Gauge invariance of many-body Schrödinger equation
with explicit Coulomb potential

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Abstract

A simple argument is presented which, based on the minimal coupling Lagrangian
for a many-body system, keeps the gauge invariance of the many-body Schrödinger
equation with explicit Coulomb potential. The elimination of longitudinal electric
field does not necessarily lead to the breakdown of gauge invariance. The choice of
Coulomb gauge cancels the total time derivative term caused by gauge transforma-
tion in the Lagrangian. All the linear and nonlinear responses are described only
by transverse vector potential and external longitudinal electric field.

1 Introduction

Quantum mechanical description of electromagnetic (EM) response of matter re-
quires the use of scalar and vector potentials for EM field. A general formulation
starts usually from the so-called minimal coupling Lagrangian $\mathcal{L}$ for the system of
charged particles and EM field. It is the sum of particles Lagrangian and that of
free EM field. The particle part is a sum of single particle Lagrangian in a given
EM field, $v^2/2m - e\phi + (e/c)v \cdot A$, over all the particles in consideration. (See
eq.(1) for notations.) The minimum action principle leads to [a] Newton equa-
tion of motion of each particle under Lorentz force, and [b] Maxwell equations for EM
field. This fact guarantees the soundness of the Lagrangian. A gauge transforma-
tion of the Lagrangian leads to an addition of a total time derivative to the original
Lagrangian. Since the minimum action principle is not affected by such a term, we
get a gauge invariant EM response.

The Hamiltonian corresponding to $\mathcal{L}$ is derived via standard procedure, and the
Schrödinger equation in terms of this Hamiltonian allows us to calculate the expecta-
tion values of various physical quantities. Among them, that of induced current
density gives the constitutive equation, which, together with Maxwell equations,
makes up the fundamental equations to calculate the EM response of matter. In
semiclassical theory where EM field is treated as classical (non-quantized) quan-
tity, these fundamental equations are solved as simultaneous equations for a given
initial condition of matter and EM field. Maxwell equations give EM field as a
functional of current and charge densities, while constitutive equation gives current
density as a functional of EM field.

According to our standard conception about matter, the Coulomb potential
among charged particles is a part of matter Hamiltonian. The energy levels of a
matter are given as the eigenvalues of the matter Hamiltonian consisting of the
kinetic energies and the Coulomb potential of all the particles in the system, as
typically seen in the Rydberg series of a hydrogen atom. However, $\mathcal{L}$ does not
contain the Coulomb potential explicitly. It emerges from rewriting the self-energy of longitudinal electric field in terms of Gauss law $\nabla \cdot \mathbf{E} = \rho/\varepsilon_0$. When we derive the matter Hamiltonian with explicit Coulomb potential from the minimal coupling Lagrangian, it is necessary to keep gauge invariance, eqs. (21, 22) below, of the many-body Schrödinger equation. But there seems to be no example of doing this in literatures, to the author’s knowledge. Some people even argue that gauge invariance is broken if we eliminate the longitudinal electric field to derive Coulomb potential. In this note, we will present a reasonable argument which enables us to keep the gauge invariance in the many-body Schrödinger equation.

In order to keep gauge invariance in this rewriting, it is essential to note that the EM field variables in $\mathcal{L}$ for an isolated system of charged particles contain both internal and external origins, although particle variables are limited to the internal system alone. A typical situation of EM response consists of steps [A] to apply an incident EM field to a matter sample, which induces a current density, and [B] the induced current density produces EM field according to Maxwell equations. The EM field in the step [A] is external origin, and the one in [B] is internal origin. By choosing the dynamical variables in such a way, we can keep the gauge invariance in the Schrödinger equation of a many-particle system with explicit Coulomb potential, as shown below.

Once we derive the matter Schrödinger equation in a gauge invariant form, the expectation value of an arbitrary physical quantity should be gauge-independent. Among all, Coulomb gauge is a special one in the sense that the Hamiltonian is already written in terms of the gauge independent components of EM field, i.e., the transverse (T) vector potential $\mathbf{A}^{(T)}$ and external longitudinal (L) electric field $\mathbf{E}_{\text{ext}}^{(L)}$. Hence the result obtained in Coulomb gauge directly gives the gauge independent form. This conclusion applies, not only to linear, but also to all the nonlinear EM responses.

