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The ‘Quantal Newtonian’ First Law: A Complementary Perspective to the Stationary-state Quantum Theory of Electrons

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Abstract

A complementary perspective to the Göttingen-Copenhagen interpretation of stationary-state quantum theory of electrons in an electromagnetic field is described. The perspective, derived from Schrödinger-Pauli theory, is that of the *individual* electron via its equation of motion or ‘Quantal Newtonian’ First Law. The Law is in terms of ‘classical’ fields experienced by *each* electron: the sum of the external and internal fields vanishes. The external field is a sum of the electrostatic and Lorentz fields. The internal field is a sum of fields’ representative of Pauli and Coulomb correlations; kinetic effects; electron density; and internal magnetic component. The energy is obtained from these fields. The sources of the fields are expectation values of Hermitian operators. The perspective is elucidated by application to quantum dots in a magnetic field in a ground, excited singlet and triplet states. The relationship of the perspective to Quantal and traditional density functional theories is briefly explained.

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Introduction

The manner in which we understand and employ quantum mechanics presently is based on the Born-Heisenberg-Bohr^[1] Göttingen-Copenhagen interpretation. According to the Born Rule, the state of a quantum system or wave function $\Psi(\mathbf{X})$ represents a ‘probability amplitude’ such that $|\Psi(\mathbf{X})|^2$ determines the probability that a certain result will be obtained when an observation is made. Thus, the average value of measurements of an observable $O(\mathbf{r})$ represented by a Hermitian operator $\hat{O}(\mathbf{r})$ carried out on a very large number of equivalent systems, independent of each other, and represented by the same wave function $\Psi(\mathbf{X})$, is the expectation value $\langle \Psi(\mathbf{X}) | \hat{O}(\mathbf{r}) | \Psi(\mathbf{X}) \rangle$.

In this paper, which is a description of the talk at the Theoretical Chemistry Symposium 2021, a complementary perspective to the stationary-state quantum theory of electrons in an electromagnetic field is described. Whereas the solution $\Psi(\mathbf{X})$ to the Schrödinger^[2] or Schrödinger-Pauli^[3] theory equation of a system of electrons in a particular state is descriptive of the *many-electron* system, the complementary perspective is that of the *individual* electron in the sea of electrons. The new perspective lies within the rubric of the Born Rule, but provides the equation of motion or ‘Quantal Newtonian’ First Law (QNFL) of *each electron*. The QNFL is derived^[4] from the Schrödinger-Pauli equation. The corresponding Law for Schrödinger theory constitutes a special case. This equation of motion parallels that of Newton’s First Law for the individual classical charged particle amongst many such interacting particles in an electromagnetic field. There are, of course, distinct differences as a consequence of being a quantum law.

The focus of the paper is thus the QNFL and the new physics it reveals. The description of the QNFL is in terms of ‘classical’ fields experienced by *each electron*. These fields are similar to those of classical physics in that they pervade all space and are tangible. The complementary perspective further proves that the energy and its components are determined from these fields. The ‘sources’ of these fields are quantum-mechanical expectation values of Hermitian operators or complex operators whose real and imaginary parts are Hermitian. It is in this context that the QNFL falls within the Born probabilistic interpretation. On the other hand, the equation satisfied by the fields is classical. In this context, one may attribute a determinism to these fields, but that is the subject matter of a separate paper^[5]. The complementary perspective is then elucidated by examples.

The quantum-mechanical system considered is one of N electrons of mass m , charge $-e$, spin moment $\boldsymbol{\mu}_s = -(g\mu_B/\hbar)\mathbf{s}$ (with gyromagnetic ratio $g = 2$, the Bohr magneton $\mu_B = e\hbar/2mc$, the velocity of light c , and \mathbf{s} the spin angular momentum vector) in a static electric $\boldsymbol{\mathcal{E}}(\mathbf{r}) = -\nabla v(\mathbf{r})/e$ and magnetic $\boldsymbol{\mathcal{B}}(\mathbf{r}) = \nabla \times \mathbf{A}(\mathbf{r})$ field, where $v(\mathbf{r})$ and $\mathbf{A}(\mathbf{r})$ are the scalar and vector potentials, respectively. The corresponding Schrödinger-Pauli theory equation is

$$\hat{H}_{spin}\Psi(\mathbf{X}) = E\Psi(\mathbf{X}), \quad (1)$$

where the Hamiltonian \hat{H}_{spin} is

$$\hat{H}_{spin} = \hat{T}_F + \hat{W} + \hat{V}, \quad (2)$$

with \hat{T}_F the Feynman kinetic energy operator:

$$\hat{T}_F = \frac{1}{2m} \sum_k \left(\boldsymbol{\sigma}_k \cdot \hat{\mathbf{p}}_{k,phys} \right) \left(\boldsymbol{\sigma}_k \cdot \hat{\mathbf{p}}_{k,phys} \right) \quad (3)$$

$$= \frac{1}{2m} \sum_k \hat{p}_{k,phys}^2 + \frac{g\mu_B}{\hbar} \sum_k \boldsymbol{\mathcal{B}}(\mathbf{r}_k) \cdot \mathbf{s}_k, \quad (4)$$

where $\hat{\mathbf{p}}_{phys} = (\hat{\mathbf{p}} + \frac{e}{c}\mathbf{A}(\mathbf{r}))$ is the physical momentum operator, $\hat{\mathbf{p}} = -i\hbar\nabla$ the canonical momentum operator, $\boldsymbol{\sigma} = \frac{2}{\hbar}\mathbf{s}$ is the Pauli spin matrix; \hat{W} is the electron-interaction operator:

$$\hat{W} = \frac{1}{2} \sum'_{k,\ell} \frac{e^2}{|\mathbf{r}_k - \mathbf{r}_\ell|} \quad (5)$$

and \hat{V} the external binding potential operator:

$$\hat{V} = \sum_k v(\mathbf{r}_k). \quad (6)$$

The $\{\Psi(\mathbf{X}), E\}$ are the eigenfunctions and eigenvalues, respectively, with $\mathbf{X} = \mathbf{x}_1, \dots, \mathbf{x}_N$; $\mathbf{x} = \mathbf{r}\zeta$; \mathbf{r} and ζ the spatial and spin coordinates. Due to the lack of spin-orbit coupling in the Hamiltonian, the solutions of the Schrödinger-Pauli equation are of the form

$$\Psi(\mathbf{X}) = \psi(\mathbf{R})\chi(Z), \quad (7)$$

where $\psi(\mathbf{R})$ is the spatial component of the wave function with $\mathbf{R} = \mathbf{r}_1, \dots, \mathbf{r}_N$; and $\chi(Z)$ the spin component with $Z = \zeta_1, \dots, \zeta_N$.

The Schrödinger theory equation constitutes a special case of the Schrödinger-Pauli equation in that the spin moment of the electron is not included in the corresponding Hamiltonian $\hat{H}_{spinless}$. Thus,

$$\hat{H}_{spinless} = \hat{T}_A + \hat{W} + \hat{V}, \quad (8)$$

where the kinetic energy operator \hat{T}_A represents only the physical momentum:

$$\hat{T}_A = \frac{1}{2} \sum_k \hat{p}_{k,phys}^2. \quad (9)$$

Yet another special case of the Schrödinger-Pauli theory equation is when there is no magnetic field present, *i.e.* $\mathbf{B}(\mathbf{r}) = 0$, in which case the spinless Hamiltonian $\hat{H}_{spinless}$ is

$$\hat{H}_{spinless} = \hat{T} + \hat{W} + \hat{V}, \quad (10)$$

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

$$\hat{T} = \frac{1}{2} \sum_k \hat{p}_k^2. \quad (11)$$

In each of the above cases, one is concerned with spin $\frac{1}{2}$ particles which obey the Pauli exclusion principle^[6]. This constraint is satisfied by the Dirac-Heisenberg^[7,8] requirement that the wave functions $\Psi(\mathbf{X})$ must be antisymmetric in an interchange of the coordinates of any two electrons. This property of $\Psi(\mathbf{X})$ is the Pauli principle.

