Publications and Research   CUNY Graduate Center

2017

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Abstract

The Schrödinger theory for a system of electrons in the presence of both a static and time-dependent electromagnetic field is generalized so as to exhibit the intrinsic self-consistent nature of the corresponding Schrödinger equations. This is accomplished by proving that the Hamiltonian in the stationary-state and time-dependent cases $\{\hat{H}; \hat{H}(t)\}$ are *exactly known* functionals of the corresponding wave functions $\{\Psi; \Psi(t)\}$, *i.e.* $\hat{H} = \hat{H}[\Psi]$ and $\hat{H}(t) = \hat{H}[\Psi(t)]$. Thus, the Schrödinger equations may be written as $\hat{H}[\Psi]\Psi = E[\Psi]\Psi$ and $\hat{H}[\Psi(t)]\Psi(t) = i\partial\Psi(t)/\partial t$. As a consequence the eiegenfunctions and energy eigenvalues $\{\Psi, E\}$ of the stationary-state equation, and the wave function $\Psi(t)$ of the temporal equation, can be determined self-consistently. The proofs are based on the 'Quantal Newtonian' first and second laws which are the equations of motion for the *individual* electron amongst the sea of electrons in the external fields. The generalization of the Schrödinger equation in this manner leads to additional new physics. The traditional description of the Schrödinger theory of electrons with the Hamiltonians $\{\hat{H}; \hat{H}(t)\}$ known constitutes a special case.

I am very pleased to write this paper in honor of Lou Massa. I first met Lou in January of 1972 at the Sanibel Symposium. At that time the Symposium was still being held at Sanibel Island. I was a graduate student at the Polytechnic Institute of Brooklyn, and Lou was an Assistant Professor at Hunter College of the City University of New York. At the Symposium I was presenting work on a variational method for the determination of the coherent atomic scattering factor, the Fourier transform of the electron density. Lou's interest at that time was on developing methods for obtaining the single-particle density matrix from x-ray diffraction data. (The density is the diagonal matrix element of the density matrix.) I vaguely recall our conversation, but little did I know at that time that we would be colleagues and friends at the same University very soon thereafter, as I joined Brooklyn College in 1973. There was not much interaction between us till 1990 when we met again at the Sanibel Symposium, now held at St. Augustine. Having published a paper on the physical interpretation of the Kohn-Sham 'exchange-correlation' potential, I was presenting the work at the Symposium. Lou showed a keen interest in the underlying physics, and this turned out to be the catalyst for our future collaboration and relationship. We have spent countless hours talking physics for the past nearly three decades, each hour as enjoyable as the next. But there are two key attributes of the discussions with Lou which have made a mark. The first are his insightful questions. In addressing those queries, one invariably comes away with further clarifications and understandings. For those questions and discussions, I am grateful. The second attribute, equally important for me, has been his support of my work over the years. The value of his encouragement cannot be expressed in words. The present paper is one I have been discussing with Lou over the past year, and hence I thought it best to write about the work for this special issue dedicated to him.

I. INTRODUCTION

The paper generalizes the Schrödinger theory of electrons in an electromagnetic field. This is accomplished by proving the intrinsic self-consistent nature of the time-dependent Schrödinger equation. The generalization in turn leads to new physics, and to the self-consistent determination of the wave function. The corresponding generalization of stationary-state theory constitutes a special case. As a consequence, the eigenfunctions and energy eigenvalues of the time-independent Schrödinger equation can be obtained in a self-consistent manner.

To put the present work in perspective, let us initially consider our present-day understanding of the stationary-state Schrödinger theory of electrons. For a system of N electrons in a static electric field $\boldsymbol{\mathcal{E}}(\mathbf{r}) = -\boldsymbol{\nabla}v(\mathbf{r})$ and magnetostatic field $\boldsymbol{\mathcal{B}}(\mathbf{r}) = \boldsymbol{\nabla} \times \mathbf{A}(\mathbf{r})$, with $v(\mathbf{r})$ and $\mathbf{A}(\mathbf{r})$ the respective scalar and vector potentials, the Schrödinger equation in atomic units (charge of electron $-e, |e| = \hbar = m = 1$) together with the assumption $c = 1$, is

$$\hat{H}\Psi(\mathbf{X}) = E\Psi(\mathbf{X}), \tag{1}$$

where the Hamiltonian $\hat{H}$ is the sum of the physical kinetic $\hat{T}_A$, electron-interaction $\hat{U}$, and external potential $\hat{V}$ energy operators:

$$\hat{H} = \hat{T}_A + \hat{U} + \hat{V}, \tag{2}$$

where

$$\hat{T}_A = \frac{1}{2}\sum_k (\hat{\mathbf{p}}_k + \mathbf{A}(\mathbf{r}_k))^2 \;\; ; \;\; \hat{U} = \frac{1}{2}{\sum_{k,l}}' \frac{1}{|\mathbf{r}_k - \mathbf{r}_l|} \;\; ; \;\; \hat{V} = \sum_k v(\mathbf{r}_k), \tag{3}$$

$\hat{\mathbf{p}} = -i\boldsymbol{\nabla}$ the canonical momentum operator; $\{\Psi(\mathbf{X}), E\}$ the eigenfunctions and energy eigenvalues; $\mathbf{X} = \mathbf{x}_1, \ldots \mathbf{x}_N; \mathbf{x} = \mathbf{r}\sigma; \mathbf{r}\sigma$ the spatial and spin coordinates.

The Schrödinger equation of Eq. (1) is the traditional manner in which the equation is written in its most general form. The magnetic field $\boldsymbol{\mathcal{B}}(\mathbf{r})$ appears in the equation via the choice of gauge, e. g. $\mathbf{A}(\mathbf{r}) = \frac{1}{2}\boldsymbol{\mathcal{B}}(\mathbf{r}) \times \mathbf{r}$, the symmetric gauge, or $\mathbf{A}(\mathbf{r}) = -Bxi_y$, the Landau gauge. The field $\boldsymbol{\mathcal{E}}(\mathbf{r})$ is assumed to be conservative so that the potential $v(\mathbf{r})$ is path independent. The choice of the external field $\boldsymbol{\mathcal{E}}(\mathbf{r})$, or equivalently the potential $v(\mathbf{r})$ that confines the electrons, then defines the physical system being considered. Thus, for example, the Schrödinger equation for matter – atoms, molecules, and solids – is defined with $\boldsymbol{\mathcal{B}}(\mathbf{r}) = 0$ and $v(\mathbf{r})$ as being Coulombic. For the two-dimensional 'artificial atom' or

quantum dot [1–3], the confining potential $v(\mathbf{r})$ has been determined [3] via experiment and theory to be harmonic. Once the electric field $\boldsymbol{\mathcal{E}}(\mathbf{r})$, or equivalently the potential $v(\mathbf{r})$, and the magnetic field $\boldsymbol{\mathcal{B}}(\mathbf{r})$ are specified, the Hamiltonian $\hat{H}$ operator is fully defined, and *known*. What remains then is the determination of the solution $\{\Psi(\mathbf{X}), E\}$ for a particular state.

