phi \;+\; q\nabla(\mathbf{v}\cdot\mathbf{A}) \tag{11}$$

and hence

$$m\frac{d\mathbf{v}}{dt} \;=\; +q\mathbf{E}(\mathbf{x}) \;+\; q\Big(\nabla(\mathbf{v}\cdot\mathbf{A}) \;-\; (\mathbf{v}\cdot\nabla)\mathbf{A}\Big)(\mathbf{x}), \tag{12}$$

where $\mathbf{E}(\mathbf{x}) = -\nabla\Phi(\mathbf{x})$ is the electric field. As to the second term on the RHS of eq. (12), it amounts to the Lorentz force $q\mathbf{v}\times\mathbf{B}(\mathbf{x})$. Indeed, by the double-vector-product formula

$$\nabla(\mathbf{v}\cdot\mathbf{A}) \;-\; (\mathbf{v}\cdot\nabla)\mathbf{A} \;=\; \mathbf{v}\times(\nabla\times\mathbf{A}) \;=\; \mathbf{v}\times\mathbf{B}, \tag{13}$$

thus altogether

$$m\frac{d\mathbf{v}}{dt} \;=\; +q\mathbf{E}(\mathbf{x}) \;+\; q\mathbf{v}\times\mathbf{B}(\mathbf{x}), \tag{14}$$

where the net force is the sum of the electrostatic force and the Lorentz magnetic force. Physically, this is the correct equation of motion for a charged particle in combined EM fields, and that completes our justification of the Lagrangian (3).

Next, consider the classical Hamiltonian for the charged particle. By the usual rules of classical mechanics, the Hamiltonian follows from the Lagrangian as

$$H(\mathbf{x},\mathbf{p}) \;=\; \frac{\partial L(\mathbf{x},\mathbf{v})}{\partial\mathbf{v}}\cdot\mathbf{v} \;-\; L(\mathbf{x},\mathbf{v}), \tag{15}$$

where the RHS should be re-expressed in terms of the position $\mathbf{x}$ and the *canonical momentum* $\mathbf{p} = \partial L/\partial\mathbf{v}$ rather than the position and the velocity. For the Lagrangian (3), the canonical momentum

$$\mathbf{p} \;=\; m\mathbf{v} \;+\; q\mathbf{A}(\mathbf{x}) \tag{7}$$

is different from the usual kinematic momentum $m\mathbf{v}$. Consequently, while

$$H \;=\; \mathbf{p}\cdot\mathbf{v} \;-\; L \;=\; m\mathbf{v}^2 \;+\; q\mathbf{A}\cdot\mathbf{v} \;-\; \tfrac{1}{2}m\mathbf{v}^2 \;+\; q\Phi \;-\; q\mathbf{v}\cdot\mathbf{A} \;=\; \tfrac{1}{2}m\mathbf{v}^2 \;+\; q\Phi(\mathbf{x}) \tag{16}$$

seems to be independent of the vector potential, this is an artefact of writing H as a function of the velocity and position. When we rewrite this Hamiltonian as a function of the canonical momentum instead of the velocity, the **A**–dependence becomes manifest:

$$\mathbf{v} \;=\; \frac{\mathbf{p} - q\mathbf{A}(\mathbf{x})}{m} \tag{17}$$

and therefore

$$H(\mathbf{x},\mathbf{p}) \;=\; \frac{1}{2m}\bigl(\mathbf{p} \,-\, q\mathbf{A}(\mathbf{x})\bigr)^2 \;+\; q\Phi(\mathbf{x}). \tag{18}$$

Quantum Mechanics

In quantum mechanics, the classical dynamical variables like positions and momenta become linear operators in the Hilbert space of quantum states. Some of these linear operators do not commute with each other, $\hat{A}\hat{B} \neq \hat{B}\hat{A}$. In particular, the position and the canonical momentum operators obey the canonical commutation relations

$$\begin{aligned} \hat{x}_i\hat{x}_j \;-\; \hat{x}_j\hat{x}_i \;&=\; 0, \\ \hat{p}_i\hat{p}_j \;-\; \hat{p}_j\hat{p}_i \;&=\; 0, \\ \hat{x}_i\hat{p}_j \;-\; \hat{p}_j\hat{x}_i \;&=\; i\hbar\delta_{i,j}\,. \end{aligned} \tag{19}$$

In terms of the wave-functions of coordinates $\psi(\mathbf{x})$, the position operators act by multiplication

$$\hat{x}_i\psi(\mathbf{x}) \;=\; x_i \times \psi(\mathbf{x}) \tag{20}$$

while the *canonical momenta* act as space derivatives

$$\hat{p}_i\psi \;=\; -i\hbar\frac{\partial\psi(\mathbf{x})}{\partial x_i}\,. \tag{21}$$

