PHYSICAL REVIEW D VOLUME 26, NUMBER 8 15 OCTOBER 1982

Power operator in quantum mechanics

Donald H. Kobe and Edward C.-T. Wen
Department of Physics, North Texas State University, Denton, Texas 76203

K.-H. Yang
Theoretical Chemistry Institute,
University of Wisconsin—Madison, Madison, Wisconsin 53706

(Received 14 January 1981; revised manuscript received 19 October 1981)

For a system consisting of a classical electromagnetic field and a charged quantum-mechanical particle, Poynting's theorem holds for the energy density of the electromagnetic field. For local energy conservation to hold, the power lost by the field is the power gained by the quantum-mechanical particle. The power per unit volume transferred from the field to the particle is $\vec{E}\cdot\vec{J}$, which is shown to be the density of the quantum-mechanical power operator. For the particle an energy theorem, similar to Poynting's theorem for the field, is satisfied in such a way that the energy of the total isolated system is conserved. The energy density of the particle is the density of the energy operator for the particle, which in this time-dependent problem is not the same as the Hamiltonian. The energy operator is gauge invariant, while the Hamiltonian is not. When the combined conditions of gauge invariance and local energy conservation are used, the appropriate basis functions to use are the eigenstates of the energy operator. Transitions between these eigenstates are determined by matrix elements of the power operator.

I. INTRODUCTION

A manifestly gauge-invariant formulation of charged quantum-mechanical particles interacting with an external classical electromagnetic field has recently been given.[1,2] In addition to the criterion of gauge invariance, the correspondence principle in its Newtonian form was used to construct gauge-invariant operators for observables with classical counterparts. This formulation of a gauge-invariant theory was criticized by Olariu *et al.*[3] as being too restrictive. They claim that the gauge invariance of the theory is insufficient to determine its form uniquely, and that the basis-determining Hamiltonian can be chosen in a quite general way. They thus say that the gauge-invariant formulation developed previously[1,2] "simply exchange(s) a dependence upon the gauge of the electromagnetic potentials for a previously unrecognized dependence upon the representation of basis states... that is equivalent to a dependence upon gauge." They recommend a choice of a basis-determining operator on intuitive grounds, in such a way that the dynamic Stark shift and dynamic Zeeman shift are apparently taken into account.

In this paper it is shown that the principles of energy conservation and gauge invariance when applied at every time are sufficient to determine the theory uniquely to be the theory of Yang[1] and Kobe and Smirl.[2] Operators corresponding to observables are constructed from the correspondence principle in its Newtonian form.[4] The physical interpretation of the theory is then made using a generalized form of Ehrenfest's theorem.[5]

The role of energy conservation is emphasized in this paper. When the classical electromagnetic field and the quantum-mechanical particle are considered together as an isolated system, the energy of the total system is conserved. For this semiclassical formulation of the field-particle problem we assume that Poynting's theorem holds. Poynting's theorem for the electromagnetic field[6] states that the energy of the field in an arbitrary volume can change either by flow of energy through the surface or by loss (gain) of energy to the charged particle. A similar energy theorem is assumed to hold for the quantum-mechanical particle, which states that the energy of the particle in an arbitrary volume can change either by flow of energy through the surface or by gain (loss) of energy

from the field. The energy lost by the field is the energy gained by the particle. Thus energy is conserved locally as well as for the whole volume. The energy operator of the particle in this time-dependent problem is shown to be the operator corresponding to the classical energy, not the Hamiltonian. Failure to recognize this distinction in time-dependent problems involving electromagnetic radiation has previously led to confusion,[7] which was resolved when the distinction between the energy operator and Hamiltonian was made.[8]

In the next section the basic ideas of the gauge-invariant formulation are discussed, and the energy operator defined. The role of energy conservation is discussed in Sec. III and it is shown that the power lost by the field is the power gained by the charged particle. In Sec. IV the time dependence of eigenvalues of different basis-determining operators is discussed. The interpretation of expansion coefficients is discussed in Sec. V. The conclusion is given in Sec. VI.

II. GAUGE INVARIANCE

In this section we review the concept of manifest gauge invariance for a single quantum-mechanical particle in a classical electromagnetic field.[9] The Hamiltonian for the particle is not a gauge-invariant operator, in the sense that it does not have a gauge-invariant expectation value. Thus the Hamiltonian cannot be the energy operator for the particle, since all operators corresponding to observables must be gauge invariant.[10] The energy operator is obtained from the correspondence principle from the classical energy consisting of kinetic and potential energies.[11]

The Hamiltonian describes the time evolution of the wave function ψ in such a way that the Schrödinger equation is form invariant under gauge transformations. The Hamiltonian for a single particle of mass m and charge q coupled minimally to an external electromagnetic radiation field characterized by the vector potential $\vec{A}$ and scalar potential A_0 is

$$H(\vec{A},A_0)=\frac{1}{2m}\left[\vec{p}-\frac{q}{c}\vec{A}\right]^2 + V+qA_0 \ . \tag{2.1}$$

