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# Dissipation Effects in Schrödinger and Quantal Density Functional Theories of Electrons in an Electromagnetic Field

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**Abstract:** Dissipative effects arise in an electronic system when it interacts with a time-dependent environment. Here, the Schrödinger theory of electrons in an electromagnetic field including dissipative effects is described from a new perspective. Dissipation is accounted for via the effective Hamiltonian approach in which the electron mass is time-dependent. The perspective is that of the individual electron: the corresponding equation of motion for the electron or time-dependent differential virial theorem—the ‘Quantal Newtonian’ second law—is derived. According to the law, each electron experiences an external field comprised of a binding electric field, the Lorentz field, and the electromagnetic field. In addition, there is an internal field whose components are representative of electron correlations due to the Pauli exclusion principle and Coulomb repulsion, kinetic effects, and density. There is also an internal contribution due to the magnetic field. The response of the electron is governed by the current density field in which a damping coefficient appears. The law leads to further insights into Schrödinger theory, and in particular the intrinsic self-consistent nature of the Schrödinger equation. It is proved that in the presence of dissipative effects, the basic variables (gauge-invariant properties, knowledge of which determines the Hamiltonian) are the density and physical current density. Finally, a local effective potential theory of dissipative systems—quantal density functional theory (QDFT)—is developed. This constitutes the mapping from the interacting dissipative electronic system to one of noninteracting fermions possessing the same dissipation and basic variables. Attributes of QDFT are the separation of the electron correlations due to the Pauli exclusion principle and Coulomb repulsion, and the determination of the correlation contributions to the kinetic energy. Hence, Schrödinger theory in conjunction with QDFT leads to additional insights into the dissipative system.

**Keywords:** dissipation effects in quantum mechanics; dissipation in Schrödinger theory; dissipation in quantal density functional theory; density functional theory

## 1. Introduction

If a quantum electronic system interacts with an environment that is time-varying, then the system is modified during the interaction, and dissipative effects within the system arise. The changing environment could correspond to a change in temperature, pressure, or stress, such that there is an input or removal of energy, thereby modifying the evolution of the quantum system. Dissipation is described by two effects [1]. One corresponds to damping or friction effects due to the dissipation of energy stored in the system. The second corresponds to the fluctuations of the systems’ degree of freedom caused by fluctuations in the environment, which can manifest as Brownian motion. There are two primary approaches to dealing with quantum dissipation. One approach is to put the system in a bath of harmonic oscillators which interact with the system via a certain coupling. The second is

to employ an effective Hamiltonian. In this latter approach, dissipative effects are simulated by the assumption that the effective mass of the electron changes with time, i.e.,  $m = m(t)$ . There is vast literature [2–19] based on this assumption, which is concerned primarily with the quantum damped harmonic oscillator, the time-dependent harmonic oscillator, and other such oscillators in the presence of various external time-varying electric and magnetic fields. Typical physical systems addressed by such calculations are, for example, an electromagnetic field being pumped into a Fabry-Pérot cavity with dissipation occurring at the walls of the cavity [20–22], or the trapping and focusing of charged and neutral particles with electric or magnetic multipole fields [23,24].

In this paper we consider dissipative effects using the effective Hamiltonian approach but from a different perspective. The perspective is that of the *individual* electron within a sea of electrons in the presence of a binding field as well as a time-dependent electromagnetic field. Assuming dissipative effects are accounted for by an electron mass that is a function of time:  $m = m(t)$ , we derive the equation of motion or time-dependent differential virial theorem—the ‘Quantal Newtonian’ second law—for the electron. To explain further, in recent work [25–35], it has been possible to describe the Schrödinger theory of electrons in an external static or time-dependent electromagnetic field from this perspective of the corresponding ‘Quantal Newtonian’ second law for the individual electron. The ‘Quantal Newtonian’ first law, a special case for time-independent phenomena, is a description of stationary-state Schrödinger theory. The laws are a description of the electronic system in terms of ‘classical’ fields experienced by each electron. The sources of these fields are quantal in that they are quantum-mechanical expectations of Hermitian operators taken with respect to the wave function. There is the external field comprised of the binding electric field, the Lorentz field, and the electromagnetic field components. The internal field experienced by each electron is comprised of components that are representative of properties of the system such as electron correlations due to the Pauli exclusion principle and Coulomb repulsion, kinetic effects, electron density, and an internal magnetic field component. In addition to the external and internal fields, there is the response of the electron as exhibited by the current density field. The laws are general in that they are valid for arbitrary state and arbitrary binding potential, and are gauge-invariant.

The terminology of ‘Quantal Newtonian’ second and first laws follows from the equivalence with the corresponding classical equations of motion for a particle amongst  $N$  particles that obey Newton’s third law of action and reaction, exert forces on each other that are equal and opposite, and lie along the line joining them. Newton’s second law for the  $i$ th particle is then  $\mathbf{F}_i^{\text{ext}} + \sum_j \mathbf{F}_{ji} = d\mathbf{p}_i/dt$ , where  $\mathbf{F}_i^{\text{ext}}$  is the external force, and  $\mathbf{F}_{ji}$  the internal force on the  $i$ th particle due to the  $j$ th particle, with the response of the particle given by the right hand side where  $\mathbf{p}_i$  is the particle momentum. The time-independent Newton’s first law for the  $i$ th particle constitutes a special case. The ‘Quantal Newtonian’ second law (see Equation (3)), and its time-independent version, the ‘Quantal Newtonian’ first law, written in terms of the ‘classical’ fields instead of forces constitute the quantum-mechanical equivalent of the classical equations of motion. These are fields experienced by *each* electron. The sources of these fields are *local* and *nonlocal* quantal collective properties. Thus, for example, the electronic density and physical current density are the local sources for the Hartree and current density fields. The pair correlation function and the single-particle density matrix are the nonlocal sources for the electron interaction and kinetic fields, respectively. Stationary-state properties such as the components of the total energy can be written in integral virial form in terms of these fields. The new perspective of a quantum-mechanical system in terms of these ‘classical’ fields which pervade all space then makes the description tangible in the rigorous classical sense.

The ‘Quantal Newtonian’ second and first laws also lead to further insights [34,35] into Schrödinger theory. A key understanding achieved is that the Hamiltonian  $\hat{H}$  is a functional of the wave function  $\psi$ , i.e.,  $\hat{H} = \hat{H}[\psi]$ . This is a new idea with many consequences, which we here explain further. Consider a stationary-state system composed of  $N$  electrons in an arbitrary binding field  $\mathcal{E}(\mathbf{r}) = -\nabla v(\mathbf{r})/e$ , with  $v(\mathbf{r})$  the binding potential. As the system is one of electrons, the kinetic  $\hat{T}$  and electron interaction  $\hat{U}$  operators are assumed to be known. If the binding potential  $v(\mathbf{r})$  is

known, the Hamiltonian  $\hat{H} = \hat{T} + \hat{U} + \hat{V}$  is known, and the wave functions  $\psi$  of the system, ground and excited, are obtained by solution of the Schrödinger equation  $\hat{H}\psi = E\psi$ . We refer to this equation as the non-self-consistent form of the Schrödinger equation. Now, from the ‘Quantal Newtonian’ first law for the system, it can be proved that the binding potential  $v(\mathbf{r})$  is a *universal* and *exactly known* functional of the wave function, *i.e.*  $v(\mathbf{r}) = v[\psi](\mathbf{r})$ . In other words, the *closed-form analytical* expression of the functional  $v[\psi](\mathbf{r})$  is known. Therefore, the Schrödinger equation can then be written as  $\hat{H}[\psi]\psi = E[\psi]\psi$ . The Schrödinger equation written in this form is also valid for *arbitrary* states, ground or excited. Because the functional  $v[\psi](\mathbf{r})$  is known, if one knows the wave function  $\psi$ , then the binding potential can be exactly determined. Now suppose there exists a system in which both the binding potential  $v(\mathbf{r})$  and the wave function  $\psi$  are unknown. One could obtain both  $v(\mathbf{r})$  and  $\psi$  by self-consistent solution of the Schrödinger equation written in functional form. One begins with an approximate form of the wave function  $\psi$  and determines the corresponding approximate potential  $v[\psi](\mathbf{r})$ . The Schrödinger equation is then solved to obtain a new wave function  $\psi$ , and the new potential  $v[\psi](\mathbf{r})$  obtained. This procedure is continued until the output and input wave functions and potential are the same or equivalently until self-consistency is achieved. The self-consistent form of the Schrödinger equation is entirely akin to that of the Hartree–Fock theory [36,37] equations  $\hat{H}^{HF}[\phi_i]\phi_i = \epsilon_i\phi_i$ , where  $\phi_i$  and  $\epsilon_i$  are the eigenfunctions and eigenvalues of the equation. The only difference between the self-consistent form of the Schrödinger equation and the Hartree–Fock theory equations is that the latter is for single-particle orbitals leading to a Slater determinant wave function, whereas the former leads to the fully interacting system wave function. As an example, due to the recent advances in semiconductor technology, it has been possible to create ‘artificial atoms’ (quantum dots) in two dimensions [38,39]. The question which then had to be addressed was what the binding potential was for these electrons confined to a plane. As a result of a Hartree level calculation as well as experiments [40,41], it is now accepted that in this case the binding potential is harmonic. Had the functional form of the Schrödinger equation existed at that time, this conclusion could have been arrived at self-consistently. For examples of the final iteration of the self-consistency procedure for a quantum dot in a magnetic field in both a ground and excited state, see [34]. In the future, there could be other systems created for which the potential  $v(\mathbf{r})$  and the wave function  $\psi$  are both unknown. With the self-consistent form of the Schrödinger equation, the corresponding wave functions and potential could then be determined. Yet another advantage of the self-consistent form of the Schrödinger equation is the following. Suppose one knows a good approximation to a wave function of a system. Then, through self-consistency, one can obtain the exact wave function as described above. The various other insights, which too are general, will be described with reference to the dissipative system of the present work.

