Electron Charge and Current Densities, the Geometric Phase and Cellular Automata *

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Some consequences of the quantum fluid dynamics formulation are discussed for excited states of atoms and molecules and for time-dependent processes. It is shown that the conservation of electronic current density $\boldsymbol{j}(\boldsymbol{r})$ allows us to manufacture a gauge potential for each excited state of an atom, molecule or atom in a molecule. This potential gives rise to a tube of magnetic flux carried around by the many-electron system. In time-dependent situations, the evolution of the electronic density distribution can be followed with simple, site-dependent cellular automaton (CA) rules. The CA consists of a lattice of sites, each with a finite set of possible values, here representing finite localized elements of electronic charge and current density (since the charge density ϱ no longer suffices to fully characterize a time-dependent system, it needs to be supplemented with information about the current density $\boldsymbol{j}$). Our numerical results are presented elsewhere and further development is in progress.

Key words: Electronic phase; Current density; Anyons; QFD; Cellular automata.

Some consequences of the fluid dynamical formulation of density functional theory [1–9] are discussed, with particular reference to excited states and time-dependent situations. The Hohenberg-Kohn theorem [10, 11] established that the ground-state energy of a many-particle system is a unique functional $E[\varrho]$ of the single-particle density $\varrho(\boldsymbol{r})$, promising an enormous simplification in theoretical studies of quantum systems, by-passing the complexities of the many-electron wavefunction. In excited states of atoms and molecules, however, as well as in time-dependent situations, the one-electron density no longer suffices to completely characterize the electronic states; in addition one now requires information about the electronic phases $S_i(\boldsymbol{r})$ or current density $\boldsymbol{j}(\boldsymbol{r})$.

Quantum fluid dynamics (QFD) views the electron cloud in a many-electron system as a "classical" fluid moving under the action of classical Coulomb forces augmented by forces of quantum origin. In an earlier paper [1] it was shown that, for a stationary electronic state, the continuity equation of QFD,

$$\nabla \cdot \boldsymbol{j} = 0\,, \tag{1}$$

represents a differential equation for the orbital electronic phases,

$$\nabla^2 S_i + (\nabla \varrho_i \cdot \nabla S_i)/\varrho_i = 0\,, \tag{2}$$

where $\varrho_i(\boldsymbol{r})$ and $S_i(\boldsymbol{r})$ are the orbital densities and orbital phases, respectively. This must be solved subject to certain periodicity conditions, which arise from the nodal topology of the wavefunctions [12–17] and give rise to vortices of orbital current, with quantized circulation.

Rather than using such an orbital treatment, it is also possible to describe a many-electron atom or molecule in terms of a *single* function in three-dimensional space,

$$\Phi(\boldsymbol{r}) = \varrho^{1/2}(\boldsymbol{r}) \exp[i S(\boldsymbol{r})/\hbar], \tag{3}$$

which satisfies a generalized non-linear Schrödinger-type equation (GNLSE). When this is done for an excited state with current-density vortices, it is evident that the velocity field, defined as

$$\boldsymbol{v}(\boldsymbol{r}) = \boldsymbol{j}(\boldsymbol{r})/\varrho(\boldsymbol{r}) \tag{4}$$

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is not irrotational, so that $\boldsymbol{v}(\boldsymbol{r})$ can be separated into an irrotational gauge term, arising from the gradient of the net electronic phase $S(\boldsymbol{r})$, and a solenoidal or transverse field term. This is equivalent to introducing an "internal magnetic vector potential" $\boldsymbol{A}_{\text{int}}(\boldsymbol{r})$ [1] into the defining equation for the electronic current density,

$$\boldsymbol{j}(\boldsymbol{r}) = (1/m)\,\varrho(\boldsymbol{r})\,[\nabla S(\boldsymbol{r}) + (e/c)\,\boldsymbol{A}_{\text{int}}(\boldsymbol{r})]. \tag{5}$$

The conservation of $j(\boldsymbol{r})$ thus allows us to manufacture a gauge potential. For each excited state of an atom or molecule, there corresponds a specific, unique configuration of internal magnetic field in the GNLSE. For each vortex of current, the internal magnetic vector potential $\boldsymbol{A}_{\text{int}}(\boldsymbol{r})$ in equation (5) gives rise to a tube of magnetic flux carried around by the pseudo-particle described by the function $\Phi(\boldsymbol{r})$. Such charged-particle-flux-tube composites have been employed theoretically to construct anyons, obeying fractional statistics [18, 19], in two dimensions. These concepts could fruitfully be employed to describe an atom in a molecule [20].

In time-dependent situations, the evolution of the electronic density distribution can be followed with simple, site-dependent cellular automaton rules. Cellular automata (CA) [21] are discrete dynamical systems constructed from many similar components, each simple, but together capable of complex self-organizing behaviour. The complexity is generated by the co-operative effect of many localized elements of electron density on a lattice of sites, each with a *finite* set of possible values. The CA evolves in discrete time steps. At each time step, the value of each site is updated according to a definite rule, which specifies the new site value in terms of its own old value and those of sites in some neighbourhood around it. The rule is applied synchronously to each site at each time step.

In an earlier work [22], we had formulated a CA simulation rule based on density functional theory (DFT) in the Thomas-Fermi local density approximation, by dividing space into a large number of discrete volume elements ("sites") labelled by n, each with density $\varrho(n)$. For small disturbances from the ground state, the evolution of the density is given by CA rules at each site governing the flow of electrons from regions of higher chemical potential (lower electronegativity) to regions of lower chemical potential (higher electronegativity) [23]. The equilibrium density is recovered through a Class II CA [21, 24]. Our numerical results, for one- and two-dimensional systems, are presented elsewhere [22].

The above treatment would be valid for a near-equilibrium situation. In a truly time-dependent situation, however, the charge density $\varrho(n)$ alone no longer suffices to fully characterize the system, as discussed above, and needs to be supplemented with information about the current density $\boldsymbol{j}(n)$. CA simulations have been used extensively in modelling reaction-diffusion systems [25, 26] and fluid dynamical equations [27–29]. These CA techniques are now being adapted to model the QFD equations of motion [2–9].

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