

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

CLASSICAL MECHANICS

In this section I describe the Lagrangian and the Hamiltonian formulations of classical mechanics of a charged particle moving in general electric and magnetic fields. The fields $\mathbf{E}(\mathbf{r}, t)$ and $\mathbf{B}(\mathbf{r}, t)$ may be time-dependent, but I take their time-dependence as given; the effects of a moving charged particle on the EM fields themselves will be explored in the second half of the classical electrodynamics class (PHY 352 L).

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

$$L(\mathbf{r}, \mathbf{v}) = \frac{m}{2} \mathbf{v}^2 - qV(\mathbf{r}), \quad (1)$$

$$H(\mathbf{r}, \mathbf{p}) = \frac{\mathbf{p}^2}{2m} + qV(\mathbf{r}). \quad (2)$$

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

$$L(\mathbf{r}, \mathbf{v}) = \frac{m}{2} \mathbf{v}^2 - qV(\mathbf{r}) + q\mathbf{v} \cdot \mathbf{A}(\mathbf{r}) \quad (3)$$

in MKSA units, or

$$L(\mathbf{r}, \mathbf{v}) = \frac{m}{2} \mathbf{v}^2 - qV(\mathbf{r}) + \frac{q}{c} \mathbf{v} \cdot \mathbf{A}(\mathbf{r}) \quad (4)$$

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 special relativity in these notes. 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,

$$m\mathbf{a} = \mathbf{F}_{\text{net}} = q\mathbf{E}(\mathbf{r}) + q\mathbf{v} \times \mathbf{B}(\mathbf{r}). \quad (5)$$

But first, let me remind you that for the time-dependent electromagnetic fields

$$\mathbf{B} = \nabla \times \mathbf{A}, \quad (6)$$

$$\mathbf{E} = -\frac{\partial \mathbf{A}}{\partial t} - \nabla V, \quad (7)$$

where the first equation assures $\nabla \cdot \mathbf{B} = 0$, come hell or high water, while the second equation leads to the Induction Law

$$\nabla \times \mathbf{E} = -\nabla \times \frac{\partial \mathbf{A}}{\partial t} - \nabla \times \nabla V = -\frac{\partial}{\partial t}(\nabla \times \mathbf{A}) - 0 = -\frac{\partial}{\partial t} \mathbf{B}. \quad (8)$$

Now, with these relations in mind, let's derive the Euler-Lagrange equations of motion

$$\frac{d}{dt} \left(\frac{\partial L(\mathbf{r}, \mathbf{v})}{\partial \mathbf{v}} \right) = + \frac{\partial L(\mathbf{r}, \mathbf{v})}{\partial \mathbf{r}} \quad (9)$$

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

$$\mathbf{p} \stackrel{\text{def}}{=} \frac{\partial L}{\partial \mathbf{v}} = m\mathbf{v} + q\mathbf{A}(\mathbf{r}). \quad (10)$$

Note: In the vector potential term $q\mathbf{A}(\mathbf{r})$, the \mathbf{r} is the time-dependent particle's position rather than some fixed point in space. Making the time dependence explicit, we have

$$\mathbf{p}(t) = m\mathbf{v}(t) + q\mathbf{A}(\mathbf{r}(t), t) \quad (11)$$

where the second argument of the vector potential allows for a time-dependent magnetic

field. Consequently,

$$\frac{d}{dt}\mathbf{A}(\mathbf{r}(t), t) = \left(\frac{\partial\mathbf{A}}{\partial t}\right)_{\text{@fixed}\mathbf{r}} + \left(\frac{d\mathbf{r}}{dt} \cdot \nabla\right)\mathbf{A} = \frac{\partial\mathbf{A}}{\partial t} + (\mathbf{v} \cdot \nabla)\mathbf{A} \quad (12)$$

and therefore

$$\frac{d\mathbf{p}}{dt} = m\frac{d\mathbf{v}}{dt} + q\frac{\partial\mathbf{A}}{\partial t} + (\mathbf{v} \cdot \nabla)\mathbf{A}. \quad (13)$$