The reason for considering the special Schrödinger theory cases is that the corresponding QNFLs and the complementary perspective each constitute special cases^[9] of the more general perspective derived for the Schrödinger-Pauli theory.

The outline and sections of the paper are the following: (a) In order to demonstrate the parallelism and contrast between the equations of motion in classical and stationary state quantum physics, we discuss Newton's First Law for an *individual* charged particle amongst other such particles in an external static electromagnetic field; (b) The complementary perspective to Schrödinger-Pauli theory via the 'Quantal Newtonian' First Law for the individual electron is described; (c) The new physics gleaned from the complementary perspective is explained; (d) The new perspective is then elucidated by application to 2-electron 2-dimensional 'artificial atoms' or semiconductor quantum dots^[10,11,12] in a magnetic field in their ground 1^1S , first excited singlet 2^1S , and the spin-correlated first excited triplet 2^3S states; (e) The relationship between the complementary perspective and the local effective potential theories of Quantal density functional (QDFT)^[13,14] and Hohenberg-Kohn-Sham density functional (DFT)^[15,16] theories is briefly discussed; (f) Finally, concluding remarks are made.

Newton's First Law for Individual Classical Charged Particle in an Electromagnetic Field

Consider N classical particles each of charge q and velocity \mathbf{v} in an external electric $\mathcal{E}(\mathbf{r})$ and magnetic $\mathcal{B}(\mathbf{r})$ field as shown in Fig. 1. Then Newton's First Law for the particle of charge q_i at \mathbf{r} moving with velocity \mathbf{v}_i is given by the vanishing of the sum of the external $\mathbf{F}_i^{ext}(\mathbf{r})$ and internal $\mathbf{F}_i^{int}(\mathbf{r})$ forces acting on it:

$$\mathbf{F}_i^{ext}(\mathbf{r}) + \mathbf{F}_i^{int}(\mathbf{r}) = 0. \quad (12)$$

The external force is given by the Coulomb-Lorentz force law (with $c = 1$) as

$$\mathbf{F}_i^{ext}(\mathbf{r}) = q_i(\mathcal{E}(\mathbf{r}) + \mathcal{L}(\mathbf{r})) \quad (13)$$

where the Lorentz field $\mathcal{L}(\mathbf{r})$ is

$$\mathcal{L}(\mathbf{r}) = \mathbf{v}_i \times \mathcal{B}(\mathbf{r}). \quad (14)$$

The internal force on the i th charge q_i due to the other charges q_j at \mathbf{r}_j is given by Coulomb's Law which satisfies the principle of superposition. Thus,

$$\mathbf{F}_i^{int}(\mathbf{r}) = \sum_j' \mathbf{F}_{ji} = q_i \sum_j' q_j \frac{(\mathbf{r} - \mathbf{r}_j)}{|\mathbf{r} - \mathbf{r}_j|^3}. \quad (15)$$

Newton's First Law for the individual charge q_i is then

$$q_i(\mathcal{E}(\mathbf{r}) + \mathcal{L}(\mathbf{r})) + q_i \sum_j' q_j \frac{(\mathbf{r} - \mathbf{r}_j)}{|\mathbf{r} - \mathbf{r}_j|^3} = 0. \quad (16)$$

On summing over all the charges, and on employing the fact that Coulomb's Law obeys Newton's Third Law so that

$$\sum_{i,j}' \mathbf{F}_{ji} = \sum_i q_i \sum_j' q_j \frac{(\mathbf{r} - \mathbf{r}_j)}{|\mathbf{r} - \mathbf{r}_j|^3} = 0, \quad (17)$$

we recover Newton's First Law for the system of charges

$$\sum_i \mathbf{F}_i^{ext}(\mathbf{r}) = 0, \quad (18)$$

or

$$\sum_i q_i(\mathcal{E}(\mathbf{r}) + \mathcal{L}(\mathbf{r})) = 0. \quad (19)$$

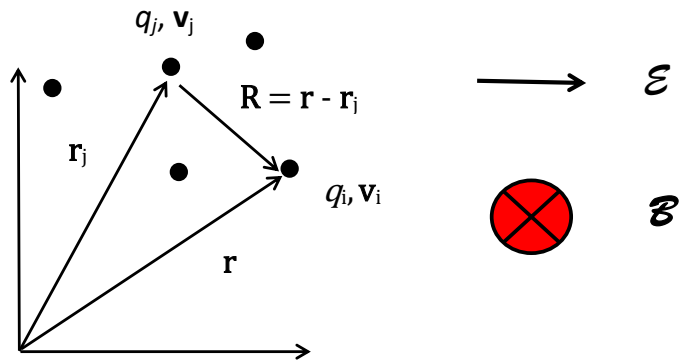


FIG. 1: A system of N classical particles each of charge q and velocity \mathbf{v} in the presence of a static external electric $\mathcal{E}(\mathbf{r})$ and magnetic $\mathcal{B}(\mathbf{r})$ field.

‘Quantal Newtonian’ First Law for the Individual Electron: A Complementary Perspective

The ‘Quantal Newtonian’ First Law

The complementary perspective to stationary-state Schrödinger-Pauli theory as defined by Eqs. (1-7) is founded in the ‘Quantal Newtonian’ First Law. In a manner similar to Newton’s First Law of Eq. (12), the statement of the QNFL is that the sum of the external $\mathcal{F}^{ext}(\mathbf{r})$ and internal $\mathcal{F}^{int}(\mathbf{r})$ fields experienced by *each* electron vanishes: (Units of $e = \hbar = m = c = 1$),

$$\mathcal{F}^{ext}(\mathbf{r}) + \mathcal{F}^{int}(\mathbf{r}) = 0. \quad (20)$$

As in classical physics (Eq. (13)), the external field $\mathcal{F}^{ext}(\mathbf{r})$ is comprised of the sum of the electrostatic $\mathcal{E}(\mathbf{r})$ and Lorentz $\mathcal{L}(\mathbf{r})$ fields:

$$\mathcal{F}^{ext}(\mathbf{r}) = \mathcal{E}(\mathbf{r}) - \mathcal{L}(\mathbf{r}) = -\nabla v(\mathbf{r}) - \mathcal{L}(\mathbf{r}). \quad (21)$$

The internal field $\mathcal{F}^{int}(\mathbf{r})$ of the QNFL differs from that of classical physics (Eq. (15)) in that it is comprised of a *sum* of fields representative of properties of the quantum-mechanical system: the electron-interaction $\mathcal{E}_{ee}(\mathbf{r})$, kinetic $\mathcal{Z}(\mathbf{r})$, differential density $\mathcal{D}(\mathbf{r})$, and internal magnetic $\mathcal{I}_m(\mathbf{r})$ field components:

$$\mathcal{F}^{int}(\mathbf{r}) = \mathcal{E}_{ee}(\mathbf{r}) - \mathcal{Z}(\mathbf{r}) - \mathcal{D}(\mathbf{r}) - \mathcal{I}_m(\mathbf{r}). \quad (22)$$

Prior to discussing the fields, we note that each field is expressed as in classical physics as the force/charge or in the quantum case as

$$\text{Field} = \text{‘force’/electron density } \rho(\mathbf{r}). \quad (23)$$

The local $O(\mathbf{r})$ or nonlocal $O(\mathbf{r}\mathbf{r}')$ sources of the individual fields or the ‘forces’ are quantum-mechanical in that they are expectation values of the corresponding $\hat{O}(\mathbf{r})$ or $\hat{O}(\mathbf{r}\mathbf{r}')$ Hermitian operators: $\langle \Psi(\mathbf{X}) | \hat{O}(\mathbf{r}) | \Psi(\mathbf{X}) \rangle$ or $\langle \Psi(\mathbf{X}) | \hat{O}(\mathbf{r}\mathbf{r}') | \Psi(\mathbf{X}) \rangle$.