A second component of the paper is the mapping via quantal density functional theory (QDFT) [25,26] of the interacting dissipative system to one of noninteracting fermions with the same dissipative effects, *i.e.*, the same  $m(t)$ . The idea of mapping the interacting system to one of noninteracting fermions harks back to the stationary-state theories of Slater [42], Sharp and Horton [43], Kohn and Sham [44], and Slater et al. [45]. These are thus local effective potential theories with the many-body effects incorporated in the potential. The model system is also designed to possess the same basic variables. The basic variables are fundamental properties of the interacting system, as explained below. QDFT differs from Schrödinger theory in the following ways. Firstly, it is a local effective potential theory [33,42–45] with the attendant advantage of easier numerical solution of the corresponding differential equation for the constituent single-particle spin orbitals of the resulting Slater determinant wave function. Secondly, it allows for the separation of the electron correlations due to the Pauli exclusion principle and Coulomb repulsion, and thereby the determination of their separate contributions to the properties of the system. In quantum chemistry, a separate Hartree–Fock theory calculation must be performed. The separation of the correlations in this manner is different because the properties derived via Hartree–Fock theory differ from those of the original fully interacting system. Thirdly, it is possible to determine the contribution of these correlations to the kinetic energy—the

correlation-kinetic contribution. QDFT is a description of the model system in terms of ‘classical’ fields and quantal sources. There is a corresponding ‘Quantal Newtonian’ second law for each model fermion. The component of the local effective potential in which all the many-body effects are incorporated is explicitly defined in terms of a *conservative* effective field: it is the work done in this field. Hence, in this second component of the paper, the ‘Quantal Newtonian’ second law for the model fermion with time-dependent mass is derived, and the corresponding QDFT equations developed. It is evident that QDFT in conjunction with Schrödinger theory leads to further insights into the physical system.

Finally, we address the issue of what properties constitute the basic variables for the interacting electronic system with dissipation as described by Schrödinger theory. This is important because in the QDFT mapping to the model fermionic system, it is important to know the properties that the Slater determinant wave function must reproduce. The concept of a basic variable stems from the stationary-state theorem of Hohenberg–Kohn [46]. Accordingly, for a system of electrons in an external electrostatic field  $\mathcal{E}(\mathbf{r}) = -\nabla v(\mathbf{r})/e$ , knowledge of the nondegenerate ground state density  $\rho(\mathbf{r})$  uniquely determines the scalar potential  $v(\mathbf{r})$  to within a constant. The proof is for fixed electron number  $N$ . As a consequence, since for the electrons the kinetic and electron interaction operators are assumed known, the Hamiltonian  $\hat{H}$  is known. Solution of the resulting time-independent Schrödinger equation then leads to the ground and excited state wave functions of the system. Thus, a basic variable is a gauge-invariant property of an electronic system, knowledge of which determines its Hamiltonian and thereby all the properties of the system. In recent work we have proved [25,47] that in the added presence of a *uniform* magnetostatic field  $\mathcal{B}(\mathbf{r}) = \nabla \times \mathbf{A}(\mathbf{r})$ , the basic variables are the nondegenerate ground state density  $\rho(\mathbf{r})$  and physical current density  $\mathbf{j}(\mathbf{r})$ . The constraints in this case are the fixed electron number  $N$ , orbital  $\mathbf{L}$ , and spin  $\mathbf{S}$  angular momentum. Knowledge of  $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$  uniquely determines the potentials  $\{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\}$  to within a constant and the gradient of a scalar function, and thereby the Hamiltonian  $\hat{H}$ . In a manner similar to the Hohenberg–Kohn theorem, it has been proved by Runge–Gross [48] that for electrons in a time-dependent electric field  $\mathcal{E}(\mathbf{y}) = -\nabla v(\mathbf{y})/e$ ,  $\mathbf{y} = \mathbf{r}t \equiv (\mathbf{r}, t)$ , knowledge of the density  $\rho(\mathbf{y})$  uniquely determines the potential  $v(\mathbf{y})$  to within a time-dependent function—hence the Hamiltonian  $\hat{H}(t)$ , and the wave function by solution of the Schrödinger equation. For electrons in a time-dependent electromagnetic field, it has been proved by Ghosh–Dhara [49] and Vignale [50] that the corresponding basic variables are  $\{\rho(\mathbf{y}), \mathbf{j}(\mathbf{y})\}$ . As the final component of the paper, by employing the arguments of Vignale, we prove that the basic variables for the electronic system in a time-dependent electromagnetic field with dissipation are  $\{\rho(\mathbf{y}), \mathbf{j}(\mathbf{y})\}$  (the work of Vignale [50] is for constant electron mass). A consequence of the proof, as in the work of Vignale, is the existence of a system of noninteracting fermions possessing the same  $\{\rho(\mathbf{y}), \mathbf{j}(\mathbf{y})\}$ . Thus, in the QDFT mapping to the model system, the Slater determinant wave function of the model fermions is constrained to reproduce the properties  $\{\rho(\mathbf{y}), \mathbf{j}(\mathbf{y})\}$ .

In Section 2 we derive the ‘Quantal Newtonian’ second law for the interacting dissipative system of electrons in an electromagnetic field. New perspectives on Schrödinger theory that arise as a consequence of the second law are described in Section 3. The proof that the basic variables for such dissipative systems are  $\{\rho(\mathbf{y}), \mathbf{j}(\mathbf{y})\}$  is given in Section 4. In Section 5 we develop the corresponding QDFT. The key facets of the paper are summarized in Section 6 together with remarks on current work.

## 2. Single Electron Perspective of Schrödinger Theory: The ‘Quantal Newtonian’ Second Law

Consider a *dissipative* system of  $N$  electrons of mass  $m = m(t)$  of charge  $-e$  (with  $e > 0$ ) in a time-dependent binding electric field  $\mathcal{E}(\mathbf{y}) = -\nabla v(\mathbf{y})/e$ , with  $\mathbf{y} = \mathbf{r}t \equiv (\mathbf{r}, t)$ . The time-dependence of the field  $\mathcal{E}(\mathbf{y})$  (or scalar potential  $v(\mathbf{y})$ ) could correspond, for example, to the time-independent binding potential and zero-point motion of the nuclei. In the added presence of a time-dependent electromagnetic field:  $\mathcal{B}(\mathbf{y}) = \nabla \times \mathbf{A}(\mathbf{y})$ ,  $\mathbf{E}(\mathbf{y}) = -\nabla\Phi(\mathbf{y}) - \frac{1}{c}\frac{\partial\mathbf{A}(\mathbf{y})}{\partial t}$ , where  $\Phi(\mathbf{y})$  and  $\mathbf{A}(\mathbf{y})$  are scalar and vector potentials, respectively, the Hamiltonian  $\hat{H}(t)$  of the system is

$$\hat{H}(t) = \frac{1}{2m(t)} \sum_k (\hat{\mathbf{p}}_k + \frac{e}{c} \mathbf{A}(\mathbf{y}_k))^2 + \sum_k [v(\mathbf{y}_k) - e\Phi(\mathbf{y}_k)] + \frac{1}{2} \sum_{k,\ell} \frac{e^2}{|\mathbf{r}_k - \mathbf{r}_\ell|}, \tag{1}$$

where the separate terms correspond to the physical kinetic  $\hat{T}_A$ , scalar potential  $\hat{V}$ , and electron interaction potential  $\hat{U}$  operators;  $\hat{\mathbf{p}}_k = -i\hbar \nabla_{\mathbf{r}_k}$  (the canonical momentum operator),  $c$  is the velocity of light, and  $\mathbf{y}_k = \mathbf{r}_k t$ . The corresponding time-dependent Schrödinger equation is

$$\hat{H}(t)\Psi(\mathbf{Y}) = i\hbar \frac{\partial \Psi(\mathbf{Y})}{\partial t}, \tag{2}$$

with  $\Psi(\mathbf{Y})$  the wave function; the coordinate  $\mathbf{Y} = \mathbf{X}t$ ;  $\mathbf{X} = \mathbf{x}_1, \dots, \mathbf{x}_N$ ; and  $\mathbf{x} = \mathbf{r}\sigma$  with  $\mathbf{r}$  and  $\sigma$  are the spatial and spin coordinates of each electron. The scalar potentials  $v(\mathbf{y})$  and  $e\Phi(\mathbf{y})$  could be combined, but we keep them separate because of the difference in their origins. Fields arising from the zero-point motion of the nuclei which could be included in  $ev(\mathbf{y})$  are small and will be ignored.

The above physical system can also be described from the perspective of the individual electron. For a complete discussion of this perspective for a non-dissipative system, we refer the reader to Chapter 2 of [25]. The single electron perspective is described by the ‘Quantal Newtonian’ second law. This law is the equation of motion for each electron in terms of the fields experienced by it and a corresponding field representing its response. In turn, the fields are obtained from quantal sources that are expectations of Hermitian operators taken with respect to the wave function  $\Psi(\mathbf{Y})$ .

