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Dirac's Equation in Semiclassical Physics

Lee W. Casperson
Portland State University

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Dirac's equation in semiclassical physics

Lee W. Casperson
Department of Electrical Engineering, Portland State University, P.O. Box 751, Portland, Oregon 97207-0751
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Dirac's equation provides the most rigorous basis known for many calculations in relativistic quantum mechanics. A set of dynamical equations having greater intuitive content can be derived from Dirac's equation without any approximations. These secondary equations govern the properties of a Dirac particle as functions of time and space and are similar to the corresponding equations governing a classical charged fluid. Several new density functions are implied by these equations and are appropriate for incorporation into the various semiclassical models of physics.

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I. INTRODUCTION

Dirac's equation is the starting point for many calculations in quantum mechanics [1]. With appropriate density definitions it is possible to derive from Dirac's equation a set of dynamical equations that resembles very closely the macroscopic equations of classical fluid mechanics [2]. Dirac's equation is linear in the wave-function variables, but by means of suitable manipulations one can obtain as exact theorems a set of equations that are quadratic in the wave functions. This process is analogous to the manner in which Poynting's theorem, which is quadratic in the electromagnetic field variables, is derived from the linear Maxwell-Heaviside equations. The Dirac-equation-based theorems may be used to infer the form of several operators and their corresponding density functions.

The idea that the wave functions of quantum mechanics might behave like a fluid is not new. This concept was implied in Schrödinger's models, and hydrodynamical interpretations of the wave function were first emphasized explicitly by Madelung [3]. While this line of interpretation by itself did not lead to dramatic new insights, it did become an integral part of the hidden-variable models of de Broglie, Bohm, and others [4–16]. The more specific question of the relationship of the wave function for a Dirac particle to the equations of a classical fluid is explored here, and the extraction of the resulting density functions and their incorporation in semiclassical models is also considered.

It is shown in Sec. II that if one employs appropriate definitions of charge density, momentum density, etc., one obtains classical-appearing results such as conservation of charge or momentum for a charged fluid. Most of the densities and the equations that interrelate these densities have not been considered previously, and the results are summarized and discussed in Sec. III.

II. THEORY

Dirac's equation can be written

$$i\hbar\frac{\partial\psi}{\partial t}=(-i\hbar c\boldsymbol{\alpha}\cdot\nabla-ec\boldsymbol{\alpha}\cdot\mathbf{A}+e\phi+\beta mc^2)\psi\ , \tag{1}$$

where c is the speed of light, m is the electron mass, $\hbar$ is Planck's constant divided by 2π, and ϕ and $\mathbf{A}$ are the ordinary scalar and vector electromagnetic potentials. In the simplest formulations the electron wave function ψ in Eq. (1) is represented by a four-component one-column matrix. The dot product notation in Eq. (1) would seem to suggest that the term $\boldsymbol{\alpha}$ represents a vector, which would have the Cartesian components α_x, α_y, and α_z. However, in the same way that the wave function ψ is a one-column matrix, the terms α_x, α_y, and α_z, as well as β must be understood as four-by-four matrices. It is a further requirement of the theory that these matrices must satisfy the relationships [17]

$$\alpha_x^2=\alpha_y^2=\alpha_z^2=\beta^2=1\ , \tag{2}$$

$$\alpha_x\alpha_y+\alpha_y\alpha_x=\alpha_y\alpha_z+a_z\alpha_y=\alpha_z\alpha_x+\alpha_x\alpha_z=0\ , \tag{3}$$

$$\alpha_x\beta+\beta\alpha_x=\alpha_y\beta+\beta\alpha_y=\alpha_z\beta+\beta\alpha_z=0\ . \tag{4}$$

Neither the representation of the wave function ψ in Eq. (1) nor the detailed representations of the $\boldsymbol{\alpha}$ and β matrices are unique in Dirac's model, and if possible it is usually considered preferable not to express these equations in an expanded form when solving problems [18]. In terms of the electromagnetic potentials, the electric field $\mathbf{E}$ and the magnetic-flux density $\mathbf{B}$ are given by [19]

