PHYSICAL REVIEW A VOLUME 42, NUMBER 7 1 OCTOBER 1990

Self-fields in semiclassical radiation theory

Michael D. Crisp
9113 Fairview Road, Silver Spring, Maryland 20910
(Received 16 January 1990)

The interaction of an atomic system with an unquantized electromagnetic field is studied by means of the Heisenberg-operator equations of motion. The electromagnetic fields created by the atom are taken into account by assuming that the charge and probability current densities are the actual charge and current source terms in Maxwell's equation. When Ehrenfest's theorem is written to order $(1/c)^2$, the equations of motion are found to have a constant of motion that can be interpreted as stating that the sum of the atomic energy, energy of interaction, and energy stored in the electromagnetic field is constant. This constant of integration can be expressed as an expectation of a new semiclassical Hamiltonian that now includes the effects of the atomic self-fields to order $1/c^2$. This Hamiltonian is related to the classical Darwin Lagrangian. Since the new approximate Hamiltonian is the sum of an atomic and a field Hamiltonian, it provides a formulation of semiclassical radiation theory that is formally close to the usual formulation of quantum electrodynamics. A Schrödinger equation can be derived by applying the variational principle to the expectation of the new Hamiltonian. The result is a nonlinear integro-differential equation, in Ψ, which is somewhat similar to Hartree's self-consistent equation for a multielectron atom. When the Heisenberg equations are written to include the next-higher-order terms, $1/c^3$, it is found that the total energy of the atom and the electromagnetic field in the vicinity of the atom decreases at a rate that is given by the Larmor power formula $(2e^2/3c^3)(d\langle \mathbf{v}\rangle/dt)^2$, where $\langle \mathbf{v}\rangle$ is the quantum-mechanical expectation of the electron's velocity operator. This approximate formulation of semiclassical radiation theory is applied to semiclassical calculations of atomic radiative shifts. It is then shown that, if some retardation effects are included to all orders of $1/c$ in the vector potential, the semiclassical analysis provides a formula for radiative energy-level shifts that are time dependent and that contain coefficients similar to the starting point of the Bethe calculation of the Lamb shift. The incorporation of mass renormalization in semiclassical theory is then discussed.

INTRODUCTION

In order to apply his equation to the interaction of electromagnetic radiation and matter, Schrödinger[1] first interpreted the absolute value squared of his wave function, $\Psi^*\Psi$, to be an actual charge density. This interpretation was based, in part, on his discovery of the quantum-mechanical continuity equation, which could then be reinterpreted as the classical continuity equation relating electrical current and charge. According to this "electrodynamic" hypothesis, the charge of an electron is not located at a point within an atom. Instead, it is spread out through a volume according to a charge density given by $e\Psi^*\Psi$. If the electron was not in a stationary state, then the Schrödinger charge cloud would oscillate and, in accordance with classical electrodynamics, radiate at frequencies equal to the difference in the electronic energy levels.

This electrodynamic interpretation of the wave function met with moderate success in explaining the interaction of bound states with an electromagnetic field. It provided direct methods for computing the frequency, relative intensities, and polarization of radiation emitted or scattered by an atom. Furthermore, it provided surprisingly accurate energy values when Hartree[2] applied it to the calculation of the energy levels of a multielectron atom. The use of Schrödinger's electrodynamic interpretation in the Hartree self-consistent method will be discussed in more detail below.

Schrödinger's interpretation of Ψ was found to be seriously flawed when used to explain the behavior of a free particle. The general spreading of a particle's wave packet made it too transient to be as stable as particles that are found in nature. Furthermore, the application of this interpretation of quantum mechanics to a scattering experiment suggested a splitting, or division, of particles which is not experimentally observed. Also, the details of electromagnetic radiation were not adequately explained by the electrodynamic hypothesis. For example, the electrodynamic hypothesis leads to the prediction that the relative intensity of two different spectral lines, which originate from the same initial state, could be altered by changing the relative populations in the two different final states. This was found to be inconsistent with experiment.[3]

A satisfactory explanation of spontaneous emission was not found by Schrödinger using his interpretation of Ψ. Later, Fermi[4] extended Schrödinger's formulation by including the effects of an atom's classical radiation reaction field back upon the atom. This assumption led to a form of spontaneous decay which had the time dependence of a truncated hyperbolic secant. This time dependence was different from the exponential decay found by Weisskopf and Wigner[5] using a quantum electrodynamic calculation. The exponential time dependence of the decay has been experimentally verified.[6]

Born's statistical interpretation of the wave function has proven capable of explaining the phenomena that Schrödinger's analysis does and, at the same time, it accounts for the free particle and scattering experiments and others which the electrodynamic hypothesis was unable to explain. Thus the Born probabilistic interpretation of Ψ has become a cornerstone of the generally accepted Copenhagen interpretation of quantum mechanics. In the case of large numbers of quantum particles occupying the same state, the Born and original Schrödinger interpretation give the same predictions. In other circumstances, the Born probabilistic interpretation provides the predictions that agree with experiment.

NEOCLASSICAL RADIATION THEORY

Quantum electrodynamics (QED) is not a perfectly consistent theory.[7] It is plagued by divergences, some of which are carried over from the classical theory of electromagnetic fields, and some of which are introduced by the procedure of quantizing the electromagnetic field. Quantizing a field that has an infinite number of degrees of freedom seems to lead unavoidably to an infinite amount of energy in the zero-point oscillations. Furthermore, the usual QED derivation of spontaneous decay, the Lamb shift, and the calculation of the anomalous moment of the electron seem to require these zero-point oscillations. Nevertheless, it is difficult to rationalize that these zero-point oscillations actually exist in nature.

In order to explore the prediction of a theoretical alternative to QED, Jaynes and his co-workers[8–11] have built upon the ideas of Schrödinger and Fermi and further developed what they have named the neoclassical theory (NCT). However, this program has not, to date, been able to point to any new crucial experimental tests of QED. Whenever the predictions of NCT and QED were different and could be practically tested, the QED predictions were found to be correct. Nevertheless, the Jaynes NCT is intuitively appealing and, where it does agree with the QED, it provides helpful physical insight concerning the process of interaction of radiation and matter.

NEOCLASSICAL HAMILTONIAN

The current analysis will begin with the conventional quantum-mechanical description of an electron of charge e, which is subject to a time-independent potential $U(\mathbf{r})$. The system will also be perturbed by an electromagnetic field which is characterized by a scalar potential $\phi(\mathbf{r},t)$ and a vector potential $\mathbf{A}(\mathbf{r},t)$. The electromagnetic field is envisioned to include both the self-fields of the electron acting back upon itself and the possibility of an external field. The Hamiltonian has the form

$$H=(\mathbf{p}-e\,\mathbf{A}/c)^2/2m+U(\mathbf{r})+e\phi\ . \tag{1}$$

The time evolution of the position operator $\mathbf{r}$ may be obtained from the Heisenberg equations of motion:

$$\frac{d\mathbf{r}}{dt}=\mathbf{v}=(\mathbf{p}-e\,\mathbf{A}/c)/m\ , \tag{2}$$

which will serve as a definition of the velocity operator, and

$$m\frac{d\mathbf{v}}{dt}=-e\left[\nabla\phi+\frac{\partial\mathbf{A}}{c\partial t}\right]+(e/2c)[\mathbf{v}\times(\nabla\times\mathbf{A})-(\nabla\times\mathbf{A})\times\mathbf{v}]-\nabla U\ . \tag{3}$$

Equations (2) and (3) constitute a generalized Ehrenfest's theorem for a charged particle in an electromagnetic field.

The sum of the two equations, obtained by applying the vector dot product with the Hermitian operator $\mathbf{v}$ once on the right and once on the left of Eq. (3), can be rewritten as

$$\frac{d[(m\mathbf{v}^2/2)+U]}{dt}=-(e/2)(\nabla\phi\cdot\mathbf{v}+\mathbf{v}\cdot\nabla\phi)-(e/2c)\left[\mathbf{v}\cdot\frac{\partial\mathbf{A}}{\partial t}+\frac{\partial\mathbf{A}}{\partial t}\cdot\mathbf{v}\right]\ . \tag{4}$$

The fact that $\mathbf{v}\cdot(\mathbf{v}\times\mathbf{H}-\mathbf{H}\times\mathbf{v})=(\mathbf{H}\times\mathbf{v}-\mathbf{v}\times\mathbf{H})\cdot\mathbf{v}\neq 0$, where $\mathbf{H}=\nabla\times\mathbf{A}$, and that $dU/dt=\mathbf{v}\cdot\nabla U+\nabla U\cdot\mathbf{v}$ when $\partial U/\partial t=0$, has been used in deriving Eq. (4).

The essential assumption of neoclassical theory is that the product of e times the quantum-mechanical probability density $\Psi^*\Psi$ acts as an actual electrical charge density $\rho(\mathbf{r},t)$ that can be used for analyzing the interaction with electromagnetic fields. In other words, it is assumed that real charge and current densities that can be written as

$$\rho(\mathbf{r},t)=e\Psi^*\Psi\ , \tag{5a}$$

and

$$\mathbf{J}(\mathbf{r},t)=(e/2)[\Psi^*(\mathbf{v}\Psi)+(\mathbf{v}\Psi)^*\Psi] \tag{5b}$$

can be used as the source terms in Maxwell's equations. It will follow, from this assumption, that the radiation field at a distance from an atom, that is large compared with the wavelength, is equivalent to that of a classical electric dipole whose value is given by the quantum-mechanical expectation value $\langle e\mathbf{r}\rangle$. But the basic assumptions of NCT are contained in Eq. (5), and the observation that electromagnetic fields are the same as if the expectation of the atom's dipole moment were an actual dipole moment is a consequence of this assumption.

In the Coulomb gauge, the fields which result from these charges can be expressed in terms of the retarded vector potential and the instantaneous Coulomb potential:

$$\mathbf{A}(\mathbf{r},t)=\frac{1}{c}\int\frac{\mathbf{J}_t(\mathbf{r}',t-R/c)}{R}d\mathbf{r}'+\mathbf{A}_0(\mathbf{r},t)\ , \tag{6a}$$

$$\phi(\mathbf{r},t)=\int\frac{\rho(\mathbf{r}',t)}{R}d\mathbf{r}'+\phi_0(\mathbf{r},t)\ , \tag{6b}$$

where $\mathbf{A}_0$ and ϕ_0 are solutions of the homogeneous wave equation, which correspond to any externally applied fields. The self-fields $\mathbf{A}_s$ and ϕ_s correspond to setting the externally applied fields to zero. $\mathbf{J}_t$ refers to the transverse component of the current density and $R=|\mathbf{R}|=|\mathbf{r}-\mathbf{r}'|$.

