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Fluid-dynamical representations of the Dirac equation

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Abstract. A relative kinetic mass operator is defined by $m = c^{-2}(E - e\Phi)$, and it is shown that by using it in a symmetric form one can correlate the (charge) velocity operator α in the Dirac theory exactly with the general quantum mechanical momentum $-i\hbar\nabla$. Then the net force, defined as the rate of change of the relative momentum with time, is exactly equal to the Lorentz force. The contribution due to the time variation of mass equals the negative of space variation of the scalar potential, the Newtonian force, whereas the time variation of the charge current absorbs the entire vector potential dependence. The analogous Euler equations can be written either in terms of the charge current or in terms of the mass current. For a many particle system one needs the usual net single particle parameters and the consideration of both the direct and exchange contributions of the two particle interaction. These Euler equations yield two different conditions of the stationary state. It is shown that the charge-current condition is necessary but not sufficient, whereas the mass-current condition retains the appropriate scalar potential dependence. These two conditions are compared for the spherically symmetric case. The charge density, charge current and relative mass current are tabulated for atomic spinors. Differences between the quantum and classical forces for the H_2^+ molecular ion exhibit the inadequacy of ordinary atomic spinor basis in forming molecular spinors.

Keywords. Relativistic; fluid dynamics; kinetic mass; force; Euler equation.

1. Introduction

The growth of relativistic molecular quantum mechanics (Pitzer 1979; Pyykkö and Desclaux 1979; Sucher 1980) and that of the relativistic density functional formalism (Rajgopal 1980; McDonald 1979) have by now sufficiently matured. At present it is of theoretical interest to examine fluid-dynamical interpretations of the relativistic equations of motions such that a consistent relationship between (charge) density (ρ), (charge) current ($\mathcal{J}$) and stress tensors should emerge.

Some related treatments are already available in the literature. Jehle considered the background of a theory with quantized flux as the primary phenomenon, and 'loop form' of it for a charged lepton, in terms of superpositions of quantum flux lines 'associated' with solutions of the Dirac equation (Jehle 1968, 1969). 'Hydrodynamical' formulations led Birula to prepare a theory for 'dyons' (Birula 1971a, b). In the nonrelativistic version Riess and Primas (1968) discussed a variation principle for the phase of wavefunctions and Riess (1970) discussed the quantization of magnetic flux. Hirschfelder and coworkers defined quantum mechanical streamlines forming quantized vortices (Hirschfelder *et al* 1974). In all these works closed loops of

quantum flux lines follow directly from the mere existence of a current density defined in the equation of continuity.

The aim of this work is to show that Dirac's equation gives rise to two possible forms of fluid-dynamical equations, and that there is an inherent relationship in going from the ' charge ' picture to the ' mass ' picture.

On the other hand the *reverse* idea, fluid-dynamical *formulation* of the Dirac equation, is already available. This formulation is in general made through a stochastic approach. For example, definition of a mean acceleration leads to a formulation of the wave equations, the Schrödinger equation in a nonrelativistic treatment (Nelson 1966) and with relativistic adjustments (discrete time and speed of light to stochastic particles), the relativistic generalization of the Fokker-Planck equation (Lehr and Park 1977). New internal variables (classical counterparts of spins) in an extended relativistic fluid droplet can be defined to obtain the Feynman-Gell-Mann wave equation by quantization (Depaquit *et al* 1972). Depletion velocity, rotational in form, of a superfluid flow in an annular region generates quantum mechanical vortex lines by drawing analogy with Dirac's theory of a magnetic monopole (Ichiyanagi 1979). Perhaps the most comprehensive stochastic approach is made by Aron (1979) in showing the generalization of classical diffusion theory to the relativistic domain by a convenient choice of the basic constants: this elegant treatment gives rise to a model of the Dirac fluid and clarifies several concepts like spin, nonlocalization and local rotations. In a recent work Petroni and Vigier (1981) show that stochastic behaviour of classical rigid tops embedded in Dirac's ether generates results comparable to the Feynman-Gell-Mann equation.

In this paper instead of deriving the Dirac equation from a classical stochastic approach, fluid-dynamical representations of the Dirac equation are made. It must be mentioned that Hestenes (Hestenes 1973, 1975, 1979) carried out an elaborate discussion on fluid-dynamical representations using a geometrical reformulation of the Dirac theory, in terms of Lorentz-rotated axes. Here derivation of appropriate conditions for the stationary states is taken up. Whenever it is felt necessary, comparisons with the results of Hestenes (Hestenes 1973, 1975, 1979) are included.

In special relativity one considers a (kinetic) relative mass dependent on the speed of the system with respect to a suitable Galilean frame of reference. This should affect the descriptions of the Newtonian 3-force (**F**) and the relative momentum density or relative mass current (**J**). A (kinetic) relative mass operator is being defined as

$$\hat{\mathbf{m}} = c^{-2}\,(\hat{E} - e\Phi). \tag{1}$$

The same operator is used here in examining Newtonian and fluid-dynamical characteristics of a Dirac system.

