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Remarks on the conventional formulation for interaction of radiation with matter

Shang-wu Qian
Department of Physics, Peking University, Beijing, China

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Abstract. The conventional formulation for interaction of radiation with matter uses a zero-potential Hamiltonian H_0 as an unperturbed Hamiltonian and this procedure leads to a conflict between the gauge invariance of probability amplitudes and the Born rule. It is pointed out that if we use a dark Hamiltonian H_d as the unperturbed Hamiltonian and consider its gauge dependence, then this conflict no longer exists. From this point of view we prove that the Lamb gauge and the Coulomb gauge in the electric dipole approximation give the same gauge-independent probability amplitudes, and thus the $\boldsymbol{A}\cdot\boldsymbol{p}$ against $\boldsymbol{r}\cdot\boldsymbol{E}$ controversy becomes unimportant.

1. Introduction

The Hamiltonian for a particle of mass m, charge q and momentum $\boldsymbol{p}=-\mathrm{i}\hbar\nabla$ in a time-varying electromagnetic field described by the vector potential $\boldsymbol{A}$ and scalar potential A_0 is

$$H=H(\boldsymbol{A}, A_0)=(\boldsymbol{p}-q\boldsymbol{A}/c)^2/2m+V+qA_0. \tag{1}$$

Conventionally, we use the complete set of orthonormal eigenfunctions $\{|\phi_n\rangle\}$ of the Hamiltonian

$$H_0=H(0,0)=\boldsymbol{p}^2/2m+V \tag{2}$$

to express the state vector of the system at time t:

$$|\psi(t)\rangle=\sum_n c_n(t)|\phi_n\rangle \tag{3}$$

the modulus square of the expansion coefficient

$$c_n(t)=\langle\phi_n|\psi(t)\rangle \tag{4}$$

defining the probability of finding the particle in an eigenstate with eigenvalue ε_n at time t. Since $|\psi\rangle$ is in general gauge dependent, and $|\phi_n\rangle$ is gauge independent, the expansion coefficients $\{c_n(t)\}$ are in general gauge dependent. As a result, the modulus square $\{|c_n(t)|^2\}$ are in general (though not necessarily) gauge dependent and consequently $\{c_n(t)\}$ cannot be interpreted in general as probability amplitudes (Yang 1976, Kobe and Smirl 1978). This conclusion seems to be in conflict with the Born rule, which is derived by Cohen (1973) using characteristic functions. This conflict comes from the fact that we have used different gauges for finding $|\psi\rangle$ and $|\phi_n\rangle$. From the physical point of view, we should use the field-free (dark) Hamiltonian as the

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unperturbed Hamiltonian, which is in general different from H_0. When we make the following gauge transformation on the potential:

$$A' = A + \nabla\Lambda \qquad A_0' = A_0 - \frac{1}{c}\frac{\partial\Lambda}{\partial t} \tag{5}$$

the Hamiltonian $H(A, A_0)$ changes to $H(A+\nabla\Lambda, A_0-(1/c)(\partial\Lambda/\partial t))$ and, consequently, the dark Hamiltonian $H(0,0)$ should become $H(\nabla\Lambda, -(1/c)(\partial\Lambda/\partial t))$, i.e. the dark Hamiltonian H_d is gauge dependent, and its expression is

$$H_d = (p - q\nabla\Lambda/c)^2/2m + V - (q/c)(\partial\Lambda/\partial t). \tag{6}$$

It should be emphasised that only in certain special cases does the operator H_d yield a complete set of eigenfunctions, and in these cases we can apply the Born rule to interpret the expansion coefficients as probability amplitudes, which are automatically gauge independent. In fact, when we can identify H_d with an energy operator introduced by Yang (1976), H_d yields a complete set of eigenfunctions. This conclusion is readily obtained from the gauge-invariant formulation (GIF) of quantum mechanics recently developed by Yang and Kobe (Yang 1976, 1982, 1983, 1985, Kobe and Smirl 1978, Kobe 1982, 1984a, b, Kobe and Yang 1985, Lee and Albrecht 1983a, b, Leubner and Zoller 1980). Therefore, if we replace H_0 by H_d in the conventional formulation (CF), then there is no conflict between gauge invariance of probability and the Born rule, and CF is just a particular case of GIF. Hereafter we shall call this revised form of CF 'RCF'.

The electric dipole approximation (EDA) is widely used in quantum optics to treat the interaction of electromagnetic radiation with matter in the long-wavelength limit. There are two widely used gauges in EDA: the Lamb gauge and the Coulomb gauge. In § 2 we shall use RCF to discuss the Lamb gauge and in § 3 we use it to discuss the Coulomb gauge. All these gauges give the same RCF expansion coefficients, and hence the $A \cdot p$ against $r \cdot E$ controversy becomes unimportant from the viewpoint of RCF.