The potential energy $V=V(\vec{r})$ is of electrostatic or nonelectromagnetic origin. The Schrödinger equation for the particle is

$$H(\vec{A},A_0)\psi=i\hbar\partial\psi/\partial t \ . \tag{2.2}$$

A gauge transformation on the wave function is

$$\psi'=\exp(iq\Lambda/\hbar c)\psi \ , \tag{2.3}$$

and the corresponding gauge transformation on the potentials is

$$\vec{A}'=\vec{A}+\nabla\Lambda \tag{2.4}$$

and

$$A_0'=A_0-\frac{1}{c}\frac{\partial\Lambda}{\partial t} \ , \tag{2.5}$$

where Λ is an arbitrary differentiable function of $\vec{r}$ and t called a gauge function. Under the combined gauge transformations in Eqs. (2.3)–(2.5) the Schrödinger equation is form invariant,[12]

$$H(\vec{A}',A_0')\psi'=i\hbar\partial\psi'/\partial t \ . \tag{2.6}$$

For an operator $\theta(\vec{A},A_0)$ to correspond to an observable quantity, its expectation value must be gauge invariant,[8,10]

$$\langle\psi\,|\,\theta(\vec{A},A_0)\psi\rangle=\langle\psi'\,|\,\theta(\vec{A}',A_0')\psi'\rangle \ , \tag{2.7}$$

where the new wave function ψ' is given in Eq. (2.3). The operator $\theta(\vec{A}',A_0')$ is the same *form* as the operator $\theta(\vec{A},A_0)$, but the new potentials in Eqs. (2.4) and (2.5) replace the old ones. The expectation value on the left-hand side in Eq. (2.7) can always be written as

$$\langle\psi\,|\,\theta(\vec{A},A_0)\psi\rangle=\langle\psi'\,|\,\theta'(\vec{A},A_0)\psi'\rangle \ , \tag{2.8}$$

where the prime on the operator denotes a unitary transformation

$$\theta'(\vec{A},A_0)=\exp(iq\Lambda/\hbar c)\theta(\vec{A},A_0) \times\exp(-iq\Lambda/\hbar c) \ . \tag{2.9}$$

By a comparison of Eqs. (2.7) and (2.8), an operator is called gauge invariant if it is form invariant under a unitary transformation,

$$\theta'(\vec{A},A_0)=\theta(\vec{A}',A_0') \ . \tag{2.10}$$

In other words, an operator is gauge invariant if a unitary transformation on the operator induces a gauge transformation on the electromagnetic potentials on which the operator depends.

As an example of a gauge-invariant operator,

consider the kinetic momentum $\vec{\pi}=\vec{p}-q\vec{A}/c$. Under a unitary transformation the kinetic momentum transforms as

$$(\vec{\pi})'=\left[\vec{p}-\frac{q}{c}\vec{A}\right]'=\vec{p}-\frac{q}{c}\vec{A}'=\vec{\pi}' , \tag{2.11}$$

and is thus form invariant under a unitary transformation. The operator corresponding to the energy, the zero component of the energy-momentum four-vector, is $\pi_0=i\hbar\partial/\partial t-qA_0$. It transforms under a unitary transformation as

$$\begin{aligned}(\pi_0)'&=(i\hbar\partial/\partial t-qA_0)'\\&=i\hbar\partial/\partial t-qA_0'=\pi_0' ,\end{aligned} \tag{2.12}$$

and is also form invariant under a unitary transformation.

In terms of the gauge-invariant operators $\vec{\pi}$ and π_0, the Schrödinger equation in Eq. (2.2) can be rewritten as

$$H(\vec{A},0)\psi=\pi_0\psi , \tag{2.13}$$

where the operator

$$H(\vec{A},0)=\frac{\pi^2}{2m}+V=\mathscr{E}(\vec{A}) \tag{2.14}$$

will be called the energy operator.[1] The energy operator is the kinetic energy operator plus the potential energy, which is the same form as the classical energy.[13] It is the Hermitian operator corresponding to π_0 in Eq. (2.13). Since π_0 and $\vec{\pi}$ are gauge invariant, $H(\vec{A},0)$ is also,

$$H'(\vec{A},0)=H(\vec{A}',0) . \tag{2.15}$$

The Hamiltonian $H(\vec{A},A_0)$, however, is not gauge invariant because

$$\begin{aligned}H'(\vec{A},A_0)=H(\vec{A}',A_0)&=H(\vec{A}',A_0')+\frac{1}{c}\frac{\partial\Lambda}{\partial t}\\&\neq H(\vec{A}',A_0') ,\end{aligned} \tag{2.16}$$

since the scalar potential is unchanged under the unitary transformation.