Note that for a charged particle in EM fields, these derivative operators correspond to the canonical momenta $p_i = mv_i + qA_i(\mathbf{x})$ rather that to the kinematic momenta $\pi_i = mv_i$. The kinematic momenta operators $\hat{\pi}_i$ act in a more complicated way as

$$\hat{\pi}_i \psi(\mathbf{x}) \;=\; -i\hbar\,\frac{\partial\psi}{\partial x_i} \;-\; qA_i(\mathbf{x}) \times \psi(\mathbf{x}), \tag{22}$$

or in vector notations

$$\vec{\hat{\pi}}\psi(\mathbf{x}) \;=\; -i\hbar\nabla\psi(\mathbf{x}) \;-\; q\mathbf{A}(\mathbf{x})\psi(\mathbf{x}). \tag{23}$$

Consequently, the classical Hamiltonian (18) of the charged particle becomes the quantum Hamiltonian operator

$$\begin{aligned} \hat{H} \;&=\; \frac{1}{2m}\left(\hat{\mathbf{p}} \,-\, q\mathbf{A}(\hat{\mathbf{x}})\right)^2 \;+\; q\Phi(\hat{\mathbf{x}}), \\ \hat{H}\psi(\mathbf{x}) \;&=\; \frac{1}{2m}\left(-i\hbar\nabla \,-\, qA(\mathbf{x})\right)^2\psi(\mathbf{x}) \;+\; q\Phi(\mathbf{x})\psi(\mathbf{x}). \end{aligned} \tag{24}$$

This Hamiltonian operator governs the time-dependence of the wave function $\psi(\mathbf{x},t)$ according to the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{x},t) \;=\; \hat{H}\psi(\mathbf{x},t) \;=\; \frac{1}{2m}\left(-i\hbar\nabla \,-\, qA(\mathbf{x},t)\right)^2\psi(\mathbf{x},t) \;+\; q\Phi(\mathbf{x},t)\psi(\mathbf{x},t). \tag{25}$$

Gauge Transforms.

The magnetic field $\mathbf{B}(\mathbf{x})$ does not uniquely determine the vector potential $\mathbf{A}(\mathbf{x})$. Instead, the fields determine the potentials up to a *gauge transform:* Pick any function $\Lambda(\mathbf{x})$ of of position and change the vector potential by its gradient,

$$\mathbf{A}(\mathbf{x}) \;\to\; \mathbf{A}'(\mathbf{x}) \;=\; \mathbf{A}(\mathbf{x}) \;+\; \nabla\Lambda(\mathbf{x}), \tag{26}$$

and the magnetic field $\mathbf{B}(\mathbf{x})$ would remain completely unchanged,

$$\mathbf{B}' \;=\; \nabla\times\mathbf{A}' \;=\; \nabla\times\left(\mathbf{A}+\nabla\Lambda\right) \;=\; \nabla\times\mathbf{A} \;+\; \nabla\times\nabla\Lambda \;=\; \mathbf{B} \;+\; 0. \tag{27}$$

In classical mechanics, a gauge transform of the potentials has no effect on the equation of motion (5) for the charged particle. In quantum mechanics, a gauge transform also does not have any effect on any *physically measurable* quantities. However, to keep the Schrödinger equation (25) working, a gauge transform (26) of the potentials should be accompanied by a *local phase transform* of the wave-function,

$$\psi(\mathbf{x}) \;\to\; \psi'(\mathbf{x}) \;=\; \psi(\mathbf{x}) \times \exp\bigl(i\,\tfrac{q}{\hbar}\,\Lambda(\mathbf{x})\bigr). \tag{28}$$

To see how this works, let me show that the combined gauge transform (26) and the local phase transform (28) is a symmetry of the Schrödinger equation for any $\Lambda(\mathbf{x})$.

