Comments on Gauge Invariance

Kuo-Ho Yang
Department of Engineering and Physics, St. Ambrose University, Davenport, IA 52803

Kirk T. McDonald
Joseph Henry Laboratories, Princeton University, Princeton, NJ 08544
(June 12, 2021; updated March 16, 2022)

1 Introduction

This note was inspired by misuse of gauge invariance in ref. [1] by H.R. Reiss, and elaborates on the general theme of this concept. A key assumption of this note is that "physical observables" must be gauge invariant. It is in this context that Reiss and others misuse gauge invariance.

(a) Reiss did not distinguish the **canonical** momentum, which is **not** gauge invariant, from the **mechanical** momentum, which **is** gauge invariant. Also, he appeared to believe that the **canonical** momentum was a physical **observable** in **any** gauge.[1]

(b) Reiss did not distinguish the **Hamiltonian**, which is **not** gauge invariant, from the **mechanical** kinetic energy or the total energy.[2] While the mechanical kinetic energy is gauge invariant, the potential energy is not. Not only that, he appeared to believe that the **Hamiltonian** was a physical **observable** in **any** gauge.[3]

(c) As they are gauge invariant, the canonical momentum and the Hamiltonian are different in different gauges. Reiss appeared to be baffled by such differences. He cited the Aharonov-Bohm (A-B) effect [3] as the justification for his statement that "gauge transformations alter physical properties", despite the fact that his simple field situation (a static, uniform electric field) would not cause any A-B effects. He failed to note that the difference between the canonical momenta in two different gauges was solely caused by the difference in the vector potentials used.

(d) Reiss claimed that the statement, "Electromagnetic potentials are more fundamental than electromagnetic fields", was supported by the A-B effects. But, he failed to appreciate the gauge **invariance** of the A-B effects. Logically, it would be difficult to use the gauge-**invariant** A-B effects to justify the physical observability of the canonical momenta and Hamiltonians that are **not** gauge **invariant**.

    We believe that potentials affect gauge-**dependent** phases (which are **not** physical observables) and cause gauge-**invariant** phase **interferences** (which **are** physical observables), so far also supported by the (quantum-mechanical or classical) A-B effects.

[1] In [1], Reiss used "momentum" to refer to the canonical momentum.

[2] The total energy of an electric charge q is defined to be the sum of its mechanical kinetic energy and potential energy qV, where V is the electric scalar potential in some gauge [2].

[3] In [1], Reiss used "energy" to refer to the Hamiltonian.

It is true that if the Lagrangian is independent of time, the Hamiltonian can be called the (total) energy.

(e) The challenges we face in the Lagrangian or the Hamiltonian formalism, whether in classical or quantum mechanics, are:

  (i) to preserve the fundamental role of the EM potentials in the coupling of EM fields to charged particles while conforming to the accepted understanding that: (1) EM potentials are not physical observables, unless we can prove otherwise in some particular cases; (2) the EM fields are physical observables; and (3) quantities that are not gauge invariant are not physical observables.

  (ii) to identify gauge-invariant physical observables (*i.e.*, physically measurable quantities) using well established knowledge and principles in physics;

  (iii) to formulate a mathematical procedure through which we can calculate the changes in particles' physical states caused by the interaction with fields through potentials.

In particular, we want to show that the **mechanical** momentum $\mathbf{P}_{\rm mech} = m\mathbf{v}$ and the **mechanical** kinetic energy KE $= \mathbf{P}^2_{\rm mech}/2m = m\mathbf{v}^2/2$ of a (nonrelativistic) charged particle in external electromagnetic fields both have gauge-invariant equations of motion.

We take the viewpoint that only gauge-invariant quantities can be physical observables in **all** gauges, and for **all** field situations [4], simple or complicated, even though gauge-dependent quantities can be calculated from gauge-invariant quantities such as charge, time, position, velocity, acceleration, *etc.*[4] In this view, electromagnetic gauge transformations cannot change the physical properties of a system. The Lagrangian, and hence the Hamiltonian, formalisms, when explicitly expressed via EM potentials rather than EM fields, are not physical observables, but do lead to gauge-invariant equations of motion.

When we talk about **physical** momenta and energies, we are talking about the **mechanical** momenta and kinetic energy, as well as electromagnetic field momentum and field energy. However, the concept of electromagnetic potential energy is not gauge invariant, and hence total energy is not a gauge-invariant concept nor a physical observable in electromagnetic examples.

2 Basics of Gauge Invariance

Let us assume that we have a particle with mass m and charge q in the presence of an electric field $\mathbf{E}(\mathbf{r}, t)$ and a magnetic field $\mathbf{B}(\mathbf{r}, t)$. We use the EM potentials in an arbitrary gauge, called gauge a, with potentials $\mathbf{A}_{\rm a}$ and $\Phi_{\rm a}$ to represent the fields, *i.e.*,

$$\mathbf{E} = -\boldsymbol{\nabla}\Phi_{\rm a} - \frac{1}{c}\frac{\partial \mathbf{A}_{\rm a}}{\partial t}, \qquad \mathbf{B} = \boldsymbol{\nabla} \times \mathbf{A}_{\rm a}. \tag{1}$$

[4]Time, position, velocity and acceleration do not have absolute values, but are defined only with respect to some frame of reference. We follow the usual convention that these quantities are nonetheless "physical observables."

In quantum theory, the term "observable" is associated with a Hermitian operator, which is not necessary a "physical observable" in the sense of being gauge invariant.

The (nonrelativistic) Lagrangian in gauge a is,

$$L_{\rm a}({\bf r},{\bf v},t) = \frac{1}{2}m{\bf v}^2 + \frac{1}{c}q{\bf v}\cdot{\bf A}_{\rm a} - q\Phi_{\rm a}, \tag{2}$$

where $\mathbf{r}$ is the position and $\mathbf{v} = d\mathbf{r}/dt$ is the (mechanical) velocity of the particle.