The description of the Newtonian 3-force is important since its expression must correlate with $\dot{\mathbf{r}}$ which can be derived in the Heisenberg picture, thus removing certain ambiguity that exists in the theoretical description of the velocity and linear momentum operator (Feynman 1961). In fact the present work stems from the idea of removing this ambiguity in a *constructive* fashion.

The form of the charge current in the Dirac theory implies that its time variation is *independent* of the scalar potential, resulting in an insufficient condition of the

stationary states. One requires a suitable definition of the relative mass current (or, momentum density) and the Euler equation should be described as its time variation such that the physical dependence on the scalar field is retained. Moreover, the relative mass current must correspond to the usual quantum mechanical linear momentum operator $-i\hbar\nabla$.

In concluding remarks fluid-dynamical parameters of a spherically symmetric system are tabulated, and the conditions for stationary states are illustrated for the atomic case and for the H_2^+ molecule ion using an approximate basis.

2. The Dirac equation

The Dirac equation is

$$i\hbar\frac{\partial}{\partial t}\psi = H_D\,\psi \equiv c\left(-i\hbar\nabla - \frac{e}{c}\mathbf{A}\right)\cdot\boldsymbol{\alpha}\,\psi + \beta\, m_0\, c^2\,\psi + e\,\Phi\,\psi \tag{2}$$

where m_0 is the proper mass, $(-\mathbf{A}, \Phi)$ is the 4-potential and $\boldsymbol{\alpha}$, β are Dirac matrices. ψ is a 4-component spinor. It is almost a trivial task to derive the equation of continuity

$$\dot{\rho} + \nabla\cdot\mathcal{J} = 0 \tag{3}$$

with $\rho = \psi^\dagger\,\psi$

and $\mathcal{J} = \psi^\dagger\, c\,\boldsymbol{\alpha}\,\psi.$

This corresponds to a velocity field (Bohm 1952; Madelung 1926; Landau 1945; Wong 1976)

$$\mathbf{v} = \psi^\dagger\, c\,\boldsymbol{\alpha}\,\psi/\rho$$

with the comparable velocity operator that can be derived by the Heisenberg equation of motion

$$\hat{\mathbf{v}} = \dot{\mathbf{r}} = c\,\boldsymbol{\alpha}.$$

There is some controversy in this regard. As Feynman (1961) puts it, the operator form of $\hat{\mathbf{v}}$ is "different from $\hat{\mathbf{p}}/m$" $\equiv -i\hbar/m\,\nabla$; furthermore since $\hat{\mathbf{v}}$ and $\hat{\mathbf{p}}$ commute, they become simultaneously measurable. Using the Maxwell relationship

$$\mathcal{E} = -\frac{1}{c}\dot{\mathbf{A}} - \nabla\Phi \tag{4}$$

one obtains

$$\frac{\partial}{\partial t}\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right) = e\,(\mathcal{E} + c\,\boldsymbol{\alpha}\times\mathcal{H}) \equiv F_L, \tag{5}$$

the analogous Lorentz force, where $\mathscr{E}$ and $\mathscr{H} = \nabla \times \mathbf{A}$ are the conventional electric and magnetic fields. But since there is no direct connection between $\dot{\mathbf{r}}$ and (5), it is difficult to accept it ' as a suitable analogue ' of Newton's equations.

This apparent discrepancy arises because of the wrong interpretation of ρ and $\mathscr{J}$ as being particle probability density and current. This becomes obvious by comparing the nonrelativistic limit (the Pauli equation) where one has a *different* particle density and current. In fact, $e\rho$ and $e\,\mathscr{J}$ should represent the *charge* density and *charge* current. $\mathbf{v}$ should indicate the velocity field for a unit *charge* (cf. charge conjugation). Interestingly enough, the same point about two different probability densities is also discussed by Aron (1979) in a stochastic formulation of the Klein-Gordon equation. Nevertheless, a relation between the velocity of charge and linear momentum of relative mass is desired.

The difficulty is removed if one can show that the combination of $\hat{\mathbf{v}}$ with $\hat{m}$ leads to the result $\hat{\mathbf{p}}$. One recalls that m itself depends on speed and thereby should be evaluated in the status of an operator, as given by (1). In the Dirac case equation (1) reduces to

$$\hat{m} = c^{-2}(H_D - e\,\Phi). \tag{6}$$

The momentum operator should be hermitean; but $\hat{m}$ and $\hat{\mathbf{v}}$ do not commute. Hence one requires that $\hat{m}$ and $\hat{\mathbf{v}}$ should be bound together in a symmetric form to yield the net relative momentum

$$\hat{\mathbf{M}} = \tfrac{1}{2}(\hat{m}\,\hat{\mathbf{v}} + \hat{\mathbf{v}}\,\hat{m}). \tag{7a}$$

Using (6) and the anticommutations $[\mathbf{X}\cdot\boldsymbol{\alpha}, \boldsymbol{\alpha}]_+ = 2\,\mathbf{X}$ and $[\boldsymbol{\alpha}, \beta]_+ = 0$, one obtains

$$\hat{\mathbf{M}} = \left(-i\,\hbar\,\nabla - \frac{e}{c}\mathbf{A}\right) \tag{7b}$$

so that it is identical to the definition of the linear momentum operator.