The ‘Quantal Newtonian’ second law for dissipative systems is

$$\mathcal{F}^{\text{ext}}(\mathbf{y}) + \mathcal{F}^{\text{int}}(\mathbf{y}) = \mathcal{J}(\mathbf{y}), \tag{3}$$

where the respective fields are: external  $\mathcal{F}^{\text{ext}}(\mathbf{y})$ , internal  $\mathcal{F}^{\text{int}}(\mathbf{y})$ , and current density response  $\mathcal{J}(\mathbf{y})$ . The law is gauge-invariant, and is derived with the constraint of the equation of continuity:

$$\nabla \cdot \mathbf{j}(\mathbf{y}) + \frac{\partial \rho(\mathbf{y})}{\partial t} = 0. \tag{4}$$

Here,  $\mathbf{j}(\mathbf{y})$  is the physical current density which is the expectation

$$\mathbf{j}(\mathbf{y}) = \langle \Psi(\mathbf{Y}) | \hat{\mathbf{j}}(\mathbf{y}) | \Psi(\mathbf{Y}) \rangle, \tag{5}$$

with  $\hat{\mathbf{j}}(\mathbf{y})$  (the physical current density operator) being the sum of its paramagnetic  $\hat{\mathbf{j}}_p(\mathbf{y})$  and diamagnetic  $\hat{\mathbf{j}}_d(\mathbf{y})$  components:

$$\hat{\mathbf{j}}(\mathbf{y}) = \hat{\mathbf{j}}_p(\mathbf{y}) + \hat{\mathbf{j}}_d(\mathbf{y}), \tag{6}$$

$$\hat{\mathbf{j}}_p(\mathbf{y}) = \frac{i\hbar}{2m(t)} \sum_k [\nabla_{\mathbf{r}_k} \delta(\mathbf{r}_k - \mathbf{r}) + \delta(\mathbf{r}_k - \mathbf{r}) \nabla_{\mathbf{r}_k}], \tag{7}$$

$$\hat{\mathbf{j}}_d(\mathbf{y}) = \frac{e\hat{\rho}(\mathbf{r})\mathbf{A}(\mathbf{y})}{m(t)c}, \tag{8}$$

with the density  $\rho(\mathbf{y})$  being the expectation

$$\rho(\mathbf{y}) = \langle \Psi(\mathbf{Y}) | \hat{\rho}(\mathbf{r}) | \Psi(\mathbf{Y}) \rangle \tag{9}$$

of the density operator

$$\hat{\rho}(\mathbf{r}) = \sum_k \delta(\mathbf{r}_k - \mathbf{r}). \tag{10}$$

The external field  $\mathcal{F}^{\text{ext}}(\mathbf{y})$  experienced by each electron is

$$\mathcal{F}^{\text{ext}}(\mathbf{y}) = \mathcal{E}(\mathbf{y}) - \mathcal{L}(\mathbf{y}) - e\mathbf{E}(\mathbf{y}), \tag{11}$$

where the Lorentz field  $\mathcal{L}(\mathbf{y})$  is defined in terms of the Lorentz ‘force’  $\ell(\mathbf{r})$  as

$$\mathcal{L}(\mathbf{y}) = \frac{\ell(\mathbf{y})}{\rho(\mathbf{y})}, \tag{12}$$

with

$$\ell(\mathbf{y}) = \frac{e}{c} \mathbf{j}(\mathbf{y}) \times \mathcal{B}(\mathbf{y}). \tag{13}$$

The internal field  $\mathcal{F}^{\text{int}}(\mathbf{y})$  experienced by each electron is the sum of the electron interaction  $\mathcal{E}_{ee}(\mathbf{y})$ , kinetic  $\mathcal{Z}(\mathbf{y})$ , differential density  $\mathcal{D}(\mathbf{y})$ , and internal magnetic  $\mathcal{I}(\mathbf{y})$  fields:

$$\mathcal{F}^{\text{int}}(\mathbf{y}) = \mathcal{E}_{ee}(\mathbf{y}) - \mathcal{Z}(\mathbf{y}) - \mathcal{D}(\mathbf{y}) - \mathcal{I}(\mathbf{y}). \tag{14}$$

The fields are defined in terms of the corresponding ‘forces’  $\mathbf{e}_{ee}(\mathbf{y})$ ,  $\mathbf{z}(\mathbf{y})$ ,  $\mathbf{d}(\mathbf{y})$ , and  $\mathbf{i}(\mathbf{y})$  as

$$\mathcal{E}_{ee}(\mathbf{y}) = \frac{\mathbf{e}_{ee}(\mathbf{y})}{\rho(\mathbf{y})}; \quad \mathcal{Z}(\mathbf{y}) = \frac{\mathbf{z}(\mathbf{y})}{\rho(\mathbf{y})}; \quad \mathcal{D}(\mathbf{y}) = \frac{\mathbf{d}(\mathbf{y})}{\rho(\mathbf{y})}; \quad \mathcal{I}(\mathbf{y}) = \frac{\mathbf{i}(\mathbf{y})}{\rho(\mathbf{y})}. \tag{15}$$

The electron interaction ‘force’  $\mathbf{e}_{ee}(\mathbf{y})$  is representative of electron correlations due to the Pauli exclusion principle and Coulomb repulsion, and is obtained from its quantal source—the pair correlation function  $P(\mathbf{r}\mathbf{r}'t)$ —via Coulomb’s law:

$$\mathbf{e}_{ee}(\mathbf{y}) = \int \frac{P(\mathbf{r}\mathbf{r}'t)(\mathbf{r} - \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|^3} d\mathbf{r}', \tag{16}$$

with  $P(\mathbf{r}\mathbf{r}'t)$  the expectation

$$P(\mathbf{r}\mathbf{r}'t) = \langle \Psi(\mathbf{Y}) | \hat{P}(\mathbf{r}\mathbf{r}') | \Psi(\mathbf{Y}) \rangle, \tag{17}$$

of the pair correlation operator

$$\hat{P}(\mathbf{r}\mathbf{r}') = \sum_{k,\ell}' \delta(\mathbf{r}_k - \mathbf{r}) \delta(\mathbf{r}_\ell - \mathbf{r}'). \tag{18}$$

The kinetic ‘force’  $\mathbf{z}(\mathbf{r})$ , representative of kinetic effects, is obtained from its quantal source, the single-particle density matrix  $\gamma(\mathbf{r}\mathbf{r}'t)$  as

$$z_\alpha(\mathbf{y}) = 2 \sum_{\beta} \nabla_{\beta} t_{\alpha\beta}(\mathbf{y}), \tag{19}$$

where the kinetic energy tensor  $t_{\alpha\beta}(\mathbf{y})$  is

$$t_{\alpha\beta}(\mathbf{y}) = \frac{1}{4} \left[ \frac{\partial^2}{\partial r'_\alpha \partial r''_\beta} + \frac{\partial^2}{\partial r'_\beta \partial r''_\alpha} \right] \gamma(\mathbf{r}'\mathbf{r}''t) \Big|_{\mathbf{r}'=\mathbf{r}''=\mathbf{r}}, \tag{20}$$

with  $\gamma(\mathbf{r}\mathbf{r}'t)$  the expectation

$$\gamma(\mathbf{r}\mathbf{r}'t) = \langle \Psi(\mathbf{Y}) | \hat{\gamma}(\mathbf{r}\mathbf{r}') | \Psi(\mathbf{Y}) \rangle \tag{21}$$

of the density matrix operator

$$\hat{\gamma}(\mathbf{r}\mathbf{r}') = \hat{A} + i\hat{B}, \tag{22}$$

$$\begin{aligned} \hat{A} &= \frac{1}{2} \sum_k [\delta(\mathbf{r}_k - \mathbf{r}) T_k(\mathbf{a}) + \delta(\mathbf{r}_k - \mathbf{r}') T_k(-\mathbf{a})], \\ \hat{B} &= \frac{i}{2} \sum_k [\delta(\mathbf{r}_k - \mathbf{r}) T_k(\mathbf{a}) - \delta(\mathbf{r}_k - \mathbf{r}') T_k(-\mathbf{a})], \end{aligned} \tag{23}$$

with  $T_k(\mathbf{a})$  being a translation operator such that  $T_k(\mathbf{a})\psi(\dots \mathbf{r}_k \dots) = \psi(\dots \mathbf{r}_k + \mathbf{a} \dots)$ , and  $\mathbf{a} = \mathbf{r}' - \mathbf{r}$ . The differential density ‘force’, representative of the density, is

$$\mathbf{d}(\mathbf{y}) = -\frac{1}{4}\nabla\nabla^2\rho(\mathbf{y}), \tag{24}$$

with the quantal source being the density  $\rho(\mathbf{y})$ . Finally, the magnetic field contribution to the internal ‘force’  $\mathbf{i}(\mathbf{y})$  whose quantal source is the current density  $\mathbf{j}(\mathbf{y})$  is

$$i_\alpha(\mathbf{y}) = \frac{e}{c}\sum_{\beta}\nabla_{\beta}I_{\alpha\beta}(\mathbf{y}), \tag{25}$$

where the tensor

$$I_{\alpha\beta}(\mathbf{y}) = [j_{\alpha}(\mathbf{y})A_{\beta}(\mathbf{y}) + j_{\beta}(\mathbf{y})A_{\alpha}(\mathbf{y})] - \frac{e}{m(t)c}\rho(\mathbf{y})A_{\alpha}(\mathbf{y})A_{\beta}(\mathbf{y}). \tag{26}$$

The response of the electron to the external  $\mathcal{F}^{\text{ext}}(\mathbf{y})$  and internal  $\mathcal{F}^{\text{int}}(\mathbf{y})$  fields is described by the current density field  $\mathcal{J}(\mathbf{y})$ , defined as

$$\mathcal{J}(\mathbf{y}) = \frac{1}{\rho(\mathbf{y})}\frac{\partial[m(t)\mathbf{j}(\mathbf{y})]}{\partial t}. \tag{27}$$

The field  $\mathcal{J}(\mathbf{y})$  can be written as the sum of a zeroth-order term  $\mathcal{J}_0(\mathbf{y})$  and a dissipative term  $\mathcal{J}^{\text{diss}}(\mathbf{y})$  involving a damping coefficient  $\zeta(t)$ . Thus,

$$\mathcal{J}(\mathbf{y}) = \mathcal{J}_0(\mathbf{y}) + \mathcal{J}^{\text{diss}}(\mathbf{y}), \tag{28}$$

where

$$\mathcal{J}_0(\mathbf{y}) = \frac{m(t)}{\rho(\mathbf{y})}\frac{\partial\mathbf{j}(\mathbf{y})}{\partial t}, \tag{29}$$

$$\mathcal{J}^{\text{diss}}(\mathbf{y}) = \zeta(t)\left(\frac{m(t)\mathbf{j}(\mathbf{y})}{\rho(\mathbf{y})}\right) \tag{30}$$

with

$$\zeta(t) = \frac{d}{dt}\ln m(t). \tag{31}$$

The ‘Quantal Newtonian’ second law of Equation (3), the proof of which is given in Appendix A, is an equivalent description of the physical system of Hamiltonian  $\hat{H}(t)$  of Equation (1) but from the perspective of the individual electron. In addition to the external binding  $\mathcal{E}(\mathbf{y})$ , Lorentz  $\mathcal{L}(\mathbf{y})$ , and electromagnetic  $\{e\mathbf{E}(\mathbf{y}), \mathcal{B}(\mathbf{y})\}$  fields, each electron experiences an internal field  $\mathcal{F}^{\text{int}}(\mathbf{y})$  representative of the properties of the system. These properties, described via component fields, are those of electron correlations due to the Pauli exclusion principle and Coulomb repulsion  $\mathcal{E}_{ee}(\mathbf{y})$ , kinetic effects  $\mathcal{Z}(\mathbf{y})$ , density  $\mathcal{D}(\mathbf{y})$ , and an internal contribution  $\mathcal{I}(\mathbf{y})$  due to the presence of the magnetic field  $\mathcal{B}(\mathbf{y})$ . The electron interaction field  $\mathcal{E}_{ee}(\mathbf{y})$  can be further decomposed into a sum of its Hartree  $\mathcal{E}_H(\mathbf{y})$  and Pauli-Coulomb  $\mathcal{E}_{xc}(\mathbf{y})$  components:

$$\mathcal{E}_{ee}(\mathbf{y}) = \mathcal{E}_H(\mathbf{y}) + \mathcal{E}_{xc}(\mathbf{y}). \tag{32}$$

