Gauge-invariant hydrogen-atom Hamiltonian

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For quantum mechanics of a charged particle in a classical external electromagnetic field, there is an apparent puzzle that the matrix element of the canonical momentum and Hamiltonian operators is gauge dependent. A resolution to this puzzle was recently provided by us [X.-S. Chen *et al.*, Phys. Rev. Lett. **100**, 232002 (2008)]. Based on the separation of the electromagnetic potential into pure-gauge and gauge-invariant parts, we have proposed a new set of momentum and Hamiltonian operators which satisfy both the requirement of gauge invariance and the relevant commutation relations. In this paper we report a check for the case of the hydrogen-atom problem: Starting from the Hamiltonian of the coupled electron, proton, and electromagnetic field, under the infinite proton mass approximation, we derive the gauge-invariant hydrogen-atom Hamiltonian and verify explicitly that this Hamiltonian is different from the Dirac Hamiltonian, which is the time translation generator of the system. The gauge-invariant Hamiltonian is the energy operator, whose eigenvalue is the energy of the hydrogen atom. It is generally time dependent. In this case, one can solve the energy eigenvalue equation at any specific instant of time. It is shown that the energy eigenvalues are gauge independent, and by suitably choosing the phase factor of the time-dependent eigenfunction, one can ensure that the time-dependent eigenfunction satisfies the Dirac equation.

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I. INTRODUCTION

In quantum mechanics, the momentum and Hamiltonian are the fundamental physical quantities of a system. The momentum (Hamiltonian) operators are the space (time) translation generators of the system. The momentum operators satisfy the canonical momentum commutation relations.

Gauge invariance has been recognized as a first principle through the development of the standard model. For a charged particle in a classical external electromagnetic field, the gauge-invariance principle requires that the matrix element of any physical observable of the system should be gauge invariant. However, there are apparent puzzles concerning the momentum and Hamiltonian operators of the charged particle. For example, the expectation value of the Hamiltonian of the hydrogen atom is gauge dependent under a time-dependent gauge transformation [1]. The matrix element of the canonical momentum operator is also gauge dependent.

A resolution to this puzzle was recently given by us in [2] (see X.-S. Chen *et al.*, 2008). The key idea of our resolution is to separate the electromagnetic potential into pure-gauge and gauge-invariant parts. Based on this separation, we have proposed a new set of momentum and Hamiltonian operators which satisfy both the requirement of gauge invariance and the relevant commutation relations.

In the present paper, following our previous work, we show an explicit check for the case of the hydrogen-atom problem: Starting from the total Hamiltonian of the coupled electron, proton, and electromagnetic field, under the infinite proton mass approximation, we derive the gauge-invariant Hamiltonian of the hydrogen atom and verify the difference between this Hamiltonian and the time translation generator, the Dirac Hamiltonian.

In Sec. II, we describe the conflict between gauge invariance and canonical quantization of the momentum and Hamiltonian operators for a charged particle in an external electromagnetic field and our resolution to this problem. In Sec. III, we give the explicit check for the case of the hydrogen-atom problem. The last section provides a summary.

II. GAUGE INVARIANCE AND CANONICAL QUANTIZATION OF THE MOMENTUM AND HAMILTONIAN OPERATORS

In classical mechanics, the canonical momentum and Hamiltonian for a nonrelativistic particle in an external electromagnetic field A^μ are

$$\vec{p} = m\vec{v} - e\vec{A}, \quad H = \frac{1}{2m}(\vec{p} + e\vec{A})^2 - eA^0, \tag{1}$$

where the charge of the particle is $-e$. These two dynamical variables are gauge dependent and so are not observables in classical gauge theory. After quantization, the momentum $\vec{p}$ is quantized as $\vec{p} = -i\vec{\nabla}$ (in coordinate representation), irrespective of which gauge is chosen, even though the classical canonical momentum is gauge dependent. The Hamiltonian is quantized by replacing $\vec{p}$ with $-i\vec{\nabla}$. The quantized momentum operators satisfy the canonical momentum commutation relations $[p^i, p^j] = 0$.