With the Hamiltonian $\hat{H}$ known, the solutions of the Schrödinger equation Eq. (1) in closed-analytical form is possible only for the simplest of systems, as in the one-electron case. Such an analytical solution is not known even for the ground state of the He atom, the second element of the Periodic Table. However, more recently, it has been shown that closed-form analytical solutions for both the ground and excited states of the two-electron Hooke's atom [4] and the two-electron quantum dot in a magnetic field [5] can be determined for a denumerable infinite set of force constants. For the cases for which the Schrödinger equation cannot be solved analytically, one must resort to various approximation methods [6] such as many-body perturbation theory, the variational principle for the energy, the Monte Carlo method, and a host of other schemes. Of these, the energy variational method is possibly the most powerful: An approximate wave function correct to $O(\delta)$ leads to a rigorous upper bound to the ground state energy that is correct to $O(\delta^2)$. An improved wave function thus corresponds to one that yields a lower energy value. However, other observables – expectations of different Hermitian operators – are correct only to the same order as the wave function itself, *i.e.* to $O(\delta)$. The variational wave function is thus accurate in the region of configuration space from which the principal contribution to the energy arises, such as the interior of atoms. It is not accurate for properties such as the diamagnetic susceptibility which samples the classically forbidden region, or the Fermi contact term obtained from the deep interior of the atom. However, there exist variational principles whereby single-particle properties such as the coherent atomic scattering factor [7], and hence the density; and the single-particle density matrix [8], and therefore the momentum density, can be obtained correct to $O(\delta^2)$ while beginning with a trial wave function correct to $O(\delta)$.

It will be shown that the Hamiltonian $\hat{H}$ of Eq. (2) is an *exactly known* functional of the wave function $\Psi(\mathbf{X})$, *i.e.* $\hat{H} = \hat{H}[\Psi(\mathbf{X})]$. This result is arrived at via the 'Quantal Newtonian' first law [9–12] for each electron. Hence, the Schrödinger equation of Eq. (1)

can now be written in a more general form as

$$\hat{H}[\Psi(\mathbf{X})]\Psi(\mathbf{X}) = E[\Psi]\Psi(\mathbf{X}), \tag{4}$$

which then exhibits its intrinsic self-consistent nature. Solutions of equations of the form $\hat{L}[\xi]\xi = \lambda\xi$, where $\{\xi, \lambda\}$ are the eigenfunctions and eigenvalues, respectively, of the operator $\hat{L}$, are obtained self-consistently. The Hartree [13] and Hartree-Fock [14] theory equations constitute examples of this form: $\hat{H}^{\mathrm{HF}}[\phi_i(\mathbf{x})]\phi_i(\mathbf{x}) = \epsilon_i\phi_i(\mathbf{x})$, where $\hat{H}^{\mathrm{HF}}$ is the Hartree-Fock theory integro-differential operator, and $\{\phi_i(\mathbf{x}), \epsilon_i\}$ the single-particle spin-orbitals and eigenvalues, respectively. The equations of local effective potential theories such as Kohn-Sham theory [15], the Optimized Potential method [16], Quantal density functional theory [9, 10], etc., are all also of the same form. There is, however, one point of difference between the self-consistent equations of these theories and that of the Schrödinger equation of Eq. (4). Whereas the solutions of equations of these theories are single-particle orbitals $\phi_i(\mathbf{x})$, the self-consistent solution of the Schrödinger equation is the many-particle wave function $\Psi(\mathbf{X})$. Finally, the non-self-consistent version of the Schrödinger equation of Eq. (1) with known Hamiltonian $\hat{H}$, then constitutes a special case of the more general self-consistent form of the equation as expressed by Eq. (4). The manner by which this is the case will be explained in Sect. III.

It is worth noting here that in the presence of solely an electrostatic field $\boldsymbol{\mathcal{E}}(\mathbf{r})$, the fact that the Hamiltonian $\hat{H}$ is a functional of the *nondegenerate ground* state wave function $\Psi_g(\mathbf{X})$ is known from the proof of the Hohenberg-Kohn (HK) theorem [17]. For N electrons, HK first prove a bijective relationship between the potential $v(\mathbf{r})$ and the nondegenerate ground state wave function $\Psi_g(\mathbf{X})$. Hence, the potential $v(\mathbf{r})$ is a functional of $\Psi_g(\mathbf{X})$, *i.e.* $v(\mathbf{r}) = v[\Psi_g(\mathbf{X})](\mathbf{r})$. Thus, $\hat{H}$ is a functional of $\Psi_g(\mathbf{X})$. *The theorem, however, does not provide what that functional is.* In the second part of the theorem, HK prove a bijective relationship between the nondegenerate ground state wave function $\Psi_g(\mathbf{X})$ and the corresponding nondegenerate ground state density $\rho(\mathbf{r})$. Thus, knowledge of this density uniquely determines the potential $v(\mathbf{r})$ to within a constant. Now, as the momentum and electron-interaction operators are assumed known, the Hamiltonian $\hat{H}$ is hence known. The solution of the resulting Schrödinger equation then leads to the wave functions $\Psi(\mathbf{X})$, both ground and excited state, of the system. (The nondegenerate ground state density $\rho(\mathbf{r})$ is thus said to be a *basic variable* of quantum mechanics.) Yet another way to arrive at

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this conclusion is due to E. Bright Wilson [9, 18] who also noted that knowledge of the ground state density leads to the Hamiltonian of the system: Integration of the density gives the electron number N; the Kato [9, 10, 19] electron-nucleus coalescence differential cusp condition on this density leads to knowledge of the nuclear charge Z and their positions.

In the added presence of a magnetostatic field $\boldsymbol{\mathcal{B}}(\mathbf{r}) = \nabla \times \mathbf{A}(\mathbf{r})$, the relationship between the scalar $v(\mathbf{r})$ and vector $\mathbf{A}(\mathbf{r})$ potentials and the nondegenerate ground state wave function $\Psi_g(\mathbf{X})$ is not one-to-one but *many-to-one* and could be *infinite-to-one*. Hence, it is not possible in this case to prove that the $\hat{H}$ is a functional of the wave function $\Psi_g(\mathbf{X})$. For a uniform magnetostatic field $\boldsymbol{\mathcal{B}}(\mathbf{r}) = \mathcal{B}\hat{\mathbf{i}}_z$, it has been proved [9, 20] in a manner different from that of the original HK theorem, that the *basic variables* are the nondegenerate ground state density $\rho(\mathbf{r})$ and the physical current density $\mathbf{j}(\mathbf{r})$. Hence, knowledge of $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$ determines the potentials $\{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\}$ to within a constant and the gradient of a scalar function, respectively. Thus, the Hamiltonian $\hat{H}$ is known, and thereby via the solution of the Schrödinger equation, the wave functions of the system.