$$\mathbf{E}=-\nabla\phi-\frac{\partial\mathbf{A}}{\partial t}\ , \tag{5}$$

$$\mathbf{B}=\nabla\times\mathbf{A}\ . \tag{6}$$

Useful theorems can be obtained from Eqs. (1)–(6) by exploring the derivative

$$\frac{\partial}{\partial t}(\psi^\dagger\mathbf{o}\psi)=\psi^\dagger\frac{\partial\mathbf{o}}{\partial t}\psi+\psi^\dagger\mathbf{o}\frac{\partial\psi}{\partial t}+\frac{\partial\psi^\dagger}{\partial t}\mathbf{o}\psi\ , \tag{7}$$

where the symbol $\mathbf{o}$ represents an as yet unspecified operator. As a shorthand, it is convenient to introduce the Hamiltonian operator

$$H=-i\hbar c\boldsymbol{\alpha}\cdot\nabla-ec\boldsymbol{\alpha}\cdot\mathbf{A}+e\phi+\beta mc^2\ , \tag{8}$$

and with this definition Eq. (1) can be written more compactly as

$$i\hbar\frac{\partial\psi}{\partial t}=H\psi\ . \tag{9}$$

With this formula, Eq. (7) becomes

$$\frac{\partial}{\partial t}(\psi^\dagger \mathbf{o}\psi)=\psi^\dagger\frac{\partial \mathbf{o}}{\partial t}\psi+\frac{i}{\hbar}[(H\psi)^\dagger \mathbf{o}\psi-\psi^\dagger \mathbf{o}H\psi]\ . \tag{10}$$

After some calculations using Eq. (8), this result can be written in the form

$$\frac{\partial}{\partial t}(\psi^\dagger \mathbf{o}\psi)=\psi^\dagger\frac{\partial \mathbf{o}}{\partial t}\psi+\frac{i}{\hbar}\psi^\dagger(H\mathbf{o}-\mathbf{o}H)\psi-\nabla\cdot(\psi^\dagger \mathbf{v}\mathbf{o}\psi)\ , \tag{11}$$

where the velocity operator

$$\mathbf{v}=c\boldsymbol{\alpha} \tag{12}$$

has been introduced in the last term.

If there is every ambiguity about the interpretation of an operation sequence, as in the last term in Eq. (11), one can always check the analysis by first replacing a vector operator $\mathbf{o}$ by one of its scalar Cartesian components and then later reassembling the vector equation from its components. More specifically, one can write the spatial aspects of the operator $\mathbf{j}_0=\mathbf{v}\mathbf{o}$ in Eq. (11) as a tensor operator current

$$\mathbf{j}_0=\begin{bmatrix} v_x o_x \mathbf{i}_x & v_x o_y \mathbf{i}_y & v_x o_z \mathbf{i}_z \\ v_y o_x \mathbf{i}_x & v_y o_y \mathbf{i}_y & v_y o_z \mathbf{i}_z \\ v_z o_x \mathbf{i}_x & v_z o_y \mathbf{i}_y & v_z o_z \mathbf{i}_z \end{bmatrix}\ , \tag{13}$$

provided that the ∇ operator is understood to mean the row vector

$$\nabla=\begin{bmatrix}\frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z}\end{bmatrix}\ . \tag{14}$$

Alternatively, the last term in Eq. (11) could be written in shorthand as $\nabla\cdot(\Psi^\dagger \mathbf{v}\mathbf{o}\Psi)=\partial_i(\Psi^\dagger v^i \mathbf{o}\Psi)$.

Equation (11) is a general theorem concerning the effect of an operator on the quantum-mechanical wave function of an electron. As specific examples, we will let the function $\mathbf{o}$ in Eq. (11) represent the scalar constant e, the vector $\boldsymbol{\mu}=e\mathbf{r}$, the differential operators $\mathbf{p}=-i\hbar\nabla-e\mathbf{A}$, $\boldsymbol{l}=\mathbf{r}\times\mathbf{p}$, $u=i\hbar\partial/\partial t-e\phi$, and the matrix operator $\mathbf{s}=(-i\hbar/4)\boldsymbol{\alpha}\times\boldsymbol{\alpha}$. The results of these substitutions are given in Table I. The first of the equations in the table is the familiar result ensuring conservation of charge; and, as will be discussed in Sec. III, the forms of the $\boldsymbol{\alpha}$ and β matrices were chosen in part to ensure that this conservation equation would result. The quantity $\boldsymbol{\rho}_\mu$ in the second equation in the table can be recognized as the electric dipole moment density, and a similar equation arises in discussions of Hertzian dipoles.

