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Quantum fluid dynamics within a relativistic density-functional framework

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Abstract. In this paper we explore certain interconnections between density-functional theory and quantum fluid dynamics of many-electron systems, in the relativistic domain, following the hydrodynamical approach adopted by Takabayashi for the one-particle Dirac equation. In order to build a 'classical' hydrodynamical interpretation, the spinor formulation is transformed into a tensor formulation by defining a number of density functions (local observables). These lead to six 'classical' fluid dynamical equations, together with two subsidiary conditions, for a complete specification of the system. The various density functions and the hydrodynamical equations are physically interpreted. The relativistic hydrodynamics discussed here correspond to a 'spinning' fluid. The *net* many-electron fluid consists of components each of which is characterised by fluid dynamical quantities corresponding to each spinor. The *net* hydrodynamical quantities are obtained by summing over the occupied spinors. Thus, our earlier non-relativistic 'classical' picture of the many-electron fluid as a collection of individual fluid components is also valid in the relativistic domain.

1. Introduction

In our earlier works (e.g., Deb and Bamzai 1979, Deb and Ghosh 1979, 1982, 1983, Bamzai and Deb 1981, Ghosh and Deb 1982a, b, c, 1983, Deb 1984) we have attempted to find some of the basic quantum mechanical (non-relativistic) and interpretative aspects of the single-particle density in order to provide further justification to the search for an alternative quantum mechanics of many-electron systems in terms of the charge density in 3D space, $\rho(\boldsymbol{r})$, and associated quantities. The great advantages of discussing the structures and properties of many-electron systems in 3D space are well known (see, e.g., Bamzai and Deb 1981, Ghosh and Deb 1982b, Deb 1984, Bader 1981). This view point essentially describes a system in terms of local quantities (which can lead to the corresponding global quantities by integration) such as charge density, current density, energy density, force density, an electric or magnetic property density (taking care about the choice of origin), etc. Many of these local quantities, e.g., charge density and current density, are hydrodynamical quantities and we have been exploring (Deb and Bamzai 1979, Deb and Ghosh 1979, 1982, 1983, Bamzai and Deb 1981, Ghosh and Deb 1982a, b, c, 1983, Deb 1984) certain interconnections, in the 3D

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space, between the density-functional, hydrodynamical and property density approaches in an attempt to unify, interlink and strengthen the theoretical formulations for a density-based alternative quantum mechanics of many-electron systems.

In this paper we extend our earlier non-relativistic work by presenting a hydrodynamical analogy to the relativistic density-functional theory (Rajagopal and Callaway 1973, Rajagopal 1978, McDonald and Vosko 1979), following the approach adopted by Takabayashi (1957) in his hydrodynamical interpretation of the one-particle Dirac equation†. The present work thus preserves the link, even in the relativistic domain, between density-functional theory (DFT) and quantum fluid dynamics (QFD). This link is likely to have promising applications, e.g., in high-energy collision phenomena (Amsden *et al* 1977, Nix 1979, Nix and Strottman 1981, Csernai and Barz 1980).

We first define a number of density functions (local observables) which lead to several 'classical'-like fluid dynamical equations. The spinor formulation is thus completely transformed into a tensor formulation. This is necessary in order to draw the hydrodynamical picture in a 'classical' sense. In the non-relativistic limit, the relativistic QFD equations conform to the spin-DFT. Note that, since in the covariant formulation of relativistic equations space and time are treated on equal footing, we are dealing here with 4D quantities instead of the 3D quantities in the non-relativistic situation.

Below, § 2 of this paper briefly outlines the relativistic DFT. The corresponding QFD equations are developed in § 3. Section 4 discusses the physical implications of the equations while § 5 makes a few concluding remarks.

2. Relativistic DFT: a summary

In relativistic DFT (Rajagopal 1978, McDonald and Vosko 1979), the energy of the system is a functional of the four-current density‡ J_μ. Consider a system of electrons moving under the influence of an external potential $v^{\text{ext}}(\boldsymbol{r}, t)$—arising due to the nuclei as well as an additional scalar potential $\phi^0(\boldsymbol{r}, t)$ such that $v^{\text{ext}}(\boldsymbol{r}, t) = v_{\text{nuc}}(\boldsymbol{r}) + e\phi^0(\boldsymbol{r}, t) = e\phi_0^{\text{ext}}(\boldsymbol{r}, t)$—and a vector potential $\boldsymbol{A}^{\text{ext}}(\boldsymbol{r}, t)$, namely the four-potential $\phi_\mu^{\text{ext}} \equiv (\phi_0^{\text{ext}}, A_k^{\text{ext}})$. Instead of the non-relativistic Kohn–Sham one-particle equations, we now have the one-particle Dirac-like equations