The equation of motion of the charged particle is given by,

$$\begin{aligned}\frac{d}{dt}\frac{\partial L}{\partial{\bf v}} &= \frac{d{\bf p}}{dt} = \frac{d}{dt}\left(m{\bf v}+\frac{q}{c}{\bf A}_a\right) = m\dot{\bf v} + \frac{q}{c}\frac{d{\bf A}_a}{dt} = \frac{d{\bf P}_{\rm mech}}{dt} + \frac{q}{c}\frac{\partial A_a}{\partial t} + \frac{q}{c}({\bf v}\cdot{\boldsymbol\nabla}){\bf A}_a \\ &= \frac{\partial L}{\partial r} = {\boldsymbol\nabla}L = \frac{q}{c}{\boldsymbol\nabla}({\bf v}\cdot{\bf A}_a) - q{\boldsymbol\nabla}\Phi_a = \frac{q}{c}({\bf v}\cdot{\boldsymbol\nabla}){\bf A}_a + \frac{q}{c}{\bf v}\times({\boldsymbol\nabla}\times{\bf A}_a) - q{\boldsymbol\nabla}\Phi_a, \end{aligned}\tag{3}$$

$$\frac{d{\bf P}_{\rm mech}}{dt} = -q{\boldsymbol\nabla}\Phi_a - \frac{q}{c}\frac{\partial A_a}{\partial t} + + \frac{q}{c}{\bf v}\times({\boldsymbol\nabla}\times{\bf A}_a) = q\left({\bf E} + \frac{\bf v}{c}\times{\bf B}\right), \tag{4}$$

which is the gauge-invariant Lorentz-force law. Note that $\mathbf{p} = \partial L/\partial\mathbf{v} = \mathbf{P}_{\rm mech} + q\mathbf{A}_a/c$ is the canonical momentum, whose equation of motion is not, in general, gauge invariant,

$$\frac{d{\bf p}}{dt} = q\left({\bf E}+\frac{\bf v}{c}\times{\bf B}\right) + \frac{q}{c}\frac{d{\bf A}_a}{dt}\,. \tag{5}$$

However, the equation of motion of the mechanical kinetic energy,

$$\frac{d{\rm KE}}{dt} = \frac{{\bf P}_{\rm mech}}{m}\cdot\frac{d{\bf P}_{\rm mech}}{dt} = q{\bf v}\cdot{\bf E}, \tag{6}$$

is gauge invariant.

The (nonrelativistic) Hamiltonian is,

$$H_{\rm a} = {\bf p}\cdot{\bf v} - L_{\rm a} = \frac{m{\bf v}^2}{2} + q\Phi_{\rm a} = {\rm KE} + q\Phi_{\rm a}, \tag{7}$$

which is not gauge invariant. If the potential $\Phi_{\rm a}$ depends on time, then $dH_{\rm a}/dt$ is also not gauge invariant.

2.1 Two Different Gauges

We now consider another set of potentials $\mathbf{A}_{\rm b}$ and $\Phi_{\rm b}$ in a different gauge, labeled gauge b, to represent the same fields $\mathbf{E}$ and $\mathbf{B}$. Then, these new potentials are related to the old potentials by a gauge transformation:

$${\bf A}_{\rm b}({\bf r},t) = {\bf A}_{\rm a}({\bf r},t) + {\boldsymbol\nabla}\chi({\bf r},t), \qquad \Phi_{\rm b}({\bf r},t) = \Phi_{\rm a}({\bf r},t) - \frac{1}{c}\frac{\partial}{\partial t}\chi({\bf r},t), \tag{8}$$

with the gauge function $\chi(\mathbf{r},t)$ having the following properties: $\boldsymbol\nabla\times(\boldsymbol\nabla\chi) = 0$ and $\partial(\boldsymbol\nabla\chi)/\partial t = \boldsymbol\nabla(\partial\chi/\partial t)$.

The Lagrangian in this other arbitrary gauge b is,

$$L_{\rm b}({\bf r},{\bf v},t) = \frac{1}{2}m{\bf v}^2 + \frac{1}{c}q{\bf v}\cdot{\bf A}_{\rm b} - q\Phi_{\rm b}. \tag{9}$$

The difference between the two Lagrangians is,

$$L_{\rm b} - L_{\rm a} = \frac{1}{c}q\mathbf{v}\cdot(\mathbf{A}_{\rm b} - \mathbf{A}_{\rm a}) - q(\Phi_{\rm b} - \Phi_{\rm a}) = \frac{q}{c}\mathbf{v}\cdot\boldsymbol{\nabla}\chi + \frac{q}{c}\frac{\partial\chi}{\partial t} = \frac{q}{c}\frac{d\chi}{dt}. \tag{10}$$

It is obvious that the Lagrangian is **not** gauge invariant.

We note that, in eqs. (2) and (9), the very **same** $\mathbf{r}$, $\mathbf{v}$, and t are used for the Lagrangian in any gauge. That is, $\mathbf{r}$, $\mathbf{v}$, and t (as well as $\mathbf{P}_{\rm mech} = m\mathbf{v}$) are gauge invariant in the Lagrangian formalism and, consequently, also in the Hamiltonian formalism.[5]

2.2 Canonical Momentum

Now we investigate the **canonical** momentum.