After a gauge transformation,

$$\psi' = e^{-ief(x)}\psi, \quad A'^\mu = A^\mu - \partial^\mu f(x), \tag{2}$$

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the expectation value of the foregoing operators transform as follows:

$$\langle\psi'|\vec{p}|\psi'\rangle = \langle\psi|\vec{p}|\psi\rangle - e\langle\psi|\vec{\nabla} f|\psi\rangle,$$
$$\langle\psi'|H'|\psi'\rangle = \langle\psi|H|\psi\rangle + e\langle\psi|\frac{\partial f}{\partial t}|\psi\rangle. \tag{3}$$

The expectation values of these two operators are gauge dependent. Therefore these expectation values are not measurable and hence these operators are not observables.

The same problem also exists in relativistic quantum mechanics. The gauge dependence of the expectation value of the Hamiltonian of the electron in an external electromagnetic field under a time-dependent gauge transformation was discussed in [1].

To resolve the puzzle of gauge invariance of the expectation value of canonical momentum, one introduces the gauge-invariant operator

$$\vec{\mathcal{P}} = \vec{p} + e\vec{A}. \tag{4}$$

It is easy to check that the expectation value of this operator is gauge invariant. However, the commutators between the components of $\vec{\mathcal{P}}$ are

$$[\mathcal{P}^i,\mathcal{P}^j] = ie(\partial^i A^j - \partial^j A^i) = ieF^{ij}, \tag{5}$$

therefore $\vec{\mathcal{P}}$ does not satisfy the Lie algebra of canonical momentum, so it cannot be the proper momentum opearator.

A resolution to this problem is given by us in [2]. Our idea is to seek a unique separation $A^\mu = A^\mu_{\rm pure} + A^\mu_{\rm phys}$, with $A^\mu_{\rm pure}$ a pure-gauge term having the same transformation property as the full A^μ and giving null field strength, and $A^\mu_{\rm phys}$ a physical term which is gauge invariant. The condition that $A_{\rm pure}$ gives null field strength reads

$$\partial^\mu A^\nu_{\rm pure} - \partial^\nu A^\mu_{\rm pure} = 0. \tag{6}$$

This equation cannot fix $A_{\rm pure}$ uniquely. One needs to find an additional condition to fix it. The spatial part of Eq. (6) is

$$\vec{\nabla} \times \vec{A}_{\rm pure} = \vec{0}. \tag{7}$$

A natural choice of the additional condition is

$$\vec{\nabla} \cdot \vec{A}_{\rm phys} = 0. \tag{8}$$

That is, $\vec{A}_{\rm phys}$ and $\vec{A}_{\rm pure}$ are the transverse component $\vec{A}_\perp$ and longitudinal component $\vec{A}_\parallel$, respectively. The time component A^0 can be decomposed in the same manner. From the condition $F^{i0}_{\rm pure} = 0$, one obtains

$$\partial_i A^0_{\rm phys} = \partial_i A^0 + \partial_t\big(A^i - A^i_{\rm phys}\big). \tag{9}$$

From Eq. (9) one can derive

$$A^0_{\rm phys} = \int_{-\infty}^{x} dx^i\big(\partial_i A^0 + \partial_t A^i - \partial_t A^i_{\rm phys}\big). \tag{10}$$

(Here no summation over the index i is implied.)

Based on the preceding gauge field decomposition, we introduce another momentum operator:

$$\vec{p}_{\rm pure} = \vec{p} + e\vec{A}_{\rm pure}. \tag{11}$$

This operator satifies both the requirement of gauge invariance (because $\vec{A}_{\rm pure}$ has the same gauge transformation property as the full $\vec{A}$) and the Lie algebra for the canonical momentum (because $A^\mu_{\rm pure}$ gives null field strength).

The long-standing puzzle of the gauge noninvariance of the expectation value of the Hamiltonian [1] can be solved in the same manner. For nonrelativistic quantum mechanics, we define a new Hamiltonian:

$$H = \frac{(\vec{p}+e\vec{A})^2}{2m} - eA^0 + eA^0_{\rm pure} = \frac{(\vec{p}+e\vec{A})^2}{2m} - eA^0_{\rm phys}. \tag{12}$$

The term $eA^0_{\rm pure}$ is a pure gauge term which cancels the unphysical energy appearing in $-eA^0$ and then guarantees that the expectation value of this Hamiltonian is gauge invariant. It is a direct extension of Eq. (11) to the zeroth momentum component.