Thus there is no ambiguity. One can easily show that the net 3-force defined as $\mathbf{F} = \dot{\mathbf{M}}$ equals the Lorentz force $\mathbf{F}_L$. Still, it is interesting to dissect the two parts of this force, particularly the part ($\mathbf{F}_1$) arising out of the time variation of mass

$$\mathbf{F} = \mathbf{F}_1 + \mathbf{F}_2 = \mathbf{F}_L, \tag{8}$$

where $\mathbf{F}_1 = \tfrac{1}{2}(\dot{m}\,c\,\boldsymbol{\alpha} + c\,\boldsymbol{\alpha}\,m)$,

and $\mathbf{F}_2 = \tfrac{1}{2}(m\,c\,\dot{\boldsymbol{\alpha}} + c\,\dot{\boldsymbol{\alpha}}\,m) \equiv \mathbf{F}_L - \mathbf{F}_1$.

Equation (6) leads to the result $\mathbf{F}_1 = -e\,\nabla\,\Phi$. Consequently, $\mathbf{F}_2 = -e/c\,\dot{\mathbf{A}} + ec\,\boldsymbol{\alpha} \times \mathscr{H}$. Thus *the entire scalar potential dependence is correlated to the variation of mass, and the vector potential dependence is totally absorbed by the variation of the speed of charge.* This derivation is *exact.*

The time dependence of the (charge) velocity operator α is given by

$$\dot{\alpha} = -\frac{i}{\hbar}[\alpha, H_D]_- = \frac{2ic}{\hbar}\left(-i\hbar\nabla - \frac{e}{c}\mathbf{A}\right) - \frac{2i}{\hbar}\alpha H_D^0,$$

where H_D^0 is the free particle Dirac hamiltonian. The general solution is

$$\alpha(t) = \alpha(0)\exp\left(-\frac{2i}{\hbar}H_D^0 t\right) + c\left[\mathbf{p}(0) - \frac{e}{c}\mathbf{A}(0)\right]H_D^{0\,-1}$$

$$\left[1 - \exp\left(-\frac{2i}{\hbar}H_D^0 t\right)\right] + \frac{2ic}{\hbar}\int_0^t d\tau \int_0^\tau d\tau'\, \mathbf{F}_L(\tau')$$

$$\exp\left(-\frac{2i}{\hbar}H_D^0(t-\tau)\right). \tag{9}$$

In the field-free case (A = 0)

$$\alpha(t) = \alpha(0) + \{\alpha(0) - c\,\mathbf{p}_0 H_D^{0\,-1}\}\left\{\exp\left(-\frac{2i}{\hbar}H_D^0 t\right) - 1\right\}$$

as given by Messiah (1962). These results show an oscillatory time dependence. The (charge) accelaration equals $c\dot{\alpha}$ which can be correlated to the 3-force.

In view of the present formalism the non-collinearity of the local velocity and momentum operators, that is, the asymmetry in the Dirac theory (Hestenes 1973, 1975, 1979; Gutler and Hestenes 1975) is to be compared with the requirement of symmetrically combining $\hat{m}$ and $\hat{v}$ in order to reproduce a hermitean $\hat{p}$. The present study does not examine this comparison, instead it is left as a subject for yet another (future) discussion. That the local 3-force is the Lorentz force is also a finding of Hestenes (Hestenes 1973, 1975, 1979) starting with the definition of an energy-momentum tensor. Here, however, it appears out of the symmetric combination of $\hat{m}$ with α.

3. Analogues of the Euler equation

The nonrelativistic form of the analogous Euler equation considers variation of the probability current with respect to time such that an expression involving stress tensors and the scalar force is obtained; the mass m remains independent of speed.

From the Dirac equation the charge current is determined by the speed of the charge and its time variation involves only the vector potential. Using the commutation $[\alpha_i, \alpha_j]_- = 2i\epsilon_{ijk}\sigma_k$ one obtains

$$\dot{\mathcal{J}}_i + \sum_{j=1}^{3}\nabla_j(\psi^\dagger v_j v_i \psi + \delta_{ij}^{(q)}) = 0, \tag{10}$$

where the quantum stress density $\nabla_j \delta_{ij}^{(q)}$ is given by

$$\nabla_i \delta_{ii}^{(q)} = -\frac{2i}{\hbar} m_0 c^2 \psi^\dagger \beta v_i \psi - \frac{2ec}{\hbar} \psi^\dagger (\sigma \times \mathbf{A})_i \psi,$$

and $$\nabla_j \delta_{ij}^{(q)} = 2ic^2 \psi^\dagger \sigma_k \nabla_j \psi \epsilon_{ijk}.$$

Here stress densities are only kinetic in nature. Hence the *kinetic* Euler equation (10) with $\dot{\mathcal{J}} = 0$ generates a necessary but *not* a sufficient condition for stationary states belonging to a specific scalar potential:

$$\text{Im}\{\psi^\dagger \alpha H_D^0 \psi\} = 0. \tag{11}$$

In other words, every stationary state satisfies (11), but every ψ satisfying (11) is *not* necessarily a stationary state for a given scalar potential. That (11) is satisfied by every stationary state is not difficult to see, since in that case the condition (11) reappears as Im $(Te - TW)$, T, W and ϵ being the kinetic energy scalar potential energy and the total energy and the equality is achieved by considering the relativistic Virial theorem (Schiff 1968) and the hermitean nature of H_D.