The canonical momenta in gauges a and b are, respectively,

$$\mathbf{p}_{\rm a} = \frac{\partial L_{\rm a}(\mathbf{r},\mathbf{v},t)}{\partial\mathbf{v}} = m\mathbf{v} + \frac{q}{c}\mathbf{A}_{\rm a}(\mathbf{r},t), \tag{11}$$

$$\mathbf{p}_{\rm b} = \frac{\partial L_{\rm b}(\mathbf{r},\mathbf{v},t)}{\partial\mathbf{v}} = m\mathbf{v} + \frac{q}{c}\mathbf{A}_{\rm b}(\mathbf{r},t). \tag{12}$$

Thus, the canonical momentum is **not** gauge invariant because,

$$\mathbf{p}_{\rm b} - \mathbf{p}_{\rm a} = \frac{q}{c}(\mathbf{A}_{\rm b} - \mathbf{A}_{\rm a}) = \frac{q}{c}\boldsymbol{\nabla}\chi. \tag{13}$$

The Hamiltonians in gauge a and gauge b are, respectively,

$$H_{\rm a}(\mathbf{r},\mathbf{p}_{\rm a},t) = \mathbf{v}\cdot\mathbf{p}_{\rm a} - L_{\rm a} = \frac{1}{2m}\left(\mathbf{p}_{\rm a} - \frac{q}{c}\mathbf{A}_{\rm a}\right)^2 + q\Phi_{\rm a} = \frac{1}{2}m\mathbf{v}^2 + q\Phi_{\rm a}, \tag{14}$$

$$H_{\rm b}(\mathbf{r},\mathbf{p}_{\rm b},t) = \mathbf{v}\cdot\mathbf{p}_{\rm b} - L_{\rm b} = \frac{1}{2m}\left(\mathbf{p}_{\rm b} - \frac{q}{c}\mathbf{A}_{\rm b}\right)^2 + q\Phi_{\rm b} = \frac{1}{2}m\mathbf{v}^2 + q\Phi_{\rm b}. \tag{15}$$

Thus, we see that the Hamiltonian is **not** gauge invariant:

$$H_{\rm b}(\mathbf{r},\mathbf{p}_{\rm b},t) - H_{\rm a}(\mathbf{r},\mathbf{p}_{\rm a},t) = q\Phi_{\rm b} - q\Phi_{\rm a} = -\frac{q}{c}\frac{\partial\chi}{\partial t}\,. \tag{16}$$

2.3 Physical Interpretation

So, what is the essence of gauge invariance, especially in the Hamiltonian formalism where quantities are expressed in terms of the canonical variables $\mathbf{r}$ (which is gauge invariant) and $\mathbf{p}$ (which is not gauge invariant)? A gauge-invariant quantity, for example, the combination $\mathbf{p} - q\mathbf{A}/c$, has the **same form**, **same value** and **same interpretation** in **all** gauges. In

[5] Throughout this note, we **always** use the symbol $\mathbf{P}_{\rm mech}$ to denotes the **mechanical** momentum, $\mathbf{P}_{\rm mech} = m\mathbf{v}$. Please notice the subscript "mech" in $\mathbf{P}_{\rm mech}$ and other mechanical (Newtonian) quantities such as $K_{\rm mech}$. In Hamiltonian mechanics (as emphasized in quantum mechanics) the symbol **p always** denotes the **canonical** momentum, $\partial L/\partial\dot{\mathbf{r}}$, associated with coordinate $\mathbf{r}$ in the Lagrangian L. The relation between the mechanical momentum $\mathbf{P}_{\rm mech} = m\mathbf{v}$ and the canonical momentum $\mathbf{p}$ for a particle with mass m and charge q is $\mathbf{P}_{\rm mech} = \mathbf{p} - q\mathbf{A}/c$, or equivalently, $\mathbf{p} = \mathbf{P}_{\rm mech} + q\mathbf{A}/c$.

the non-relativistic examples investigated here, the gauge invariance of $\mathbf{p}-q\mathbf{A}/c$ means that $\mathbf{p}_\mathrm{a} - q\mathbf{A}_\mathrm{a}/c$ is $m\mathbf{v}$ in gauge a and $\mathbf{p}_\mathrm{b} - q\mathbf{A}_\mathrm{b}/c$ is $m\mathbf{v}$ in gauge b. They also have the same value because according to eqs. (11)-(12): $\mathbf{p}_\mathrm{a} - q\mathbf{A}_\mathrm{a}/c = m\mathbf{v} = \mathbf{p}_\mathrm{b} - q\mathbf{A}_\mathrm{b}/c$.

The interpretation of a quantity, gauge invariant or not, is determined by its **equation of motion**. That is because the equation of motion shows how the quantity **behaves** during the interaction with fields. For example, both $\mathbf{p}$ and $\mathbf{p} - q\mathbf{A}/c$ **look like** a linear momentum. The most reliable way to decide which one, if any, behaves like the mechanical linear momentum as prescribed by Newton's second law is through the physics contained in the equations of motion. We use $\mathbf{p}_\mathrm{a} - q\mathbf{A}_\mathrm{a}/c$ in gauge a in eq. (11) as an example:

$$\frac{d}{dt}(\mathbf{p}_\mathrm{a} - q\mathbf{A}_\mathrm{a}/c) = q\mathbf{E} + \frac{q}{c}\frac{(\mathbf{p}_\mathrm{a} - q\mathbf{A}_\mathrm{a}/c)}{m} \times \mathbf{B} = q\mathbf{E} + q\frac{\mathbf{v}}{c} \times \mathbf{B}. \tag{17}$$

It is the total force on the right-hand side of eq. (17) that firmly establishes the physics behind the interpretation of $(\mathbf{p}_\mathrm{a} - q\mathbf{A}_\mathrm{a}/c)$ as the mechanical linear momentum in gauge a. Since $(\mathbf{p} - q\mathbf{A}/c)$ is gauge invariant, eq. (17) also means that the same interpretation is true in all other gauges, *i.e.*, $(\mathbf{p}_\mathrm{b} - q\mathbf{A}_\mathrm{b}/c)$ is the mechanical linear momentum in gauge b, *etc.*. Another example is a charged particle in a static, uniform electric field considered in Sec. 3 below, particularly eqs. (26), (28), (38), and (52).

Then, what should we do about quantities that are **not** gauge invariant? When we say that a quantity is not gauge invariant, we mean that it will have **different values** and **different interpretations** in two **different** gauges. In other words, the values and the interpretations are done on a **gauge-by-gauge** basis. It may or may not have a physically meaningful interpretation in one gauge, but, if it does, the **same** physical interpretation can **not** be applied to a **different** gauge. Or equivalently, the **same** physical interpretation will **not** be valid in a **different** gauge.