For the time-dependent case, consider N electrons in an external electrostatic field $\boldsymbol{\mathcal{E}}(\mathbf{r}) = -\boldsymbol{\nabla} v(\mathbf{r})$ which defines the physical system, and an external electromagnetic field $\mathbf{E}(\mathbf{y}) = -\boldsymbol{\nabla}\Phi(\mathbf{y}) - \partial\mathbf{A}(\mathbf{y})/\partial t$, $\boldsymbol{\mathcal{B}}(\mathbf{y}) = \boldsymbol{\nabla} \times \mathbf{A}(\mathbf{y})$; $\mathbf{y} = \mathbf{r}t$. Combining $v(\mathbf{r}) + \Phi(\mathbf{y})$ as $v(\mathbf{y})$, and defining $\mathbf{Y} = \mathbf{X}t$ and $\mathbf{y}_k = \mathbf{r}_k t$, the Schrödinger equation is

$$\hat{H}(t)\Psi(\mathbf{Y}) = i\frac{\partial\Psi(\mathbf{Y})}{\partial t}, \tag{5}$$

with the time-dependent Hamiltonian $\hat{H}(t)$ being

$$\hat{H}(t) = \hat{T}_A(t) + \hat{U} + \hat{V}(t), \tag{6}$$

where the physical kinetic $\hat{T}_A(t)$, electron-interaction $\hat{U}$, and potential $\hat{V}(t)$ energy operators are

$$\hat{T}_A(t) = \frac{1}{2}\sum_k(\hat{\mathbf{p}}_k + \mathbf{A}(\mathbf{y}_k))^2 \;\; ; \;\; \hat{U} = \frac{1}{2}\sum_{k,l}{}' \frac{1}{|\mathbf{r}_k - \mathbf{r}_l|} \;\; ; \;\; \hat{V}(t) = \sum_k v(\mathbf{y}_k), \tag{7}$$

and $\Psi(\mathbf{Y})$ is the wave function.

From the 'Quantal Newtonian' second law [9, 21, 22], it can be shown that the Hamiltonian $\hat{H}(t)$ is an *exactly known* functional of $\Psi(\mathbf{Y})$, *i.e.* $\hat{H}(t) = \hat{H}[\Psi(\mathbf{Y})]$. The time-dependent Schrödinger equation in self-consistent form is then

$$\hat{H}[\Psi(\mathbf{Y})]\Psi(\mathbf{Y}) = i\frac{\partial\Psi(\mathbf{Y})}{\partial t}. \tag{8}$$

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In this manner, the Schrödinger equation is written in a more general form. The Schrödinger equation of Eq. (5) with the Hamiltonian $\hat{H}(t)$ known, then constitutes a special case.

The 'Quantal Newtonian' first and second laws which are the equations of motion for the individual electron are described in Sect. II. The derivation of the self-consistent form of the stationary-state and time-dependent Schrödinger equations, and the description of the self-consistent procedure for the former, are given in Sect. III. The new physics gleaned thereby is explained in Section IV. Concluding remarks are made in Section V.

II. 'QUANTAL NEWTONIAN' FIRST AND SECOND LAWS

As noted in the Introduction, the conclusion that the Schrödinger equation is intrinsically a self-consistent one stems from the 'Quantal Newtonian' first and second laws, those for the stationary-state and time-dependent cases, respectively. These are equations of motion for the *individual electron* in the sea of electrons that are subjected to an external field. (These equations are the quantum-mechanical analogs of Newton's equations for an individual particle amongst a group of interacting particles with an external force present.) The laws are stated in terms of 'classical' fields whose sources are quantum-mechanical expectations of Hermitian operators taken with respect to the wave function. The quantal sources, and hence the fields, are representative of properties of the system. The fields can also be expressed in terms of the ratio of the corresponding 'force' to the electron (charge) density.

We begin with a description of the 'Quantal Newtonian' first law [9, 11, 12] for the physical system described by the Hamiltonian of Eq. (1). For completeness, a brief outline of the proof [9, 11] of this law is given in the Appendix. According to the law, the sum of the external $\boldsymbol{\mathcal{F}}^{\text{ext}}(\mathbf{r})$ and internal $\boldsymbol{\mathcal{F}}^{\text{int}}(\mathbf{r})$ fields experienced by each electron vanish:

$$\boldsymbol{\mathcal{F}}^{\text{ext}}(\mathbf{r}) + \boldsymbol{\mathcal{F}}^{\text{int}}(\mathbf{r}) = 0. \tag{9}$$

The external field $\boldsymbol{\mathcal{F}}^{\text{ext}}(\mathbf{r})$ is the sum of the electrostatic $\boldsymbol{\mathcal{E}}(\mathbf{r})$ and Lorentz $\boldsymbol{\mathcal{L}}(\mathbf{r})$ fields:

$$\boldsymbol{\mathcal{F}}^{\text{ext}}(\mathbf{r}) = \boldsymbol{\mathcal{E}}(\mathbf{r}) - \boldsymbol{\mathcal{L}}(\mathbf{r}) = -\boldsymbol{\nabla}v(\mathbf{r}) - \boldsymbol{\mathcal{L}}(\mathbf{r}). \tag{10}$$

The internal field $\boldsymbol{\mathcal{F}}^{\text{int}}(\mathbf{r})$ is the sum of the following fields: an electron-interaction field $\boldsymbol{\mathcal{E}}_{\text{ee}}(\mathbf{r})$ representative of electron correlations due to the Pauli exclusion principle and Coulomb repulsion; a kinetic field $\boldsymbol{\mathcal{Z}}(\mathbf{r})$ representative of kinetic effects; a differential density field

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$\mathcal{D}(\mathbf{r})$ representative of the density; and an internal magnetic field $\mathcal{I}(\mathbf{r})$ component:

$$\mathcal{F}^{\text{int}}(\mathbf{r}) = \mathcal{E}_{\text{ee}}(\mathbf{r}) - \mathcal{Z}(\mathbf{r}) - \mathcal{D}(\mathbf{r}) - \mathcal{I}(\mathbf{r}). \tag{11}$$

