MASTER

ORO 5126-24

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Kuo-Ho Yang
Department of Physics and Astronomy
University of Maryland, College Park, Maryland 20742

August 1977

U. of Md. TR #78-013
U. of Md. PP #78-037

UNIVERSITY OF MARYLAND
DEPARTMENT OF PHYSICS AND ASTRONOMY
COLLEGE PARK, MARYLAND

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Kuo-Ho Yang^{*†}
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ABSTRACT

We show that the two-component spin of a nonrelativistic electron causes no conceptual difficulty to the gauge invariant formulation of quantum mechanics proposed previously by the author.

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* Supported in part by the National Science Foundation and the U. S. Energy Research and Development Administration.

† Present address: Theoretical Chemistry Institute, University of Wisconsin, Madison, Wisconsin 53706.

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It has recently been brought to my attention that there are worries whether a previously proposed gauge invariant interpretation of quantum mechanics is applicable to systems more complicated than the two simple systems investigated before.^[1] (These two simple systems are a spinless, nonrelativistic and a Dirac charged particle.) The worries center on whether the basic idea of the gauge invariant formulation--the Poynting theorem--can be applied, for example, to a nonrelativistic charged particle with spin, with or without spin-orbit interaction. We believe that this issue has been settled because a charged particle spin-1/2 can be considered as an approximation of a Dirac particle.^[2] Nevertheless, we think it constructive to demonstrate explicitly how one should go about in trying to incorporate the Poynting theorem into such a system.

Consider a charged particle with mass m , charge e , and spin $\mathbf{s}$ moving in the presence of a conservative electrostatic field $\mathbf{E}_0(\mathbf{r})$, and a time-varying electromagnetic field $\mathbf{E}(\mathbf{r}, t)$ and $\mathbf{B}(\mathbf{r}, t)$. The Schrödinger equation in an arbitrary gauge g is

$$i\hbar \dot{\psi} = H \psi \quad (1)$$

where

$$H = \frac{1}{2m} \left(\mathbf{p} - \frac{e}{c} \mathbf{A} \right)^2 + eV_0(\mathbf{r}) + e\phi - \mu_0 \mathbf{s} \cdot \mathbf{B}(\mathbf{r}, t) \quad (2)$$

where $\mathbf{A}$ and ϕ are the potentials in gauge g and describe the fields $\mathbf{E}$ and $\mathbf{B}$ through the usual relations^[3]

$$\mathbf{B}(\mathbf{r}, t) = \nabla \times \mathbf{A}(\mathbf{r}, t), \quad \mathbf{E}(\mathbf{r}, t) = -\nabla \phi(\mathbf{r}, t) - \frac{1}{c} \dot{\mathbf{A}}(\mathbf{r}, t). \quad (3)$$

Throughout this paper, a dot over a quantity implies a partial differentiation with respect to time. The constant μ_0 has the usual meaning (watch out for a factor of 2 difference). We stress here that the potential energy $eV_0(\mathbf{r})$ must

be constructed strictly according to the procedure discussed in Ref. [1] or in Ref. [4].

The current density is^[5]

$$\mathbf{J}(\mathbf{r}, t) \equiv \frac{1}{2} \{ [\psi^\dagger (e\mathbf{v} \psi)] + [\psi^\dagger (e\mathbf{v} \psi)]^* \} + c\mu_0 \nabla \times (\psi^\dagger \mathbf{s} \psi) \quad (4)$$

where $\dagger$ is the symbol for Hermitian conjugate and $*$ for complex conjugate.

The velocity operator $\mathbf{v}(t)$ for our system described by the Hamiltonian in Eq. (1) is

$$\mathbf{v}(t) = \frac{1}{m} (\mathbf{p} - \frac{e}{c} \mathbf{A}). \quad (5)$$

Using Eqs. (4), (5) and the following definitions

$$\rho(\mathbf{r}, t) \equiv e\psi^\dagger(\mathbf{r}, t)\psi(\mathbf{r}, t), \quad (6)$$

$$H_B \equiv \frac{1}{2m} (\mathbf{p} - \frac{e}{c} \mathbf{A})^2 + eV_0 - \mu_0 \mathbf{s} \cdot \mathbf{B}, \quad (7)$$

we can easily show

$$\frac{\partial}{\partial t} \rho(\mathbf{r}, t) + \nabla \cdot \mathbf{J}(\mathbf{r}, t) = 0, \quad (8)$$

$$\frac{d}{dt} \langle \psi | H_B | \psi \rangle = \int d\mathbf{r} \mathbf{J}(\mathbf{r}, t) \cdot \mathbf{E}(\mathbf{r}, t). \quad (9)$$

Equation (8) is then interpreted as the equation of continuity and Eq. (9) is interpreted as corresponding to the interaction of electromagnetic waves and matter as prescribed by the Poynting theorem.