On the other hand, the Euler–Lagrange equation (9) for the Lagrangian (3) reads

$$\frac{d\mathbf{p}}{dt} = +\frac{\partial L}{\partial\mathbf{r}} = -q\nabla V + q\nabla(\mathbf{v} \cdot \mathbf{A}). \quad (14)$$

Equating the right hand sides of the last two formulae, we arrive at

$$m\frac{d\mathbf{v}}{dt} + q\frac{\partial\mathbf{A}}{\partial t} + (\mathbf{v} \cdot \nabla)\mathbf{A} = -q\nabla V + q\nabla(\mathbf{v} \cdot \mathbf{A}) \quad (15)$$

and hence

$$m\mathbf{a} \stackrel{\text{def}}{=} m\frac{d\mathbf{v}}{dt} = q\left(-\nabla V - \frac{\partial\mathbf{A}}{\partial t}\right) + q\left(\nabla(\mathbf{v} \cdot \mathbf{A}) - (\mathbf{v} \cdot \nabla)\mathbf{A}\right). \quad (16)$$

In light of eq. (7), the first group of terms on the RHS here is simply the electric force $q\mathbf{E}$. As to the second group of terms, it amounts to the Lorentz magnetic force $q\mathbf{v} \times \mathbf{B}$. Indeed, by the $B(AC) - C(AB)$ rule for a double vector product $A \times (B \times C)$, we have

$$\mathbf{v} \times \mathbf{B} = \mathbf{v} \times (\nabla \times \mathbf{A}) = \nabla(\mathbf{v} \cdot \mathbf{A}) - (\mathbf{v} \cdot \nabla)\mathbf{A}, \quad (17)$$

exactly as in eq. (16). Altogether, the Lagrangian (3) and hence eq. (16) gives a simple equation of motion for the charged particle in EM fields,

$$m\mathbf{a}(t) = q\mathbf{E}(\mathbf{r}, t) + q\mathbf{v}(t) \times \mathbf{B}(\mathbf{r}, t). \quad (18)$$

Physically, we know this equation of motion is correct, and that's what justifies 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

$$H(\mathbf{r}, \mathbf{p}) = \frac{\partial L(\mathbf{r}, \mathbf{v})}{\partial \mathbf{v}} \cdot \mathbf{v} - L(\mathbf{r}, \mathbf{v}), \quad (19)$$

where the RHS should be re-expressed in terms of the position \mathbf{r} 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

$$\mathbf{p} = m\mathbf{v} + q\mathbf{A}(\mathbf{r}) \quad (10)$$

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

$$H = \mathbf{p} \cdot \mathbf{v} - L = m\mathbf{v}^2 + q\mathbf{A} \cdot \mathbf{v} - \frac{1}{2}m\mathbf{v}^2 + qV - q\mathbf{v} \cdot \mathbf{A} = \frac{1}{2}m\mathbf{v}^2 + qV(\mathbf{r}) \quad (20)$$

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 \mathbf{A} -dependence becomes manifest:

$$\mathbf{v} = \frac{\mathbf{p} - q\mathbf{A}(\mathbf{r})}{m} \quad (21)$$

and therefore

$$H(\mathbf{r}, \mathbf{p}) = \frac{1}{2m} (\mathbf{p} - q\mathbf{A}(\mathbf{r}))^2 + qV(\mathbf{r}). \quad (22)$$

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

$$\begin{aligned}\hat{r}_i\hat{r}_j - \hat{r}_j\hat{r}_i &= 0, \\ \hat{p}_i\hat{p}_j - \hat{p}_j\hat{p}_i &= 0, \\ \hat{r}_i\hat{p}_j - \hat{p}_j\hat{r}_i &= i\hbar\delta_{i,j},\end{aligned}\tag{23}$$

for $i, j = x, y, z$.