This follows from the fact that the pair correlation density  $g(\mathbf{r}\mathbf{r}'t)$  at  $\mathbf{r}'$  for an electron at  $\mathbf{r}$  which is  $g(\mathbf{r}\mathbf{r}'t) = P(\mathbf{r}\mathbf{r}'t)/\rho(\mathbf{y})$  may be expressed as  $g(\mathbf{r}\mathbf{r}'t) = \rho(\mathbf{r}'t) + \rho_{xc}(\mathbf{r}\mathbf{r}'t)$ , where  $\rho_{xc}(\mathbf{r}\mathbf{r}'t)$  is the Fermi-Coulomb hole charge, the quantal source of the field  $\mathcal{E}_{xc}(\mathbf{y})$ . The quantal source for the Hartree field  $\mathcal{E}_H(\mathbf{y})$  is the density  $\rho(\mathbf{y})$ . The response of the electron in turn is described by the current density component fields  $\mathcal{J}_0(\mathbf{y})$  and  $\mathcal{J}^{\text{diss}}(\mathbf{y})$ . The ‘Quantal Newtonian’ second law for constant electron mass for which the term  $\mathcal{J}^{\text{diss}}(\mathbf{y})$  vanishes then constitutes a special case [33].

The ‘Quantal Newtonian’ second law of Equation (3) constitutes the basis for the remaining sections of the paper.

### 3. New Perspectives on the Schrödinger Equation

The Schrödinger equation of Equation (2) is written in traditional form. The Hamiltonian  $\hat{H}(t)$  is assumed as known: it is a first-order differential equation in time which can be solved for the evolution of the wave function  $\Psi(\mathbf{Y})$  given an initial condition at  $t = 0$ . We refer to Equation (2) as the non-self-consistent form of the Schrödinger equation. In this section we describe new perspectives on the Schrödinger equation as arrived at via the ‘Quantal Newtonian’ second law. *In particular, the law helps to exhibit the intrinsic self-consistent nature of the equation.*

To explain further, consider the Hamiltonian  $\hat{H}(t)$  of Equation (1). In it, the binding scalar potential  $v(\mathbf{y})$  represents a potential energy viz. that of an electron (at time  $t$ ). Furthermore, as it is a potential energy, it is *path-independent*. The potential is also thought of as being *extrinsic* to the system of electrons. The ‘Quantal Newtonian’ second law proves  $v(\mathbf{y})$  to be a potential in the rigorous classical sense. From Equation (3) it follows that  $v(\mathbf{y})$  is the work done (at time  $t$ ) to move an electron from some reference point at infinity to its position at  $\mathbf{r}$  in a conservative field  $\mathcal{F}(\mathbf{y})$ :

$$v(\mathbf{y}) = \int_{\infty}^{\mathbf{r}} \mathcal{F}(\mathbf{y}') \cdot d\ell' ; (\mathbf{y}' = \mathbf{r}'t) \tag{33}$$

where  $\mathcal{F}(\mathbf{y}) = \mathcal{F}^{\text{int}}(\mathbf{y}) - \mathcal{L}(\mathbf{y}) - e\mathbf{E}(\mathbf{y}) - \mathcal{J}(\mathbf{y}) = \mathcal{E}_{ee}(\mathbf{y}) - \mathcal{Z}(\mathbf{y}) - \mathcal{D}(\mathbf{y}) - \mathcal{I}(\mathbf{y}) - \mathcal{L}(\mathbf{y}) - e\mathbf{E}(\mathbf{y}) - \mathcal{J}(\mathbf{y})$ . As  $\nabla \times \mathcal{F}(\mathbf{y}) = 0$ , the function  $v(\mathbf{y})$  is *path-independent*. The expression for the potential  $v(\mathbf{y})$  of Equation (33) shows that it is inherently related to the properties of the system via the conservative field  $\mathcal{F}(\mathbf{y})$ . Thus, for example, it depends on the Pauli and Coulomb correlations via the electron interaction field  $\mathcal{E}_{ee}(\mathbf{y})$ , kinetic effects via the kinetic field  $\mathcal{Z}(\mathbf{y})$ , and so on. Therefore, the potential  $v(\mathbf{y})$  is a sum of functions each representative of a property of the system. The relationship between the properties of the system and the potential  $v(\mathbf{y})$  then shows the latter to be an *intrinsic* constituent of the system. This statement is further substantiated in the following paragraphs.

Finally, what the expression for  $v(\mathbf{y})$  shows is that it is an *exactly known* functional of the wave function:  $v(\mathbf{y}) = v[\Psi(\mathbf{Y})](\mathbf{y})$ . This is the case because the components of the field  $\mathcal{F}(\mathbf{y})$  are obtained from quantal sources that are expectations of Hermitian operators taken with respect to the wave function  $\Psi(\mathbf{Y})$ . As a consequence, the Hamiltonian  $\hat{H}(t)$  is then an exactly known functional of  $\Psi(\mathbf{Y})$ , i.e.,  $\hat{H}(t) = \hat{H}[\Psi(\mathbf{Y})](t)$ . This then demonstrates the intrinsic self-consistent nature of the Schrödinger equation which can now be written as

$$\hat{H}[\Psi(\mathbf{Y})]\Psi(\mathbf{Y}) = i\hbar \frac{\partial \Psi(\mathbf{Y})}{\partial t}, \tag{34}$$

where the Hamiltonian functional  $\hat{H}[\Psi(\mathbf{Y})]$  is

$$\begin{aligned} \hat{H}[\Psi(\mathbf{Y})] &= \frac{1}{2m(t)} \sum_k (\hat{\mathbf{p}}_k + \frac{e}{c} \mathbf{A}(\mathbf{y}_k))^2 + \sum_k v[\Psi(\mathbf{Y})](\mathbf{y}_k) \\ &- e \sum_k \Phi(\mathbf{y}_k) + \frac{1}{2} \sum'_{k,\ell} \frac{e^2}{|\mathbf{r}_k - \mathbf{r}_\ell|}, \end{aligned} \tag{35}$$

or equivalently

$$\begin{aligned} \hat{H}[\Psi(\mathbf{Y})] &= \frac{1}{2m(t)} \sum_k (\hat{\mathbf{p}}_k + \frac{e}{c} \mathbf{A}(\mathbf{y}_k))^2 + \sum_k \int_{\infty}^{\mathbf{r}_k} \mathcal{F}[\Psi](\mathbf{y}) \cdot d\ell \\ &- e \sum_k \Phi(\mathbf{y}_k) + \frac{1}{2} \sum'_{k,\ell} \frac{e^2}{|\mathbf{r}_k - \mathbf{r}_\ell|}. \end{aligned} \tag{36}$$

Recall that the meaning of the functional  $v[\Psi(\mathbf{Y})](\mathbf{y})$  is that for each new  $\Psi(\mathbf{Y})$  a new  $v(\mathbf{y})$  is obtained.

The self-consistency procedure is then as follows (see also Figure 1). One begins with an initial approximate input wave function  $\Psi^{\text{in}}(\mathbf{Y})$  and initial condition  $\Psi^{\text{in}}(\mathbf{Y}; t = 0)$ . With this choice of  $\Psi^{\text{in}}(\mathbf{Y})$ , one determines the various quantal sources, and from these sources the corresponding fields to construct the field  $\mathcal{F}(\mathbf{y})$ . The work done in this field in turn leads to a potential  $v[\Psi^{\text{in}}(\mathbf{Y})](\mathbf{y})$  via Equation (33). The Schrödinger equation Equation (34) is then solved to obtain a  $\Psi^{\text{out}}(\mathbf{Y})$ . With this  $\Psi^{\text{out}}(\mathbf{Y})$  a new  $v(\mathbf{y})$  is obtained in a similar way, and the procedure continued until  $\Psi^{\text{in}}(\mathbf{Y}) = \Psi^{\text{out}}(\mathbf{Y})$ . In this manner, the wave function  $\Psi(\mathbf{Y})$  as well as the potential  $v(\mathbf{y})$  can be determined self-consistently. As in the stationary-state case discussed in the Introduction, if the binding potential  $v(\mathbf{y})$  is known, the wave function  $\Psi(\mathbf{Y})$  can be obtained via solution of the Schrödinger equation (Equation (2)). Conversely, if the wave function  $\Psi(\mathbf{Y})$  is known, then the potential  $v(\mathbf{y})$  can be determined via Equation (33). If both  $v(\mathbf{y})$  and  $\Psi(\mathbf{Y})$  are *unknown*, then they can be determined by solution of the self-consistent form of the Schrödinger equation (Equation (34)). Or, if the wave function  $\Psi(\mathbf{Y})$  is known approximately, then the exact wave function can be obtained via the self-consistent procedure.)