Our past experience tells us that most have difficulty deriving equations necessary for gauge invariant formulation. As an example, we shall demonstrate how to get to Eq. (9) in the following. First, we split up H_B into two components.

$$H_B = H_B^{\text{orbit}} + H_B^{\text{spin}} \quad (10)$$

with

$$H_B^{\text{orbit}} \equiv \frac{1}{2m} (\mathbf{p} - \frac{e}{c} \mathbf{A})^2 + eV_0 \quad (11)$$

$$H_B^{\text{spin}} \equiv -\mu_0 \mathbf{s} \cdot \mathbf{B}.$$

We also observe that the following relation is true

$$H = H_B + e\phi. \quad (12)$$

Using all of the equations above, we get

$$\begin{aligned} \frac{d}{dt} \langle \psi | H_B | \psi \rangle &= \langle \psi | \frac{\partial H_B}{\partial t} + \frac{1}{i\hbar} [H_B, H] | \psi \rangle \\ &= \langle \psi | \frac{\partial H_B^{\text{orbit}}}{\partial t} + \frac{1}{i\hbar} [H_B^{\text{orbit}}, e\phi] | \psi \rangle + \langle \psi | \frac{\partial H_B^{\text{spin}}}{\partial t} | \psi \rangle, \end{aligned} \quad (13)$$

where we have already assumed that the wave function ψ behaves so nicely that all the surface terms encountered vanish.

The orbital term in Eq. (13) is well known from previous investigation.^[1]

We therefore only quote the result here:

$$\begin{aligned} &\langle \psi | \frac{\partial H_B^{\text{orbit}}}{\partial t} + \frac{1}{i\hbar} [H_B^{\text{orbit}}, e\phi] | \psi \rangle \\ &= \int d\mathbf{r} \, \mathbf{E}(\mathbf{r}, t) \cdot \frac{1}{2} \left\{ \left[\psi^\dagger \left(\frac{e(\mathbf{p} - \frac{e}{c} \mathbf{A})}{m} \psi \right) \right] + \left[\psi^\dagger \left(\frac{e(\mathbf{p} - \frac{e}{c} \mathbf{A})}{m} \psi \right) \right]^* \right\}. \end{aligned} \quad (14)$$

The spin term can be converted into the desired form as follows.

$$\begin{aligned} \langle \psi | \frac{\partial H_B^{\text{spin}}}{\partial t} | \psi \rangle &= -\mu_0 \int d\mathbf{r} (\psi^\dagger \mathbf{s} \psi) \cdot \frac{\partial \mathbf{B}}{\partial t} = c\mu_0 \int d\mathbf{r} (\psi^\dagger \mathbf{s} \psi) \cdot \nabla \times \mathbf{E} \\ &= c\mu_0 \int d\mathbf{r} \{ \nabla \cdot (\mathbf{E} \times (\psi^\dagger \mathbf{s} \psi)) + \mathbf{E} \cdot \nabla \times (\psi^\dagger \mathbf{s} \psi) \}. \end{aligned} \quad (15)$$

If we invoked again the nice behavior of ψ so that the surface term vanishes, then Eq. (9) is obvious by Eqs. (14) and (15).

Suppose now the spin-orbit interaction is turned on. The Hamiltonian in gauge g will be

$$H = \frac{1}{2m} \left(\mathbf{p} - \frac{e}{c} \mathbf{A} \right)^2 + eV_0 + e\phi - \mu_0 \mathbf{s} \cdot \mathbf{B} + f(r) \mathbf{s} \cdot \mathbf{r} \times \left(\mathbf{p} - \frac{e}{c} \mathbf{A} \right) \quad (16)$$

where we have added another assumption that V_0 is a central potential and where the function $f(r)$ is related to V_0 in the usual way.^[2] It should perhaps be mentioned that the gauge invariance of the Schrödinger equation demands $(\mathbf{p} - \frac{e}{c} \mathbf{A})$ instead of $\mathbf{p}$ in the spin-orbit interaction. We believe that this

point is well known.^[6] The velocity operator for this Hamiltonian will be

$$\mathbf{v}(t) = \frac{1}{m} \left(\mathbf{p} - \frac{e}{c} \mathbf{A} \right) + f(r) \mathbf{s} \times \mathbf{r}. \quad (17)$$

The current density is still defined by Eq. (4). One can easily obtain Eqs. (8) and (9) if

$$H_B = \frac{1}{2m} \left(\mathbf{p} - \frac{e}{c} \mathbf{A} \right)^2 + eV_0 - \mu_0 \mathbf{s} \cdot \mathbf{B} + f(r) \mathbf{s} \cdot \mathbf{r} \times \left(\mathbf{p} - \frac{e}{c} \mathbf{A} \right). \quad (18)$$

In conclusion, we have shown that there is no conceptual difficulty in incorporating the Poynting theorem--the central idea of the gauge invariant interpretation--into the quantum system of a nonrelativistic charged particle with spin, with or without spin-orbit interaction. It is then straightforward how to proceed from here to construct gauge invariant energy spectrum and probability amplitudes.^[1]

The author wishes to thank the Nuclear Theory Group for the hospitality extended to him during the past two years.

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