Therefore, for a charged particle in a classical external electromagnetic field, the gauge-invariant momentum (Hamiltonian) operator is not the space (time) translation generator of the system. The gauge-invariant momentum and Hamiltonian are observables, whereas the space and time translation generators are not.

The Dirac Hamiltonian has the same unphysical energy part, which must be canceled in the same manner as for the Schroedinger Hamiltonian. (The distinction between the gauge-invariant Hamiltonian and the time translation generator in this case was also pointed out by Kobe and Yang in [3].) In the rest of this paper, we do a check for the case of the hydrogen-atom problem: Starting from the Hamiltonian of the coupled electron, proton, and electromagnetic field, under the infinite proton mass approximation, we derive the gauge-invariant hydrogen-atom Hamiltonian and verify the difference between this Hamiltonian and the time translation generator, the Dirac Hamiltonian.

III. DERIVATION OF THE GAUGE-INVARIANT HYDROGEN-ATOM HAMILTONIAN

Let us start from the coupled-field Lagrangian for electron, proton, and electromagnetic field,

$$\mathcal{L} = -\tfrac{1}{4}F_{\mu\nu}F^{\mu\nu} + \bar{\psi}_e\big(i\gamma^\mu D^{(e)}_\mu - m\big)\psi_e + \bar{\psi}_p\big(i\gamma^\mu D^{(p)}_\mu - M\big)\psi_p, \tag{13}$$

with $D^{(e)}_\mu = \partial_\mu - ieA_\mu$ and $D^{(p)}_\mu = \partial_\mu + ieA_\mu$ (here e is the charge of the proton). From this Lagrangian one can derive the total energy of the system:

$$H = \int d^3x\left[\psi_e^\dagger(i\vec{\alpha}\cdot\vec{D}^{(e)} + \beta m)\psi_e + \psi_p^\dagger(i\vec{\alpha}\cdot\vec{D}^{(p)} + \beta M)\psi_p + \frac{1}{2}(E^2 + B^2)\right]. \tag{14}$$

To proceed, we decompose the gauge potential $\vec{A}$ in terms of its transverse and longitudinal parts:

$$\vec{A} = \vec{A}_{\rm phys} + \vec{A}_{\rm pure} = \vec{A}_\perp + \vec{A}_\parallel.$$

Then one has

$$\begin{aligned}\vec{E} &= -\vec{\nabla}A^0 - \frac{\partial}{\partial t}\vec{A}_{\text{pure}} - \frac{\partial}{\partial t}\vec{A}_{\text{phys}}\\ &= -\vec{\nabla}A^0_{\text{phys}} - \vec{\nabla}A^0_{\text{pure}} - \frac{\partial}{\partial t}\vec{A}_{\text{pure}} - \frac{\partial}{\partial t}\vec{A}_{\text{phys}}\\ &= -\vec{\nabla}A^0_{\text{phys}} - \frac{\partial}{\partial t}\vec{A}_{\text{phys}}\\ &= -\vec{\nabla}A^0_{\text{phys}} - \frac{\partial}{\partial t}\vec{A}_{\perp}\\ &\equiv \vec{E}_{\parallel} + \vec{E}_{\perp},\end{aligned} \tag{15}$$

where we have used the condition that A^μ_{pure} gives null field strength. The total electromagnetic field energy then separates into two terms,

$$\frac{1}{2}\int d^3x(E^2+B^2) = \frac{1}{2}\int d^3x E_{\parallel}^2 + \frac{1}{2}\int d^3x(E_{\perp}^2 + B^2), \tag{16}$$

where the cross term $\vec{E}_{\parallel}\cdot\vec{E}_{\perp}$ vanishes by an integration by parts. The first term on the right-hand side of (16) is the total energy associated with the Coulomb field. In fact, from the Gauss law $\vec{\nabla}\cdot\vec{E} = e\psi_p^\dagger\psi_p - e\psi_e^\dagger\psi_e = \rho_p + \rho_e$, one has

$$\vec{\nabla}\cdot\vec{E}_{\parallel} = -\nabla^2 A^0_{\text{phys}} = \rho_p + \rho_e. \tag{17}$$