In terms of 'forces', the individual fields are written as

$$\mathcal{L}(\mathbf{r}) = \frac{\boldsymbol{\ell}(\mathbf{r})}{\rho(\mathbf{r})} \ ; \ \mathcal{E}_{\text{ee}}(\mathbf{r}) = \frac{\mathbf{e}_{\text{ee}}(\mathbf{r})}{\rho(\mathbf{r})} \ ; \ \mathcal{Z}(\mathbf{r}) = \frac{\mathbf{z}(\mathbf{r})}{\rho(\mathbf{r})} \ ; \ \mathcal{D}(\mathbf{r}) = \frac{\mathbf{d}(\mathbf{r})}{\rho(\mathbf{r})} \ ; \ \mathcal{I}(\mathbf{r}) = \frac{\mathbf{i}(\mathbf{r})}{\rho(\mathbf{r})}, \tag{12}$$

where the density $\rho(\mathbf{r})$, a quantal source, is the expectation

$$\rho(\mathbf{r}) = \langle \Psi(\mathbf{X}) | \hat{\rho}(\mathbf{r}) | \Psi(\mathbf{X}) \rangle, \tag{13}$$

of the density operator $\hat{\rho}(\mathbf{r}) = \sum_k \delta(\mathbf{r}_k - \mathbf{r})$. The Lorentz 'force' $\boldsymbol{\ell}(\mathbf{r})$ is obtained from its quantal source, the physical current density $\mathbf{j}(\mathbf{r})$ as

$$\boldsymbol{\ell}(\mathbf{r}) = \mathbf{j}(\mathbf{r}) \times \boldsymbol{\mathcal{B}}(\mathbf{r}), \tag{14}$$

with $\mathbf{j}(\mathbf{r})$ the expectation

$$\mathbf{j}(\mathbf{r}) = \langle \Psi(\mathbf{X}) | \hat{\mathbf{j}}(\mathbf{r}) | \Psi(\mathbf{X}) \rangle, \tag{15}$$

of the physical current density operator $\hat{\mathbf{j}}(\mathbf{r}) = \frac{1}{2i} \sum_k [\boldsymbol{\nabla}_{\mathbf{r}_k} \delta(\mathbf{r}_k - \mathbf{r}) + \delta(\mathbf{r}_k - \mathbf{r}) \boldsymbol{\nabla}_{\mathbf{r}_k}] + \hat{\rho}(\mathbf{r}) \mathbf{A}(\mathbf{r})$. The electron-interaction 'force' $\mathbf{e}_{\text{ee}}(\mathbf{r})$ is obtained by Coulomb's law via its quantal source, the pair-correlation function $P(\mathbf{rr}')$ as

$$\mathbf{e}_{\text{ee}}(\mathbf{r}) = \int \frac{\mathbf{P}(\mathbf{rr}')(\mathbf{r} - \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|^3} d\mathbf{r}', \tag{16}$$

with $P(\mathbf{rr}')$ the expectation

$$P(\mathbf{rr}') = \langle \Psi(\mathbf{X}) | \hat{\mathbf{P}}(\mathbf{rr}') | \Psi(\mathbf{X}) \rangle, \tag{17}$$

of the pair-operator $\hat{\mathbf{P}}(\mathbf{rr}') = \sum'_{k,l} \delta(\mathbf{r}_k - \mathbf{r}) \delta(\mathbf{r}_l - \mathbf{r}')$. The kinetic 'force' is obtained from its quantal source, the single-particle density matrix $\gamma(\mathbf{rr}')$ as

$$z_\alpha(\mathbf{r}) = 2 \sum_\beta \nabla_\beta t_{\alpha\beta}(\mathbf{r}), \tag{18}$$

where the kinetic energy tensor is

$$t_{\alpha\beta}(\mathbf{r}) = \frac{1}{4} \left[\frac{\partial^2}{\partial r'_\alpha \partial r''_\beta} + \frac{\partial^2}{\partial r'_\beta \partial r''_\alpha} \right] \gamma(\mathbf{r}'\mathbf{r}'') \Big|_{\mathbf{r}'=\mathbf{r}''=\mathbf{r}}, \tag{19}$$

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with $\gamma(\mathbf{rr'})$ the expectation

$$\gamma(\mathbf{rr'}) = \langle\Psi(\mathbf{X})|\hat{\gamma}(\mathbf{rr'})|\Psi(\mathbf{X})\rangle, \tag{20}$$

of the density matrix operator $\hat{\gamma}(\mathbf{rr'}) = \hat{A} + i\hat{B}$, $\hat{A} = \frac{1}{2}\sum_j[\delta(\mathbf{r}_j - \mathbf{r})T_j(\mathbf{a}) + \delta(\mathbf{r}_j - \mathbf{r'})T_j(-\mathbf{a})]$, $\hat{B} = -\frac{i}{2}\sum_j[\delta(\mathbf{r}_j - \mathbf{r})T_j(\mathbf{a}) - \delta(\mathbf{r}_j - \mathbf{r'})T_j(-\mathbf{a})]$, with $T_j(\mathbf{a})$ a translation operator such that $T_j(\mathbf{a})\Psi(\ldots\mathbf{r}_j,\ldots) = \Psi(\ldots\mathbf{r}_j + \mathbf{a},\ldots)$. The differential density 'force' is obtained from its quantal source, the density $\rho(\mathbf{r})$ as

$$\mathbf{d}(\mathbf{r}) = -\frac{1}{4}\boldsymbol{\nabla}\nabla^2\rho(\mathbf{r}). \tag{21}$$

The internal magnetic 'force' whose quantal source is the physical current density $\mathbf{j}(\mathbf{r})$ is

$$i_\alpha(\mathbf{r}) = \sum_\beta \nabla_\beta I_{\alpha\beta}(\mathbf{r}), \tag{22}$$

with the tensor

$$I_{\alpha\beta}(\mathbf{r}) = [j_\alpha(\mathbf{r})A_\beta(\mathbf{r}) + j_\beta(\mathbf{r})A_\alpha(\mathbf{r})] - \rho(\mathbf{r})A_\alpha(\mathbf{r})A_\beta(\mathbf{r}). \tag{23}$$

It is important to note that the 'Quantal Newtonian' first law is valid for *arbitrary* state, and is gauge invariant. It also satisfies the continuity equation $\boldsymbol{\nabla}\cdot\mathbf{j}(\mathbf{r}) = 0$.

For completeness, the components of the total energy – the kinetic T, electron-interaction E_{ee}, the internal magnetic I, and external E_{ext} – can each be expressed in integral virial form in terms of the respective fields [9, 11]:

$$T = -\frac{1}{2}\int\rho(\mathbf{r})\mathbf{r}\cdot\boldsymbol{\mathcal{Z}}(\mathbf{r})d\mathbf{r}, \tag{24}$$

$$E_{ee} = \int\rho(\mathbf{r})\mathbf{r}\cdot\boldsymbol{\mathcal{E}}_{ee}(\mathbf{r})d\mathbf{r}, \tag{25}$$

$$I = \int\rho(\mathbf{r})\mathbf{r}\cdot\boldsymbol{\mathcal{I}}(\mathbf{r})d\mathbf{r}, \tag{26}$$

$$E_{ext} = \int\rho(\mathbf{r})\mathbf{r}\cdot\boldsymbol{\mathcal{F}}^{ext}(\mathbf{r})d\mathbf{r}. \tag{27}$$

These energy component expressions together with the 'Quantal Newtonian' first law then provide a tangible description of stationary-state Schrödinger theory in terms of fields and quantal sources.

