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Wigner high-electron-correlation regime of nonuniform density systems: A quantal-density-functional-theory study

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The Wigner regime of a system of electrons in an external field is characterized by a low electron density and a high electron-interaction energy relative to the kinetic energy. The low-correlation regime is in turn described by a high electron density and an electron-interaction energy smaller than the kinetic energy. The Wigner regime of a nonuniform-electron-density system is investigated via quantal density functional theory (QDFT). Within QDFT, the contributions of electron correlations due to the Pauli exclusion principle, Coulomb repulsion, and correlation-kinetic effects are separately delineated and explicitly defined. The nonuniform-electron-density system studied is that of the Hooke's atom in the Wigner regime, for which the exact wave function is derived. As such, the results of the QDFT analysis are exact. It is observed that in comparison to the low-correlation case, not only is the electron-interaction energy greater than the kinetic energy as a fraction of the total energy, but so are its individual Hartree, Pauli, and Coulomb components. The ionization potential as a fraction of the total energy too is greater. But most significantly, in the Wigner regime, the correlation-kinetic energy as a fraction of both the electron-interaction and the total energy is substantially greater than in the low-correlation case. Hence, we propose that the Wigner regime now also be characterized by a high correlation-kinetic energy. The kinetic energy as a fraction of the total energy, however, is less than in the low-correlation case. This fact and the high correlation-kinetic energy value in the Wigner regime is explained by the concept of "quantal compression" of the kinetic energy density derived from QDFT. The corresponding results for the low-correlation case are in turn a consequence of a "quantal decompression" of the kinetic energy density. From the QDFT analysis, the exact values for the Kohn-Sham theory "exchange-correlation" and "correlation" energy functionals of the density and their respective functional derivatives are also obtained. These results ought to be of value in the construction and testing of approximate energy functionals valid for the Wigner regime.

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I. INTRODUCTION

The state of matter comprised of a low-electron-density gas in the presence of an external field $\mathcal{F}^{\text{ext}} = -\nabla v(\mathbf{r})$ due to a neutralizing uniform positive charge (jellium) background was originally proposed by Wigner [1,2]. As the electron density becomes lower, the kinetic energy of the electrons becomes negligible in comparison to the electron-interaction potential energy. It is the latter term of the Hamiltonian that then dominates in the determination of the wave function and leads to a crystallization of the electronic assembly into a body-centered cubic structure. The difference between the energy per particle for this structure [2,3] compared to the value for the cubic [4], face-centered cubic [3], and hexagonal [5] structures is very small. In his work, Wigner also determined the correction to the energy due to the zero-point oscillations of the electrons about the lattice points. The Wigner regime of the electron gas is thus characterized in the literature by a low electronic density and an electron-interaction energy that is much greater than the kinetic energy. This state of matter has been observed experimentally in a two-dimensional (2D) electron gas on the surface of liquid helium and in GaAs-GaAlAs heterostructures in the presence of strong magnetic fields [6–9].

Since the original papers by Wigner, there has been considerable work done on this and other systems in this

regime. Carr [4] extended Wigner's work by taking account of lattice vibrations to determine the energy, specific heat, and magnetic properties. There have been many studies, more recently employing quantum Monte Carlo methods, on the determination of the transition density for the onset of Wigner crystallization [10–13]. An atomic model that also allows for study of the Wigner regime is the Hooke's atom [14–16]. The atom is comprised of two electrons that interact Coulombically but are confined harmonically. The Wigner regime is achieved in this model for weak confinement. For this model atom, closed-form analytical solutions for the wave function can be obtained [16] for both ground and excited states for a denumerably infinite set of harmonic force constants. There has also been work employing this model [16–20] to determine the critical force constant k for transition to this regime ($k_{\text{crit}} \approx 1.6093 \times 10^{-3}$) and analysis in the limit of vanishing force constant.

The Wigner regime of a nonuniform electron gas has also been addressed within the context of Kohn-Sham (KS) density functional theory (DFT) [21]. It turns out that the available approximations for the KS "exchange-correlation" energy functional fail in this regime [22]. As stated by Malet and Gori-Giorgi [23],

Indeed, it is very counterintuitive that strongly correlated systems, in which the electron-electron repulsion plays a prominent role, can be exactly represented in terms of noninteracting electrons. For this reason, several authors have used accurate many-body solutions of prototypical strongly

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correlated systems to obtain (by inversion) and characterize the exact noninteracting KS system. These works make it all the more evident how difficult it is to find adequate approximations of the exact KS system, so that, albeit theoretically possible, it may seem unrealistic to describe strongly correlated systems with KS DFT.

More recently, the strictly correlated electron functional [24–31] has been related [22,23] to KS DFT, and the new framework applied to various systems such as 2D quantum dots [22]. For work on the construction of energy functionals based on the calibration of results on the spin- and spatially-symmetrized open-shell atoms in the first to third rows see [32] and references therein.