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

$$\hat{x}\psi(x, y, z) = x \times \psi(x, y, z), \quad \hat{y}\psi(x, y, z) = y \times \psi(x, y, z), \quad \hat{z}\psi(x, y, z) = z \times \psi(x, y, z),\tag{24}$$

while the *canonical momenta* act as space derivatives

$$\hat{p}_x\psi(x, y, z) = -i\hbar\frac{\partial\psi}{\partial x}, \quad \hat{p}_y\psi(x, y, z) = -i\hbar\frac{\partial\psi}{\partial y}, \quad \hat{p}_z\psi(x, y, z) = -i\hbar\frac{\partial\psi}{\partial z}.\tag{25}$$

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

$$\hat{\pi}_i\psi(\mathbf{r}) = -i\hbar\frac{\partial\psi}{\partial r_i} - qA_i(\mathbf{r})\psi(\mathbf{r}),\tag{26}$$

or in vector notations

$$\vec{\hat{\pi}}\psi(\mathbf{r}) = -i\hbar\nabla\psi(\mathbf{r}) - q\mathbf{A}(\mathbf{r})\psi(\mathbf{r}).\tag{27}$$

Consequently, the classical Hamiltonian (22) of the charged particle becomes the quantum

Hamiltonian operator

$$\begin{aligned}\hat{H} &= \frac{1}{2m} (\hat{\mathbf{p}} - q\mathbf{A}(\hat{\mathbf{r}}))^2 + qV(\hat{\mathbf{r}}), \\ \hat{H}\psi(\mathbf{r}) &= \frac{1}{2m} (-i\hbar\nabla - qA(\mathbf{r}))^2\psi(\mathbf{r}) + qV(\mathbf{r})\psi(\mathbf{r}).\end{aligned}\tag{28}$$

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

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r}, t) = \hat{H}\psi(\mathbf{r}, t) = \frac{1}{2m} (-i\hbar\nabla - qA(\mathbf{r}, t))^2\psi(\mathbf{r}, t) + qV(\mathbf{r}, t)\psi(\mathbf{r}, t).\tag{29}$$

GAUGE TRANSFORMS.

The electric and the magnetic fields $\mathbf{E}(\mathbf{r}, t)$ and $\mathbf{B}(\mathbf{r}, t)$ do not uniquely determine the vector and the scalar potentials $V(\mathbf{r}, t)$ and $\mathbf{A}(\mathbf{r}, t)$. Instead, the fields determine the potentials up to a *gauge transform*: Pick any function $\Lambda(x, y, z, t)$ of space and time and let

$$\begin{aligned}\mathbf{A}(\mathbf{r}, t) &\rightarrow \mathbf{A}'(\mathbf{r}, t) = \mathbf{A}(\mathbf{r}, t) + \nabla\Lambda(\mathbf{r}, t), \\ V(\mathbf{r}, t) &\rightarrow V'(\mathbf{r}, t) = V(\mathbf{r}, t) - \frac{\partial}{\partial t}\Lambda(\mathbf{r}, t).\end{aligned}\tag{30}$$

Regardless of $\Lambda(\mathbf{r}, t)$, the new potential \mathbf{A}' and V' yield exactly the same electric and magnetic fields as the old potentials:

$$\begin{aligned}\mathbf{E}' &= -\nabla V' - \frac{\partial \mathbf{A}'}{\partial t} \\ &= -\nabla \left(V - \frac{\partial \Lambda}{\partial t} \right) - \frac{\partial}{\partial t} (\mathbf{A} + \nabla \Lambda) \\ &= -\nabla V - \frac{\partial \mathbf{A}}{\partial t} + \left(\frac{\partial}{\partial t} (\nabla \Lambda) - \nabla \left(\frac{\partial \Lambda}{\partial t} \right) \right) \\ &= \mathbf{E} + 0,\end{aligned}\tag{31}$$

$$\begin{aligned}\mathbf{B}' &= \nabla \times \mathbf{A}' = \nabla \times (\mathbf{A} + \nabla \Lambda) \\ &= \nabla \times \mathbf{A} + \nabla \times \nabla \Lambda \\ &= \mathbf{B} + 0.\end{aligned}\tag{32}$$

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 (29) working, a gauge transform (30) of the potentials should be accompanied by a *local phase transform* of the wave-function,

$$\psi(x, y, z, t) \rightarrow \psi'(x, y, z, t) = \psi(x, y, z, t) \times \exp\left(i \frac{q}{\hbar} \Lambda(x, y, z, t)\right). \quad (33)$$

To see how this works, let me show that the combined gauge transform (30) and the local phase transform (33) is a symmetry of the Schrödinger equation for any position-and-time-dependent $\Lambda(x, y, z, t)$.