This result enforces the foundation of the first-principles theory of micro- [1] and macroscopic EM response [2], where a single $3\times 3$ susceptibility tensor describes all the electric, magnetic and chiral polarizations for linear response. The susceptibility is expressed, through the explicit use of Coulomb gauge, in a quantum mechanical form. The choice of a partial system from a global one as an object for considering EM response does not spoil the gauge invariance.

Since the arguments and logical steps for establishing the gauge invariance of many-body Schrödinger equation is rather simple, as will be seen below, it might well be given elsewhere. However, no reference of this kind is known to the present author and many of his colleagues working with electromagnetism. Thus, the author considers it useful to give the details of arguments in this note.

## 2 Formulation

We start from the minimal coupling Lagrangian to describe an isolated system of interacting charged particles and EM field as

$$
\mathcal{L} = \sum_\ell \left\{ \frac{1}{2} m_\ell v_\ell^2 - e_\ell \phi(\mathbf{r}_\ell) + e_\ell \mathbf{v}_\ell \cdot \mathbf{A}(\mathbf{r}_\ell) \right\} + \frac{\varepsilon_0}{2} \int d\mathbf{r} \left\{ \left( \frac{\partial \mathbf{A}}{\partial t} + \nabla \phi \right)^2 - c^2 (\nabla \times \mathbf{A})^2 \right\},
$$

(1)
where \( m_\ell, e_\ell, r_\ell, v_\ell \) are the mass, charge, coordinate, and velocity, respectively, of the \( \ell \)-th particle, and \( \phi \) and \( A \) scalar and vector potential, respectively. The interaction terms in \( \mathcal{L} \) can be rewritten as
\[
\sum \ell \left\{ -e_\ell \phi(r_\ell) + e_\ell v_\ell \cdot A(r_\ell) \right\} = \int d\mathbf{r} \left\{ -\rho(\mathbf{r}) \phi(\mathbf{r}) + \mathbf{J}(\mathbf{r}) \cdot A(\mathbf{r}) \right\},
\]
where
\[
\rho(\mathbf{r}) = \sum \ell e_\ell \delta(\mathbf{r} - \mathbf{r}_\ell),
\]
\[
\mathbf{J}(\mathbf{r}) = \sum \ell e_\ell v_\ell \delta(\mathbf{r} - \mathbf{r}_\ell)
\]
are charge and current densities, respectively.

As well known, the Lagrange equations due to this \( \mathcal{L} \) lead to the Newton equation of motion of the \( \ell \)-th particle
\[
m_\ell \frac{d^2 \mathbf{r}_\ell}{dt^2} = e_\ell \left\{ \mathbf{E}(\mathbf{r}_\ell) + \mathbf{v}_\ell \times \mathbf{B}(\mathbf{r}_\ell) \right\},
\]
and the Maxwell equations for EM field
\[
\nabla \cdot \left[ \frac{\partial \mathbf{A}}{\partial t} + \nabla \phi \right] = -\frac{\rho}{\varepsilon_0} \quad (\nabla \cdot \mathbf{E} = \frac{\rho}{\varepsilon_0}),
\]
\[
\frac{1}{c^2} \frac{\partial^2 \mathbf{A}}{\partial t^2} - \nabla^2 \mathbf{A} + \nabla(\nabla \cdot \mathbf{A} + \frac{1}{c^2} \frac{\partial \phi}{\partial t}) = \mu_0 \mathbf{J}.
\]
Maxwell equations give EM field as a functional of \( \rho \) and \( \mathbf{J} \), which also contains the solution of the homogeneous equations (for \( \rho = 0 \), \( \mathbf{J} = 0 \)). The existence of the field component independent of the internal charges is important for the gauge invariant rewriting of \( \mathcal{L} \) into many-body Hamiltonian with explicit Coulomb potential.

