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# Quantal Density Functional Theory in the Presence of a Magnetic Field

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We generalize the quantal density functional theory (QDFT) of electrons in the presence of an external electrostatic field  $\mathcal{E}(\mathbf{r}) = -\nabla v(\mathbf{r})$  to include an external magnetostatic field  $\mathbf{B}(\mathbf{r}) = \nabla \times \mathbf{A}(\mathbf{r})$ , where  $\{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\}$  are the respective scalar and vector potentials. The generalized QDFT, valid for nondegenerate ground and excited states, is the mapping from the interacting system of electrons to a model of noninteracting fermions with the same density  $\rho(\mathbf{r})$  and physical current density  $\mathbf{j}(\mathbf{r})$ , and from which the total energy can be obtained. The properties  $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$  constitute the basic quantum mechanical variables because, as proved previously, for a nondegenerate ground state they uniquely determine the potentials  $\{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\}$ . The mapping to the noninteracting system is arbitrary in that the model fermions may be either in their ground or excited state. The theory is explicated by application to a ground state of the exactly solvable (2-dimensional) Hooke's atom in a magnetic field, with the mapping being to a model system also in its ground state. The majority of properties of the model are obtained in closed analytical or semi-analytical form. A comparison with the corresponding mapping from a ground state of the (3-dimensional) Hooke's atom in the absence of a magnetic field is also made.

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## I. INTRODUCTION

The study of the electronic properties of matter in the presence of both an external electrostatic field  $\mathcal{E}(\mathbf{r}) = -\nabla v(\mathbf{r})$  and a magnetostatic field  $\mathbf{B}(\mathbf{r}) = \nabla \times \mathbf{A}(\mathbf{r})$ , where  $\{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\}$  are the scalar and vector potentials, continues to be of interest. Properties such as the Zeeman effect in atoms and molecules, and the de Haas-van Alphen effect, the Hall effect and magnetoresistance in solids, have been studied. The more recent interest has focused on electrons confined to two dimensions: metal-oxide-semiconductor structures, quantum wells and super lattices, the integer and fractional Quantum Hall effects, and quantum dots.

In this paper we generalize the conventional quantal density functional theory [1, 2] (QDFT) of a system of electrons in the presence of an external electrostatic field  $\mathcal{E}(\mathbf{r})$  to now include an external magnetostatic field  $\mathbf{B}(\mathbf{r})$ . In the presence of a magnetic field, QDFT is the mapping from the true interacting system of electrons in a nondegenerate ground or excited state to a model  $S$  system of noninteracting fermions having the same density  $\rho(\mathbf{r})$  and physical current density  $\mathbf{j}(\mathbf{r})$ . From the model system the same total energy  $E$  may be obtained. The state of the model system is arbitrary in that it may be in a ground or excited state configuration. The existence of the model fermionic system is an assumption. Due to the present interest in two-dimensional electronic systems, we then explicate this QDFT by application to the exactly solvable Hooke's atom [3] in which the electrons are confined to a plane by a magnetic field.

The choice of the properties  $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$  is governed by the fact that they constitute the basic variables in the quantum mechanics of electrons in static external potentials  $\{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\}$ . They are the basic variables because as we have proved previously [4], for the nondegenerate ground state, the ground state  $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$  uniquely determines the external potentials  $\{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\}$ . In other words, the relationship between  $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$  and  $\{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\}$  is one-to-one. Thus,  $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$  uniquely determine the Hamiltonian, and hence by solution of the Schrödinger equation, all the properties of the system. (In Hohenberg-Kohn [5] theory, *i.e.* in the absence of a magnetic field, the basic variable is the ground state density  $\rho(\mathbf{r})$  because it uniquely determines the external potential  $v(\mathbf{r})$ . The relationship between  $\rho(\mathbf{r})$  and  $v(\mathbf{r})$  is one-to-one.) We have also proved [4] that in general the wave function  $\Psi$  is a functional of  $\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})$ , and a smooth gauge function  $\alpha(\mathbf{R})$  with  $\mathbf{R} = \mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N$ . As  $\rho(\mathbf{r})$  and  $\mathbf{j}(\mathbf{r})$  are gauge invariant properties, it is the functional dependence on the gauge function  $\alpha(\mathbf{R})$  that ensures the wave function written as a functional is gauge

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variant. However, as the choice of the gauge function is usually arbitrary because all gauge functions correspond to the same physical system, it can be chosen to be zero. Hence, the choice of the basic variables  $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$  for the properties that the  $S$  system must reproduce.

For completeness we note that the Hohenberg-Kohn theorem [5] was generalized by Rajagopal and Callaway [6] to the relativistic case in which the variables are the four-potential  $\{v(\mathbf{rt}), \mathbf{A}(\mathbf{rt})\}$  and the four-current  $\{\rho(\mathbf{rt}), \mathbf{j}(\mathbf{rt})\}$ . For stationary state theory, the idea of employing  $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$  within the context of Kohn-Sham theory [7] in which the mapping is in terms of energy functionals and functional derivatives was due to Ghosh and Dhara [8] and Diener [8]. The former employ these variables without proving the one-to-one relationship between  $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$  and  $\{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\}$ . The latter does not account for the fact that in the presence of a magnetic field, the relationship between the potentials  $\{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\}$  and the wave function  $\Psi$  can be many-to-one and not one-to-one. See also our work of Ref. [4] for a Kohn-Sham  $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$  functional theory. There is also the work of Vignale and Rasolt [9] who employ the density  $\rho(\mathbf{r})$  and the paramagnetic current density  $\mathbf{j}_p(\mathbf{r})$  as the variables. (The current density  $\mathbf{j}_p(\mathbf{r})$  is not a basic variable in the rigorous sense defined above.) However, as  $\mathbf{j}_p(\mathbf{r})$  is gauge variant, these authors employ instead the vorticity  $\boldsymbol{\nu}(\mathbf{r}) = \nabla \times (\mathbf{j}_p(\mathbf{r})/\rho(\mathbf{r}))$  in their theory. For additional work on this latter theory, see Refs. [10–13]. There is also a magnetic field density functional theory [14] in which the variables employed are the density  $\rho(\mathbf{r})$  and the magnetic field  $\mathbf{B}(\mathbf{r})$ .

In Sect. II, we present the equations governing the QDFT in the presence of a magnetic field. In Sect. III, we apply the generalized QDFT to map a ground state of the Hooke's atom in a magnetic field to one of noninteracting fermions in their ground state with the same density  $\rho(\mathbf{r})$  and physical current density  $\mathbf{j}(\mathbf{r})$ . The majority of the properties describing the model  $S$  system can be obtained in closed analytical or semi-analytical form. The contrast of the properties with the case when the magnetic field is absent [1, 15] is made. Concluding remarks follow in Sect. IV.

## II. QUANTAL DENSITY FUNCTIONAL THEORY

As in conventional QDFT [1, 2], the description of the mapping in the presence of an external magnetostatic field to an  $S$  system with the same  $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$  is in terms of ‘classical’ fields whose sources are quantal in that they are expectations of Hermitian operators. In addition to the fields representative of correlations due to the Pauli exclusion principle, Coulomb repulsion, and correlation-kinetic effects, there now exists a field representative of correlation-magnetic effects. The new field is a consequence of the difference between the vector potentials for the interacting and model systems. The equations of the QDFT are derived from the generalized ‘quantal Newtonian’ first law (or differential virial theorem) and the integral virial theorem as written in terms of fields for both the interacting [10, 16] and  $S$  systems. As QDFT is based on the virial theorems, the theory is valid for both a nondegenerate ground or excited state of the interacting electrons. Additionally, the state of the model  $S$  system is arbitrary, in that it may be in a ground or excited state configuration. We begin with a description of the interacting system.

### A. Interacting System of Electrons

Consider a system of  $N$  electrons in the presence of an external electrostatic field  $\mathcal{E}(\mathbf{r}) = -\nabla v(\mathbf{r})$  and a magnetostatic field  $\mathbf{B}(\mathbf{r}) = \nabla \times \mathbf{A}(\mathbf{r})$ , where  $v(\mathbf{r})$  and  $\mathbf{A}(\mathbf{r})$  are the corresponding scalar and vector potentials, respectively. (For simplicity of equation writing we assume  $e = \hbar = m = c = 1$ . To obtain the expressions in atomic units, replace  $\mathbf{A}(\mathbf{r})$  by  $\mathbf{A}(\mathbf{r})/c$ .) The Hamiltonian  $\hat{H}$  is then

$$\hat{H} = \hat{T}_A + \hat{U} + \hat{V}, \quad (1)$$

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

$$\hat{T}_A = \frac{1}{2} \sum_{i=1}^N (\hat{\mathbf{p}}_i + A(\mathbf{r}_i))^2 \quad (2)$$

$$= T + \sum_{i=1}^N \hat{\omega}(\mathbf{r}_i; \mathbf{A}(\mathbf{r}_i)), \quad (3)$$

with  $\hat{T}$  the ‘canonical’ kinetic energy operator

$$\hat{T} = \sum_{i=1}^N \frac{p_i^2}{2} = - \sum_{i=1}^N \frac{1}{2} \nabla_i^2, \quad (4)$$

and the operator  $\hat{\omega}(\mathbf{r}; \mathbf{A})$  defined as

$$\hat{\omega}(\mathbf{r}; \mathbf{A}(\mathbf{r})) = \frac{1}{2}A^2(\mathbf{r}) - i\hat{\Omega}(\mathbf{r}; \mathbf{A}) \quad (5)$$

with

$$\hat{\Omega}(\mathbf{r}; \mathbf{A}(\mathbf{r})) = \frac{1}{2}\{\nabla \cdot \mathbf{A}(\mathbf{r}) + 2\mathbf{A}(\mathbf{r}) \cdot \nabla\}. \quad (6)$$

The electron-interaction potential energy operator  $\hat{U}$  is

$$\hat{U} = \sum_{i,j=1}^N u(\mathbf{r}_i \mathbf{r}_j) = \frac{1}{2} \sum_{i,j=1}^N \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}, \quad (7)$$

and the external electrostatic potential energy operator  $\hat{V}$  is

$$\hat{V} = \sum_{i=1}^N v(\mathbf{r}_i). \quad (8)$$

The time-independent Schrödinger equation is

$$\hat{H}(\mathbf{R}; \mathbf{A})\Psi(\mathbf{X}) = E\Psi(\mathbf{X}), \quad (9)$$

where  $\{\Psi(\mathbf{X}), E\}$  are the eigenfunctions and eigenenergies of the system, with  $\mathbf{R} = \mathbf{r}_1, \dots, \mathbf{r}_N$ ;  $\mathbf{X} = \mathbf{x}_1, \dots, \mathbf{x}_N$ ;  $\mathbf{x} = \mathbf{r}\sigma$ ,  $\{\mathbf{r}\sigma\}$  being the spatial and spin coordinates.

The system of interacting electrons can equivalently be described in terms of the ‘quantal Newtonian’ first law [10] according to which the sum of the external  $\mathcal{F}^{\text{ext}}(\mathbf{r})$  and internal  $\mathcal{F}^{\text{int}}(\mathbf{r})$  fields experienced by each electron vanishes. Thus,

$$\mathcal{F}^{\text{ext}}(\mathbf{r}) + \mathcal{F}^{\text{int}}(\mathbf{r}) = 0. \quad (10)$$

This law is valid for arbitrary gauge and derived employing the continuity condition

$$\nabla \cdot \mathbf{j}(\mathbf{r}) = 0. \quad (11)$$

In Appendix A we provide a different derivation of the generalized ‘quantal Newtonian’ first law based on the approach originated by Holas and March [17] for the zero magnetic field case. (In [10] these authors derived the first law via the equation of motion for the single particle density matrix.)

The components of these fields arise from local and nonlocal quantal sources such as the density  $\rho(\mathbf{r})$ , the pair-correlation function  $P(\mathbf{r}\mathbf{r}')$ , the reduced single-particle density matrix  $\gamma(\mathbf{r}\mathbf{r}')$  and the physical current density  $\mathbf{j}(\mathbf{r})$ , which in turn are expectations of Hermitian operators or the complex sum of Hermitian operators taken with respect to the wave function  $\Psi(\mathbf{X})$ . Thus,

$$\rho(\mathbf{r}) = \langle \Psi(\mathbf{X}) | \hat{\rho}(\mathbf{r}) | \Psi(\mathbf{X}) \rangle, \quad (12)$$

$$P(\mathbf{r}\mathbf{r}') = \langle \Psi(\mathbf{X}) | \hat{P}(\mathbf{r}\mathbf{r}') | \Psi(\mathbf{X}) \rangle, \quad (13)$$

$$\gamma(\mathbf{r}\mathbf{r}') = \langle \Psi(\mathbf{X}) | \hat{\gamma}(\mathbf{r}\mathbf{r}') | \Psi(\mathbf{X}) \rangle, \quad (14)$$

$$j(\mathbf{r}) = \langle \Psi(\mathbf{X}) | \hat{\mathbf{j}}(\mathbf{r}) | \Psi(\mathbf{X}) \rangle = \mathbf{j}_p(\mathbf{r}) + \mathbf{j}_d(\mathbf{r}), \quad (15)$$

with  $\mathbf{j}_p(\mathbf{r})$  and  $\mathbf{j}_d(\mathbf{r})$  the paramagnetic and diamagnetic components, and where the density  $\hat{\rho}(\mathbf{r})$ , pair-correlation  $\hat{P}(\mathbf{r}\mathbf{r}')$ , single-particle density matrix  $\hat{\gamma}(\mathbf{r}\mathbf{r}')$ , and current density  $\hat{\mathbf{j}}(\mathbf{r})$  operators are defined as

$$\hat{\rho}(\mathbf{r}) = \sum_{i=1}^N \delta(\mathbf{r}_i - \mathbf{r}), \quad (16)$$

$$\hat{P}(\mathbf{r}\mathbf{r}') = \sum_{i,j=1}^N \delta(\mathbf{r}_i - \mathbf{r}) \delta(\mathbf{r}_j - \mathbf{r}'), \quad (17)$$

$$\hat{\gamma}(\mathbf{r}\mathbf{r}') = \hat{A} + i\hat{B}, \quad (18)$$

$$\hat{A} = \frac{1}{2} \sum_{j=1}^N [\delta(\mathbf{r}_j - \mathbf{r}) T_j(\mathbf{a}) + \delta(\mathbf{r}_j - \mathbf{r}') T_j(-\mathbf{a})], \quad (19)$$

$$\hat{B} = -\frac{i}{2} \sum_{j=1}^N [\delta(\mathbf{r}_j - \mathbf{r}) T_j(\mathbf{a}) - \delta(\mathbf{r}_j - \mathbf{r}') T_j(-\mathbf{a})], \quad (20)$$

$T_j(\mathbf{a})$  is a translation operator such that  $T_j(\mathbf{a})\psi(\dots \mathbf{r}_j, \dots) = \psi(\dots \mathbf{r}_j + \mathbf{a}, \dots)$ , and  $\mathbf{a} = \mathbf{r}' - \mathbf{r}$ , and

$$\hat{\mathbf{j}}(\mathbf{r}) = \hat{\mathbf{j}}_p(\mathbf{r}) + \hat{\mathbf{j}}_d(\mathbf{r}), \quad (21)$$

with the paramagnetic density operator

$$\hat{\mathbf{j}}_p(\mathbf{r}) = \frac{1}{2i} \sum_{k=1}^N [\nabla_{\mathbf{r}_k} \delta(\mathbf{r}_k - \mathbf{r}) + \delta(\mathbf{r}_k - \mathbf{r}) \nabla_{\mathbf{r}_k}] \quad (22)$$

and the diamagnetic current density operator

$$\hat{\mathbf{j}}_d = \hat{\rho}(\mathbf{r}) \mathbf{A}(\mathbf{r}). \quad (23)$$

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

$$\mathcal{F}^{\text{ext}}(\mathbf{r}) = \mathcal{E}(\mathbf{r}) - \mathcal{L}(\mathbf{r}), \quad (24)$$

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

$$\mathcal{L}(\mathbf{r}) = \frac{\mathbf{l}(\mathbf{r})}{\rho(\mathbf{r})}, \quad (25)$$

and where

$$\mathbf{l}(\mathbf{r}) = \mathbf{j}(\mathbf{r}) \times \mathbf{B}(\mathbf{r}), \quad (26)$$

with its components given as

$$l_\alpha(\mathbf{r}) = \sum_{\beta=1}^3 [j_\beta(\mathbf{r}) \nabla_\alpha A_\beta(\mathbf{r}) - j_\beta(\mathbf{r}) \nabla_\beta A_\alpha(\mathbf{r})]. \quad (27)$$

The internal field  $\mathcal{F}^{\text{int}}(\mathbf{r})$  is the sum of the electron-interaction  $\mathcal{E}_{ee}(\mathbf{r})$ , kinetic  $\mathcal{Z}(\mathbf{r})$ , differential density  $\mathcal{D}(\mathbf{r})$ , and internal magnetic  $\mathcal{I}(\mathbf{r})$  fields. These fields are defined in terms of the corresponding ‘forces’  $\mathbf{e}_{ee}(\mathbf{r})$ ,  $\mathbf{z}(\mathbf{r}; \gamma)$ ,  $\mathbf{d}(\mathbf{r})$ ,  $\mathbf{i}(\mathbf{r}; \mathbf{j}\mathbf{A})$ , respectively, as

$$\mathcal{E}_{ee}(\mathbf{r}) = \frac{\mathbf{e}_{ee}(\mathbf{r})}{\rho(\mathbf{r})}; \quad \mathcal{Z}(\mathbf{r}) = \frac{\mathbf{z}(\mathbf{r}; \gamma)}{\rho(\mathbf{r})}; \quad \mathcal{D}(\mathbf{r}) = \frac{\mathbf{d}(\mathbf{r})}{\rho(\mathbf{r})}; \quad \mathcal{I}(\mathbf{r}) = \frac{\mathbf{i}(\mathbf{r}; \mathbf{j}\mathbf{A})}{\rho(\mathbf{r})}. \quad (28)$$

The electron-interaction ‘force’  $\mathbf{e}_{ee}(\mathbf{r})$ , representative of electron correlations due to the Pauli exclusion principle and Coulomb repulsion, is obtained via Coulomb’s law via its quantal source, the pair-correlation function  $P(\mathbf{r}\mathbf{r}')$ :

$$\mathbf{e}_{ee}(\mathbf{r}) = \int \frac{P(\mathbf{r}\mathbf{r}')(\mathbf{r} - \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|^3} d\mathbf{r}'. \quad (29)$$

The kinetic ‘force’  $\mathbf{z}(\mathbf{r}; \gamma)$ , representative of kinetic effects, is obtained from its quantal source, the reduced single-particle density matrix  $\gamma(\mathbf{r}\mathbf{r}')$ . It is defined in terms of its components as

$$z_\alpha(\mathbf{r}; \gamma) = 2 \sum_{\beta=1}^3 \nabla_\beta t_{\alpha\beta}(\mathbf{r}; \gamma), \quad (30)$$

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

$$t_{\alpha\beta}(\mathbf{r}; \gamma) = \frac{1}{4} \left( \frac{\partial^2}{\partial r'_\alpha \partial r''_\beta} + \frac{\partial^2}{\partial r'_\beta \partial r''_\alpha} \right) \gamma(\mathbf{r}'\mathbf{r}'') \Big|_{\mathbf{r}'=\mathbf{r}''=\mathbf{r}}. \quad (31)$$

The differential density ‘force’  $\mathbf{d}(\mathbf{r})$  whose quantal source is the density  $\rho(\mathbf{r})$ , is defined as

$$\mathbf{d}(\mathbf{r}) = -\frac{1}{4} \nabla \nabla^2 \rho(\mathbf{r}). \quad (32)$$

Finally, the contribution of the magnetic field to the internal ‘force’  $\mathbf{i}(\mathbf{r}; \mathbf{j}\mathbf{A})$  for which the quantal source is the physical current density  $\mathbf{j}(\mathbf{r})$  is defined in terms of its components as

$$i_\alpha(\mathbf{r}; \mathbf{j}\mathbf{A}) = \sum_{\beta=1}^3 \nabla_\beta I_{\alpha\beta}(\mathbf{r}; \mathbf{j}\mathbf{A}), \quad (33)$$

with

$$I_{\alpha\beta}(\mathbf{r}; \mathbf{j}\mathbf{A}) = [j_\alpha(\mathbf{r})A_\beta(\mathbf{r}) + j_\beta(\mathbf{r})A_\alpha(\mathbf{r})] - \rho(\mathbf{r})A_\alpha(\mathbf{r})A_\beta(\mathbf{r}). \quad (34)$$

The fields  $\mathcal{L}(\mathbf{r})$ ,  $\mathcal{E}_{ee}(\mathbf{r})$ ,  $\mathcal{D}(\mathbf{r})$ , and the sum  $[\mathcal{Z}(\mathbf{r}) + \mathcal{I}(\mathbf{r})]$  are gauge invariant [10].