The definitions of the above ‘classical’ fields, their quantal sources, the corresponding Hermitian operators, and the ‘forces’, are summarized in Table 1.

We next discuss the various fields.

(a) The external electrostatic field $\mathcal{E}(\mathbf{r}) = -\nabla v(\mathbf{r})$ is the field binding the electrons. The binding potential $v(\mathbf{r})$ is Coulombic for natural atoms, molecules and solids; harmonic for

TABLE I: Definitions of the ‘classical’ fields of the complementary perspective, their quantal sources, the corresponding Hermitian operators, and the ‘forces’. The quantal sources are the expectation values of the operators taken with respect to the wave function.

‘Classical’ Field	Quantal Source	Operator	‘Force’
<i>Electron – interaction</i>	<i>Pair – correlation function</i>	<i>Pair – correlation</i>	
$\mathcal{E}_{ee}(\mathbf{r}) = \mathbf{e}_{ee}(\mathbf{r})/\rho(\mathbf{r})$	$P(\mathbf{r}\mathbf{r}')$	$\hat{P}(\mathbf{r}\mathbf{r}') = \sum'_{k,\ell} \delta(\mathbf{r}_k - \mathbf{r})\delta(\mathbf{r}_\ell - \mathbf{r}')$	$\mathbf{e}_{ee}(\mathbf{r}) = \int \frac{P(\mathbf{r}\mathbf{r}')(\mathbf{r}-\mathbf{r}')}{ \mathbf{r}-\mathbf{r}' ^3} d\mathbf{r}'$
<i>Kinetic</i> $\mathcal{Z}(\mathbf{r}) = \mathbf{z}(\mathbf{r})/\rho(\mathbf{r})$	<i>Single – Particle Density Matrix</i> $\gamma(\mathbf{r}\mathbf{r}')$	<i>Density Matrix</i> $\hat{\gamma}(\mathbf{r}\mathbf{r}') = \hat{A} + i\hat{B}$ $\hat{A} = \frac{1}{2} \sum_k [\delta(\mathbf{r}_k - \mathbf{r})T_k(\mathbf{a}) + \delta(\mathbf{r}_k - \mathbf{r}')T_k(-\mathbf{a})]$ $\hat{B} = -\frac{i}{2} \sum_k [\delta(\mathbf{r}_k - \mathbf{r})T_k(\mathbf{a}) - \delta(\mathbf{r}_k - \mathbf{r}')T_k(-\mathbf{a})]$ $T_k(\mathbf{a})\psi(\dots\mathbf{r}_k\dots) = \psi(\dots\mathbf{r}_k + \mathbf{a}\dots)$ $\mathbf{a} = \mathbf{r}' - \mathbf{r}$	$z_\alpha(\mathbf{r}) = 2 \sum_\beta \nabla_\beta t_{\alpha\beta}(\mathbf{r}; \gamma)$ $t_{\alpha\beta}(\mathbf{r}; \gamma) = \frac{1}{4} [\frac{\partial^2}{\partial r'_\alpha \partial r''_\beta} + \frac{\partial^2}{\partial r'_\beta \partial r''_\alpha}] \gamma(\mathbf{r}'\mathbf{r}'') _{\mathbf{r}'=\mathbf{r}''=\mathbf{r}}$
<i>Differential Density</i> $\mathcal{D}(\mathbf{r}) = \mathbf{d}(\mathbf{r})/\rho(\mathbf{r})$	<i>Density</i> $\rho(\mathbf{r})$	<i>Density</i> $\hat{\rho}(\mathbf{r}) = \sum_k \delta(\mathbf{r}_k - \mathbf{r})$	$\mathbf{d}(\mathbf{r}) = -\frac{1}{4} \nabla \nabla^2 \rho(\mathbf{r})$
<i>Lorentz</i> $\mathcal{L}(\mathbf{r}) = \boldsymbol{\ell}(\mathbf{r})/\rho(\mathbf{r})$	<i>Current Density</i> $\mathbf{j}(\mathbf{r})$	<i>Current Density</i> $\hat{\mathbf{j}}(\mathbf{r}) = \hat{\mathbf{j}}_p(\mathbf{r}) + \hat{\mathbf{j}}_d(\mathbf{r}) + \hat{\mathbf{j}}_m(\mathbf{r})$ $\hat{\mathbf{j}}_p(\mathbf{r}) = \frac{1}{2} \sum_k [\hat{\mathbf{p}}_k \delta(\mathbf{r}_k - \mathbf{r}) + \delta(\mathbf{r}_k - \mathbf{r})\hat{\mathbf{p}}_k]$ $\hat{\mathbf{j}}_d(\mathbf{r}) = \frac{1}{c} \hat{\rho}(\mathbf{r}) \mathbf{A}(\mathbf{r})$ $\hat{\mathbf{j}}_m(\mathbf{r}) = -c \nabla \times \hat{\mathbf{m}}(\mathbf{r})$ $\hat{\mathbf{m}}(\mathbf{r}) = -\frac{1}{c} \sum_k \mathbf{s}_k \delta(\mathbf{r}_k - \mathbf{r})$	$\boldsymbol{\ell}(\mathbf{r}) = \mathbf{j}(\mathbf{r}) \times \boldsymbol{\mathcal{B}}(\mathbf{r})$
<i>Internal Magnetic</i> $\mathcal{I}_m(\mathbf{r}) = \mathbf{i}_m(\mathbf{r})/\rho(\mathbf{r})$	<i>Current Density</i> $\mathbf{j}(\mathbf{r})$	<i>Current Density</i> $\hat{\mathbf{j}}(\mathbf{r}) = \hat{\mathbf{j}}_p(\mathbf{r}) + \hat{\mathbf{j}}_d(\mathbf{r}) + \hat{\mathbf{j}}_m(\mathbf{r})$	$i_{m,\alpha}(\mathbf{r}) = \sum_\beta \nabla_\beta I_{\alpha\beta}(\mathbf{r})$ $I_{\alpha\beta}(\mathbf{r}) = [j_\alpha(\mathbf{r})A_\beta(\mathbf{r}) + j_\beta(\mathbf{r})A_\alpha(\mathbf{r})] - \rho(\mathbf{r})A_\alpha(\mathbf{r})A_\beta(\mathbf{r})$

‘artificial atoms’ or semiconductor quantum dots^[10,11,12], or ‘artificial molecules’ or quantum dot molecules and quantum dot lattices^[17]; or if screening by the electrons is considered, it is the Yukawa potential, and so on. The QNFL is valid for arbitrary field $\mathcal{E}(\mathbf{r})$ or potential $v(\mathbf{r})$.

(b) Each electron experiences a Lorentz field $\mathcal{L}(\mathbf{r})$ as might be expected. After all, if there is a charged particle in a magnetic field, it must experience a Lorentz force. However, the Lorentz field $\mathcal{L}(\mathbf{r})$ appears naturally via the derivation of the QNFL. Its quantal source is the *local* physical current density $\mathbf{j}(\mathbf{r})$, the expectation value of the current density operator $\hat{\mathbf{j}}(\mathbf{r})$. The current density $\mathbf{j}(\mathbf{r})$ in turn is a sum of its paramagnetic $\mathbf{j}_p(\mathbf{r})$, diamagnetic $\mathbf{j}_d(\mathbf{r})$, and magnetization (spin) $\mathbf{j}_m(\mathbf{r})$ components. (Note that for the Schrödinger theory Hamiltonian $\hat{H}_{spinless}$ of Eq. (8), there is no magnetization component $\mathbf{j}_m(\mathbf{r})$; for the $\hat{H}_{spinless}$ of Eq. (10), there is additionally no diamagnetic component $\mathbf{j}_d(\mathbf{r})$.)