Let's start with the local phase transform (28) for a position-dependent Λ and consider what happens to the gradient of the wave function:

$$\begin{aligned}
\nabla\psi' &= \nabla\Bigl(\psi \times \exp\bigl(i\tfrac{q}{\hbar}\Lambda\bigr)\Bigr)\\
&= (\nabla\psi) \times \exp\bigl(i\tfrac{q}{\hbar}\Lambda\bigr) \;+\; \psi \times \nabla\bigl(\exp\bigl(i\tfrac{q}{\hbar}\Lambda\bigr)\bigr)\\
&= (\nabla\psi) \times \exp\bigl(i\tfrac{q}{\hbar}\Lambda\bigr) \;+\; \psi \times \Bigl(\exp\bigl(i\tfrac{q}{\hbar}\Lambda\bigr) \times i\tfrac{q}{\hbar}\,\nabla\Lambda\Bigr)\\
&= \exp\bigl(i\tfrac{q}{\hbar}\Lambda\bigr) \times \Bigl(\nabla\psi \;+\; i\tfrac{q}{\hbar}\,(\nabla\Lambda) \times \psi\Bigr).
\end{aligned} \tag{29}$$

Note that the gradient $\nabla\psi$ does not transform *covariantly, i.e.* like the ψ itself. Instead, there is an extra inhomogeneous term $(\nabla\Lambda)\psi$ inside the big $(\cdots)$. To remedy this non-covariance, let's define *the covariant derivative*

$$\vec{\mathcal{D}}\psi(\mathbf{x}) = \;\nabla\psi(\mathbf{x}) \;-\; i\tfrac{q}{\hbar}\,\mathbf{A}(\mathbf{x})\psi(\mathbf{x}). \tag{30}$$

This derivative does transform covariantly under the local phase transforms (28), provided the vector potential $\mathbf{A}(\mathbf{x})$ is gauge-transformed for the same $\Lambda(\mathbf{x})$. Indeed,

$$\begin{aligned}
\bigl[\vec{\mathcal{D}}\psi\bigr]' &= \vec{\mathcal{D}}'\psi' \;=\; \nabla\psi' \;-\; i\tfrac{q}{\hbar}\,\mathbf{A}'\psi' \qquad \langle\!\langle\,\text{note } \mathbf{A}' \text{ as well as } \psi' \text{ here}\,\rangle\!\rangle\\
&= \exp\bigl(i\tfrac{q}{\hbar}\Lambda\bigr) \times \Bigl(\nabla\psi \;+\; i\tfrac{q}{\hbar}\,(\nabla\Lambda) \times \psi\Bigr) \;-\; i\tfrac{q}{\hbar}\bigl(\mathbf{A} \;+\; \nabla\Lambda\bigr) \times \exp\bigl(i\tfrac{q}{\hbar}\Lambda\bigr) \times \psi\\
&= \exp\bigl(i\tfrac{q}{\hbar}\Lambda\bigr) \times \Bigl[\nabla\psi \;+\; i\tfrac{q}{\hbar}\,(\nabla\Lambda) \times \psi \;-\; i\tfrac{q}{\hbar}\,\mathbf{A} \times \psi \;-\; i\tfrac{q}{\hbar}\,(\nabla\Lambda) \times \psi\Bigr]\\
&= \exp\bigl(i\tfrac{q}{\hbar}\Lambda\bigr) \times \Bigl[\nabla\psi \;-\; i\tfrac{q}{\hbar}\,\mathbf{A} \times \psi\Bigr]\\
&= \exp\bigl(i\tfrac{q}{\hbar}\Lambda\bigr) \times \vec{\mathcal{D}}\psi.
\end{aligned} \tag{31}$$

Multiple covariant derivatives of the wave function also transform covariantly, for example

$$[\mathcal{D}_i\mathcal{D}_j\psi]' \;=\; \mathcal{D}'_i[\mathcal{D}_j\psi]' \;=\; \mathcal{D}'_i\bigl[\exp(\bigl(i\tfrac{q}{\hbar}\Lambda\bigr)\times D_j\psi\bigr] \;=\; \exp\bigl(i\tfrac{q}{\hbar}\Lambda\bigr)\times\mathcal{D}_i\mathcal{D}_|\psi, \tag{32}$$

in particular

$$\bigl[\vec{\mathcal{D}}^2\psi\bigr] \;=\; \exp(\bigl(i\tfrac{q}{\hbar}\Lambda\bigr)\times\vec{\mathcal{D}}^2\psi. \tag{33}$$

In the coordinate basis for the wave functions, the covariant gradient (30) — or rather $-i\hbar\vec{\mathcal{D}}$ — is the kinematic momentum operator,

$$\vec{\hat{\pi}} \;=\; \hat{\mathbf{p}} \;-\; q\mathbf{A}(\hat{\mathbf{x}}) \;=\; -i\hbar\nabla \;-\; q\mathbf{A}(\mathbf{x}) \;=\; -i\hbar\vec{\mathcal{D}}. \tag{34}$$