The energy  $E$  is then the sum of the kinetic  $T$ , external  $E_{\text{ext}}$ , electron-interaction  $E_{ee}$ , and internal magnetic contribution  $I$  energies:

$$E = E_{\text{ext}} + (T + E_{ee} + I), \quad (35)$$

where in integral virial form in terms of the respective fields

$$T = -\frac{1}{2} \int \rho(\mathbf{r}) \mathbf{r} \cdot \mathcal{Z}(\mathbf{r}) d\mathbf{r} \quad (36)$$

$$E_{\text{ext}} = \int \rho(\mathbf{r}) \mathbf{r} \cdot \mathcal{F}^{\text{ext}}(\mathbf{r}) d\mathbf{r} \quad (37)$$

$$E_{ee} = \int \rho(\mathbf{r}) \mathbf{r} \cdot \mathcal{E}_{ee}(\mathbf{r}) d\mathbf{r} \quad (38)$$

$$I = \int \rho(\mathbf{r}) \mathbf{r} \cdot \mathcal{I}(\mathbf{r}) d\mathbf{r}. \quad (39)$$

By operating on the first law by  $\int d\mathbf{r} \rho(\mathbf{r}) \mathbf{r} \cdot$  one obtains the integral virial theorem [7]:

$$2T + E_{ee} - I = -E_{\text{ext}}. \quad (40)$$

## B. Model System of Noninteracting Fermions

We next assume that there exists a model system of *noninteracting* fermions – an  $S$  system – that possesses the same ground state density  $\rho(\mathbf{r})$  and physical current density  $\mathbf{j}(\mathbf{r})$  as that of the interacting system of electrons described above. In constructing the  $S$  system one needs to then determine an effective scalar potential  $v_s(\mathbf{r})$  and an effective vector potential  $\mathbf{A}_s(\mathbf{r})$  such that on substitution into the corresponding Schrödinger equation, the resulting Slater determinantal wave function will reproduce the  $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$ . In essence, one thus assumes there exists an effective magnetic field  $\mathbf{B}_s(\mathbf{r}) = \nabla \times \mathbf{A}_s(\mathbf{r})$ .

The  $S$  system Hamiltonian is

$$\hat{H}_s = \hat{T}_{A,s} + \hat{V}_s = \sum_{i=1}^N h_s(\mathbf{r}_i), \quad (41)$$

where

$$\hat{T}_{A,s} = \frac{1}{2} \sum_{i=1}^N (\hat{\mathbf{p}}_i + \mathbf{A}_s(\mathbf{r}_i))^2, \quad (42)$$

$$\hat{V}_s = \sum_{i=1}^N v_s(\mathbf{r}_i), \quad (43)$$

so that

$$h_s(\mathbf{r}) = \frac{1}{2} (\hat{\mathbf{p}} + \mathbf{A}_s(\mathbf{r}))^2 + v_s(\mathbf{r}). \quad (44)$$

The  $S$  system orbital equation is

$$\left[ \frac{1}{2} (\hat{\mathbf{p}}_i + \mathbf{A}_s(\mathbf{r}))^2 + v_s(\mathbf{r}) \right] \phi_i(\mathbf{x}) = \epsilon_i \phi_i(\mathbf{x}), \quad (45)$$

and its wave function is a Slater determinant  $\Phi\{\phi_i\}$  of the orbitals  $\phi_i(\mathbf{x})$  occupying the lowest states if the  $S$  system is in its ground state. Assuming the model fermions are subject to the same external electrostatic field  $\mathcal{E}(\mathbf{r}) = -\nabla v(\mathbf{r})$ , we write

$$v_s(\mathbf{r}) = v(\mathbf{r}) + v_{ee}(\mathbf{r}), \quad (46)$$

where  $v_{ee}(\mathbf{r})$  is an effective scalar electron-interaction potential energy whose rigorous physical interpretation will be given below. The  $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$  as obtained from the  $S$  system are the expectations

$$\rho(\mathbf{r}) = \langle \Phi\{\phi_i\} | \hat{\rho}(\mathbf{r}) | \Phi\{\phi_i\} \rangle = \sum_{\sigma} \sum_{i=1}^N \phi_i^*(\mathbf{r}\sigma) \phi_i^*(\mathbf{r}\sigma), \quad (47)$$

and

$$\mathbf{j}(\mathbf{r}) = \langle \Phi\{\phi_i\} | \hat{\mathbf{j}}_s(\mathbf{r}) | \Phi\{\phi_i\} \rangle = \mathbf{j}_{p,s}(\mathbf{r}) + \mathbf{j}_{d,s}(\mathbf{r}), \quad (48)$$

with  $\mathbf{j}_{p,s}(\mathbf{r}), \mathbf{j}_{d,s}(\mathbf{r})$  the  $S$  system paramagnetic and diamagnetic current density components, and where the operator  $\hat{\mathbf{j}}_s(\mathbf{r})$  is defined as

$$\hat{\mathbf{j}}_s(\mathbf{r}) = \hat{\mathbf{j}}_p(\mathbf{r}) + \hat{\mathbf{j}}_{d,s}(\mathbf{r}), \quad (49)$$

with

$$\hat{\mathbf{j}}_{d,s}(\mathbf{r}) = \hat{\rho}(\mathbf{r}) \mathbf{A}_s(\mathbf{r}). \quad (50)$$

The ‘quantal Newtonian’ first law for the  $S$  system derived employing the continuity condition of Eq. (11) is

$$\mathcal{F}_s^{\text{ext}}(\mathbf{r}) + \mathcal{F}_s^{\text{int}}(\mathbf{r}) = 0, \quad (51)$$

where

$$\mathcal{F}_s^{\text{ext}}(\mathbf{r}) = \mathcal{E}(\mathbf{r}) - \mathcal{L}_s(\mathbf{r}). \quad (52)$$

Here  $\mathcal{L}_s(\mathbf{r})$  is the corresponding effective Lorentz field defined in terms of the Lorentz ‘force’ as

$$\mathcal{L}_s(\mathbf{r}) = \frac{\mathbf{l}_s(\mathbf{r})}{\rho(\mathbf{r})}, \quad (53)$$

with

$$\mathbf{l}_s(\mathbf{r}) = \mathbf{j}(\mathbf{r}) \times \mathbf{B}_s(\mathbf{r}), \quad (54)$$

and where the components of the ‘force’ are

$$l_{s,\alpha}(\mathbf{r}) = \sum_{\beta=1}^3 \left[ j_{\beta}(\mathbf{r}) \nabla_{\alpha} A_{s,\beta}(\mathbf{r}) - j_{\beta}(\mathbf{r}) \nabla_{\beta} A_{s,\alpha}(\mathbf{r}) \right]. \quad (55)$$

The internal field  $\mathcal{F}_s^{\text{int}}(\mathbf{r})$  of the  $S$  system is

$$\mathcal{F}_s^{\text{int}}(\mathbf{r}) = -\nabla v_{ee}(\mathbf{r}) - \mathcal{D}(\mathbf{r}) - \mathcal{Z}_s(\mathbf{r}) - \mathcal{I}_s(\mathbf{r}), \quad (56)$$

where the kinetic  $\mathcal{Z}_s(\mathbf{r})$  and internal magnetic  $\mathcal{I}_s(\mathbf{r})$  fields are defined in terms of the ‘forces’  $\mathbf{z}_s(\mathbf{r}; \gamma_s)$  and  $\mathbf{i}_s(\mathbf{r}; \mathbf{j}\mathbf{A}_s)$  as

$$\mathcal{Z}_s(\mathbf{r}) = \frac{\mathbf{z}(\mathbf{r}; \gamma_s)}{\rho(\mathbf{r})} \quad \text{and} \quad \mathcal{I}_s(\mathbf{r}) = \frac{\mathbf{i}_s(\mathbf{r}; \mathbf{j}\mathbf{A}_s)}{\rho(\mathbf{r})}. \quad (57)$$

The  $S$  system kinetic ‘force’ in turn is defined in terms of its quantal source, the Dirac density matrix  $\gamma_s(\mathbf{r}\mathbf{r}')$  as

$$z_{s,\alpha}(\mathbf{r}; \gamma_s) = 2 \sum_{\beta=1}^3 \nabla_{\beta} t_{s,\alpha\beta}(\mathbf{r}; \gamma_s) \quad (58)$$

where the kinetic energy tensor  $t_{s,\alpha\beta}(\mathbf{r}; \gamma_s)$  is

$$t_{s,\alpha\beta}(\mathbf{r}; \gamma_s) = \frac{1}{4} \left[ \frac{\partial^2}{\partial r'_{\alpha} \partial r''_{\beta}} + \frac{\partial^2}{\partial r'_{\beta} \partial r''_{\alpha}} \right] \gamma_s(\mathbf{r}'\mathbf{r}'') \Big|_{\mathbf{r}'=\mathbf{r}''=\mathbf{r}}, \quad (59)$$

and the source

$$\gamma_s(\mathbf{r}\mathbf{r}') = \langle \Phi\{\phi_i\} | \hat{\gamma}(\mathbf{r}\mathbf{r}') | \Phi\{\phi_i\} \rangle = \sum_{\sigma} \sum_{i=1}^N \phi_i^*(\mathbf{r}\sigma) \phi_i^*(\mathbf{r}'\sigma). \quad (60)$$

The internal magnetic ‘force’  $\mathbf{i}_s(\mathbf{r}; \mathbf{j}\mathbf{A}_s)$  is defined as

$$i_{s,\alpha}(\mathbf{r}; \mathbf{j}\mathbf{A}_s) = \sum_{\beta} \nabla_{\beta} I_{s,\alpha\beta}(\mathbf{r}; \mathbf{j}\mathbf{A}_s), \quad (61)$$

with

$$I_{s,\alpha\beta}(\mathbf{r}; \mathbf{j}\mathbf{A}_s) = \left[ j_{\alpha}(\mathbf{r}) A_{s,\beta}(\mathbf{r}) + j_{\beta}(\mathbf{r}) A_{s,\alpha}(\mathbf{r}) \right] - \rho(\mathbf{r}) A_{s,\alpha}(\mathbf{r}) A_{s,\beta}(\mathbf{r}). \quad (62)$$

The effective scalar and vector potentials  $\{v_s(\mathbf{r}), \mathbf{A}_s(\mathbf{r})\}$  of the  $S$  system differential equation Eq. (45) are determined as follows:

(a) The effective vector potential  $\mathbf{A}_s(\mathbf{r})$  is obtained from the requirement that the physical current density  $\mathbf{j}(\mathbf{r})$  of the  $S$  system Eq. (48) is the same as that of the interacting system Eq. (15).

(b) The effective scalar potential  $v_s(\mathbf{r})$  and the effective electron-interaction potential  $v_{ee}(\mathbf{r})$  are determined as explained next. As the external electrostatic field  $\mathcal{E}(\mathbf{r})$  is the same for the interacting and model systems, we equate the corresponding expressions for this field given by the ‘quantal Newtonian’ first law for each system. Thus, we obtain *the effective electron-interaction potential energy  $v_{ee}(\mathbf{r})$  to be the work done to move a model fermion from some reference point at infinity to its position at  $\mathbf{r}$  in the force of a conservative effective field  $\mathcal{F}^{\text{eff}}(\mathbf{r})$ :*

$$v_{ee}(\mathbf{r}) = - \int_{\infty}^{\mathbf{r}} \mathcal{F}^{\text{eff}}(\mathbf{r}) \cdot d\ell', \quad (63)$$

where  $\mathcal{F}^{\text{eff}}(\mathbf{r})$  is the sum of the electron-interaction  $\mathcal{E}_{ee}(\mathbf{r})$ , correlation-kinetic  $\mathcal{Z}_{tc}(\mathbf{r})$ , and correlation-magnetic  $\mathcal{M}_c(\mathbf{r})$  fields:

$$\mathcal{F}^{\text{eff}}(\mathbf{r}) = \mathcal{E}_{ee}(\mathbf{r}) + \mathcal{Z}_{tc}(\mathbf{r}) + \mathcal{M}_c(\mathbf{r}), \quad (64)$$

and where

$$\mathcal{Z}_{tc}(\mathbf{r}) = \mathcal{Z}_s(\mathbf{r}) - \mathcal{Z}(\mathbf{r}), \quad (65)$$

$$\mathcal{M}_c(\mathbf{r}) = \mathcal{L}_s(\mathbf{r}) - \mathcal{L}(\mathbf{r}) + \mathcal{I}_s(\mathbf{r}) - \mathcal{I}(\mathbf{r}). \quad (66)$$

As in the  $\mathbf{B} = 0$  case [1, 2], the field  $\mathcal{E}_{ee}(\mathbf{r})$  may be subdivided into its Hartree  $\mathcal{E}_H(\mathbf{r})$ , Pauli  $\mathcal{E}_x(\mathbf{r})$ , and Coulomb  $\mathcal{E}_c(\mathbf{r})$  field components. The quantal sources for these fields are the density  $\rho(\mathbf{r})$ , the Fermi hole  $\rho_x(\mathbf{r}\mathbf{r}')$ , and the Coulomb hole  $\rho_c(\mathbf{r}\mathbf{r}')$ , respectively. Thus, the effective field may be expressed as

$$\mathcal{F}^{\text{eff}}(\mathbf{r}) = \mathcal{E}_H(\mathbf{r}) + \mathcal{E}_x(\mathbf{r}) + \mathcal{E}_c(\mathbf{r}) + \mathcal{Z}_{tc}(\mathbf{r}) + \mathcal{M}_c(\mathbf{r}), \quad (67)$$



with each field being representative of a specific electron correlation. Note that  $\nabla \times \mathcal{F}^{\text{eff}}(\mathbf{r}) = 0$  so that the work done  $v_{ee}(\mathbf{r})$  is *path-independent*. The individual components of  $\mathcal{F}^{\text{eff}}(\mathbf{r})$  are separately curl free for systems with certain symmetry, as in the example of the following section which is one of cylindrical symmetry. The work done in each field is then path-independent.

Writing the effective vector potential  $A_s(\mathbf{r})$  as

$$\mathbf{A}_s(\mathbf{r}) = \mathbf{A}(\mathbf{r}) + \mathbf{A}_{ee}(\mathbf{r}), \quad (68)$$

where  $\mathbf{A}_{ee}(\mathbf{r})$  is an effective electron-interaction vector potential, the expression for the ground state energy in terms of  $S$  system properties is

$$E = \sum_i \epsilon_i - \int \rho(\mathbf{r}) v_{ee}(\mathbf{r}) d\mathbf{r} - \int \mathbf{j}(\mathbf{r}) \cdot \mathbf{A}_{ee}(\mathbf{r}) d\mathbf{r} + E_{ee} + T_c, \quad (69)$$

where the correlation-kinetic energy  $T_c$  is

$$T_c = \frac{1}{2} \int \rho(\mathbf{r}) \mathbf{r} \cdot \mathcal{Z}_{t_c}(\mathbf{r}) d\mathbf{r}. \quad (70)$$

On applying  $\int d\mathbf{r} \rho(\mathbf{r}) \mathbf{r} \cdot \nabla$  to Eq. (63) one obtains the corresponding integral virial theorem for the  $S$  system:

$$E_{ee} + 2T_c + M_c = \int \rho(\mathbf{r}) \mathbf{r} \cdot \mathcal{F}^{\text{eff}}(\mathbf{r}) d\mathbf{r}, \quad (71)$$

where

$$M_c = \int \rho(\mathbf{r}) \mathbf{r} \cdot \mathcal{M}_c(\mathbf{r}) d\mathbf{r}, \quad (72)$$

The ‘quantal Newtonian’ first law is of course valid for both ground and excited states. Hence, the mapping via QDFT is applicable to ground and excited states. Furthermore, as in the  $\mathbf{B} = 0$  case [1, 2], the mapping to the  $S$  system is arbitrary in that the model fermions may be in a ground or excited state.

