Some aspects about gauge transformations in non-relativistic QED

J. A. Sanchez-Monroy\(^1\)\(^*\), and J. Morales\(^1,2\)†

Grupo de Campos y Partículas \(^1\), and
Centro Internacional de Física \(^2\)

Bogotá, Colombia

D. E. Zambrano‡

Centro Brasileiro de Pesquisas Físicas - CBPF, Rio de Janeiro Brazil

The wave mechanical formulation of quantum electrodynamics is investigated under gauge transformations. For this purpose we observe the structure of Schrödinger equation and matricial elements under these transformations. We conclude this theory is not gauge invariant since the eiger-energies may depend of gauge function, since that the Hamiltonian is operator gauge dependent and cannot represent the observable energy.

I. INTRODUCTION

Is a well-known fact that physical laws cannot depend of arbitrarities arisen from mathematical formalism. There are some cases where arbitrarities are introduced to make easy the calculations, but these quantities cannot be experimentally measured [1, 2].

Gauge transformations in electrodynamics are an example of mathematical arbitrariness. Classically this theory is gauge invariant [3, 4], A. M. Stewart studied the effect of gauge transformations over Hamiltonian and Schrödinger equation with classical potentials (semiclassical electrodynamics regime [1, 2]), he found that only one class of gauge functions can leave the results invariant [1]. There are a stronger restriction for conservative systems [5], which is perhaps due to some troubles in the interpretation of the Hamiltonian as energy [6, 7].

In this work we show that semiclassical electrodynamics is not gauge invariant[1, 5], and we obtain the restriction for gauge functions to preserve the invariance[2] (see section II). We prove in section III that although there exists a restriction, which relates potentials that produce some troubles in the interpretation of the Hamiltonian operator under a gauge transformation is

\[ A \rightarrow A' = A + \nabla \chi, \quad \phi \rightarrow \phi' = \phi - \frac{\partial \chi}{\partial t} \]  (1)

where \( \chi \) is a scalar function called gauge function. If the equations of motion do not change, the dynamics of the system is conserved and the theory is invariant under gauge transformations. Classical electrodynamics is gauge invariant[2, 3].

In quantum mechanics with the Schrödinger picture, Schrödinger equations gives the temporal evolution of the system,

\[ H \Psi(r, t) = i\hbar \frac{\partial \Psi(r, t)}{\partial t}. \]  (2)

Hamiltonian operator under a gauge transformation is

\[ H_{\chi}(p, r, t) = \left( \frac{p - e(A + \nabla \chi)}{2m} \right)^2 + e\left( \phi - \frac{\partial \chi}{\partial t} \right), \]  (3)

where subindex \( \chi \) denotes the gauge function, it is clear that this gauge transformation does not change the picture. For \( \chi = 0 \),

\[ H_0 = \frac{1}{2m} \left( p - \frac{e}{c} A \right)^2 + e\phi. \]  (4)

We assume that exist an unitary operator \( U(\chi) \) such that \( \Psi'(r, t) = U \Psi_0(r, t) \). In general \( U \) is not time-independent, since \( \chi \) may depend explicitly of time. Multiplying to the left the Schrödinger equation for \( \Psi_0 \) by \( U \), we obtain that

\[ i\hbar U \frac{\partial U \Psi_0}{\partial t} = U H_0 \Psi_0. \]  (5)

The chain rule for derivatives provides us the identity

\[ U \frac{\partial U \Psi_0}{\partial t} = \frac{\partial (U \Psi_0)}{\partial t} - \frac{\partial U}{\partial t} \Psi_0. \]  (6)