3 Charged Particle in a Static, Uniform Electric Field

Consider a nonrelativistic particle with mass m and charge q in the presence of a static, uniform electric field $\mathbf{E}_0$. There exist gauges in which the potentials are time dependent, so the Hamiltonian is not necessarily the total energy (in that gauge), although Hamiltonian is constant in any gauge.

3.1 Newtonian Formalism

Newton's equation of motion for this example is,

$$\mathbf{P}_\mathrm{mech} = m\mathbf{v}, \qquad \frac{d}{dt}\mathbf{P}_\mathrm{mech} = q\mathbf{E}_0, \tag{18}$$

where $\mathbf{P}_\mathrm{mech}$ is the **mechanical** linear momentum with a **mechanical** velocity $\mathbf{v} = d\mathbf{r}/dt$ and $\mathbf{r}$ is the position of the particle. It is naïvely appealing to define a potential energy as in [2], PE $= -q\mathbf{r} \cdot \mathbf{E}_0$, which involves an implicit choice of a gauge. It follows that the mechanical kinetic energy K_mech and total energy E_T associated with mass m (sum of the mechanical kinetic energy $K_{\rm mech}$ and the potential energy $-q\mathbf{r}\cdot\mathbf{E}_0$ due to the static, uniform electric force $q\mathbf{E}_0$ on the particle [2]) have the equations of motion,[6]

$$K_{\rm mech} = \frac{1}{2}m\mathbf{v}^2, \qquad \frac{d}{dt}K_{\rm mech} = \mathbf{v}\cdot q\mathbf{E}_0, \tag{19}$$

$$E_{\rm T} = \frac{1}{2}m\mathbf{v}^2 - q\mathbf{r}\cdot\mathbf{E}_0, \qquad \frac{d}{dt}E_{\rm T} = 0. \tag{20}$$

3.2 Lagrangian and Hamiltonian Formalisms in Three Gauges

3.2.1 Gauge 1

The static, uniform electric field $\mathbf{E}_0$ can be represented by a set of potentials in gauge 1,

$$\mathbf{A}_1 = 0, \qquad \Phi_1 = -\mathbf{r}\cdot\mathbf{E}_0. \tag{21}$$

The Lagrangian constructed with this set of potentials is,

$$L_1(\mathbf{r},\mathbf{v},t) = \frac{1}{2}m\mathbf{v}^2 + \frac{1}{c}q\mathbf{v}\cdot\mathbf{A}_1 - q\Phi_1 = \frac{1}{2}m\mathbf{v}^2 + q\mathbf{r}\cdot\mathbf{E}_0. \tag{22}$$

The **canonical** (linear) momentum $\mathbf{p}_1$ in gauge 1 is,

$$\mathbf{p}_1 = \frac{\partial L_1}{\partial\mathbf{v}} = m\mathbf{v} + \frac{q}{c}\mathbf{A}_1 = m\mathbf{v}. \tag{23}$$

The Hamiltonian H_1 in gauge 1 is,

$$H_1(\mathbf{r},\mathbf{p}_1,t) = \mathbf{v}\cdot\mathbf{p}_1 - L_1 = \frac{1}{2m}\mathbf{p}_1^2 - q\mathbf{r}\cdot\mathbf{E}_0. \tag{24}$$

Hamilton's equations of motion for the position $\mathbf{r}$, the canonical momentum $\mathbf{p}_1$ and Hamiltonian H_1 in gauge 1 are,

$$\frac{d\mathbf{r}}{dt} = \frac{\partial H_1}{\partial\mathbf{p}_1} \qquad \Rightarrow \qquad \mathbf{v} = \frac{\mathbf{p}_1}{m}, \tag{25}$$

$$\frac{d\mathbf{p_1}}{dt} = -\frac{\partial H_1}{\partial\mathbf{r}} = q\mathbf{E}_0, \tag{26}$$

$$\frac{dH_1}{dt} = -\frac{\partial H_1}{\partial t} = 0. \tag{27}$$

We note that eq. (25) is just eq. (23). Also, the (mechanical) velocity $\mathbf{v}$ is gauge invariant because both the position $\mathbf{r}$ and the time t are gauge invariant.

In gauge 1, the **mechanical** linear momentum, kinetic energy and total energy in eqs. (18)-(20), and their equations of motion are, from eqs. (25)-(27),

$$(\mathbf{P}_{\rm mech})_1 = m\mathbf{v} = \mathbf{p}_1, \qquad \frac{d}{dt}(\mathbf{P}_{\rm mech})_1 = \frac{d\mathbf{p}_1}{dt} = q\mathbf{E}_0, \tag{28}$$

[6]Note that we could also take the potential energy to be PE $= -q\mathbf{r}\cdot\mathbf{E}_0 + f(t)$ for any function f not dependent on $\mathbf{r}$, and the force $-\boldsymbol{\nabla}$ PE on charge q would be the same.

But then, the energy E_T would, in general, depend on time.

$$(K_{\text{mech}})_1 = \frac{m\mathbf{v}^2}{2} = \frac{\mathbf{p}_1^2}{2m}, \qquad \frac{d}{dt}(K_{\text{mech}})_1 = \frac{\mathbf{p_1}}{m} \cdot \frac{d\mathbf{p}_1}{dt} = \mathbf{v} \cdot q\mathbf{E}_0, \tag{29}$$

$$(E_{\text{T}})_1 = \frac{m\mathbf{v}^2}{2} - q\mathbf{r} \cdot \mathbf{E} = \frac{\mathbf{p}_1^2}{2m} - q\mathbf{r} \cdot \mathbf{E}, \qquad \frac{d}{dt}(E_{\text{T}})_1 = \frac{dH_1}{dt} = 0, \tag{30}$$

These three equations of motion above are identical to the Newtonian equations in eqs. (18)-(20). We note in gauge 1, the Hamiltonian H_1 in eq. (24) is identical to the total energy $(E_{\text{T}})_1$ in eq. (30).