In this paper, we perform an analysis of the electron correlations in the Wigner regime of a nonuniform-electron-density system as described by the Hooke’s atom via quantal density functional theory (QDFT) [33,34]. (Also see [33] and [34] for references to the original literature.) QDFT provides the mapping, based on the “quantal Newtonian” first law [33–35], from the interacting system in any state, ground or excited, to a model system of noninteracting fermions with the same electronic density. The state of the model system to which the mapping is performed is arbitrary. With the assumption of the existence of the model system, the mapping described via QDFT is *direct*. In the present work, we map from the ground state of the Hooke’s atom to a model system also in its ground state. (The choice of density for the equivalence follows from the Hohenberg-Kohn theorem, according to which the nondegenerate ground-state density is a basic variable of quantum mechanics [36,37]. Knowledge of the density, a gauge-invariant property, uniquely determines the external potential, thereby the Hamiltonian and, by solution of the Schrödinger equation, the wave function.) The QDFT description is in terms of quantal sources that are expectations of Hermitian operators or of their complex sums. These quantal sources lead to “classical” fields that are representative of the different electron correlations that must be accounted for in the mapping, viz., those due to the Pauli exclusion principle, Coulomb repulsion, and correlation-kinetic effects. As in classical physics, the local effective potential of the model fermions is obtained as the work done on these fermions in the force of a *conservative effective field* which is the sum of the individual fields. The components of the total energy are in turn determined, again as in classical physics, via the corresponding integral virial expressions in terms of the individual fields. Within QDFT, the contributions of the different correlations to the local effective potential of the model fermions, and to the total energy, are *separately* delineated and *explicitly* defined.

In a short communication [38] based on our present work, and with a focus on the kinetic and correlation-kinetic aspects, two additional results that differ significantly from prior understandings were noted. First, there is a “quantal compression” of the kinetic energy density (KED) towards and about the nucleus in the Wigner regime. This explains the lowering of the kinetic energy as a fraction of the total energy. (In the low-electron-correlation regime, there is a “quantal decompression” of the KED away from the nucleus. The terminology quantal compression and quantal decompression is employed because the source of the kinetic energy, viz., the

single-particle density matrix, is quantum mechanical in nature in that it is the expectation of a complex sum of Hermitian operators taken with respect to the system wave function.) Second, the correlation-kinetic energy as a fraction of both the electron-interaction and the total energy was discovered to be large. Thus, we proposed that the Wigner regime be characterized not only by a high electron-interaction energy compared to the kinetic energy, but also by a high value of the correlation-kinetic energy. The details of the derivation of these results are given in the present work.

In Sec. II we provide the general equations of time-independent QDFT. In Sec. III the interacting Wigner system is described. The system Hamiltonian, together with the analytical expression for the *exact* wave function derived, and the corresponding orbitals of the model system are given. The quantal sources, the resulting fields, and the potentials and energies that arise from these fields are presented in Secs. IV–VI, respectively. An analysis of the results is provided in Sec. VII. Concluding remarks are made and future work described in Sec. VIII.

The calculations are performed numerically. For this purpose, we have developed accurate codes employing, in particular, the Fourier and Chebyshev pseudospectral method [39,40]. This allows for the accurate determination of nonlocal quantal sources and up to third-order derivatives of these sources. The details of the code and of the accuracy achieved by it are given elsewhere [41]. One purpose of developing these programs is to employ them in fully self-consistent calculations in the future as described in [34].

II. QUANTAL DENSITY FUNCTIONAL THEORY

The equations of QDFT are derived from the “quantal Newtonian” first law for the interacting and the model noninteracting fermion systems. For details of the derivation and references to the original literature, see [33] and [34].

Consider a system of N electrons in an external field $\mathcal{F}^{\text{ext}} = -\nabla v(\mathbf{r})$. The Schrödinger equation for this system is (in atomic units $e = \hbar = m = 1$)

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

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

$$\hat{H} = \hat{T} + \hat{U} + \hat{V}, \quad (2)$$

with $\hat{T} = -\frac{1}{2} \sum_i \nabla_i^2$, $\hat{U} = \frac{1}{2} \sum_{i,j}' 1/|\mathbf{r}_i - \mathbf{r}_j|$, $\hat{V} = \sum_i v(\mathbf{r}_i)$; $\Psi(\mathbf{X})$, and E the eigenfunctions and eigenvalues, and where $\mathbf{X} = \mathbf{x}_1, \dots, \mathbf{x}_N$, with $\mathbf{x} = \mathbf{r}\sigma$ the spatial and spin coordinates. In QDFT, this interacting system is mapped into one of noninteracting fermions having the same density $\rho(\mathbf{r})$ and the same external potential $v(\mathbf{r})$. The corresponding Schrödinger equation for these model fermions is then

$$\left(-\frac{1}{2}\nabla^2 + v(\mathbf{r}) + v_{ee}(\mathbf{r})\right)\phi_i(\mathbf{x}) = \epsilon_i\phi_i(\mathbf{x}), \quad i = 1, \dots, N, \quad (3)$$

where $\phi_i(\mathbf{x})$ and ϵ_i are the corresponding single-particle orbitals and eigenvalues. The wave function of the model system is a Slater determinant $\Phi\{\phi_i\}$ of these orbitals, which are not necessarily all in the lowest occupied states [33,34]. The