In terms of the Hamiltonian, the energy operator in Eq. (2.14) is

$$\mathscr{E}(\vec{A})=H(\vec{A},A_0)-qA_0 . \tag{2.17}$$

For time-dependent electromagnetic fields qA_0 is not a potential energy, and must therefore be subtracted from the Hamiltonian to obtain the energy. The negative gradient of qA_0,

$$-\nabla qA_0=q\vec{E}+\frac{q}{c}\frac{\partial\vec{A}}{\partial t} , \tag{2.18}$$

where $\vec{E}$ is the electric field, is not a force $q\vec{E}$ because of the vector potential term on the right-hand side. A potential energy, like V in Eq. (2.1), is defined such that its negative gradient,

$$-\nabla V=\vec{F}_0 , \tag{2.19}$$

is a conservative force.

In the gauge-invariant formulation of quantum mechanics developed by Yang[1] use is made of the eigenvalue problem for the energy operator

$$\mathscr{E}(\vec{A})\psi_n=\epsilon_n\psi_n , \tag{2.20}$$

where ψ_n are the eigenfunctions and ϵ_n are the eigenvalues which may depend on the time as a parameter. The wave function in Eq. (2.2) is expanded in terms of the eigenfunctions of the energy operator

$$\psi=\sum_n c_n\psi_n . \tag{2.21}$$

The expansion coefficients c_n are gauge invariant, and satisfy the set of equations

$$i\hbar\dot{c}_n-\tilde{\epsilon}_n c_n=-\sum_{m\neq n}\langle\psi_n\,|\,\pi_0\psi_m\rangle c_m , \tag{2.22}$$

where

$$\tilde{\epsilon}_n=\epsilon_n-\langle\psi_n\,|\,\pi_0\psi_n\rangle \tag{2.23}$$

is a "dressed" energy.[2]

Since the wave function is not an observable and is not unique because gauge transformations in Eq. (2.3) can be made on it, the *state* of the system cannot be unambiguously specified by specifying a wave function. A state can, however, be specified by giving the equivalence class of all wave functions gauge equivalent to a given wave function. For the case of eigenstates of observable operators, the *eigenvalues* are gauge invariant, and can thus be used to specify the quantum-mechanical states in the absence of degeneracy. In the more general case, the equivalence class of eigenstates of an operator corresponding to an observable can be used to specify the states. The phase factor in Eq. (2.3) does not depend on the state, so the concept of state is gauge invariant, while the wave function is not. For example, in Eq. (2.20) the eigenvalue ϵ_n is gauge invariant, the energy operator is form invariant under gauge transformation, but the wave function ψ_n is not gauge invariant. We shall use n

to denote the equivalence class $[\psi_n]$ of all wave functions differing from ψ_n only by a phase factor, generally depending on space and time, as in Eq. (2.3).

To show definitively that $\mathscr{E}(\vec{A})$ is indeed the energy operator for the particle, we shall show in the next section that it is the operator required in the energy conservation theorem.

III. POWER OPERATOR

The system we consider in this paper is a single charged quantum particle interacting with a classical electromagnetic field. In this section we shall show that the energy operator obtained in Sec. II can be used to construct the energy density of the particle. The time rate of change of the energy of the particle in a small volume is due to the energy flux of the particle through the surface and the power the particle gains from the electromagnetic field. The corresponding time rate of change in the energy of the electromagnetic field in the same small volume is due to the energy flux of the field through the surface and the power lost to the particle. Since Poynting's theorem[6] applies to the classical electromagnetic field, the power lost by the field is $\vec{J}\cdot\vec{E}$ where $\vec{J}$ is the current density. Energy conservation requires that the energy lost by the field is equal to the energy gained by the particle. We shall show that this energy is given in terms of the quantum-mechanical power operator, first introduced by Yang.[1]

A. Energy of the field

For the electromagnetic field characterized by the electric field $\vec{E}$ and magnetic induction $\vec{B}$, the energy density (in Gaussian units) is

$$\mathscr{U}_{\rm em}=\frac{1}{8\pi}(E^2+B^2)\ . \tag{3.1}$$

From Maxwell's equations the electromagnetic field satisfies Poynting's theorem[6]

$$\partial\mathscr{U}_{\rm em}/\partial t+\nabla\cdot\vec{\mathscr{S}}_{\rm em}=-\vec{J}\cdot\vec{E}\ , \tag{3.2}$$

where the energy flux $\vec{\mathscr{S}}_{\rm em}$ is the Poynting vector

$$\vec{\mathscr{S}}_{\rm em}=\frac{c}{4\pi}\vec{E}\times\vec{B}\ . \tag{3.3}$$

The electromagnetic field loses energy to the charged particle at the rate $\vec{J}\cdot\vec{E}$ per unit volume, where $\vec{J}$ is the current density inside the volume. In quantum mechanics, the current density due to a single particle can be written as