$$\{-\mathrm{i}\hbar c\boldsymbol{\alpha}\cdot\nabla + \beta mc^2 + V^{\text{eff}}[\rho(\boldsymbol{r}, t)] + e\boldsymbol{\alpha}\cdot\boldsymbol{A}^{\text{eff}}[\boldsymbol{J}(\boldsymbol{r}, t)]\}\Psi_j(\boldsymbol{r}, t) = \mathrm{i}\hbar\,\partial\Psi_j/\partial t \tag{1}$$

where

$$V^{\text{eff}}[\rho(\boldsymbol{r}, t)] = v^{\text{ext}}(\boldsymbol{r}, t) + e^2\int\frac{\rho(\boldsymbol{r}', t)}{|\boldsymbol{r}-\boldsymbol{r}'|}\,\mathrm{d}\boldsymbol{r}' + \frac{\delta E_{\text{xc}}[\rho, \boldsymbol{J}]}{\delta\rho} \tag{2}$$

$$\boldsymbol{A}^{\text{eff}}[\boldsymbol{J}(\boldsymbol{r}, t)] = \boldsymbol{A}^{\text{ext}}(\boldsymbol{r}, t) + e\int\frac{\boldsymbol{J}(\boldsymbol{r}', t)}{|\boldsymbol{r}-\boldsymbol{r}'|}\,\mathrm{d}\boldsymbol{r}' + \frac{1}{c}\frac{\delta E_{\text{xc}}[\rho, \boldsymbol{J}]}{\delta\boldsymbol{J}}. \tag{3}$$

The particle density and the current density are defined through the four-component

† Alternative formulations of relativistic hydrodynamics have been provided by, e.g., Gurtler and Hestenes (1975) using space–time algebra and by Bialynicki-Birula (1971) using the Klein–Gordon equation.

‡ Unless otherwise specified, Greek subscripts (e.g., μ) run from one to four whereas the Latin subscripts (e.g., k) run from one to three. The subscript j is reserved for the one-particle DFT orbitals $\{\Psi_j\}$. A vectorial notation (boldface) is employed only for three-vectors.

spinors $\Psi_j(\boldsymbol{r}, t)$ as

$$\rho(\boldsymbol{r}, t) = \sum_j^{\text{occ}} \Psi_j^\dagger \Psi_j \tag{4}$$

$$J_k(\boldsymbol{r}, t) = \sum_j^{\text{occ}} \Psi_j^\dagger \alpha_k \Psi_j. \tag{5}$$

Note that J_k is related to the actual current density S_k through the relation $S_k = cJ_k$. In this paper, we shall use the term 'current density' for both J_k and S_k.

Now, introduce the Dirac γ-matrices

$$\gamma_k = -\mathrm{i}\beta\alpha_k, \qquad \gamma_4 = \beta \tag{6}$$

and the four-vectors

$$x_\mu \equiv (x_1, x_2, x_3, \mathrm{i}ct) \tag{7}$$

$$p_\mu \equiv (p_1, p_2, p_3, \mathrm{i}E/c) \tag{8}$$

for position and momentum, respectively. Equation (1) can now be compactly written as

$$\sum_\mu \gamma_\mu [\partial_\mu + (\mathrm{i}e/\hbar c)\phi_\mu^{\text{eff}}]\Psi_j + (mc/\hbar)\Psi_j = 0. \tag{9}$$

In equation (9), the electronic charge is taken as $-e$ and $\partial_\mu \equiv \partial/\partial x_\mu$. This equation represents the motion of the jth particle in the presence of an effective force (Pauli 1958) arising out of an effective four-potential $\phi_\mu^{\text{eff}} \equiv (\phi_0^{\text{eff}}, A_k^{\text{eff}})$, where $e\phi_0^{\text{eff}} = V^{\text{eff}}$.

The net particle and current densities may be written in terms of the four-vector $J_\mu \equiv (\rho, J_k)$, where

$$\begin{aligned} J_0 \equiv \rho &= \sum_j^{\text{occ}} \Psi_j^\dagger \Psi_j = \sum_j^{\text{occ}} \bar{\Psi}_j \gamma_4 \Psi_j \\ J_k &\equiv \sum_j^{\text{occ}} \Psi_j^\dagger \alpha_k \Psi_j = \mathrm{i} \sum_j^{\text{occ}} \bar{\Psi}_j \gamma_k \Psi_j \\ J_\mu &= \mathrm{i} \sum_j^{\text{occ}} \bar{\Psi}_j \gamma_\mu \Psi_j. \end{aligned} \tag{10}$$