Replacing the last expression in Eq. (5) we obtain that

\[ i\hbar \frac{\partial (U \Psi_0)}{\partial t} = U H_0 \Psi_0 + i\hbar \frac{\partial U}{\partial t} \Psi_0 \]

\[ = \left( U H_0 U^\dagger + i\hbar \frac{\partial U}{\partial t} U^\dagger \right) (U \Psi_0). \]  (7)
The relation between $\Psi_0$ and $\Psi'$ allows us to write that

$$i\hbar \frac{\partial \Psi'}{\partial t} = H' \Psi' = \left( U H_0 U^\dagger + i \hbar \frac{\partial U}{\partial t} U^\dagger \right) \Psi', \quad (8)$$

then the form of the Schrödinger equation’s remains invariant under any transformation with the form

$$H' = U H U^\dagger + i \hbar \frac{\partial U}{\partial t} U^\dagger. \quad (9)$$

Taking $U(\chi) = e^{ie\chi(r,t)/\hbar}$, we obtain the Hamiltonian under a gauge transformation Eq. (3). Explicitly, $\Psi_0$ transforms as

$$\Psi_0 \rightarrow \Psi_\chi = U(\chi) \Psi_0(r,t) = \Psi_0(r,t) e^{ie\chi(r,t)/\hbar}. \quad (10)$$

Here is important to emphasize that wavefunctions and Hamiltonian change locally with a gauge transformation then Schrödinger equation may change and thus the physics of the system. In order to see this we calculate the matricial elements of the Hamiltonian operator. Taking $|n_0\rangle$ and $|m_0\rangle$, which are two elements of the basis of Hamiltonian $H_0$, the matricial element after a gauge transformation is given by

$$\langle n_\chi | H_\chi | m_\chi \rangle = \langle n_0 | H_0 | m_0 \rangle - e \langle n_0 | \frac{\partial \chi}{\partial t} | m_0 \rangle$$

$$= E_{n,0} \delta_{n,m} - e \int \frac{\partial \chi}{\partial t} \psi_{n,0}^* \psi_{m,0}(r,t) \, dr \quad (11)$$

where $|n_\chi \rangle := e^{ie\chi/\hbar} \psi_{n,0}(r,t)$ and $E_{n,0}$ is the eigenvalue related to $|n_0\rangle$. Hence the Hamiltonian might be not diagonal in the transformed basis.

In the other hand, the experimental measures correspond to energy differences, which must be invariant. From Eq. (11) we can see that

$$E_{n,\chi} - E_{m,\chi} = E_{n,0} - E_{m,0}$$

$$+ e \int \frac{\partial \chi}{\partial t} \left[ |\rho_{m,0}(r,t)|^2 - |\rho_{n,0}(r,t)|^2 \right] \, dr \quad (12)$$

where $\rho_{n,0}(r,t)$ is the probability density related to $|n_0\rangle$. In conclusion, energy differences eventually are not invariant. If we restrict to $\chi$ by means

$$\chi(r,t) = f(r) + g(t), \quad (13)$$

we guarantee the invariance of energy differences.

We have another trouble when we consider a time-independent Hamiltonian, which we transform by means a gauge function as in Eq. (13). Eq. (11) implies that

$$E_{n,\chi} = E_{n,0} - e \int \psi_{n,0}^* \psi_{n,0}(r,t) \, dr$$

$$= E_{n,0} - e \frac{dg(t)}{dt}, \quad (14)$$

so in order to keep eigenvalues time-independent of a time-independent Hamiltonian under a gauge transformation, the gauge function should fulfills

$$\frac{\partial \chi}{\partial t} = \text{const.}$$

This equation implies that

$$\chi(r,t) = f(r) + kt \quad (15)$$

with $k = \text{const.}$ Eq. (15) is the restriction for gauge functions that guarantee the invariance of the theory.

### III. DEEP INSIDE TROUBLE

We define $\Phi$ as set of all electrodynamical potentials possible that describe a given system. Eq. (15) divides the set $\Phi$ in equivalence classes. Each equivalence class has associated a family of Hamiltonians, which produce the same physical results.

If we take two different equivalence classes, we obtain two different families of Hamiltonians that yield contradictory results. Since there not exist a physical criterion to choose the correct family, thus we have two different solutions for the same system. Eq. (1) allow us to obtain an infinity (non-numerable) number of families of Hamiltonians, that in principle describe the same electromagnetic field, but from a mathematical point of view we may obtain infinite number of distinct solutions for the same system (see FIG 1).