Expressions for the self-fields are only needed over the small region for which the atomic wave function is appreciably different from zero. This makes an expansion of the time-dependent current in powers of $1/c$ useful:

$$\mathbf{A}_s(\mathbf{r},t)=\frac{1}{c}\int\frac{\mathbf{J}_t(\mathbf{r}',t)}{R}d\mathbf{r}'-\frac{2}{3c^2}\frac{d}{dt}\int\mathbf{J}(\mathbf{r}',t)d\mathbf{r}'+\frac{1}{2c^3}\frac{d^2}{dt^2}\int R\,\mathbf{J}_t(\mathbf{r}',t)d\mathbf{r}'+\cdots\ , \tag{7}$$

where the identity

$$\int\mathbf{J}_t(\mathbf{r},t)d\mathbf{r}=\tfrac{2}{3}\int\mathbf{J}(\mathbf{r},t)d\mathbf{r}\ , \tag{8}$$

which is derived in Appendix A, has been used to obtain the second term of Eq. (7). It would be more precise to view the expansion of Eq. (7) as an expansion in (v/c), where v is a characteristic velocity of the charge elements that make up $\mathbf{J}$, or in terms of $(a\omega/c)$ where a is a characteristic dimension of the charge distribution and ω is characteristic of the frequencies contained in the Fourier transform of $\mathbf{J}$. However, such an approach would be cumbersome, and it is sufficient to just carefully keep track of powers of $1/c$ throughout this paper. In a relativistic analysis, $\mathbf{J}$ could have velocity components equal to the speed of light, c, and the expansion of Eq. (7) would have to be looked at more critically. The first term in the expansion of Eq. (7) is the Coulomb gauge vector potential, which gives the magnetic field that corresponds to the law of Biot-Savart.

Because Eq. (6) involves integrals over space, substitution of the expressions for charge and current density of Eqs. (5) leads naturally to expressions for the self-fields in terms of quantum-mechanical expectation values. When this is done the result obtained from Eqs. (7) and (6) is

$$\mathbf{A}_s(\mathbf{r},t)=\frac{e}{2\pi^2c}\int\frac{d\mathbf{k}}{k^2}e^{i\mathbf{k}\cdot\mathbf{r}}\langle e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}\rangle_\perp$$

$$-\frac{2e}{3c^2}\frac{d\langle\mathbf{v}\rangle}{dt}+\cdots\ , \tag{9a}$$

$$\phi_s(\mathbf{r},t)=\frac{e}{2\pi^2}\int\frac{d\mathbf{k}}{k^2}e^{i\mathbf{k}\cdot\mathbf{r}}\langle e^{-i\mathbf{k}\cdot\mathbf{r}}\rangle\ , \tag{9b}$$

where the Hermitian property of $\mathbf{v}$ ensures that

$$\int\mathbf{J}(\mathbf{r},t)d\mathbf{r}=(e/2)\int[\Psi^*(\mathbf{v}\Psi)+(\mathbf{v}\Psi)^*\Psi]d\mathbf{r}$$

$$=e\int\Psi^*(\mathbf{v}\Psi)d\mathbf{r}=e\langle\mathbf{v}\rangle\ . \tag{10}$$

Other quantum-mechanical expectation values are given by

$$\langle e^{i\mathbf{k}\cdot\mathbf{r}}\rangle=\int\Psi^*(e^{i\mathbf{k}\cdot\mathbf{r}}\Psi)d\mathbf{r}\ , \tag{11a}$$

$$\langle e^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}\rangle=\int\Psi^*(e^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}\Psi)d\mathbf{r}\ , \tag{11b}$$

$$\int\mathbf{J}_t(\mathbf{r},t)e^{i\mathbf{k}\cdot\mathbf{r}}d\mathbf{r}=e\langle e^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}\rangle_\perp$$

$$=-e\frac{\mathbf{k}}{k}\times\left[\frac{\mathbf{k}}{k}\times\int\Psi^*(e^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}\Psi)d\mathbf{r}\right]\ , \tag{11c}$$

and the identity

$$1/R=(1/2\pi^2)\int d\mathbf{k}e^{i\mathbf{k}\cdot\mathbf{R}}/k^2 \tag{12}$$

has been used. Equation (11c) was derived with the aid of results of Appendix A.

The expression for the Hamiltonian of Eq. (1) can be rewritten in terms of the Hermitian velocity operator $\mathbf{v}$ of Eq. (2).

$$H=H_0+H_I=m\mathbf{v}^2/2+U+e\phi\ , \tag{13}$$

where the Hamiltonian in the absence of all fields is

$$H_0=\mathbf{p}^2/2m+U\ , \tag{14a}$$

and the interaction Hamiltonian is

$$H_I=e\phi-(e/2c)(\mathbf{A}\cdot\mathbf{v}+\mathbf{v}\cdot\mathbf{A})-(e^2/2mc^2)\mathbf{A}^2 \tag{14b}$$

or

$$H_I=e\phi-(e/c)(\mathbf{A}\cdot\mathbf{v})-(e^2/2mc^2)\mathbf{A}^2 \tag{14c}$$

for the Coulomb gauge.

When the expressions for the self-fields given in Eq. (9) are substituted into operator equations of motion, such as the Heisenberg equations of Eqs. (3) and (4), one gets an expression that is a mixture of quantum-mechanical operators and expectation values. An expression that just involves quantum-mechanical expectation values can be obtained by taking the expectation of this mixed equation. For example, taking the expectation value of Eq. (4) when there are no external fields, one gets

$$\frac{d}{dt}\langle m\mathbf{v}^2/2+U\rangle=-(e/2)\langle\nabla\phi_s\cdot\mathbf{v}+\mathbf{v}\cdot\nabla\phi_s\rangle$$

$$-(e/2c)\left\langle\mathbf{v}\cdot\frac{\partial\mathbf{A}_s}{\partial t}+\frac{\partial\mathbf{A}_s}{\partial t}\cdot\mathbf{v}\right\rangle\ . \tag{15}$$

The use of expressions of Eq. (9) reveals that

$$-(e/2)\langle \nabla\phi_s\cdot\mathbf{v}+\mathbf{v}\cdot\nabla\phi_s\rangle = -e\frac{d\langle\phi_s\rangle}{dt}+e\left\langle\frac{\partial\phi_s}{\partial t}\right\rangle = -(e/2)\frac{d\langle\phi_s\rangle}{dt}$$
$$= -\frac{e^2}{4\pi^2}\frac{d}{dt}\int\frac{d\mathbf{k}}{k^2}\langle e^{i\mathbf{k}\cdot\mathbf{r}}\rangle\langle e^{-i\mathbf{k}\cdot\mathbf{r}}\rangle\ , \tag{16a}$$

where the identity $d\langle\phi_s\rangle/dt=2\langle\partial\phi_s/\partial t\rangle$, which is derived from Eq. (9b) in Appendix B, has been used to obtain Eq. (16a). Similarly, the quantum-mechanical expectation values are given by

$$-(e/2c)\left\langle\mathbf{v}\cdot\frac{\partial\mathbf{A}_s}{\partial t}+\frac{\partial\mathbf{A}_s}{\partial t}\cdot\mathbf{v}\right\rangle = -\frac{e^2}{4\pi^2c^2}\frac{d}{dt}\int\frac{d\mathbf{k}}{k^2}\langle e^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}\rangle_\perp\cdot\langle e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}\rangle_\perp+\frac{2e^2}{3c^3}\langle\mathbf{v}\rangle\cdot\frac{d^2\langle\mathbf{v}\rangle}{dt^2}+\cdots\ , \tag{16b}$$

$$-(e/c)\langle\mathbf{A}_s\cdot\mathbf{v}\rangle = -\frac{e^2}{2\pi^2c^2}\int\frac{d\mathbf{k}}{k^2}\langle e^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}\rangle_\perp\cdot\langle e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}\rangle_\perp+\frac{2e^2}{3c^3}\langle\mathbf{v}\rangle\cdot\frac{d\langle\mathbf{v}\rangle}{dt}+\cdots\ . \tag{16c}$$

The last term in Eq. (16c) is proportional to $d\langle\mathbf{v}\rangle^2/dt$. Such a term appears in many classical derivations of radiation reaction. In these classical derivations it is neglected because its average contribution can be exactly zero for a periodic system or go to zero when averaged over an increasingly longer time period for a bound system.

The expression of Eqs. (16), which are given in terms of quantum-mechanical expectation values, can be rewritten in terms of the current and charge densities of Eq. (5) as follows:

$$\frac{1}{4\pi^2c^2}\int\frac{d\mathbf{k}}{k^2}\langle e^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}\rangle_\perp\cdot\langle e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}\rangle_\perp = \frac{1}{2c^2}\int\int\frac{\mathbf{J}_t(\mathbf{r},t)\cdot\mathbf{J}_t(\mathbf{r}',t)}{R}d\mathbf{r}\,d\mathbf{r}'$$
$$= \frac{1}{4c^2}\int\int\left[\frac{\mathbf{J}(\mathbf{r},t)\cdot\mathbf{J}(\mathbf{r}',t)}{R}+\frac{[\mathbf{J}(\mathbf{r},t)\cdot\mathbf{R}][\mathbf{J}(\mathbf{r}',t)\cdot\mathbf{R}]}{R^3}\right]d\mathbf{r}\,d\mathbf{r}'\ , \tag{17a}$$

$$\frac{1}{4\pi^2}\int\frac{d\mathbf{k}}{k^2}\langle e^{i\mathbf{k}\cdot\mathbf{r}}\rangle\langle e^{-i\mathbf{k}\cdot\mathbf{r}}\rangle = \tfrac{1}{2}\int\int\frac{\rho(\mathbf{r},t)\rho(\mathbf{r}',t)}{R}d\mathbf{r}\,d\mathbf{r}'\ . \tag{17b}$$

LARMOR FORMULA

From classical electrodynamics, the energy contained in an electromagnetic field is

$$H_F=(1/8\pi)\int(\mathbf{E}^2+\mathbf{H}^2)d\mathbf{r}\ . \tag{18}$$

If only the self-fields are present, this may be evaluated approximately by substituting in from the fields that are calculated from the potentials of Eq. (6):

$$H_F\approx\tfrac{1}{2}\int\int\frac{\rho(\mathbf{r},t)\rho(\mathbf{r}',t)}{R}d\mathbf{r}\,d\mathbf{r}'+\frac{1}{2c^2}\int\int\frac{\mathbf{J}_t(\mathbf{r},t)\cdot\mathbf{J}_t(\mathbf{r}',t)}{R}d\mathbf{r}\,d\mathbf{r}'\ . \tag{19}$$

In the absence of externally applied fields, Eq. (19) is equal to Eq. (18) when terms of order of $1/c^4$ and higher are neglected.

In Appendix B, it is shown that Eqs. (15), (16), and (19) can be combined to give an expression for the time rate of change of the expectation of the Hamiltonian defined in Eq. (1):

$$\frac{d\langle H\rangle}{dt}=\frac{d\langle H_0+H_I\rangle}{dt}=-\frac{dH_F}{dt}-\frac{2e^2}{3c^3}\left[\frac{d\langle\mathbf{v}\rangle}{dt}\right]^2, \tag{20a}$$

which can be rewritten as

$$\frac{d(\langle H_0\rangle+\langle H_I\rangle+H_F)}{dt}=-\frac{2e^2}{3c^3}\left[\frac{d\langle\mathbf{v}\rangle}{dt}\right]^2. \tag{20b}$$

The term on the right-hand side of Eq. (20b) is recognized as the Larmor formula,[12] which describes the power radiated by an electrical charge subject to an acceleration $d\langle\mathbf{v}\rangle/dt$. Equation (20b) is an expression of conservation of energy during the emission of radiation by the atomic system. Equation (20b) is a generalization of Ehrenfest's theorem to include self-fields so that it can be applied to the radiation of energy away from an atomic system. If the $1/c^3$ terms are neglected, it can be thought of as a generalization of Eq. (72b) of Jaynes and Cummings.[8] Equation (20) covers a general atomic system instead of the two-level system of Ref. 8; it does not rely on the dipole approximation and includes a multitude of electromagnetic modes instead of a single mode. The left-hand side consists of the sum of $\langle H_0\rangle$, which is the expectation value of the unperturbed atomic Hamiltonian (without self-fields), the expectation of the interaction Hamiltonian of the atomic system with the self-fields $\langle H_I\rangle$, which is obtained from Eq. (14b), and the energy contained in the electromagnetic self-field surrounding the atom, H_F [which is given to an approximation that includes terms of order $1/c^3$ by Eq. (19)]. The right-hand side of Eq. (20b) is equal to the classical Larmor formula for the emission of radiation from an accelerated charge, provided that the acceleration is equal to the expectation of the velocity operator $\langle \mathbf{v} \rangle$.