In equations (10), we have used

$$\Psi_j^\dagger = \bar{\Psi}_j \gamma_4$$

which means that if

$$\Psi_j = \begin{pmatrix} \Psi_j^1 \\ \Psi_j^2 \\ \Psi_j^3 \\ \Psi_j^4 \end{pmatrix}$$

then

$$\begin{aligned} \Psi_j^\dagger &= (\Psi_j^{1*} \Psi_j^{2*} \Psi_j^{3*} \Psi_j^{4*}) \\ \bar{\Psi}_j &= (\Psi_j^{1*} \Psi_j^{2*} - \Psi_j^{3*} - \Psi_j^{4*}). \end{aligned} \tag{11}$$

The effective four-potential is ϕ_μ^{eff}, where

$$\begin{aligned} e\phi_0^{\text{eff}} &= v^{\text{ext}}(\boldsymbol{r}, t) + v^{\text{int}}[\rho(\boldsymbol{r}, t)] + v_{\text{xc}}[\rho(\boldsymbol{r}, t)] \\ &= e(\phi_0^{\text{ext}} + \phi_0^{\text{int}} + \phi_0^{\text{xc}}) \\ \phi_k^{\text{eff}} \equiv A_k^{\text{eff}} &= A_k^{\text{ext}}(\boldsymbol{r}, t) + A_k^{\text{int}}[J_k(\boldsymbol{r}, t)] + A_k^{\text{xc}}[J_k(\boldsymbol{r}, t)]. \end{aligned} \tag{12}$$

In equations (12), we have

$$\begin{aligned} v^{\text{int}}[\rho(\boldsymbol{r}, t)] &= e^2 \int \frac{\rho(\boldsymbol{r}', t)}{|\boldsymbol{r} - \boldsymbol{r}'|} \, \mathrm{d}\boldsymbol{r}' \\ A_k^{\text{int}}[J_k(\boldsymbol{r}, t)] &= e \int \frac{J_k(\boldsymbol{r}', t)}{|\boldsymbol{r} - \boldsymbol{r}'|} \, \mathrm{d}\boldsymbol{r}' \\ v^{\text{xc}}[\rho(\boldsymbol{r}, t)] &= \delta E_{\text{xc}}[\rho, \boldsymbol{J}]/\delta\rho \\ A_k^{\text{xc}}[\boldsymbol{J}(\boldsymbol{r}, t)] &= (1/e)\, \delta E_{\text{xc}}[\rho, \boldsymbol{J}]/\delta J_k. \end{aligned} \tag{13}$$

Thus, we find

$$\begin{aligned} \phi_\mu^{\text{int}} &\equiv (\phi_0^{\text{int}}, A_k^{\text{int}}) \\ \phi_\mu^{\text{xc}} &\equiv (\phi_0^{\text{xc}}, A_k^{\text{xc}}). \end{aligned} \tag{14}$$

3. Analogous relativistic QFD quantities and equations

The hydrodynamical analogy to the non-relativistic quantum mechanics of many-electron systems involves (Deb and Ghosh 1979, 1982, Ghosh and Deb 1982a, c, Bartolotti 1981) only the electronic charge and current densities while the incorporation of spin brings in addition the polarisation density (Takabayashi 1955c, Janossy and Ziegler-Naray 1966). In the relativistic situation, however, a number of density functions or local observables (Hestenes 1973) are to be defined, e.g., bilinear quantities of the form $\bar{\Psi}_j \gamma^A \Psi_j$, where γ^A is a suitable linear combination of γ_μ's. Although there is no *unique* way of choosing γ^A (see, e.g., Takabayashi 1955a), a particularly convenient scheme originally due to Pauli (1958) is found to be convenient (Takabayashi 1955b) for dealing with relativistic hydrodynamics.

Following Takabayashi (1957), the quantities below are defined:

(a) Scalar: $$(Q)_j = \bar{\Psi}_j \Psi_j; \qquad Q = \sum_j^{\text{occ}} (Q)_j \tag{15}$$

(b) Pseudoscalar: $$(Q')_j = \mathrm{i}\bar{\Psi}_j \gamma_5 \Psi_j; \qquad Q' = \sum_j^{\text{occ}} (Q')_j \quad \text{with } \gamma_5 = \gamma_1\gamma_2\gamma_3\gamma_4 \tag{16}$$

(c) Vector: $$(J_\mu)_j = \mathrm{i}\bar{\Psi}_j \gamma_\mu \Psi_j; \qquad J_\mu = \sum_j^{\text{occ}} (J_\mu)_j \tag{17}$$

(d) Pseudovector: $$(J'_\mu)_j = -\mathrm{i}\bar{\Psi}_j \gamma_5 \gamma_\mu \Psi_j; \qquad J'_\mu = \sum_j^{\text{occ}} (J'_\mu)_j \tag{18}$$

(e) Antisymmetric tensor: $(M_{\mu\nu})_j = \mathrm{i}\bar{\Psi}_j \gamma_\mu \gamma_\nu \Psi_j, \qquad \mu \neq \nu;$

$$M_{\mu\nu} = -M_{\nu\mu} = \sum_j^{\text{occ}} (M_{\mu\nu})_j. \tag{19}$$

In equations (15)–(19), quantities with subscript j correspond to the jth spinor while the *net* quantities are obtained by summing over the spinors.