$$\vec{J}=\mathrm{Re}\psi^*(\vec{r},t)q\vec{v}\psi(\vec{r},t)\ , \tag{3.4}$$

where Re denotes the real part. The velocity operator $\vec{v}$ is defined as

$$\vec{v}=m^{-1}\vec{\pi}\ , \tag{3.5}$$

where $\vec{\pi}$ is the kinetic momentum in Eq. (2.11). The power density $\vec{J}\cdot\vec{E}$ on the right-hand side of Eq. (3.2) may be rewritten as

$$\vec{J}\cdot\vec{E}=\mathscr{P}=\mathrm{Re}\psi^*P\psi\ , \tag{3.6}$$

where the Hermitian power operator P is defined as

$$P=\frac{q}{2}(\vec{v}\cdot\vec{E}+\vec{E}\cdot\vec{v})\ . \tag{3.7}$$

In order to write Eq. (3.6) in this form we have used the identity

$$\mathrm{Re}\psi^*\vec{v}\cdot\vec{E}\psi=\mathrm{Re}\{\psi^*[\vec{E}\cdot\vec{v}-m^{-1}i\hbar\nabla\cdot\vec{E}]\psi\}\ . \tag{3.8}$$

Since by Gauss's law

$$\nabla\cdot\vec{E}=4\pi\rho\ , \tag{3.9}$$

where the charge density is $\rho=q\psi^*\psi$, the last term in the square brackets on the right-hand side of Eq. (3.8) vanishes when the real part is taken. Poynting's theorem in Eq. (3.2) can thus be rewritten as

$$\partial\mathscr{U}_{\rm em}/\partial t+\nabla\cdot\vec{\mathscr{S}}_{\rm em}=-\mathscr{P}\ , \tag{3.10}$$

from Eq. (3.6).

B. Energy of the particle

If the operator $\mathscr{E}(\vec{A})$ in Eq. (2.14) is the energy operator for the particle, the energy density of the particle is[14]

$$\mathscr{U}_p=\mathrm{Re}\psi^*\mathscr{E}(\vec{A})\psi\ . \tag{3.11}$$

From the Schrödinger equation in Eq. (2.2) it can be shown that the energy density of the particle satisfies

$$\partial\mathscr{U}_p/\partial t+\nabla\cdot\vec{\mathscr{S}}_p=\mathscr{P}\ . \tag{3.12}$$

The power density $\mathscr{P}$ is given by Eq. (3.6) and the energy flux of the particle is

$$\vec{\mathscr{S}}_p = \tfrac{1}{2}\,\mathrm{Re}[(\vec{\nabla}\psi)^* \mathscr{E}(\vec{A})\psi + \psi^* \vec{\nabla}\mathscr{E}(\vec{A})\psi] \,. \tag{3.13}$$

The right-hand side of Eq. (3.12) is the power per unit volume absorbed from the electromagnetic field. For this reason we can identify $\mathscr{E}(\vec{A})$ as the energy operator. Relativistic electrons[8] and nonrelativistic electrons with spin[15] have previously been treated.

C. Energy conservation

By adding Eqs. (3.2) and (3.12) the condition of total energy conservation can be obtained. The total energy density

$$\mathscr{U} = \mathscr{U}_{\mathrm{em}} + \mathscr{U}_p \,, \tag{3.14}$$

and the total energy flux

$$\vec{\mathscr{S}} = \vec{\mathscr{S}}_{\mathrm{em}} + \vec{\mathscr{S}}_p \,, \tag{3.15}$$

satisfy an equation of continuity

$$\partial \mathscr{U} / \partial t + \nabla \cdot \mathscr{S} = 0 \,. \tag{3.16}$$

Thus the total energy of the field and the particle is conserved *locally,* because the power per unit volume lost by the electromagnetic field is the power per unit volume gained by the particle.

The physical significance of the conservation of energy at all times can be illustrated by integrating Eq. (3.16) over a volume Ω enclosed by a surface σ. If we assume that Ω is sufficiently large that the particle is completely confined within σ at the times of interest, then using Eqs. (3.11), (3.14), and (3.15) we get

$$\frac{d}{dt}\int_{\Omega} d^3r\, \mathscr{U}_{\mathrm{em}} + \oint_{\sigma} d\vec{\sigma}\cdot\vec{\mathscr{S}}_{\mathrm{em}} = -\frac{d}{dt}\langle\psi \,|\, \mathscr{E}(\vec{A})\psi\rangle \,. \tag{3.17}$$

Under steady-state conditions, the electromagnetic field energy in the volume Ω is constant, so

$$\frac{d}{dt}\langle\psi \,|\, \mathscr{E}(\vec{A})\psi\rangle = -\oint_{\sigma} d\vec{\sigma}\cdot\vec{\mathscr{S}}_{\mathrm{em}} \,. \tag{3.18}$$

Thus, the measurement of the total net flow of the electromagnetic energy across the entire surface σ is a measurement of the change of the average value of the energy of the particle.

