Energy operator for non-relativistic and relativistic quantum mechanics revisited

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Abstract

For quantum mechanics of a charged particle in a classical external electromagnetic field the momentum and Hamiltonian operators are gauge dependent. For overcome this difficulty we reexamined the effect of a gauge transformation on Schrödinger and Dirac equations. We show that the gauge invariance of the operator $H - i\hbar\frac{\partial}{\partial t}$ provides a way to find the energy operator from first principles. In particular, when the system has stationary states the energy operator can be identified without ambiguities for non-relativistic and relativistic quantum mechanics. Finally, we examine other approaches finding that in the case in which the electromagnetic field is time independent, the energy operator obtained here is the same as one recently proposed by Chen et al. [1].

1 Introduction

The physical description of nature must not depend on arbitrariness arisen from mathematical formalism. Typically some non-physical quantities (NPQ) are introduced in order to find a solution for the equations which governs the dynamics of a given system. In electrodynamics a gauge transformation of the electromagnetic fields is a well known example of such an arbitrariness. Classical mechanics with electromagnetic fields, via Lorentz force, is gauge invariant [2, 3]. However, there are apparent problems concerning the momentum and Hamiltonian operators of the charged particle in quantum mechanics, due to the fact that the expectation values of these two operators are gauge dependent [1, 4]-[21].

Experimental results are gauge independent, therefore it is necessary to find a gauge invariant quantity to represent physical energy. In the literature, there are some suggestions for this purpose. One of them consists in a gauge invariant energy operator which was proposed by Yang [7]. This approach frequently has been used in literature [8]-[16]. However, as we will show, it is possible to find counterexamples in which this approach does not represent the energy. A different proposal suggests to restricting the gauge function to be a sum of a purely spatial function plus a linear function of time [18]-[21]. We will show that this approach yield to contradictory results.

On the other hand, finding a definition of gluon spin and orbital angular momentum has been a long standing problem [22, 23]. Recently Chen et al. proposed a gauge invariant decomposition of the total nucleon

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angular momentum into quark and gluon constituents [24, 25]. The decomposition is based on the separation of the electromagnetic potential into pure gauge and gauge invariant parts, which simultaneously satisfies the requirement of gauge invariance and the relevant commutation relations. With this decomposition a new energy operator was proposed in the non-relativistic and relativistic quantum mechanics [1, 4, 5].

The purpose of this paper is of set forth the gauge invariance of quantum mechanics. For this we will show, in section 2, that the operator $H - i\hbar \frac{\partial}{\partial t}$ is gauge invariant, even for relativistic quantum mechanics. At the same time we will show how to derive the gauge invariant energy operator from first principles explicitly when the system has stationary states in section 2. In section 3, we will discuss other approaches. Additionally, we will demonstrate that for time independent electromagnetic fields, our approach is consistent with the decomposition of the potential into a pure gauge and a gauge invariant parts, proposed in [1, 4, 5], is consistent with our approach. Finally we summarize our conclusions in section 4.

2 Gauge invariance

Let us describe the electrodynamics using the potentials $A$ and $A^0$, the classical electrodynamics is invariant by the so-called gauge transformations

$$ A \rightarrow A' = A + \nabla \chi, \quad A^0 \rightarrow A^0' = A^0 - \frac{\partial \chi}{\partial t}, $$

where the scalar function $\chi$ is the gauge function. Due to the fact that classical equations of motion are given in terms of the fields, the transformation Eq. (1) does not change anything in the dynamics, i.e. classical theory is gauge invariant.