The 'Quantal Newtonian' second law [22] for each electron corresponding to the time-dependent Hamiltonian of Eq. (6) is the generalization of the first law of Eq. (9), and reads

$$\boldsymbol{\mathcal{F}}^{ext}(\mathbf{y}) + \boldsymbol{\mathcal{F}}^{int}(\mathbf{y}) = \boldsymbol{\mathcal{J}}(\mathbf{y}), \tag{28}$$

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where the external field is

$$\boldsymbol{\mathcal{F}}^{\text{ext}}(\mathbf{y}) = \boldsymbol{\mathcal{E}}(\mathbf{r}) - \boldsymbol{\mathcal{L}}(\mathbf{r}) - \mathbf{E}(\mathbf{r}) \tag{29}$$

$$= -\boldsymbol{\nabla}v(\mathbf{y}) - \boldsymbol{\mathcal{L}}(\mathbf{r}) + \frac{\partial \mathbf{A}(\mathbf{y})}{\partial t}, \tag{30}$$

the internal field is

$$\boldsymbol{\mathcal{F}}^{\text{int}}(\mathbf{y}) = \boldsymbol{\mathcal{E}}_{\text{ee}}(\mathbf{y}) - \boldsymbol{\mathcal{Z}}(\mathbf{y}) - \boldsymbol{\mathcal{D}}(\mathbf{y}) - \boldsymbol{\mathcal{I}}(\mathbf{y}), \tag{31}$$

and where the response of the electron to the external and internal fields is the current density field

$$\boldsymbol{\mathcal{J}}(\mathbf{y}) = \frac{1}{\rho(\mathbf{y})} \frac{\partial \mathbf{j}(\mathbf{y})}{\partial t}. \tag{32}$$

The definitions of the fields, and the expressions for the (nonconserved) energy components, are the same as for the stationary state case but with a temporal dependence. The second law is also gauge invariant, and satisfies the continuity condition $\boldsymbol{\nabla} \cdot \mathbf{j}(\mathbf{y}) + \partial\rho(\mathbf{y})/\partial t = 0$.

III. SCHRÖDINGER EQUATION IN SELF-CONSISTENT FORM

The self-consistent forms of the stationary-state (Eq. (4)) and time-dependent (Eq. (8)) Schrödinger equations follow from the 'Quantal Newtonian' first and second laws, respectively.

A. Stationary-state Case

From the first law of Eq. (9) corresponding to the Hamiltonian of Eq. (2), we see that the external scalar potential $v(\mathbf{r})$ is the work done to move an electron from a reference point at infinity to its position at $\mathbf{r}$ in the force of a conservative field $\boldsymbol{\mathcal{F}}(\mathbf{r})$:

$$v(\mathbf{r}) = \int_{\infty}^{\mathbf{r}} \boldsymbol{\mathcal{F}}(\mathbf{r}') \cdot d\boldsymbol{\ell}', \tag{33}$$

where $\boldsymbol{\mathcal{F}}(\mathbf{r}) = \boldsymbol{\mathcal{F}}^{\text{int}}(\mathbf{r}) - \boldsymbol{\mathcal{L}}(\mathbf{r}) = \boldsymbol{\mathcal{E}}_{\text{ee}}(\mathbf{r}) - \boldsymbol{\mathcal{Z}}(\mathbf{r}) - \boldsymbol{\mathcal{D}}(\mathbf{r}) - \boldsymbol{\mathcal{J}}(\mathbf{r}) - \boldsymbol{\mathcal{L}}(\mathbf{r})$. As the components of the field $\boldsymbol{\mathcal{F}}(\mathbf{r})$ are obtained from quantal sources that are expectations of Hermitian operators taken with respect to the wave function $\Psi(\mathbf{X})$, the field $\boldsymbol{\mathcal{F}}(\mathbf{r})$ is a functional of $\Psi(\mathbf{X})$, $i.e.$ $\boldsymbol{\mathcal{F}}(\mathbf{r}) = \boldsymbol{\mathcal{F}}[\Psi(\mathbf{X})](\mathbf{r})$. Hence, the scalar potential $v(\mathbf{r})$ is such a functional:

$$v(\mathbf{r}) = v[\Psi(\mathbf{X})](\mathbf{r}) = \int_{\infty}^{\mathbf{r}} \boldsymbol{\mathcal{F}}(\mathbf{r})[\Psi](\mathbf{r}') \cdot d\boldsymbol{\ell}'. \tag{34}$$

On substitution of the functional of Eq. (34) into Eq. (1) then leads to the self-consistent form of the Schrödinger equation, *viz.* that of Eq. (4) rewritten fully as

$$\left[\frac{1}{2}\sum_k \left(\hat{\mathbf{p}}_k + \mathbf{A}(\mathbf{r}_k)\right)^2 + \frac{1}{2}\sum_{k,l}{}' \frac{1}{|\mathbf{r}_k - \mathbf{r}_l|} + \sum_k v[\Psi](\mathbf{r}_k)\right]\Psi(\mathbf{X}) = E[\Psi]\Psi(\mathbf{X}), \qquad (35)$$

or equivalently as

$$\left[\frac{1}{2}\sum_k \left(\hat{\mathbf{p}}_k + \mathbf{A}(\mathbf{r}_k)\right)^2 + \frac{1}{2}\sum_{k,l}{}' \frac{1}{|\mathbf{r}_k - \mathbf{r}_l|} + \sum_k \int_\infty^{\mathbf{r_k}} \boldsymbol{\mathcal{F}}[\Psi](\mathbf{r}) \cdot d\boldsymbol{\ell}\right]\Psi(\mathbf{X}) = E[\Psi]\Psi(\mathbf{X}). \quad (36)$$

The intrinsic self-consistent nature of the Schrödinger equation then becomes evident. Recall that the meaning of the functional $v[\Psi(\mathbf{X})](\mathbf{r})$ is that for each different $\Psi(\mathbf{X})$ one obtains a different $v(\mathbf{r})$. The self-consistent procedure for the solution of Eq. (35) or (36) is then as follows (see also Fig. 1): One begins with an approximate input $\Psi^{\text{in}}(\mathbf{X})$. For this $\Psi^{\text{in}}(\mathbf{X})$ one obtains the various quantal sources, and from these quantal sources the field $\boldsymbol{\mathcal{F}}[\Psi^{\text{in}}(\mathbf{X})](\mathbf{r})$, and from the field the potential $v[\Psi^{\text{in}}(\mathbf{X})](\mathbf{r})$. The Schrödinger equation is then solved to obtain a new output approximate solution $\Psi^{\text{out}}(\mathbf{X})$ and eigenenergy $E[\Psi^{\text{out}}]$. The output solution $\Psi^{\text{out}}(\mathbf{X})$ is then treated as the new approximate input wave function $\Psi^{\text{in}}(\mathbf{X})$, and the entire process repeated until the $\Psi^{\text{in}}(\mathbf{X}) = \Psi^{\text{out}}(\mathbf{X})$, or when self-consistency is achieved. In this manner, the *exact* $\hat{H}[\Psi]$, $\Psi(\mathbf{X})$, and E are obtained in the final iteration of the self-consistent procedure.