### III. APPLICATION TO AN EXACTLY SOLVABLE MODEL

For the application of QDFT we consider the Hooke’s atom [3] comprised of two electrons in a harmonic external potential of frequency  $\omega_0$  in which the electrons are confined to the  $x-y$  plane by a magnetic field  $\mathbf{B}$  applied in the  $z$ -direction. With the vector potential chosen such that  $\mathbf{A} = \frac{1}{2}\mathbf{B} \times \mathbf{r}$ , the Coulomb gauge  $\nabla \cdot \mathbf{A} = 0$  is satisfied. The Hamiltonian for this system (in a.u. with  $e = \hbar = m = 1$ ) is

$$\hat{H} = \sum_{i=1}^2 \left\{ \frac{1}{2} \left( \hat{\mathbf{p}}_i + \frac{1}{c} \mathbf{A}(\mathbf{r}_i) \right)^2 + \frac{1}{2} \omega_0^2 r_i^2 \right\} + \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}. \quad (73)$$

There exist analytical solutions to the corresponding Schrödinger equation for effective oscillator frequencies  $\tilde{\omega} = \sqrt{\omega_0^2 + \omega_L^2}$  belonging to certain denumerably infinite set of values, where  $\omega_L = B/2c$  is the Larmor frequency. For  $\tilde{\omega} = 1$ , the ground state wave function is

$$\Psi(\mathbf{r}_1 \mathbf{r}_2) = C(1 + r_{12}) e^{-\frac{1}{2}(r_1^2 + r_2^2)}, \quad (74)$$

where  $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$  and  $C^2 = 1/\pi^2(3 + 2\pi)$ . The corresponding ground state energy is  $E = 3$  a.u.

For the wave function of Eq. (74), many properties of the QDFT mapping to the model fermion system are obtained in closed analytical or semi-analytical form. These expressions and their asymptotic behavior near and at the nucleus and in the classically forbidden region are given in Appendix B. We next discuss the individual properties.

#### A. Quantal Sources

##### 1. Electron Density $\rho(\mathbf{r})$ and Physical Current Density $\mathbf{j}(\mathbf{r})$

The ground state electron density  $\rho(\mathbf{r})$  is

$$\rho(\mathbf{r}) = \frac{2}{\pi(3 + \sqrt{2\pi})} e^{-r^2} \left\{ \sqrt{\pi} e^{-\frac{1}{2}r^2} \left[ (1 + r^2) I_0\left(\frac{1}{2}r^2\right) + r^2 I_1\left(\frac{1}{2}r^2\right) \right] + (2 + r^2) \right\}, \quad (75)$$

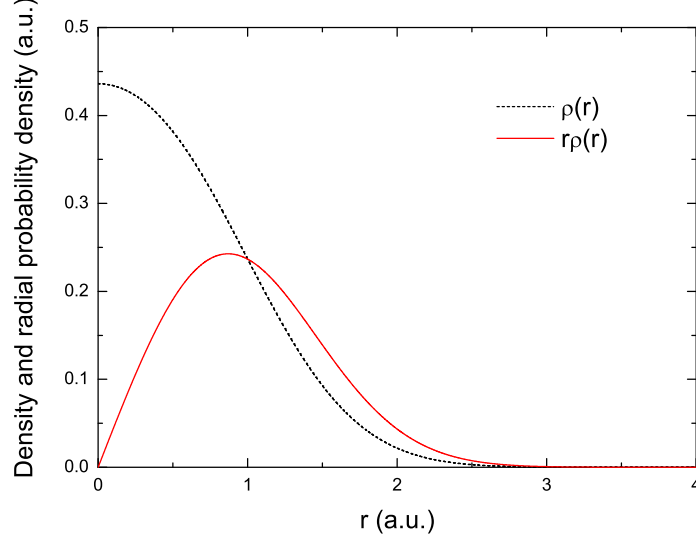


FIG. 1: (Color Online) Electron density  $\rho(r)$  and radial probability density  $r\rho(r)$ .

where  $I_0(x)$  and  $I_1(x)$  are the zeroth- and first-order modified Bessel functions [18]. (Note that the expression given in [19] is incorrect.) The density has cylindrical symmetry:  $\rho(\mathbf{r}) = \rho(r)$ . The density  $\rho(r)$  and the radial probability density  $r\rho(r)$  are plotted in Fig 1. As expected for this harmonic external potential, the density does not exhibit a cusp at the nucleus. The asymptotic structure of the density near the nucleus and in the classically forbidden region are given in Appendix B. As the wave function is real, the paramagnetic current density  $\mathbf{j}_p(\mathbf{r}) = 0$ . Thus, the physical current density

$$\mathbf{j}(\mathbf{r}) = \frac{1}{c}\rho(\mathbf{r})\mathbf{A}(\mathbf{r}), \quad (76)$$

and satisfies the continuity condition  $\nabla \cdot \mathbf{j}(\mathbf{r}) = 0$ .

For the mapping of the above interacting system in its ground state to an  $S$  system also in its ground state, the corresponding  $S$  system orbitals  $\phi_i(\mathbf{x})$  are of the general form

$$\phi_i(\mathbf{r}) = \sqrt{\frac{\rho(\mathbf{r})}{2}} e^{i\theta(\mathbf{r})} \quad ; \quad i = 1, 2 \quad (77)$$

where  $\theta(\mathbf{r})$  is an arbitrary real phase factor. The  $S$  system paramagnetic current density  $\mathbf{j}_{p,s}(\mathbf{r})$  is then

$$\mathbf{j}_{p,s}(\mathbf{r}) = -\rho(\mathbf{r})\nabla\theta(\mathbf{r}). \quad (78)$$

The phase factor  $\theta(\mathbf{r})$  may be incorporated into a gauge transformation so that for the resulting  $S$  system the effective vector and scalar potentials are  $\mathbf{A}'_s(\mathbf{r}) = \mathbf{A}_s(\mathbf{r}) + \nabla\theta(\mathbf{r})$  and  $v'_s(\mathbf{r}) = v_s(\mathbf{r})$  with the orbitals being  $\phi_i(\mathbf{r}) = \sqrt{\rho(\mathbf{r})/2}$ . Thus, for different gauge functions, the corresponding  $S$  systems differ only by a gauge transformation. We emphasize, however, that the mapping from the ground state of the interacting system to the model system in its ground state is *unique*. The unique  $S$  system reproduces the density and physical current density of the interacting system.

As the phase factor is arbitrary, for convenience we set  $\theta(\mathbf{r}) = 0$ , so that  $\mathbf{j}_{p,s}(\mathbf{r}) = 0$ . The requirement that the  $S$  system produce the same physical current density  $\mathbf{j}(\mathbf{r})$  then leads to the effective vector potential  $\mathbf{A}_s(\mathbf{r})$  to be

$$\mathbf{A}_s(\mathbf{r}) = \mathbf{A}(\mathbf{r}). \quad (79)$$

The  $S$  system differential equation is then

$$\left[ \frac{1}{2}\hat{p}^2 + \frac{1}{2}\tilde{\omega}^2 r^2 + v_{ee}(\mathbf{r}) \right] \sqrt{\rho(\mathbf{r})} = \epsilon \sqrt{\rho(\mathbf{r})}. \quad (80)$$

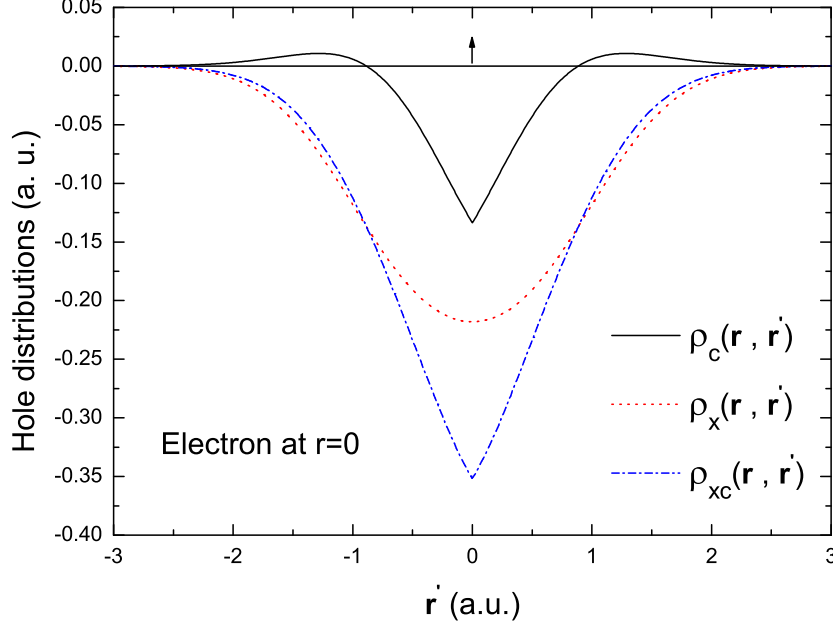


FIG. 2: (Color Online) Cross-sections through the quantal Fermi-Coulomb  $\rho_{xc}(\mathbf{r}\mathbf{r}')$ , Fermi  $\rho_x(\mathbf{r}\mathbf{r}')$ , and Coulomb  $\rho_c(\mathbf{r}\mathbf{r}')$  holes for an electron at the nucleus as indicated by the arrow.

Note that as a consequence of Eq. (79), the contribution of the correlation-magnetic field  $\mathcal{M}_c(\mathbf{r})$  to the potential energy  $v_{ee}(\mathbf{r})$  vanishes, as does the contribution of  $\mathbf{A}_{ee}(\mathbf{r})$  to the total energy  $E$ . Thus, it is only the electron-interaction  $\mathcal{E}_{ee}(\mathbf{r})$  and correlation-kinetic  $\mathcal{Z}_{tc}(\mathbf{r})$  fields that contribute to  $v_{ee}(\mathbf{r})$  and  $E$ .

## 2. Pair-correlation density $g(\mathbf{r}\mathbf{r}')$ , Fermi $\rho_x(\mathbf{r}\mathbf{r}')$ and Coulomb $\rho_c(\mathbf{r}\mathbf{r}')$ holes

It is best to study the electron-interaction properties due to the Pauli exclusion principle and Coulomb repulsion via the pair-correlation density  $g(\mathbf{r}\mathbf{r}')$  which is defined in terms of the quantal source  $P(\mathbf{r}\mathbf{r}')$  as  $g(\mathbf{r}\mathbf{r}') = P(\mathbf{r}\mathbf{r}')/\rho(\mathbf{r})$ . The pair-density may be separated into its local and non-local components as  $g(\mathbf{r}\mathbf{r}') = \rho(\mathbf{r}') + \rho_{xc}(\mathbf{r}\mathbf{r}')$ , where  $\rho_{xc}(\mathbf{r}\mathbf{r}')$  is the Fermi-Coulomb hole charge distribution. In turn  $\rho_{xc}(\mathbf{r}\mathbf{r}')$  may be further subdivided into its Fermi  $\rho_x(\mathbf{r}\mathbf{r}')$  and Coulomb  $\rho_c(\mathbf{r}\mathbf{r}')$  hole charge components. The Fermi hole is defined in terms of the  $S$  system Dirac density matrix as  $\rho_x(\mathbf{r}\mathbf{r}') = -|\gamma_s(\mathbf{r}\mathbf{r}')|^2/2\rho(\mathbf{r})$ . These charge distributions satisfy the sum rules:  $\int g(\mathbf{r}\mathbf{r}')d\mathbf{r}' = N-1$ ;  $\int \rho_{xc}(\mathbf{r}\mathbf{r}')d\mathbf{r}' = -1$ ;  $\int \rho_x(\mathbf{r}\mathbf{r}')d\mathbf{r}' = -1$ ;  $\rho_x(\mathbf{r}\mathbf{r}') \leq 0$ ;  $\rho_x(\mathbf{r}\mathbf{r}') = -\rho(\mathbf{r})/2$ ;  $\int \rho_c(\mathbf{r}\mathbf{r}')d\mathbf{r}' = 0$ .

For the ground state then  $\rho_x(\mathbf{r}\mathbf{r}') = -\rho(\mathbf{r}')/2$  independent of the electron position  $\mathbf{r}$ , so that the non-local nature of the pair-correlation density is exhibited by the dynamic Coulomb hole  $\rho_c(\mathbf{r}\mathbf{r}')$ . In Fig 2 cross-sections of the Fermi-Coulomb  $\rho_{xc}(\mathbf{r}\mathbf{r}')$ , Fermi  $\rho_x(\mathbf{r}\mathbf{r}')$ , and Coulomb  $\rho_c(\mathbf{r}\mathbf{r}')$  holes are plotted for an electron at the nucleus. Observe that for this electron position, all the holes are spherically symmetric about it. Also observe that both the Fermi-Coulomb and Coulomb holes exhibit a cusp at the electron position representative of the two-dimensional electron-electron coalescence condition on the wave function [2, 20].

In Figs 3-6 cross-sections through the Coulomb hole  $\rho_c(\mathbf{r}\mathbf{r}')$  in different directions corresponding to  $\theta' = 0^\circ, 45^\circ, 90^\circ$  with respect to the nucleus-electron direction are plotted. The electron positions considered, as indicated by arrows, are  $\mathbf{r} = 0.5, 1.585, 3.0$ , and  $18.0$  a.u. Observe the dynamic structure of the Coulomb hole and the fact that it is not symmetric about the electron. For asymptotic electron positions (Fig. 6), the Coulomb hole becomes more and more spherically symmetric about the nucleus. The cusp [2, 20] in the hole at the electron position is also clearly evident in Fig 3. The Coulomb hole also becomes an essentially static charge distribution for far asymptotic positions of the electron.

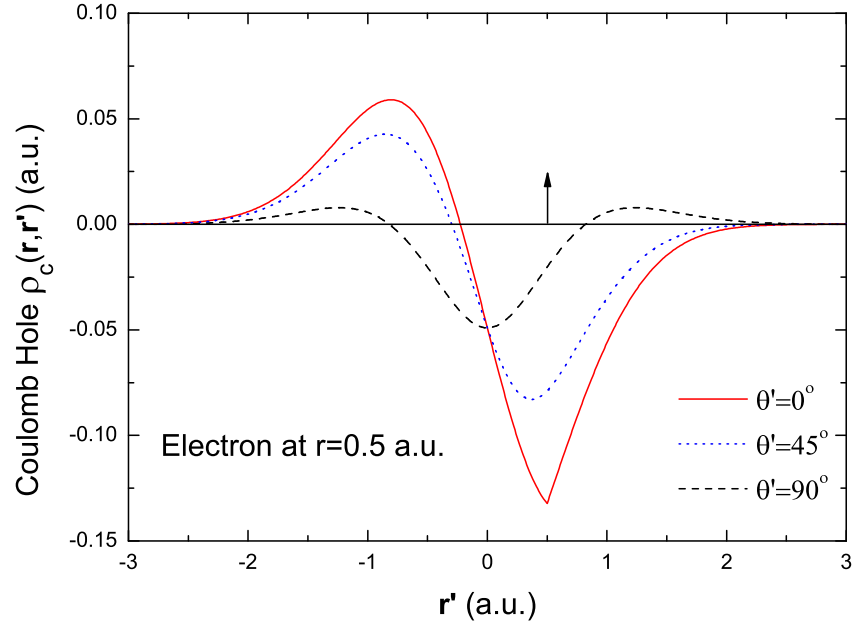


FIG. 3: (Color Online) Cross-sections through the Coulomb hole  $\rho_c(\mathbf{r}, \mathbf{r}')$  in different directions corresponding to  $\theta' = 0^\circ, 45^\circ, 90^\circ$  with respect to the nucleus-electron direction. The electron is at  $r = 0.5$  a.u.

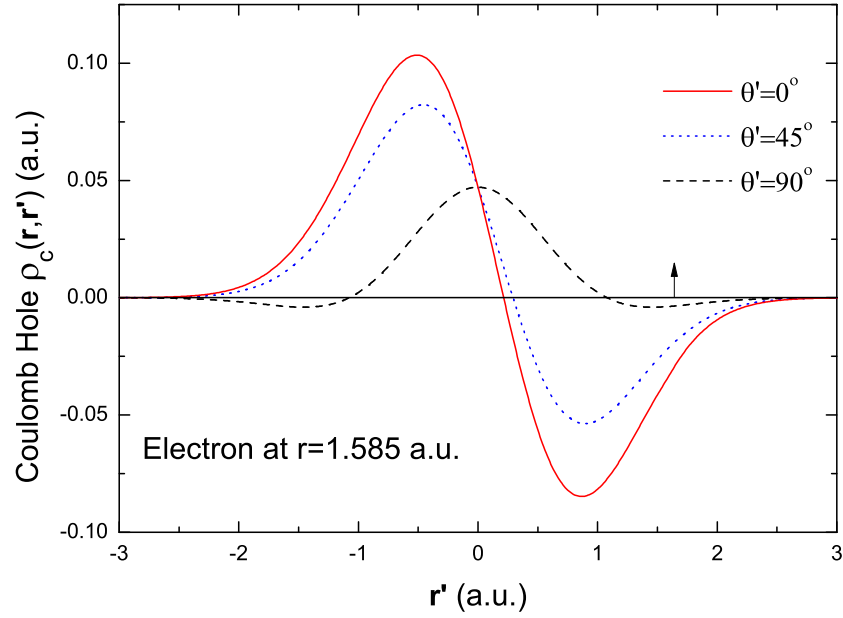


FIG. 4: (Color Online) Same as in Fig. 3 except that the electron is at  $r = 1.585$  a.u.