Let's start with the local phase transform (33) for a position-dependent Λ and consider what happens to the gradient of the wave function:

$$\begin{aligned} \nabla\psi' &= \nabla\left(\psi \times \exp\left(i\frac{q}{\hbar}\Lambda\right)\right) \\ &= (\nabla\psi) \times \exp\left(i\frac{q}{\hbar}\Lambda\right) + \psi \times \nabla\left(\exp\left(i\frac{q}{\hbar}\Lambda\right)\right) \\ &= (\nabla\psi) \times \exp\left(i\frac{q}{\hbar}\Lambda\right) + \psi \times \left(\exp\left(i\frac{q}{\hbar}\Lambda\right) \times i\frac{q}{\hbar} \nabla\Lambda\right) \\ &= \exp\left(i\frac{q}{\hbar}\Lambda\right) \times \left(\nabla\psi + i\frac{q}{\hbar} (\nabla\Lambda) \times \psi\right). \end{aligned} \quad (34)$$

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

$$\vec{\mathcal{D}}\psi(\mathbf{r}) = \nabla\psi(\mathbf{r}) - i\frac{q}{\hbar} \mathbf{A}(\mathbf{r})\psi(\mathbf{r}). \quad (35)$$

This derivative does transform covariantly under the local phase transforms (33), provided the vector potential $\mathbf{A}(\mathbf{r})$ is gauge-transformed for the same $\Lambda(\mathbf{r})$. Indeed,

$$\begin{aligned} [\vec{\mathcal{D}}\psi]' &= \vec{\mathcal{D}}'\psi' = \nabla\psi' - i\frac{q}{\hbar} \mathbf{A}'\psi' \quad \langle\langle \text{note } \mathbf{A}' \text{ as well as } \psi' \text{ here} \rangle\rangle \\ &= \exp\left(i\frac{q}{\hbar}\Lambda\right) \times \left(\nabla\psi + i\frac{q}{\hbar} (\nabla\Lambda) \times \psi\right) - i\frac{q}{\hbar} (\mathbf{A} + \nabla\Lambda) \times \exp\left(i\frac{q}{\hbar}\Lambda\right) \times \psi \\ &= \exp\left(i\frac{q}{\hbar}\Lambda\right) \times \left[\nabla\psi + i\frac{q}{\hbar} (\nabla\Lambda) \times \psi - i\frac{q}{\hbar} \mathbf{A} \times \psi - i\frac{q}{\hbar} (\nabla\Lambda) \times \psi\right] \\ &= \exp\left(i\frac{q}{\hbar}\Lambda\right) \times \left[\nabla\psi - i\frac{q}{\hbar} \mathbf{A} \times \psi\right] \\ &= \exp\left(i\frac{q}{\hbar}\Lambda\right) \times \vec{\mathcal{D}}\psi. \end{aligned} \quad (36)$$

In the same way, for a time-dependent $\Lambda(\mathbf{r}, t)$, we define the *covariant time derivative*

$$\mathcal{D}_t\psi(\mathbf{r}, t) = \frac{\partial\psi(\mathbf{r}, t)}{\partial t} + i\frac{q}{\hbar}V(\mathbf{r}, t)\psi(\mathbf{r}, t), \quad (37)$$

then after a combined phase and gauge transform

$$[\mathcal{D}_t\psi(\mathbf{r}, t)]' = \exp(i\frac{q}{\hbar}\Lambda(\mathbf{r}, t)) \times \mathcal{D}_t\psi(\mathbf{r}, t). \quad (38)$$

As an operator acting on the wave functions, the covariant gradient (35) — or rather $-i\hbar\vec{\mathcal{D}}$ — is the kinematic momentum operator,

$$\vec{\pi} = \hat{\mathbf{p}} - q\mathbf{A}(\hat{\mathbf{r}}) = -i\hbar\nabla - q\mathbf{A}(\mathbf{r}) = -i\hbar\vec{\mathcal{D}}. \quad (39)$$

Consequently, the Hamiltonian operator (28) for the charged particles can be written in terms of covariant derivatives as

$$\hat{H}\psi(\mathbf{r}) = -\frac{\hbar^2}{2m}\vec{\mathcal{D}}^2\psi(\mathbf{r}) + V(\mathbf{r})\psi(\mathbf{r}). \quad (40)$$