Of these sixteen quantities, the six components of $(M_{\mu\nu})_j$ can be expressed in terms of the others (see equation (44)). Also, there exist the following three relations among the $(J_\mu)_j$ and $J'_\mu)_j$; note that, unless otherwise specified, summation over repeated Greek symbols is implied.

$$\begin{aligned} (J_\mu)_j (J_\mu)_j &= -(P)_j^2 \\ (J'_\mu)_j (J'_\mu)_j &= (P)_j^2 \\ (J_\mu)_j (J'_\mu)_j &= 0 \end{aligned} \tag{20}$$

where

$$(P)_j^2 = (Q)_j^2 + (Q')_j^2. \tag{20a}$$

This indicates that the time-like vector $(J_\mu)_j$ and the space-like vector $(J'_\mu)_j$ are mutually orthogonal (see, e.g., Takabayashi 1956a). Hence, we are led to only seven independent quantities. However, since a spinor contains *four* complex components, *eight* real quantities are required for complete specification. The missing quantity which is actually related to the phase parts of the spinor components can be obtained (Takabayashi 1957) by defining quantities involving differentiation, e.g., of the gauge-invariant form

$$D_\mu(\bar{\Psi}_j \gamma^A \Psi_j) = \mathrm{i}\{[\partial_\mu + (\mathrm{i}e/\hbar c)\phi_\mu^{\text{eff}}]\bar{\Psi}_j \gamma^A \Psi_j - \bar{\Psi}_j \gamma^A [\partial_\mu - (\mathrm{i}e/\hbar c)\phi_\mu^{\text{eff}}]\Psi_j\}. \tag{21}$$

Then, corresponding to each γ^A used in writing equations (15)–(19), one obtains a quantity defined by equation (21), namely

(a) Vector: $$(\bar{Q}_\mu)_j = \frac{\hbar}{2mc} D_\mu(Q)_j; \qquad \bar{Q}_\mu = \sum_j^{\text{occ}} (\bar{Q}_\mu)_j \tag{22}$$

(b) Pseudovector: $$(\bar{Q}'_\mu)_j = \frac{\hbar}{2mc} D_\mu(Q')_j; \qquad \bar{Q}'_\mu = \sum_j^{\text{occ}} (\bar{Q}'_\mu)_j \tag{23}$$

(c) Tensor: $$(T_{\mu\nu})_j = \frac{\hbar}{2mc} D_\mu(J_\nu)_j; \qquad T_{\mu\nu} = \sum_j^{\text{occ}} (T_{\mu\nu})_j \tag{24}$$

(d) Pseudotensor: $$(T'_{\mu\nu})_j = \frac{\hbar}{2mc} D_\mu(J'_\nu)_j; \qquad T'_{\mu\nu} = \sum_j^{\text{occ}} (T'_{\mu\nu})_j \tag{25}$$

(e) Three-rank tensor: $$(N_{\mu\nu\lambda})_j = \frac{\hbar}{2mc} D_\mu(M_{\nu\lambda})_j; \qquad N_{\mu\nu\lambda} = \sum_j^{\text{occ}} (N_{\mu\nu\lambda})_j. \tag{26}$$

However, there also exist several relations among these quantities so that, in effect, only one additional new quantity (the missing one) is introduced. Therefore, it suffices to consider only the following independent quantities

Set A: $(Q)_j, (Q')_j, (J_\mu)_j, (J'_\mu)_j, (\bar{Q}_\mu)_j$

in terms of which the complete theory can be formulated. Note, however, that in addition to the subsidiary condition, equations (20), the following kinematic identity must be satisfied (Takabayashi 1957, 1955b)

$$\begin{aligned}\{(e/mc^2)(P)_j F^{\text{eff}}_{\mu\nu} &+(Q)_j[\partial_\mu((\bar{Q}_\nu)_j/(P)_j)-\partial_\nu((\bar{Q}_\mu)_j/(P)_j)]\\ &+(Q')_j[\partial_\mu((\bar{Q}'_\nu)_j/(P)_j)-\partial_\nu((\bar{Q}'_\mu)_j/(P)_j)]\}\\ &=(\hbar/2mc)(P)_j^{-3}\{[(R_\mu)_j(Z_\nu)_j-(R_\nu)_j(Z_\mu)_j]\\ &-i\varepsilon_{\alpha\beta\gamma\delta}(J_\alpha)_j(J_\beta)_j[\partial_\mu(J_\gamma)_j\partial_\nu(J_\delta)_j-\partial_\mu(J'_\gamma)_j\partial_\nu(J'_\delta)_j]\},\end{aligned} \tag{27}$$