From Eq. (17) one can obtain A^0_{phys}

$$A^0_{\text{phys}} = -\frac{1}{\nabla^2}(\rho_p + \rho_e). \tag{18}$$

One then has

$$\begin{aligned}\frac{1}{2}\int d^3x E_{\parallel}^2 &= -\frac{1}{2}\int d^3x \vec{E}_{\parallel}\cdot\vec{\nabla}A^0_{\text{phys}}\\ &= \frac{1}{2}\int d^3x \vec{\nabla}\cdot\vec{E}_{\parallel}A^0_{\text{phys}}\\ &= -\frac{1}{2}\int d^3x(\rho_p+\rho_e)\frac{1}{\nabla^2}(\rho_p+\rho_e)\\ &= \frac{1}{4\pi}\int d^3xd^3y\rho_e(\vec{x},t)\frac{1}{|\vec{x}-\vec{y}|}\rho_p(\vec{y},t)\\ &\quad + \frac{1}{8\pi}\int d^3xd^3y\rho_e(\vec{x},t)\frac{1}{|\vec{x}-\vec{y}|}\rho_e(\vec{y},t)\\ &\quad + \frac{1}{8\pi}\int d^3xd^3y\rho_p(\vec{x},t)\frac{1}{|\vec{x}-\vec{y}|}\rho_p(\vec{y},t).\end{aligned} \tag{19}$$

The second term on the right-hand side of (16) is the energy of the transverse electromagnetic field. The total energy of the system then separates into the following terms:

$$\begin{aligned}H &= \int d^3x\psi_e^\dagger(i\vec{\alpha}\cdot\vec{D}^{(e)} + \beta m)\psi_e\\ &\quad + \int d^3x\psi_p^\dagger(i\vec{\alpha}\cdot\vec{D}^{(p)} + \beta M)\psi_p\\ &\quad + \frac{1}{4\pi}\int d^3xd^3y\rho_e(\vec{x},t)\frac{1}{|\vec{x}-\vec{y}|}\rho_p(\vec{y},t)\\ &\quad + \frac{1}{8\pi}\int d^3xd^3y\rho_e(\vec{x},t)\frac{1}{|\vec{x}-\vec{y}|}\rho_e(\vec{y},t)\\ &\quad + \frac{1}{8\pi}\int d^3xd^3y\rho_p(\vec{x},t)\frac{1}{|\vec{x}-\vec{y}|}\rho_p(\vec{y},t)\\ &\quad + \frac{1}{2}\int d^3x(\vec{E}_{\perp}^2 + \vec{B}^2).\end{aligned} \tag{20}$$

Now let us turn to the hydrogen-atom problem. Here one assumes that the proton is infinitely massive, that is, $M\to\infty$. In this limit the proton plays the role of a static source situated at a fixed point in space which, for convenience, one takes to be the origin. The electromagnetic current of the proton is then

$$j_p^\mu(\vec{x},t) = (\rho_p(\vec{x},t),\vec{j}_p(\vec{x},t)) = (e\delta^3(\vec{x}),\vec{0}). \tag{21}$$

To find out the energy of the electron in the electromagnetic field of the proton, one needs to derive the electromagnetic potential A^μ. The equation of motion for A^μ is

$$\partial^2 A^\mu - \partial^\mu(\partial\cdot A) = j_p^\mu + j_e^\mu. \tag{22}$$

Using Eqs. (21) and (22) can be written as

$$\begin{aligned}\partial^2 A^0 - \frac{\partial}{\partial t}\left(\frac{\partial A^0}{\partial t} + \vec{\nabla}\cdot\vec{A}\right) &= -\nabla^2 A^0 - \frac{\partial}{\partial t}(\vec{\nabla}\cdot\vec{A})\\ &= e\delta^3(\vec{x}) + \rho_e,\end{aligned} \tag{23}$$

$$\partial^2\vec{A} + \vec{\nabla}\left(\frac{\partial A^0}{\partial t} + \vec{\nabla}\cdot\vec{A}\right) = \vec{j}_e. \tag{24}$$