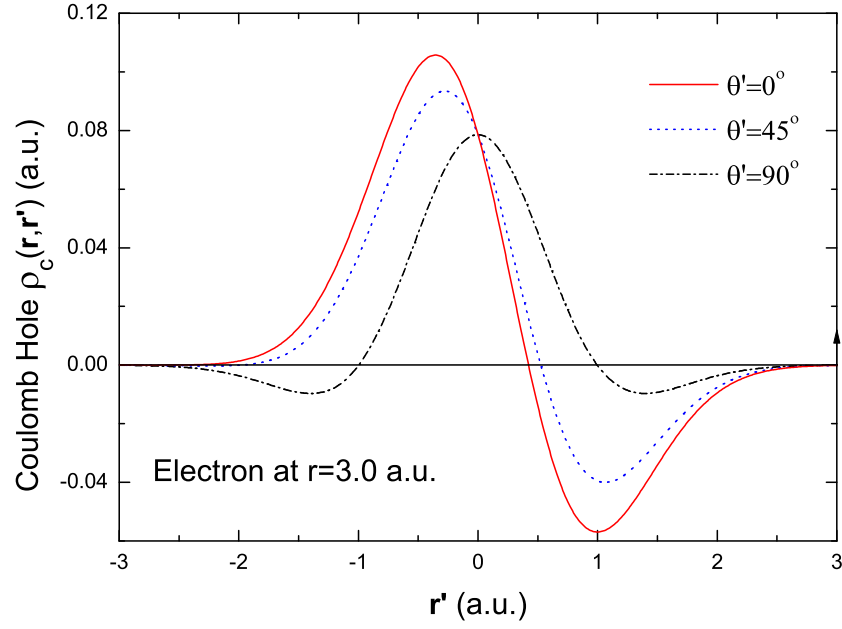


FIG. 5: (Color Online) Same as in Fig. 3 except that the electron is at  $r = 3$  a.u.

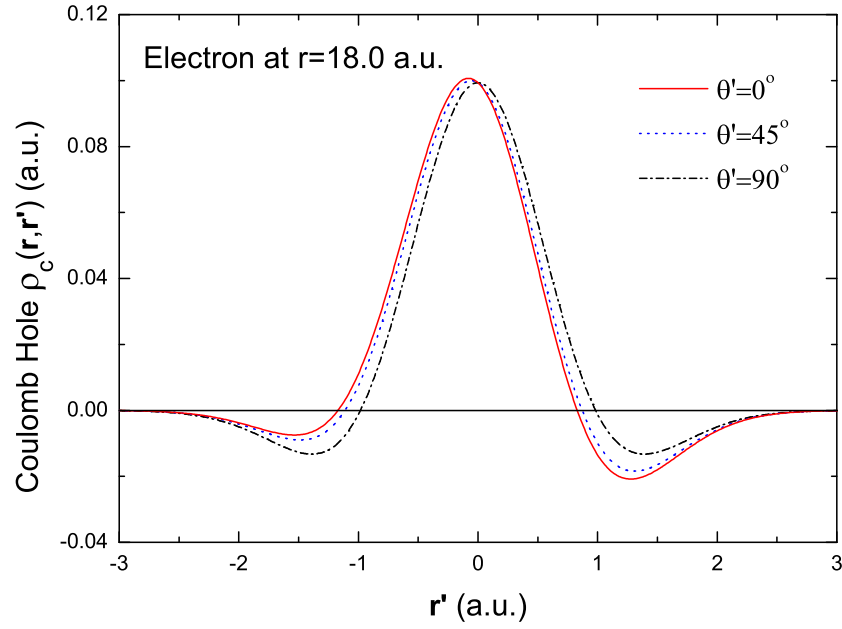


FIG. 6: (Color Online) Same as in Fig. 3 except that the electron is at  $r = 18$  a.u.

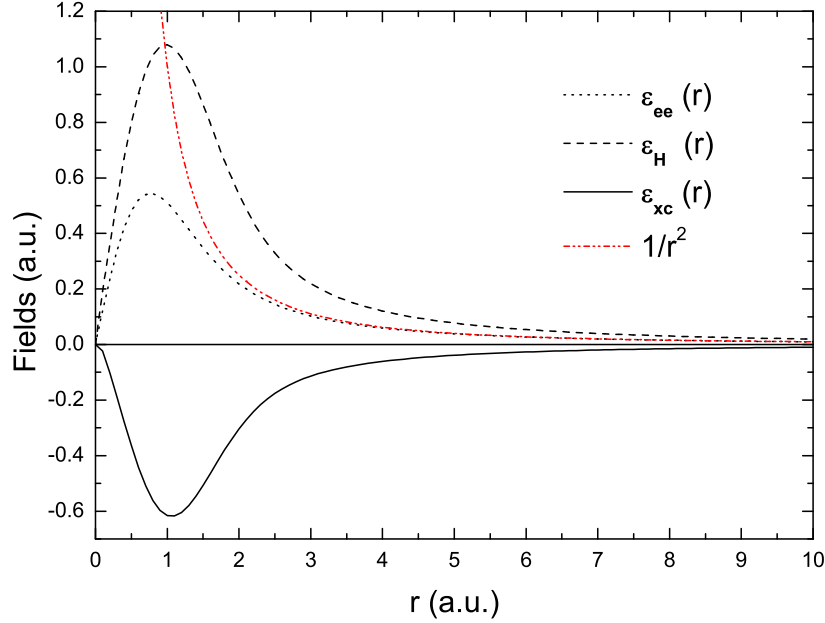


FIG. 7: (Color Online) The electron-interaction  $\mathcal{E}_{ee}(r)$ , and its Hartree  $\mathcal{E}_H(r)$  and Pauli-Coulomb  $\mathcal{E}_{xc}(r)$  components. The function  $1/r^2$  is also plotted.

### 3. Single-particle $\gamma(\mathbf{r}\mathbf{r}')$ and Dirac $\gamma_s(\mathbf{r}\mathbf{r}')$ Density Matrices

The expressions for the reduced single-particle  $\gamma(\mathbf{r}\mathbf{r}')$  and Dirac  $\gamma_s(\mathbf{r}\mathbf{r}')$  density matrices are given in Appendix B.

## B. Fields and Energies

### 1. Electron-interaction field $\mathcal{E}_{ee}(\mathbf{r})$ and Energy $E_{ee}$

The analytical expression for the electron-interaction field  $\mathcal{E}_{ee}(\mathbf{r})$  and the corresponding value of the energy  $E_{ee}$  are given in Appendix B (see also Table 1). The field  $\mathcal{E}_{ee}(\mathbf{r})$  and energy  $E_{ee}$  can be split into their Hartree  $[\mathcal{E}_H(\mathbf{r}), E_H]$ , Pauli-Coulomb  $[\mathcal{E}_{xc}(\mathbf{r}), E_{xc}]$ , Pauli  $[\mathcal{E}_x(\mathbf{r}), E_x]$ , and Coulomb  $[\mathcal{E}_c(\mathbf{r}), E_c]$  components. As the respective quantal sources for the fields are all spherically symmetric about the electron position at the nucleus, all the fields vanish at the origin. The asymptotic structure of the fields in the classically forbidden region is

$$\begin{aligned} \mathcal{E}_{ee}(r) &\underset{r \rightarrow \infty}{\sim} \frac{1}{r^2} + \frac{2}{r^3}, \quad \mathcal{E}_H(r) \underset{r \rightarrow \infty}{\sim} \frac{2}{r^2} + \frac{5}{r^3}, \quad \mathcal{E}_{xc}(r) \underset{r \rightarrow \infty}{\sim} -\frac{1}{r^2} - \frac{3}{r^3} \\ \mathcal{E}_x(r) &\underset{r \rightarrow \infty}{\sim} -\frac{1}{r^2} - \frac{5}{2r^3}, \quad \mathcal{E}_c(r) \underset{r \rightarrow \infty}{\sim} -\frac{1}{2r^3}. \end{aligned} \quad (81)$$

The asymptotic structure is a consequence of the quantal source charge sum rules and the fact that these dynamic charge distributions become static for asymptotic positions of the electron. The asymptotic structure of  $\mathcal{E}_{ee}(r)$  near the nucleus is

$$\mathcal{E}_{ee}(r) \underset{r \rightarrow \infty}{\sim} \frac{1}{2(2 + \sqrt{\pi})} \left[ (4 + 3\sqrt{\pi})r - \frac{1}{4}(13\sqrt{\pi} + 16)r^3 \right]. \quad (82)$$

The fields are plotted in Figs 7-9. The corresponding energies obtained from these fields are quoted in Table 1. It is interesting to note that in contrast to the Hooke's atom in the absence of a magnetic field [1, 15] for which

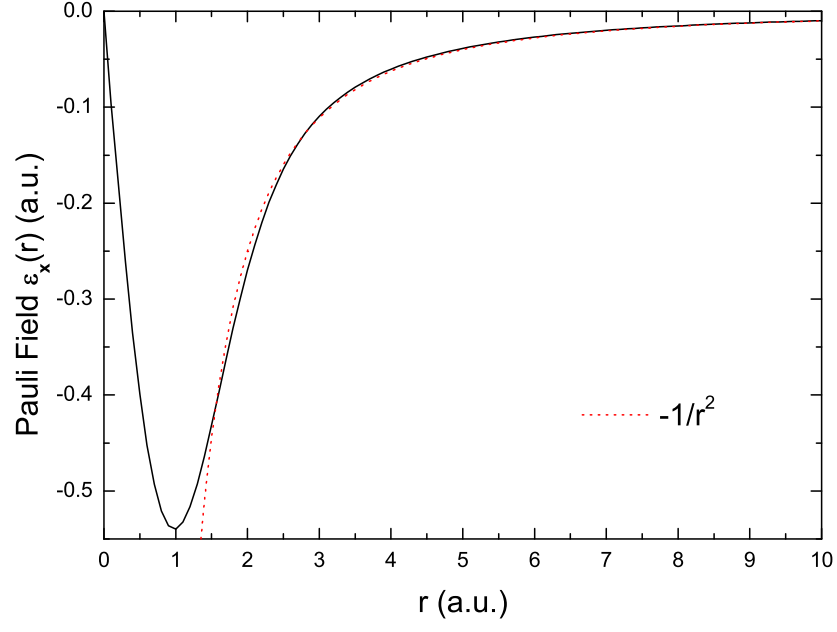


FIG. 8: (Color Online) The Pauli field  $\mathcal{E}_x(r)$ . The function  $-1/r^2$  is also plotted.

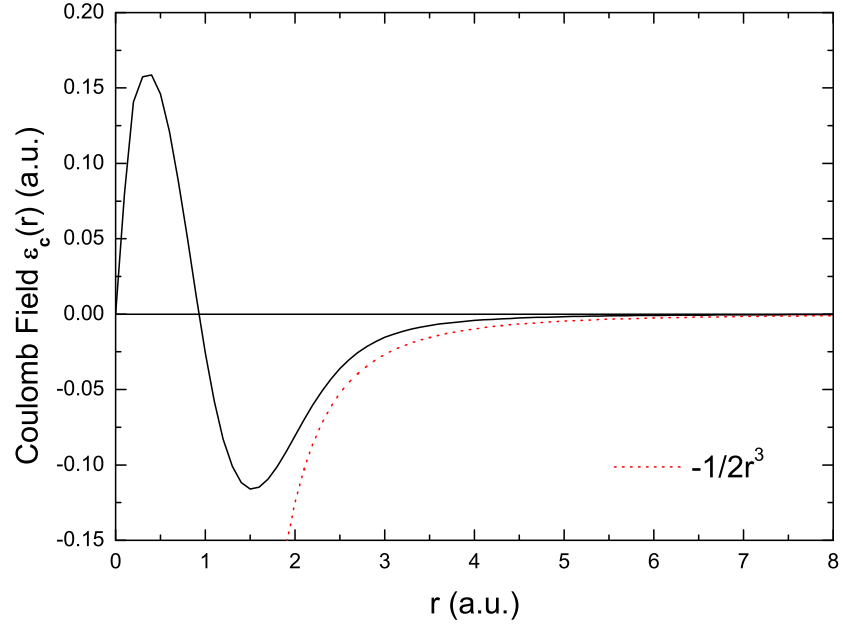


FIG. 9: (Color Online) The Coulomb field  $\mathcal{E}_c(r)$ . The function  $-1/2r^3$  is also plotted.

TABLE I: Quantal density functional theory properties of the ground state  $S$  system that reproduces the density, physical current density, and total energy of the Hooke's atom in a magnetic field in a ground state with effective oscillator frequency  $\tilde{\omega} = 1$ .

| Property   | Value (a.u.) |
|------------|--------------|
| $E$        | 3.000 000    |
| $E_{ee}$   | 0.818 401    |
| $E_H$      | 1.789 832    |
| $E_{xc}$   | -0.971 431   |
| $E_x$      | -0.894 916   |
| $E_c$      | -0.076 515   |
| $E_{ext}$  | 1.295 400    |
| $T_s$      | 0.780 987    |
| $T_c$      | 0.105 212    |
| $\epsilon$ | 2.000 000    |

the Coulomb field is an order of magnitude smaller than the Pauli field, the Coulomb field in the presence of the magnetic field though still smaller is of the same order of magnitude as the corresponding Pauli field. Nevertheless, the Coulomb energy is again an order of magnitude smaller than the Pauli energy (see Table 1). The reason for this is that the Coulomb field (see Fig. 9) is both positive and negative. Yet another point of contrast is that in the case when the magnetic field is present, the Coulomb field decays asymptotically as  $O(-\frac{1}{r^3})$  whereas in the absence of the magnetic field it decays as  $O(-\frac{1}{r^4})$ .

## 2. Correlation-kinetic field $\mathcal{Z}_{t_c}(\mathbf{r})$ and energy $T_c$

The correlation-kinetic field  $\mathcal{Z}_{t_c}(\mathbf{r})$  and energy  $T_c$  are obtained from the interacting and  $S$  system kinetic-energy tensors  $t_{\alpha\beta}(\mathbf{r}; \gamma)$  and  $t_{s,\alpha\beta}(\mathbf{r}; \gamma_s)$ , respectively. As a consequence of the cylindrical symmetry, these tensors are of the form

$$t_{\alpha\beta}(\mathbf{r}; \gamma) = \frac{r_\alpha r_\beta}{r^2} f(r) + \delta_{\alpha\beta} f(r) \quad (83)$$

and

$$t_{s,\alpha\beta}(\mathbf{r}; \gamma_s) = \frac{r_\alpha r_\beta}{r^2} h(r) \quad (84)$$

where the functions  $f(r)$ ,  $k(r)$ , and  $h(r)$  are given in Appendix B. To compare the off-diagonal matrix elements of the tensors, we plot in Fig 10 the functions  $f(r)$  and  $h(r)$ . Observe that they are extremely close, both vanishing at the nucleus, and decaying in a similar manner asymptotically. Hence, the contribution of the off-diagonal elements to the corresponding kinetic ‘forces’ are similar, and therefore their contribution to the correlation-kinetic field  $\mathcal{Z}_{t_c}(\mathbf{r})$  very small. To compare the diagonal matrix elements of the tensors, we plot in Fig. 11 the functions  $f(r) + 2k(r)$  and  $h(r)$ . Observe that the diagonal matrix element of the interacting system tensor is now finite at the nucleus and differs from that of the  $S$  system in the interior region of the atom. Hence, the contribution to the correlation-kinetic field  $\mathcal{Z}_{t_c}(\mathbf{r})$  arises principally from the diagonal matrix elements and from the interior of the atom. This is also the region from which the contribution to the correlation-kinetic energy  $T_c$  arises.

The expressions for the interacting and  $S$  system kinetic ‘forces’  $\mathbf{z}_\alpha(\mathbf{r}; \gamma)$  and  $\mathbf{z}_{s,\alpha}(\mathbf{r}; \gamma_s)$ , respectively, and their corresponding asymptotic structure are given in Appendix B. The correlation-kinetic field  $\mathcal{Z}_{t_c}(\mathbf{r})$  and its components  $\mathcal{Z}_s(\mathbf{r})$  and  $\mathcal{Z}(\mathbf{r})$  are plotted in Fig. 12. Observe that  $\mathcal{Z}_{t_c}(\mathbf{r})$  is positive throughout space. Its asymptotic structure obtained from Eqs. (B7), (B20) and (B23) is

$$\mathcal{Z}_{t_c}(r) \underset{r \rightarrow \infty}{\sim} \frac{3}{r^3} - \frac{12}{r^5}. \quad (85)$$



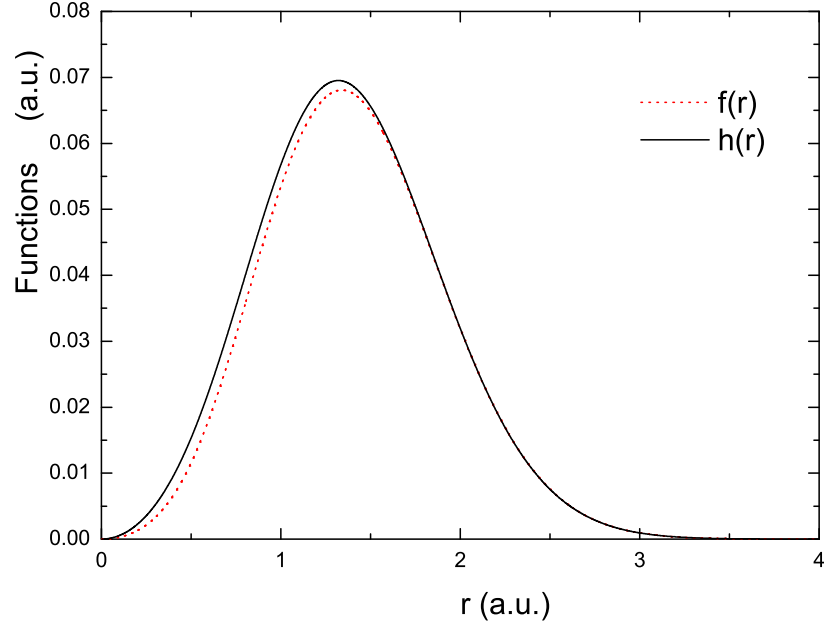


FIG. 10: (Color Online) Functions  $f(r)$  and  $h(r)$  of the off-diagonal elements of the interacting and non-interacting kinetic energy tensors  $t_{\alpha\beta}(\mathbf{r}; \gamma)$  and  $t_{s,\alpha\beta}(\mathbf{r}; \gamma_s)$ , respectively.