(c) The electron-interaction field $\mathcal{E}_{ee}(\mathbf{r})$ is obtained via Coulomb’s Law from its *nonlocal* quantal source, the pair-correlation function $P(\mathbf{r}\mathbf{r}')$ which is the expectation value of the pair operator $\hat{P}(\mathbf{r}\mathbf{r}')$. The field is representative of electron correlations due to Coulomb repulsion and those due to the Pauli principle. Again, one might expect such a field representing the Coulomb repulsion between electrons to exist as in the classical case. But since, the pair function $P(\mathbf{r}\mathbf{r}')$ is the expectation value of the pair-correlation operator $\hat{P}(\mathbf{r}\mathbf{r}')$, and the wave function $\Psi(\mathbf{X})$ is antisymmetric in an interchange of the coordinates of the electrons, the field also accounts for correlations due to the Pauli principle. Thus, the contribution of the correlations due to the Pauli principle to the field $\mathcal{E}_{ee}(\mathbf{r})$ are also accounted for via Coulomb’s Law.

(d) According to the QNFL, there exists a kinetic field $\mathcal{Z}(\mathbf{r})$ experienced by each electron. The field is representative of kinetic effects. Its *nonlocal* quantal source is the reduced single-particle density matrix $\gamma(\mathbf{r}\mathbf{r}')$, the expectation value of the density matrix operator $\hat{\gamma}(\mathbf{r}\mathbf{r}')$. The fact that each electron experiences such a field is strictly a quantum-mechanical feature.

(e) The QNFL also shows that each electron experiences a field representative of the electron density $\rho(\mathbf{r})$, the differential density field $\mathcal{D}(\mathbf{r})$. Its *local* quantal source is the density $\rho(\mathbf{r})$, the expectation of the density operator $\hat{\rho}(\mathbf{r})$.

(f) Finally, another way that the quantum system is distinguished from its classical counter-part, is that there exists in addition to the Lorentz field $\mathcal{L}(\mathbf{r})$, an internal magnetic field $\mathcal{I}_m(\mathbf{r})$ component whose quantal source is also the physical current density $\mathbf{j}(\mathbf{r})$.

Additional salient features of the QNFL are the following:

(i) The QNFL is derived from the Schrödinger-Pauli equation by ensuring the satisfaction of the equation of continuity: $\nabla \cdot \mathbf{j}(\mathbf{r}) = 0$.

(ii) The QNFL is gauge invariant.

(iii) As is the case for the Schrödinger-Pauli equation, the QNFL is valid for *arbitrary* potential function $v(\mathbf{r})$, state, and dimensionality.

(iv) On summing over all the electrons, it can be proved that as in the classical case (see Eq. (17)), the contribution of the internal field $\mathcal{F}^{int}(\mathbf{r})$ vanishes:

$$\int \rho(\mathbf{r})\mathcal{F}^{int}(\mathbf{r})d\mathbf{r} = 0. \quad (24)$$

In fact it can be shown that the contribution of each component of the internal field $\mathcal{F}^{int}(\mathbf{r})$ separately vanishes. This then leads to the stationary-state Ehrenfest's Theorem^[18]:

$$\int \rho(\mathbf{r})\mathcal{F}^{ext}(\mathbf{r})d\mathbf{r} = 0, \quad (25)$$

the quantum equivalent to Newton's First Law (see Eq. (18)).

(v) With the exception of the external field $\mathcal{E}(\mathbf{r}) = -\nabla v(\mathbf{r})$, the remaining fields are in general not conservative. However, their sum $\mathcal{F}(\mathbf{r}) = \mathcal{F}^{int}(\mathbf{r}) - \mathcal{L}(\mathbf{r})$ is always conservative, *i.e.* $\nabla \times \mathcal{F}(\mathbf{r}) = 0$. For certain symmetries, the individual fields are conservative. Or, if a certain symmetry is imposed, as in the central field approximation, then the individual fields can each be made to be conservative.

The Total Energy

To complete the complementary perspective, once again in a manner similar to that of classical physics, the energy E of the quantum system, as described by the Schrödinger-Pauli equation, and its components may be expressed in integral virial form in terms of the component-fields experienced by each electron. Thus, the kinetic T , electron-interaction E_{ee} , the external electrostatic E_{es} , and magnetostatic E_{mag} energies are

$$T = -\frac{1}{2} \int \rho(\mathbf{r})\mathbf{r} \cdot \mathcal{Z}(\mathbf{r})d\mathbf{r}, \quad (26)$$

$$E_{ee} = \int \rho(\mathbf{r})\mathbf{r} \cdot \mathcal{E}_{ee}(\mathbf{r})d\mathbf{r}, \quad (27)$$

$$E_{es} = \int \rho(\mathbf{r})v(\mathbf{r})d\mathbf{r}, \quad (28)$$

$$E_{mag} = \int \rho(\mathbf{r})\mathbf{r} \cdot \mathcal{M}(\mathbf{r})d\mathbf{r}, \quad (29)$$

where $\mathcal{M}(\mathbf{r}) = -[\mathcal{L}(\mathbf{r}) + \mathcal{I}_m(\mathbf{r})]$. The above expressions are valid irrespective of whether or not the individual fields are conservative. The total energy E may then be written as

$$E = T + E_{ee} + E_{em}, \quad (30)$$

with $E_{em} = E_{es} + E_{mag}$, the electromagnetic energy.

Note that the energy E_{es} may also be expressed in virial form in terms of the electrostatic field $\mathcal{E}(\mathbf{r})$, but with a coefficient that depends on the degree of the homogeneous function $v(\mathbf{r})$. Additionally, if the field $\mathcal{M}(\mathbf{r})$ is conservative, *i.e.* $\nabla \times \mathcal{M}(\mathbf{r}) = 0$, then E_{mag} may be expressed as

$$E_{mag} = \int \rho(\mathbf{r})v_m(\mathbf{r})d\mathbf{r}, \quad (31)$$

where the magnetic scalar potential $v_m(\mathbf{r})$ is defined as $\mathcal{M}(\mathbf{r}) = -\nabla v_m(\mathbf{r})$. (Note that both the scalar electrostatic $v(\mathbf{r})$ and magnetostatic $v_m(\mathbf{r})$ potentials are *path independent*.)

This then is the complementary perspective to our present understanding and usage of the quantum mechanics of electrons. In the following section we describe the new physics revealed by this alternate perspective.

New Physics

We describe here the new physics arrived at via the complementary perspective. These new concepts are not a feature of and cannot be surmised via our traditional understanding of quantum mechanics.

1. The QNFL establishes, as in classical physics, that each electron in a magnetostatic field $\mathcal{B}(\mathbf{r})$ experiences a Lorentz field $\mathcal{L}(\mathbf{r})$. Although it is implicitly understood that such a field must exist, it is now *explicitly* shown to be the case. Furthermore, the *individual* contributions of the paramagnetic $\mathbf{j}_p(\mathbf{r})$, diamagnetic $\mathbf{j}_d(\mathbf{r})$, and magnetization $\mathbf{j}_m(\mathbf{r})$ current density components to the Lorentz field $\mathcal{L}(\mathbf{r})$ can be separately determined. (See ^[19].)