where

$$F^{\text{eff}}_{\mu\nu}=\partial_\mu\phi^{\text{eff}}_\nu-\partial_\nu\phi^{\text{eff}}_\mu \tag{28}$$

$$\begin{aligned}(Z_\mu)_j &=(Q')_j(\bar{Q}_\mu)_j-(Q)_j(\bar{Q}'_\mu)_j\\ &=(J'_\nu)_j\partial_\mu(J_\nu)_j\end{aligned} \tag{29}$$

$$(K_\mu)_j=(Q)_j(\bar{Q}_\mu)_j+(Q')_j(\bar{Q}'_\mu)_j \qquad \text{(used later in (37))} \tag{30}$$

$$(R_\mu)_j=(Q)_j\partial_\mu(Q')_j-(Q')_j\partial_\mu(Q)_j. \tag{31}$$

It is now possible to derive the *equations of motion* in terms of the above basic quantities. We start with the one-particle Dirac equation and its conjugate, namely

$$\gamma_\mu[\partial_\mu+(ie/\hbar c)\phi^{\text{eff}}_\mu]\Psi_j+(mc/\hbar)\Psi_j=0 \tag{9}$$

and

$$[\partial_\mu-(ie/\hbar c)\phi^{\text{eff}}_\mu]\bar{\Psi}_j\gamma_\mu-(mc/\hbar)\bar{\Psi}_j=0. \tag{32}$$

By premultiplying equation (9) by $\bar{\Psi}_j\gamma^A$ and postmultiplying equation (32) by $\gamma^A\Psi_j$, followed by addition and subtraction, one obtains 32 equations not all of which are independent. After taking proper combinations, one can obtain the following set of independent hydrodynamical equations; their significance is discussed in § 4.

(a) Scalar equation: $$\partial_\mu(J_\mu)_j=0 \tag{33}$$

(b) Pseudoscalar equation: $$\partial_\mu(J'_\mu)_j+(2mc/\hbar)(Q')_j=0 \tag{34}$$

(c) Scalar equation: $$(T_{\mu\mu})_j+(Q)_j=0 \tag{35}$$

(d) Pseudoscalar equation: $$(T'_{\mu\mu})_j=0 \tag{36}$$

(e) Vector equation:
$$\begin{aligned}&(J_\nu)_j\partial_\nu(J_\mu)_j-(J'_\nu)_j\partial_\nu(J'_\mu)_j\\ &=-(P)_j\partial_\mu(P)_j-(P)_j^{-2}\{(J_\mu)_j(J'_\nu)_j-(J_\nu)_j(J'_\mu)_j\}(Z_\nu)_j\\ &\quad+i(P)_j^{-2}\varepsilon_{\mu\nu\kappa\lambda}(J_\nu)_j(J'_\kappa)_j(K_\lambda)_j\end{aligned} \tag{37}$$

(f) Pseudovector equation:
$$\begin{aligned}&(J_\nu)_j\partial_\nu(J'_\mu)_j-(J'_\nu)_j\partial_\nu(J_\mu)_j\\ &=-(Z_\mu)_j-(P)_j^{-1}\partial_\nu(P)_j\{(J_\mu)_j(J'_\nu)_j-(J_\nu)_j(J'_\mu)_j\}\\ &\quad+i(P)_j^{-2}\varepsilon_{\mu\nu\kappa\lambda}(J_\nu)_j(J'_\kappa)_j(R_\lambda)_j.\end{aligned} \tag{38}$$

Each of equations (37) and (38) represents only two linearly independent equations because of the restrictions, equations (20). Thus, there are only eight independent equations, as expected.

Equations (33)–(38), together with the subsidiary conditions (20) and (27), form the basis of relativistic hydrodynamics of many-electron systems. The whole treatment can be developed in terms of the set A of density functions described before. For one-electron systems, however, the following set of quantities has been found to be more convenient (Takabayashi 1956b):