If one is content with an accuracy that neglects terms of order $1/c^3$, Eq. (20b) provides a constant of motion that is equal to the sum of the expectation values of the energy of the atomic system, the energy of interaction with the self-field, and the energy stored in the self-field. This suggests that the right-hand side of Eq. (20b) could be considered to be the expectation value of a Hamiltonian, for the combined atomic system and electromagnetic field, which is accurate as long as terms of order $1/c^3$ can be neglected. The $1/c^3$ terms, of course, give the effects of the atom irreversibly radiating into the electromagnetic field.

Writing out the constant given by the left-hand side of Eq. (20b) as a quantum-mechanical expectation, one has, to an accuracy of $1/c^2$, that

$$\begin{aligned}\langle H_{\text{tot}} \rangle = \langle H_0 \rangle + \langle H_I \rangle + H_F = \int \Psi^* \left[\frac{\mathbf{p}^2}{2m} + U \right] \Psi \, d\mathbf{r} + (e^2/2) \int \int [\Psi^*(\mathbf{r}')\Psi^*(\mathbf{r})(1/R)\Psi(\mathbf{r}')\Psi(\mathbf{r})] d\mathbf{r}' \, d\mathbf{r} \\ -(e^2/4c^2) \int \int \{ [\Psi^*(\mathbf{r}')\mathbf{v}'\Psi(\mathbf{r}')] \cdot [\Psi^*(\mathbf{r})\mathbf{v}\Psi(\mathbf{r})]/R \\ +[\Psi^*(\mathbf{r}')\mathbf{v}'\Psi(\mathbf{r}')] \cdot \mathbf{R} [\Psi^*(\mathbf{r})\mathbf{v}\Psi(\mathbf{r})] \cdot \mathbf{R}/R^3 \} d\mathbf{r}' \, d\mathbf{r} \ .\end{aligned} \tag{21}$$

Note that the expectation of the above Hamiltonian is expressed completely in terms of the particle variables without the aid of the radiation variables. Since the electromagnetic field is not contained in the Hamiltonian describing the system, the same predictions will be made from it, whether the electromagnetic field is quantized or not. In other words, to order $1/c^2$, quantization does not matter, and there are no zero-point oscillations.

An expression formally similar to Eq. (21) is obtained in second quantized theories of matter-field interactions. However, the analysis contained here remains a one-particle, nonrelativistic, first quantized analysis. The wave functions that are contained in Eq. (21) are not to be interpreted as noncommuting operators.

The expectation expressed by Eq. (21) can be written in an alternate form using the Fourier transform of $1/R$ which is given in Eq. (12):

$$\begin{aligned}\langle H_{\text{tot}} \rangle = \langle H_0 \rangle + (e^2/4\pi^2) \\ \times \int \left[\frac{d\mathbf{k}}{k^2} \right] \left[\langle e^{i\mathbf{k}\cdot\mathbf{r}} \rangle \langle e^{-i\mathbf{k}\cdot\mathbf{r}} \rangle \right. \\ \left. - \frac{\langle e^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{v} \rangle_\perp \cdot \langle e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{v} \rangle_\perp}{c^2} \right] .\end{aligned} \tag{22}$$

QED IN THE COULOMB GAUGE

In 1932, Fermi[13] proposed a formulation of quantum electrodynamics (QED) which was based upon a Hamiltonian from which the longitudinal components of the electromagnetic field had been eliminated. In Fermi's formulation, the effects of the longitudinal electric field are contained in the instantaneous Coulomb potential of Eq. (6b). The scalar potential is given exactly by the expression of Eq. (6b) in the Coulomb gauge. The scalar potential ϕ in Eq. (1) is then replaced by an expression involving only the distribution of charge at some time t. Thus use of the Coulomb gauge in QED allows elimination of the degrees of freedom accompanying the longitudinal electric field at the expense of Lorentz invariance. The remaining dynamical variables associated with the degrees of freedom of the transverse electromagnetic field must then be quantized.

Use of the approximation Hamiltonian, whose expectation is given by Eq. (21), goes one step beyond the Fermi formulation of QED. Not only have the degrees of freedom associated with the longitudinal field been eliminated, but the use of the first term of Eq. (7) for the vector potential provides an approximation (good to order $1/c^2$) for the effects of self-fields on the atom. This approximately eliminates the degrees of freedom associated with the transverse field. The complete elimination of the electromagnetic fields from the Hamiltonian allows treatment of the entire system, consisting of atom plus electromagnetic interactions, in a thoroughly quantum-mechanical fashion without the need to separately quantize the Maxwell field. Quantizing the electromagnetic field, with its infinite number of degrees of freedom, is a procedure that results in a awkwardly divergent zero-point energy when followed in QED. Of course the Fermi formulation of QED is exact, while the approximate Hamiltonian of Eq. (21) has limited application, because it neglects terms of order $1/c^3$ and higher. While within its range of validity, the approximate Hamiltonian of Eq. (21) allows a complete determination of the state of the system in terms of the instantaneous charge and current distributions without reference to the electromagnetic fields; it does result in a nonlinear, integrodifferential equation that is difficult to solve.

There is no known exact many-body Hamiltonian describing the interaction of charged particles. Breit[14] and others have developed an approximate Hamiltonian, which is related to the one in Eq. (21), and applied it to obtain fairly accurate calculations of the energy levels of the helium atom. However, the Breit interaction term is intended to account, approximately, for the effect of the electric and magnetic fields of one electron on the other electron, while present application is directed toward understanding the interaction of an electron with itself.

Because all of the electromagnetic fields have been eliminated in the approximate Hamiltonian of Eq. (21), it is a useful common ground for comparing QED and NCT calculations. Since the electromagnetic field has been eliminated, it is irrelevant whether it is quantized or not. Only the assumptions of Eq. (5) remain to distinguish such a semiclassical calculation from QED.

CLASSICAL DARWIN HAMILTONIAN

When the finite speed of propagation of the electromagnetic field is taken into account, an exact classical Lagrangian cannot be written down for two or more interacting charged particles. The interaction of charged particles, with velocities v small compared with the speed of light, can be approximately described by a Lagrangian. Such an approximate Lagrangian was first derived by Darwin[15] by neglecting retardation effects associated with terms of order $(v/c)^3$ or smaller. As was done in deriving Eq. (21), the Darwin Lagrangian essentially neglects the radiation modes and describes the interaction between moving charged particles in terms of an approximate instantaneous action-at-a-distance term which depends on velocity. Later, Breit applied an interaction of this form to quantum-mechanical calculations. Although Darwin's work was originally applied to a collection of individual particles, it can be readily generalized to a classical expression for the Hamiltonian of a continuous charge distribution which is spread out in space. The resulting classical Hamiltonian may be written:

$$H_{\text{Darwin}}=\frac{1}{4c^2}\int\int\left\{\frac{\mathbf{J}(\mathbf{r},t)\cdot\mathbf{J}(\mathbf{r}',t)}{R}+\frac{[\mathbf{J}(\mathbf{r},t)\cdot\mathbf{R}][\mathbf{J}(\mathbf{r}',t)\cdot\mathbf{R}]}{R^3}\right]d\mathbf{r}\,d\mathbf{r}'+\tfrac{1}{2}\int\int\frac{\rho(\mathbf{r},t)\rho(\mathbf{r}',t)}{R}d\mathbf{r}\,d\mathbf{r}'+H_0\ . \tag{23}$$

The classical current that would be used in Eq. (23) is given by $\mathbf{J}=\rho\mathbf{v}$. To be consistent, the classical particle Hamiltonian H_0 would have to be relativistically accurate to the same order of $1/c^2$ as the Darwin interaction terms. Thus an expression of the form

$$H_0=\mathbf{p}^2/2m-\mathbf{p}^4/8m^3c^2+U(\mathbf{r}) \tag{24}$$

should replace Eq. (14a). This would lead to a correction for Eq. (2). It will be assumed that the unperturbed eigenfunctions ψ_α and eigenenergies E_α are correct to an order consistent with the other approximations used in this paper.

VARIATIONAL METHOD

There is a close connection between quantum theory and the variational principle. Schrödinger first obtained his wave equation from an application of the variational method to the Hamilton-Jacobi equation. It has been shown that the Schrödinger equation is mathematically equivalent to the Euler's equation, obtained by applying the variational principle to minimize the expectation of the Hamiltonian.

Ordinarily, one would think that most of the quantum-mechanical information had been lost when the expectations values were taken. However, a wave equation can be derived from the condition that the expectation of the Hamiltonian of Eq. (21) should be minimum under arbitrary independent variations in the wave function Ψ and its complex conjugate Ψ^*.

The wave equation can be derived as an Euler-Lagrange equation resulting from the condition that

$$\delta\langle H_{\text{tot}}\rangle=0\ , \tag{25a}$$

subject to the constraint that the wave function remains normalized. The resulting equation is

$$\left\{H_0+e^2\int\left[\Psi^*(\mathbf{r}')\left[\frac{1}{R}\right]\Psi(\mathbf{r}')\right]d\mathbf{r}'-(1/2c^2)\int\left[\left[\frac{1}{R}\right][\Psi^*(\mathbf{r}')\mathbf{v}'\Psi(\mathbf{r}')]+(\mathbf{R}/R^3)\cdot[\Psi^*(\mathbf{r}')\mathbf{v}'\Psi(\mathbf{r}')]\mathbf{R}\right]d\mathbf{r}'\cdot\mathbf{v}\right\}\Psi(\mathbf{r})=E\Psi(\mathbf{r})\ . \tag{25b}$$

Alternately, this wave equation may be rewritten:

$$H\Psi=E\Psi\ , \tag{26a}$$

where the Hamiltonian is given by

$$H=H_0+e\int\frac{\rho}{R}d\mathbf{r}'-\frac{e}{c^2}\left[\int\left[\frac{\mathbf{J}_t}{R}\right]d\mathbf{r}'\right]\cdot\mathbf{v}\ , \tag{26b}$$

or, using the Fourier expression of Eq. (12) again,

$$H=H_0+\frac{e}{2\pi^2}\int\frac{d\mathbf{k}}{k^2}\left[e^{i\mathbf{k}\cdot\mathbf{r}}\left\{\langle e^{-i\mathbf{k}\cdot\mathbf{r}}\rangle-\frac{\langle e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}\rangle_\perp\cdot\mathbf{v}}{c^2}\right]\right]\ . \tag{26c}$$

Although Eq. (26a) looks formally like an eigenvalue equation, it is not because the Hamiltonian operator H depends on Ψ.