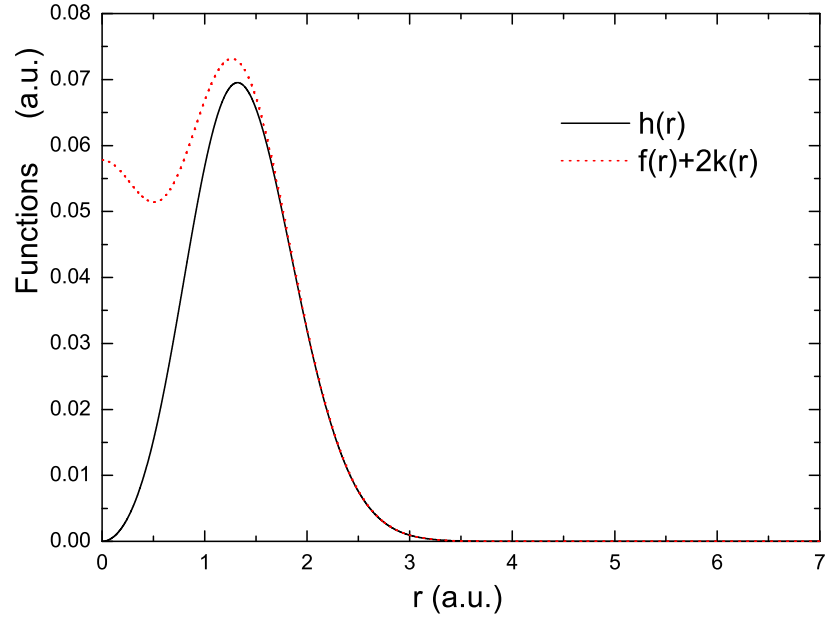


FIG. 11: (Color Online) The functions  $f(r) + 2k(r)$  and  $h(r)$  of the diagonal elements of the tensors  $t_{\alpha\beta}(\mathbf{r}; \gamma)$  and  $t_{s,\alpha\beta}(\mathbf{r}; \gamma_s)$ , respectively.

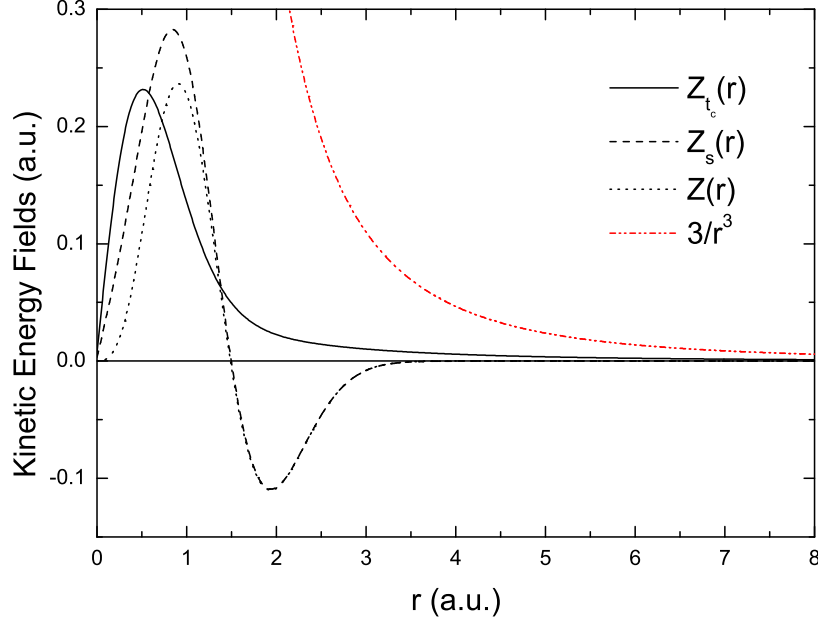


FIG. 12: (Color Online) Correlation-kinetic field  $Z_{tc}(r)$ , and its components  $Z_s(r)$  and  $Z(r)$  for the noninteracting and interacting systems. The function  $3/r^3$  is also plotted.

(Note the cancelation of the asymptotic structure of the ‘forces’  $z(r)$  and  $z_s(r)$  from terms of  $O(r^5)$  to  $O(r^0)$ .)

The kinetic energy of the interacting and  $S$  systems,  $T$  and  $T_s$ , may be obtained either from the fields  $\mathcal{Z}(\mathbf{r})$  and  $\mathcal{Z}_s(\mathbf{r})$ , respectively, or from the corresponding system kinetic energy densities  $t(\mathbf{r})$  and  $t_s(\mathbf{r})$ . (The kinetic energy density is the trace of the kinetic energy tensor.) The value of  $T = 0.886\,199$  a.u.;  $T_s = 0.780\,987$  a.u.;  $T_c = 0.105\,212$  a.u. In contrast to the case with no magnetic field [1, 15] for which  $T_c$  is an order of magnitude smaller than  $T_s$ , in the present case the  $T_c$  though still smaller is of the same order of magnitude as  $T_s$ .

### C. Potentials

#### 1. Electron-interaction potential $W_{ee}(\mathbf{r})$

Due to cylindrical symmetry, the electron-interaction field  $\mathcal{E}_{ee}(\mathbf{r})$  is conservative. Hence, the contribution of Pauli and Coulomb correlations  $W_{ee}(\mathbf{r})$  to the effective electron-interaction potential energy  $v_{ee}(\mathbf{r})$  is the work done in this field:

$$W_{ee}(\mathbf{r}) = - \int_{\infty}^{\mathbf{r}} \mathcal{E}_{ee}(\mathbf{r}') \cdot d\ell'. \quad (86)$$

This work done is path-independent. The electron-interaction potential  $W_{ee}(\mathbf{r})$  may be further subdivided into its Hartree  $W_H(\mathbf{r})$ , Pauli-Coulomb  $W_{xc}(\mathbf{r})$ , Pauli  $W_x(\mathbf{r})$  and Coulomb  $W_c(\mathbf{r})$  components, each being the work done in the conservative fields  $\mathcal{E}_H(\mathbf{r})$ ,  $\mathcal{E}_{xc}(\mathbf{r})$ ,  $\mathcal{E}_x(\mathbf{r})$ , and  $\mathcal{E}_c(\mathbf{r})$ , respectively.

The structure of the individual potentials follows directly from the corresponding fields. Thus, for example, since the field  $\mathcal{E}_{xc}(\mathbf{r})$  is negative throughout space and vanishes at the nucleus, the corresponding potential  $W_{xc}(\mathbf{r})$  is negative and has zero slope at the nucleus. The asymptotic structure of the potentials follows from Eq. (81):

$$\begin{aligned} W_{ee}(r) &\underset{r \rightarrow \infty}{\sim} \frac{1}{r} + \frac{1}{r^2}, & W_H(r) &\underset{r \rightarrow \infty}{\sim} \frac{2}{r} + \frac{5}{2r^2}, & W_{xc}(r) &\underset{r \rightarrow \infty}{\sim} -\frac{1}{r} - \frac{3}{2r^2} \\ W_x(r) &\underset{r \rightarrow \infty}{\sim} -\frac{1}{r} - \frac{5}{4r^2}, & W_c(r) &\underset{r \rightarrow \infty}{\sim} -\frac{1}{4r^2}. \end{aligned} \quad (87)$$

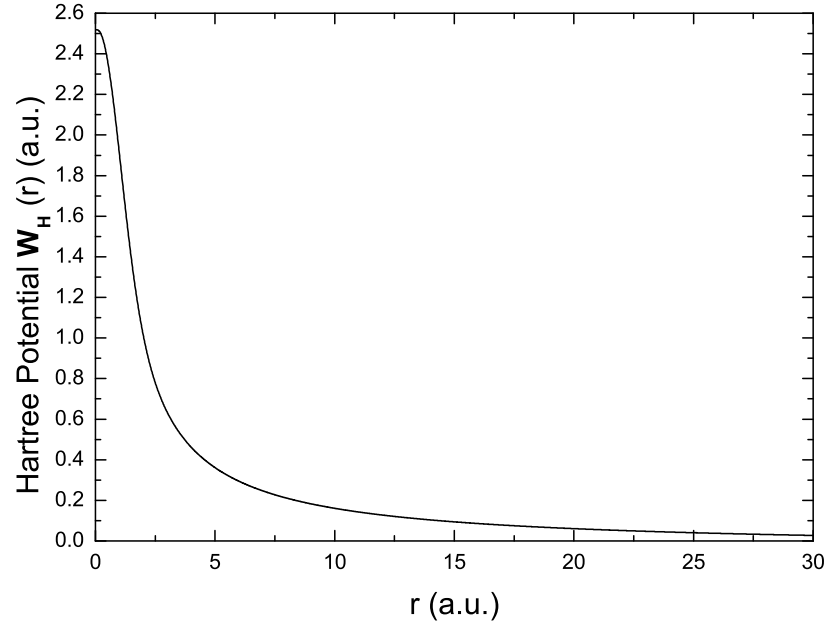


FIG. 13: (Color Online) The Hartree potential energy  $W_H(r)$

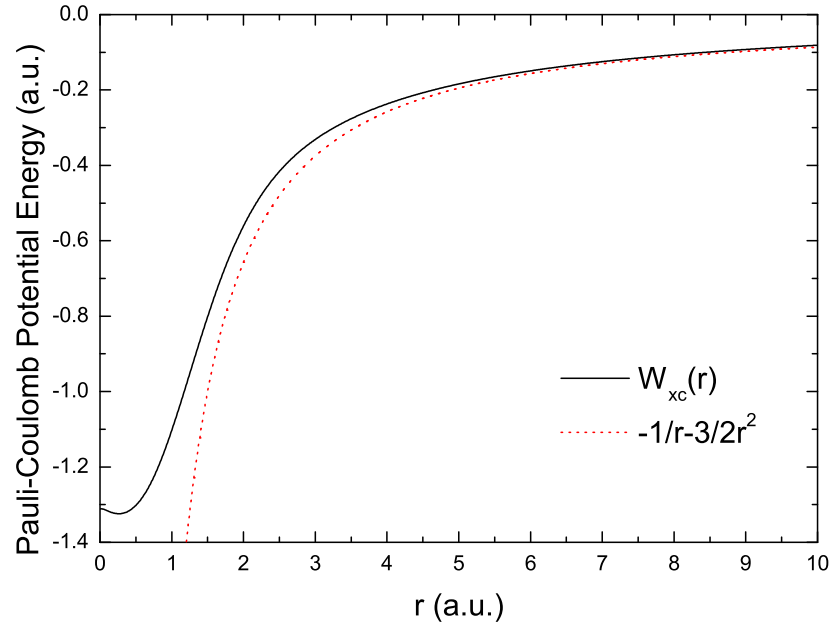


FIG. 14: (Color Online) The Pauli-Coulomb potential energy  $W_{xc}(r)$ . The function  $-1/r - 3/2r^2$  is also plotted.

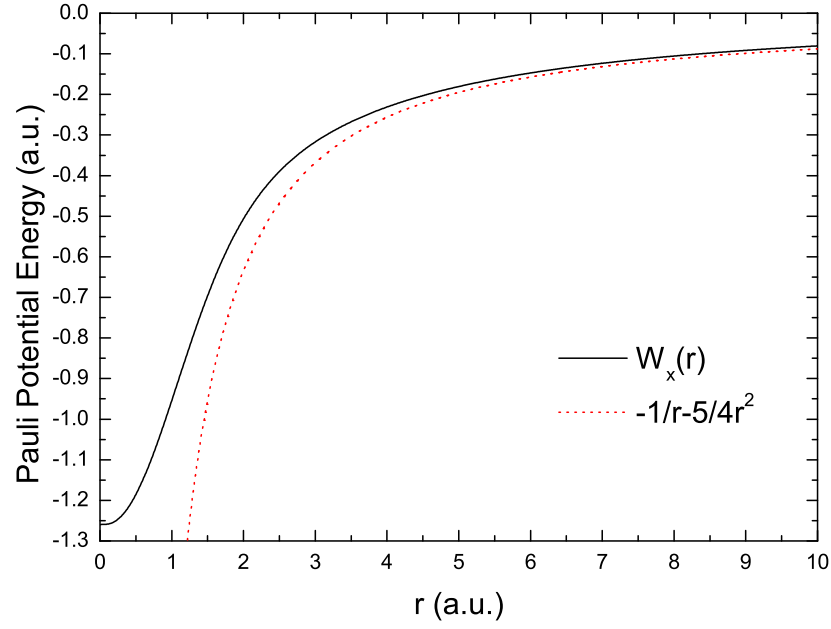


FIG. 15: (Color Online) The Pauli potential energy  $W_x(r)$ . The function  $-1/r - 5/4r^2$  is also plotted.

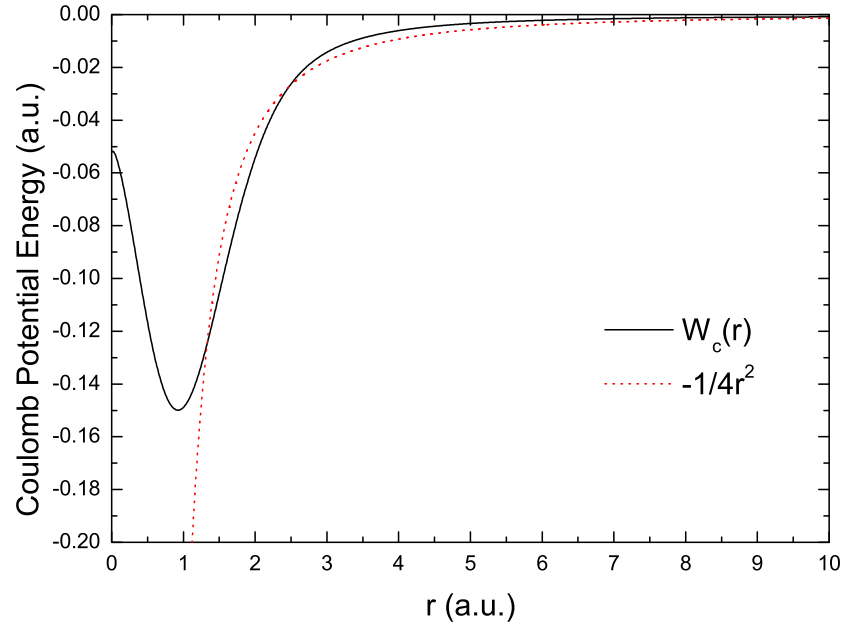


FIG. 16: (Color Online) The Coulomb potential energy  $W_c(r)$ . The function  $-1/4r^2$  is also plotted.

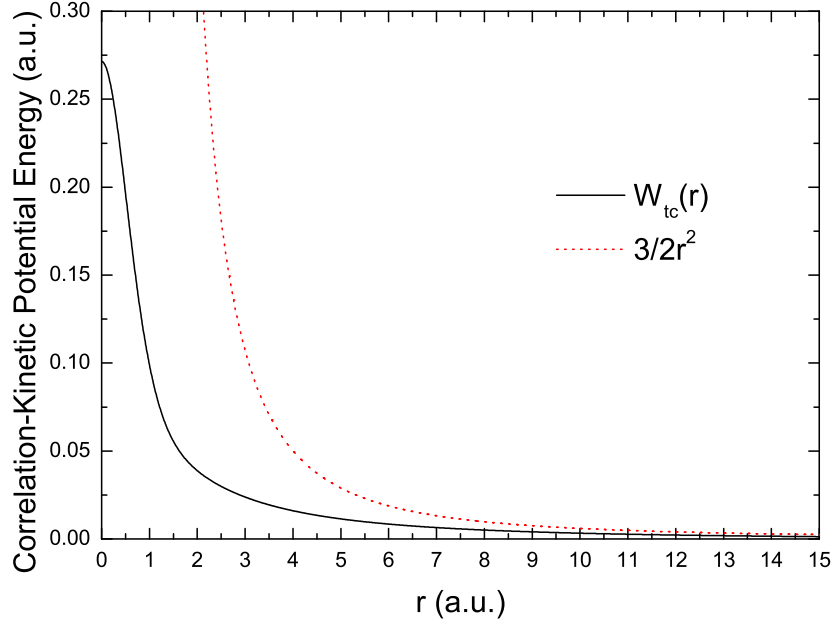


FIG. 17: (Color Online) The correlation-kinetic potential energy  $W_{tc}(r)$ . The function  $3/2r^2$  is also plotted.

Note that the Coulomb potential  $W_c(r)$  decays as  $O(-1/r^2)$ , whereas in the absence of a magnetic field  $W_c(\mathbf{r})$  decays as  $O(-1/r^3)$ .

The potentials  $W_H(r)$ ,  $W_{xc}(r)$ ,  $W_x(r)$ ,  $W_c(r)$ , and  $W_{ee}(r)$  are plotted in Figs 13-16, 18.

### 2. Correlation-kinetic potential $W_{tc}(\mathbf{r})$

Once again, as a consequence of cylindrical symmetry, the correlation-kinetic field  $\mathcal{Z}_{tc}(\mathbf{r})$  is conservative, and therefore the contribution of this effect to the effective electron-interaction potential energy  $v_{ee}(\mathbf{r})$  is the work done in this field:

$$W_{tc}(\mathbf{r}) = - \int_{\infty}^{\mathbf{r}} \mathcal{Z}_{tc}(\mathbf{r}') \cdot d\ell'. \quad (88)$$

This work done is also path-independent. The potential energy  $W_{tc}(r)$  is plotted in Figs. 17, 18. It is positive throughout space as a result of the field  $\mathcal{Z}_{tc}(\mathbf{r})$  being positive. Its asymptotic structure obtained from Eq. (85) is

$$W_{tc}(r) \underset{r \rightarrow \infty}{\sim} \frac{3}{2r^2}. \quad (89)$$

It is evident from Eqs. (87) and (89) (see also Fig. 18) that  $W_{tc}(r)$  decays asymptotically much faster than the electron-interaction potential  $W_{ee}(r)$ . This decay of  $W_{tc}(\mathbf{r})$  of  $O(\frac{1}{r^2})$  is the same as in the absence of a magnetic field.