2. One further learns that in addition to the external Coulomb $\mathcal{E}(\mathbf{r})$ and Lorentz $\mathcal{L}(\mathbf{r})$ fields, each electron also experiences an internal field $\mathcal{F}^{int}(\mathbf{r})$. This field is comprised of its electron-interaction $\mathcal{E}_{ee}(\mathbf{r})$, kinetic $\mathcal{Z}(\mathbf{r})$, differential density $\mathcal{D}(\mathbf{r})$, and internal magnetic $\mathcal{I}_m(\mathbf{r})$ components with each field being representative of a property of the system. The existence of the Lorentz $\mathcal{L}(\mathbf{r})$ and the various internal fields are arrived at solely via the QNFL.

3. The existence of the fields experienced by each electron then leads to *new* expressions for the total energy E and of its components. Furthermore, as in classical physics, the structure of the fields informs as to the regions of configuration space from which the principal contributions to the energy and of its components arises. (The expression for the kinetic energy T of Eq. (26) is the third expression in the literature^[20] for the kinetic energy density as obtained from the single-particle density matrix $\gamma(\mathbf{r}\mathbf{r}')$. This should be of value in Kohn-Sham^[16] density functional theory (see e.g.^[21,22], and work^[23,24,25] in which information-entropic measures are used within quantum mechanics. It also plays a significant role in Quantal density functional theory^[13,14].)

4. In writing the Hamiltonian of bound electrons, it is assumed that the binding field $\mathcal{E}(\mathbf{r})$ is conservative, which means that the corresponding potential $v(\mathbf{r})$ is *path independent*. This is rigorously shown to be the case via the QNFL (see No. 5 below).

5. The QNFL (Eq. (20)) provides a rigorous physical interpretation of the binding potential $v(\mathbf{r})$ in the Hamiltonian. Accordingly, $v(\mathbf{r})$ is *the work done to move an electron from some reference point at infinity to its position at \mathbf{r} in the force of the conservative field $\mathcal{F}(\mathbf{r})$* :

$$v(\mathbf{r}) = \int_{\infty}^{\mathbf{r}} \mathcal{F}(\mathbf{r}') \cdot d\ell', \quad (32)$$

where $\mathcal{F}(\mathbf{r}) = \mathcal{F}^{int}(\mathbf{r}) - \mathcal{L}(\mathbf{r}) = \mathcal{E}_{ee}(\mathbf{r}) - \mathcal{Z}(\mathbf{r}) - \mathcal{D}(\mathbf{r}) - \mathcal{I}_m(\mathbf{r}) - \mathcal{L}(\mathbf{r})$. Since $\nabla \times \mathcal{F}(\mathbf{r}) = 0$, this work done is *path independent*. This definition is consistent with the classical physics description of a potential energy being the work done in a conservative field. This then can be thought of as being *the quantum-mechanical definition of the operator $v(\mathbf{r})$* (see also No. 7 below).

6. Traditionally, the analytical structure of the binding potential function $v(\mathbf{r})$ in a Hamiltonian is assumed known, and thought of as being an independent extrinsic input to it. The QNFL as expressed by Eq. (32), however, provides a more fundamental insight to this potential. The expression shows that the potential $v(\mathbf{r})$ depends upon the internal field $\mathcal{F}^{int}(\mathbf{r})$ components and the Lorentz field $\mathcal{L}(\mathbf{r})$. The potential $v(\mathbf{r})$ is therefore inherently related to the properties of the system. It can no longer be thought of as being independent of the system of bound electrons. In fact it is constructed via these properties via Eq. (32). If the various internal fields are separately conservative, the function $v(\mathbf{r})$ is then a sum of constituent functions each representative of a property of the system.

7. The potential $v(\mathbf{r})$ is an *exactly known universal functional* of the wave function $\Psi(\mathbf{X})$, *i.e.* $v(\mathbf{r}) = v[\Psi](\mathbf{r})$. To understand this, note that the field $\mathcal{F}(\mathbf{r})$ of Eq. (32) is a sum of constituent fields whose sources are expectation values of Hermitian operators taken with respect to the wave function $\Psi(\mathbf{X})$. Thus, the field $\mathcal{F}(\mathbf{r})$ is a functional of $\Psi(\mathbf{X})$, *i.e.* $\mathcal{F}(\mathbf{r}) = \mathcal{F}[\Psi](\mathbf{r})$. Hence, the potential $v(\mathbf{r})$ is a functional of $\Psi(\mathbf{X})$:

$$v[\Psi](\mathbf{r}) = \int_{-\infty}^{\mathbf{r}} \mathcal{F}[\Psi](\mathbf{r}') \cdot d\ell'. \quad (33)$$

The functional $v[\Psi](\mathbf{r})$ is valid for *arbitrary* state, *nondegenerate* or *degenerate ground* or *excited*. It is *universal* in that the functional $v[\Psi](\mathbf{r})$ is the same for *arbitrary* system whether natural or artificial as defined by the Schrödinger-Pauli or Schrödinger Hamiltonians. (We note the statement that the potential $v(\mathbf{r})$ is a functional of the *nondegenerate ground* state wave function $\Psi_g(\mathbf{X})$ for the case when only an external electrostatic field $\mathcal{E}(\mathbf{r})$ is present was proved by Hohenberg and Kohn^[15]. However, the functional was not provided. The explicit functional is given via the QNFL by Eq. (33).) To reiterate, Eq. (33) explicitly demonstrates that it is the quantum-mechanical definition of the potential operator $v(\mathbf{r})$.

Elucidation of Complementary Perspective by Application to ‘Artificial Atoms’ in a Magnetic Field

We elucidate the complementary perspective by application to ‘artificial atoms’ or semiconductor quantum dots in a magnetic field. These are 2-dimensional atoms in a quantum well in a thin layer of semiconductor such as *GaAs* sandwiched between two layers of another semiconductor *AlGaAs*. The 2-dimensional motion is restricted by an electrostatic field. The magnetic field is perpendicular to this plane of motion. As the ‘atom’ is housed in a semiconductor, the free electron mass m must be replaced by the band-effective mass m^* , and the electron interaction modified by the dielectric constant ϵ . For *GaAs*, the effective mass $m^* = 0.067m$ and $\epsilon = 12.4$. The binding potential $v(\mathbf{r})$ of such ‘atoms’ is harmonic: $v(\mathbf{r}) = \frac{1}{2}k_0r^2$ with k_0 the binding force constant; $k_0 = m^*\omega_0^2$ and ω_0 the binding frequency.

For a 2-electron ‘artificial atom’ in a magnetic field $\mathcal{B}(\mathbf{r})$ the Schrödinger-Pauli theory

equation is then

$$\left[\frac{1}{2m^*} \sum_{k=1}^2 (\hat{\mathbf{p}}_k + \frac{e}{c} \mathbf{A}(\mathbf{r}_k))^2 + \frac{g^* \mu_B}{\hbar} \sum_{k=1}^2 \mathbf{B}(\mathbf{r}_k) \cdot \mathbf{s}_k + \frac{1}{\epsilon} \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} + \frac{1}{2} m^* \omega_0^2 \sum_{k=1}^2 r_k^2 \right] \Psi(\mathbf{x}_1, \mathbf{x}_2) = E \Psi(\mathbf{x}_1, \mathbf{x}_2), \quad (34)$$

with g^* the gyromagnetic ration; $\mathbf{x} = \mathbf{r}\zeta$. The wave functions $\Psi(\mathbf{x}_1, \mathbf{x}_2)$ are of the form of Eq. (7):

$$\Psi(\mathbf{x}_1, \mathbf{x}_2) = \psi(\mathbf{r}_1, \mathbf{r}_2) \chi(\zeta_1, \zeta_2), \quad (35)$$