2. The Lamb gauge in EDA

In EDA only the effect of the electric field on the system is considered, i.e. magnetic effects are neglected. The wavelength of the electromagnetic radiation is taken to be long compared with the spatial dimensions of the system. Only the electric field at the origin need be considered and the spatial variation of the field can be neglected. Thus, in EDA we have

$$E(r, t) \approx E(0, t) = E(t) \qquad B(r, t) \approx 0. \tag{7}$$

In the Lamb gauge, the vector potential A^L is chosen to be zero, and the scalar potential A_0^L is chosen to be $-r \cdot E(t)$, i.e.

$$A^L(r, t) = 0 \qquad A_0^L(r, t) = -r \cdot E(t). \tag{8}$$

Hence the Hamiltonian in the Lamb gauge is (Lamb 1952)

$$H^L = H_0 - qr \cdot E(t) \tag{9}$$

From (9) it is apparent that in the Lamb gauge the Hamiltonian is gauge independent and, moreover, the dark Hamiltonian is also gauge independent and always equal to H_0, i.e.

$$H_d^L = p^2/2m + V. \tag{10}$$

Hence in the Lamb gauge there is no difference between RCF and CF, and the CF expansion coefficients are gauge independent and can be interpreted as probability amplitudes which are given by expression (4).

3. The Coulomb gauge in EDA

In the Coulomb gauge the vector potential $\boldsymbol{A}^c$ is chosen to be a transverse field and the scalar potential A_0^c is chosen to be zero, i.e.

$$\nabla \cdot \boldsymbol{A}^c(\boldsymbol{r}, t) = 0 \qquad A_0^c = 0. \tag{11}$$

Hence the Hamiltonian in the Coulomb gauge is

$$H^c = (\boldsymbol{p} - q\boldsymbol{A}^c/c)^2/2m + V. \tag{12}$$

From (12) it is readily seen that in the Coulomb gauge the Hamiltonian (12) can be identified with the energy operator introduced by Yang (1976), and the dark Hamiltonian is just the field-free energy operator, i.e.

$$H_d^c = (\boldsymbol{p} + q\nabla\Lambda/c)^2/2m + V. \tag{13}$$

Since the last term $-(q/c)(\partial\Lambda/\partial t)$ in (6) is chosen to be zero in the Coulomb gauge, we can only make a gauge transformation with a gauge function Λ which is independent of time t. Since we can write out the eigenvalue equation of the energy operator, we have the following eigenvalue equation for the dark Hamiltonian:

$$H_d^c|\phi_n^c\rangle = \varepsilon_n|\phi_n^c\rangle. \tag{14}$$

In the Coulomb gauge in EDA, the vector potential can be replaced by its value at the origin, i.e.

$$\boldsymbol{A}^c(\boldsymbol{r}, t) = \boldsymbol{A}^c(0, t) = \boldsymbol{A}(t). \tag{15}$$

In EDA the Lamb gauge transforms to the Coulomb gauge according to the gauge function

$$\Lambda(\boldsymbol{r}, t) = \boldsymbol{r} \cdot \boldsymbol{A}(t). \tag{16}$$

The Schrödinger equation and eigenvalue equation of the dark Hamiltonian in these two gauges are

Lamb gauge: $\quad i\hbar\, \partial|\psi^L\rangle/\partial t = H^L\psi^L \qquad H_0|\phi_n^L\rangle = \varepsilon_n|\phi_n^L\rangle \qquad (17)$

Coulomb gauge: $\quad i\hbar\, \partial|\psi^c\rangle/\partial t = H^c\psi^c \qquad H_d^c|\phi_n^c\rangle = \varepsilon_n|\phi_n^c\rangle. \qquad (18)$

The relations between the two wavefunctions and the two sets of eigenstates are

$$|\psi^c\rangle = U|\psi^L\rangle \tag{19}$$

$$|\phi_n^c\rangle = \mathrm{U}|\phi_n^L\rangle \tag{20}$$

where the unitary operator U is

$$U = \exp(\mathrm{i}q\boldsymbol{r} \cdot \boldsymbol{A}(t)/\hbar c). \tag{21}$$

The RCF expansion coefficients in the Coulomb gauge are

$$c_n^c(t) = \langle\phi_n^c|\psi^c\rangle \tag{22}$$

which are gauge independent and from (19) and (20) we readily obtain

$$c_n^c(t) = \langle\phi_n^L|\psi^L\rangle = c_n^L(t) = c_n(t).$$

Therefore, in RCF, the Lamb and Coulomb gauges are equally applicable, they give the same probability amplitudes which are gauge invariant, and thus the $\boldsymbol{A}\cdot\boldsymbol{p}$ against $\boldsymbol{r}\cdot\boldsymbol{E}$ controversy becomes unimportant.

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