3.2.2 Gauge 2

The static, uniform electric field $\mathbf{E}_0$ can be represented by a different set of potentials in gauge 2 (which is sometimes called the Gibbs gauge [5]),

$$\mathbf{A}_2 = -c\mathbf{E}_0 t, \qquad \Phi_2 = 0. \tag{31}$$

The Lagrangian constructed with this new set of potentials is then,

$$L_2(\mathbf{r}, \mathbf{v}, t) = \frac{1}{2}m\mathbf{v}^2 + \frac{1}{c}q\mathbf{v} \cdot \mathbf{A}_2 - q\Phi_2 = \frac{1}{2}m\mathbf{v}^2 - q\mathbf{v} \cdot \mathbf{E}_0 t. \tag{32}$$

The canonical momentum $\mathbf{p}_2$ in gauge 2 is,

$$\mathbf{p}_2 = \frac{\partial L_2}{\partial \mathbf{v}} = m\mathbf{v} + \frac{q}{c}\mathbf{A}_2 = m\mathbf{v} - q\mathbf{E}_0 t. \tag{33}$$

The Hamiltonian H_2 in gauge 2 is then,

$$H_2(\mathbf{r}, \mathbf{p}_2, t) = \mathbf{v} \cdot \mathbf{p}_2 - L_2 = \frac{1}{2m}(\mathbf{p}_2 + q\mathbf{E}_0 t)^2. \tag{34}$$

Hamilton's equations of motion for the canonical momentum $\mathbf{p}_2$ and the Hamiltonian H_2 in gauge 2 are,

$$\frac{d\mathbf{r}}{dt} = \frac{\partial H_2}{\partial \mathbf{p}_2} \qquad \Rightarrow \qquad \mathbf{v} = \frac{(\mathbf{p}_2 + q\mathbf{E}_0 t)}{m}. \tag{35}$$

$$\frac{d\mathbf{p}_2}{dt} = -\frac{\partial H_2}{\partial \mathbf{r}} = 0, \qquad \mathbf{p}_2 = m\mathbf{v}_{\text{init}}. \tag{36}$$

$$\frac{dH_2}{dt} = \frac{\partial H_2}{\partial t} = \frac{(\mathbf{p}_2 + q\mathbf{E}_0 t)}{m} \cdot (q\mathbf{E}_0) = \mathbf{v} \cdot (q\mathbf{E}_0), \tag{37}$$

where $\mathbf{v}_{\text{init}}$ in eq. (36) is the particle's initial velocity at $t = 0$.

In gauge 2, the **mechanical** quantities in eqs. (18)-(20) and their equations of motion are,

$$(\mathbf{P}_{\text{mech}})_2 = m\mathbf{v} = \mathbf{p}_2 + q\mathbf{E}_0 t, \qquad \frac{d}{dt}(\mathbf{P}_{\text{mech}})_2 = \frac{d}{dt}(\mathbf{p}_2 + q\mathbf{E}_0 t) = q\mathbf{E}_0, \tag{38}$$

$$(K_{\text{mech}})_2 = \frac{m\mathbf{v}^2}{2} = \frac{(\mathbf{p}_2 + q\mathbf{E}_0 t)^2}{2m}, \qquad \frac{d}{dt}(K_{\text{mech}})_2 = \frac{\mathbf{p}_2 + q\mathbf{E}_0 t}{m} \cdot q\mathbf{E}_0 = \mathbf{v} \cdot q\mathbf{E}_0, \tag{39}$$

$$(E_{\text{T}})_2 = \frac{m\mathbf{v}^2}{2} - q\mathbf{r} \cdot \mathbf{E} = \frac{(\mathbf{p}_2 + q\mathbf{E}_0 t)^2}{2m} - q\mathbf{r} \cdot \mathbf{E}, \qquad \frac{d}{dt}(E_{\text{T}})_2 = 0. \tag{40}$$

It is instructive to note that the Hamiltonian H_2 in eq. (34) is identical to the mechanical kinetic energy $(K_{\text{mech}})_2$ in eq. (39). This is in contrast to the fact that the Hamiltonian H_1 in eq. (24) in gauge 1 is identical to the total energy $(E_{\text{T}})_1$ in eq. (30).

3.2.3 Gauge α

Let us consider the following potentials of gauge α,

$$\mathbf{A}_\alpha = (\alpha - 1)(-c\mathbf{E}_0 t), \qquad \Phi_\alpha = (2-\alpha)(-\mathbf{r}\cdot\mathbf{E}_0). \tag{41}$$

for any real α. When $\alpha = 1$, the potentials reduce to those in gauge 1, and when $\alpha = 2$, the potentials reduce to those in gauge 2. They also generate the correct static, uniform electric field $\mathbf{E}_0$,

$$-\boldsymbol{\nabla}\Phi_\alpha - \frac{1}{c}\frac{\partial \mathbf{A}_\alpha}{\partial t} = (2-\alpha)\mathbf{E}_0 + (\alpha-1)\mathbf{E}_0 = \mathbf{E}_0. \tag{42}$$

In gauge α, the Lagrangian is,

$$L_\alpha(\mathbf{r},\mathbf{v},t) = \frac{1}{2}m\mathbf{v}^2 + \frac{1}{c}q\mathbf{v}\cdot\mathbf{A}_\alpha - q\Phi_\alpha = \frac{1}{2}m\mathbf{v}^2 - (\alpha-1)q\mathbf{v}\cdot\mathbf{E}_0 t + (2-\alpha)q\mathbf{r}\cdot\mathbf{E}_0, \tag{43}$$

the canonical momentum is,

$$\mathbf{p}_\alpha = \frac{\partial L_\alpha}{\partial \mathbf{v}} = m\mathbf{v} + \frac{q}{c}\mathbf{A}_\alpha = m\mathbf{v} - (\alpha-1)q\mathbf{E}_0 t, \tag{44}$$

and the Hamiltonian is,

$$H_\alpha(\mathbf{r},\mathbf{p}_\alpha,t) = \mathbf{v}\cdot\mathbf{p}_\alpha - L_\alpha = \frac{1}{2m}[\mathbf{p}_\alpha + (\alpha-1)q\mathbf{E}_0 t]^2 - (2-\alpha)q\mathbf{r}\cdot\mathbf{E}_0. \tag{45}$$