A more complete form of the Euler equation is obtained in terms of the relative mass current (or relative momentum density) **J** defined as

$$\mathbf{J} = \text{Re}\{\psi^\dagger \hat{\mathbf{M}} \psi\}. \tag{12}$$

Substituting the expression of $\hat{\mathbf{M}}$ from (6) one obtains the Gordon current

$$\mathbf{J} = \frac{1}{2}\left[\left\{\left(i\hbar \nabla - \frac{e}{c}\mathbf{A}\right)\psi^\dagger\right\}\psi + \psi^\dagger\left(-i\hbar \nabla - \frac{e}{c}\mathbf{A}\right)\psi\right], \tag{12a}$$

identical with the *nonrelativistic* expression of $m\mathcal{J}$. Using Dirac equation and the result $[\alpha \cdot \mathbf{X}, \alpha]_- = 2i\sigma \times X$, one obtains the analogous Euler equation

$$\dot{J}_i + \sum_{j=1}^{3} \nabla_j \left[\text{Re}\left\{\psi^\dagger v_j \left(p_i - \frac{e}{c}A_i\right)\psi\right\} + \mathcal{T}_{ij}^{(q)}\right] = \rho e \mathcal{E}_i \tag{13}$$

with the associated stress densities

$$\nabla_j \mathcal{T}_{ij}^{(q)} = -e\psi^\dagger \alpha_j \mathcal{H}_k \psi \epsilon_{ijk}.$$

For a stationary state stress densities must balance the kinetic term (since $\dot{J}_i + (e/c)\rho \dot{\mathbf{A}}_i = 0$) and the force density:

$$\sum_{j=1}^{3} \nabla_j \left[\text{Re}\left\{\psi^\dagger v_j \left(p_i - \frac{e}{c}A_i\right)\psi\right\} + \mathcal{T}_{ij}^{(q)}\right] = -e\rho \nabla_i \Phi. \tag{14}$$

This is a more restrictive condition than (11) and stationary states are now characteristic of a scalar potential.

Net current density in the Dirac theory is the sum of the relative mass (Gordon) current and the magnetic moment density due to the electron spin. Conservation laws for local p, S (spin) and E are not repeated here since they have already been considered by Gurtler and Hestenes (1975). Conservation laws for J and S are expected to describe the Dirac stationary state. Therefore, the following discussion is limited to the comparison of the conservations of $\mathcal{J}$ and J.

4. Many-particle systems

In the time dependent Dirac-Fock scheme the Dirac hamiltonian is modified by the two particle interaction

$$i\hbar\,\dot{\psi} = [H_D + V(\mathbf{r}, t)]\,\psi \tag{15}$$

where $V(\mathbf{r}, t)$ encompasses both the direct and exchange interactions

$$\begin{aligned} &V(\mathbf{r}, t)\,\psi(\mathbf{r}, t) \\ &= \int \mathrm{d}^3\,\mathbf{r}_2 \sum_k \{\psi_k^\dagger(\mathbf{r}_2, t)\,\psi_k(\mathbf{r}_2, t) f_k\,\tilde{V}(\mathbf{r}, \mathbf{r}_2)\,\psi(\mathbf{r}, t) \\ &\quad - \psi_k^\dagger(\mathbf{r}_2, t)\,\psi_k(\mathbf{r}, t) f_k\,\tilde{V}(\mathbf{r}, \mathbf{r}_2)\,\psi(\mathbf{r}_2, t)\}, \end{aligned}$$

f_k being the (fractional) occupancy of the kth spinor. The equation of continuity, (3), is now achieved by considering the net single particle parameters

$$\begin{aligned} &\dot{n} + \nabla \cdot \mathcal{J} = 0, \\ &n(\mathbf{r}, t) = \sum_k \rho_k(\mathbf{r}, t) f_k, \qquad (16) \\ \text{and} \quad &\mathcal{J}(\mathbf{r}, t) = \sum_k \mathcal{J}^{(k)}(\mathbf{r}, t) f_k. \end{aligned}$$