D. Electric dipole approximation

In the limit that the wavelength is long compared to the atomic dimensions, the power density $\mathscr{P}$ in Eq. (3.6) that the particle gains from the electromagnetic field can be written as

$$\mathscr{P} = q\vec{E}(0,t)\cdot \mathrm{Re}\psi^* \vec{\nabla}\psi \,. \tag{3.19}$$

The displacement density $\psi^* \vec{r}\psi$ satisfies

$$\frac{\partial}{\partial t}\psi^* x_i \psi + \nabla\cdot\vec{\mathscr{S}}_i = \mathrm{Re}\psi^* v_i \psi \,, \tag{3.20}$$

where x_i is the ith component of the displacement $\vec{r}$ $(i=1,2,3)$. The "flux of displacement x_i" $\vec{\mathscr{S}}_i$ is defined as

$$\vec{\mathscr{S}}_i = \tfrac{1}{2}\,\mathrm{Re}[(\vec{\nabla}\psi)^* x_i\psi + \psi^* \vec{\nabla} x_i \psi] \tag{3.21}$$

for $i=1,2,3$. If Eqs. (3.19) and (3.20) are used in the right-hand side of Eq. (3.12), and some rearrangements are made, we obtain

$$\frac{\partial}{\partial t}\,\mathrm{Re}\psi^*[H(\vec{A},0) - q\vec{E}(0,t)\cdot\vec{r}]\psi + \nabla\cdot[\vec{\mathscr{S}}_p - qE_i(0,t)\vec{\mathscr{S}}_i] = -q\dot{\vec{E}}(0,t)\cdot\psi^*\vec{r}\psi \,, \tag{3.22}$$

where summation on repeated indices from 1 to 3 is implied. Thus it might be thought that the operator $H(\vec{A},0) - q\vec{E}(0,t)\cdot\vec{r}$ could be interpreted as the energy operator in this case. However, the right-hand side of Eq. (3.22) is not $\mathscr{P} = \vec{E}\cdot\vec{J}$, the power density supplied to the particle by the field. Therefore, $H(\vec{A},0) - q\vec{E}(0,t)\cdot\vec{r}$ cannot in general be interpreted as the energy operator since the conservation of total energy is violated. However, in the case of a static field $\vec{E}_0$ the right-hand side of Eq. (3.22) vanishes. The term $-q\vec{E}_0\cdot\vec{r}$ can then be absorbed into the potential energy of the particle, and the energy operator is $H(\vec{A},0) - q\vec{E}_0\cdot\vec{r}$.

IV. BASIS-DETERMINING OPERATOR

When dealing with a time-dependent problem it is often useful to expand the wave function in a complete set of eigenstates of an appropriate operator. In the manifestly gauge-invariant formulation the wave function is expanded in terms of the

eigenstates of the energy operator $\mathscr{E}(\vec{A})=H(\vec{A},0)$. On the other hand, Olariu *et al.* propose expanding the wave function in terms of eigenstates of a basis-determining operator which involves two arbitrary functions. In this section we compare the two approaches.

Olariu *et al.* use for their representation eigenstates of a basis-determining operator

$$H_B=\frac{1}{2m}\left[\vec{p}-\frac{q}{c}\vec{A}-\frac{q}{c}\nabla\lambda\right]^2 + V+q\phi_0 , \tag{4.1}$$

where λ and ϕ_0 are arbitrary *fixed* functions of $\vec{r}$ and t. The eigenvalue problem for the Hermitian operator H_B is

$$H_B\chi_n=E_n\chi_n , \tag{4.2}$$

where χ_n are the (orthonormal) eigenfunctions and E_n are the corresponding eigenvalues, both of which depend on the time as a parameter.

The wave function ψ can be expanded in terms of these eigenfunctions

$$\psi=\sum_n b_n\chi_n , \tag{4.3}$$

where the expansion coefficients b_n are conventionally interpreted as the probability amplitudes of finding the system in the state χ_n. Olariu *et al.* say that by a judicious choice of λ and ϕ_0, the eigenvalues E_n can describe the energies in a more physical way than when H_B is the energy operator (i.e., when $\lambda=0$, $\phi_0=0$). We shall now contrast the behavior of H_B and E_n with $\mathscr{E}(\vec{A})$ and ϵ_n in Eq. (2.20), respectively.

If we consider the density of H_B in a manner analogous to Eq. (3.11),

$$\mathscr{U}_B=\mathrm{Re}\psi^*H_B\psi , \tag{4.4}$$

then the time rate of change of $\mathscr{U}_B$ can be written as

$$\frac{\partial\mathscr{U}_B}{\partial t}+\nabla\cdot\vec{\mathscr{S}}_B=s_B . \tag{4.5}$$

The flux of H_B is $\vec{\mathscr{S}}_B$, defined as

$$\vec{\mathscr{S}}_B=\tfrac{1}{2}[(\vec{v}\psi)^*H_B\psi+\psi^*\vec{v}H_B\psi] . \tag{4.6}$$