Hamilton's equations of motion are,

$$\frac{d\mathbf{r}}{dt} = \frac{\partial H_\alpha}{\partial \mathbf{p}_\alpha} \qquad \Rightarrow \qquad \mathbf{v} = \frac{1}{m}[\mathbf{p}_\alpha + (\alpha-1)q\mathbf{E}_0 t], \tag{46}$$

$$\frac{d\mathbf{p}_\alpha}{dt} = -\frac{\partial H_\alpha}{\partial \mathbf{r}} = (2-\alpha)q\mathbf{E}_0, \tag{47}$$

$$\frac{dH_\alpha}{dt} = \frac{\partial H_\alpha}{\partial t} = \frac{1}{m}[\mathbf{p}_\alpha + (\alpha-1)q\mathbf{E}_0 t]\cdot[(\alpha-1)q\mathbf{E}_0] = (\alpha-1)\mathbf{v}\cdot(q\mathbf{E}_0). \tag{48}$$

The mechanical quantities in eqs. (18)-(20) have the following expressions in gauge α,

$$(\mathbf{P}_{\text{mech}})_\alpha = m\mathbf{v} = \mathbf{p}_\alpha + (\alpha-1)q\mathbf{E}_0 t, \tag{49}$$

$$(K_{\text{mech}})_\alpha = \frac{m\mathbf{v}^2}{2} = \frac{1}{2m}[\mathbf{p}_\alpha + (\alpha-1)q\mathbf{E}_0 t]^2, \tag{50}$$

$$(U_{\text{mech}})_\alpha = \frac{m\mathbf{v}^2}{2} - q\mathbf{r}\cdot\mathbf{E} = \frac{1}{2m}[\mathbf{p}_\alpha + (\alpha-1)q\mathbf{E}_0 t]^2 - q\mathbf{r}\cdot\mathbf{E}. \tag{51}$$

Their equations of motion are,

$$\frac{d}{dt}(\mathbf{P}_{\text{mech}})_\alpha = \frac{d}{dt}[\mathbf{p}_\alpha + (\alpha-1)q\mathbf{E}_0 t] = (2-\alpha)q\mathbf{E}_0 + (\alpha-1)q\mathbf{E}_0 = q\mathbf{E}_0, \tag{52}$$

$$\frac{d}{dt}(K_{\text{mech}})_\alpha = \frac{1}{m}[\mathbf{p}_\alpha + (\alpha-1)q\mathbf{E}_0 t]\cdot\frac{d}{dt}[\mathbf{p}_\alpha + (\alpha-1)q\mathbf{E}_0 t] = \mathbf{v}\cdot q\mathbf{E}_0, \tag{53}$$

$$\frac{d}{dt}(E_{\text{T}})_\alpha = \frac{d}{dt}(K_{\text{mech}})_\alpha - q\frac{d\mathbf{r}}{dt}\cdot\mathbf{E}_0 = \mathbf{v}\cdot q\mathbf{E}_0 - q\mathbf{v}\cdot\mathbf{E}_0 = 0. \tag{54}$$

3.3 Comments on Physical Interpretations

The simple field situation (static, uniform electric field) discussed above provides us with several good learning examples about quantities that are not gauge invariant.

3.3.1 Canonical Momentum

First, consider the canonical momentum $\mathbf{p}$. From eqs. (25) and (26), the canonical momentum $\mathbf{p}_1$ in gauge 1 **is** also the **mechanical** momentum for all t. This happens because there is no magnetic field, and gauge 1 has a vanishing vector potential $\mathbf{A}_1 = 0$. So, $\mathbf{p}_1$ is a special case of a gauge-invariant $\mathbf{p}_1 - q\mathbf{A}_1/c$ with $\mathbf{A}_1 = 0$. Of course, when a magnetic field is present, $\mathbf{p}$ can never be the mechanical momentum in any gauge because then there does not exist a gauge with $\mathbf{A} = 0$.

But, by eqs. (35) and (36), the canonical momentum $\mathbf{p}_2$ in gauge 2 **is** the **initial** mechanical momentum at $t = 0$, not the mechanical linear momentum at all times. The only reason for $\mathbf{p}_2$ being the initial mechanical momentum is because the electric field is **not position** dependent. Then, Newton's equation of motion eq. (18) (or eq. (38)) has the solution,

$$m\mathbf{v}(t) = m\mathbf{v}_{\text{init}} + q\mathbf{E}_0 t. \tag{55}$$

In gauge 2, the gauge-invariant mechanical momentum is $m\mathbf{v} = \mathbf{p}_2 - q\mathbf{A}_2/c = \mathbf{p}_2 + q\mathbf{E}_0 t$. Thus, we deduce from eq. (55) that the canonical momentum $\mathbf{p}_2$ is the initial mechanical momentum at $t = 0$. Obviously, if the electric field is position dependent, or if a magnetic field is present, the canonical momentum will not be the initial mechanical momentum.

3.3.2 The Hamiltonian

Now, let us now look at the Hamiltonian H.

In gauge 1, the Hamiltonian H_1 in eq. (24) **is** the **total energy** as indicated in eqs. (27) and (30). This is a consequence of the canonical momentum $\mathbf{p}_1$ being the mechanical momentum as explained earlier. On the other hand, the Hamiltonian H_2 in eq. (34) in gauge 2 is the **mechanical kinetic** energy as indicated in eqs. (34), (37) and (39). This comes about because $\Phi_2 = 0$. See also eqs. (14) and (15).

We note from the above discussions that the physical interpretabilities of $\mathbf{p}_1$, $\mathbf{p}_2$, H_1 and H_2 are just special cases of gauge-invariant quantities in some particular gauges for a very simple field situation.