It is clear from fluid mechanical analogies that the parameter $\boldsymbol{\rho}_p$ appearing in the third equation in the table represents the momentum density, while the term $\mathbf{f}=\rho_e\mathbf{E}+\mathbf{J}_e\times\mathbf{B}$ represents the force density, and $\mathbf{J}_p$ is the momentum-current density. In tensor notation the momentum equation for a classical uncharged fluid has been written [20]

$$\frac{\partial}{\partial t}(\rho_m v_i)=-\frac{\partial p}{\partial x_i}-\frac{\partial(v_k\rho_m v_i)}{\partial x_k}\ , \tag{15}$$

TABLE I. Fluid equations for a Dirac wave function.

Density definitions		Equations
Charge:	$\rho_e=\psi^\dagger e\psi$	$\frac{\partial\rho_e}{\partial t}=-\nabla\cdot\mathbf{J}_e$
Charge current:	$\mathbf{J}_e=\psi^\dagger \mathbf{v}e\psi$	
Dipole moment:	$\boldsymbol{\rho}_\mu=\psi^\dagger e\mathbf{r}\psi$	$\frac{\partial\boldsymbol{\rho}_\mu}{\partial t}=\mathbf{J}_e-\nabla\cdot\mathbf{J}_\mu$
Dipole moment current:	$\mathbf{J}_\mu=\psi^\dagger \mathbf{v}e\mathbf{r}\psi$	
Momentum:	$\boldsymbol{\rho}_p=\mathrm{Re}(\psi^\dagger\mathbf{p}\psi)$	$\frac{\partial\boldsymbol{\rho}_p}{\partial t}=\rho_e\mathbf{E}+\mathbf{J}_e\times\mathbf{B}-\nabla\cdot\mathbf{J}_p$
Momentum current:	$\mathbf{J}_p=\mathrm{Re}(\psi^\dagger\mathbf{v}\mathbf{p}\psi)$	
Orbital angular momentum:	$\boldsymbol{\rho}_l=\mathbf{r}\times\mathrm{Re}(\psi^\dagger\mathbf{p}\psi)$	$\frac{\partial\boldsymbol{\rho}_l}{\partial t}=\mathbf{r}\times(\rho_e\mathbf{E}+\mathbf{J}_e\times\mathbf{B})+\mathbf{C}-\nabla\cdot\mathbf{J}_l$
Orbital angular momentum current:	$\mathbf{J}_l=\mathrm{Re}(\psi^\dagger\mathbf{v}\mathbf{r}\times\mathbf{p}\psi)$	
Spin-orbit coupling:	$\mathbf{C}=\mathrm{Re}(\psi^\dagger\mathbf{v}\times\mathbf{p}\psi)$	
Spin angular momentum:	$\boldsymbol{\rho}_s=\mathrm{Re}(\psi^\dagger\mathbf{s}\psi)$	$\frac{\partial\boldsymbol{\rho}_s}{\partial t}=-\mathbf{C}-\nabla\cdot\mathbf{J}_s$
Spin angular momentum current:	$\mathbf{J}_s=\mathrm{Re}(\psi^\dagger\mathbf{v}\mathbf{s}\psi)$	
Energy:	$\rho_u=\mathrm{Re}(\Psi^\dagger u\Psi)$	$\frac{\partial\rho_u}{\partial t}=\mathbf{J}_e\cdot\mathbf{E}-\nabla\cdot\mathbf{J}_u$
Energy current:	$\mathbf{J}_u=\mathrm{Re}(\Psi^\dagger\mathbf{v}u\Psi)$	

where v_i is the i component of the velocity, ρ_m is the mass density, p is the pressure, and a summation over repeated indices is implied. It is clear that the Dirac momentum equation is exactly parallel to Eq. (15) if the electromagnetic forcing terms are replaced by the pressure gradient. Thus, the equation in the table may be regarded as an equation for the momentum density of a charged uniform pressure fluid in the presence of electric and magnetic fields.

It follows from the form of the fourth equation in Table I that ρ_l represents an orbital angular momentum density, $\mathbf{r}\times\mathbf{f}$ is a torque density, and the last term results from the spatial distribution of the angular momentum density. The "unexpected" term is the coupling $\mathbf{C}$, and this term is related to an intrinsic spin angular momentum density. In an ordinary classical fluid one would expect the velocity and momentum density to be parallel, but with a Dirac particle the density of the velocity-momentum operator cross product does not vanish.