The expectation of the Hamiltonian in Eq. (26) will not give the same value as the expectation of Eqs. (21) or (22), because the expectation of the Hamiltonian of Eq. (26) would count the energy of interaction between different parts of the charge distribution twice. A similar situation arose in the application of the self-consistent method, where direct calculation of the expectation from the Hartree Hamiltonian would count the electrostatic energy of interaction between pairs of electrons twice. As in the case of the self-consistent method, the correct and unambiguous procedure is to solve Eq. (26a) for the wave function and then substitute the result into Eqs. (21) or (22) to compute the expectation of the energy.

HARTREE SELF-CONSISTENT METHOD

Equation (25b) is reminiscent of the equation which Hartree[2] first wrote down, based only on intuitive arguments, to calculate the energy levels of multielectron atoms. In addition to Hartree's average electrostatic repulsion term, which is equal to the quantum-mechanical expectation $e\langle 1/R\rangle$, a new term has appeared in Eq. (24) which corresponds to the expectation of $(e/c)\langle \mathbf{A}\cdot\mathbf{v}\rangle$.

Hartree originally assumed that each electron in a multielectron atom is described by its own independent wave function. This wave function is determined by the effect of an equivalent potential, which takes into account the combined effects of the nucleus and the "average" effects of all the other atomic electrons. The average effect of all the other electrons was calculated by using Schrödinger's electrodynamic hypothesis. In other words, Hartree assumed that all the other electrons' charges were smeared out over the volume of the atom according to their probability densities $\Psi^*\Psi$.

Hartree went on to point out that this electron cloud picture provided an intuitive understanding of the first-order perturbation-theory calculation of the energy levels of multielectron atoms. It follows from first-order perturbation theory that a perturbed energy equals the exact Hamiltonian average over the unperturbed state. When independent electron wave functions are used as the unperturbed states, first-order perturbation yields a perturbed energy which is the same as would be obtained for electrostatic energy of interaction of smeared out electrons acting as classical charge distributions. The perturbation of the electrostatic repulsion of the two electrons within a helium atom is by no means small compared with the attraction of the nucleus. It is thus somewhat surprising that first-order perturbation theory gives the correct ground-state energy to about 5% for light atoms. Of course, perturbation theory can be derived from a variational principle; so this observation is not logically independent from ones about the self-consistent method.

In spite of the initial successes of the application of the Hartree method, it was considered to ". . . stand rather apart from the main current of quantum theory . . ."[16] until it was shown by Slater,[16] and independently by Fock,[17] that the Hartree method is mathematically equivalent to the variational principle, applied to minimize the expectation of the atomic Hamiltonian, when the trial function is taken to be a simple product of single-particle wave functions. The variational principle ensures the highest accuracy of results consistent with the other assumptions that are implicit in the choice of the trial wave function. Single-particle wave functions are not the most general choice for describing a multielectron atom; thus the Hartree method remains only an approximation.

In order to get agreement with experiment, Hartree took care not to allow each electron to act electrostatically on itself. Hartree obtained satisfactory results only if the interaction of each electron with its own self-field was subtracted from the total energy. Equation (25b) is meant to represent a one-electron atom; so the self-energy effects, which were eliminated when using the Hartree self-consistent method, are the important effects in Eq. (25b).

Application of the Hartree method to the helium atom provides surprisingly good results when one considers that it is tantamount to assuming that the effects of electrostatic repulsion of the second electron are equivalent to those obtained if that single electron's charge distribution were smeared out over the volume of the atom. Once again, the Schrödinger electrodynamic interpretation provides a useful and intuitively appealing method for computing the bound-state energy levels that are perturbed by electromagnetic fields. Although the variational principle provides a mathematical justification for the validity of this assumption, the intuitive picture appears to fly in the face of the Born probabilistic interpretation of Ψ.

RADIATIVE LEVEL SHIFTS

The neglect of $1/c^3$ terms in the derivation of Eq. (25b) has the consequence that its solution will include some of the level shifts which are due to the coupling of an atomic system to an electromagnetic field, but none of the effects connected with loss of energy to the radiation field. A description of the transfer of energy, from the atomic system and its neighboring electromagnetic field to the electromagnetic far field, requires retention of terms of order $1/c^3$, such as the one on the right-hand side of Eq. (20b). The semiclassical effects introduced when terms of order $1/c^3$ and higher are kept include the nonexponential spontaneous decay of NCT, which does not agree with experiment. An approximate calculation of level shifts that are present when terms of order $1/c^2$ are kept will follow.

In the Schrödinger picture, one can express the atomic state Ψ in terms of a complete set of unperturbed eigenfunctions ψ_α as

$$\Psi=\sum_{\alpha} a_\alpha \psi_\alpha \;, \tag{27a}$$

where

$$H_0\psi_\alpha=E_\alpha\psi_\alpha \;, \tag{27b}$$

and the atomic transition frequency between the level α and β, $\Omega_{\alpha\beta}$, is given by

$$\hbar\Omega_{\alpha\beta}=E_\alpha-E_\beta \;. \tag{27c}$$

The coefficients a_α are time dependent, corresponding to the Schrödinger picture. Then the terms in the Hamiltonian of Eq. (26) can be written:

$$\langle e^{-i\mathbf{k}\cdot\mathbf{r}}\rangle=\sum_{\alpha,\beta} a_\alpha a_\beta^* (\beta|e^{-i\mathbf{k}\cdot\mathbf{r}}|\alpha) \;, \tag{28a}$$

$$\langle e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}\rangle_\perp=\sum_{\alpha,\beta} a_\alpha a_\beta^* (\beta|e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}|\alpha)_\perp \;. \tag{28b}$$

This allows expression of the total Hamiltonian as

$$H=H_0+(e^2/2\pi^2)\sum_{\alpha,\beta} a_\alpha a_\beta^* \times\int \frac{d\mathbf{k}}{k^2} e^{i\mathbf{k}\cdot\mathbf{r}} \left[(\beta|e^{-i\mathbf{k}\cdot\mathbf{r}}|\alpha) - \frac{(\beta|e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}|\alpha)_\perp\cdot\mathbf{v}}{c^2} \right] . \tag{28c}$$

The matrix elements of this Hamiltonian are

$$H_{rs}=(r|H|s)\equiv\int\psi_r^* H\psi_s d\mathbf{r}$$

$$=E_r\delta_{rs}+V_{rs}\ ,\tag{29a}$$

introducing the definitions

$$V_{rs}\equiv\sum a_\alpha(t)a_\beta(t)^*\hbar K_{rs}^{\alpha\beta}\ ,\tag{29b}$$

and

$$K_{rs}^{\alpha\beta}\equiv W_{rs}^{\alpha\beta}-\Gamma_{rs}^{\alpha\beta}\ ,\tag{29c}$$

where $\Gamma_{rs}^{\alpha\beta}$ was first introduced in Eq. (A4) of Ref. 9 as

$$\hbar\Gamma_{rs}^{\alpha\beta}\equiv(e^2/2\pi^2m^2c^2)\int\frac{d\mathbf{k}}{k^2}(\beta|e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{p}|\alpha)_\perp\cdot(r|e^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{p}|s)_\perp\ ,\tag{29d}$$

and $W_{lm}^{\alpha\beta}$ corresponds to a contribution from the electrostatic self-energy that was subtracted from the Hamiltonian, in an attempt to include mass renormalization in that semiclassical calculation, at the beginning of Ref. 9.

$$\hbar W_{rs}^{\alpha\beta}\equiv+\frac{e^2}{2\pi^2}\int\frac{d\mathbf{k}}{k^2}(\beta|e^{-i\mathbf{k}\cdot\mathbf{r}}|\alpha)(r|e^{i\mathbf{k}\cdot\mathbf{r}}|s)\ .\tag{29e}$$

The justification for the "renormalization" which is accomplished by subtracting the electrostatic term of Eq. (29e) in Ref. 9 was that it was associated with the electron's electromagnetic mass and therefore already included in the electron mass m. This argument is weak because, if the electron goes from a well-localized particle to a charge cloud spread throughout the atom's volume, the electromagnetic mass changes drastically. Thus the concept of a charged particle's electromagnetic mass is difficult to reconcile with the Schrödinger electrodynamic interpretation of $\Psi^*\Psi$. A consistent treatment of the electrostatic self-energy of a charged particle has thus far eluded NCT.

Replacing the operator $\mathbf{v}$ by the operator $\mathbf{p}$ in Eq. (29d) introduces, according to Eqs. (2) and (7), an error of neglecting terms of order $1/c^4$ and higher, which is consistent with previous approximations.

The Schrödinger equation that results from the use of the Hamiltonian of Eq. (29a) may be written:

$$i\hbar\frac{da_l}{dt}=E_la_l+\hbar\sum_{j\alpha\beta}[K_{lj}^{\alpha\beta}(a_\alpha a_\beta^*)]a_j\ ,\tag{30a}$$

which can be transformed to the interaction picture by

$$a_k(t)=c_k(t)\exp[-i(E_kt/\hbar)]\ ,\tag{30b}$$

$$i\frac{dc_l}{dt}=\sum_{j\alpha\beta}[K_{lj}^{\alpha\beta}(c_\alpha c_\beta^*)]c_j$$

$$\times\exp[-i(E_\beta-E_\alpha+E_l-E_j)t/\hbar]\ .\tag{30c}$$

The right-hand side of Eq. (30c) will oscillate rapidly unless the condition

$$E_\beta-E_\alpha+E_l-E_j=0\ .\tag{30d}$$

If there is no degeneracy, this is satisfied only if $\beta=j$ and $\alpha=l$, or $\alpha=\beta$ and $l=j$. Including both possibilities, Eq. (30c) reduces to

$$i\frac{dc_l}{dt}=\sum_j(K_{lj}^{lj}+K_{ll}^{jj})(c_jc_j^*)c_l\ .\tag{31a}$$

Since the K's on the right-hand side of Eq. (30a) are real, it follows that

$$\frac{d(c_jc_j^*)}{dt}=\frac{d(a_ja_j^*)}{dt}=0\ ,\tag{31b}$$

and all the $c_jc_j^*=a_ja_j^*$ are constant in time. Substituting the constant $c_jc_j^*$ into Eq. (31a) and using Eq. (30b) to transform back into the Schrödinger picture, Eq. (30a) becomes

$$i\hbar\frac{da_l}{dt}=\left[E_l+\hbar\sum_j(K_{lj}^{lj}+K_{ll}^{jj})a_j(0)a_j(0)^*\right]a_l(t)\ ,\tag{32a}$$

from which the energy-level shifts can be identified as

$$\Delta E_l=\hbar\sum_j(K_{lj}^{lj}+K_{ll}^{jj})a_j(0)a_j(0)^*\ .\tag{32b}$$

If the same semiclassical mass-renormalization argument used in Ref. 9 is applied to eliminate the electrostatic terms $W_{rs}^{\alpha\beta}$ from $K_{rs}^{\alpha\beta}$ in Eq. (32b), then the resulting energy shift is

$$\Delta E_l=-\sum_j\hbar\Gamma_{lj}^{lj}a_j(0)a_j(0)^*\ .\tag{32c}$$

In addition to subtracting the term corresponding to the electrostatic self-energy of the electron, matrix elements of the form $(l|e^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}|l)_\perp$, which would be exactly equal to zero if the electric dipole approximation was made, are neglected because they are small compared with $(l|e^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}|j)_\perp$ when $l\neq j$. The difference in energy shifts, or transition frequency, between the lth and mth level is then

$$\Delta E_l-\Delta E_m=\hbar\delta\Omega_{lm}$$

$$=-\sum_j\hbar(\Gamma_{lj}^{lj}-\Gamma_{jm}^{jm})a_j(0)a_j(0)^*\ ,\tag{32d}$$

which is in agreement with Eq. (18) of Ref. 9. If $a_m(0)a_m(0)^*=1$, Eq. (32d) reduces to $\delta\Omega_{lm}=-\Gamma_{lm}^{lm}$, because Γ_{mm}^{mm} is negligible. Reference 9 does not neglect the terms of order $1/c^3$, and as a result a nonexponential spontaneous decay is introduced. This causes the coefficients $a_j(t)a_j^*(t)$ to vary in time resulting in the time-dependent frequency shift which is characteristic of the neoclassical theory.