The canonical momentum $\mathbf{p}_\alpha$ and the Hamiltonian H_α in gauge α, with $\alpha \neq 1$ and $\alpha \neq 2$, are good examples of non-gauge-invariant quantities having no readily-available physically meaningful interpretations.

In general, a quantity that is not gauge invariant usually cannot be physically interpreted in any gauge. There are exceptions for some simple field situations as explained earlier.

As a consequence of the above discussions, if we want to assign a physical interpretation to a gauge-**invariant** quantity, the usual way to justify the physical interpretation is to derive the **equation of motion** of the quantity in **only one gauge** and justify the interpretation by the physics contained in that equation of motion. The reason is that the same interpretation will be valid in all other gauges.

On the other hand, if we want to assign a physical interpretation to a quantity that is **not** gauge invariant, there are **two** things that must be done to accompany such a physical interpretation: (1) we **must specify a specific gauge** in which such a physical interpretation is valid, and (2) we **must justify** such an interpretation based on the contents of the equation of motion in that specific gauge. For example, in case of the physical (mechanical) linear momentum, the total force on the particle must be present in the equation of motion, *e.g.*, eq. (26) for $\mathbf{p}_1$. As mentioned earlier, a quantity that is not gauge invariant but happens to have a physical interpretation in a particular gauge usually is a special case of a gauge-invariant quantity (*e.g.*, $\mathbf{p}_1 = \mathbf{p}_1 - q\mathbf{A}_1/c$ where $\mathbf{A}_1 = 0$), or it happens to be identical to another gauge-variant quantity in the same gauge (*e.g.*, $H_2 = (K_{\rm mech})_2$ in Sec. 4).

The following **mechanical** quantities, some with the subscript "mech", are gauge invariant: $t, \mathbf{r}$, the mechanical velocity $\mathbf{v} = d\mathbf{r}/dt$, the mechanical linear momentum, $\mathbf{P}_{\rm mech} = m\mathbf{v}$, the mechanical angular momentum $\mathbf{L}_{\rm mech} = \mathbf{r} \times \mathbf{P}_{\rm mech}$, and the mechanical kinetic energy $K_{\rm mech} = m\mathbf{v}^2/2$.

3.3.3 Equations of Motion

In the following, we investigate their equations of motion in the Hamiltonian formalism.

The Hamiltonian for a particle with mass m and charge q coupling to the potentials $\mathbf{A}$ and Φ in an arbitrary gauge is,

$$H = \frac{1}{2m}\left(\mathbf{p} - \frac{q}{c}\mathbf{A}\right)^2 + q\Phi, \tag{56}$$

with the fields $\mathbf{E}$ and $\mathbf{B}$ being related to the potentials by,

$$\mathbf{E} = -\boldsymbol{\nabla}\Phi - \frac{1}{c}\frac{\partial \mathbf{A}}{\partial t}, \qquad \mathbf{B} = \boldsymbol{\nabla} \times \mathbf{A}. \tag{57}$$

Then,

$$\mathbf{v} = \frac{\partial H}{\partial \mathbf{p}} = \frac{1}{m}\left(\mathbf{p} - \frac{q}{c}\mathbf{A}\right), \tag{58}$$

$$\mathbf{P}_{\rm mech} = m\mathbf{v} = \mathbf{p} - \frac{q}{c}\mathbf{A}\,, \tag{59}$$

$$\frac{d}{dt}\mathbf{P}_{\rm mech} = q\mathbf{E} + \frac{q}{mc}\left(\mathbf{p} - \frac{q}{c}\mathbf{A}\right) \times \mathbf{B} = q\mathbf{E} + \frac{1}{c}q\mathbf{v} \times \mathbf{B}, \tag{60}$$

$$\mathbf{L}_{\rm mech} = \mathbf{r} \times \mathbf{P}_{\rm mech} = \mathbf{r} \times \left(\mathbf{p} - \frac{q}{c}\mathbf{A}\right), \tag{61}$$

$$\frac{d}{dt}\mathbf{L}_{\rm mech} = \mathbf{r} \times \left\{q\mathbf{E} + \frac{q}{mc}\left(\mathbf{p} - \frac{q}{c}\mathbf{A}\right) \times \mathbf{B}\right\} = \mathbf{r} \times \left\{q\mathbf{E} + \frac{1}{c}q\mathbf{v} \times \mathbf{B}\right\}, \tag{62}$$

$$K_{\rm mech} = \frac{1}{2}m\mathbf{v}^2 = \frac{1}{2m}\left(\mathbf{p} - \frac{q}{c}\mathbf{A}\right)^2, \tag{63}$$

$$\frac{d}{dt}K_{\rm mech} = \frac{q}{m}\left(\mathbf{p} - \frac{q}{c}\mathbf{A}\right) \cdot \mathbf{E} = q\mathbf{v} \cdot \mathbf{E}. \tag{64}$$

Use of the Radiation Gauge

For certain problems (*e.g.*, a hydrogen atom in an external laser field where the electron interacts with the Coulomb field of the proton and external radiation fields), the total fields can be regarded to consist of a static electric field $\mathbf{E}_{\rm s}(\mathbf{r}) = -\boldsymbol{\nabla} V_{\rm s}(\mathbf{r})$ and an EM radiation field with $\mathbf{E}_{\rm rad}(\mathbf{r}, t)$ and $\mathbf{B}_{\rm rad}(\mathbf{r}, t)$:

$$\mathbf{E} = \mathbf{E}_{\rm s}(\mathbf{r}) + \mathbf{E}_{\rm rad}(\mathbf{r}, t), \qquad \mathbf{B} = \mathbf{B}_{\rm rad}(\mathbf{r}, t), \tag{65}$$

We can define a static (scalar) potential energy $qV_{\rm s}$ as in [2], and then define the total energy associated with mass m with charge q by,

$$E_{\rm T} = K_{\rm mech} + qV_{\rm s}(\mathbf{r}) = \frac{1}{2m}\left(\mathbf{p} - \frac{q}{c}\mathbf{A}\right)^2 + qV_{\rm s}(\mathbf{r}). \tag{66}$$