The fifth equation in the table governs the spin density. Spin is, of course, not usually associated with a classical fluid, but one can contemplate the possibility of a fluid of small gyroscopes. The fourth and fifth equations may be combined to obtain the equation

$$\frac{\partial}{\partial t}(\rho_l+\rho_s)=\mathbf{r}\times\mathbf{f}-\nabla\cdot(\mathbf{J}_l+\mathbf{J}_s)\ . \tag{16}$$

This result governs the total angular momentum in the presence of forces due to electric and magnetic fields. The sixth equation in the table governs the energy density, and this equation may be recognized as the wave-function complement of Poynting's theorem.

III. DISCUSSION

In the previous section Dirac's equation has been used as a basis for deriving several equations that govern the wave functions of a Dirac particle. These equations are listed in Table I together with the definitions of the densities involved. For greater symmetry the indicator Re for real part could be included in all of the density definitions, even though some of the densities are intrinsically real. It should be emphasized that these formulas have been derived from Dirac's equation without approximation. A striking feature of these results is their close resemblance to the equations of classical fluid mechanics. In all cases the time derivative of a density function has been related to the divergence of an appropriate tensor source current density and sometimes also to electromagnetic forcing terms.

One of the greatest difficulties with quantum mechanics is that interpretations of the wave functions and the way in which they represent physical variables are largely lacking in intuitive content. One of the few intuitive features of the conventional theory is conservation of charge $\partial\rho_e/\partial t=-\nabla\cdot\mathbf{J}_e$, but this feature was built in at the outset. In the words of Morse and Feshbach, "We used the choice of charge and current density expressions and the requirement that they satisfy the equation of continuity to guide us in our choice of the Dirac equation" [21]. We see now that this choice of charge continuity is an arbitrary basis for that derivation. Dirac's equation is actually a package deal. That equation implies a variety of other conservation theorems, and conversely any of those theorems could be considered a basis for constructing the equation.

The theorems discussed here provide new insight into the behavior of the wave function at the microscopic level. We find that the wave function of a Dirac particle in the presence of applied fields seems to flow about in much the same way as a classical charged fluid, carrying with it momentum and angular momentum densities in the same sense that it carries charge. These results are in contrast to the Ehrenfest theorems that involve integrals over all space, require that the wave function be well behaved at large distances, and require that any electromagnetic fields be constant over the dimensions of the wave packet. In fact, Ehrenfest-like theorems can be obtained in the appropriate limits by integrating the equations shown in Table I.

When the results developed here are combined with the Maxwell-Heaviside equations, various practical semiclassical problems involving the interaction of charges and fields can be addressed. As an early example, the charge density shown in the table is the basis of Hartree's self-consistent-field method for calculating the wave functions of multielectron atoms [22]. The current density in the table can be used to calculate the magnetic field associated with an electron in an atom in a manner analogous to the field calculation for an orbiting electron in the Bohr model [23]. Similarly, in the interaction of light with atoms the dipole moment density in the table leads directly to the polarization source term in the electromagnetic field equations, and calculations of this type are the basis for treatments of light absorption and laser amplification. The momentum density functions in the table can be used for dynamical calculations, and for example the momentum distribution or trajectory of an orbiting electron wave packet in a Rydberg atom could be calculated [24].

While the results of calculations such as some of those that have just been mentioned may ultimately be the same as in previous semiclassical models, the derivations suggested here are conceptually more direct. The interpretation of the density functions follows unambiguously from the form of theorems that are themselves exact consequences of Dirac's equation. By contrast, in conventional semiclassical models the form of the operators may be determined in a more roundabout way, and the justification for introducing the expectation values of those operators into the classical fluid or electromagnetic equations is more obscure.

As a final observation, it may be remarked that though the theorems described here have been derived in an exact and straightforward way from Dirac's equation; for the most part these theorems do not have close parallels starting from Schrödinger's equation. The reason for this limitation of the Schrödinger model may be understood from a consideration of Poynting's theorem of electromagnetics. In studies of electromagnetic wave propagation in free space, one commonly begins by constructing from the Maxwell-Heaviside equations an exact wave

equation that is second order in time and space. Some of the higher derivatives may then be eliminated from this equation by means of slowly varying envelope (SVE) or paraxial approximations. It is evident that after these approximations one could no longer derive Poynting's theorem, which is an exact consequence of the original Maxwell-Heaviside equations. In the same way, the exact theorems developed here are not necessarily consistent with the more approximate Schrödinger equation.

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