The canonical momentum and Hamiltonian are defined by

$$ p = mv + qA, \quad \text{and} \quad H = \frac{1}{2m} \left( p - \frac{q}{c} A \right)^2 + qA^0, $$

respectively. Here $q$ denotes the charge of the particle. The Hamiltonian is quantized if $p$ is replaced by $-i\hbar \nabla$. After a gauge transformation Eq. (1), the expectation value of the operators in Eq. (2) are transformed as:

$$ \langle \Psi' | p' | \Psi' \rangle = \langle \Psi | p | \Psi \rangle + q \langle \Psi | \nabla \chi | \Psi \rangle $$

and

$$ \langle \Psi' | H' | \Psi' \rangle = \langle \Psi | H | \Psi \rangle + q \langle \Psi | \frac{\partial \chi}{\partial t} | \Psi \rangle $$

where $| \Psi' \rangle = e^{iq\chi(r,t)/\hbar} | \Psi \rangle$. Notice that the expectation values of these two operators are gauge dependent. In order to remove the gauge dependence of the expectation value of canonical momentum, one introduces the gauge invariant operator,

$$ P = p - qA. $$

It is straightforward to check that the expectation value of this operator is gauge invariant, since the expectation value of $qA$ cancels the additional term in the right side of in Eq. (3). However, the commutators between the components of $P$ are

$$ [P^i, P^j] = -iq(\partial^i A^j - \partial^j A^i) = -iqF^{ij}. $$

therefore $P$ does not satisfy the Lie algebra of canonical momentum (i.e. $[P^i, P^j] = 0$), then it cannot be the proper momentum operator [1, 5].
On the other hand, the dynamics of a quantum particle is described by its (complex) wavefunction \( \Psi(r, t) \), and its evolution is determined by the equation [26]:

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

where \( \hbar \) is the Planck constant and \( H \) is the Hamiltonian. Denoting by \( A = (A^0, A) \) to the external electromagnetic potential, for non-relativistic quantum mechanics we have the Hamiltonian

\[
H_S = \frac{1}{2m} \left( \mathbf{p} - \frac{q}{c} \mathbf{A} \right)^2 + qA^0, \tag{8}
\]

and so we obtain the known Schrödinger equation. Meanwhile, for relativistic quantum mechanics we have the Dirac Hamiltonian

\[
H_D = \bar{\alpha} \cdot \left( \mathbf{p} - \frac{q}{c} \mathbf{A} \right) + \beta m + qA^0, \tag{9}
\]

where \( \bar{\alpha} \) and \( \beta \) are \( 4 \times 4 \) Dirac matrices.

Let us consider the effect of a unitary transformation \( U(\chi) \) on Eq. (7),

\[
i\hbar U(\chi) \frac{\partial}{\partial t} \Psi = U(\chi) H \Psi. \tag{10}
\]

From the Leibniz’s law for derivatives we have that

\[
U(\chi) \frac{\partial \Psi}{\partial t} = \frac{\partial}{\partial t} [U(\chi) \Psi] - \frac{\partial U(\chi)}{\partial t} \Psi. \tag{11}
\]

Thus Eq. (10) which becomes

\[
i\hbar \frac{\partial}{\partial t} [U(\chi) \Psi] = U(\chi) H \Psi + i\hbar \frac{\partial U(\chi)}{\partial t} \Psi = \left[ U(\chi) H U^\dagger(\chi) + i\hbar \frac{\partial U(\chi)}{\partial t} U^\dagger(\chi) \right] (U(\chi) \Psi). \tag{12}
\]

Let us define the transformed wavefunction as \( \Psi'(r, t) \equiv U(\chi) \Psi(r, t) \), hence the transformed Hamiltonian is given by

\[
H' \equiv U(\chi) H U^\dagger(\chi) + i\hbar \frac{\partial U(\chi)}{\partial t} U^\dagger(\chi) \tag{13}
\]

in order to obtain the transformed Schrödinger (or Dirac) equation

\[
H' \Psi' = i\hbar \frac{\partial \Psi'}{\partial t}, \tag{14}
\]