The kinetic Euler equation is almost trivially generated from (10); however, presence of the operator α in $\mathcal{J}^{(k)}$ provides a contribution from the two particle interaction

$$\begin{aligned} &\dot{\mathcal{J}}_i + \sum_{j=1}^{3} \nabla_j \sum_k \{\psi_k^\dagger v_j v_i \psi_k + S_{ij}^{(k)})\} f_k \\ &= \frac{2c}{\hbar}\,\mathrm{Im} \int \mathrm{d}^3\,\mathbf{r}_2\,\mathcal{N}(\mathbf{r}_2, \mathbf{r}; t)\,\tilde{V}(\mathbf{r}, \mathbf{r}_2)\,\mathcal{J}_i(\mathbf{r}, \mathbf{r}_2; t), \end{aligned} \tag{17}$$

where $\mathcal{N}(\mathbf{r}, \mathbf{r}'; t)$ and $\mathcal{J}(\mathbf{r}, \mathbf{r}'; t)$ are conventional Dirac-Fock (charge) density and (charge) current

$$\mathcal{N}(\mathbf{r}, \mathbf{r}'; t) = \sum_k \psi_k^\dagger(\mathbf{r}', t)\, \psi_k(\mathbf{r}, t)\, f_k, \tag{17a}$$

and

$$\mathcal{J}(\mathbf{r}, \mathbf{r}'; t) = C \sum_k \psi_k^\dagger(\mathbf{r}', t) \propto \psi_k(\mathbf{r}, t)\, f_k. \tag{17b}$$

A similar treatment with the relative momentum density $J^{(k)}(\mathbf{r}, t)$ using the electric field $\mathcal{E}$ converts (13) into

$$\dot{j}_i^{(k)} + \sum_{j=1}^{3} \nabla_j \left[\mathrm{Re} \left\{ \psi_k^\dagger v_j \left(p_i - \frac{e}{c} A_i \right) \psi_k \right\} + \mathfrak{T}_{ij}^{(k)} \right] = e\, \rho_k\, \mathcal{E}_i$$

$$+ \text{direct term} + \text{exchange term},$$

where the direct term $= -\,\mathrm{Re} \int \mathrm{d}^3 \mathbf{r}_2\, \rho(\mathbf{r}_2, t)\, \nabla_i \tilde{V}(\mathbf{r}, \mathbf{r}_2)\, \rho_k(\mathbf{r}, t)$,

and the exchange term $= -\,\mathrm{Re} \int \mathrm{d}^3 \mathbf{r}_2 \{ \mathcal{N}(\mathbf{r}_2, \mathbf{r}; t)\, \tilde{V}(\mathbf{r}, \mathbf{r}_2)\, \psi_k^\dagger(\mathbf{r}_2, t)$

$$\nabla_i \psi_k(\mathbf{r}, t) - \nabla_i (\mathcal{N}(\mathbf{r}, \mathbf{r}_2; t)\, \tilde{V}(\mathbf{r}, \mathbf{r}_2))\, \psi_k^\dagger(\mathbf{r}, t)\, \psi_k(\mathbf{r}_2, t) \},$$

for a *real* and *symmetric* two particle interaction, $\tilde{V}(\mathbf{r}, \mathbf{r}_2) = \tilde{V}(\mathbf{r}_2, \mathbf{r})$. The net relative momentum density J,

$$J(\mathbf{r}, t) = \sum_k J^{(k)}(\mathbf{r}, t)\, f_k,$$

can be utilized to write the net Euler equation

$$\dot{J}_i + \sum_{j=1}^{3} \nabla_j \sum_k \left[f_k\, \mathrm{Re} \left\{ \psi_k^\dagger v_j \left(p_i - \frac{e}{c} A_i \right) \psi_k \right\} + \mathfrak{T}_{ij}^{(k)} \right]$$

$$= e\rho\, \mathcal{E}_i - \mathrm{Re} \int \mathrm{d}^3 \mathbf{r}_2 \{ \rho(\mathbf{r}_2, t)\, \rho(\mathbf{r}, t) - |N(\mathbf{r}, \mathbf{r}_2; t)|^2 \}$$

$$\otimes \nabla_i \tilde{V}(\mathbf{r}, \mathbf{r}_2). \tag{18}$$

As usual, the change for a many particle system has been two-fold; (i) one needs to consider the net single particle parameters and (ii) the force density is suitably

modified to add the direct and exchange contribution of two-electron interactions to the external force density.

5. Discussion

In § 2 a mass operator has been defined which is hermitean and which, in combination with the velocity operator $c\alpha$, reproduces a consistent linear momentum operator $\mathbf{p}=-i\hbar\nabla$. The net 3-force is therefore identical with the Lorentz force $\mathbf{F}_L$, whereas the time variation of *only* relative mass in $\mathbf{p}$ is given by $\mathbf{F}_1 = -e\nabla\Phi$.