Thanks to its covariance, the expectation value of the kinematic momentum is gauge invariant,

$$\langle\psi|\,\vec{\hat{\pi}}\,|\psi\rangle \;=\; \iiint d^3\mathbf{x}\,\psi^*(\mathbf{x})\vec{\hat{\pi}}\psi(\mathbf{x}) \;\longrightarrow\; \text{itself} \tag{35}$$

because

$$\begin{aligned}
\psi'(\mathbf{x}) \;&=\; \exp\bigl(+i\tfrac{q}{\hbar}\Lambda(\mathbf{x})\bigr)*\psi(\mathbf{x}),\\
\bigl[\vec{\hat{\pi}}\psi(\mathbf{x})\bigr]' \;&=\; \exp\bigl(+i\tfrac{q}{\hbar}\Lambda(\mathbf{x})\bigr)*\vec{\hat{\pi}}\psi(\mathbf{x}),\\
\bigl[\psi^*(\mathbf{x})\bigr]' \;&=\; \exp\bigl(-i\tfrac{q}{\hbar}\Lambda(\mathbf{x})\bigr)*\psi^*(\mathbf{x}),\\
\text{hence}\quad \bigl[\psi^*(\mathbf{x})\vec{\hat{\pi}}\psi(\mathbf{x})\bigr] \;&=\; \psi^*(\mathbf{x})\vec{\hat{\pi}}\psi(\mathbf{x}).
\end{aligned} \tag{36}$$

As to the Hamiltonian operator (24), in the coordinate basis it can also be expressed in terms of the covariant derivatives as

$$\hat{H}\psi(\mathbf{x}) \;=\; -\frac{\hbar^2}{2m}\vec{\mathcal{D}}^2\psi(\mathbf{x}) \;+\; \Phi(\mathbf{x})\psi(\mathbf{x}). \tag{37}$$

Consequently, this Hamiltonian operator acts covariantly under all time-independent gauge transforms $\Lambda(\mathbf{x})$,

$$\bigl[\hat{H}\psi(\mathbf{x})\bigr]' \;=\; \exp\bigl(+i\tfrac{q}{\hbar}\Lambda(\mathbf{x})\bigr)\times\hat{H}\psi(\mathbf{x}), \tag{38}$$

so both sides of the Schrödinger equation transform in the same way: The time-dependent

Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{x},t) \;=\; \hat{H}\psi \tag{39}$$

becomes

$$i\hbar\frac{\partial}{\partial t}\Big(\psi'(\mathbf{x},t) \;=\; \exp\bigl(i\tfrac{q}{\hbar}\Lambda(\mathbf{x})\bigr)\times\psi(\mathbf{x},t)\Big) \;=\; \hat{H}'\psi'(\mathbf{x},t) \;=\; \exp\bigl(i\tfrac{q}{\hbar}\Lambda(\mathbf{x})\bigr)\times\hat{H}\psi(\mathbf{x},t) \tag{40}$$

and hence (for a time-independent $\Lambda(\mathbf{x})$)

$$\exp\bigl(i\tfrac{q}{\hbar}\Lambda(\mathbf{x})\bigr)\times i\hbar\frac{\partial}{\partial t}\psi(\mathbf{x},t) \;=\; \exp\bigl(i\tfrac{q}{\hbar}\Lambda(\mathbf{x})\bigr)\times\hat{H}\psi(\mathbf{x},t),$$

which is completely equivalent to the original equation (39). Likewise, the time-independent Schrödinger eigenstate equation

$$E\psi(\mathbf{x}) \;=\; \hat{H}\psi(\mathbf{x}) \tag{41}$$

becomes

$$E\psi'(\mathbf{x}) \;=\; \exp\bigl(i\tfrac{q}{\hbar}\Lambda(\mathbf{x})\bigr)\times E\psi(\mathbf{x}) \;=\; \hat{H}'\psi'(\mathbf{x}) \;=\; \exp\bigl(i\tfrac{q}{\hbar}\Lambda(\mathbf{x})\bigr)\times\hat{H}\psi(\mathbf{x}), \tag{42}$$

which is completely equivalent to the original eq. (41). Therefore, if the wave function $\psi(\mathbf{x},t)$ obeys the Schrödinger equation before the combined gauge/phase transform, then after the transform the new $\psi'(\mathbf{x},t)$ also obeys the new Schrödinger equation. And that's why *the local phase transform* (28) *should be accompanied by the gauge transform* (26) *and vice verse.*

This issue of the gauge/phase transforms may seem rather technical, but it is the key to understanding the Aharonov–Bohm effect (*cf.* my notes on the subject) and the Dirac quantization condition for the magnetic charges (*cf.*my notes electric-magnetic duality and magnetic monopoles).