When solving Eqs. (23) and (24), one needs to choose a gauge. In the following we choose the gauge

$$\vec{\nabla}\cdot\vec{A}(\vec{x},t) = \chi(\vec{x},t) = \nabla^2 f(\vec{x},t), \tag{25}$$

where $f(\vec{x},t)$ is an arbitrary function. From Eq. (23) one can derive A^0:

$$A^0(\vec{x},t) = \frac{e}{4\pi r} - \frac{\partial}{\partial t}f(\vec{x},t) + \frac{1}{4\pi}\int d^3y\frac{\rho_e(\vec{y},t)}{|\vec{x}-\vec{y}|}. \tag{26}$$

Substituting (26) into Eq. (24) gives

$$\begin{aligned}&\partial^2\vec{A}(\vec{x},t) + \vec{\nabla}\left(-\partial^2 f(\vec{x},t) + \frac{1}{4\pi}\int d^3y\frac{1}{|\vec{x}-\vec{y}|}\frac{\partial}{\partial t}\rho_e(\vec{y},t)\right)\\ &\quad = \vec{j}_e(\vec{x},t),\end{aligned} \tag{27}$$

whereby one can derive $\vec{A}$:

$$\begin{aligned}\vec{A}(\vec{x},t) &= \vec{\nabla}f(\vec{x},t) + (\partial^2)^{-1}\vec{j}_e(\vec{x},t)\\ &\quad + \frac{1}{4\pi}\int d^3y(\partial^2)^{-1}\left(\frac{\vec{x}-\vec{y}}{|\vec{x}-\vec{y}|^3}\frac{\partial}{\partial t}\rho_e(\vec{y},t)\right).\end{aligned} \tag{28}$$

From Eqs. (26) and (28) we can attribute $(\frac{e}{4\pi r} - \frac{\partial f}{\partial t}, \vec{\nabla}f)$ to be the electromagnetic potential produced by the static proton source in the gauge (25).

Now we can isolate the energy of the electron in the electromagnetic field of the proton from the total energy of the system Eq. (20). We only need to consider terms involving the electron field. These are $\int d^3x\psi_e^\dagger(i\vec{\alpha}\cdot\vec{D}^{(e)} + \beta m)\psi_e$ and $\frac{1}{4\pi}\int d^3xd^3y\rho_e(\vec{x},t)\frac{1}{|\vec{x}-\vec{y}|}\rho_p(\vec{y},t)$. The term $\frac{1}{8\pi}\int d^3xd^3y\rho_e(\vec{x},t)\frac{1}{|\vec{x}-\vec{y}|}\rho_e(\vec{y},t)$ represents the electron self-energy and one does not need to take it into account.

The term $\int d^3x\psi_e^\dagger(i\vec{\alpha}\cdot\vec{D}^{(e)}+\beta m)\psi_e$ can be written as

$$\begin{aligned}\int d^3x\psi_e^\dagger(i\vec{\alpha}\cdot\vec{D}^{(e)}+\beta m)\psi_e\\ &= \int d^3x\psi_e^\dagger(-i\vec{\alpha}\cdot\vec{\nabla}+e\vec{\alpha}\cdot\vec{A}+\beta m)\psi_e\\ &= \int d^3x\psi_e^\dagger(-i\vec{\alpha}\cdot\vec{\nabla}+e\vec{\alpha}\cdot\vec{\nabla}f+\beta m)\psi_e\\ &\quad -\int d^3x\vec{j}_e(\vec{x},t)\cdot\left(\partial_x^2\right)^{-1}\vec{j}_e(\vec{x},t)\\ &\quad -\frac{1}{4\pi}\int d^3xd^3y\vec{j}_e(\vec{x},t)\cdot\left(\partial_x^2\right)^{-1}\left(\frac{\vec{x}-\vec{y}}{|\vec{x}-\vec{y}|^3}\frac{\partial}{\partial t}\rho_e(\vec{y},t)\right).\end{aligned} \tag{29}$$

Here the first term on the right-hand side of Eq. (29) is the kinetic energy of the electron and the $\vec{j}\cdot\vec{A}$ part of the interaction energy of the electron with the electromagnetic field of the proton. The second and third terms on the right-hand side of Eq. (29) represent the self-interaction energy of the electron field, which we do not need to consider.