In the nonrelativisitic limit $mc^2 \simeq m_0c^2 + \frac{1}{2m_0}\left(-i\hbar\nabla - \frac{e}{c}\mathbf{A}\right)^2 + \ldots$, such that to the lowest order (c^{-2}) $\dot{m} = -(i/2\,\hbar m_0 c^2)\left[\left(-i\hbar\nabla - \frac{e}{c}\mathbf{A}\right)^2, H_D\right]_-$. The force $\mathbf{F}_1$ can then be described as (to order c^{-2})

$$\mathbf{F}_1 = \mathbf{F}_{11} + \mathbf{F}_{12} + \mathbf{F}_{13}$$

where $$\mathbf{F}_{11} = -\frac{e}{m_0c^2}\,\mathbf{v}\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)\cdot\nabla\Phi,$$

$$\mathbf{F}_{12} = -\frac{i\hbar}{2m_0\,c}\,e\,\nabla^2\mathbf{A},$$

and $$\mathbf{F}_{13} = \frac{e}{m_0c}\,\mathcal{H}\times\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right).$$

The first term describes the kinetic modification of the gradient of the scalar potential and the second term similarly describes the kinetic modification of the gradient of the vector potential; the third term represents coupling of the magnetic field with the particle momentum spaced over the Compton wavelength. In this fashion one may attempt to reveal different interactions that contribute to the variation of mass.

The time variation of speed takes a simple appearance in case the Lorentz force is chosen to be invariant of time. In this case (9) reduces to the form

$$\alpha(t) - \alpha(0) = -\left\{\alpha(0) - c\left(\mathbf{p}(0) - \frac{e}{c}\mathbf{A}(0)\right)H_D^{0\,-1}\right.$$

$$\left. - c\,\mathbf{F}_L\,H_D^{0\,-1}\left(1 - \frac{2i}{\hbar}H_D^0\right)^{-1}\right\}\left\{1 - \exp\left(-\frac{2i}{\hbar}H_D^0\,t\right)\right\}.$$

The definition of the mass operator in (6) thus appears to satisfy all related theoretical expressions in a consistent fashion. A word of caution is included here. For example, for a stationary state in the region $E - e\Phi < 0$, $(m - m_0)$ appears to be negative and one should refrain from interpreting it as an admixture of negative energy states. The same phenomenon occurs with negative kinetic energy in the

nonrelativistic case, and this is to be physically interpreted as the uncertainty involved with the determination of kinetic energy. The positional uncertainty in this region creates an uncertainty in momentum which gives rise to an uncertainty in kinetic energy that supersedes the decreasing amount of the relative mass.

The fluid-dynamical representation offers a simple description in terms of macroscopic parameters like ρ (r, t), v (r, t) and stress densities. As in the nonrelativistic situation (Bohm 1952; Madelung 1926; Landau 1945; Wong 1976) these may find applications in the description of collision processes or in relativistic density functional formalism. For stationary states one obtains the requirement that stresses must balance the force densities appearing in the Euler equation. The non-diagonal components of the stress tensors are responsible for vorticity in the system.

We now examine the difference between the two Euler conditions, equations (11) and (14), for a centrally symmetric system retaining atomic symmetry for the single-particle states, given by

$$\psi_p (r, \theta, \phi; t) = r^{-1} \begin{bmatrix} P_{n_p k_p} (r, t) & \chi_{k_p m_p} (\theta, \phi) \\ i\, Q_{n_p k_p} (r, t) & \chi_{-k_p m_p} (\theta, \phi) \end{bmatrix} \tag{19a}$$

in the notation of Rose (1957). P and Q are respectively the 'upper' and 'lower' components. For a stationary state one obtains (Rose 1957):

$$c \left[\frac{\partial}{\partial r} \left(\frac{P}{r} \right) + \frac{K+1}{r^2} P \right] = (E - V + m_0 c^2) \frac{P}{r}, \tag{19b}$$

and

$$c \left[\frac{\partial}{\partial r} \left(\frac{Q}{r} \right) - \frac{K-1}{r^2} Q \right] = - (E - V - m_0 c^2) \frac{Q}{r}.$$

For a vanishing vector potential

$$\psi^{\dagger}_{nj\mu}\ \alpha \left\{ c\ \alpha \cdot \mathbf{p}\ \psi_{nj\mu} + m_0 c^2 \beta\ \psi_{nj\mu} \right\}$$

$$= \mathrm{Im}\, (\chi^{*}_{-k\mu}\ \tau\ \chi_{k\mu})\ (E_n - V)\ P_n\ Q_n / r^2;$$

τ = Pauli spin matrix; V = scalar potential.

Thus (11) is satisfied for any stationary state of any centrally symmetric scalar potential without any guarantee that $\psi_{nj\mu}$ is a stationary state of a particular potential. The validity depends only on the spherical symmetry of the system, rather than the exact form of the potential.

Under similar conditions

$$\sum_{j=1}^{3} \nabla_j\, \mathrm{Re} \left\{ \psi^{\dagger}\, v_j\, p_i\, \psi \right\} = c \left[\psi^{\dagger}\, \nabla_i\, \alpha \cdot p\, \psi - (\alpha \cdot p\ \psi)^{\dagger}\, \nabla_i \psi \right] = - \rho\, \nabla_i\, e\, \Phi,$$

the last result being derive for a stationary state. Then (14) is satisfied for stationary states of a particular scalar potential.