Here, the radiation fields have no scalar potential, and this convention, sometimes called the radiation gauge is a form of the Coulomb gauge. Consideration of the total energy (66) is useful in experiments measuring stimulated absorption or emission by external radiation fields because changes of $E_{\rm T}$ depend **only** the effects of the radiation fields on the particle's physical states:

$$\frac{d}{dt}E_{\rm T} = \frac{q}{m}\left(\mathbf{p} - \frac{q}{c}\mathbf{A}\right)\cdot(\mathbf{E} + \boldsymbol{\nabla} V_{\rm s}) = \frac{q}{m}\left(\mathbf{p} - \frac{q}{c}\mathbf{A}\right)\cdot \mathbf{E}_{\rm rad} = q\mathbf{v}\cdot\mathbf{E}_{\rm rad}. \tag{67}$$

We note that the $\mathbf{v}$ in eq. (58), $\mathbf{P}_{\rm mech}$ in eq. (59), $\mathbf{L}_{\rm mech}$ in eq. (61), $K_{\rm mech}$ in eq. (63) [but not $E_{\rm T}$ in eq. (66)] all have the same values in all gauges and that the equations of motion in eqs. (60), (62), (64) and (67) are all gauge invariant.

References

[1] H.R. Reiss, *Fundamental formulation of light-matter interactions revisited*, Phys. Rev. A **100**, 052105 (2019), http://kirkmcd.princeton.edu/examples/QED/reiss_pra_100_052105_19.pdf

[2] We can construct a static electric potential $V_{\rm s}(\mathbf{r})$ from an electrostatic field $\mathbf{E}_{\rm s}(\mathbf{r})$ by the **path-independent** line-integral,

$$V_{\rm s}(\mathbf{r}_2) - V_{\rm s}(\mathbf{r}_1) = -\int_{\mathbf{r}_1}^{\mathbf{r}_2} \mathbf{E}_{\rm s}(\mathbf{s})\cdot d\mathbf{s}, \tag{68}$$

because $\boldsymbol{\nabla}\times\mathbf{E}_{\rm s} = 0$. Hence, $\mathbf{E}_{\rm s}(\mathbf{r}) = -\boldsymbol{\nabla} V_{\rm s}(\mathbf{r})$. In Newtonian mechanics, the quantity $qV_{\rm s}(\mathbf{r})$ is called the electric **potential energy** of a particle (of mass m and charge q) due to $\mathbf{E}_{\rm s}(\mathbf{r})$. The static electric potential energy can be converted to the interaction energy between the external static field $\mathbf{E}_{\rm s}(\mathbf{x})$ and the electric field $\mathbf{E}_q(\mathbf{x}, t)$ produced by the charge q through Maxwell's equations. If we use $\rho_q(\mathbf{x}, t) = q\,\delta(\mathbf{x} - \mathbf{r}(t))$ to denote the charge density of point-charge q at position $\mathbf{r}(t)$, then

$$4\pi\rho_q(\mathbf{x}, t)V_{\rm s}(\mathbf{x}) = (\boldsymbol{\nabla}\cdot\mathbf{E}_q)V_{\rm s} = \boldsymbol{\nabla}\cdot(V_{\rm s}\mathbf{E}_q) - \mathbf{E}_q\cdot(\boldsymbol{\nabla} V_{\rm s}) = \mathbf{E}_q\cdot\mathbf{E}_{\rm s} + \boldsymbol{\nabla}\cdot(V_{\rm s}\mathbf{E}_q). \tag{69}$$

We integrate the above equation over the whole space and divide both sides by 4π, we get

$$qV_{\rm s}(\mathbf{r}) = \frac{1}{4\pi}\int \mathbf{E}_q \cdot \mathbf{E}_{\rm s}\, d^3\mathbf{x} + \frac{1}{4\pi}\oint_\Sigma \mathbf{n}\cdot(V_{\rm s}\mathbf{E}_q)\, d\sigma. \tag{70}$$

where Σ is the surface enclosing the whole space at infinity, $d\sigma$ is a surface element of Σ and $\mathbf{n}$ is a unit vector normal to $d\sigma$ pointing outward.

The potential energy $qV_{\rm s}(\mathbf{r})$ is constructed only from the static electric field $\mathbf{E}_{\rm s}(\mathbf{r})$ through path-independent line-integrals, which implicitly is a use of the Coulomb gauge. Importantly, its time-derivative, $d(qV_{\rm s})/dt = q\mathbf{v}\cdot\boldsymbol{\nabla}V_{\rm s} = -q\mathbf{v}\cdot\mathbf{E}_0$, contains only gauge-invariant, physically measurable quantities ($\mathbf{v}$ and $\mathbf{E}_{\rm s}$), which is a common characteristic of Newtonian physical observables, although the potential $V_{\rm s}$ is not gauge invariant.

Finally, we see that we can take the potential energy to be PE $= qV_{\rm s}(\mathbf{r}) = -q\mathbf{r}\cdot\mathbf{E}_s$.

[3] Y. Aharonov and D. Bohm, *Significance of Electromagnetic Potentials in Quantum Theory*, Phys. Rev. **115**, 485 (1959),
http://kirkmcd.princeton.edu/examples/QM/aharonov_pr_115_485_59.pdf

[4] C. Cohen-Tannoudji, B. Diu and F. Laloë, *Quantum Mechanics* (Hermann/Wiley, Paris, 1977), especially "$\mathrm{H_{III}}$: gauge invariance", pp. 315-328,
http://kirkmcd.princeton.edu/examples/QM/cohen-tannoudji_qm1.pdf

[5] K.-H. Yang and K.T. McDonald, *Formal Expressions for the Electromagnetic Potentials in Any Gauge* (Feb. 25, 2015), http://kirkmcd.princeton.edu/examples/gauge.pdf