Therefore, a unitary transformation \( U(\chi) \) does not affect the form of the Schrödinger (or Dirac) equation and the notion of probability, since \(|\Psi'(r, t)|^2 = |\Psi(r, t)|^2\). However, the Hamiltonian has been changed by Eq. (13), which means that it is not measurable and cannot be seen as an energy operator [17]. The particular choice of \( U(\chi) = e^{iq\chi(r,t)/\hbar} \) reproduces the gauge transformations Eq. (1). So the Hamiltonian is modified by the gauge transformation according to Eq. (13) and it does not constraint that their eigenvalues remain unchanged. Consequently, the eigenvalue problem of the Hamiltonian, in general, does not give the energy spectrum: The set of eigenvalues of \( H \), denoted by \( \alpha_n \), are different from the energy levels of the system. This set is defined as by the equation

\[
H(A^0, A)u_n = \alpha_n u_n, \tag{15}
\]
where \( u_n \) are the eigenfunctions of \( H(A^0, A) \). Notice that \( \{\alpha_n\} \) in general are not the energy. In order to clarify the ideas above enunciated, consider the equation of eigenvalues of \( H' \),

\[
H'(A^0', A')v_j(x, t) = \beta_j v_j(x, t).
\] (16)

The sets \( \{\alpha_k\}_{k \in I} \) and \( \{\beta_j\}_{j \in I'} \) are not necessary the same and so the index sets \( I \) and \( I' \) may be different (e.g., a spectrum may be discrete and the other not). Then, omitting the functional dependencies,

\[
H'(A^0', A')v_j = \left[ UH(A^0, A)U^\dagger + i\hbar \frac{\partial U}{\partial t} U^\dagger \right] v_j = \beta_j v_j,
\] (17)

and so

\[
\left[ H + i\hbar U^\dagger (\chi) \frac{\partial U(\chi)}{\partial t} \right] (U^\dagger(\chi)v_j) = \beta_j (U^\dagger(\chi)v_j).
\] (18)

Now, if we define \( f_j(x, t) = U^\dagger(\chi)v_j(x, t) \) and remarking that \( U = e^{i\eta x (r, t)/\hbar} \), one has

\[
\left[ H - q \frac{\partial \chi(x, t)}{\partial t} \right] f_j = \beta_j f_j.
\] (19)

Note that the eigenvalues \( \beta \) in Eqs. (16) and (19) are the same, thus \( H' \) and \( H - q \frac{\partial \chi(x, t)}{\partial t} \) are equivalent operators\(^1\). However, \( H \) and \( H' \) are not equivalent operators, thus they do not have the same eigenvalues. We conclude that in general the Hamiltonian does not represent the energy. On the other hand, the procedure performed to obtain Eq. (14) from Eq. (10) ensures that the operator \( H - i\hbar \frac{\partial}{\partial t} \) is equivalent to \( H' - i\hbar \frac{\partial}{\partial t} \). This equivalence implies that the solutions of the Schrödinger (or Dirac) equation for \( H \) and \( H' \) are the same. In this sense, the quantum mechanics of a charged particle in a classical external electromagnetic field is gauge invariant.

So far we had demonstrated the gauge invariance of quantum mechanics. Now some questions rest: If the Hamiltonian does not represent the energy, which operator does? Can a time-dependent gauge transformation change the energy spectrum?

First, let us review the recipe to obtain the energy spectrum of a particular system. Suppose that Eq. (7) allows the separation of variables as

\[
\Psi_k(r, t) = e^{-i\alpha_k t/\hbar} \psi_k(r),
\] (20)

thus Schrödinger (or Dirac) equation is read as the eigenvalues equation of \( H(A^0, A) \)

\[
H(A^0, A)\psi_k(r) = \alpha_k \psi_k(r).
\] (21)

These \( \psi_k(r) \) correspond to the stationary states of \( H \). After applying a transformation Eq. (1), the transformed wavefunction is

\[
\Psi_{k\chi}(r, t) = e^{i\chi(r, t)} \Psi_k(r, t) = e^{i\chi(r, t)} e^{i\alpha_k t} \psi_k(r)
\] (22)

and the transformed Hamiltonian is \( H'(A', A'^0) = H(A^0 - \partial \chi, A + \nabla \chi) \). Notice that the transformed wavefunction is also stationary, because \( |\Psi_{k\chi}(r, t)| = |\psi_k(r)| \). If we substitute these transformed wavefunction