HIGHER-ORDER TERMS

In the nonrelativistic limit, each successive term in the expansion of Eq. (7) is less than the preceding term by less than a factor[9] of $\omega a/c\approx\alpha=e^2/\hbar c$, where ω is the maximum frequency contained in the atomic current $\mathbf{J}$, and α is the fine-structure constant. The Dirac theory of the electron implies that $\mathbf{J}=ec\Psi^*\boldsymbol{\alpha}\Psi$ can contain velocity components equal to the speed of light c, if both positive and negative energy states are present. Thus an expansion of the form shown in Eq. (7) might not be valid in a relativistic theory.

Retardation effects will now be taken into account to a higher degree of accuracy by performing the expansion of Eq. (7) in the interaction picture. This will replace the expansion in terms of powers of $\omega a/c$ by an expansion in terms of $a/c\tau$, where τ is the characteristic time in which the density-matrix elements $c_l c_m^*$, in the interaction picture, change. Thus $1/\tau$ will be the order of the radiative level shift ($\sim\alpha^4 mc^2/\hbar$) or the spontaneous lifetime of the atomic state ($\sim\alpha^5 mc^2/\hbar$). It will be seen that an expansion more accurate than that of Eq. (7) leads to the appearance of radiative level shifts that contain coefficients similar to the Bethe logarithm expression for the Lamb shift.[18] In addition the improved approximation will be useful for comparison of the results of this paper with those of others.

Ackerhalt and his collaborators[19] have formulated QED in terms of the Heisenberg equations of motion. They obviated the need for quantization of the electromagnetic field by eliminating these fields from their equations. In this way, Ackerhalt *et al.* studied radiative level shifts and spontaneous decay in the absence of a quantized field and its accompanying zero-point oscillations. A discussion of this work is contained in the book by Allen and Eberly.[20]

Barut and his collaborators,[21,22] have also formulated QED in terms of the self-fields of charge and current density sources. They use the standard electromagnetic Green's functions to remove the need for quantization of the electromagnetic field. They solve the resulting nonlinear integro-differential equations by an iteration procedure, in a manner reminiscent of Hartree's solution of his self-consistent equations. In so doing, Barut avoided perturbation techniques which have been identified as a source of trouble in QED. Barut's work uses a current $j_\mu = e\Psi^*\gamma_\mu\Psi$, which would reduce to the NCT source terms of Eq. (5) in the nonrelativistic limit provided that second quantization is not applied to the Dirac field, Ψ. The Coulomb gauge and an expansion of the self-fields such as the one used in Eq. (7) are not Lorentz invariant, but one would expect the Barut analysis to parallel the work presented here in the nonrelativistic limit.

In the Coulomb gauge, the vector potential is related to the transverse component of the charge current through the wave equation:

$$\nabla^2 \mathbf{A} - (1/c^2)\frac{\partial^2 \mathbf{A}}{\partial t^2} = -4\pi \mathbf{J}_t/c\ . \tag{33}$$

The vector potential and the charge current can be written in terms of Fourier transforms:

$$\mathbf{A}(\mathbf{r},t) = (1/2\pi)^4 \int d\mathbf{k} \int d\omega\, \mathbf{A}(\mathbf{k},\omega) \exp[i(\mathbf{k}\cdot\mathbf{r} - \omega t)]\ , \tag{34a}$$

and

$$\mathbf{J}(\mathbf{r},t) = (1/2\pi)^4 \int d\mathbf{k} \int d\omega \mathbf{J}(\mathbf{k},\omega) \exp[i(\mathbf{k}\cdot\mathbf{r} - \omega t)]\ , \tag{34b}$$

where the inverse transform is such that

$$\begin{aligned}\mathbf{J}_\perp(\mathbf{k},\omega) &= \int d\mathbf{r} \int dt \mathbf{J}_t(\mathbf{r},t) \exp[-i(\mathbf{k}\cdot\mathbf{r} - \omega t)] \\ &= -(\mathbf{k}/k) \times \left[\left[\frac{\mathbf{k}}{k} \right] \times \int d\mathbf{r} \int dt \mathbf{J}(\mathbf{r},t) \exp[-i(\mathbf{k}\cdot\mathbf{r} - \omega t)] \right] \\ &= -(\mathbf{k}/k) \times [(\mathbf{k}/k) \times \mathbf{J}(\mathbf{k},\omega)]\ .\end{aligned} \tag{34c}$$

Substituting from Eq. (34) into Eq. (33), one has

$$\mathbf{A}(\mathbf{k},\omega) = 4\pi c[1/(c^2k^2 - \omega^2)]\mathbf{J}_\perp(\mathbf{k},\omega)\ , \tag{35}$$

which defines the Fourier transform of the vector potential, for a fixed $\mathbf{k}$, everywhere in the complex ω plane, except at the simple poles $\omega = \pm ck$.

In classical electrodynamics, a particular solution for the vector potential, which satisfies Eq. (33), is usually found by first finding the Green's function response of Eq. (33) with $J_{tx} = J_{ty} = J_{tz} = \delta(\mathbf{r})\delta(t)$. This would mean that $\mathbf{J}_\perp(\mathbf{k},\omega) = 1$ in Eq. (35). The contour integration for ω is then caried out over a path which can give a retarded or advanced Green's function or some combination of the two. Finally, the integration over $\mathbf{k}$ is carried out and, if the ω contour of integration is taken to run below the two poles, the retarded vector potential of Eq. (6a) results as a particular solution of Eq. (33).

For the purposes of this paper, the contour that gives the retarded potential is the one that gives the particular solution of Eq. (33) which corresponds to the self-field. However, for the present analysis it is useful to explicitly carry out the ω integration, but not the integration over $\mathbf{k}$. The approach for carrying out the integration over ω will be to use the convolution theorem, which says that the inverse Fourier transform of the product of the Fourier transforms of two functions is the convolution of the two functions. Except for the coefficient $4\pi c$, the inverse of the Fourier transform of the first factor of Eq. (35) is

$$(1/2\pi)\int d\omega \exp(-i\omega t)/(c^2k^2 - \omega^2) = -(1/ck)\sin(ckt)U(t)\ , \tag{36a}$$

where the unit step function, $U(t)$, is a consequence of the selection of the retarded potential's contour of integration.

The inverse Fourier transform of the second factor of Eq. (35) is given by

$$\begin{aligned}(1/2\pi)\int_{-\infty}^{\infty} d\omega \exp(-i\omega t)\mathbf{J}_\perp(\mathbf{k},\omega) &\equiv \mathbf{j}_\perp(\mathbf{k},t)\\ &= \int \mathbf{J}_t(\mathbf{r},t)e^{-i\mathbf{k}\cdot\mathbf{r}}d\mathbf{r}\\ &= e\langle e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}\rangle_\perp\ , \end{aligned} \tag{36b}$$

where Eqs. (34b) and (11c) have been used to relate this term to a quantum-mechanical expectation value. The term $\mathbf{j}(\mathbf{k},t)$ can be rewritten in the interaction picture using Eqs. (28b) and (30b) as

$$\mathbf{j}_\perp(\mathbf{k},t)=e\sum_{\alpha\beta}(\beta|e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}|\alpha)_\perp \exp(-i\Omega_{\alpha\beta}t)c_\alpha(t)c_\beta(t)^*\ , \tag{37}$$

where the transition frequencies $\Omega_{\alpha\beta}$ are defined in Eq. (27c). Using the expression of Eqs. (36) and (37) to invert Eq. (35) by using the convolution theorem, the Fourier transform of Eq. (34a) can be written:

$$\mathbf{A}_s(\mathbf{r},t)=(e/2\pi^2)\sum_{\alpha\beta}\int\frac{d\mathbf{k}}{k}e^{i\mathbf{k}\cdot\mathbf{r}}(\beta|e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}|\alpha)_\perp\int_0^\infty \sin(ckt')\exp[-i\Omega_{\alpha\beta}(t-t')]c_\alpha(t-t')c_\beta(t-t')^*\,dt'\ . \tag{38a}$$

If we compare Eqs. (30a) and (30c), it is seen that the coefficients in the interaction picture vary much more slowly than the coefficients in the Schrödinger picture. Thus it is a better approximate to expand $c_\alpha(t-t')c_\beta(t-t')^*$ in a Taylor series than to expand $a_\alpha(t-t')a_\beta(t-t')^*$, as was originally done in Eq. (7). The first term of such an expansion can be obtained by integrating the last integral in Eq. (38a) by parts and assuming that $c_\alpha(\infty)c_\beta(\infty)^*=0$:

$$\begin{aligned}\mathbf{A}_s(\mathbf{r},t)=\frac{e}{4\pi^2}\sum_{\alpha\beta}\int e^{i\mathbf{k}\cdot\mathbf{r}}(\beta|e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}|\alpha)_\perp\\ \times\Bigg[[1/(ck-\Omega_{\alpha\beta})+1/(ck+\Omega_{\alpha\beta})]c_\alpha(t)c_\beta(t)^*\exp(-i\Omega_{\alpha\beta}t)\\ +\int_0^\infty\frac{d[c_\alpha(t-t')c_\beta(t-t')^*]}{dt'}\left[\frac{\exp[i(ck+\Omega_{\alpha\beta})t']}{(ck+\Omega_{\alpha\beta})}+\frac{\exp[-i(ck-\Omega_{\alpha\beta})t']}{(ck-\Omega_{\alpha\beta})}\right]dt'\Bigg]\frac{d\mathbf{k}}{k}\ .\end{aligned} \tag{38b}$$

No approximation has been made in going from Eq. (38a) to Eq. (38b). The time integral in Eq. (38b) can be thought of as the remainder which would be neglected if only the first term in the Taylor expansion were kept. In other words, making the approximation

$$c_\alpha(t-t')c_\beta(t-t')^*\approx c_\alpha(t)c_\beta(t)^* \tag{38c}$$

and taking the term $c_\alpha(t)c_\beta(t)^*$ outside of the integral sign in Eq. (38a) would neglect the second term in Eq. (38b). Neglecting the second term in Eq. (38b) allows explicit integration over time in Eq. (38a), with the result being

$$\mathbf{A}_s(\mathbf{r},t)=\frac{e}{4\pi^2}\sum_{\alpha\beta}\exp(-i\Omega_{\alpha\beta}t)c_\alpha(t)c_\beta(t)^*\int\frac{d\mathbf{k}}{k}e^{i\mathbf{k}\cdot\mathbf{r}}(\beta|e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}|\alpha)_\perp[1/(ck-\Omega_{\alpha\beta})+1/(ck+\Omega_{\alpha\beta})]\ . \tag{38d}$$