For the purpose of future reference it is useful to calculate $\mathcal{J}$ and **J** corresponding to the atomic symmetry, equation (19a):

$$\mathcal{J}(\mathbf{r}, \theta, \phi) = 2c\, r^{-2}\, P(r, t)\, Q(r, t)\, \mathrm{Im}\, \{\chi^*_{-k,\mu}\, \tau\, \chi_{k,\mu}\},$$

and $$\mathbf{J}(r, \theta, \phi) = -\hbar\, \mathrm{Im}\, \{\psi^\dagger\, \nabla\, \psi\}.$$

Table 1 summarizes ρ_k, $\mathcal{J}^{(k)}$ and $\mathbf{J}^{(k)}$ for different angular symmetries. The currents illustrate vortices or circulations as readily expected from the mere existence of the current density (Jehle 1968, 1969; Birula 1971a, b; Riess and Primas 1968; Riess 1970; Hirschfelder *et al* 1974). These currents vanish for a relativistically closed shell.

Hydrogen atomic basis is given by (Pavlik and Blinder 1967)

$$\psi_{1s_{1/2}} = \begin{Bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{Bmatrix} \quad \text{with} \quad \begin{Bmatrix} \psi_3 \\ \psi_4 \end{Bmatrix} = (2m_0\, c)^{-1} \left\{1 + \frac{E - e\,\Phi}{2m_0\, c^2}\right\}^{-1} \tau \cdot \mathbf{p} \begin{Bmatrix} \psi_1 \\ \psi_2 \end{Bmatrix}$$

where $$\begin{Bmatrix} \psi_1 \\ \psi_2 \end{Bmatrix} = \begin{Bmatrix} e^{-Zr}\, r^{\gamma-1} \\ 0 \end{Bmatrix},$$

and $$\gamma = (1 - \alpha^2\, Z^2)^{1/2}.$$

Z is the effective nuclear charge divided by the Bohr radius and α is the fine structure constant. $r^{\gamma-1}$ is necessary to generate the correct behaviours near nucleus. For simplicity we may disregard this term to obtain the approximate $1s_{1/2}$ spinor

$$\psi = \left(\frac{(1+\gamma)\, Z^3}{2\pi}\right)^{1/2} \begin{Bmatrix} e^{-Zr} \\ 0 \\ -i\left(\dfrac{1-\gamma}{1+\gamma}\right)^{1/2} e^{-Zr} \cos\theta \\ -i\left(\dfrac{1-\gamma}{1+\gamma}\right)^{1/2} e^{-Zr} \sin\theta\, e^{i\phi} \end{Bmatrix},$$

where both the charge and spin symmetry is retained. A straightforward treatment with this description of an atomic system shows that the quantum force

$$\mathbf{F}^Q_x = -\frac{i\hbar c}{\rho} \sum_{j=1}^{3} \nabla_j\, (\psi^\dagger\, \alpha_j\, \nabla_x\, \psi)$$

Table 1. Relative (charge) density n, current density $\mathcal{J}$ and mass current J for atomic symmetry.

Spinors (Angular symmetry)	n	$\mathcal{J}$ in terms of the unit vector ϕ	J in terms of the unit vector ϕ
$s \pm \frac{1}{2}$	$(P^2 + Q^2)/4\pi r^2$	$\pm (cPQ \sin \theta/2\pi r^2)$	$\pm (\hbar Q^2 \sin \theta/4\pi r^3)$
$p^* \pm \frac{1}{2}$	$(P^2 + Q^2)/4\pi r^2$	$\mp (cPQ \sin \theta/2\pi r^2)$	$\pm (\hbar P^2 \sin \theta/4\pi r^3)$
$p \pm 3/2$	$3 \sin^2 \theta (P^2 + Q^2)/8\pi r^2$	$\pm (3\, cPQ \sin^2 \theta/4\pi r^2)$	$\pm (3\hbar (P^2 + (1 + \sin^2 \theta)Q^2) \sin \theta/8\pi r^3)$
$p \pm \frac{1}{2}$	$(3 \cos^2 \theta + 1)(P^2 + Q^2)/8\pi r^2$	$\pm (cPQ (9 \cos^2 \theta - 1) \sin \theta/4\pi r^2)$	$\pm (\hbar (P^2 + 9Q^2 \cos^2 \theta) \sin \theta/8\pi r^3)$
$d^* \pm 3/2$	$3 \sin^2 \theta (P^2 + Q^2)/8\pi r^2$	$\mp (3\, cPQ \sin^2 \theta/4\pi r^2)$	$\pm (3\hbar ((1 + \sin^2 \theta) P^2 + Q^2) \sin \theta/8\pi r^3)$
$d^* \pm \frac{1}{2}$	$(3 \cos^2 \theta + 1)(P^2 + Q^2)/8\pi r^2$	$\mp (cPQ (9 \cos^2 \theta - 1) \sin \theta/4\pi r^2)$	$\pm (\hbar (9P^2 \cos^2 \theta + Q^2) \sin \theta/8\pi r^3)$
Relativistic closed shell	$(P^2 + Q^2)/2\pi r^2$	0	0

$P(r, t)$ and $Q(r, t)$ are upper and lower (radial) components. Polar coordinates (r, θ, ϕ) have been employed.

equals the classical force, F_x^{cl},

$$F_x^Q = -\frac{Z e^2 x}{r^3} \equiv F_x^{\mathrm{cl}}$$

which is consistent with (14) (simply because of the correct symmetry rather than the accurate radial behaviour).