\(^1\)A linear operator \( C \) in a Hilbert space \( \mathcal{H} \) and a linear operator \( C' \) in a Hilbert space \( \mathcal{H}' \) are called equivalent if there exist an isomorphism \( U \) of \( \mathcal{H} \) onto \( \mathcal{H}' \) (or an automorphism \( U \) of \( \mathcal{H} \) if \( \mathcal{H} = \mathcal{H}' \)) such that \( C = U^{-1} C' U \) \([27]\).
and Hamiltonian in the Schrödinger (or Dirac) equation Eq. (7), it is easy to check that the time-independent eigenvalue equation associated is
\[
\left[ H \left( A^0 - \frac{\partial \chi}{\partial t}, A \right) + q \frac{\partial \chi}{\partial t} \right] \psi_k(r) = \alpha_k \psi_k(r). \tag{23}
\]
We see that the left-hand side of the above equation is equal to left-hand side of the Eq. (21)
\[
H \left( A^0 - \frac{\partial \chi}{\partial t}, A \right) + q \frac{\partial \chi}{\partial t} = H(A^0, A), \tag{24}
\]
and therefore Eqs. (23) and (21) have the same solutions. Therefore, the operator obtained from the separation of variables is gauge invariant and represents the energy. We conclude that in the particular case in which the Schrödinger (or Dirac) equation allows a separation of variables as in Eq. (20), the energies are given by the eigenvalues \(\alpha_k\) of the Hamiltonian whose eigenfunctions are a product of an spatial function by \(e^{-i\alpha_k t}\). Additionally, if another Hamiltonian \(H'\) is related with the separable one \(H\) by means a gauge transformation, the eigenvalue equation of \(H'\) must be modified by introducing the term \(\partial/\partial t\), in order to perform the separation of variables. Hence this new eigenvalue equation in terms of \(H'\) (Eq. (23)) provides the actual energies.

### 3 Discussion about other interpretations

As we mentioned in the Introduction, there are other attempts to resolve the gauge invariance of quantum mechanics, though, as we will show in this section, some of these approaches lead to wrong conclusions, whereas thee most recent proposal by Chen et al [1, 4, 5, 24, 25] is consistent with our present approach.

#### 3.1 Yang’s energy-operator

First we will consider the Yang’s energy-operator, then we will discuss the restrictions on the gauge function [18] and we will finish by explaining the approach of Refs. [1, 4, 5, 24, 25].

The fact that the Hamiltonian is not a gauge invariant quantity, and so a NPQ, strikes against the common meaning of the Hamiltonian as the energy. A different proposal is given by Yang and it has been used in literature [7, 8, 9, 10, 11, 12, 13, 14, 15, 16]: in order define a gauge invariant operator representing the energy is introduced the Yang’s energy-operator \(\mathcal{Y}(A)\),
\[
\mathcal{Y}(A) = H(A^0, A) - qA^0. \tag{25}
\]
A simple application of Eq. (13) shows its invariance. However, a typical system, as the Hydrogen atom denies its plausibility. For instance, consider the \(n\)-th level of an Hydrogen atom
\[
E_n = \frac{-1}{2} \left( \frac{me^4}{(4\pi\epsilon_0\hbar)^2} \right) \frac{1}{n^2}. \tag{26}
\]
This standard result is obtained by using the Hamiltonian of the form \(H(A^0, A = 0)\), with an electrostatic potential \(A^0(r) = -e/4\pi\epsilon_0|\mathbf{r}|\). This Hamiltonian does not depend on time, and so the solutions of its time-dependent Schrödinger equation may be calculated by using a separation of variables
\[
\Psi(r, t) = e^{-iE_n/\hbar t} \psi(r). \tag{27}
\]
For this case, the eigenvalue equation of the Yang’s energy-operator is:

\[ \mathcal{Y}(A = 0)\psi(r, t) = [H(A^0, A = 0) - eA^0]\psi(r, t) = \frac{p^2}{2m}\psi(r) = \epsilon\psi(r, t). \]  
(28)