Essentially, the same approximation was made by Ackerhalt[19] in order to obtain approximate solutions of their time-dependent Heisenberg equations. The appearance of both terms, $1/(ck\pm\Omega_{\alpha\beta})$, in self-field calculations was noted and extensively discussed by Ackerhalt. The matrix element of the atomic interaction for the vector potential of Eq. (38c) is

$$(r|\mathbf{A}_s\cdot\mathbf{v}|s)=\frac{e}{4\pi^2}\sum_{\alpha\beta}\exp(-i\Omega_{\alpha\beta}t)c_\alpha(t)c_\beta(t)^*\int(r|e^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}|s)_\perp\cdot(\beta|e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}|\alpha)_\perp[1/(ck-\Omega_{\alpha\beta})+1/(ck+\Omega_{\alpha\beta})]\frac{d\mathbf{k}}{k}\ . \tag{39}$$

Nonrelativistic QED calculations of radiative level shifts are usually carried out with only the transverse field taken into account. In order to facilitate comparison with these QED calculations, the longitudinal field will not be included in the NCT calculations to follow. In addition, the diamagnetic term $(e^2/2mc^2)\mathbf{A}^2$ is usually ignored in QED calculations because its contribution to the energy shift is independent of particle momentum. However, in semiclassical theory the expectation of the diamagnetic energy, which is proportional to $\langle\mathbf{A}_s^2\rangle$, is dependent on the atomic state. Nevertheless, comparison between QED and NCT predictions will be made without including diamagnetic effects.

Writing Eq. (25b) without the electrostatic term $e^2\int[\Psi^*(\mathbf{r}')(1/R)\Psi(\mathbf{r}')]d\mathbf{r}'$ and the diamagnetic term, the Schrödinger equation takes the form

$$i\hbar\frac{da_l}{dt}=E_la_l-(e/c)\sum_j(l|\mathbf{A}_s\cdot\mathbf{v}|j)a_j\ . \tag{40a}$$

Using Eq. (39) in Eq. (40a), one obtains

$$i\hbar\frac{dc_l}{dt}=-\frac{e^2}{4\pi^2}\sum_{\alpha,\beta,j}\left\{c_\alpha(t)c_\beta(t)^*\exp[i(\Omega_{lj}-\Omega_{\alpha\beta})t]\int[1/(ck-\Omega_{\alpha\beta})+1/(ck+\Omega_{\alpha\beta})]\times(\beta|e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}|\alpha)_\perp\cdot(l|e^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}|j)_\perp\frac{d\mathbf{k}}{ck}\right\}c_j(t)\ . \tag{40b}$$

Following the reasoning of Ref. 9, the rapidly oscillating terms of the form $\exp[-i(\Omega_{\alpha\beta}-\Omega_{lj})t]$ are neglected unless $l=\alpha$ and $j=\beta$, or $l=j$ and $\alpha=\beta$, resulting in a simplified expression:

$$i\hbar\frac{dc_l}{dt}=-\frac{e^2}{4\pi^2}\sum_j c_j(t)c_j(t)^*\left\{\int[1/(ck-\Omega_{lj})+1/(ck+\Omega_{lj})](l|e^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}|j)_\perp\cdot(j|e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}|l)_\perp\frac{d\mathbf{k}}{ck}+2\int(l|e^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}|l)_\perp\cdot(j|e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}|j)_\perp\frac{d\mathbf{k}}{c^2k^2}\right\}c_l(t)\ . \tag{40c}$$

In the same way that ΔE_l of Eqs. (32b) and (32c) was identitied from Eq. (32a), a level shift can be identified from Eq. (40c) when the latter is written in the Schrödinger picture. The resulting energy shift is

$$\Delta E_l=-\frac{e^2}{4\pi^2}\sum_j c_j(t)c_j(t)^*\left\{\int[1/(ck-\Omega_{lj})+1/(ck+\Omega_{lj})](l|e^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}|j)_\perp\cdot(j|e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}|l)_\perp\frac{d\mathbf{k}}{ck}+2\int(l|e^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}|l)_\perp\cdot(j|e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}|j)_\perp\frac{d\mathbf{k}}{c^2k^2}\right\}\ . \tag{41}$$

Ackerhalt and co-workers[19] also obtain both the $1/(ck-\Omega_{lj})$ and $1/(ck+\Omega_{lj})$ terms in their Heisenberg equation of motion treatment of radiative level shifts. They point out that the second terms are neglected when the Wigner-Weisskopf[5] approximation is made. In QED, the Wigner-Weisskopf approximation consists of neglecting transitions to states which do not conserve energy. This approximation is acceptable for calculating the time dependence of spontaneous decay, but neglects significant terms when calculating level shifts which are essential due to "virtual" transitions which may not necessarily conserve energy. The additional $1/(ck+\Omega_{lj})$ term is also present in the work of Barut and Kraus.[21] The two terms, $1/(ck-\Omega_{lj})$ and $1/(ck+\Omega_{lj})$, first appear in the expression for the self-field's vector potential of Eq. (38d). From the semiclassical derivation contained in this paper, it is apparent that there is nothing which is essentially quantum mechanical that leads to the appearance of both factors in Eq. (41). They would appear as a consequence of Eqs. (33) or (35) for any classical current source that could be written as the sum of harmonic components.

Use of the identities

$$1/(ck-\Omega_{lj})=(1/ck)[1+\Omega_{lj}/(ck-\Omega_{lj})] \tag{42a}$$

and

$$1/(ck+\Omega_{lj})=(1/ck)[1-\Omega_{lj}/(ck+\Omega_{lj})] \tag{42b}$$

allows the rewriting of the energy shift as

$$\Delta E_l=-\frac{e^2}{4\pi^2}\sum_j c_j(t)c_j(t)^*\left\{2\int[(l|e^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}|j)_\perp\cdot(j|e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}|l)_\perp+(l|e^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}|l)_\perp\cdot(j|e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}|j)_\perp]\frac{d\mathbf{k}}{c^2k^2}+\int\Omega_{lj}[1/(ck-\Omega_{lj})-1/(ck+\Omega_{lj})](l|e^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}|j)_\perp\cdot(j|e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}|l)_\perp\frac{d\mathbf{k}}{c^2k^2}\right\}\ . \tag{42c}$$

COMPARISON WITH BETHE'S CALCULATION

Bethe's[18] calculation of the Lamb shift starts with the electric dipole approximation, which sets the terms $e^{i\mathbf{k}\cdot\mathbf{r}}\approx 1$. In QED, this assumption can be justified when mass renormalization, which also involves retardation terms of the form $e^{i\mathbf{k}\cdot\mathbf{r}}$, is carried out. If the dipole approximation is not made, then retardation causes the integrals of Eq. (42c) to converge. This observation was made in the first footnote in the work of Kroll and Lamb,[23] which contains a relativistic quantum electrodynamic Lamb shift calculation. They report that the resulting S-$P_{1/2}$ shift is calculated to be 1135 Mc/s which is within 10% of the observed Lamb shift. The radiative shifts that are found to converge when retardation is included in Ref. 9 are similarly of the same order of magnitude as the observed Lamb shifts.

The validity of the electric dipole approximation in the semiclassical theory is unclear. Indeed, the theory of electromagnetic mass, which is the motivation for mass renormalization, is difficult to reconcile with Schrödinger's electrodynamic interpretation of the wave function. Mass renormalization is carried out in Ref. 9 by subtracting off the electrostatic self-energy. It is difficult to imagine the physical electromagnetic mass decreasing in time as the wave packet of a free particle expands. Even in the case of bound states, the electrostatic self-energy, which would be given by e multiplied by the quantum-mechanical expectation of the scalar potential of Eq. (9b), would change by significant amounts as the atomic state changed.

The energy shift of Eq. (42c) expresses the radiative level shifts that are predicted from NCT to a higher accuracy than was contained in Ref. 9. It is first noted that the shift contains a sum of contributions weighted by factors $c_j(t)c_j(t)^*$. According to Born's statistical interpretation of Ψ, these weighting factors would be identified with the probability of excitation of the jth unperturbed state at t. This predicted time-dependent frequency shift appears to be an essential consequence of the NCT assumptions of Eq. (5) and is not found in nature.[24]

Some of the terms within the brackets of Eq. (42c) can be related to Bethe's QED calculation of the Lamb shift. The first integral,

$$\Delta E_{lj}^{\text{mass}} = -\frac{e^2}{2\pi^2 c^2}\int [(l|e^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}|j)_\perp\cdot(j|e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}|l)_\perp + (l|e^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}|l)_\perp\cdot(j|e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}|j)_\perp]\frac{d\mathbf{k}}{c^2k^2}\,, \tag{43a}$$

is similar to the one subtracted by Bethe during the mass-renormalization process. An expression like the first one in Eq. (43a), including retardation, does appear in the QED calculation of radiative corrections to the levels of a helium atom.[25] Physically, this QED correction to the helium energy levels, which can be identified with the Breit Hamiltonian, corresponds to one of the two electrons emitting a virtual photon which is absorbed by the other electron. However, Eq. (43a) has been derived in NCT for a one-electron system. Physically, it corresponds to the single electron interacting with its own electromagnetic field.

The second term is

$$\Delta E_{lj}^{\text{Lamb}} = -\frac{e^2}{4\pi^2}\Omega_{lj}\int [1/(ck-\Omega_{lj}) - 1/(ck+\Omega_{lj})] \times (l|e^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}|j)_\perp\cdot(j|e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}|l)_\perp\frac{d\mathbf{k}}{c^2k^2}\,. \tag{43b}$$

The expression of Eq. (43b) is the sum of two integrals, the first of which is

$$\Delta E_{lj}^{\text{Bethe}} = -\frac{e^2}{4\pi^2 c^2}(E_l - E_j) \times \int \frac{(l|e^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}|j)_\perp\cdot(j|e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}|l)_\perp}{(\hbar ck - E_l + E_j)}\frac{d\mathbf{k}}{k^2}\,, \tag{43c}$$

can be made to resemble the Bethe logarithm expression for the Lamb shift by making the electric dipole approximation, integrating over the angular coordinates, and introducing a cutoff at relativistic values of k. The transition frequencies Ω_{lj} are replaced by the unperturbed energy eigenvalues according to Eq. (27c) to facilitate comparison with Bethe's results:

$$\Delta E_{lj}^{\text{Bethe}} = -\frac{2e^2}{3\pi c^3\hbar}(E_l - E_j)\int_0^{mc^2/\hbar}\frac{(l|\mathbf{v}|j)\cdot(j|\mathbf{v}|l)\hbar c}{(\hbar ck - E_l + E_j)}dk\,. \tag{43d}$$

The NCT result of Eq. (42c) combined with Eq. (43d) differs from Bethe's[18] Eq. (5), in that the sum over the intermediate states j has to be weighted by the coefficients $c_j(t)c_j(t)^*$. This is an important difference and precludes the use of the summation rules that allowed Bethe to get his final results. It also implies that the NCT radiative level shifts will be time dependent and, at a given time, depend on the relative excitation of the atomic energy levels.