Moreover, if we put the $V\psi$ term on the other side of the time-dependent Schrödinger eqn. (29), we get

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r}, t) - V(\mathbf{r}, t)\psi(\mathbf{r}, t) = -\frac{\hbar^2}{2m}\vec{\mathcal{D}}^2\psi(\mathbf{r}, t) \quad (41)$$

where the left-hand side is the covariant time derivative $i\hbar\mathcal{D}_t\psi(\mathbf{r}, t)$. Altogether, we get the covariant form of the Schrödinger equation

$$i\hbar\mathcal{D}_t\psi(\mathbf{r}, t) = -\frac{\hbar^2}{2m}\vec{\mathcal{D}}^2\psi(\mathbf{r}, t) \quad (42)$$

where both sides transform covariantly under the local phase transforms:

$$\begin{aligned} \psi'(x, y, z, t) &= \exp(i\frac{q}{\hbar}\Lambda(x, y, z, t)) \times \psi(x, y, z, t), \\ [i\hbar\mathcal{D}_t\psi(x, y, z, t)]' &= \exp(i\frac{q}{\hbar}\Lambda(x, y, z, t)) \times [i\hbar\mathcal{D}_t\psi(x, y, z, t)], \\ \left[-\frac{\hbar^2}{2m}\vec{\mathcal{D}}^2\psi(x, y, z, t)\right]' &= \exp(i\frac{q}{\hbar}\Lambda(x, y, z, t)) \times \left[-\frac{\hbar^2}{2m}\vec{\mathcal{D}}^2\psi(x, y, z, t)\right]. \end{aligned} \quad (43)$$

Therefore, if the wave function $\psi(x, y, z, t)$ obeys the Schrödinger equation before the combined gauge/phase transform, then after the transform the new $\psi'(x, y, z, t)$ also obeys the

new Schrödinger equation. And that's why *the local phase transform* (33) *should be accompanied by the gauge transform* (30) *and vice versa*.

This issue of the gauge/phase transforms may seem rather technical, but as I show in the [next set of my notes](#), it leads to the Aharonov–Bohm effect, helps explain how SQUID magnetometers work, and even explains how magnetic monopoles might work in quantum mechanics.

For the moment, let me simply generalize the relation between the gauge and the phase transforms from ordinary quantum mechanics to quantum electrodynamics (QED) and other quantum field theories. In QED, instead of wave-functions of individual electrons we have the quantum electron field $\hat{\Psi}(x, y, z, t)$ which creates and annihilates electrons and positrons. But despite its operatorial nature, as a function of space and time coordinates — or rather, as a 4-component array of such functions — it obeys a linear Dirac equation

$$i\hbar\mathcal{D}_t\hat{\Psi} + i\hbar c\vec{\alpha}\cdot\vec{\mathcal{D}}\hat{\Psi} - mc^2\beta\hat{\Psi} = 0 \quad (44)$$

where $\vec{\mathcal{D}}$ and \mathcal{D}_t are the covariant derivatives exactly as in eqs. (35) and (37) for $q = -e$, and $\alpha_x, \alpha_y, \alpha_z$ and β are 4×4 Dirac matrices, never mind their details. In light of the covariant derivatives in the Dirac equation, QED is invariant under local phase transforms of the electron field $\hat{\Psi}(\mathbf{r}, t)$ accompanied by the gauge transforms of the EM potential fields $\hat{V}(\mathbf{r}, t)$ and $\hat{\mathbf{A}}(\mathbf{r}, t)$. This invariance — called *the gauge symmetry* — is absolutely essential to QED and helps explain many of its key features, for example the exact masslessness of the photons.

The gauge symmetry of QED can be generalized to more complicated local symmetries of other quantum field theories. For example, in QCD — quantum chromodynamics, the theory of strong interactions — there is a gauge symmetry mixing the 3 colors of the quarks, accompanied by a rather complicated transform of the EM-like gluon fields. Almost all features of QCD — and hence of the strong interactions — follow from this gauge symmetry, but the explanation is way too complicated for this class.