Being \( \epsilon \) the eigenvalues of \( \mathcal{Y}(A) \). The above expression is obviously a free-particle Hamiltonian, it means that the spectrum is continuous!. Notice that Eq. (25) is equal to the free-particle Hamiltonian for any \( H = \frac{p^2}{2m} + eA^0(x) \).

Now, if we start by taking the temporal gauge for the Hydrogen atom, we have that

\[ A^0 = 0, \quad A = \frac{et}{r^3} r, \]  
(29)

thus, the eigenvalue equation of \( \mathcal{Y} \) is

\[ \mathcal{Y}(A)\psi(r, t) = [H(A^0 = 0, A)]\psi(r, t) = \left(\frac{p - eA}{2m}\right)^2\psi(r) = \epsilon\psi(r, t). \]  
(30)

Now if we multiply both sides of Eq. (30) by \( U(\chi) = e^{iqf(r)/\hbar}e^{iqg(t)/\hbar} \), with \( \chi(r, t) = et/r \) and taking into account the identity

\[ e^{ie\chi(r, t)/\hbar}\left(\frac{p - eA}{2m}\right)^2\psi(r) = \left[\frac{p - e(A + \nabla\chi)}{2m}\right]e^{ie\chi(r, t)/\hbar}\psi(r, t), \]  
(31)

the eigenvalues equation becomes

\[ \frac{p^2}{2m}\left[ e^{ie\chi(r, t)/\hbar}\psi(r, t) \right] = \epsilon \left[ e^{ie\chi(r, t)/\hbar}\psi(r, t) \right]. \]  
(32)

Again we obtain a similar result as in Eq. (28). The above arguments proof the unsuitability of the energy-operator to describe properly the energy. Specifically, we proved that the operator \( \mathcal{Y}(A) \) in the Eq. (30) is equivalent to operator \( \frac{p^2}{2m} \), and so they have the same eigenvalues. Consequently the operator \( \mathcal{Y}(A) \) in Eq. (25) is not the energy in general.

3.2 Restrict the gauge function

Another approach, proposed by Stewart [18], consists in restricting the gauge function to the form:

\[ \chi(r, t) = f(r) + g(t). \]  
(33)

This constraint is equivalent to assume the separation of the operator:

\[ U(\chi) = e^{iqf(r)/\hbar}e^{iqg(t)/\hbar}. \]  
(34)

However, allowing this restriction leads to ambiguity when choosing the gauge potential. To see this, let us define \( \Omega \) as a set of all possible electrodynamic potentials that may represent a given system. Eq. (33) divides the set \( \Omega \) in equivalence classes (see fig. 1). According to Stewart any two Hamiltonians, \( H \) and \( H' \), yields the same physical results only if they are related by a gauge transformation of the form (33). Under this assumption, if we take two different equivalence classes, we obtain two different physical results and as there is no way to choose beforehand which is the “real” equivalence class that represents the physical system. Then the restriction on the gauge function, Eq. (33), does not gives a satisfactory solution for the gauge invariance, because it does not decide which equivalence class describes properly the physical system.
Figure 1: Potentials space $\mathcal{U}$. Each piece of this circle corresponds to a set of potentials that are related between themselves by Eq. (33). For each set we may choose a pair $(A^0, A)$ to represent it, dividing $\mathcal{U}$ on equivalence classes (sets of potentials). (We here show few classes, but actually are infinite).