The second integral appearing in Eq. (42b) contains a term, $-1/(ck+\Omega_{lj})$, which is similar to results obtained by Ackerhalt and his collaborators[19,20] when studying the QED problem of spontaneous emission and level shifts in the Heisenberg picture.

Mahanty[11] has also carried out a more complete calculation of the NCT frequency shifts than is contained in Ref. 9. He employed an approach that is different than the one above. Mahanty uses a contour integral approach and arrives at a logarithmic expression for the Lamb shift that is similar to Bethe's.

Barut and his collaborators[21,22] arrive at expressions for the QED level shifts and mass-renormalization terms very similar to those of Eq. (41). Although they appear to be using a relativistic version of the NCT assumptions of Eq. (5), they do not obtain the weighting coefficients $c_j(t)c_j(t)^*$ in their expressions for energy shifts that are derived above. A possible explanation for this may lie in the papers by Bialynicki-Birula[26] and Barut.[27]

CONCLUSIONS

Expressions similar to the Bethe logarithm calculation of the Lamb shift appear in the semiclassical calculation of radiative level shifts, in addition to terms that are similar to those that are subtracted through mass-renormalization procedure. However, the semiclassical terms are multiplied by quantum coefficients $c_l c_l^*$ in a way that makes the radiative shifts time dependent and dependent on the excitation of different energy levels. This seems to be an inescapable consequence of the NCT assumptions of Eq. (5). These coefficients also prevent the use of the matrix summation techniques that Bethe used to get his final expression for the Lamb shift. Even level shifts based upon the approximate Hamiltonian of Eq. (26), from which the electromagnetic field variables have been eliminated, imply the level and frequency shifts of Eq. (32) which depend on the degree of excitation of the atomic energy levels. Furthermore, it is more difficult to rationalize the QED arguments of mass renormalization with a semiclassical theory that is based upon Schrödinger's electrodynamic hypothesis for Ψ. The natural tendency of a free electron's wave packet to expand makes semiclassical mass renormalization ambiguous.

APPENDIX A

Equations (11c) and (8) will be derived in this appendix, starting with definition of the Fourier spatial transform, which is implicit in Eq. (34),

$$\mathbf{j}(\mathbf{k})\equiv\int\mathbf{J}(\mathbf{r})\exp(-i\mathbf{k}\cdot\mathbf{r})d\mathbf{r}\ , \tag{A1}$$

and its inverse,

$$\mathbf{J}(\mathbf{r})=(1/2\pi)^3\int\mathbf{j}(\mathbf{k})\exp(i\mathbf{k}\cdot\mathbf{r})d\mathbf{k}\ . \tag{A2}$$

Any vector $\mathbf{j}(\mathbf{k})$ can be written as the sum of a vector perpendicular to and a vector parallel to any vector $\mathbf{k}$:

$$\mathbf{j}(\mathbf{k})=(\mathbf{k}/k)[(\mathbf{k}/k)\cdot\mathbf{j}(\mathbf{k})]-(\mathbf{k}/k)\times[(\mathbf{k}/k)\times\mathbf{j}(\mathbf{k})]\ . \tag{A3}$$

Substituting this into Eq. (A2), leads to a resolution of $\mathbf{J}$ into two parts:

$$\begin{aligned}\mathbf{J}(\mathbf{r})=&\left[\frac{1}{2\pi}\right]^3\int(\mathbf{k}/k)[(\mathbf{k}/k)\cdot\mathbf{j}(\mathbf{k})\exp(i\mathbf{k}\cdot\mathbf{r})d\mathbf{k}]\\&-\left[\frac{1}{2\pi}\right]^3\int(\mathbf{k}/k)\times[(\mathbf{k}/k)\times\mathbf{j}(\mathbf{k})\exp(i\mathbf{k}\cdot\mathbf{r})d\mathbf{k}]\ .\end{aligned} \tag{A4}$$

Direct computation shows that the curl of the first integral in Eq. (A4) is zero and that the divergence of the second integral is zero. This allows the identification of the longitudinal $\mathbf{J}_l$ and transverse $\mathbf{J}_t$ parts of $\mathbf{J}$ to be

$$\mathbf{J}_l(\mathbf{r})=\left[\frac{1}{2\pi}\right]^3\int(\mathbf{k}/k)[(\mathbf{k}/k)\cdot\mathbf{j}(\mathbf{k})\exp(i\mathbf{k}\cdot\mathbf{r})d\mathbf{k}]\ , \tag{A5}$$

$$\mathbf{J}_t(\mathbf{r})=-\left[\frac{1}{2\pi}\right]^3\int(\mathbf{k}/k)\times[(\mathbf{k}/k)\times\mathbf{j}(\mathbf{k})\exp(i\mathbf{k}\cdot\mathbf{r})d\mathbf{k}]\ , \tag{A6}$$

where

$$\mathbf{J}(\mathbf{r})=\mathbf{J}_l(\mathbf{r})+\mathbf{J}_t(\mathbf{r})\ . \tag{A7}$$

Computing directly from Eq. (A6) and using the definition of Eq. (A1),

$$\int\mathbf{J}_t(\mathbf{r})e^{-i\mathbf{k}\cdot\mathbf{r}}d\mathbf{r}=-(\mathbf{k}/k)\times\left[\left[\frac{\mathbf{k}}{k}\right]\times\int\mathbf{J}(\mathbf{r})e^{-i\mathbf{k}\cdot\mathbf{r}}d\mathbf{r}\right]\ . \tag{A8}$$

Equation (11c) follows from using Eq. (5b) in Eq. (A8) and drawing on the Hermitian properties of the operator $\mathbf{v}$.

The integral of Eq. (A5) over space can be computed:

$$\int\mathbf{J}_l(\mathbf{r})d\mathbf{r}=(1/2\pi)^3\int(\mathbf{k}/k)[(\mathbf{k}/k)\cdot\mathbf{j}(\mathbf{k})\int\exp(i\mathbf{k}\cdot\mathbf{r})d\mathbf{k}]d\mathbf{r}\ . \tag{A9}$$

If the integrands are well behaved, the order of integration over $\mathbf{k}$ and $\mathbf{r}$ can be interchanged. This yields a δ-function:

$$(1/2\pi)^3\int\exp(i\mathbf{k}\cdot\mathbf{r})d\mathbf{r}=\delta(\mathbf{k})=(1/2\pi)\delta(k)/k^2\ . \tag{A10}$$

Substituting in this result and using Eq. (A1),

$$\int\mathbf{J}_l(\mathbf{r})d\mathbf{r}=(1/2\pi)\int[\delta(k)/k^2](\mathbf{k}/k)[(\mathbf{k}/k)\cdot\int\mathbf{J}(\mathbf{r}')\exp(-i\mathbf{k}\cdot\mathbf{r}')d\mathbf{r}'\,d\mathbf{k}]\ . \tag{A11}$$

The integration over $\mathbf{k}$ can be performed first, and it is simplest to consider that the vector $\mathbf{r}'$ is parallel to the k_z axis when doing this integration. Introducing unit vectors in the x, y, and z directions as $\hat{\mathbf{e}}_x$, $\hat{\mathbf{e}}_y$, and $\hat{\mathbf{e}}_z$, one can write

$$\begin{aligned}&(1/2\pi)\int[\delta(k)/k^2](\mathbf{k}/k)[(\mathbf{k}/k)\cdot\mathbf{J}\exp(-i\mathbf{k}\cdot\mathbf{r}')d\mathbf{k}]\\&\quad=(1/2\pi)\int_0^\infty\int_{-1}^1\int_0^{2\pi}\delta(k)\exp(-ikr'\cos\theta)\{[\hat{\mathbf{e}}_z\cos\theta+\sin\theta(\hat{\mathbf{e}}_x\cos\phi+\hat{\mathbf{e}}_y\sin\phi)]\\&\qquad\qquad\times[J_z\cos\theta+\sin\theta(J_x\cos\phi+J_y\sin\phi)]\}d\phi\,d(\cos\theta)dk\ ,\\&(1/2)\int_0^\infty\int_{-1}^1\delta(k)\exp(-ikr'\cos\theta)[2J_z\hat{\mathbf{e}}_z\cos^2\theta+\sin^2\theta(J_x\hat{\mathbf{e}}_x+J_y\hat{\mathbf{e}}_y)]d(\cos\theta)dk\\&\quad=\int_0^\infty(2J_z\hat{\mathbf{e}}_z\{\sin(kr')/(kr')+2[\cos(kr')/(kr')^2-\sin(kr')/(kr')^3]\}\\&\qquad-2(J_x\hat{\mathbf{e}}_x+J_y\hat{\mathbf{e}}_y)[\cos(kr')/(kr')^2-\sin(kr')/(kr')^3])\delta(k)dk\ .\end{aligned} \tag{A12}$$

The effect of completing the remaining integral over k is to take one half the limit of the integrand as k approaches zero from a positive value. Only one half the limit is used, because the integral is from 0 to ∞ instead of from $-\infty$ to $+\infty$, as is usually the case in evaluating integrals involving $\delta(k)$.[28] Substituting the result into Eq. (A11) yields the following result:

$$\int\mathbf{J}_l(\mathbf{r})d\mathbf{r}=(1/3)\int\mathbf{J}(\mathbf{r})d\mathbf{r}\ . \tag{A13}$$

Combining this with Eq. (A7) provides the result stated in Eq. (8).

APPENDIX B

First, the identity which was used in the derivation of Eq. (16a) will be derived here. Starting with the expression for the electrostatic self-potential of Eq. (9b), the quantum-mechanical expectation of the electrostatic self-energy is

$$\langle \phi_s \rangle = \frac{e}{2\pi^2} \int \frac{d\mathbf{k}}{k^2} \langle e^{i\mathbf{k}\cdot\mathbf{r}} \rangle \langle e^{-i\mathbf{k}\cdot\mathbf{r}} \rangle \ . \tag{B1}$$

The rate of change of the self-potential is

$$\frac{\partial \phi_s}{\partial t}(\mathbf{r},t) = \frac{e}{2\pi^2} \int \frac{d\mathbf{k}}{k^2} e^{i\mathbf{k}\cdot\mathbf{r}} \frac{d\langle e^{-i\mathbf{k}\cdot\mathbf{r}} \rangle}{dt} \ . \tag{B2}$$

Taking the quantum-mechanical expectation value of Eq. (B2) leads to

$$\left\langle \frac{\partial \phi_s}{\partial t} \right\rangle = \frac{e}{2\pi^2} \int \frac{d\mathbf{k}}{k^2} \langle e^{i\mathbf{k}\cdot\mathbf{r}} \rangle \frac{d\langle e^{-i\mathbf{k}\cdot\mathbf{r}} \rangle}{dt} \ , \tag{B3}$$

which can be seen to be one half of $d\langle \phi_s \rangle / dt$ by direct computation.