### 3. Effective electron-interaction potential $v_{ee}(\mathbf{r})$

The effective electron-interaction potential  $v_{ee}(\mathbf{r})$  is then the sum of the electron-interaction  $W_{ee}(\mathbf{r})$  and correlation-kinetic  $W_{tc}(\mathbf{r})$  potentials:

$$v_{ee}(\mathbf{r}) = W_{ee}(\mathbf{r}) + W_{tc}(\mathbf{r}). \quad (90)$$

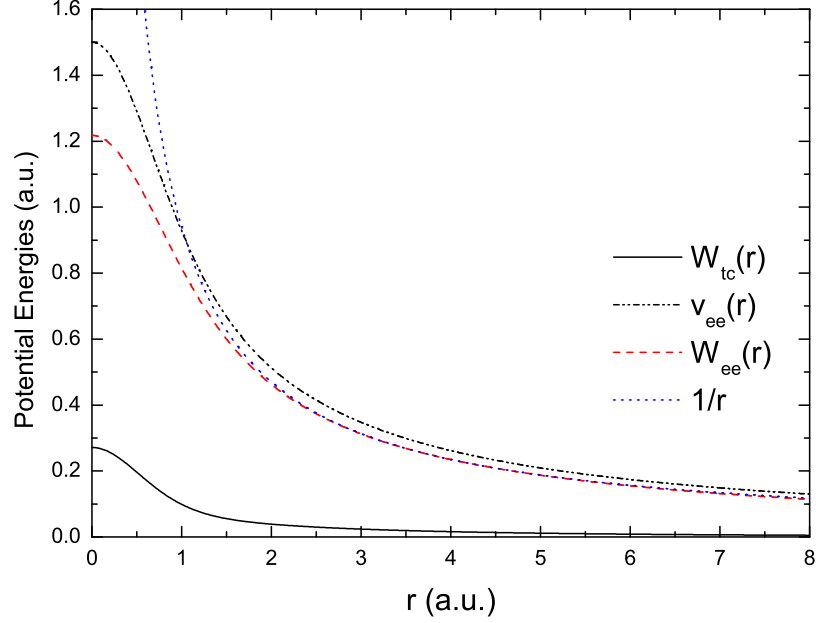


FIG. 18: (Color Online) The electron-interaction  $W_{ee}(r)$ , correlation-kinetic  $W_{tc}(r)$ , and effective electron-interaction  $v_{ee}(r)$  potential energies. The function  $1/r$  is also plotted.

The potential  $v_{ee}(r)$  is plotted in Fig. 18. Its structure near the nucleus and in the classically forbidden region are

$$v_{ee}(r) \underset{r \rightarrow 0}{\sim} 1.50 - 0.99r^2, \quad (91)$$

$$v_{ee}(r) \underset{r \rightarrow \infty}{\sim} \frac{1}{r} + \frac{5}{2r^2}. \quad (92)$$

Observe (see Figs 16 and 17), that the Coulomb  $W_c(r)$  and correlation-kinetic  $W_{tc}(r)$  components of  $v_{ee}(r)$  are of the same order of magnitude but opposite in sign. Hence, there is a substantial cancelation of these effects in the potential  $v_{ee}(r)$ . There is also a significant cancelation between the Hartree  $W_H(r)$  and Pauli  $W_x(r)$  potentials (see Figs. 13 and 14). It is due to this cancelation that the asymptotic structure of  $v_{ee}(r)$  is  $1/r$  (see Eq. 87), and is due to the residual Hartree potential. The Pauli and Coulomb correlations, and correlation-kinetic effects, all contribute to the term of  $O(1/r^2)$  of  $v_{ee}(r)$ .

#### D. Eigenvalue $\epsilon$

The eigenvalue of the  $S$  system differential equation Eq. (80) can be obtained directly from it since the solution  $\sqrt{\rho(\mathbf{r})}$  is known. Or it may be determined by writing  $v_{ee}(\mathbf{r})$  with  $\tilde{\omega} = 1$  as

$$v_{ee}(\mathbf{r}) = \epsilon + \frac{1}{2} \frac{\nabla^2 \sqrt{\rho}}{\sqrt{\rho}} - \frac{1}{2} r^2. \quad (93)$$

Since  $v_{ee}(\mathbf{r})$  vanishes at infinity, and  $\nabla^2 = \partial^2/\partial r^2 + (1/r)\partial/\partial r$ , we obtain  $\epsilon = 2$  a.u.

#### E. Single-particle expectations

With the density  $\rho(\mathbf{r})$  known, the expectations of the single-particle operators  $\hat{O} = \sum_i r_i^n, n = 2, 1, -1$  and  $\hat{O} = \sum_i \delta(\mathbf{r}_i)$  may be determined and are given in Appendix B.

#### IV. CONCLUDING REMARKS

We have extended the QDFT of electrons to the case where there exists both a static external scalar and vector potential  $\{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\}$ . The QDFT, based on the ‘quantal Newtonian’ first law, maps the interacting system to one of noninteracting fermions with the same density and physical current density  $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$ , which properties constitute the basic quantum mechanical variables. The QDFT is general in that it is valid for both ground and excited nondegenerate states of the interacting system. The mapping to the model system is arbitrary in that it could be either in a ground or excited state. A principle attribute of the theory is that the separate contributions to a property of the different electron correlations that must be accounted for in the mapping, *viz.* those due to the Pauli Exclusion Principle and Coulomb repulsion, and the correlation-kinetic and correlation-magnetic effects, are explicitly defined. As such, the contribution of each individual electron correlation to a property can be separately obtained and studied.

To explicate the theory, we have applied it to the Hooke’s atom in the presence of an external magnetic field. Thereby, we have explicitly constructed a noninteracting fermionic system which possesses the same ground state  $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$  as that of the atom. In this example, the mapping demonstrated is from a singlet ground state of the atom to a model system also in its singlet ground state [21].

The role played by each individual electron correlation is clearly demonstrated in the above application. Thus, for example, correlation-kinetic effects contribute positively to the effective electron-interaction potential energy  $v_{ee}(\mathbf{r})$  of the model system, whereas the correlations due to Coulomb repulsion contribute negatively. Both these potentials are also of the same order of magnitude. Additionally, it also turns out that the lowest-order contribution of both the correlation-kinetic and Coulomb potentials in the classically forbidden region is of  $O(1/r^2)$ . As a consequence, there is a significant cancellation of the contributions of these two correlations to both the potential energy  $v_{ee}(\mathbf{r})$  as well as to the total energy  $E$ . In a similar manner, contributions of correlations arising from the Pauli exclusion principle and those due to the Coulomb self-energy, also tend to cancel.

A comparison of the present results with those of the mapping for the Hooke’s atom in the absence of a magnetic field [1, 2, 15] shows both similarities and differences, the latter arising as a consequence of the difference in dimensionality. Thus, for example, the 3-dimensional dynamic Coulomb hole for the Hooke’s atom exhibits a cusp at the position of the electron thereby indicating the satisfaction of the electron-electron coalescence condition for the wave function in 3-dimensions [20, 23]. Similarly, the 2-dimensional Coulomb hole of the present work exhibits a cusp at each electron position representative of the 2-dimensional electron-electron coalescence constraint [20]. On the other hand, the asymptotic decay structure of the corresponding Coulomb fields and potentials in the classically forbidden region differ in spite of the fact that in each case the Coulomb hole satisfies the same sum rule of having a total charge of zero. This difference in the structure is a result of the difference in dimensionality. Another striking difference due to the reduced dimensionality is that correlation-kinetic effects which are relatively insignificant in the 3-dimensional case are far more significant in 2-dimensions. The correlation-kinetic energy in the latter case is greater in magnitude than the Coulomb energy and over ten percent of the Pauli energy. This fact is important in the Kohn-Sham description of the mapping [4] the application of which requires the construction of approximate energy functionals of  $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$  and their functional derivatives. Contributions due to correlation-kinetic effects cannot therefore be ignored in a first approximation.

Finally, we are presently extending the QDFT described in the present work to the case of external time-dependent electromagnetic fields. In this case it has been shown [24] that the basic variables are the time-dependent density and physical current density  $\{\rho(\mathbf{r}, t), \mathbf{j}(\mathbf{r}, t)\}$ . Such a QDFT will then make possible, for example, the study of the interaction of radiation with matter from the perspective of the separate contributions of the various electron correlations present.

#### Acknowledgments

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#### Appendix A: Proof of the ‘Quantal Newtonian’ First Law in the Presence of a Magnetic Field

Consider the Hamiltonian  $\hat{H}$  of Eq. (1) and the corresponding Schrödinger equation Eq. (9). Writing the wave function as  $\Psi = \Psi^R + i\Psi^I$ , where  $\Psi^R$  and  $\Psi^I$  are the real and imaginary parts, we have on substitution into Eq. (9)

$$[\hat{U} + \hat{V} + \frac{1}{2}\mathbf{A}^2(\mathbf{r}) - E](\Psi^R + i\Psi^I) = [-\hat{T} + i\hat{\Omega}](\Psi^R + i\Psi^I), \quad (\text{A1})$$

or, since  $\hat{T}$  and  $\hat{\Omega}$  have differential operators:

$$\hat{U} + \hat{V} + \frac{1}{2}\mathbf{A}^2(\mathbf{r}) - E = \frac{(-\hat{T}\Psi^R - \hat{\Omega}\Psi^I)}{\Psi^R} = \frac{(-\hat{T}\Psi^I + \hat{\Omega}\Psi^R)}{\Psi^I}. \quad (\text{A2})$$

With  $\nabla_i^2 = \sum_{\beta=1}^3 \frac{\partial^2}{\partial r_{i\beta}^2}$ , we have on differentiating the individual terms on the right hand side of (A2) with respect to  $r_{1\alpha}$

$$\frac{\partial}{\partial r_{1\alpha}} \left[ \frac{\hat{T}\Psi^R}{\Psi^R} \right] = -\frac{1}{2\Psi^R} \sum_{i=1}^N \sum_{\beta=1}^3 \frac{\partial^3 \Psi^R}{\partial r_{i\beta} \partial r_{i\beta} \partial r_{1\alpha}} + \frac{1}{2(\Psi^R)^2} \frac{\partial \Psi^R}{\partial r_{1\alpha}} \sum_{i=1}^N \sum_{\beta=1}^3 \frac{\partial^2 \Psi^R}{\partial r_{i\beta}^2}, \quad (\text{A3})$$

and

$$\begin{aligned} \frac{\partial}{\partial r_{1\alpha}} \left[ \frac{\hat{\Omega}\Psi^I}{\Psi^R} \right] &= \sum_{i=1}^N \sum_{\beta=1}^3 \left\{ \frac{1}{\Psi^R} \frac{\partial}{\partial r_{1\alpha}} (A_{i\beta} \frac{\partial \Psi^I}{\partial r_{i\beta}}) - \frac{1}{(\Psi^R)^2} A_{i\beta} \frac{\partial \Psi^I}{\partial r_{i\beta}} \frac{\partial \Psi^R}{\partial r_{1\alpha}} \right\} \\ &+ \frac{1}{2} \sum_{i=1}^N \sum_{\beta=1}^3 \left\{ \frac{1}{\Psi^R} \frac{\partial}{\partial r_{1\alpha}} (\Psi^I \frac{\partial A_{i\beta}}{\partial r_{i\beta}}) - \frac{1}{(\Psi^R)^2} \Psi^I \frac{\partial A_{i\beta}}{\partial r_{i\beta}} \frac{\partial \Psi^R}{\partial r_{1\alpha}} \right\}. \end{aligned} \quad (\text{A4})$$

Differentiating the left hand side of (A2) with respect to  $r_{1\alpha}$ , employing Eq.(A3) and (A4), we arrive at

$$\begin{aligned} \left[ \frac{\partial}{\partial r_{1\alpha}} \{v(\mathbf{r}_1) + \frac{1}{2}A^2(\mathbf{r}_1) + \sum_{j=2}^N u(\mathbf{r}_1, \mathbf{r}_j)\} \right] (\Psi^R)^2 \\ = \sum_{i=1}^N \sum_{\beta=1}^3 \left[ \frac{1}{2} \Psi^R \frac{\partial^3 \Psi^R}{\partial r_{i\beta} \partial r_{i\beta} \partial r_{1\alpha}} - \frac{1}{2} \frac{\partial \Psi^R}{\partial r_{1\alpha}} \frac{\partial^2 \Psi^R}{\partial r_{i\beta}^2} \right] \\ - \sum_{i=1}^N \sum_{\beta=1}^3 \left[ \Psi^R \frac{\partial}{\partial r_{1\alpha}} (A_{i\beta} \frac{\partial \Psi^I}{\partial r_{i\beta}}) - A_{i\beta} \frac{\partial \Psi^I}{\partial r_{i\beta}} \frac{\partial \Psi^R}{\partial r_{1\alpha}} \right] \\ - \frac{1}{2} \sum_{i=1}^N \sum_{\beta=1}^3 \left\{ \Psi^R \frac{\partial}{\partial r_{1\alpha}} (\Psi^I \frac{\partial A_{i\beta}}{\partial r_{i\beta}}) - \Psi^I \frac{\partial A_{i\beta}}{\partial r_{i\beta}} \frac{\partial \Psi^R}{\partial r_{1\alpha}} \right\}. \end{aligned} \quad (\text{A5})$$

The right hand side of (A5) can be further simplified by using the following relations:

$$\frac{1}{4} \frac{\partial^3 \Psi^R \Psi^R}{\partial r_{i\beta} \partial r_{i\beta} \partial r_{1\alpha}} = \frac{1}{2} \frac{\partial^2 \Psi^R}{\partial r_{i\beta}^2} \frac{\partial \Psi^R}{\partial r_{1\alpha}} + \frac{\partial \Psi^R}{\partial r_{i\beta}} \frac{\partial^2 \Psi^R}{\partial r_{i\beta} \partial r_{1\alpha}} + \frac{1}{2} \Psi^R \frac{\partial^3 \Psi^R}{\partial r_{i\beta} \partial r_{i\beta} \partial r_{1\alpha}}, \quad (\text{A6})$$

and

$$-\frac{\partial}{\partial r_{i\beta}} \left[ \frac{\partial \Psi^R}{\partial r_{1\alpha}} \frac{\partial \Psi^R}{\partial r_{i\beta}} \right] = -\frac{\partial \Psi^R}{\partial r_{1\alpha}} \frac{\partial^2 \Psi^R}{\partial r_{i\beta} \partial r_{i\beta}} - \frac{\partial^2 \Psi^R}{\partial r_{1\alpha} \partial r_{i\beta}} \frac{\partial \Psi^R}{\partial r_{i\beta}}. \quad (\text{A7})$$

Adding (A6) and (A7) we obtain

$$\frac{1}{4} \frac{\partial^3 \Psi^R \Psi^R}{\partial r_{i\beta} \partial r_{i\beta} \partial r_{1\alpha}} - \frac{\partial}{\partial r_{i\beta}} \left[ \frac{\partial \Psi^R}{\partial r_{1\alpha}} \frac{\partial \Psi^R}{\partial r_{i\beta}} \right] = \frac{1}{2} \Psi^R \frac{\partial^3 \Psi^R}{\partial r_{i\beta} \partial r_{i\beta} \partial r_{1\alpha}} - \frac{1}{2} \frac{\partial \Psi^R}{\partial r_{1\alpha}} \frac{\partial^2 \Psi^R}{\partial r_{i\beta}^2}, \quad (\text{A8})$$

where the right hand side of (A8) then corresponds to the terms in the first parenthesis of (A5).



Thus, (A5) for the real part of the wave function  $\Psi^R$  becomes

$$\begin{aligned}
& \left[ \frac{\partial}{\partial r_{1\alpha}} \{v(\mathbf{r}_1) + \frac{1}{2}A^2(\mathbf{r}_1) + \sum_{j=2}^N u(\mathbf{r}_1, \mathbf{r}_j)\} \right] (\Psi^R)^2 \\
&= \sum_{i=1}^N \sum_{\beta=1}^3 \left\{ \frac{1}{4} \frac{\partial^3 (\Psi^R \Psi^R)}{\partial r_{i\beta} \partial r_{i\beta} \partial r_{1\alpha}} - \frac{\partial}{\partial r_{i\beta}} \left( \frac{\partial \Psi^R}{\partial r_{1\alpha}} \frac{\partial \Psi^R}{\partial r_{i\beta}} \right) \right\} \\
&\quad - \sum_{i=1}^N \sum_{\beta=1}^3 \left[ \Psi^R \frac{\partial}{\partial r_{1\alpha}} \left( A_{i\beta} \frac{\partial \Psi^I}{\partial r_{i\beta}} \right) - A_{i\beta} \frac{\partial \Psi^I}{\partial r_{i\beta}} \frac{\partial \Psi^R}{\partial r_{1\alpha}} \right] \\
&\quad - \frac{1}{2} \sum_{i=1}^N \sum_{\beta=1}^3 \left\{ \Psi^R \frac{\partial}{\partial r_{1\alpha}} \left( \Psi^I \frac{\partial A_{i\beta}}{\partial r_{i\beta}} \right) - \Psi^I \frac{\partial A_{i\beta}}{\partial r_{i\beta}} \frac{\partial \Psi^R}{\partial r_{1\alpha}} \right\}. \tag{A9}
\end{aligned}$$

Similarly, the equation for the imaginary part of the wave function  $\Psi^I$  is

$$\begin{aligned}
& \left[ \frac{\partial}{\partial r_{1\alpha}} \{v(\mathbf{r}_1) + \frac{1}{2}A^2(\mathbf{r}_1) + \sum_{j=2}^N u(\mathbf{r}_1, \mathbf{r}_j)\} \right] (\Psi^I)^2 \\
&= \sum_{i=1}^N \sum_{\beta=1}^3 \left\{ \frac{1}{4} \frac{\partial^3 (\Psi^I \Psi^I)}{\partial r_{i\beta} \partial r_{i\beta} \partial r_{1\alpha}} - \frac{\partial}{\partial r_{i\beta}} \left( \frac{\partial \Psi^I}{\partial r_{1\alpha}} \frac{\partial \Psi^I}{\partial r_{i\beta}} \right) \right\} \\
&\quad + \sum_{i=1}^N \sum_{\beta=1}^3 \left[ \Psi^I \frac{\partial}{\partial r_{1\alpha}} \left( A_{i\beta} \frac{\partial \Psi^R}{\partial r_{i\beta}} \right) - A_{i\beta} \frac{\partial \Psi^R}{\partial r_{i\beta}} \frac{\partial \Psi^I}{\partial r_{1\alpha}} \right] \\
&\quad + \frac{1}{2} \sum_{i=1}^N \sum_{\beta=1}^3 \left\{ \Psi^I \frac{\partial}{\partial r_{1\alpha}} \left( \Psi^R \frac{\partial A_{i\beta}}{\partial r_{i\beta}} \right) - \Psi^R \frac{\partial A_{i\beta}}{\partial r_{i\beta}} \frac{\partial \Psi^I}{\partial r_{1\alpha}} \right\}. \tag{A10}
\end{aligned}$$

Note that the terms in the first parenthesis in (A9) and (A10) correspond to the derivation in the  $\mathbf{B} = 0$  case. The terms in the second two parenthesis are the additional terms in the presence of a vector potential.