Set B: $P, \theta, v_\mu, \omega_\mu, k_\mu$

where

(a) Scalar: $$P = [(Q)^2 + (Q')^2]^{1/2} \tag{39}$$

(b) Pseudoscalar: $$\theta = \tan^{-1}[Q'/Q] \tag{40}$$

(c) Vector: $$v_\mu = J_\mu / P \tag{41}$$

(d) Pseudovector: $$\omega_\mu = J'_\mu / P \tag{42}$$

(e) Vector: $$k_\mu = K_\mu / P^2. \tag{43}$$

The subsidiary conditions as well as all the hydrodynamical equations can be expressed in terms of these quantities (see, e.g., Takabayashi 1956a, 1957). For instance, the subsidiary condition (27) may be written more simply as

$$[\partial_\mu k_\nu - \partial_\nu k_\mu] = -(i\hbar/2mc)\varepsilon_{\alpha\beta\gamma\delta} v_\alpha \omega_\beta [\partial_\mu v_\gamma \partial_\nu v_\delta - \partial_\mu \omega_\gamma \partial_\nu \omega_\delta] - (e/mc^2) F^{\text{eff}}_{\mu\nu}. \tag{44}$$

Note, however, that for a many-electron system, set A quantities are more convenient since then the net quantities Q, Q', $J_\mu, \ldots$ etc can be obtained directly by summing over the individual spinor contributions, unlike the quantities in set B. Further, it is the net quantities—and not the individual spinor contributions—which are local observables and therefore have direct physical significance. All other quantities defined in equations (19), (22)–(26) can be expressed in terms of the fundamental quantities of set A. For example,

$$(M_{\mu\nu})_j = (P_j)^{-2}\{-(Q')_j[(J_\mu)_j (J'_\nu)_j - (J_\nu)_j (J'_\mu)_j] + i(Q)_j[(J_k)_j (J'_\lambda)_j - (J_\lambda)_j (J'_k)_j]\} \tag{45}$$

and

$$(T_{\mu\nu})_j = (P_j)^{-2}\{(K_\mu)_j (J_\nu)_j + (\hbar/2mc)[(R_\mu)_j (J'_\nu)_j + i\varepsilon_{\nu\alpha\beta\gamma}(J_\alpha)_j (J'_\beta)_j \partial_\mu (J_\gamma)_j]\}. \tag{46}$$

Therefore, within relativistic DFT, the many-electron system can be completely characterised by the quantities of set A through the hydrodynamical equations (33)–(38), together with the subsidiary conditions (20) and (27).

Interestingly, the above hydrodynamical equations can also be derived from a variation principle. One obtains the following form of the Lagrangian density (Takabayashi 1956b) by expressing the symmetrised Lagrangian density (Takabayashi 1957) for the original Dirac-like DFT equation (9) in terms of the basic hydrodynamic quantities and adding to it the Lagrangian densities corresponding to the subsidiary conditions:

$$\mathscr{L} = \sum_j (\mathscr{L})_j \tag{47}$$

$$
\begin{aligned}
(\mathscr{L})_j = &-mc^2(P_j)^{-2}\{(K_\mu)_j(J_\nu)_j + (P)_j^2(Q)_j \\
&+(\hbar/2mc)[(R_\mu)_j(J'_\nu)_j + i\varepsilon_{\nu\alpha\beta\gamma}(J_\alpha)_j(J'_\beta)_j\partial_\mu(J_\gamma)_j]\} \\
&+\tfrac{1}{2}(mc^2/e)F^{\text{eff}}_{\mu\nu}\{(\partial_\mu[(P)_j^{-2}(K_\nu)_j - \partial_\nu[(P)_j^{-2}(K_\mu)_j]) \\
&+(i\hbar/2mc)\varepsilon_{\alpha\beta\gamma\delta}(P)_j^2(J_\alpha)_j(J'_\beta)_j[\partial_\mu\{(J_\gamma)_j/(P)_j\}\partial_\nu\{(J_\delta)_j/(P)_j\} \\
&-\partial_\mu\{(J'_\gamma)_j/(P)_j\}\partial_\nu\{(J'_\delta)_j/(P)_j\}]\} + \tfrac{1}{4}(F^{\text{eff}}_{\mu\nu})^2. \qquad (48)
\end{aligned}
$$

The variation of this Lagrangian density with respect to the basic quantities leads to the hydrodynamical equations.

4. Physical significance of relativistic QFD quantities and equations

In this section we will first discuss the physical significance of the quantities of set A as well as the tensors $M_{\mu\nu}$ and $T_{\mu\nu}$ given in equations (45) and (46) respectively. This will pave the way towards a physical interpretation of the relativistic QFD equations given above.