In order to illustrate this situation, we consider the Harmonic Oscillator: a particle inside of an electric field $E = -m u^2 x/e$. Two possible Hamiltonians for this system are

$$H_0 = -\frac{\hbar^2}{2m} \nabla^2 + \frac{1}{2} m u^2 x^2, \quad (16)$$

$$H_1 = -\frac{\hbar^2}{2m} \nabla^2 + \frac{1}{2} m u^2 x^2 - 2ekt, \quad (17)$$
where $k$ is a constant that adjusts the units. Is clear that $H_0$ and $H_1$ are related by the gauge transformation $\chi = kt^2$ and thus two both belong to two different families of Hamiltonians. Eigenvalues for each Hamiltonian are

$$E_n^0 = \hbar \omega \left(n + \frac{1}{2}\right), \quad n = 0, 1, 2, \ldots , \quad (18)$$

$$E_n^1 = \hbar \omega \left(n + \frac{1}{2}\right) + 2ekt, \quad n = 0, 1, 2, \ldots , \quad (19)$$

respectively. The last results are distinct and contradictory, since first one describes a conservative system and the other one does not.

At this point, we cannot decide which family of Hamiltonian are correct, there are two different families of Hamiltonians that yield contradictory results. We obtain that the Hamiltonian is operator gauge dependent and cannot represent the observable energy. If we consider the hamiltonian of free particle now we see

$$H = \frac{-\hbar^2}{2m} \nabla^2, \quad (20)$$

which represents the energy. Another hamiltoniano like (which one can obtain by means of a gauge transformation)

$$H = -\frac{\hbar^2}{2m} \nabla^2 + e\phi(t), \quad (21)$$

it does not represent the energy for the case of a free particle. Motivated by this case in the Appendix we propose to fix the gauge searching.

**IV. CONCLUSIONS**

Non-relativistic QED is not gauge invariant since the eiger-energies may depend of gauge function. In order to maintain the same physical results, gauge function must be have the form

$$\chi = f(r) + kt, \quad (12)$$

hence, we cannot take arbitrarily the electrodynamical potentials $A$ and $\phi$. Restriction (15) divides the set of potentials of a physical system in equivalence classes, this implies the existence of infinite number of distinct solutions for the same system. Since there not exists a physics-theoretical criterion to decide which family of Hamiltonians is proper to describe the system, only experimental result can do it.

With this panorama, we should think to find a theoretical procedure such that selects an unique equivalence class and be suitable for any physical system. In the Appendix we propose to fix the gauge searching for, where we find a method that allows us to choose an unique family of Hamiltonians.

**Appendix**

Fixing the gauge, maybe we could restrict the potentials to an unique equivalence class. We only must to impose to the set of potentials that fulfills the gauge condition that be a subset of an unique equivalence class defined by (15) and this set contains at least a couple of potentials $(A, \phi)$ for each physical problem. The last condition means that the gauge does not restrict the potentials at the point that these potentials just only work for particular cases.

It is easy to prove that Lorentz gauge

$$\nabla \cdot A + \frac{1}{c} \frac{\partial \phi}{\partial t} = 0$$

and time-independent gauge

$$\frac{\partial \phi}{\partial t} = 0$$

do not satisfy these condition. But the modified temporal gauge $(\phi = \text{const.})$, fulfills it, since

$$\frac{\partial \chi}{\partial t} = \text{const}, \quad (18)$$

and for any pair of potentials $(A, \phi)$ we can build the potentials $(A', \phi')$ by means

$$\phi' = 0, \quad (19)$$

$$A' = A + \int_T^T \nabla \phi' \, dt', \quad (20)$$

where it is clear that $A'$ and $\phi'$ describe the same electromagnetic field that $A$ and $\phi$ and belong to the equivalence class of modified temporal gauge.

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