The source (or sink) of H_B is

$$s_B=\mathscr{P}+\mathrm{Re}\psi^*\left\{(4m^2i\hbar)^{-1}\left[\left[\vec{\pi}-\frac{q}{c}\nabla\lambda\right]^2,\pi^2\right]+\frac{q}{2}\left[\vec{v}\cdot\nabla\left[\phi_0-\frac{1}{c}\dot{\lambda}\right]+\nabla\left[\phi_0-\frac{1}{c}\dot{\lambda}\right]\cdot\vec{v}\right]\right.$$
$$\left.-\frac{q}{mc}\nabla\lambda\cdot\left[q\vec{E}-\frac{q}{c}\nabla\dot{\lambda}-\nabla V\right]+q\dot{\phi}_0\right\}\psi , \tag{4.7}$$

where the power density $\mathscr{P}$ is defined in Eq. (3.6) and the dot over a quantity denotes the partial time derivative. There are many terms in Eq. (4.7) which are difficult to interpret physically. If we choose $\nabla\lambda=0$, then Eq. (4.7) simplifies to

$$s_B=\mathscr{P}+\mathrm{Re}\psi^*\left[\frac{q}{2}(\vec{v}\cdot\nabla\phi_0+\nabla\phi_0\cdot\vec{v})+q\dot{\phi}_0\right]\psi . \tag{4.8}$$

The only term which we can interpret physically in Eq. (4.8) is $\mathscr{P}$, the power density, since the quantity in the square brackets in Eq. (4.8) is not a power. If we wish Eq. (4.8) to reduce to a power density we must choose both $\dot{\phi}_0=0$ and $\nabla\phi_0=0$, so ϕ_0 is a constant which can be chosen to be zero. Since we have chosen both $\nabla\lambda=0$ and $\phi_0=0$, H_B in Eq. (4.1) becomes the energy operator in Eq. (2.14). The conservation law in Eq. (4.5) reduces to Eq. (3.12), and Eq. (4.6) for the flux reduces to Eq. (3.13).

We can also consider the time rate of change of the eigenvalue E_n in Eq. (4.2). If the time derivative of Eq. (4.2) is taken, then

$$\dot{H}_B\chi_n+H_B\dot{\chi}_n=\dot{E}_n\chi_n+E_n\dot{\chi}_n , \tag{4.9}$$

where the dot denotes the partial time derivative. If the inner product of Eq. (4.9) is taken with χ_n, we obtain

$$\dot{E}_n=\langle\chi_n\,|\,\dot{H}_B\chi_n\rangle . \tag{4.10}$$

Substituting the time derivative of Eq. (4.1) into Eq. (4.10), we obtain

$$\dot{E}_n = \left\langle \chi_n \left| \left[P - \frac{q^2}{mc} \nabla\lambda \cdot \vec{E} + q\dot{\phi}_0 \right] \right| \chi_n \right\rangle . \tag{4.11}$$

where P is the power operator in Eq. (3.7). The time rate of change of the eigenvalue E_n is the expectation value of a sum of the power operator P, $-(q^2/mc)\nabla\lambda\cdot\vec{E}$, and $q\dot{\phi}_0$. It is only the power operator P that has physical significance. In particular if $\dot{\phi}_0 \neq 0$ when $\vec{E}=0$, the eigenvalue E_n continues to change in time even though no power is being absorbed from the field.

On the other hand, the time rate of change of the eigenvalue ϵ_n of the energy operator in Eq. (2.20) is

$$\begin{aligned} \dot{\epsilon}_n &= \langle \psi_n | P \psi_n \rangle \\ &= \int d^3r \, \vec{E}\cdot q \, \mathrm{Re}\psi_n^* \vec{v} \psi_n , \end{aligned} \tag{4.12}$$

which is the expectation value of the power operator in the state ψ_n. Equation (4.12) states that the energy eigenvalue for an electron in the state ψ_n changes at a rate given by the power absorbed from the field. Equation (4.11) reduces to Eq. (4.12) if we choose $\nabla\lambda=0$ and $\dot{\phi}_0=0$. If $q\phi_0$ is a function of $\vec{r}$ alone, it is a potential energy. However, the potential energies of the problem are all included in V. Therefore, the function $\phi_0=0$. The basis-determining operator H_B in Eq. (4.1) then reduces to the energy operator in Eq. (2.14). The eigenfunctions χ_n and eigenvalues E_n in Eq. (4.2) reduce to ψ_n and ϵ_n, respectively, in Eq. (2.20).

V. PHYSICAL INTERPRETATION OF EXPANSION COEFFICIENTS

We shall show in this section that in the formulation of Olariu *et al.*[3] the operator which couples the states χ_n in Eq. (4.2) can in general couple the states even when the field is zero. In contrast, the quantity which couples states in the gauge-invariant formulation of Yang[1] is related to matrix elements of the quantum-mechanical power operator. When the electromagnetic field is zero there is no coupling between the eigenstates of the energy operator.