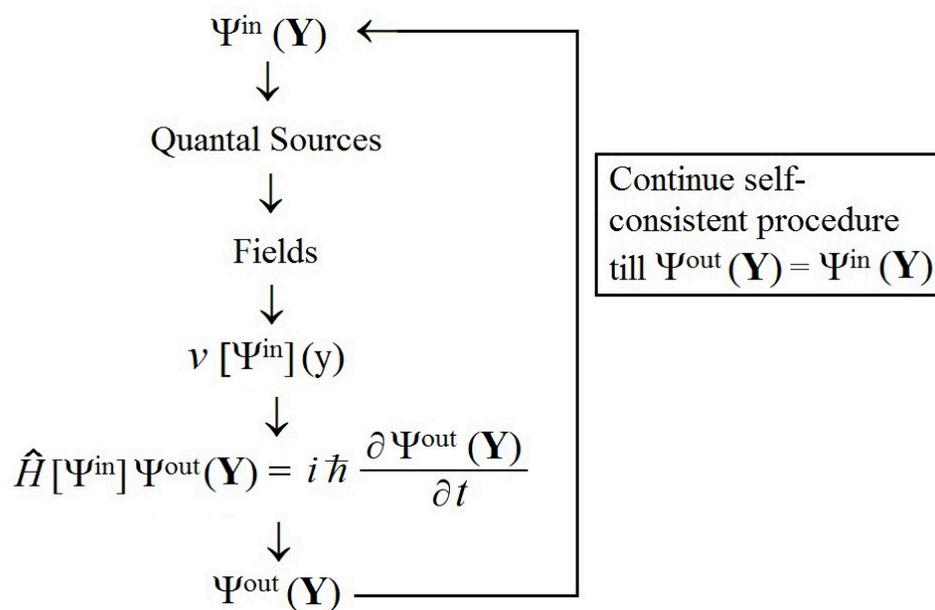


Figure 1. Procedure for the self-consistent solution of the Schrödinger equation at each instant of time.

The Schrödinger equation, as written in its non-self-consistent (Equation (2)) and self-consistent (Equation (34)) versions, also differ in another fundamental way (see also [34,35]). Observe that due to the correspondence principle, it is the vector potential  $\mathbf{A}(\mathbf{y})$  that appears in the Hamiltonian of Equation (1). The magnetic field  $\mathbf{B}(\mathbf{y})$  appears in it only following the choice of gauge. However, in the Hamiltonian functional of Equations (35) or (36), the magnetic field  $\mathbf{B}(\mathbf{y})$  appears explicitly via the Lorentz field  $\mathcal{L}(\mathbf{y})$  contribution to the potential  $v(\mathbf{y})$  (see Equation (33)). That this must be the case follows from the fact that in any self-consistent procedure, all the physical information must be present in the corresponding differential equation.

The above remarks for the dissipative Schrödinger system are general in that they are equally applicable to the case of constant electron mass, as well as to the stationary state case.

#### 4. Basic Variables in Dissipative Systems

Within Schrödinger theory, there are properties that are termed basic variables. These are gauge-invariant properties, knowledge of which determines the external scalar and vector

potentials—the property of invertibility. With the canonical kinetic energy and electron interaction potential energy operators assumed known, the system Hamiltonian is thus fully defined. The solution of the corresponding Schrödinger equation then leads to the system wave function. In this manner, the basic variables thereby determine the properties of the system. In this section we prove, by employing the ‘Quantal Newtonian’ second law derived in Section 2, that the basic variables for dissipative systems as defined by the Hamiltonian of Equation (1) are the density  $\rho(\mathbf{y})$  and the physical current density  $\mathbf{j}(\mathbf{y})$ .

The knowledge of which properties constitute the basic variables is also of significance in local effective potential theory [33,42–45]. Such theories constitute the mapping from the interacting system of electrons to one of noninteracting fermions possessing the same basic variables. The proof that  $\{\rho(\mathbf{y}), \mathbf{j}(\mathbf{y})\}$  constitute the basic variables is equivalent to the proof of existence of such model systems [50–52]. In the section to follow, we develop the QDFT equations for noninteracting fermions possessing the same  $\{\rho(\mathbf{y}), \mathbf{j}(\mathbf{y})\}$ .

The proof the  $\{\rho(\mathbf{y}), \mathbf{j}(\mathbf{y})\}$  are the basic variables is similar to that of Vignale [50] for non-dissipative systems for which the electron mass is a constant. Hence, we provide here only a brief outline of the proof.

One begins by considering the dissipative Hamiltonian  $\hat{H}(t)$  of the form of Equation (1):

$$\hat{H}(t) = \frac{1}{2m(t)} \sum_k (\hat{\mathbf{p}}_k + \frac{e}{c} \mathbf{A}(\mathbf{y}_k))^2 + \sum_k v(\mathbf{y}_k) + \sum_{k,\ell}' \hat{U}(\mathbf{r}_k - \mathbf{r}_\ell), \tag{37}$$

where  $\{v(\mathbf{y}), \mathbf{A}(\mathbf{y})\}$  are the external scalar and vector potentials, and  $\hat{U}(\mathbf{r}_k - \mathbf{r}_\ell)$  an arbitrary electron interaction potential energy operator. The solution of the Schrödinger equation  $\hat{H}(t)\Psi(\mathbf{Y}) = i\hbar\partial\Psi(\mathbf{Y})/\partial t$  with initial state  $\Psi(\mathbf{Y}; t = 0)$  leads to the densities  $\{\rho(\mathbf{y}), \mathbf{j}(\mathbf{y})\}$ . What is proved is that there exist other many-particle dissipative systems with Hamiltonian  $\hat{H}'(t)$ , potentials  $\{v'(\mathbf{y}), \mathbf{A}'(\mathbf{y})\}$ , and  $U'(\mathbf{r}_k - \mathbf{r}_\ell)$ , and Schrödinger equation  $\hat{H}'\Psi'(\mathbf{Y}) = i\hbar\partial\Psi'(\mathbf{Y})/\partial t$  with initial state  $\Psi'(\mathbf{Y}; t = 0)$  which generate the same  $\{\rho(\mathbf{y}), \mathbf{j}(\mathbf{y})\}$  as that of  $\hat{H}(t)$ . The potentials  $\{v'(\mathbf{y}), \mathbf{A}'(\mathbf{y})\}$  are determined by  $\{v(\mathbf{y}), \mathbf{A}(\mathbf{y})\}$ ,  $\Psi(\mathbf{Y}; t = 0)$  and  $\Psi'(\mathbf{Y}; t = 0)$  to within a time-dependent scalar function  $\partial C(\mathbf{y})/\partial t$  and the gradient of  $C(\mathbf{y})$ , respectively. It follows [50–52] that if one considers the primed system to be that of noninteracting fermions but with the same dissipative mass  $m(t)$ , then *the theorem allows for the existence of a local effective potential system which can then reproduce the  $\{\rho(\mathbf{y}), \mathbf{j}(\mathbf{y})\}$  of the interacting system.* The scalar potentials  $v(\mathbf{y})$  and  $v'(\mathbf{y})$  are eliminated from the Hamiltonians by a gauge transformation of the form  $\partial C(\mathbf{y})/\partial t = v(\mathbf{y})$  with  $C(\mathbf{y}; t = 0) = 0$  in each case. The potential  $\Phi(\mathbf{y})$  may also be put to zero. The corresponding ‘Quantal Newtonian’ second law of Equation (3) for the unprimed and primed systems assuming the same dissipative  $\{\rho(\mathbf{y}), \mathbf{j}(\mathbf{y})\}$  and  $m(t)$  are

$$-\mathcal{E}_{ee}(\mathbf{y}) + \mathcal{Z}(\mathbf{y}) + \mathcal{D}(\mathbf{y}) + \mathcal{I}(\mathbf{y}) - \frac{e}{c} \frac{\partial \mathbf{A}(\mathbf{y})}{\partial t} + \mathcal{L}(\mathbf{y}) = \mathcal{J}(\mathbf{y}), \tag{38}$$

and

$$-\mathcal{E}'_{ee}(\mathbf{y}) + \mathcal{Z}'(\mathbf{y}) + \mathcal{D}(\mathbf{y}) + \mathcal{I}'(\mathbf{y}) - \frac{e}{c} \frac{\partial \mathbf{A}'(\mathbf{y})}{\partial t} + \mathcal{L}'(\mathbf{y}) = \mathcal{J}(\mathbf{y}). \tag{39}$$

On subtracting Equation (38) from Equation (39) one obtains

$$\frac{e}{c} \frac{\partial \Delta \mathbf{A}(\mathbf{y})}{\partial t} = \frac{e}{c} \mathbf{j}(\mathbf{y}) \times [\nabla \times \Delta \mathbf{A}(\mathbf{y})] + \Delta \mathbf{Q}(\mathbf{y}), \tag{40}$$

where  $\Delta \mathbf{A}(\mathbf{y}) = \mathbf{A}(\mathbf{y}) - \mathbf{A}'(\mathbf{y})$  and  $\Delta \mathbf{Q}(\mathbf{y}) = \mathbf{Q}(\mathbf{y}) - \mathbf{Q}'(\mathbf{y})$  with  $\mathbf{Q}(\mathbf{y}) = -\mathcal{E}_{ee}(\mathbf{y}) + \mathcal{Z}(\mathbf{y}) + \mathcal{I}(\mathbf{y})$ . The solution to Equation (40) for  $\Delta \mathbf{A}(\mathbf{y})$  then determines  $\mathbf{A}'(\mathbf{y})$  which produces the same current density  $\mathbf{j}(\mathbf{y})$  of  $\mathbf{A}(\mathbf{y})$ . Equation (40) may also be derived via the equation of motion for the physical current density  $\mathbf{j}(\mathbf{y})$  as done by Vignale [50] for the non-dissipative system. We do not provide here the details of that derivation. The equation is the dissipative system equivalent of Equation (11) of Vignale.