To describe an isolated system of particles by this Lagrangian, we restrict \( \ell \) only to the particles in the system, while vector and scalar potentials are allowed to have the components of internal and external origins. The external components are treated as given quantities.

Coulomb potential is derived from the self-energy of the L electric field. The solution of \( \nabla \cdot \mathbf{E} = \rho/\varepsilon_0 \) has the form
\[
\mathbf{E}^{(L)}(\mathbf{r}) = \mathbf{E}_0^{(L)}(\mathbf{r}) - \frac{1}{4\pi\varepsilon_0} \nabla \int d\mathbf{r}' \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|},
\]
where \( \mathbf{E}_0^{(L)}(\mathbf{r}) \) is the solution of the homogeneous equation
\[
\nabla \cdot \mathbf{E}_0^{(L)}(\mathbf{r}) = -\nabla \cdot \left[ \frac{\partial \mathbf{A}_0^{(L)}}{\partial t} + \nabla \phi_0 \right] = 0
\]
given as a constant vector
\[
\mathbf{E}_0^{(L)}(\mathbf{r}) = \mathbf{C}_0 = -\frac{\partial \mathbf{A}_0^{(L)}}{\partial t} - \nabla \phi_0.
\]
For a given $C_0$, there are infinite sets of $A_0^{(L)}$ and $\phi_0$, corresponding to gauge transformation. (See eqs.(21, 22).)

The Lagrangian of electric field can be divided into $T$ and $L$ components as

$$\frac{\epsilon_0}{2} \int dr [E^{(L)}(r)^2 + E^{(T)}(r)^2]. \tag{11}$$

The integral of the $L$ component is evaluated as

$$\frac{\epsilon_0}{2} \int dr [E^{(L)}(r)]^2 = U_C + \frac{\epsilon_0}{2} \int dr C_0^2, \tag{12}$$

$$U_C = \frac{1}{8\pi\epsilon_0} \int \int dr'dr \frac{\rho(r')\rho(r)}{|r-r'|}, \tag{13}$$

where $U_C$ is the Coulomb potential among the internal charges.

The $T$ component of vector potential is, like the $L$ component, the sum of the component $A_0^{(T)}$ induced by current density and the component of the external origin $A_0^{(T)}$. The latter is the solution of the homogeneous equation

$$\frac{1}{c^2} \frac{\partial^2 A_0^{(T)}}{\partial t^2} - \nabla^2 A_0^{(T)} = 0. \tag{14}$$

Writing the $L$ field induced by $\rho$, in terms of $A$ and $\phi$, as

$$- \nabla \int dr' \frac{\rho(r')}{|r-r'|} = - \frac{\partial A^{(L)}_{\text{ind}}}{\partial t} - \nabla \phi_{\text{ind}}, \tag{15}$$

we have

$$\phi = \phi_0 + \phi_{\text{ind}}, \quad A^{(L)} = A_0^{(L)} + A^{(L)}_{\text{ind}}, \quad A^{(T)} = A_0^{(T)} + A^{(T)}_{\text{ind}}. \tag{16}$$

In terms of these variables, $\mathcal{L}$ is written as

$$\mathcal{L} = \sum \frac{1}{2} m_\ell v_\ell^2 + U_C + \int dr [-\rho(r)\phi(r) + J(r) \cdot A(r)]$$

$$+ \frac{\epsilon_0}{2} \int dr \left[ C_0^2 + (\frac{\partial A^{(T)}}{\partial t})^2 - c^2(\nabla \times A^{(T)})^2 \right]. \tag{17}$$

for a general gauge. The $L$ components of $A$ and $\phi$ remain only in the interaction term. Hereafter, we drop the constant term $\sim \int dr C_0^2$, since it does not affect the motion of internal particles. The corresponding Hamiltonian is obtained as

$$\mathcal{H} = \sum \frac{1}{2m_\ell} \{ p_\ell - e_\ell A(r_\ell) \}^2 - U_C + \int dr \rho(r)\phi(r)$$

$$+ \frac{\epsilon_0}{2} \int dr \left\{ (\frac{\partial A^{(T)}}{\partial t})^2 + c^2(\nabla \times A^{(T)})^2 \right\}. \tag{18}$$