The electron-proton Coulomb energy term is

$$\begin{aligned}\frac{1}{4\pi}\int d^3xd^3y\rho_e(\vec{x},t)\frac{1}{|\vec{x}-\vec{y}|}\rho_p(\vec{y},t)\\ &= \frac{e}{4\pi}\int d^3x\rho_e(\vec{x},t)\frac{1}{|\vec{x}|}\\ &= \int d^3x\psi_e^\dagger\left(-\frac{e^2}{4\pi r}\right)\psi_e.\end{aligned} \tag{30}$$

So the energy of the electron in the electromagnetic field of the proton is

$$\int d^3x\psi_e^\dagger\left(-i\vec{\alpha}\cdot\vec{\nabla}+e\vec{\alpha}\cdot\vec{\nabla}f+\beta m-\frac{e^2}{4\pi r}\right)\psi_e. \tag{31}$$

From this expression one reads out the hydrogen-atom Hamiltonian:

$$H=\vec{\alpha}\cdot(\vec{p}+e\vec{\nabla}f)+\beta m-\frac{e^2}{4\pi r}. \tag{32}$$

In contrast, from the Lagrangian (13) one can derive the equation of motion of the electron field:

$$(i\gamma^\mu\partial_\mu+e\gamma^\mu A_\mu-m)\psi_e=0. \tag{33}$$

Substituting Eqs. (26) and (28) into Eq. (33) and dropping all terms nonlinear in ψ_e, one obtains the linearized equation of motion of the electron field:

$$\left[i\gamma^\mu\partial_\mu+e\gamma^0\left(\frac{e}{4\pi r}-\frac{\partial f}{\partial t}\right)-e\vec{\gamma}\cdot\vec{\nabla}f-m\right]\psi_e=0. \tag{34}$$

Equation (34) is just the Dirac equation of an electron in the external electromagnetic field of the proton source:

$$\begin{aligned}i\frac{\partial}{\partial t}\psi_e &= \left(-i\vec{\alpha}\cdot\vec{\nabla}+e\vec{\alpha}\cdot\vec{\nabla}f+\beta m-\frac{e^2}{4\pi r}+e\frac{\partial f}{\partial t}\right)\psi_e\\ &= H_D\psi_e,\end{aligned} \tag{35}$$

where H_D is the Dirac Hamiltonian, which is the time translation generator. Here one notes that the presence of the term $e\frac{\partial f}{\partial t}$ in H_D is necessary for the gauge invariance of the Dirac equation under time-dependent gauge transformation.

Denoting the electromagnetic potential produced by the static proton source as $A^\mu=(A^0,\vec{A})=(\frac{e}{4\pi r}-\frac{\partial f}{\partial t},\vec{\nabla}f)$, one can write

$$H=\vec{\alpha}\cdot(\vec{p}+e\vec{A})+\beta m-eA^0_{\text{phys}} \tag{36}$$

and

$$H_D=\vec{\alpha}\cdot(\vec{p}+e\vec{A})+\beta m-eA^0. \tag{37}$$

Thus we have explicitly verified that the gauge-invariant hydrogen-atom Hamiltonian is different from the Dirac Hamiltonian.

Here we give some further discussion on the Dirac Hamiltonian and the gauge-invariant Hamiltonian. In our approach we use the Dirac Hamiltonian in the time-dependent Dirac equation, because the Dirac Hamiltonian is the time translation generator. The gauge-invariant Hamiltonian is the energy operator of the system, whose eigenvalue is the energy of the hydrogen atom. The gauge-invariant Hamiltonian is generally time dependent. In this case, one can solve the energy eigenvalue equation at any specific instant of time. It can be shown that the energy eigenvalues are gauge independent, and by suitably choosing the phase factor of the time-dependent eigenfunction, one can ensure that the time-dependent eigenfunction satisfies the Dirac equation. The proof is as follows.