As both  $\mathbf{A}(\mathbf{y})$  and  $\mathbf{A}'(\mathbf{y})$  are expandable in a Taylor series of time near  $t = 0$ , so is  $\Delta\mathbf{A}(\mathbf{y})$ . Substitution of this expansion of  $\Delta\mathbf{A}(\mathbf{y})$  into Equation (40) then leads to a recursion relationship for the coefficients of the expansion, together with the initial value constraint of  $\Delta\mathbf{A}(\mathbf{y}; t = 0) = \mathbf{A}(\mathbf{y}; t = 0) - \mathbf{A}'(\mathbf{y}; t = 0)$ . With the coefficients of the expansion determined, the vector potential  $\mathbf{A}'(\mathbf{y})$  is known. There is the added constraint that the Taylor series converges within a radius  $t_c > 0$  [50]. The potential  $\mathbf{A}'(\mathbf{y})$  can be determined up to  $t_c$ , and then  $t_c$  can be considered the new initial time, and the process repeated. Implicit in all this is the assumption that the radius of convergence cannot be zero. Hence, the vector potential  $\mathbf{A}'(\mathbf{y})$  is determined to within the gradient of a scalar function. To put another way, if there exist two vector potentials  $\mathbf{A}(\mathbf{y})$  and  $\mathbf{A}'(\mathbf{y})$  that generate the same current density  $\mathbf{j}(\mathbf{y})$ , then they differ by a gauge transformation. The present proof for dissipative systems is a generalization of the proof of Vignale [50] which in turn is a generalization of that due to van Leeuwen [51] for the case when the time-dependent magnetic field  $\mathcal{B}(\mathbf{y})$  is absent (we refer to our work as a generalization of that of Vignale, because a new term involving a dissipation coefficient now appears). In a similar manner it can be proved that if two external scalar potentials  $v(\mathbf{y})$  and  $v'(\mathbf{y})$  lead to the same dissipative density  $\rho(\mathbf{y})$ , then they can only differ by a time-dependent function  $\partial C(t)/\partial t$ . Thus, the basic variables for dissipative systems are  $\{\rho(\mathbf{y}), \mathbf{j}(\mathbf{y})\}$ .

### 5. Quantal Density Functional Theory of Dissipative Systems

In this section we develop the equations for the QDFT of dissipative systems. As noted in the Introduction, a key purpose of developing a QDFT is to enable a separation of the electron correlations due to the Pauli exclusion principle and Coulomb repulsion, and to determine the contribution of these correlations to the kinetic energy. Such a separation is of particular significance for lower-dimensional systems such as quantum dots [25,31,53] and in the high electron correlation Wigner regime [54,55]. In such systems, correlation-kinetic effects play a very significant role in comparison to those of the exclusion principle and Coulomb repulsion. Additionally, QDFT is a local effective potential theory with the attendant attributes of the latter.

QDFT is the mapping from the interacting dissipative system defined by the Hamiltonian of Equation (1) to a model dissipative  $S$  system of noninteracting fermions possessing the same basic variables  $\{\rho(\mathbf{y}), \mathbf{j}(\mathbf{y})\}$ . This implies that the model fermions also have the same time-dependent mass  $m(t)$ . Finally, the model fermions experience the same external electromagnetic fields. Hence, the electron potentials  $\{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\}$  are also the same. The principal advantage of requiring [33] the model fermions to possess the same basic variables and experience the same potentials is that then the only correlations that must be accounted for by the  $S$  system are those due to the Pauli exclusion principle, Coulomb repulsion, and correlation-kinetic effects.

The dissipative  $S$  system Schrödinger equation for the single-particle orbitals  $\phi_k(\mathbf{y})$  of the Slater determinant wave function  $\Omega\{\phi_k\}$  is

$$\left[ \frac{1}{2m(t)} \left( \hat{\mathbf{p}} + \frac{e}{c} \mathbf{A}(\mathbf{y}) \right)^2 + v_s(\mathbf{y}) \right] \phi_k(\mathbf{y}) = i\hbar \frac{\partial \phi_k(\mathbf{y})}{\partial t}; \quad k = 1, \dots, N, \tag{41}$$

where the local effective potential  $v_s(\mathbf{y})$  is

$$v_s(\mathbf{y}) = v(\mathbf{y}) - e\Phi(\mathbf{y}) + v_{ee}(\mathbf{y}), \tag{42}$$

and where all the many body effects are incorporated in the local electron interaction potential  $v_{ee}(\mathbf{y})$ . The resulting properties—the Dirac density matrix  $\gamma_s(\mathbf{r}\mathbf{r}'t)$ , density  $\rho_s(\mathbf{y})$ , physical current density  $\mathbf{j}_s(\mathbf{y})$ , and pair correlation density  $g_s(\mathbf{r}\mathbf{r}'t) = P_s(\mathbf{r}\mathbf{r}'t)/\rho_s(\mathbf{y})$  with  $P_s(\mathbf{r}\mathbf{r}'t)$  the pair correlation function—are expectations of the corresponding operators  $\hat{\gamma}(\mathbf{r}\mathbf{r}')$ ,  $\hat{\rho}(\mathbf{r})$ ,  $\hat{\mathbf{j}}(\mathbf{r})$ ,  $\hat{P}(\mathbf{r}\mathbf{r}')$  taken with respect to the Slater determinant  $\Omega\{\phi_k(\mathbf{y})\}$ .

With the requirement that  $\rho_s(\mathbf{y}) \equiv \rho(\mathbf{y})$  and  $\mathbf{j}_s(\mathbf{y}) \equiv \mathbf{j}(\mathbf{y})$ , the ‘Quantal Newtonian’ second law for each dissipative  $S$  system fermion is as follows (see Appendix A)

$$\mathcal{F}^{\text{ext}}(\mathbf{y}) + \mathcal{F}_s^{\text{int}}(\mathbf{y}) = \mathcal{J}(\mathbf{y}), \tag{43}$$

where the external field  $\mathcal{F}^{\text{ext}}(\mathbf{y})$  is given by Equation (11), and the response field  $\mathcal{J}(\mathbf{y})$  by Equation (28). The internal field experienced by each model fermion is

$$\mathcal{F}_s^{\text{int}}(\mathbf{y}) = -\nabla v_{ee}(\mathbf{y}) - \mathcal{Z}_s(\mathbf{y}) - \mathcal{D}(\mathbf{y}) - \mathcal{I}(\mathbf{y}), \tag{44}$$

where the kinetic field  $\mathcal{Z}_s(\mathbf{y})$  is defined in a manner similar to that for  $\mathcal{Z}(\mathbf{y})$  of Equation (19) but in terms of the Dirac density matrix  $\gamma_s(\mathbf{r}\mathbf{r}'t)$ . The fields  $\mathcal{D}(\mathbf{y})$  and  $\mathcal{I}(\mathbf{y})$  too are the same as those for the interacting system.

On subtracting the ‘Quantal Newtonian’ law Equation (43) from that for the interacting system Equation (3), one obtains the electron interaction potential  $v_{ee}(\mathbf{y})$  as to be the work done (at each instant of time  $t$ ) to move the model fermion from some reference point at infinity to its position at  $\mathbf{r}$  in the conservative effective field  $\mathcal{F}^{\text{eff}}(\mathbf{y})$ :

$$v_{ee}(\mathbf{y}) = - \int_{\infty}^{\mathbf{r}} \mathcal{F}^{\text{eff}}(\mathbf{y}') \cdot d\ell', \tag{45}$$

where

$$\mathcal{F}^{\text{eff}}(\mathbf{y}) = \mathcal{E}_{ee}(\mathbf{y}) + \mathcal{Z}_{t_c}(\mathbf{y}), \tag{46}$$

with  $\mathcal{E}_{ee}(\mathbf{y})$  defined by Equations (15) and (16), and where  $\mathcal{Z}_{t_c}(\mathbf{y})$  is the correlation-kinetic field defined as

$$\mathcal{Z}_{t_c}(\mathbf{y}) = \mathcal{Z}_s(\mathbf{y}) - \mathcal{Z}(\mathbf{y}). \tag{47}$$

As  $\nabla \times \mathcal{F}^{\text{eff}}(\mathbf{y}) = 0$ , the work done  $v_{ee}(\mathbf{y})$  is *path-independent*. With this  $v_{ee}(\mathbf{y})$ , the solutions  $\phi_k(\mathbf{y})$  of Equation (41) for the model system reproduce the same dissipative  $\{\rho(\mathbf{y}), \mathbf{j}(\mathbf{y})\}$  as that of the interacting system.

Next, writing the  $S$  system pair correlation density as  $g_s(\mathbf{r}\mathbf{r}'t) = \rho(\mathbf{y}') + \rho_x(\mathbf{r}\mathbf{r}'t)$ , where the Fermi hole charge  $\rho_x(\mathbf{r}\mathbf{r}'t)$  is  $\rho_x(\mathbf{r}\mathbf{r}'t) = -|\gamma_s(\mathbf{r}\mathbf{r}'t)|^2/2\rho(\mathbf{y})$ , one defines the Coulomb hole charge as  $\rho_c(\mathbf{r}\mathbf{r}'t) = g(\mathbf{r}\mathbf{r}'t) - g_s(\mathbf{r}\mathbf{r}'t) = \rho_{xc}(\mathbf{r}\mathbf{r}'t) - \rho_x(\mathbf{r}\mathbf{r}'t)$ . Thus, the electron interaction field  $\mathcal{E}_{ee}(\mathbf{y})$  subdivision of Equation (32) can be further decomposed as

$$\mathcal{E}_{ee}(\mathbf{y}) = \mathcal{E}_H(\mathbf{y}) + \mathcal{E}_x(\mathbf{y}) + \mathcal{E}_c(\mathbf{y}), \tag{48}$$

where  $\mathcal{E}_x(\mathbf{y})$  and  $\mathcal{E}_c(\mathbf{y})$  are the Pauli and Coulomb fields, as obtained from the Fermi and Coulomb hole charges, respectively. In this manner, the effective field  $\mathcal{F}^{\text{eff}}(\mathbf{y})$  can be written as a sum of its Hartree, Pauli, Coulomb, and correlation-kinetic components:

$$\mathcal{F}^{\text{eff}}(\mathbf{y}) = \mathcal{E}_H(\mathbf{y}) + \mathcal{E}_x(\mathbf{y}) + \mathcal{E}_c(\mathbf{y}) + \mathcal{Z}_{t_c}(\mathbf{y}). \tag{49}$$

Note that the fields  $\mathcal{E}_x(\mathbf{y})$ ,  $\mathcal{E}_c(\mathbf{y})$ ,  $\mathcal{Z}_{t_c}(\mathbf{y})$  may not be separately conservative. Their sum always is.