Adding (A9), and (A10) yields

$$\begin{aligned}
& \left[ \frac{\partial}{\partial r_{1\alpha}} \{v(\mathbf{r}_1) + \frac{1}{2}A^2(\mathbf{r}_1) + \sum_{j=2}^N u(\mathbf{r}_1, \mathbf{r}_j)\} \right] |\Psi|^2 \\
&= \sum_{i=1}^N \sum_{\beta=1}^3 \left\{ \frac{1}{4} \frac{\partial^3 |\Psi|^2}{\partial r_{i\beta} \partial r_{i\beta} \partial r_{1\alpha}} - \frac{\partial}{\partial r_{i\beta}} \left( \frac{\partial \Psi^R}{\partial r_{1\alpha}} \frac{\partial \Psi^R}{\partial r_{i\beta}} + \frac{\partial \Psi^I}{\partial r_{1\alpha}} \frac{\partial \Psi^I}{\partial r_{i\beta}} \right) \right\} \\
&\quad + \left[ A_{i\beta} \left( \frac{\partial \Psi^I}{\partial r_{i\beta}} \frac{\partial \Psi^R}{\partial r_{1\alpha}} - \frac{\partial \Psi^R}{\partial r_{i\beta}} \frac{\partial \Psi^I}{\partial r_{1\alpha}} \right) + \left( \Psi^I \frac{\partial}{\partial r_{1\alpha}} \left( A_{i\beta} \frac{\partial \Psi^R}{\partial r_{i\beta}} \right) - \Psi^R \frac{\partial}{\partial r_{1\alpha}} \left( A_{i\beta} \frac{\partial \Psi^I}{\partial r_{i\beta}} \right) \right) \right] \\
&\quad + \frac{1}{2} \sum_{i=1}^N \sum_{\beta=1}^3 \left\{ \Psi^I \frac{\partial}{\partial r_{1\alpha}} \left( \Psi^R \frac{\partial A_{i\beta}}{\partial r_{i\beta}} \right) - \Psi^R \frac{\partial A_{i\beta}}{\partial r_{i\beta}} \frac{\partial \Psi^I}{\partial r_{1\alpha}} \right. \\
&\quad \left. - \Psi^R \frac{\partial}{\partial r_{1\alpha}} \left( \Psi^I \frac{\partial A_{i\beta}}{\partial r_{i\beta}} \right) + \Psi^I \frac{\partial A_{i\beta}}{\partial r_{i\beta}} \frac{\partial \Psi^R}{\partial r_{1\alpha}} \right\}. \tag{A11}
\end{aligned}$$

The terms of the first parenthesis on the right hand side of (A11) may be rewritten by splitting each term into its  $i = 1$  and  $i \geq 2$  contributions as

$$\sum_{i=1}^N \sum_{\beta=1}^3 \frac{1}{4} \frac{\partial}{\partial r_{i\beta}} \frac{\partial}{\partial r_{i\beta}} \frac{\partial}{\partial r_{1\alpha}} |\Psi|^2 = \left[ \frac{1}{4} \nabla_1^2 \frac{\partial}{\partial r_{1\alpha}} |\Psi|^2 + \frac{1}{4} \sum_{j=2}^N \sum_{\beta=1}^3 \frac{\partial}{\partial r_{j\beta}} \frac{\partial}{\partial r_{j\beta}} \frac{\partial}{\partial r_{1\alpha}} |\Psi|^2 \right], \tag{A12}$$

and

$$\begin{aligned}
& \sum_{i=1}^N \sum_{\beta=1}^3 \frac{\partial}{\partial r_{i\beta}} \left( \frac{\partial \Psi^R}{\partial r_{1\alpha}} \frac{\partial \Psi^R}{\partial r_{i\beta}} + \frac{\partial \Psi^I}{\partial r_{1\alpha}} \frac{\partial \Psi^I}{\partial r_{i\beta}} \right) \\
&= \left[ \sum_{\beta=1}^3 \frac{\partial}{\partial r_{1\beta}} \left( \frac{\partial \Psi^R}{\partial r_{1\alpha}} \frac{\partial \Psi^R}{\partial r_{1\beta}} + \frac{\partial \Psi^I}{\partial r_{1\alpha}} \frac{\partial \Psi^I}{\partial r_{1\beta}} \right) \right. \\
&\quad \left. + \sum_{j=2}^N \sum_{\beta=1}^3 \frac{\partial}{\partial r_{j\beta}} \left( \frac{\partial \Psi^R}{\partial r_{1\alpha}} \frac{\partial \Psi^R}{\partial r_{j\beta}} + \frac{\partial \Psi^I}{\partial r_{1\alpha}} \frac{\partial \Psi^I}{\partial r_{j\beta}} \right) \right]. \tag{A13}
\end{aligned}$$

Again, the only new terms in (A11) that arise on the right hand side due to the presence of the magnetic field or vector potential  $\mathbf{A}$  are those of the second two parentheses of (A11). These terms can be further simplified to

$$\begin{aligned}
& \sum_{i=1}^N \sum_{\beta=1}^3 [A_{i\beta} \left( \frac{\partial \Psi^I}{\partial r_{i\beta}} \frac{\partial \Psi^R}{\partial r_{1\alpha}} - \frac{\partial \Psi^R}{\partial r_{i\beta}} \frac{\partial \Psi^I}{\partial r_{1\alpha}} \right) + (\Psi^I \frac{\partial}{\partial r_{1\alpha}} (A_{i\beta} \frac{\partial \Psi^R}{\partial r_{i\beta}}) - \Psi^R \frac{\partial}{\partial r_{1\alpha}} (A_{i\beta} \frac{\partial \Psi^I}{\partial r_{i\beta}})) \\
&+ \Psi^I \frac{\partial A_{i\beta}}{\partial r_{i\beta}} \frac{\partial \Psi^R}{\partial r_{1\alpha}} - \Psi^R \frac{\partial A_{i\beta}}{\partial r_{i\beta}} \frac{\partial \Psi^I}{\partial r_{1\alpha}}]. \tag{A14}
\end{aligned}$$

Once again, we split these terms into their  $i = 1$  and  $i \geq 2$  contributions. The  $i = 1$  term of Eq. (A14) is

$$\begin{aligned}
& \sum_{\beta=1}^3 [A_{1\beta} \left( \frac{\partial \Psi^I}{\partial r_{1\beta}} \frac{\partial \Psi^R}{\partial r_{1\alpha}} - \frac{\partial \Psi^R}{\partial r_{1\beta}} \frac{\partial \Psi^I}{\partial r_{1\alpha}} \right) + (\Psi^I \frac{\partial}{\partial r_{1\alpha}} (A_{1\beta} \frac{\partial \Psi^R}{\partial r_{1\beta}}) - \Psi^R \frac{\partial}{\partial r_{1\alpha}} (A_{1\beta} \frac{\partial \Psi^I}{\partial r_{1\beta}})) \\
&= [\frac{\partial A_{1\beta}}{\partial r_{1\alpha}} (\Psi^I \frac{\partial \Psi^R}{\partial r_{1\beta}} - \Psi^R \frac{\partial \Psi^I}{\partial r_{1\beta}}) + (\frac{\partial}{\partial r_{1\beta}} (A_{1\beta} \Psi^I \frac{\partial \Psi^R}{\partial r_{1\alpha}} - A_{1\beta} \Psi^R \frac{\partial \Psi^I}{\partial r_{1\alpha}}))]. \tag{A15}
\end{aligned}$$

The  $i \geq 2$  contribution of (A14) is

$$= \sum_{i=2}^N \sum_{\beta=1}^3 \frac{\partial}{\partial r_{i\beta}} [A_{i\beta} (\Psi^I \frac{\partial \Psi^R}{\partial r_{1\alpha}} - \Psi^R \frac{\partial \Psi^I}{\partial r_{1\alpha}}) + \Psi^I \frac{\partial A_{i\beta}}{\partial r_{i\beta}} \frac{\partial \Psi^R}{\partial r_{1\alpha}} - \Psi^R \frac{\partial A_{i\beta}}{\partial r_{i\beta}} \frac{\partial \Psi^I}{\partial r_{1\alpha}}]. \tag{A16}$$

We next operate by  $N \sum_{\sigma_1} \int d\mathbf{X}^{N-1}$  on (A11) employing (A12, A13, A15, A16) for its right hand side. For the left hand side of (A11) one obtains

$$\frac{\partial}{\partial r_{1\alpha}} \{v(\mathbf{r}_1) + A^2(\mathbf{r}_1)\} \rho(\mathbf{r}_1) + N \sum_{j=2}^N \sum_{\sigma_1} \int \frac{\partial u(\mathbf{r}_1 \mathbf{r}_j)}{\partial r_{1\alpha}} |\Psi|^2 d\mathbf{X}^{N-1}. \tag{A17}$$

For the right hand side of (A11) we note that the contributions of the second terms of (A12) and (A13), and that of the term (A16) vanish for  $|r_j| \rightarrow \infty$ . Thus, the result of the above operation on the right hand side of (A11) is

$$\begin{aligned}
& \frac{1}{4} \nabla_1^2 \frac{\partial}{\partial r_{1\alpha}} \rho(\mathbf{r}_1) - 2N \sum_{\beta=1}^3 \sum_{\sigma_1} \int \frac{1}{2} \frac{\partial}{\partial r_{1\beta}} \left( \frac{\partial \Psi^R}{\partial r_{1\alpha}} \frac{\partial \Psi^R}{\partial r_{1\beta}} + \frac{\partial \Psi^I}{\partial r_{1\alpha}} \frac{\partial \Psi^I}{\partial r_{1\beta}} \right) d\mathbf{X}^{N-1} \\
&+ N \sum_{\beta=1}^3 \sum_{\sigma_1} \int \left[ \frac{\partial A_{1\beta}}{\partial r_{1\alpha}} \left( \Psi^I \frac{\partial \Psi^R}{\partial r_{1\beta}} - \Psi^R \frac{\partial \Psi^I}{\partial r_{1\beta}} \right) \right. \\
&\quad \left. + \left\{ \frac{\partial}{\partial r_{1\beta}} \left( A_{1\beta} \Psi^I \frac{\partial \Psi^R}{\partial r_{1\alpha}} - A_{1\beta} \Psi^R \frac{\partial \Psi^I}{\partial r_{1\alpha}} \right) \right\} \right] d\mathbf{X}^{N-1}. \tag{A18}
\end{aligned}$$

It can be readily seen that in the second term of (A18), the terms within the parenthesis

$$N \sum_{\sigma_1} \int \frac{1}{2} \left( \frac{\partial \Psi^R}{\partial r_{1\alpha}} \frac{\partial \Psi^R}{\partial r_{1\beta}} + \frac{\partial \Psi^I}{\partial r_{1\alpha}} \frac{\partial \Psi^I}{\partial r_{1\beta}} \right) d\mathbf{X}^{N-1} = t_{\alpha\beta}(\mathbf{r}), \tag{A19}$$

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

$$t_{\alpha\beta}(\mathbf{r}) = \frac{1}{4} \left( \frac{\partial^2}{\partial r'_\alpha \partial r''_\beta} + \frac{\partial^2}{\partial r'_\beta \partial r''_\alpha} \right) \gamma(\mathbf{r}'\mathbf{r}'') \Big|_{\mathbf{r}'=\mathbf{r}''=\mathbf{r}}, \quad (\text{A20})$$

with  $\gamma(\mathbf{r}'\mathbf{r}'')$  the reduced single particle density matrix quantal source of Eq. (15). Thus, the second term of (A18) is the component  $z_\alpha(\mathbf{r})$  of the kinetic ‘force’  $\mathbf{z}(\mathbf{r}; \gamma)$ :

$$z_\alpha(\mathbf{r}) = 2 \sum_{\beta=1}^3 \frac{\partial}{\partial r_\beta} t_{\alpha\beta}(\mathbf{r}). \quad (\text{A21})$$

The third term of (A17) may be expressed in terms of the pair-correlation function  $P(\mathbf{r}\mathbf{r}')$  of Eq. (14):

$$N \sum_{j=2}^N \sum_{\sigma_1} \int \frac{\partial u(\mathbf{r}_1 \mathbf{r}_j)}{\partial r_{1\alpha}} |\Psi|^2 d\mathbf{X}^{N-1} = \int \frac{\partial u(\mathbf{r}\mathbf{r}')}{\partial r_\alpha} P(\mathbf{r}\mathbf{r}') d\mathbf{r}'. \quad (\text{A22})$$

In vector form (A22) is

$$\int \nabla u(\mathbf{r}\mathbf{r}') P(\mathbf{r}\mathbf{r}') d\mathbf{r}' = - \int \frac{P(\mathbf{r}\mathbf{r}')(\mathbf{r} - \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|^3} d\mathbf{r}' \quad (\text{A23})$$

$$= -\mathbf{e}_{ee}(\mathbf{r}), \quad (\text{A24})$$

with  $\mathbf{e}_{ee}(\mathbf{r})$  the electron-interaction ‘force’ as obtained by Coulomb’s law.

The last term of (A18) may be expressed in terms of the paramagnetic current density  $\mathbf{j}_p(\mathbf{r})$  as

$$k_\alpha(\mathbf{r}; \mathbf{j}_p \mathbf{A}) = \sum_{\beta=1}^3 \left[ \left( \frac{\partial A_{1\beta}}{\partial r_{1\alpha}} \right) \mathbf{j}_{p\beta}(\mathbf{r}_1) + \frac{\partial}{\partial r_{1\beta}} \left( A_{1\beta} j_{p\alpha}(\mathbf{r}_1) \right) \right]. \quad (\text{A25})$$

On putting together (A17) and (A18) in terms of their further simplifications expressed as ‘forces, we have in vector form

$$\rho(\mathbf{r}) \left[ \nabla v(\mathbf{r}) + \frac{1}{2} \nabla A^2(\mathbf{r}) \right] - \mathbf{e}_{ee}(\mathbf{r}) + \mathbf{z}(\mathbf{r}; \gamma) + \mathbf{d}(\mathbf{r}) + \mathbf{k}(\mathbf{r}; \mathbf{j}_p \mathbf{A}) = 0, \quad (\text{A26})$$

where the differential density ‘force’  $\mathbf{d}(\mathbf{r})$  is

$$\mathbf{d}(\mathbf{r}) = -\frac{1}{4} \nabla \nabla^2 \rho(\mathbf{r}). \quad (\text{A27})$$

Equation (A26) is the differential virial theorem derived by Holas and March [6] via the equation of motion for the single particle density matrix.

Now since the physical current density  $\mathbf{j}(\mathbf{r})$  is

$$\mathbf{j}(\mathbf{r}) = \mathbf{j}_p(\mathbf{r}) + \rho(\mathbf{r}) \mathbf{A}(\mathbf{r}), \quad (\text{A28})$$

we have

$$\mathbf{k}(\mathbf{r}; \mathbf{j}_p \mathbf{A}) + \frac{1}{2} \rho(\mathbf{r}) \nabla A^2(\mathbf{r}) = \mathbf{k}(\mathbf{r}; \mathbf{j} \mathbf{A}) - \sum_{\beta=1}^3 \nabla_\beta [\rho(\mathbf{r}) \mathbf{A}_\alpha(\mathbf{r}) \mathbf{A}_\beta(\mathbf{r})], \quad (\text{A29})$$

so that

$$k_\alpha(\mathbf{r}; \mathbf{j} \mathbf{A}) = \sum_{\beta=1}^3 [j_\beta(\mathbf{r}) \{ \nabla_\alpha A_\beta(\mathbf{r}) \} + \nabla_\beta \{ A_\beta(\mathbf{r}) j_\alpha(\mathbf{r}) \}]. \quad (\text{A30})$$

Equation (A26) is then

$$\rho(\mathbf{r}) \nabla v(\mathbf{r}) - \mathbf{e}_{ee}(\mathbf{r}) + \mathbf{z}(\mathbf{r}; \gamma) + \mathbf{d}(\mathbf{r}) + \mathbf{k}(\mathbf{r}; \mathbf{j} \mathbf{A}) - \sum_{\beta=1}^3 \nabla_\beta [\rho(\mathbf{r}) A_\alpha(\mathbf{r}) A_\beta(\mathbf{r})] = 0. \quad (\text{A31})$$

The last two terms of (A31) which are the only terms that depend upon the vector potential can be afforded a rigorous physical interpretation. Their sum can be expressed as the sum of a contribution of the external Lorentz ‘force’  $\mathbf{l}(\mathbf{r})$  and a corresponding contribution  $\mathbf{i}(\mathbf{r})$  to the internal ‘force’. The Lorentz ‘force’  $\mathbf{l}(\mathbf{r})$  defined in terms of the physical current density  $\mathbf{j}(\mathbf{r})$  is

$$\mathbf{l}(\mathbf{r}) = \mathbf{j}(\mathbf{r}) \times \mathbf{B}(\mathbf{r}). \quad (\text{A32})$$

With  $\mathbf{B} = \nabla \times \mathbf{A}$ , we have

$$l_\alpha(\mathbf{r}) = \sum_{\beta=1}^3 [j_\beta(\mathbf{r}) \nabla_\alpha A_\beta(\mathbf{r}) - j_\beta(\mathbf{r}) \nabla_\beta A_\alpha(\mathbf{r})]. \quad (\text{A33})$$

The contribution of the magnetic field to the internal force  $\mathbf{i}(\mathbf{r})$  is defined via its components as

$$i_\alpha(\mathbf{r}) = \sum_{\beta=1}^3 \nabla_\beta I_{\alpha\beta}(\mathbf{r}), \quad (\text{A34})$$

where

$$I_{\alpha\beta}(\mathbf{r}) = [j_\alpha(\mathbf{r}) A_\beta(\mathbf{r}) + j_\beta(\mathbf{r}) A_\alpha(\mathbf{r})] - \rho(\mathbf{r}) A_\alpha(\mathbf{r}) A_\beta(\mathbf{r}). \quad (\text{A35})$$

On applying the continuity condition  $\nabla \cdot \mathbf{j}(\mathbf{r}) = \sum_\beta \nabla_\beta j_\beta(\mathbf{r}) = 0$ , it is readily seen that

$$l_\alpha(\mathbf{r}) + i_\alpha(\mathbf{r}) = k_\alpha(\mathbf{r}; \mathbf{jA}) - \sum_{\beta=1}^3 \nabla_\beta [\rho(\mathbf{r}) A_\alpha(\mathbf{r}) A_\beta(\mathbf{r})]. \quad (\text{A36})$$

Thus, (A31) may be written in ‘quantal Newtonian’ form in terms of external  $\mathcal{F}^{\text{ext}}(\mathbf{r})$  and internal  $\mathcal{F}^{\text{int}}(\mathbf{r})$  fields as

$$\mathcal{F}^{\text{ext}}(\mathbf{r}) + \mathcal{F}^{\text{int}}(\mathbf{r}) = 0 \quad (\text{A37})$$

with the external field defined as

$$\mathcal{F}^{\text{ext}}(\mathbf{r}) = \mathcal{E}(\mathbf{r}) - \mathcal{L}(\mathbf{r}) \quad (\text{A38})$$

where the external electrostatic  $\mathcal{E}(\mathbf{r})$  field is

$$\mathcal{E}(\mathbf{r}) = -\nabla v(\mathbf{r}), \quad (\text{A39})$$

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

$$\mathcal{L}(\mathbf{r}) = \frac{\mathbf{l}(\mathbf{r})}{\rho(\mathbf{r})}. \quad (\text{A40})$$

The internal field  $\mathcal{F}^{\text{int}}(\mathbf{r})$  is

$$\mathcal{F}^{\text{int}}(\mathbf{r}) = \mathcal{E}_{ee}(\mathbf{r}) - \mathcal{Z}(\mathbf{r}) - \mathcal{D}(\mathbf{r}) - \mathcal{I}(\mathbf{r}), \quad (\text{A41})$$

where the electron-interaction  $\mathcal{E}_{ee}(\mathbf{r})$ , kinetic  $\mathcal{Z}(\mathbf{r})$ , differential density  $\mathcal{D}(\mathbf{r})$ , and internal magnetic  $\mathcal{I}(\mathbf{r})$  fields are defined in terms of their corresponding forces as

$$\mathcal{E}_{ee}(\mathbf{r}) = \frac{\mathbf{e}_{ee}(\mathbf{r})}{\rho(\mathbf{r})}; \mathcal{Z}(\mathbf{r}) = \frac{\mathbf{z}(\mathbf{r}; \gamma)}{\rho(\mathbf{r})}; \mathcal{D}(\mathbf{r}) = \frac{\mathbf{d}(\mathbf{r})}{\rho(\mathbf{r})}; \mathcal{I}(\mathbf{r}) = \frac{\mathbf{i}(\mathbf{r}; \mathbf{jA})}{\rho(\mathbf{r})}. \quad (\text{A42})$$

## Appendix B: QDFT Analytical Expressions for the Ground State Properties of the Hooke’s Atom in a Magnetic Field

In this appendix we give the QDFT analytical and semi-analytical expressions for the mapping from a ground state of the interacting Hooke’s atom in a magnetic field to one of noninteracting fermions in a ground state with equivalent density  $\rho(\mathbf{r})$  and physical current density  $\mathbf{j}(\mathbf{r})$ . The expressions derived are for an effective oscillator frequency  $\tilde{\omega} = 1$ .