### 3.3 Decomposition of the electromagnetic potential

Finally, let us consider a decomposition of the electromagnetic potential into pure gauge and gauge invariant parts \[1, 4, 5, 24, 25\],

$$ A = A_{\text{pure}} + A_{\text{phys}}, \quad A^0 = A^0_{\text{pure}} + A^0_{\text{phys}}, $$

with

$$ \nabla \times A_{\text{pure}} = 0, \quad \nabla \cdot A_{\text{phys}} = 0, $$

$$ \nabla A^0_{\text{pure}} = -\frac{1}{c} \frac{\partial A_{\text{pure}}}{\partial t}, \quad \nabla^2 A^0_{\text{phys}} = -\frac{\rho}{\epsilon_0}. $$

Under a gauge transformation Eq. (1) these two parts are transformed as follows,

$$ A'_{\text{pure}} = A_{\text{pure}} + \nabla \chi, \quad A'_{\text{phys}} = A_{\text{phys}}, \quad A^0_{\text{pure}}' = A^0_{\text{pure}} - \frac{\partial \chi}{\partial t}, \quad A^0_{\text{phys}}' = A^0_{\text{phys}}. $$

In this approach the energy operator is $H(A^0, A) - qA^0_{\text{pure}} = H(A^0_{\text{phys}}, A)$, where $H = H_S$ for non-relativistic quantum mechanics, and $H = H_D$ for relativistic quantum mechanics\footnote{It can be proved that the operator $H(A^0_{\text{phys}}, A)$ in [1] is the same energy operator $H(A^0, A) - \frac{q}{\epsilon_0} \frac{\partial}{\partial t} \nabla \cdot A$ in [24, 25], using that $\nabla A^0_{\text{pure}} = -\frac{1}{\epsilon_0} \frac{\partial}{\partial t} A_{\text{pure}}$, one has $A^0 = \frac{q}{\epsilon_0} \frac{\partial}{\partial t} \nabla \cdot A = A^0_{\text{phys}}$.}. It is straightforward to prove that $H - eA^0_{\text{pure}}$ is gauge independent \[7\].

Next we will show that the energy operator $H(A^0_{\text{phys}}, A)$ is consistent with our analysis of first principles, at least for the particular case of a time independent electromagnetic field. In this case

$$ E(r) = -\nabla A^0 - \frac{1}{c} \frac{\partial A}{\partial t}, \quad B(r) = \nabla \times A. $$

\[9\]
Without loss of generality we can choose $A(r)$ and $A_0(r)$ to be also time independent, because the magnetic field is time independent. By means of introducing the decomposition Eq. (35), and using Eq. (36) one can derive

$$E(r) = -\nabla A_0(r), \quad B(r) = \nabla \times A_{phys}(r),$$  \hspace{1cm} (40)

on the other hand using Eq. (37), \(\nabla A_0^{\text{pure}} = 0\) and implies that $A^{0}_{\text{pure}} = \text{const.}$ This constant can always be absorbed by $A_{\text{phys}}$. Then, Eq. (7) can be written as

$$H(A_{phys}^{0}(r), A(r))\Psi(r, t) = i\hbar \frac{\partial}{\partial t} \Psi(r, t),$$ \hspace{1cm} (41)

that allows as to have variable separation of the kind of Eq. (20). The energy operator obtained their $H(A_{phys}^{0}(r), A(r))$, is the same as one recently proposed by Chen et al. [1, 4, 5].

4 Conclusions

In this paper we have reexamined the gauge invariant of non-relativistic and relativistic quantum mechanics of a charged particle in a classical external electromagnetic field. We show how the gauge invariance of the operator $H - i\hbar \frac{\partial}{\partial t}$ provides a way to find the energy operator. In particular, when the system has stationary states the energy operator can be identified without ambiguities from first principles. We have dismissed some approaches suggested in the literature and we have found that the energy operator obtain in this paper (for time independent electromagnetic field) is the same one recently proposed by Chen et al. [1, 4, 5].

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