Next the details of the derivation of Eq. (20) will be given. Starting with the left-hand side of Eq. (4) and substituting in for $\mathbf{v}$ from Eq. (2):

$$\begin{aligned} \frac{d[(m\mathbf{v}^2/2)+U]}{dt} &= \frac{d[\mathbf{p}^2/2m - (e/2mc)(\mathbf{A}\cdot\mathbf{p}+\mathbf{p}\cdot\mathbf{A}) + (e^2/2mc^2)\mathbf{A}^2 + U]}{dt} \\ &= \frac{d[\mathbf{p}^2/2m - (e/2c)(\mathbf{A}\cdot\mathbf{v}+\mathbf{v}\cdot\mathbf{A}) - (e^2/2mc^2)\mathbf{A}^2 + U]}{dt} \ . \end{aligned} \tag{B4}$$

This allows the rewriting of Eq. (4) as

$$\frac{d[\mathbf{p}^2/2m + U - (e/2c)(\mathbf{A}\cdot\mathbf{v}+\mathbf{v}\cdot\mathbf{A}) - (e^2/2mc^2)\mathbf{A}^2]}{dt} = -(e/2)(\nabla\phi\cdot\mathbf{v}+\mathbf{v}\cdot\nabla\phi) - (e/2c)\left[\mathbf{v}\cdot\left[\frac{\partial \mathbf{A}}{\partial t}\right] + \left[\frac{\partial \mathbf{A}}{\partial t}\right]\cdot\mathbf{v}\right] \ . \tag{B5}$$

Using the approximate expressions for the self-fields shown in Eq. (9),

$$\mathbf{A}_s(\mathbf{r},t) \approx \frac{e}{2\pi^2 c} \int \frac{d\mathbf{k}}{k^2} e^{i\mathbf{k}\cdot\mathbf{r}} \langle e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{v} \rangle_\perp - \frac{2e}{3c^2}\frac{d\langle \mathbf{v} \rangle}{dt} \ , \tag{B6}$$

$$\phi_s(\mathbf{r},t) = \frac{e}{2\pi^2} \int \frac{d\mathbf{k}}{k^2} e^{i\mathbf{k}\cdot\mathbf{r}} \langle e^{-i\mathbf{k}\cdot\mathbf{r}} \rangle \ . \tag{B7}$$

In Eq. (B5) and again neglecting the diamagnetic term, $(e^2/2mc^2)\mathbf{A}_s^2$, which would be of order $1/c^4$ according to Eq. (B6), one obtains

$$\begin{aligned} &\frac{d[\mathbf{p}^2/2m + U - (e^2/4\pi^2c^2)\int (\mathbf{v}e^{i\mathbf{k}\cdot\mathbf{r}} + e^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{v})\cdot\langle e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}\rangle_\perp (d\mathbf{k}/k^2) + (2e^2/3c^3)\mathbf{v}\cdot(d\langle \mathbf{v}\rangle/dt)]}{dt} \\ &\qquad = -e\left[\frac{d\phi_s}{dt} - \frac{\partial \phi_s}{\partial t}\right] - \frac{e^2}{4\pi^2c^2}\int (\mathbf{v}e^{i\mathbf{k}\cdot\mathbf{r}} + e^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{v})\cdot\left[\frac{d\langle e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}\rangle_\perp}{dt}\right]\frac{d\mathbf{k}}{k^2} + \frac{2e^2}{3c^3}\mathbf{v}\cdot\left[\frac{d^2\langle \mathbf{v}\rangle}{dt^2}\right] \ , \end{aligned} \tag{B8}$$

where the "chain rule" for time derivatives of Heisenberg operators which evolve under the Hamiltonian of Eq. (1) is

$$\frac{d\phi}{dt} = \frac{\partial \phi}{\partial t} + \tfrac{1}{2}(\mathbf{v}\cdot\nabla\phi + \nabla\phi\cdot\mathbf{v}) \ . \tag{B9}$$

Taking quantum-mechanical expectations of both sides of Eq. (B8), identifying the atomic field in absence of self-fields H_0 defined by Eq. (14a), and using the identity $d\langle \phi_s \rangle/dt = 2\langle \partial\phi_s/\partial t \rangle$ which was derived above,

$$\begin{aligned} &\frac{d\{\langle H_0 \rangle - (e^2/2\pi^2c^2)\int \langle e^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}\rangle_\perp \cdot \langle e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}\rangle_\perp (d\mathbf{k}/k^2) + (2e^2/3c^3)\langle \mathbf{v}\rangle\cdot[d\langle \mathbf{v}\rangle/dt]\}}{dt} \\ &\qquad = -\frac{e}{2}\frac{d\phi_s}{dt} - \frac{e^2}{2\pi^2c^2}\int \langle e^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}\rangle_\perp \cdot \left[\frac{d\langle e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}\rangle_\perp}{dt}\right]\frac{d\mathbf{k}}{k^2} + \frac{2e^2}{3c^3}\langle \mathbf{v}\rangle\cdot\left[\frac{d^2\langle \mathbf{v}\rangle}{dt^2}\right] \ . \end{aligned} \tag{B10}$$

Noting the equality of

$$-(e^2/2\pi^2c^2)\int \langle e^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}\rangle_\perp \cdot \left[\frac{d\langle e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}\rangle_\perp}{dt}\right]\frac{d\mathbf{k}}{k^2} = -(e^2/2\pi^2c^2)\int \langle e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}\rangle_\perp \cdot \left[\frac{d\langle e^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}\rangle_\perp}{dt}\right]\frac{d\mathbf{k}}{k^2} \ , \tag{B11}$$

Eq. (B10) can be rewritten:

$$\frac{d[\langle H_0\rangle+(e/2)\langle\phi_s\rangle-(e^2/2\pi^2c^2)\int\langle e^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}\rangle_\perp\cdot\langle e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}\rangle_\perp(d\mathbf{k}/k^2)+(2e^2/3c^3)\langle\mathbf{v}\rangle\cdot(d\langle\mathbf{v}\rangle/dt)]}{dt}$$
$$=-(e^2/4\pi^2c^2)\int\left[\frac{d(\langle e^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}\rangle_\perp\cdot\langle e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}\rangle_\perp)}{dt}\right](d\mathbf{k}/k^2)+(2e^2/3c^3)\langle\mathbf{v}\rangle\cdot\left[\frac{d^2\langle\mathbf{v}\rangle}{dt^2}\right]. \tag{B12}$$

Rearranging so that the terms up to order $1/c^2$ are on the left and the terms of order $1/c^3$ are on the right and using the expectation of Eq. (9b) for $\langle\phi_s\rangle$, one gets

$$d\left[\langle H_0\rangle-(e^2/2\pi^2c^2)\int\langle e^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}\rangle_\perp\cdot\langle e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}\rangle_\perp(d\mathbf{k}/k^2)\right.$$
$$\left.+(e^2/4\pi^2)\int(\langle e^{i\mathbf{k}\cdot\mathbf{r}}\rangle\langle e^{-i\mathbf{k}\cdot\mathbf{r}}\rangle+\langle e^{i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}\rangle_\perp\cdot\langle e^{-i\mathbf{k}\cdot\mathbf{r}}\mathbf{v}\rangle_\perp/c^2)(d\mathbf{k}/k^2)\right]\Big/dt=-(2e^2/3c^3)\left[\frac{d\langle\mathbf{v}\rangle}{dt}\right]^2. \tag{B13}$$

Comparing with Eqs. (14c) and (16c), the second term within the braces on the left-hand side of Eq. (B13) can be identified with the expectation of the interaction energy $\langle H_I\rangle$ of the atom with its self-field $\mathbf{A}_s$ if the term

$$(2e^2/3c^3)\langle\mathbf{v}\rangle\cdot\left[\frac{d\langle\mathbf{v}\rangle}{dt}\right]=(e^2/3c^3)\left[\frac{d\langle\mathbf{v}\rangle^2}{dt}\right] \tag{B14}$$

is neglected. This term corresponds to energy that is rapidly transferred back and forth between the field and the atomic system. It is usually neglected in classical analyses of radiation reaction by averaging over a period long compared with an atomic cycle or over an exact period for a periodic system.[29] The third term within the large parentheses on the right-hand side of Eq. (B13) is identified as the energy stored in the electromagnetic field surrounding the atom which can be obtained by substituting from Eqs. (17) into Eq. (19).

[1] E. Schrödinger, Ann. Phys. (Leipzig) **79**, 361 (1926).

[2] D. R. Hartree, Proc. Cambridge Philos. Soc. **24**, 89 (1928).

[3] G. Gaviola, Nature **122**, 772 (1928).

[4] E. Fermi, Rend. Lincei **5**, 795 (1927). I am indebted to Carlos Stroud for pointing out this reference to me. Unfortunately, the work cited in Refs. 8–11 was done without the knowledge of this paper.

[5] V. Weisskopf and E. P. Wigner, Z. Phys. **63**, 54 (1930).

[6] H. M. Gibbs, in *Coherence and Quantum Optics*, edited by L. Mandel and E. Wolf (Plenum, New York, 1973).

[7] P. A. M. Dirac, Phys. Rev. **139**, B684 (1965).

[8] E. T. Jaynes and F. W. Cummings, Proc. IEEE **51**, 89 (1963).

[9] M. D. Crisp and E. T. Jaynes, Phys. Rev. **179**, 1253 (1969).

[10] C. R. Stroud and E. T. Jaynes, Phys. Rev. A **1**, 106 (1970).

[11] J. Mahanty, Nuovo Cimento B **22**, 110 (1974).

[12] J. J. Larmor, Philos. Mag. **44**, 503 (1897).

[13] E. Fermi, Rev. Mod. Phys. **4**, 87 (1932).

[14] G. Breit, Phys. Rev. **34**, 553 (1929); **36**, 383 (1930); **39**, 616 (1932).

[15] C. G. Darwin, Philos. Mag. **39**, 537 (1920).

[16] J. C. Slater, Phys. Rev. **35**, 210 (1930).

[17] V. Fock, Z. Phys. **61**, 126 (1930).

[18] H. A. Bethe, Phys. Rev. **172**, 339 (1947).

[19] J. R. Ackerhalt, P. L. Knight, and J. H. Eberly, Phys. Rev. Lett. **30**, 456 (1973); J. R. Ackerhalt, J. H. Eberly, and P. L. Knight, in *Coherence and Quantum Optics*, edited by L. Mandel and E. Wolf (Plenum, New York, 1973), p. 635; P. W. Milonni, J. R. Ackerhalt, and W. A. Smith, Phys. Rev. Lett. **31**, 958 (1973); J. R. Ackerhalt and J. H. Eberly, Phys. Rev. D **10**, 3350 (1974).

[20] L. Allen and J. H. Eberly, *Optical Resonance and Two-Level Atoms* (Wiley, New York, 1975), Chap. 7.

[21] A. O. Barut and J. Kraus, Found. Phys. **13**, 189 (1983).

[22] A. O. Barut and J. F. van Huele, Phys. Rev. A **32**, 3187 (1985).

[23] Norman M. Kroll and Willis E. Lamb, Jr., Phys. Rev. **75**, 388 (1949).

[24] M. L. Citron, H. R. Gray, C. W. Gabel, and C. R. Stroud, Jr., Phys. Rev. A **16**, 1507 (1977).

[25] H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of One- and Two-Electron Systems* (Springer-Verlag, Berlin, 1957), p. 170ff.

[26] I. Bialynicki-Birula, Phys. Rev. A **34**, 3500 (1986).

[27] A. O. Barut, Phys. Rev. A **34**, 3502 (1986).

[28] W. Heitler, *The Quantum Theory of Radiation*, 3rd ed. (Clarendon, Oxford, 1954), p. 68.

[29] J. D. Jackson, *Classical Electrodynamics* (Wiley, New York, 1963), p. 578ff.