### 1. Electron density $\rho(\mathbf{r})$

$$\rho(\mathbf{r}) = 2\pi C^2 e^{-r^2} \left\{ \sqrt{\pi} e^{-\frac{1}{2}r^2} \left[ (1+r^2) I_0\left(\frac{1}{2}r^2\right) + r^2 I_1\left(\frac{1}{2}r^2\right) \right] + (2+r^2) \right\}, \quad (\text{B1})$$

with  $C^2 = 1/\pi^2(3+2\pi)$ , and where  $I_0(x)$  and  $I_1(x)$  are the zeroth- and first-order modified Bessel functions  $I_\nu(x)$  [18] with

$$I_\nu(x) = \sum_{n=0}^{\infty} \frac{1}{n! \Gamma(n+\nu+1)} \left(\frac{1}{2}x\right)^{2n+\nu} \quad (\text{B2})$$

and  $\Gamma(x)$  the Gamma function [18]. The asymptotic structure of  $\rho(r)$  near the nucleus is

$$\rho(r) \underset{r \rightarrow 0}{\sim} \frac{2}{\pi(3+\sqrt{2\pi})} \left\{ 2 + \sqrt{\pi} - \left(1 + \frac{1}{2}\sqrt{\pi}\right)r^2 - \frac{1}{16}\sqrt{\pi}r^4 + \dots \right\}, \quad (\text{B3})$$

with

$$\rho(0) = 0.436132 \text{ a.u.} \quad (\text{B4})$$

Employing the asymptotic behavior of the Bessel functions:

$$I_0(z) \underset{r \rightarrow \infty}{\sim} \frac{e^z}{\sqrt{2\pi z}} \sum_{n=0}^{\infty} \frac{(-1)^n}{(2z)^n} \frac{\Gamma(n+\frac{1}{2})}{n! \Gamma(-n+\frac{1}{2})} + \frac{e^{-z}}{\sqrt{2\pi z}} \sum_{n=0}^{\infty} \frac{i}{(2z)^n} \frac{\Gamma(n+\frac{1}{2})}{n! \Gamma(-n+\frac{1}{2})}, \quad (\text{B5})$$

and

$$I_1(z) \underset{r \rightarrow \infty}{\sim} \frac{e^z}{\sqrt{2\pi z}} \sum_{n=0}^{\infty} \frac{(-1)^n}{(2z)^n} \frac{\Gamma(n+\frac{3}{2})}{n! \Gamma(-n+\frac{3}{2})} - \frac{e^{-z}}{\sqrt{2\pi z}} \sum_{n=0}^{\infty} \frac{i}{(2z)^n} \frac{\Gamma(n+\frac{3}{2})}{n! \Gamma(-n+\frac{3}{2})}, \quad (\text{B6})$$

the asymptotic structure of the density in the classically forbidden region is

$$\rho(r) \underset{r \rightarrow \infty}{\sim} \frac{2}{\pi(3+\sqrt{2\pi})} e^{-r^2} \left\{ r^2 + 2r + 2 + \frac{1}{2r} + \frac{1}{16r^3} + \dots \right\}. \quad (\text{B7})$$

### 2. Pair-correlation density $g(\mathbf{r}\mathbf{r}')$

$$g(\mathbf{r}\mathbf{r}') = \frac{2C^2(1+R)^2 e^{-(r^2+r'^2)}}{\rho(\mathbf{r})} \quad (\text{B8})$$

where  $R = |\mathbf{r} - \mathbf{r}'|$ .

### 3. Single-particle density matrix $\gamma(\mathbf{r}\mathbf{r}')$

$$\gamma(\mathbf{r}\mathbf{r}') = 2C^2 e^{-\frac{1}{2}(r^2+r'^2)} \int (1+|\mathbf{r}-\mathbf{y}|)(1+|\mathbf{r}'-\mathbf{y}|) d\mathbf{y} \quad (\text{B9})$$

#### 4. Dirac Density matrix $\gamma_s(\mathbf{r}\mathbf{r}')$

$$\gamma_s = \sqrt{\rho(\mathbf{r})\rho(\mathbf{r}')} \quad (\text{B10})$$

#### 5. Electron-interaction field $\mathcal{E}_{ee}(\mathbf{r})$

$$\mathcal{E}_{ee}(\mathbf{r}) = \frac{2\pi^{\frac{3}{2}}C^2}{\rho(\mathbf{r})} \frac{\mathbf{r}}{r} e^{-\frac{3}{2}r^2} [2I_{\frac{1}{2}}(\frac{1}{2}r^2) + \frac{3r}{2}I_0(\frac{1}{2}r^2) - \frac{r}{2}I_1(\frac{1}{2}r^2)] \quad (\text{B11})$$

#### 6. Electron-interaction energy $E_{ee}$

$$E_{ee} = 4\pi^{\frac{5}{2}}C^2 \int_0^\infty r^2 e^{-\frac{3}{2}r^2} [2I_{\frac{1}{2}}(\frac{1}{2}r^2) + \frac{3r}{2}I_0(\frac{1}{2}r^2) - \frac{r}{2}I_1(\frac{1}{2}r^2)] dr \quad (\text{B12})$$

$$= 4\pi^{\frac{5}{2}}C^2 \left[ \frac{\sqrt{2\pi}}{4} + \frac{1}{2} \right] = 0.818401 \text{ a.u.} \quad (\text{B13})$$

#### 7. Kinetic energy tensor $t_{\alpha\beta}(\mathbf{r}; \gamma)$

$$t_{\alpha\beta}(\mathbf{r}; \gamma) = \frac{r_\alpha r_\beta}{r^2} f(r) + \delta_{\alpha\beta} k(r), \quad (\text{B14})$$

where

$$f(r) = \pi C^2 e^{-r^2} \left\{ r^4 + 1 - \frac{1 - e^{-r^2}}{r^2} + \sqrt{\pi} e^{-r^2/2} \left[ r^4 I_0(\frac{1}{2}r^2) + (r^4 - r^2) I_1(\frac{1}{2}r^2) \right] \right\}, \quad (\text{B15})$$

and

$$k(r) = \pi C^2 e^{-r^2} \frac{(1 - e^{-r^2})}{2r^2}. \quad (\text{B16})$$

#### 8. Kinetic energy tensor $t_{s,\alpha\beta}(\mathbf{r}; \gamma_s)$

$$t_{s,\alpha\beta}(\mathbf{r}; \gamma_s) = \frac{r_\alpha r_\beta}{r^2} h(r), \quad (\text{B17})$$

where

$$h(r) = \frac{1}{8\rho(r)} \left( \frac{\partial \rho}{\partial r} \right)^2. \quad (\text{B18})$$

### 9. Kinetic ‘force’ $z_\alpha(\mathbf{r}; \gamma)$

$$\begin{aligned}
z_\alpha(\mathbf{r}; [\gamma]) &= 2 \sum_\beta \nabla_\beta t_{\alpha\beta}(\mathbf{r}; [\gamma]) = \frac{2r_\alpha}{r} \left[ \frac{\partial(f(r) + k(r))}{\partial r} + \frac{f(r)}{r} \right] \\
&= \frac{2\pi C^2 r_\alpha}{r} e^{-r^2} \left\{ [-2r^5 + 5r^3 - 2r + \frac{2(1 - e^{-r^2})}{r}] \right. \\
&\quad \left. + \sqrt{\pi} e^{-r^2/2} [(-2r^5 + 4r^3)I_0(\frac{r^2}{2}) + (-2r^5 + 6r^3 - r)I_1(\frac{r^2}{2})] \right\}.
\end{aligned} \tag{B19}$$

$$z(r) \underset{r \rightarrow \infty}{\sim} 2\pi C^2 e^{-r^2} (-2r^5 - 4r^4 + 5r^3 + 11r^2 - 2r - \frac{33}{8} + \frac{2}{r} - \frac{15}{33r^2} + \frac{6}{r^3}) \tag{B20}$$

$$z(r) \underset{r \rightarrow 0}{\sim} 2\pi C^2 \left[ (4 + \frac{15}{4}\sqrt{\pi})r^3 - (\frac{17}{3} - \frac{49}{8}\sqrt{\pi})r^5 \right]. \tag{B21}$$

### 10. Kinetic ‘force’ $z_{s,\alpha}(\mathbf{r}; \gamma_s)$

$$z_{s,\alpha}(\mathbf{r}; [\gamma_s]) = 2 \sum_\beta \nabla_\beta t_{\alpha\beta}(\mathbf{r}; [\gamma_s]) = \frac{r_\alpha}{2r\rho} \left( \frac{\partial \rho}{\partial r} \right) \left[ -\frac{1}{2\rho} \left( \frac{\partial \rho}{\partial r} \right)^2 + \frac{\partial^2 \rho}{\partial r^2} + \frac{1}{2r} \left( \frac{\partial \rho}{\partial r} \right) \right]. \tag{B22}$$

$$z_s(r) \underset{r \rightarrow \infty}{\sim} 2\pi c^2 e^{-r^2} (-2r^5 - 4r^4 + 5r^3 + 11r^2 - 2r - \frac{33}{8} + \frac{5}{r} - \frac{15}{33r^2} - \frac{5}{r^3}). \tag{B23}$$

$$z_s(r) \underset{r \rightarrow 0}{\sim} 0.33r + 0.40r^3 - 0.76r^5. \tag{B24}$$

### 11. Kinetic Energy $T$

$$T = 2\pi^2 C^2 \left[ \frac{3}{2} + \frac{3}{8}\sqrt{2\pi} \right] = 0.886199 \text{ a.u.} \tag{B25}$$

### 12. External Energy $E_{ext}$

$$E_{ext} = \int \rho(r) \frac{r^2}{2} d\mathbf{r} = 2\pi^2 C^2 \left[ 2 + \frac{5\sqrt{2\pi}}{8} \right] = 1.295400 \text{ a.u.} \tag{B26}$$

### 13. Electron-interaction potential $W_{ee}(\mathbf{r})$

$$W_{ee}(\mathbf{r}) = -2\pi^{\frac{3}{2}} C^2 \int_\infty^r \frac{1}{\rho(y)} e^{-\frac{3}{2}y^2} \left[ 2I_{\frac{1}{2}}(\frac{y^2}{2}) + \frac{3}{2}yI_0(\frac{y^2}{2}) - \frac{1}{2}yI_1(\frac{y^2}{2}) \right] dy. \tag{B27}$$

$$W_{ee}(0) = 1.217891 \text{ a.u.} \tag{B28}$$

#### 14. Hartree potential $W_H(r)$

In two-dimensions the term  $1/|\mathbf{r} - \mathbf{r}'|$  can be rewritten as

$$\begin{aligned} \frac{1}{|\mathbf{r} - \mathbf{r}'|} &= \frac{4}{\pi} \int_0^\infty \left\{ \frac{1}{2} I_0(kr_{<}) K_0(kr_{>}) + \sum_{m=1}^\infty \cos[m(\phi - \phi')] I_m(kr_{<}) K_m(kr_{>}) \right\} \\ &= \frac{4}{\pi} \left\{ \frac{1}{2r_{>}} K\left(\frac{r_{<}^2}{r_{>}^2}\right) + \sum_{m=1}^\infty \sqrt{\pi} \Gamma\left(m + \frac{1}{2}\right) \left(\frac{r_{<}^2}{r_{>}^2}\right)^m \cos[m(\phi - \phi')] \right. \\ &\quad \left. \times {}_2F_1\left(\frac{1}{2}, \frac{1}{2} + m, m + 1; \frac{r_{<}^2}{r_{>}^2}\right) \frac{1}{2r_{>} \Gamma(m + 1)} \right\}, \end{aligned} \quad (\text{B29})$$

where  $r_{<}(r_{>})$  is the smaller (larger) of  $r$  and  $r'$ ,  $I_i$  and  $K_i$  are the modified Bessel functions of  $i$ -th order,  ${}_2F_1(a, b, c; x)$  is the Hypergeometric function [18], and  $K(x)$  is the complete elliptic integral of the first kind [18]

$$K(k) = \int_0^1 dt [(1 - t^2)(1 - kt^2)]^{-1/2} = \frac{\pi}{2} {}_2F_1\left(\frac{1}{2}, \frac{1}{2}, 1; k\right). \quad (\text{B30})$$

Using the above equations and performing the angular integral, we obtain

$$\begin{aligned} W_H(\mathbf{r}) &= \int \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' \\ &= 4 \int_0^r dr' \frac{r'}{r} \rho(r') K\left(\frac{r'^2}{r^2}\right) + 4 \int_r^\infty dr' \rho(r') K\left(\frac{r^2}{r'^2}\right). \end{aligned} \quad (\text{B31})$$

#### 15. Expectations

$$\begin{aligned} \langle r \rangle &= \int \rho(r) r d\mathbf{r} \\ &= 4\pi^2 c^2 \int e^{-r^2} \{ 2r^2 + r^4 + \sqrt{\pi} e^{-\frac{1}{2}} [(r^2 + r^4) I_0\left(\frac{1}{2}r^2\right) + r^4 I_1\left(\frac{1}{2}r^2\right)] \} dr \\ &= 4\pi^2 c^2 \left[ \frac{7}{8} \sqrt{\pi} + \frac{\sqrt{6}\pi}{18} ({}_2F_1\left(\frac{3}{4}, \frac{5}{4}, 1, \frac{1}{9}\right) + {}_2F_1\left(\frac{5}{4}, \frac{7}{4}, 1, \frac{1}{9}\right)) + \frac{5\sqrt{6}\pi}{36} {}_2F_1\left(\frac{7}{4}, \frac{9}{4}, 1, \frac{1}{9}\right) \right] \\ &= 2.037 \, 89 \, a.u. \end{aligned} \quad (\text{B32})$$

$$\begin{aligned} \langle r^2 \rangle &= \int \rho(r) r^2 d\mathbf{r} \\ &= 4\pi^2 c^2 \int e^{-r^2} \{ 2r^3 + r^5 + \sqrt{\pi} e^{-\frac{1}{2}} [(r^3 + r^5) I_0\left(\frac{1}{2}r^2\right) + r^5 I_1\left(\frac{1}{2}r^2\right)] \} dr \\ &= 4\pi^2 c^2 \left[ 2 + \frac{3\sqrt{\pi}}{8\sqrt{2}} + \frac{19\sqrt{\pi}}{32\sqrt{2}} + \frac{9\sqrt{\pi}}{32\sqrt{2}} \right] \\ &= 4\pi^2 c^2 \left[ 2 + \frac{5\sqrt{2}\pi}{8} \right] \\ &= 2.590 \, 8 \, a.u. \end{aligned} \quad (\text{B33})$$



$$\begin{aligned}
\langle \frac{1}{r} \rangle &= \int \rho(r) \frac{1}{r} d\mathbf{r} \\
&= 4\pi^2 c^2 \int e^{-r^2} \{2 + r^2 + \sqrt{\pi} e^{-\frac{1}{2}} [(1 + r^2) I_0(\frac{1}{2} r^2) + r^2 I_1(\frac{1}{2} r^2)]\} dr \\
&= 4\pi^2 c^2 [\frac{5}{4} \sqrt{\pi} + \frac{\sqrt{6}}{6} \pi_2 F_1(\frac{1}{4}, \frac{3}{4}, 1, \frac{1}{9}) + \frac{\sqrt{6}}{18} \pi_2 F_1(\frac{3}{4}, \frac{5}{4}, 1, \frac{1}{9}) + \frac{\sqrt{6}}{72} \pi_2 F_1(\frac{5}{4}, \frac{7}{4}, 1, \frac{1}{9})] \\
&= 2.996\,87\, a.u.
\end{aligned} \tag{B34}$$

$$\langle \delta(\mathbf{r}) \rangle = \rho(0) = 2\pi C^2 [2 + \sqrt{\pi}] = 0.436132 \text{ a.u.} \tag{B35}$$

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