The quantity $(J_\mu)_j$ is the four-current vector corresponding to the jth spinor. The corresponding actual current density is

$$(S_k)_j = c(J_k)_j \qquad (49)$$

while the electron density associated with the jth spinor is

$$\rho_j(\boldsymbol{r}, t) = (J_0)_j = -i(J_4)_j. \qquad (50)$$

The net current and electron densities are sums over the occupied spinors, i.e.,

$$
\begin{aligned}
S_k &= \sum_j (S_k)_j \\
\rho(\boldsymbol{r}, t) &= \sum_j \rho_j(\boldsymbol{r}, t).
\end{aligned} \qquad (51)
$$

One can also write

$$(J_k)_j = (P)_j(v_k)_j, \qquad (52)$$

interpreting $(v_k)_j$ as the 'classical' hydrodynamical velocity field and $(P)_j$ as the density in the local rest frame (Takabayashi 1956a)—the reference frame moving with velocity $c(v_k)_j$ at each point in space at each instant—corresponding to the jth spinor. The link between $(P)_j$ and $(J_4)_j$ can thus be seen easily (Takabayashi 1956a). Further, the interpretation of $(Q)_j$ and $(Q')_j$ is also given through $(P)_j$. Note that each $(P)_j$ denotes density in a different frame and a net P cannot be obtained by summing over the $(P)_j$'s.

The quantity $(J'_\mu)_j$ denotes the spin (angular momentum) density four-vector and gives the correct quantum mechanical expectation value for the particle spin, i.e., $\frac{1}{2}\hbar\int(J'_k)_j\,d\boldsymbol{r}$. Thus, $\frac{1}{2}\hbar(J'_k)_j$ is the spin (angular momentum) density for the jth spinor distributed in space in a 'classical' sense. $(J'_\mu)_j$ can also be factorised as

$$(J'_\mu)_j = (P)_j(\omega_\mu)_j. \qquad (53)$$

The antisymmetric tensor $M_{\mu\nu}$ of equations (19) and (45) can be interpreted as the electric and magnetic moment density tensor. Thus, $(M_{kl})_j$ denotes the magnetic

moment density while $-\mathrm{i}(M_{k4})_j$ denotes the electric moment density for the jth spinor. The corresponding net quantities are obtained merely by summing over j.

The quantity $(\bar{Q}_\mu)_j$ can be interpreted as the convection current density for the jth spinor. $T_{\mu\nu}$ of equations (24), (46) and (47) represents the energy–momentum tensor. These expressions for $T_{\mu\nu}$ are consistent with Pauli's (1958) definition of the energy–momentum tensor, namely

$$(T_{\mu\nu})_j = (\hbar/2mc)(\partial_\mu \bar{\Psi}_j \gamma_\nu \Psi_j - \bar{\Psi}_j \gamma_\nu \partial_\mu \Psi_j) - (e/mc^2)\phi_\mu^{\text{eff}}(J_\nu)_j \tag{54}$$

and can be obtained by rewriting equation (54) in terms of the basic hydrodynamic variables. The momentum density is represented by $-(\mathrm{i}/c)T_{k4}$ and the energy density by $-T_{44}$.

Now, $(T_{\mu\nu})_j$ satisfies the conservation law

$$\partial_\nu (T_{\mu\nu})_j = (e/mc^2) F_{\mu\nu}^{\text{eff}} (J_\nu)_j. \tag{55}$$

Using equation (46), equation (55) takes the form

$$mc(P)_j (v_\nu)_j \partial_\nu \{(P)_j^{-2}(K_\mu)_j\} [\equiv m(P)_j (\mathrm{d}/\mathrm{d}\tau_j)\{(P)_j^{-2}(K_\mu)_j\}]$$
$$= -\partial_\nu \{(L_{\mu\nu})_j\} + (e/c) F_{\mu\nu}^{\text{eff}} (J_\nu)_j \tag{56}$$

by introducing the proper time τ_j by $\mathrm{d}/\mathrm{d}\tau_j \equiv c(v_\nu)_j \partial_\nu$.

One can interpret (56) as the equation of motion for the proper momentum vector. The second term on the right-hand side of (56) is the usual Lorentz-type force while the first term represents the 'quantum force' arising from the 'quantum stress tensor' $L_{\mu\nu}$, defined by

$$(L_{\mu\nu})_j = \tfrac{1}{2}\hbar (P)_j^{-2} \{(R_\mu)_j (J'_\nu)_j + \mathrm{i}\varepsilon_{\nu\alpha\beta\gamma} (J_\alpha)_j (J'_\beta)_j \partial_\mu (J_\gamma)_j\}, \tag{57}$$

corresponding to the jth spinor. The net quantum stress tensor $L_{\mu\nu}$ is also obtained by summing over the individual spinor contributions, namely

$$L_{\mu\nu} = \sum_j (L_{\mu\nu})_j. \tag{58}$$

The stress tensor $L_{\mu\nu}$ forms a part of the energy–momentum tensor, i.e.,

$$mc(T_{\mu\nu})_j = (L_{\mu\nu})_j + mc(P)_j^{-2}(K_\mu)_j (J_\nu)_j. \tag{59}$$

Equation (56) is analogous to the Navier–Stokes-type equation in non-relativistic QFD (Deb and Ghosh 1979, 1982, Ghosh and Deb 1982a, c, Bartolotti 1981, Deb 1984).