The Schrödinger equation Eq. (1) with *known* Hamiltonian $\hat{H}$ constitutes a special case of the more general self-consistent form of the equation Eq. (4 or 35). To explain this point further, we note that in speaking of the N electrons, it is assumed that their canonical momentum and electron-interaction operators are known. With the external potential $v(\mathbf{r})$ specified, the Hamiltonian $\hat{H}$ is fully defined, and the equation solved for $\{\Psi(\mathbf{X}), E\}$ for the individual states. In the self-consistent form of the Schrödinger equation, the momentum and electron-interaction operators are once again known. Hence, it is the potential $v(\mathbf{r})$, and thereby the Hamiltonian $\hat{H}[\Psi(\mathbf{X})]$, that is obtained self-consistently. Thus, the self-consistent solution of Eq. (4 or 35) determines $\{v(\mathbf{r}), \Psi(\mathbf{X}), E\}$ for the different states. It is in this context that the Schrödinger equation of Eq. (1) is a special case of the more general form of Eq. (4). The solution $\{\Psi(\mathbf{X}), E\}$ of the Schrödinger equation Eq. (1) with Hamiltonian $\hat{H}$ known is equivalent to the final iteration of the self-consistent solution of equation Eq. (4 or 35).

Ψ^{in}

$\downarrow$

Quantal Sources

$\downarrow$

Fields

$\downarrow$

$\upsilon\left[\Psi^{in}\right]$

$\downarrow$

$\hat{H}[\Psi^{in}]\Psi^{out} = E\,\Psi^{out}$

$\downarrow$

Ψ^{out}

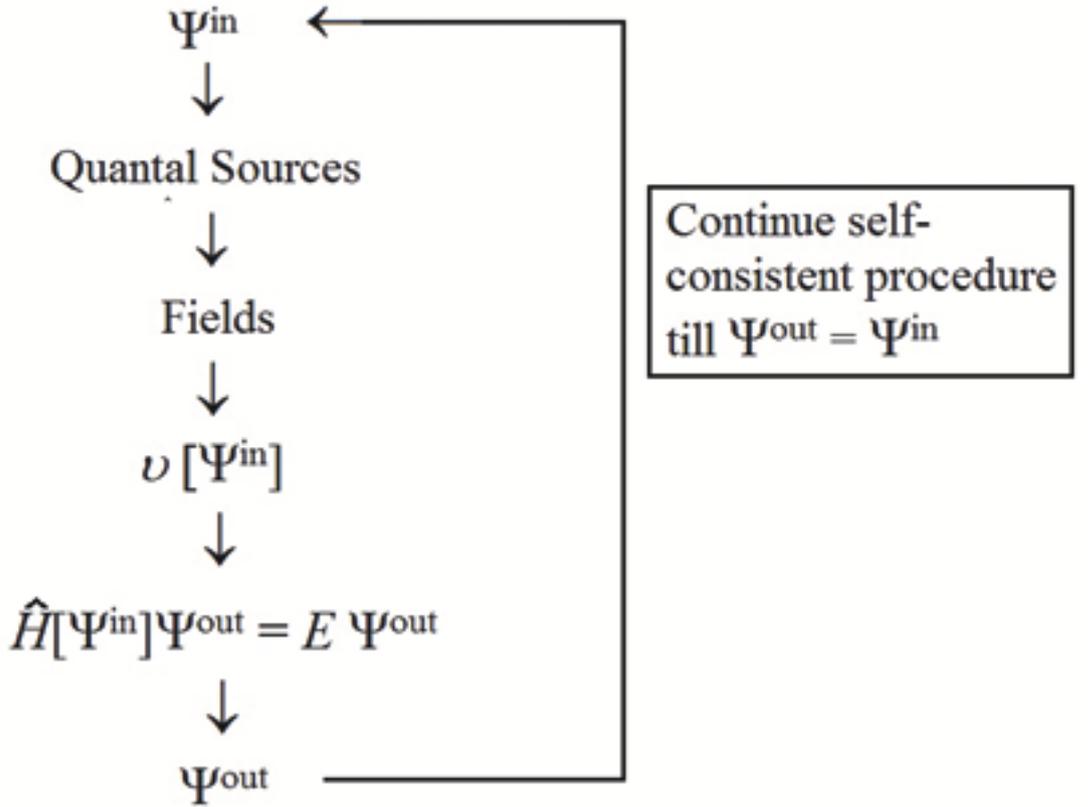Continue self-consistent procedure till $\Psi^{out} = \Psi^{in}$

FIG. 1: Procedure for the self-consistent solution of the Schrödinger equation.

As in any self-consistent procedure, the choice of the initial input wave function *apropos* to the physical system of interest is key. One would then obtain the correct corresponding scalar potential $v(\mathbf{r})$. For atoms, molecules, and solids this potential would be Coulombic. For 'artificial atoms' or quantum dots, it would be harmonic. It is quite likely that there may exist other solutions for which $v(\mathbf{r})$ is different. It is only after self-consistency is achieved that one must judge and test with experiment whether or not the solution is physically meaningful.

The self-consistency procedure is applicable for both ground and excited states. This follows from the 'Quantal Newtonian' first law which is valid for *arbitrary* state. Note that irrespective of the state of a system, the corresponding conservative field $\mathcal{F}(\mathbf{r})$ of Eq. (34) will always lead to the *same* scalar potential $v(\mathbf{r})$ for a specific system.

An attribute of the self-consistency procedure is that the wave function $\Psi(\mathbf{X})$ thus obtained, in contrast to the variational method discussed previously, is accurate throughout

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space. As self-consistent procedures are numerical, the accuracy of the wave function will be as good as that of the accuracy of the self-consistent procedure. The more numerically refined the self-consistency, the more accurate the wave function.

B. Temporal Case

From the 'Quantal Newtonian' second law of Eq. (28) corresponding to the Hamiltonian of Eq. (6), it follows that the scalar time-dependent potential $v(\mathbf{y})$ is the work done at each instant of time to move an electron from a reference point at infinity to its position at $\mathbf{r}$ in the force of a *conservative* field $\boldsymbol{\mathcal{F}}(\mathbf{y})$ that is a functional of $\Psi(\mathbf{Y})$, and that hence this potential is a functional of $\Psi(\mathbf{Y})$:

$$v(\mathbf{y}) = v[\Psi(\mathbf{Y})](\mathbf{y}) = \int_\infty^{\mathbf{r}} \boldsymbol{\mathcal{F}}[\Psi(\mathbf{Y})](\mathbf{y}') \cdot d\boldsymbol{\ell}', \tag{37}$$