Finally, we note that the model system Schrödinger equation for the orbitals  $\phi_k(\mathbf{y})$  of Equation (41) is also intrinsically self-consistent. The reason for this is that the electron interaction potential  $v_{ee}(\mathbf{y})$  of Equation (45) is a known functional of the orbitals  $\phi_k(\mathbf{y})$ , because the effective field  $\mathcal{F}^{\text{eff}}(\mathbf{y})$  is such a functional i.e.,  $v_{ee}(\mathbf{y}) = v_{ee}[\phi_k](\mathbf{y})$ . Hence, the differential equation may be written as

$$\left[ \frac{1}{2m(t)} (\hat{\mathbf{p}} + \frac{e}{c} \mathbf{A}(\mathbf{y}))^2 + \{v(\mathbf{y}) - e\Phi(\mathbf{y})\} + v_{ee}[\phi_k](\mathbf{y}) \right] \phi_k(\mathbf{y}) = i\hbar \frac{\partial \phi_k(\mathbf{y})}{\partial t}, \tag{50}$$

or equivalently

$$\left[ \frac{1}{2m(t)} \left( \hat{\mathbf{p}} + \frac{e}{c} \mathbf{A}(\mathbf{y}) \right)^2 + \{v(\mathbf{y}) - e\Phi(\mathbf{y})\} - \int_{\infty}^{\mathbf{r}} \mathcal{F}[\phi_k](\mathbf{y}) \cdot d\ell \right] \phi_k(\mathbf{y}) = i\hbar \frac{\partial \phi_k(\mathbf{y})}{\partial t}. \quad (51)$$

Thus, we note, that the Schrödinger equation for the dissipative system of interacting electrons and that of the model system of noninteracting fermions with the same densities  $\{\rho(\mathbf{y}), \mathbf{j}(\mathbf{y})\}$  can both be written so as to exhibit their intrinsic self-consistent nature.

### 6. Summary and Conclusions

This paper develops a framework by which dissipative effects are incorporated within the Schrödinger theory of electrons in electromagnetic fields. Dissipation is accounted for via the effective Hamiltonian approach by the assumption that the mass of the electron is a function of time, i.e.,  $m = m(t)$ . The perspective presented differs from that in the literature. The description is in terms of the equation of motion of the *individual electron* or equivalently, the ‘Quantal Newtonian’ second law for each electron. According to the law, the electron experiences both the external field  $\mathcal{F}^{\text{ext}}(\mathbf{y})$ —the time-dependent binding electric field, the Lorentz field, and the electromagnetic field—and an internal field  $\mathcal{F}^{\text{int}}(\mathbf{y})$  composed of components representative of the properties of the system. These component fields represent electron correlations due to the Pauli exclusion principle and Coulomb repulsion, kinetic effects, density, and a contribution to the internal field due to the external magnetic field. The response of the electron to these fields is then a current density field  $\mathcal{J}(\mathbf{y})$  which involves a damping coefficient  $\zeta(t)$  which accounts for the dissipative effects. The internal field components too are reflective of the dissipation through their dependence on the mass of the electron. These fields are ‘classical’ in the sense that they are obtained from quantal sources which in turn are expectations of Hermitian operators.

The ‘Quantal Newtonian’ second law leads to further insights into Schrödinger theory. It follows from the law that the external scalar binding potential of the electron  $v(\mathbf{y})$  can be afforded a rigorous physical interpretation in the classical sense: It is the work done to move an electron in a conservative field  $\mathcal{F}(\mathbf{y})$ . The field is the sum of the internal, Lorentz, electric and current density response fields. Hence, the components of  $v(\mathbf{y})$ —the contributions due to the individual properties of the system—are *explicitly known*. As the field  $\mathcal{F}(\mathbf{y})$  is conservative, the work done is *path-independent*. Furthermore, as the components of the field  $\mathcal{F}(\mathbf{y})$  are obtained from quantal sources that are expectations of Hermitian operators taken with respect to the wave function  $\Psi$ , it is an *exactly known* functional of  $\Psi$  i.e.,  $\mathcal{F}(\mathbf{y}) = \mathcal{F}[\Psi](\mathbf{y})$ . In turn, the potential  $v(\mathbf{y})$  is an *exactly known* functional of  $\Psi$ , i.e.,  $v(\mathbf{y}) = v[\Psi](\mathbf{y})$ . Substitution of this  $v[\Psi](\mathbf{y})$  into the Hamiltonian shows that the Hamiltonian is an *exactly known* functional of  $\Psi$ , i.e.,  $\hat{H}(t) = \hat{H}[\Psi](t)$ . The Schrödinger equation can therefore be written in a more general form as  $\hat{H}[\Psi]\Psi = i\hbar \partial \Psi / \partial t$  which then demonstrates its intrinsic self-consistent nature. Thereby, the wave function  $\Psi$  can be determined self-consistently. This constitutes a generalization of the Schrödinger theory to dissipative systems.

It is also proved that for this dissipative quantum-mechanical system, the basic variables are the density  $\rho(\mathbf{y})$  and physical current density  $\mathbf{j}(\mathbf{y})$ . Hence, knowledge of the gauge-invariant properties  $\{\rho(\mathbf{y}), \mathbf{j}(\mathbf{y})\}$  uniquely determines the external scalar  $v(\mathbf{y})$  and vector  $\mathbf{A}(\mathbf{y})$  potentials to within a time-dependent function and the gradient of this function, respectively. In other words,  $\{\rho(\mathbf{y}), \mathbf{j}(\mathbf{y})\}$  determine the wave function  $\Psi$  of the system, and thereby all properties. The proof of the one-to-one relationship  $\{v(\mathbf{y}), \mathbf{A}(\mathbf{y})\} \leftrightarrow \{\rho(\mathbf{y}), \mathbf{j}(\mathbf{y})\}$  also proves the existence of a system of noninteracting fermions possessing the same  $\{\rho(\mathbf{y}), \mathbf{j}(\mathbf{y})\}$  provided the wave functions of the interacting and model systems at the initial time  $t = 0$  lead to the same initial state  $\{\rho(\mathbf{y}), \mathbf{j}(\mathbf{y})\}$ .

Finally, with the knowledge that the basic variables are the densities  $\{\rho(\mathbf{y}), \mathbf{j}(\mathbf{y})\}$ , we develop the equations of QDFT that map the interacting dissipative system to one of noninteracting fermions with the same dissipative response  $\{\rho(\mathbf{y}), \mathbf{j}(\mathbf{y})\}$ . Provided the model fermions are subject to the same external potentials  $\{v(\mathbf{y}), \mathbf{A}(\mathbf{y})\}$ , the only correlations that need to be accounted for are those due to

the Pauli exclusion principle, Coulomb repulsion, and correlation-kinetic effects. All the many-body effects are then incorporated into a local electron interaction potential  $v_{ee}(\mathbf{y})$  which is the work done in a conservative effective field  $\mathcal{F}^{\text{eff}}(\mathbf{y})$ . The work done  $v_{ee}(\mathbf{y})$  is therefore *path-independent*. The field  $\mathcal{F}^{\text{eff}}(\mathbf{y})$  is a known functional of the orbitals  $\phi_k(\mathbf{y})$ , so that the Hamiltonian  $\hat{H}_{s,k}$  of the model fermion is a functional of  $\phi_k(\mathbf{y})$ . Thus, the Schrödinger equation of each model fermion is of the self-consistent form  $\hat{H}_{s,k}[\phi_k(\mathbf{y})]\phi_k(\mathbf{y}) = i\hbar\partial\phi_k(\mathbf{y})/\partial t$ , with the corresponding wave function  $\Omega\{\phi_k(\mathbf{y})\}$  being a Slater determinant of the orbitals  $\phi_k(\mathbf{y})$ . This equation, with a local effective potential, is of course, far easier to solve than the self-consistent Schrödinger equation.

Density functional theory (both time-independent [44,56] and time-dependent [48,52]), and QDFT are equivalent in that both map the interacting system of electrons to one of noninteracting fermions possessing the same basic variables. The former theories are mathematical in the sense that they are in terms of energy and action functionals of the density, and of their functional derivatives. In contrast, QDFT is a physical theory. It describes a quantum-mechanical system in terms of fields that arise from quantal sources, the stationary-state description being a special case of the time-dependent theory. It thus provides a rigorous physical interpretation [25,29,57,58] of the functionals and functional derivatives of density functional theory. Additionally, QDFT allows for the separation of the electron correlations due to the Pauli exclusion principle, Coulomb repulsion, and correlation-kinetic effects. The contribution of these correlations to the local electron interaction potential in which the many-body effects are incorporated, and to the total energy, is explicitly defined. For approximation methods and applications of QDFT, we refer the reader to [26].

As noted in the Introduction, the self-consistent solution of the various local effective potential theories [25,42–45] is for the single-particle spin-orbital with the resulting wave function being a Slater determinant of these orbitals. On the other hand, the solution of the self-consistent Schrödinger equation of Equation (34) is for the many-body wave function. Hence, from a numerical perspective, the solution is more difficult. In recent work [34] we have demonstrated the self-consistency procedure for the non-dissipative 2D two-electron ‘artificial atom’ or quantum dot in a magnetic field [31,53,59,60] in a ground and excited singlet state. Work on the dissipative quantum-dot is in progress and will be presented elsewhere. We believe that with present-day computing power, the solution of the self-consistent Schrödinger equation for other systems is feasible, but that is for the future. There exist many methods such as the variational and perturbative schemes for the determination of the approximate wave function of a system. The understanding that the Schrödinger equation can be solved self-consistently means that there is now a path for the determination of the exact wave function to the degree of numerical accuracy desired.