If Eq. (4.3) is substituted into the Schrödinger equation in Eq. (2.2), the resulting equation for b_n is

$$i\hbar\dot{b}_n - E_n b_n = \sum_m \langle \chi_n | [H(\vec{A},A_0) - H_B - i\hbar\partial/\partial t]\chi_m \rangle b_m . \tag{5.1}$$

In the nondegenerate case ($E_n \neq E_m$, $n \neq m$) Eq. (5.1) can be rewritten as

$$i\hbar\dot{b}_n - \langle \chi_n | [H(\vec{A},A_0) - i\hbar\partial/\partial t]\chi_n \rangle b_n = \sum_{m\neq n} (E_n - E_m)^{-1} \langle \chi_n | [H_B, H(\vec{A},A_0) - i\hbar\partial/\partial t]\chi_m \rangle b_m . \tag{5.2}$$

The commutator in Eq. (5.2) can be evaluated, and the resulting equation is

$$\begin{aligned} &i\hbar\dot{b}_n - \langle \chi_n | [H(\vec{A},A_0) - i\hbar\partial/\partial t]\chi_n \rangle b_n \\ &= \sum_{m\neq n} i\hbar(E_n - E_m)^{-1} \left\langle \chi_n \left| \left\{ P + (q/2m)(\vec{\pi}\cdot\nabla\phi_0 + \nabla\phi_0\cdot\vec{\pi}) + q\dot{\phi}_0 - (i\hbar 4m^2)^{-1} \left[\pi^2, \left[\vec{\pi} - \frac{q}{c}\nabla\lambda \right]^2 \right] \right. \right. \right. \\ &\qquad - (q/mc)\nabla\lambda\cdot(q\vec{E} - \nabla V) \\ &\qquad \left. \left. \left. - (q/2mc) \left[\left[\vec{\pi} - \frac{q}{c}\nabla\lambda \right] \cdot \nabla\dot{\lambda} + \nabla\dot{\lambda}\cdot \left[\vec{\pi} - \frac{q}{c}\nabla\lambda \right] \right] \right\} \right| \chi_m \right\rangle b_m , \end{aligned} \tag{5.3}$$

where $\vec{\pi}$ is given in Eq. (2.11) and P is the power operator in Eq. (3.7). In Eq. (5.3) the states are coupled by matrix elements of the power operator and terms which involve λ and ϕ_0. In the case where the electromagnetic field is zero, $\vec{E}=0$, Eq. (5.3) predicts that there is still coupling. Thus the eigenstates of the Olariu *et al.* basis-determining operator are not stationary states in general in the absence of the field. If we choose $\nabla\lambda=0$, then some of the terms in Eq. (5.3) vanish and it becomes

$$\begin{aligned} &i\hbar\dot{b}_n - \langle \chi_n | [H(\vec{A},A_0) - i\hbar\partial/\partial t]\chi_n \rangle b_n \\ &\qquad = \sum_{m\neq n} i\hbar(E_n - E_m)^{-1} \langle \chi_n | [P + (q/2m)(\vec{\pi}\cdot\nabla\phi_0 + \nabla\phi_0\cdot\vec{\pi}) + q\dot{\phi}_0]\chi_m \rangle b_m . \end{aligned} \tag{5.4}$$

As an example of this expression, let us make the electric dipole approximation (EDA) and take $\lambda=0$, $\phi_0(\vec{r},t)=-\vec{E}(t)\cdot\vec{r}$, as suggested by Olariu *et al.*[3] Then in Eq. (5.4) the first term in the square brackets on the right-hand side cancels the second, and it becomes

$$i\hbar\dot{b}_n-\langle\chi_n\,|\,[H(\vec{A},A_0)-i\hbar\partial/\partial t]\chi_n\rangle b_n=\sum_{m\neq n}-i\hbar(E_n-E_m)^{-1}q\dot{\vec{E}}(t)\cdot\langle\chi_n\,|\,\vec{r}\chi_m\rangle b_m\ . \tag{5.5}$$

The coupling between the states χ_n and χ_m is due to matrix elements of $\dot{\vec{E}}(t)\cdot\vec{r}$. This interaction is not a power as discussed in Sec. III D. At a time when $\vec{E}(t)=0$, $\dot{\vec{E}}$ may not be zero, so according to Eq. (5.5) the states may be coupled. Conversely, when $\dot{\vec{E}}=0$, $\vec{E}$ may not be zero, but there is no coupling according to Eq. (5.5). However, classically, it is only when $\vec{E}\neq0$ that the particle absorbs energy from the field.

On the other hand, for the nondegenerate case, Eq. (2.22) can be written as

$$i\hbar\dot{c}_n-\langle\psi_n\,|\,[H(\vec{A},0)+qA_0-i\hbar\partial/\partial t]\psi_n\rangle c_n=\sum_{m\neq n}i\tau_{nm}\langle\psi_n\,|\,P\psi_m\rangle c_m\ , \tag{5.6}$$

where

$$\tau_{nm}=\hbar(\epsilon_n-\epsilon_m)^{-1} \tag{5.7}$$

is a characteristic time associated with the transition from state m to state n. The gauge-invariant formulation shows that the state m and the state n are coupled by the quantity $\tau_{nm}\langle\psi_n\,|\,P\psi_m\rangle$, i.e., the matrix element of the power operator times the appropriate characteristic time. Thus the coupling is induced by the power operator. There is no coupling when the electromagnetic field is zero, in contrast to Eqs. (5.3)–(5.5).