Note that the sign of $U_C$ term is negative here. An additional contribution $+2U_C$ is included in the interaction terms, as we see below. This $\mathcal{H}$ can be used as a general one to deal with the interacting particles and EM field on various levels from non-relativistic QED to semi-classical micro- and macroscopic responses.
For a semiclassical theory of EM response, we define the matter Hamiltonian in an EM field

\[ H_1 = \sum_\ell \frac{1}{2m_\ell} \{ p_\ell - e_\ell A(\mathbf{r}_\ell) \}^2 - U_C + \int d\mathbf{r} \rho(\mathbf{r}) \phi(\mathbf{r}) \]  

(19)

by dropping the EM energy term from \( H \). The solution of the Schrödinger equation

\[ i\hbar \frac{\partial \Psi}{\partial t} = H_1 \Psi \]  

(20)

allows us to calculate the expectation value of induced current density for a given EM field, i.e., the constitutive equation.

It should be noted that this many-body Schrödinger equation is gauge invariant, i.e., the gauge transformation \{ \mathbf{A}, \phi, \Psi \} \rightarrow \{ \mathbf{A}', \phi', \Psi' \} mediated by an arbitrary scalar function \( \chi(\mathbf{r}, t) \)

\[
\begin{align*}
\mathbf{A}' &= \mathbf{A} + \nabla \chi, \quad \phi' = \phi - \frac{\partial \chi}{\partial t}, \quad \Psi' = \exp(i\Theta)\Psi, \\
\Theta &= \sum_\ell \frac{e_\ell}{\hbar} \chi(\mathbf{r}_\ell, t) = \frac{1}{\hbar} \int d\mathbf{r} \rho(\mathbf{r}) \chi(\mathbf{r}, t).
\end{align*}
\]

(21)

(22)

does not change the Schrödinger equation. If we denote the coordinate, velocity, and spin of an arbitrary particle as \( \hat{O} \), we have \( \hat{O}\Psi' = \exp(i\Theta)\hat{O}\Psi \), so that the expectation value

\[ \langle \Psi' | f(\hat{O}) | \Psi' \rangle = \langle \Psi | f(\hat{O}) | \Psi \rangle \]

(23)

of any physical quantity written as a function of \( \hat{O} \)'s is gauge invariant.

When we treat materials containing heavy elements, or magnetic species, etc., it is required to consider the relativistic corrections, such as spin-orbit interaction (\( \mathcal{H}_{so} \)), spin Zeeman interaction (\( \mathcal{H}_Z \)), etc. For that purpose, we simply add the corresponding terms to \( \mathcal{H}_C \). The spin Zeeman term can be included in the matter-EM field interaction term, and the rest in the matter Hamiltonian \( \mathcal{H}_M \). This correction does not change the argument about the gauge invariance, since the correction terms are written in terms of \( E \) and \( B \).

3 Meaning of Coulomb gauge

Among the terms of \( \mathcal{L} \), the only one affected by gauge transformation is the interaction term related with L field

\[
\int d\mathbf{r}[-\rho(\mathbf{r})\phi(\mathbf{r}) + \mathbf{J}^{(L)}(\mathbf{r}) \cdot \mathbf{A}^{(L)}(\mathbf{r})] = \int d\mathbf{r} \left[ \nabla \cdot \mathbf{P}^{(L)}(\mathbf{r}) + \frac{\partial \mathbf{P}^{(L)}}{\partial t} \cdot \mathbf{A}^{(L)}(\mathbf{r}) \right].
\]

(24)

This can be further rewritten as

\[
\int d\mathbf{r} \mathbf{P}^{(L)} \cdot \mathbf{E}^{(L)} + \frac{d}{dt} \int d\mathbf{r} \mathbf{P}^{(L)} \cdot \mathbf{A}^{(L)}.
\]

(25)