where $\boldsymbol{\mathcal{F}}[\Psi(\mathbf{Y})](\mathbf{y}) = \boldsymbol{\mathcal{F}}^{\mathrm{int}}(\mathbf{y}) - \boldsymbol{\mathcal{L}}(\mathbf{y}) + \partial \mathbf{A}(\mathbf{y})/\partial t - \boldsymbol{\mathcal{J}}(\mathbf{y}); \mathbf{y}' = \mathbf{r}'t$. On substitution of the functional of Eq. (37) into the Hamiltonian $\hat{H}(t)$ of Eq. (6), one obtains the self-consistent form of the time-dependent Schrödinger equation of Eq. (8) or written equivalently as

$$\left[\frac{1}{2} \sum_k \left(\hat{\mathbf{p}}_k + \mathbf{A}(\mathbf{y}_k) \right)^2 + \frac{1}{2} {\sum_{k,l}}' \frac{1}{|\mathbf{r}_k - \mathbf{r}_l|} + \sum_k v[\Psi(\mathbf{Y})](\mathbf{y}_k) \right] \Psi(\mathbf{Y}) = i \frac{\partial \Psi(\mathbf{Y})}{\partial t}, \tag{38}$$

or

$$\left[\frac{1}{2} \sum_k \left(\hat{\mathbf{p}}_k + \mathbf{A}(\mathbf{y}_k) \right)^2 + \frac{1}{2} {\sum_{k,l}}' \frac{1}{|\mathbf{r}_k - \mathbf{r}_l|} + \sum_k \int_\infty^{\mathbf{r_k}} \boldsymbol{\mathcal{F}}[\Psi](\mathbf{y}) \cdot d\boldsymbol{\ell} \right] \Psi(\mathbf{Y}) = i \frac{\partial \Psi(\mathbf{Y})}{\partial t}. \tag{39}$$

The evolution of the wave function $\Psi(\mathbf{Y})$ is then obtained by self-consistent solution of Eq. (39) for each instant of time. The Schrödinger equation of Eq. (5) with Hamiltonian $\hat{H}(\mathbf{t})$ known, then constitutes a special case of the more general form given above.

For examples of the intrinsic self-consistent nature of the Schrödinger equation and the satisfaction of the 'Quantal Newtonian' laws for the stationary-state and time-dependent cases, we refer the reader to [9, 23]. In [9], the stationary-state 3D case of two Hooke's atoms, one in a ground and the other in an excited state are considered. In [23], this is demonstrated for the 2D case of two quantum dots in a uniform magnetic field, one in a ground and the other in an excited state. The time-evolution of the wave functions for the same states of these systems is also described [9, 23] in conjunction with the Generalized Kohn theorem [24].

IV. NEW PHYSICS

The 'Quantal Newtonian' laws of Schrödinger theory of electrons in electromagnetic fields leads to new physics. We provide here a brief summary of these insights for the stationary state case. The generalization to the time-dependent case readily follows.

(1) The stationary-state Schrödinger theory equation is now understood to be intrinsically self-consistent. This constitutes a generalization of the Schrödinger equation that is valid for *arbitrary* state whether nondegenerate or degenerate, ground or excited. In turn, this then allows for the self-consistent determination of the wave functions.

(2) The Schrödinger equation $\hat{H}\Psi(\mathbf{X}) = E\Psi(\mathbf{X})$ with $\hat{H}$ known then constitutes a special case of the more general self-consistent form $\hat{H}[\Psi(\mathbf{X})]\Psi(\mathbf{X}) = E[\Psi(\mathbf{X})]\Psi(\mathbf{X})$.

(3) The function $v(\mathbf{r})$ of Eq. (33 or 34) is now understood to be a potential in the rigorous classical sense of the work done in a conservative field $\boldsymbol{\mathcal{F}}(\mathbf{r})$. Furthermore, as the $\boldsymbol{\nabla} \times \boldsymbol{\mathcal{F}}(\mathbf{r}) = 0$, this work done is *path-independent*.

(4) As the field $\boldsymbol{\mathcal{F}}(\mathbf{r})$ is the sum of the internal $\boldsymbol{\mathcal{F}}^{\text{int}}(\mathbf{r})$ and Lorentz $\boldsymbol{\mathcal{L}}(\mathbf{r})$ fields (see below Eq. (33)), the potential $v(\mathbf{r})$ depends upon all the properties of the system via the components of $\boldsymbol{\mathcal{F}}^{\text{int}}(\mathbf{r})$ and including the physical current density $\mathbf{j}(\mathbf{r})$ via $\boldsymbol{\mathcal{L}}(\mathbf{r})$. Hence, the individual contributions to $v(\mathbf{r})$ of electron correlation due to the Pauli principle and Coulomb repulsion, kinetic effects, the density, the physical current density, and the magnetic field are all explicitly known.

(5) In the traditional manner in which the Schrödinger equation is written as in Eq. (1), the electric field $\boldsymbol{\mathcal{E}}(\mathbf{r}) = -\boldsymbol{\nabla}v(\mathbf{r})$ is considered an *extrinsic* input to the system of the N electrons. From the self-consistent form of the equation Eq. (35), it becomes evident that the field $\boldsymbol{\mathcal{E}}(\mathbf{r})$ or equivalently the potential $v(\mathbf{r})$ is *intrinsic* in that it depends on the properties of the system converging to its final form as self-consistency is achieved.

(6) In the Schrödinger equation of Eq. (1) with Hamiltonian $\hat{H}$ known, it is the vector potential $\mathbf{A}(\mathbf{r})$ and not the magnetic field $\boldsymbol{\mathcal{B}}(\mathbf{r})$ that appears in it as a result of the correspondence principle. This point is significant because a vector potential can exist in a region of space where a magnetic field is not present as in the Bohm-Aharonov effect [25]. It is only following the choice of gauge that the magnetic field $\boldsymbol{\mathcal{B}}(\mathbf{r})$ then appears in the Schrödinger equation. In the self-consistent form of the Schrödinger equation Eq. (35 or 36), the magnetic field $\boldsymbol{\mathcal{B}}(\mathbf{r})$ appears explicitly in the Hamiltonian $\hat{H}[\Psi(\mathbf{X})]$ via the Lorentz

field $\boldsymbol{\mathcal{L}}(\mathbf{r})$ term in the potential $v(\mathbf{r})$. This is understandable because in order to solve the integro-differential equation self-consistently, all the information with regard to the physical system must be present within the equation.