Equation (5.3) reduces to Eq. (5.6) if we choose $\nabla\lambda=0$, $\nabla\phi_o=0$, and $\dot{\phi}_0=0$. If $\dot{\phi}_0$ and $\nabla\phi_0$ are taken to be zero, then ϕ_0 is a constant which can be taken to be zero. In this case the basis-determining operator H_B in Eq. (4.1) then reduces to the energy operator in Eq. (2.14), the eigenfunctions χ_n and eigenvalues E_n in Eq. (4.2) reduce to ψ_n and ϵ_n, respectively, in Eq. (2.20). The expansion coefficients b_n in Eq. (4.3) reduce to c_n in Eq. (2.21).

VI. CONCLUSION

This paper emphasizes Poynting's theorem and energy conservation in providing a physical interpretation of the quantum mechanics of a charged particle when an external classical electromagnetic field is applied. As a result of energy conservation, the power lost by the electromagnetic field is the power gained by the particle. This condition is satisfied if the energy operator of the particle is defined so that the time rate of change of the average energy is equal to the expectation value of the quantum-mechanical power operator. The energy operator must also be gauge invariant, which the Hamiltonian is not. In fact, all operators corresponding to observables should be gauge invariant.[10] The gauge-invariant formulation of Yang[1] and Kobe and Smirl[2] maintains gauge invariance and energy conservation at all times.

Any set of basis functions may be used to calculate the wave function $\psi(t)$ of the particle interacting with the external classical electromagnetic field. An eigenstate $\psi_n(t)$ is the eigenstate of the energy operator $\mathscr{E}$ in Eq. (2.20). The probability amplitude for finding the system in an energy eigenstate $\psi_n(t)$ at time t is $c_n(t)=\langle\psi_n(t)\,|\,\psi(t)\rangle$. If χ_n is an eigenstate of an operator H_B which is not an observable, the amplitude $b_n(t)=\langle\chi_n(t)\,|\,\psi(t)\rangle$ has no significance becasue ψ cannot be projected into the function χ_n by any measurement.

ACKNOWLEDGMENTS

The North Texas State University Faculty Research Fund has given partial support to D. H. K. and E. C.-T. W. K.-H. Y. has received support from the NSF and from the University of Wisconsin—Madison Graduate School Research Committee. D. H. K. would like to thank Professor C. B. Collins for helpful discussions.

[1]K.-H. Yang, Ann Phys. (N.Y.) 101, 62 (1976).
[2]D. H. Kobe and A. L. Smirl, Am. J. Phys. 46, 624 (1978); D. H. Kobe, Int. J. Quant. Chem. S 12, 73 (1978).
[3]S. Olariu, I. Popescu, and C. B. Collins, Phys. Rev. D 20, 3095 (1979).

[4]H. A. Kramers, *Quantum Mechanics* (Dover, New York, 1964), p. 207.

[5]See, e.g., L. I. Schiff, *Quantum Mechanics,* 3rd edition (McGraw-Hill, New York, 1968), pp. 28–30, 179.

[6]J. D. Jackson, *Classical Electrodynamics,* 2nd edition (Wiley, New York, 1975), pp. 236–240.

[7]T. Goldman, Phys. Rev. D 15, 1063 (1977).

[8]D. H. Kobe and K.-H. Yang. J. Phys. A 13, 3171 (1980).

[9]The same ideas can be used to treat systems of many particles. See D. H. Kobe, Phys. Rev. A 19, 205 (1979); 19, 1876 (1979).

[10]One of the best discussions of gauge invariance in a textbook is C. Cohen-Tannoudji, B. Diu, and F. Laloë, *Quantum Mechanics* (Wiley, New York, 1977), Vol. I, pp. 315–328.

[11]Even in the theory of classical particles and fields there is a distinction between the Hamiltonian of the particles and their energy in a time-dependent external electromagnetic field. See D. H. Kobe, Am. J. Phys. 49, 581 (1981), and G. Wentzel, *Introduction to the Quantum Theory of Fields* (Interscience, New York, 1949), p. 69.

[12]V. Fock, Z. Phys. 39, 226 (1927).

[13]Reference 4, p. 269. The treatment here resolves the problem, noticed by Kramers, that the "energy" was apparently not gauge invariant.

[14]D. H. Kobe, Am. J. Phys. 46, 342 (1978); J. O. Hirschfelder and K.-H. Yang, Int. J. Quant. Chem. S 14, 695 (1978).

[15]K.-H. Yang, Phys. Lett. 64A, 276 (1977).