Let H_C be the gauge-invariant Hamiltonian in the Coulomb gauge,

$$H_C=\vec{\alpha}\cdot\vec{p}+\beta m-\frac{e^2}{4\pi r}, \tag{38}$$

and $H_f(t)$ be the gauge-invariant Hamiltonian in a general gauge,

$$H_f(t)=\vec{\alpha}\cdot(\vec{p}+e\vec{\nabla}f)+\beta m-\frac{e^2}{4\pi r}. \tag{39}$$

It can be easily seen that $H_f(t)$ and H_C are connected by a time-dependent unitary transformation:

$$e^{-ief(\vec{x},t)}H_Ce^{ief(\vec{x},t)}=H_f(t). \tag{40}$$

H_C has the following energy eigenvalue equation,

$$H_C[e^{-iE_nt}\psi_n(\vec{x})]=E_n[e^{-iE_nt}\psi_n(\vec{x})], \tag{41}$$

where E_n is the energy eigenvalue of the hydrogen atom in the Coulomb gauge and $e^{-iE_nt}\psi_n(\vec{x})$ is the corresponding stationary-state wave function. From (40) and (41) one can derive

$$H_f(t)[e^{-ief(\vec{x},t)}e^{-iE_nt}\psi_n(\vec{x})]=E_n[e^{-ief(\vec{x},t)}e^{-iE_nt}\psi_n(\vec{x})]. \tag{42}$$

So, at each instant of time t, $H_f(t)$ has the same eigenvalues as the Coulomb gauge Hamiltonian, with $e^{-ief(\vec{x},t)}e^{-iE_nt}\psi_n(\vec{x})$ being the corresponding instantaneous eigenfunction. In addition, since $e^{-iE_nt}\psi_n(\vec{x})$ satisfies the time-dependent Dirac equation in the Coulomb gauge,

$$i\frac{\partial}{\partial t}[e^{-iE_nt}\psi_n(\vec{x})] = \left(\vec{\alpha}\cdot\vec{p} + \beta m - \frac{e^2}{4\pi r}\right)[e^{-iE_nt}\psi_n(\vec{x})], \tag{43}$$

from the gauge invariance of the Dirac equation, one has

$$\begin{aligned} i\frac{\partial}{\partial t}&[e^{-ief}e^{-iE_nt}\psi_n(\vec{x})] \\ &= \left[\vec{\alpha}\cdot(\vec{p} + e\vec{\nabla}f) + \beta m - \frac{e^2}{4\pi r} + e\frac{\partial f}{\partial t}\right] \\ &\quad\times [e^{-ief}e^{-iE_nt}\psi_n(\vec{x})]. \end{aligned} \tag{44}$$

Therefore, the instantaneous eigenfunction $e^{-ief}e^{-iE_nt}\psi_n(\vec{x})$ of the time-dependent gauge-invariant Hamiltonian $H_f(t)$ satisfies the time-dependent Dirac equation.

IV. SUMMARY

Gauge invariance has long been recognized as a first principle through the development of the standard model. However, for the quantum mechanics of a charged particle in a classical external electromagnetic field, there is an apparent puzzle that the matrix element of the canonical momentum and Hamiltonian operators is gauge dependent. A resolution to this puzzle is provided by us in [2]. Based on the separation of the electromagnetic potential into pure-gauge and gauge-invariant parts, we have proposed a new set of momentum and Hamiltonian operators which satisfy both the requirement of gauge invariance and the relevant commutation relations.

In this paper we did a check for the case of the hydrogen-atom problem: Starting from the Hamiltonian of the coupled electron, proton, and electromagnetic field, under the infinite proton mass approximation, we derive the gauge-invariant hydrogen-atom Hamiltonian and verify explicitly that this Hamiltonian is different from the Dirac Hamiltonian, which is the time translation generator of the system. Therefore, the Dirac Hamiltonian, which determines the time evolution of the system, is not an observable, whereas the gauge-invariant Hamiltonian is. The gauge-invariant Hamiltonian is the energy operator, whose eigenvalue is the energy of the hydrogen atom. It is generally time dependent. In this case, one can solve the energy eigenvalue equation at any specific instant of time. It is shown that the energy eigenvalues are gauge independent, and by suitably choosing the phase factor of the time-dependent eigenfunction, one can ensure that the time-dependent eigenfunction satisfies the Dirac equation.

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