with $\psi(\mathbf{r}_1, \mathbf{r}_2)$ the spatial and $\chi(\zeta_1, \zeta_2)$ the spin components. The analytical wave function solutions are derived in the symmetric gauge $\mathbf{A}(\mathbf{r}) = \frac{1}{2} \mathbf{B}(\mathbf{r}) \times \mathbf{r}$ with the magnetic field in the z -direction $\mathbf{B}(\mathbf{r}) = B \mathbf{i}_z$. The expressions for the spatial components $\psi(\mathbf{r}_1, \mathbf{r}_2)$ for a ground 1^1S , first excited singlet 2^1S and triplet 2^3S states derived by the method of Taut^[26] are given below. These expressions are in terms of an effective force constant $k_{eff} = \omega_0^2 + \omega_L^2$, where $\omega_L = B/2c$ is the Larmor frequency. The parameter values characterizing each wave function are given in Table 2. (Effective atomic units are employed: $e^2/\epsilon = \hbar = m^* = c = 1$. The effective Bohr radius is $a_0^* = a_0(m\epsilon/m^*)$; the effective energy unit is $(a.u.)^* = (a.u.)(m^*/m\epsilon^2)$.)

Ground 1^1S State^[27]

$$\psi(\mathbf{r}_1, \mathbf{r}_2) = N e^{-\frac{1}{2} \sqrt{k_{eff}}(r_1^2 + r_2^2)} (1 + |\mathbf{r}_1 - \mathbf{r}_2|). \quad (36)$$

First Excited Singlet 2^1S State^[28]

$$\psi(\mathbf{r}_1, \mathbf{r}_2) = N e^{-\frac{1}{2} \sqrt{k_{eff}}(r_1^2 + r_2^2)} (1 + |\mathbf{r}_1 - \mathbf{r}_2| + c_2 |\mathbf{r}_1 - \mathbf{r}_2|^2 + c_3 |\mathbf{r}_1 - \mathbf{r}_2|^3). \quad (37)$$

First Excited Triplet 2^3S State^[4,19]

$$\psi(\mathbf{r}_1, \mathbf{r}_2) = N e^{im\theta} e^{-\frac{1}{2} \sqrt{k_{eff}}(r_1^2 + r_2^2)} (|\mathbf{r}_1 - \mathbf{r}_2| + c_2 |\mathbf{r}_1 - \mathbf{r}_2|^2 + c_3 |\mathbf{r}_1 - \mathbf{r}_2|^3 + c_4 |\mathbf{r}_1 - \mathbf{r}_2|^4). \quad (38)$$

Note that the spatial part of the wave function $\psi(\mathbf{r}_1, \mathbf{r}_2)$ for the ground 1^1S and singlet 2^1S states is symmetric in an interchange of the spatial coordinates $(\mathbf{r}_1, \mathbf{r}_2)$ because the spin component $\chi(\zeta_1, \zeta_2)$ is antisymmetric in an interchange of the spin coordinates (ζ_1, ζ_2) . For the triplet 2^3S state, the spin component $\chi(\zeta_1, \zeta_2)$ is symmetric in an interchange of (ζ_1, ζ_2) ,

and therefore the spatial part $\psi(\mathbf{r}_1\mathbf{r}_2)$ is antisymmetric in the interchange of $\psi(\mathbf{r}_1\mathbf{r}_2)$. This antisymmetry is a result of the phase factor $e^{im\theta}$. When the coordinates \mathbf{r}_1 and \mathbf{r}_2 are interchanged, the magnitude of the relative coordinate vector $\mathbf{u} = \mathbf{r}_2 - \mathbf{r}_1$ does not change, but the angle θ , which is the angle of the relative coordinate \mathbf{u} , changes to $\theta + \pi$. This changes the sign of the phase factor.

In Figs. 2, 3, 4, we plot for the ground 1^1S , first excited singlet 2^1S , and the spin-correlated first excited triplet 2^3S states the electron-interaction $\mathcal{E}_{ee}(\mathbf{r})$, kinetic $\mathcal{Z}(\mathbf{r})$, the differential density $\mathcal{D}(\mathbf{r})$, Lorentz $\mathcal{L}(\mathbf{r})$, and internal magnetic $\mathcal{I}_m(\mathbf{r})$ fields. There is an evolutionary commonality in these graphs: **(a)** Shell structure is evident in each graph for the fields $\mathcal{E}_{ee}(\mathbf{r})$, $\mathcal{Z}(\mathbf{r})$, and $\mathcal{D}(\mathbf{r})$: one shell for the ground 1^1S state and two shells for the excited 2^1S and 2^3S states. (In Figs. 3 and 4, the second shell is not evident in the field $\mathcal{E}_{ee}(\mathbf{r})$ on the scale of the figure.); **(b)** For the ground 1^1S and singlet 2^1S states, the wave functions $\psi(\mathbf{r}_1\mathbf{r}_2)$ are real. As a consequence, the paramagnetic component $\mathbf{j}_p(\mathbf{r})$ of the current density vanishes. Further, as these are both singlet states, the magnetization current density $\mathbf{j}_m(\mathbf{r})$ too vanishes. The Lorentz $\mathcal{L}(\mathbf{r})$ and internal magnetic $\mathcal{I}_m(\mathbf{r})$ fields are then solely due to the diamagnetic component $\mathbf{j}_d(\mathbf{r})$ which is proportional to the electron density $\rho(\mathbf{r})$. Although the density $\rho(\mathbf{r})$, and hence $\mathbf{j}_d(\mathbf{r})$ exhibits shell structure, it can be shown analytically that the fields $\mathcal{L}(\mathbf{r})$ and $\mathcal{I}_m(\mathbf{r})$ for these states are linear (Figs. 1, 2); **(c)** For the triplet 2^3S state, the wave function $\psi(\mathbf{r}_1\mathbf{r}_2)$ is complex, and hence there exists a paramagnetic current density component $\mathbf{j}_p(\mathbf{r})$. As this is a triplet state with electron spin correlation, there also exists a magnetization component $\mathbf{j}_m(\mathbf{r})$. All three components $\mathbf{j}_p(\mathbf{r})$, $\mathbf{j}_d(\mathbf{r})$, and $\mathbf{j}_m(\mathbf{r})$ exhibit shell structure. For the triplet 2^3S state (Fig. 4), both the Lorentz $\mathcal{L}(\mathbf{r})$ and internal magnetic $\mathcal{I}_m(\mathbf{r})$ components also exhibit shell structure; **(d)** Finally, the satisfaction of the QNFL for each state is shown in the Figs. 2, 3, 4. On summing the individual fields, one then obtains the linear function $-k_0r$, the gradient of the scalar potential $v(\mathbf{r})$, in each case, *i.e.*

$$-\mathcal{E}_{ee}(\mathbf{r}) + \mathcal{Z}(\mathbf{r}) + \mathcal{D}(\mathbf{r}) + \mathcal{L}(\mathbf{r}) + \mathcal{I}_m(\mathbf{r}) = -k_0r. \quad (39)$$

Employing the fields exhibited in Figs. 2, 3, 4, the kinetic T , electron-interaction E_{ee} , electromagnetic E_{em} and total energy E are then obtained from Eqs. (26) - (30). These values are given in Table 3. (The values are the same as would be obtained by taking the expectation values of the individual terms of the Hamiltonian \hat{H}_{spin} of Eq. (34).)