As eq.(24) shows, this \( \mathbf{E}^{(L)} \) contains the L field induced by \( \rho \). Its contribution is

\[
\int d\mathbf{r} \mathbf{P}^{(L)} \cdot \mathbf{E}_{\text{ind}}^{(L)} = -2U_C.
\]

(26)
Considering this rewriting, we can express $L$ as

$$
L = \sum_{\ell} \frac{1}{2} m_\ell v_\ell^2 - U_C + \int dr P^{(L)} \cdot E^{(L)}_0 + \frac{d}{dt} \int dr P^{(L)} \cdot A^{(L)} + \int dr J^{(T)} \cdot A^{(T)} + \frac{\epsilon_0}{2} \int dr \left[ \left( \frac{\partial A^{(T)}}{\partial t} \right)^2 - c^2 (\nabla \times A^{(T)})^2 \right].
$$

A total time derivative term (of a function of coordinates) in Lagrangian is known to play no role in the minimal action principle. The physical meaning of eliminating the total time derivative term in the $L$ given above is just choosing Coulomb gauge. If we apply the gauge transformation (21) to $L$, a difference $\delta L$ arises only from (25) as

$$
\delta L = \int dr [P^{(L)} \cdot \nabla \frac{\partial \chi}{\partial t} + \frac{dP^{(L)}}{dt} \cdot \nabla \chi] = \frac{d}{dt} \int dr P^{(L)} \cdot \nabla \chi.
$$

If we choose $\chi$ satisfying $\nabla \chi = -A^{(L)}$, the total time derivative term of (27) vanishes. The choice $\nabla \chi = -A^{(L)}$ eliminates the L component of $A$, so that the elimination of the total time derivative term is equivalent to the choice of Coulomb gauge.

It should be stressed that $E^{(L)}_0$ in the interaction term is an external L field, while the contribution of the internal L field is totally included in $U_C$. Writing $E^{(L)}_0 = E^{(L)}_{\text{ext}}$ to emphasize this point, we may end up with the Lagrangian in Coulomb gauge as

$$
L_C = \sum_{\ell} \frac{1}{2} m_\ell v_\ell^2 - U_C + \int dr P^{(L)} \cdot E^{(L)}_{\text{ext}} + \int dr J^{(T)} \cdot A^{(T)} + \frac{\epsilon_0}{2} \int dr \left[ \left( \frac{\partial A^{(T)}}{\partial t} \right)^2 - c^2 (\nabla \times A^{(T)})^2 \right].
$$

Thus, the Hamiltonian in Coulomb gauge is

$$
H_C = \sum_{\ell} \frac{1}{2m_\ell} \{ p_\ell - e_\ell A^{(T)}(r_\ell) \}^2 + U_C - \int dr P^{(L)} \cdot E^{(L)}_{\text{ext}} + \frac{\epsilon_0}{2} \int dr \left\{ \left( \frac{\partial A^{(T)}}{\partial t} \right)^2 + c^2 (\nabla \times A^{(T)})^2 \right\}.
$$

This form of $H_C$ itself is well-known [5]. However, its derivation within the framework of gauge invariant many-body Schrödinger equation with explicit Coulomb potential does not seem to be found in textbooks.

It should be stressed that the EM variables in this Hamiltonian are $A^{(T)}$ and $E^{(L)}_{\text{ext}}$, which are the gauge invariant components of EM field. The response theory in terms of these EM variables is now guaranteed to be gauge invariant. The induced current density is given as the power series expansion with respect to these field variables, and their coefficients, i.e., the susceptibilities, are written in terms of the eigenvalues and eigenfunctions of the many-body Hamiltonian $H_M = \sum_\ell (p_\ell^2/2m_\ell) + U_C$. The merit of this representation is that the susceptibilities are given as separable integral kernels, which plays an essential role in solving integral equations and also carrying out the long wavelength approximation to derive macroscopic constitutive equation [1, 2].
4 Summary

In summary, we have shown that the many-body Schrödinger equation with explicit Coulomb potential can be given in a gauge invariant form, and that the EM response obtained in Coulomb gauge directly gives the gauge invariant one.

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