V.   CONCLUDING REMARKS

This paper presents a new and more general way of thinking of the Schrödinger theory of electrons in an electromagnetic field. The fundamental understanding achieved is that the Hamiltonian $\{\hat{H}; \hat{H}(t)\}$ of the Schrödinger equation for the stationary-state and time-dependent cases, respectively, is an *exactly known* functional of the corresponding wave function $\{\Psi(\mathbf{X}); \Psi(\mathbf{Y})\}$, *i.e.* $\hat{H} = \hat{H}[\Psi(\mathbf{X})]$ and $\hat{H}(t) = \hat{H}[\Psi(\mathbf{Y})]$. This conclusion is arrived at via the 'Quantal Newtonian' first and second laws which are the equations of motion for the individual electron. As a consequence of the above conclusion, the Schrödinger equation can be expressed in a manner that exhibits its intrinsic self-consistent form. Thus, the stationary-state eigenfunctions and eigenenergies $\{\Psi(\mathbf{X}), E\}$, and the time-dependent wave function $\Psi(\mathbf{Y})$, can be determined self-consistently. This constitutes a new path for the determination of the wave function of the system. A further implication of the self-consistent procedure is that the corresponding scalar potentials $\{v(\mathbf{r}); v(\mathbf{y})\}$ and hence the respective Hamiltonians $\{\hat{H}[\Psi(\mathbf{X})]; \hat{H}[\Psi(\mathbf{Y})]\}$ too are determined self-consistently. Furthermore, the separate contributions to the scalar potentials $\{v(\mathbf{r}); v(\mathbf{y})\}$ of correlations due to the Pauli exclusion principle and Coulomb repulsion, kinetic and magnetic effects, and the density and physical current density , are identified. Additionally, in self-consistent form, the Schrödinger equation in which the vector potentials $\{\mathbf{A}(\mathbf{r}); \mathbf{A}(\mathbf{y})\}$ appear in the Hamiltonian as part of the field component of the momentum, now explicitly includes a term involving the magnetic field $\{\boldsymbol{\mathcal{B}}(\mathbf{r}); \boldsymbol{\mathcal{B}}(\mathbf{y})\}$ via the potentials $\{v(\mathbf{r}); v(\mathbf{y})\}$. The above insights all contribute to the generalization of the Schrödinger theory of electrons.

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APPENDIX A: DERIVATION OF THE 'QUANTAL NEWTONIAN' FIRST LAW

In this appendix we provide an outline of the proof of the 'Quantal Newtonian' first law of Eq. (9) corresponding to the physical system described by the Hamiltonian of Eq. (2). Expressing the wavefunction Ψ in terms of its real Ψ^R and imaginary Ψ^I parts as $\Psi = \Psi^R + i\Psi^I$, the Schrödinger equation Eq. (1) may be written as

$$[\hat{T} + \hat{U} + \hat{V} + \hat{W}](\Psi^R + i\Psi^I) = E(\Psi^R + i\Psi^I), \tag{A1}$$

where $\hat{T}$ is the canonical kinetic energy operator:

$$\hat{T} = -\frac{1}{2}\sum_j \nabla_j^2, \tag{A2}$$

and the operator $\hat{W}$ is

$$\hat{W} = \sum_j \hat{\omega}(\mathbf{r}_j), \tag{A3}$$

with

$$\hat{\omega}(\mathbf{r}_j) = \frac{1}{2}A^2(\mathbf{r}) - i\hat{\Omega}(\mathbf{r}), \tag{A4}$$

and

$$\hat{\Omega}(\mathbf{r}) = \frac{1}{2}\big[\boldsymbol{\nabla}\cdot\mathbf{A} + 2\mathbf{A}\cdot\boldsymbol{\nabla}\big]. \tag{A5}$$

Following the differentiations, (as the operator $\hat{T}$ and $\hat{W}$ contain differential operators), and after considerable algebra [9, 11], one arrives at the 'force' equation

$$\rho(\mathbf{r})\boldsymbol{\nabla}(\mathbf{r}) - \mathbf{e}_{\mathrm{ee}}(\mathbf{r}) \;+\; \mathbf{z}(\mathbf{r}) + \mathbf{d}(\mathbf{r}) + \mathbf{k}(\mathbf{r})$$
$$- \sum_\beta \nabla_\beta\big[\rho(\mathbf{r})\mathbf{A}(\mathbf{r})A_\beta(\mathbf{r})\big] = 0, \tag{A6}$$

where the 'forces' $\mathbf{e}_{\mathrm{ee}}(\mathbf{r}), \mathbf{z}(\mathbf{r}), \mathbf{d}(\mathbf{r})$ are defined in the text, and where

$$k_\alpha(\mathbf{r}) = \sum_\beta \big[j_\beta(\mathbf{r})\{\nabla_\alpha A_\beta(\mathbf{r})\} + \nabla_\beta\{A_\beta(\mathbf{r})j_\alpha(\mathbf{r})\}\big]. \tag{A7}$$

Defining the Lorentz 'force' $\boldsymbol{\ell}(\mathbf{r})$ as

$$\boldsymbol{\ell}(\mathbf{r}) = \mathbf{j}(\mathbf{r}) \times \boldsymbol{\mathcal{B}}(\mathbf{r}), \tag{A8}$$

then with $\boldsymbol{\mathcal{B}}(\mathbf{r}) = \boldsymbol{\nabla} \times \mathbf{A}(\mathbf{r})$, we have

$$\ell_\alpha(\mathbf{r}) = \sum_\beta \left[j_\beta(\mathbf{r})\nabla_\alpha A_\beta(\mathbf{r}) - j_\beta(\mathbf{r})\nabla_\beta A_\alpha(\mathbf{r}) \right]. \tag{A9}$$

Similarly, one defines an internal 'force' contribution $\mathbf{i}(\mathbf{r})$ due to the magnetic field as

$$i_\alpha(\mathbf{r}) = \sum_\beta \nabla_\beta I_{\alpha\beta}(\mathbf{r}), \tag{A10}$$

where the tensor

$$I_{\alpha\beta}(\mathbf{r}) = \left[j_\alpha(\mathbf{r})A_\beta(\mathbf{r}) + j_\beta(\mathbf{r})A_\alpha(\mathbf{r}) \right] - \rho(\mathbf{r})A_\alpha(\mathbf{r})A_\beta(\mathbf{r}). \tag{A11}$$

On applying the continunity condition $\boldsymbol{\nabla} \cdot \mathbf{j}(\mathbf{r}) = 0$, it can be shown that the last two terms of (A6) are

$$k_\alpha(\mathbf{r}) - \sum_\beta \nabla_\beta \left[\rho(\mathbf{r})A_\alpha(\mathbf{r})A_\beta(\mathbf{r}) \right] = \ell_\alpha(\mathbf{r}) + i_\alpha(\mathbf{r}). \tag{A12}$$

The 'force' equation (A6) is then

$$\rho(\mathbf{r})\boldsymbol{\nabla} v(\mathbf{r}) + \boldsymbol{\ell}(\mathbf{r}) - \mathbf{e}_{\mathrm{ee}}(\mathbf{r}) + \mathbf{z}(\mathbf{r})\mathbf{d}(\mathbf{r}) + \mathbf{i}(\mathbf{r}), \tag{A13}$$

which on dividing by $\rho(\mathbf{r})$ leads to the 'Quantal Newtonian' first law of Eq. (9).

The derivation of the 'Quantal Newtonian' second law of Eq. (28) in the presence of a time-dependent electromagnetic field is similar, and we refer the reader to [22] for the details.