But the chosen atomic basis need not necessarily be a good description of molecular spinors, $\Psi_{1s\sigma 1/2} = [2(1+s)]^{-1/2} \otimes [\psi^A_{1s_{1/2}} + \psi^B_{1s_{1/2}}]$. In the limit $\mathbf{r}_B \to \mathbf{r}_A$ the atomic equality is achieved. However, in general F_x^Q need not equal F_x^{cl}.

Figure 1(a) illustrates $-F_x^Q$ to be compared with $-F_x^{\mathrm{cl}}$ in figure 1(b), for the H_2^+ molecular ion system. The difference is plotted in figure 1(c). All the forces are calculated in the xz plane ($y = 0$). In the near nuclear region $r^{\gamma-1}$ varies largely from unity, generating very poor behaviour in our approximate description of the molecular spinor. Thus the difference $(F_x^{\mathrm{cl}} - F_x^Q)$ is most pronounced [figure 1(c)]. At large distances the radial behaviour of the basis spinors improves. Yet there is a difference in magnitude between F_x^Q and F_x^{cl} in the outward region indicating the inadequacy of the description of the molecular spinor $\Psi_{1s\sigma 1/2}$ as a linear combination of only atomic $_{1s_{1/2}}$ functions.

As a future possibility, discussion on spin density is *deliberately* avoided in this work.

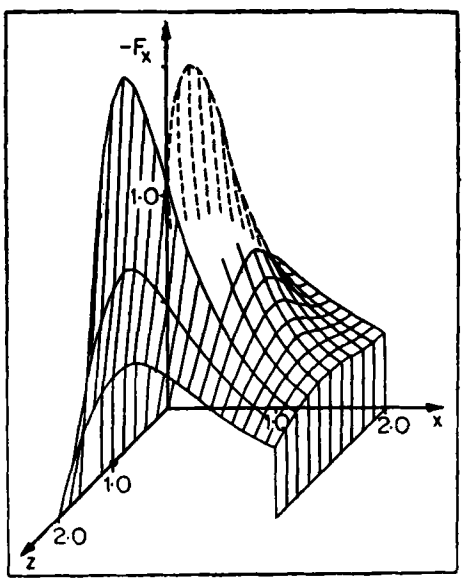

Figure 1a. F_x^{quantum} in the XZ plane. Hydrogen nuclei at $X = 0, Z = 1$ and $X = 0, Z = -1$. Atomic units have been used throughout.

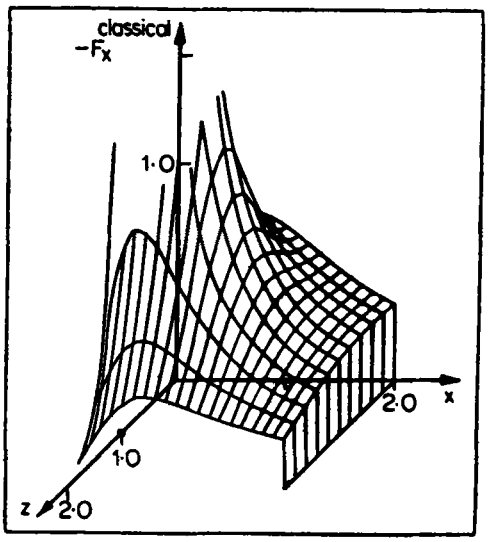

Figure 1b. $F_x^{\text{classical}}$ in the XZ plane. Hydrogen nuclei at $X = 0, Z = 1$ and $X = 0$, $Z = -1$. Atomic units have been used throughout.

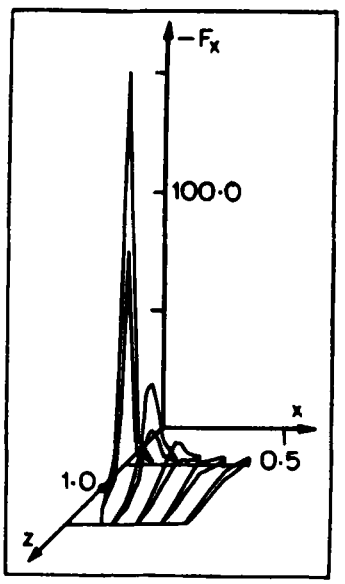

Figure 1c. F_x^{quantum} (upper surface) and $F_x^{\text{classical}}$ (lower surface) in the blown up region of XZ plane. Hydrogen nuclei at $X=0$, $Z=1$ and $X=0$, $Z=-1$. Atomic units have been used throughout.

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