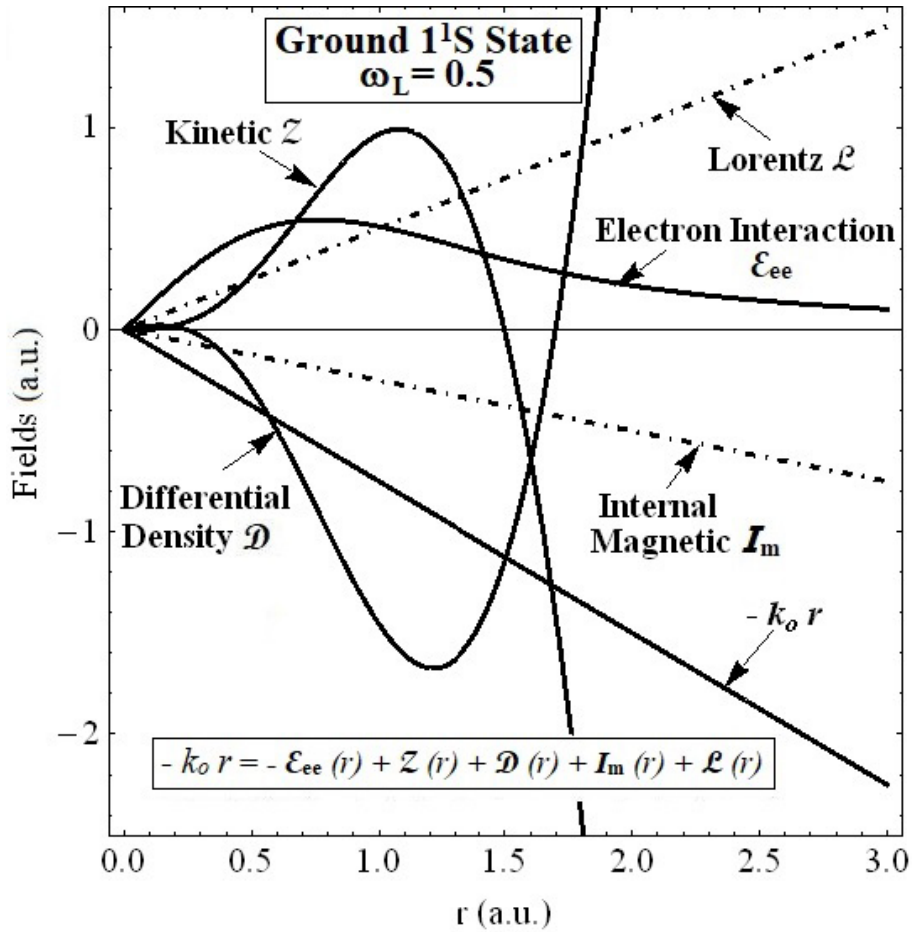


FIG. 2: The fields experienced by each electron in a ground 1^1S state of the ‘artificial atom’: electron-interaction $\mathcal{E}_{ee}(\mathbf{r})$, kinetic $\mathcal{Z}(\mathbf{r})$, differential density $\mathcal{D}(\mathbf{r})$, Lorentz $\mathcal{L}(\mathbf{r})$ and internal magnetic $\mathcal{I}_m(\mathbf{r})$. The fields $\mathcal{L}(\mathbf{r})$ and $\mathcal{I}_m(\mathbf{r})$ are plotted for a Larmor frequency $\omega_L = 0.5$. The function $-k_0 r$ is also plotted with the value of k_0 given in Table 2.

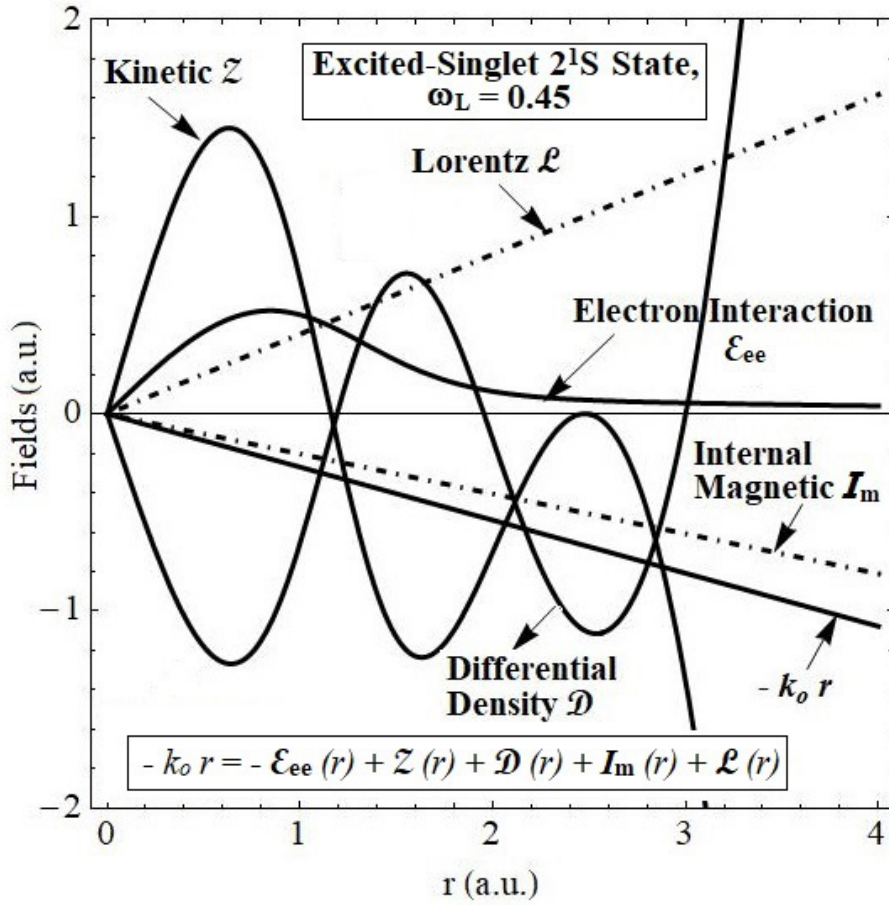


FIG. 3: The same as in Fig. 2 but for a first excited singlet 2^1S state of the ‘artificial atom. The Larmor frequency is $\omega_L = 0.45$.

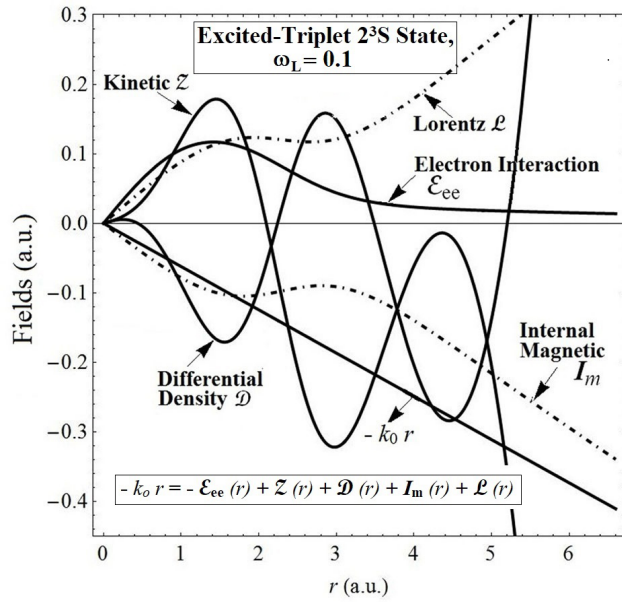


FIG. 4: The same as in Fig. 2 but for a first excited triplet 2^3S state of the ‘artificial atom’. The Larmor frequency is $\omega_L = 0.1$.

TABLE II: Wave function characteristics of the ‘artificial atoms’ in a magnetic field in their ground 1^1S , first excited singlet 2^1S and triplet 2^3S states: Normalization constant N ; effective force constant k_{eff} ; binding force constant k_0 ; Larmor frequency ω_L ; coefficients c_i ; angular momentum quantum number m .