Now, the conservation of angular momentum demands that the energy–momentum tensor be symmetric. However, $T_{\mu\nu}$, as defined here, is not symmetric. To remedy this situation, one can consider the relation (Pauli 1958, Takabayashi 1956a)

$$(T_{\mu\nu})_j - (T_{\nu\mu})_j = \tfrac{1}{2}\mathrm{i}(\hbar/mc)\varepsilon_{\mu\nu\kappa\lambda}\partial_\kappa (J'_\lambda)_j \tag{60}$$

and define a symmetric energy–momentum tensor

$$(\Theta_{\mu\nu})_j = (\Theta_{\nu\mu})_j = \tfrac{1}{2}[(T_{\mu\nu})_j + (T_{\nu\mu})_j]$$
$$= (T_{\mu\nu})_j = \tfrac{1}{4}\mathrm{i}(\hbar/mc)\varepsilon_{\mu\nu\kappa\lambda}\partial_\kappa (J'_\lambda)_j \tag{61}$$

which also obeys an equation analogous to equation (55).

The various hydrodynamic equations derived in § 3 can now be interpreted. Thus, (33) is the continuity equation for the four-current density $(J_\mu)_j$ whereas (34) is a continuity-type equation for the spin density $(J'_\mu)_j$. Equations (35) and (36) are two scalar equations involving the energy-momentum tensor $T_{\mu\nu}$, while (37) and (38) denote, respectively, the Euler equation of flow and the equation of motion for the spin distribution.

By summing each of (33)–(36) over j, one obtains the following equations involving the net quantities:

$$\text{(i)} \qquad \partial_\mu J_\mu = 0 \tag{62}$$

$$\text{(ii)} \qquad \partial_\mu J'_\mu + (2mc/\hbar)Q' = 0 \tag{63}$$

$$\text{(iii)} \qquad T_{\mu\mu} + Q = 0 \tag{64}$$

$$\text{(iv)} \qquad T'_{\mu\mu} = 0. \tag{65}$$

However, attempts to recast equations (37) and (38) in terms of net quantities lead to quite complicated equations.

The field quantity $F^{\text{eff}}_{\mu\nu}$ in equation (28) represents the effective field arising out of the potential ϕ^{eff}_μ in equation (12). It consists of the external field, the internal Coulomb field due to the charge and the current density, as well as the contribution from the xc four-potential in equation (14). Thus, the Lorentz-type effective force appearing as the last term in equation (56), arises from the external electric and magnetic fields, the internal Coulomb field and the xc field. The 'quantum force' arising from a 'quantum stress tensor' appears separately in the Navier–Stokes-type equation (56).

The relativistic hydrodynamics discussed in this paper correspond to a 'spinning' fluid. The net many-electron fluid consists of components each of which is characterised by fluid dynamical quantities corresponding to each spinor. Each fluid component obeys the set of hydrodynamical equations (33)–(38). The hydrodynamical quantities can be obtained, in principle, by solving these equations; the *net* quantities are then obtained by summing over the occupied spinors. Thus, the 'classical' picture of a many-electron fluid as a collection of individual fluid components is valid in both the non-relativistic (Ghosh and Deb 1982c, Deb and Ghosh 1982, Bartolotti 1981) and the relativistic domain. Although the relativistic QFD equations present a complicated appearance, they are nevertheless 'classical', incorporating quantities of quantum origin, e.g., quantum stress tensor, spin density, etc.

5. Conclusion

In this work, the one-particle Dirac-like density-functional equations have been re-expressed in terms of a tensor formulation, suppressing the Ψ_j-spinors and the γ-matrices. The hydrodynamical quantities and equations depict a many-electron system subjected to external fields. The relativistic hydrodynamics developed here has a conceptual advantage in that it offers a consistent 'classical' view of quantum systems in terms of local observables, thereby permitting ready visualisation and interpretation of various physicochemical phenomena in 3D (real) space or the 4D time–space. The adoption of a tensor formulation clearly reveals the covariance properties with respect to various transformations.

The present formalism extends Takabayashi's (1957) relativistic hydrodynamic formulation from one-particle to many-particle systems. It also supplements our earlier

work (Deb and Ghosh, 1979, 1982, Ghosh and Deb 1982a) on the quantum fluid dynamics of non-relativistic systems, highlighting again the advantages of a joint approach to physicochemical phenomena in terms of density-functional theory and quantum fluid dynamics. Through this approach, new aspects of relativistic quantum systems may be brought to light and useful techniques may be devised for practical applications to various problems in physics and chemistry.

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