In conclusion, we have developed the Schrödinger theory of electrons in a dissipative environment from the perspective of the individual electron via the corresponding equation of motion. As a consequence, new insights into Schrödinger theory are obtained. We have also derived the equations of quantal density functional theory, the local effective potential equivalent of the interacting dissipative system of electrons. The equations derived and conclusions arrived at for both theories are general. The non-dissipative system constitutes a special case. Stationary state systems constitute yet another special case.

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## Appendix A. Derivation of the ‘Quantal Newtonian’ Second Law

To derive the ‘Quantal Newtonian’ second law, expand the Hamiltonian of Equation (1) so as to rewrite it as

$$\hat{H}(t) = -\frac{\hbar^2}{2m(t)} \sum_k \nabla_{\mathbf{r}_k}^2 + \frac{1}{2} \sum_{k,\ell}' \frac{e^2}{|\mathbf{r}_k - \mathbf{r}_\ell|} + \sum_k [v(\mathbf{y}_k) - e\Phi(\mathbf{y}_k)] + \sum_k \hat{\omega}(\mathbf{y}_k \mathbf{A}(\mathbf{y}_k)), \tag{A1}$$

where the operator  $\hat{\omega}(\mathbf{y}_k \mathbf{A}(\mathbf{y}_k))$  is

$$\hat{\omega}(\mathbf{y}_k \mathbf{A}(\mathbf{y}_k)) = \frac{e^2}{2m(t)c^2} A^2(\mathbf{y}) - i \frac{\hbar e}{2m(t)c} [\nabla \cdot \mathbf{A}(\mathbf{y}) + 2\mathbf{A}(\mathbf{y}) \cdot \nabla]. \tag{A2}$$

Next, write the wave function as  $\Psi(\mathbf{Y}) = \Psi^R(\mathbf{Y}) + i\Psi^I(\mathbf{Y})$ , where  $\Psi^R(\mathbf{Y})$  and  $\Psi^I(\mathbf{Y})$  are its real and imaginary parts. Substitute this  $\Psi(\mathbf{Y})$  into the Schrödinger equation (Equation (2)) and perform the various differentiations. After considerable algebra, one arrives at the ‘force’ equation

$$-\mathbf{e}_{ee}(\mathbf{y}) + \mathbf{z}(\mathbf{y}) + \mathbf{d}(\mathbf{y}) + \mathbf{k}(\mathbf{y} \mathbf{j}_p \mathbf{A}) + \rho(\mathbf{y}) \nabla \left[ v(\mathbf{y}) - e\Phi(\mathbf{y}) + \frac{e^2}{2m(t)c^2} A^2(\mathbf{y}) \right] + \frac{\partial}{\partial t} [m(t) \mathbf{j}_p(\mathbf{y})] = 0, \tag{A3}$$

where the ‘forces’  $\mathbf{e}_{ee}(\mathbf{y})$ ,  $\mathbf{z}(\mathbf{y})$ ,  $\mathbf{d}(\mathbf{y})$  and paramagnetic current density  $\mathbf{j}_p(\mathbf{y})$  are defined in the text, and where  $\mathbf{k}(\mathbf{y} \mathbf{j}_p \mathbf{A})$  is

$$k_\alpha(\mathbf{y} \mathbf{j}_p \mathbf{A}) = \frac{e}{c} \sum_\beta \{ j_{p\beta}(\mathbf{y}) \nabla_\alpha A_\beta(\mathbf{y}) + \nabla_\beta [A_\beta(\mathbf{y}) j_{p\alpha}(\mathbf{y})] \}. \tag{A4}$$

We next rewrite Equation (A3) in terms of the physical current density  $\mathbf{j}(\mathbf{y})$  via Equation (6). Thus, for Equation (A4) one obtains

$$k_\alpha(\mathbf{y} \mathbf{j}_p \mathbf{A}) = k_\alpha(\mathbf{y} \mathbf{j} \mathbf{A}) - \frac{e^2}{m(t)c^2} \sum_\beta \{ \rho(\mathbf{y}) A_\beta(\mathbf{y}) [\nabla_\alpha A_\beta(\mathbf{y})] + \nabla_\beta [A_\beta(\mathbf{y}) \rho(\mathbf{y}) A_\alpha(\mathbf{y})] \} \tag{A5}$$

$$= k_\alpha(\mathbf{y} \mathbf{j} \mathbf{A}) - \frac{e^2}{2m(t)c^2} \sum_\beta \rho(\mathbf{y}) \nabla_\alpha A_\beta^2(\mathbf{y}) - \frac{e^2}{m(t)c^2} \sum_\beta \{ A_\beta(\mathbf{y}) \nabla_\beta [\rho(\mathbf{y}) A_\alpha(\mathbf{y})] + \rho(\mathbf{y}) A_\alpha(\mathbf{y}) \nabla_\beta A_\beta(\mathbf{y}) \}, \tag{A6}$$

or in vector form

$$k(\mathbf{y} \mathbf{j}_p \mathbf{A}) = k(\mathbf{y} \mathbf{j} \mathbf{A}) - \frac{e^2}{2m(t)c^2} \rho(\mathbf{y}) \nabla A^2(\mathbf{y}) - \frac{e^2}{m(t)c^2} \{ \mathbf{A}(\mathbf{y}) \cdot \nabla [\rho(\mathbf{y}) \mathbf{A}(\mathbf{y})] + \rho(\mathbf{y}) \mathbf{A}(\mathbf{y}) \nabla \cdot \mathbf{A}(\mathbf{y}) \}. \tag{A7}$$

On employing Equation (6) together with the continuity Equation (4), we have

$$\frac{\partial}{\partial t} [m(t) \mathbf{j}_p(\mathbf{y})] = \frac{\partial}{\partial t} [m(t) \mathbf{j}(\mathbf{y})] + \frac{e}{c} \mathbf{A}(\mathbf{y}) \nabla \cdot \mathbf{j}(\mathbf{y}) - \frac{e}{c} \rho(\mathbf{y}) \frac{\partial \mathbf{A}(\mathbf{y})}{\partial t}. \tag{A8}$$

Substituting Equations (A7) and (A8) into Equation (A3), and using  $\mathbf{E}(\mathbf{y}) = -\nabla\Phi(\mathbf{y}) - \frac{1}{c} \frac{\partial \mathbf{A}(\mathbf{y})}{\partial t}$  leads to

$$-\mathbf{e}_{ee}(\mathbf{y}) + \mathbf{z}(\mathbf{y}) + \mathbf{d}(\mathbf{y}) + \rho(\mathbf{y}) \nabla v(\mathbf{y}) + \rho(\mathbf{y}) e \mathbf{E}(\mathbf{y}) + \left( k(\mathbf{y} \mathbf{j} \mathbf{A}) - \frac{e^2}{m(t)c^2} \{ \mathbf{A}(\mathbf{y}) \cdot \nabla [\rho(\mathbf{y}) \mathbf{A}(\mathbf{y})] + \rho(\mathbf{y}) \mathbf{A}(\mathbf{y}) \nabla \cdot \mathbf{A}(\mathbf{y}) \} + \frac{e}{c} \mathbf{A}(\mathbf{y}) \nabla \cdot \mathbf{j}(\mathbf{y}) \right) + \frac{\partial}{\partial t} [m(t) \mathbf{j}(\mathbf{y})] = 0. \tag{A9}$$

With the Lorentz ‘force’  $\ell(\mathbf{y})$  defined as in Equation (13) and with  $\mathcal{B}(\mathbf{y}) = \nabla \times \mathbf{A}(\mathbf{y})$ , we have

$$\ell_\alpha(\mathbf{y}) = \sum_\beta [j_\beta(\mathbf{y})\nabla_\alpha A_\beta(\mathbf{y}) - j_\beta(\mathbf{y})\nabla_\beta A_\alpha(\mathbf{y})]. \tag{A10}$$

With the internal ‘force’  $\mathbf{i}(\mathbf{y})$  contribution due to the magnetic field defined as in Equation (25), it is readily seen that  $\ell(\mathbf{y}) + \mathbf{i}(\mathbf{y})$  is equivalent to the terms in Equation (A9) in the large parentheses. Thus, on dividing by  $\rho(\mathbf{y})$ , Equation (A9) becomes

$$-\mathcal{E}_{ee}(\mathbf{y}) + \mathcal{Z}(\mathbf{y}) + \mathcal{D}(\mathbf{y}) + \mathcal{I}(\mathbf{y}) - [\mathcal{E}(\mathbf{y}) - e\mathbf{E}(\mathbf{y})] + \mathcal{L}(\mathbf{y}) + \frac{1}{\rho(\mathbf{y})} \frac{\partial}{\partial t} [m(t)\mathbf{j}(\mathbf{y})] = 0. \tag{A11}$$

Finally,

$$\frac{1}{\rho(\mathbf{y})} \frac{\partial}{\partial t} [m(t)\mathbf{j}(\mathbf{y})] = \mathcal{J}_0(\mathbf{y}) + \mathcal{J}^{\text{diss}}(\mathbf{y}), \tag{A12}$$

with  $\mathcal{J}_0(\mathbf{y})$  and  $\mathcal{J}^{\text{diss}}(\mathbf{y})$  as defined by Equations (29) and (30). Equation (A11) is thus the ‘Quantal Newtonian’ second law of Equation (3) which is the equation of motion for the individual electron.

For the dissipative S system in the same external field  $\mathcal{F}^{\text{ext}}(\mathbf{y})$ , and with the same densities  $\{\rho(\mathbf{y}), \mathbf{j}(\mathbf{y})\}$ , the ‘Quantal Newtonian’ second law of Equation (43) for the noninteracting fermions is obtained in a similar manner by writing the orbital  $\phi_{\mathbf{k}}(\mathbf{y})$  as  $\phi_{\mathbf{k}}(\mathbf{y}) = \phi_{\mathbf{k}}^R(\mathbf{y}) + i\phi_{\mathbf{k}}^I(\mathbf{y})$ , where  $\phi_{\mathbf{k}}^R(\mathbf{y})$  and  $\phi_{\mathbf{k}}^I(\mathbf{y})$  are the real and imaginary components, and by substitution into the corresponding Schrödinger equation (Equation (41)).

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