State	N	k_{eff}	k_0	ω_L	c_i	m
1^1S	0.135646	1.000000	0.750000	0.500000		0
2^1S	0.108563	0.471716	0.269216	0.450000	$c_2 = -0.265111$ $c_3 = -0.182082$	0
2^3S	0.022466	0.072217	0.062217	0.1000000	$c_2 = \frac{1}{3}$ $c_3 = -0.059108$ $c_4 = -0.015884$	1

TABLE III: The total energy E and its kinetic T , electron-interaction E_{ee} , and electromagnetic E_{em} components for the ‘artificial atoms’ in a magnetic field in their ground 1^1S , first excited singlet 2^1S and triplet 2^3S states.

State	Energies (<i>a.u.</i>)*			
	T	E_{ee}	E_{em}	E
1^1S	0.886199	0.818401	1.295400	3.000000
2^1S	1.266683	0.600476	1.566907	3.434066
2^3S	0.615577	0.254158	0.742657	1.612392

RELATIONSHIP TO QUANTAL AND TRADITIONAL DENSITY FUNCTIONAL THEORIES

Stationary state Quantal Density Functional Theory (QDFT)^[4,13,14,29] is a *local effective potential* theory complement to Schrödinger-Pauli/Schrödinger theory valid for *arbitrary* state. QDFT maps the interacting system of electrons described by the Hamiltonian \hat{H}_{spin} of Eq. (1) to one of noninteracting fermions possessing the same gauge invariant properties of the electronic and physical current densities $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$. Thus, in such a theory, the many-body effects due to the Pauli principle and Coulomb repulsion are incorporated into

a *local* (multiplicative) electron-interaction potential $v_{ee}(\mathbf{r})$. The potential $v_{ee}(\mathbf{r})$ includes in addition the contributions of these correlations to the kinetic energy – the Correlation-Kinetic effects. As was the case for the interacting system, the QDFT mapping is in terms of ‘classical’ fields and quantal sources that are expectations of Hermitian operators, and is based on the corresponding ‘Quantal Newtonian’ First Law for the model fermionic system. Hence, there is a *rigorous physical* definition of the potential $v_{ee}(\mathbf{r})$: *it is the work done in a conservative effective field $\mathcal{F}^{\text{eff}}(\mathbf{r})$ in which the correlations due to the Pauli principle, Coulomb repulsion, and Correlation-Kinetic effects are incorporated.* The total energy E and its components too can be expressed in integral virial form in terms of fields descriptive of the model system. As noted, QDFT is applicable to ground and excited states whether nondegenerate or degenerate. The state of the model system is also *arbitrary*: It could be in a ground or excited state. A key attribute of QDFT is that it is possible to delineate the *separate* contributions due to the Pauli principle, Coulomb repulsion and Correlation-Kinetic effects to the potential $v_{ee}(\mathbf{r})$ and the total energy E . Another is that irrespective of the state of the model system, its highest occupied eigenvalue is the negative of the ionization potential. Of course, being a local effective potential theory, it is more amenable to numerical computation.

Ground state density functional theory (DFT) due to Kohn and Sham (KS)^[16] is also a local effective potential theory based on the ground state theorems of Hohenberg and Kohn^[15]. The mapping is from a ground state of the interacting system of electrons to a ground state of the noninteracting fermionic model system possessing the same density $\rho(\mathbf{r})$. DFT is a *mathematical* theory in that the description of the electron correlations is in terms of an unknown electron-interaction energy functional of the density $E_{ee}^{KS}[\rho]$. The corresponding local potential $v_{ee}(\mathbf{r})$ in which all the many-body effects are incorporated is then defined as the functional derivative $\delta E_{ee}^{KS}[\rho]/\delta\rho(\mathbf{r})$. In DFT too, the highest occupied eigenvalue of the model system in its ground state corresponds to the negative of the ionization potential^[30]. Based on the above description of QDFT, these mathematical definitions of the energy functional and its functional derivative within DFT can be provided a rigorous physical interpretation in terms of the fields of QDFT. The reader is referred to^[13] for the detailed derivations.

Thus, the complementary perspective to Schrödinger-Pauli/Schrödinger theory presented here helps in defining local effective potential theory in general via QDFT as well as providing

an understanding of the mathematical entities of traditional DFT.

Concluding Remarks

This work is a description of a complementary perspective to the statistical Göttingen-Copenhagen interpretation of the stationary-state quantum mechanics of electrons in an electromagnetic field. New physics is thereby arrived at. The perspective is that of the *individual* electron via its equation of motion or ‘Quantal Newtonian’ First Law (QNFL). The Law is in terms of ‘classical’ fields experienced by each electron. The fields are ‘classical’ in that their sources are quantum-mechanical expectation values of Hermitian operators. Thus, the perspective hews to the Born interpretation. There is a parallelism between the QNFL and Newton’s First Law for an *individual* classical charged particle amongst other such particles in an external electromagnetic field. The fields of classical physics pervade all space and are tangible. In an entirely similar manner, the fields experienced by each electron also pervade all space, and in that context they too are tangible.

There are, of course, fundamental differences between the classical and quantum cases. The parallelism between the two can only go so far. In a magnetic field, a moving classical particle with charge experiences a Lorentz field. Similarly, a bound electron in a magnetic field also experiences a Lorentz field. This fact is now rigorously proved to be the case via the derivation of the QNFL. What is further revealed is that each electron experiences internal fields that are separately representative of properties of the system: electron correlations due to the Pauli principle and Coulomb repulsion, kinetic effects, the electron density, and that there is an internal magnetic field component. The existence of these various fields in a quantum system is an understanding arrived at solely through the new perspective.

In classical physics, the energy of a system of charged particles in an electromagnetic field may be expressed in terms of the various existing fields. In a similar manner, the energy of a quantum system and *all* of its components may also be obtained from the quantum fields experienced by each electron. In the quantum case, this also includes the kinetic energy which is determined from the kinetic field.

A fundamental new insight achieved concerns our understanding of the scalar binding potential $v(\mathbf{r})$ of the electrons. In traditional quantum mechanics, the potential $v(\mathbf{r})$ is considered as an extrinsic input to the Hamiltonian. The complementary perspective, however,

shows the potential to be intrinsically dependent on the fields experienced by each electron. The potential can therefore no longer be thought of as being independent of the physical system. That this is the case can also be understood from a mathematical perspective. It is shown that the potential $v(\mathbf{r})$ is a functional of the system wave function $\Psi(\mathbf{X})$, *i.e.* $v(\mathbf{r}) = v[\Psi](\mathbf{r})$. Thus, the potential is *self-consistently* related to the wave function. In other words, it is the knowledge of the wave function $\Psi(\mathbf{X})$ that uniquely determines the potential $v(\mathbf{r})$.

The above new insights: the various fields experienced by each electron; the determination of the energy via these fields; the functional dependence of the potential $v(\mathbf{r})$ on the wave function $\Psi(\mathbf{X})$, are all elucidated by application to three different 2-electron ‘artificial atoms’, one in a ground state, another in a first excited singlet state, and one in the first excited triplet state. The fields of each application demonstrate the satisfaction of the QNFL, the determination of the energy via these fields, and thereby the complementary perspective.

The quantal-source – field complementary perspective to Schrödinger-Pauli/Schrödinger theory in turn leads to an understanding of local effective potential theory both ground and excited via QDFT, and thereby to the explanation of the energy density functionals and their functional derivatives of DFT.

For a system of electrons in the presence of a time-dependent electromagnetic field, there exists a ‘Quantal Newtonian’ Second Law for each electron that parallels the corresponding Newton’s Second Law. There is therefore a complementary perspective to time-dependent Schrödinger-Pauli theory. Such a description is the subject of future work.

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