many-body correlations due to the Pauli exclusion principle, Coulomb repulsion, and correlation-kinetic effects that must be accounted for in the mapping are incorporated in the local electron-interaction potential $v_{ee}(\mathbf{r})$. This potential is the work done to move the model fermion from a reference point at infinity to its position at $\mathbf{r}$ in the force of a conservative effective field $\mathcal{F}^{\text{eff}}(\mathbf{r})$:

$$v_{ee}(\mathbf{r}) = - \int_{\infty}^{\mathbf{r}} \mathcal{F}^{\text{eff}}(\mathbf{r}') \cdot d\ell', \quad \nabla \times \mathcal{F}^{\text{eff}}(\mathbf{r}) = 0. \quad (4)$$

The work done is thus path independent. The effective field $\mathcal{F}^{\text{eff}}(\mathbf{r})$ experienced by the model fermion,

$$\mathcal{F}^{\text{eff}}(\mathbf{r}) = \mathcal{E}_{ee}(\mathbf{r}) + \mathcal{Z}_{tc}(\mathbf{r}), \quad (5)$$

is the sum of an electron-interaction field $\mathcal{E}_{ee}(\mathbf{r})$ representative of Pauli and Coulomb correlations and a correlation-kinetic field $\mathcal{Z}_{tc}(\mathbf{r})$ representative of the difference in kinetic energy between the interacting and model systems. The $\mathcal{E}_{ee}(\mathbf{r})$ field can be written in terms of its Hartree $\mathcal{E}_H(\mathbf{r})$, Pauli $\mathcal{E}_x(\mathbf{r})$, and Coulomb $\mathcal{E}_c(\mathbf{r})$ components, so that

$$\mathcal{F}^{\text{eff}}(\mathbf{r}) = \mathcal{E}_H(\mathbf{r}) + \mathcal{E}_x(\mathbf{r}) + \mathcal{E}_c(\mathbf{r}) + \mathcal{Z}_{tc}(\mathbf{r}). \quad (6)$$

For systems of special symmetry, such as that considered in the present work, these individual fields are separately conservative. Therefore, the potential $v_{ee}(\mathbf{r})$ can be expressed as the sum of the work done in each field,

$$v_{ee}(\mathbf{r}) = W_H(\mathbf{r}) + W_x(\mathbf{r}) + W_c(\mathbf{r}) + W_{tc}(\mathbf{r}), \quad (7)$$

the notation being evident. Each work done is then path independent. The electron-interaction E_{ee} and correlation-kinetic T_c energies can in turn be expressed in terms of the fields $\mathcal{E}_{ee}(\mathbf{r})$ and $\mathcal{Z}_{tc}(\mathbf{r})$ in integral virial form as [33]

$$E_{ee} = \int \rho(\mathbf{r}) \mathbf{r} \cdot \mathcal{E}_{ee}(\mathbf{r}) d\mathbf{r} = E_H + E_x + E_c, \quad (8)$$

$$T_c = \frac{1}{2} \int \rho(\mathbf{r}) \mathbf{r} \cdot \mathcal{Z}_{tc}(\mathbf{r}) d\mathbf{r}, \quad (9)$$

where E_H , E_x , and E_c are the Hartree, Pauli, and Coulomb energy components, respectively, arising from their respective fields. The total energy of the interacting system is then

$$E = T_s + E_{\text{ext}} + E_H + E_x + E_c + T_c, \quad (10)$$

where

$$T_s = \langle \Phi\{\phi_i\} | \hat{T} | \Phi\{\phi_i\} \rangle, \quad (11)$$

$$E_{\text{ext}} = \int \rho(\mathbf{r}) v(\mathbf{r}) d\mathbf{r}. \quad (12)$$

The expressions for the energy components are independent of whether or not the individual fields are conservative.

The electron-interaction field $\mathcal{E}_{ee}(\mathbf{r})$ is defined as

$$\mathcal{E}_{ee}(\mathbf{r}) = \frac{\mathbf{e}_{ee}(\mathbf{r})}{\rho(\mathbf{r})}, \quad (13)$$

where the electron-interaction “force” $\mathbf{e}_{ee}(\mathbf{r})$ is obtained via Coulomb’s law from its quantal source, the pair-correlation

function $P(\mathbf{r}\mathbf{r}')$:

$$\mathbf{e}_{ee}(\mathbf{r}) = \int \frac{P(\mathbf{r}\mathbf{r}')(\mathbf{r} - \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|^3} d\mathbf{r}'. \quad (14)$$

The correlation-kinetic field $\mathcal{Z}_{tc}(\mathbf{r})$ is defined as

$$\mathcal{Z}_{tc}(\mathbf{r}) = \frac{\mathbf{z}_{tc}(\mathbf{r})}{\rho(\mathbf{r})}, \quad (15)$$

where the correlation-kinetic force is obtained from its quantal source, the difference between the single-particle $\gamma(\mathbf{r}\mathbf{r}')$ and the Dirac $\gamma_s(\mathbf{r}\mathbf{r}')$ density matrices, as

$$z_{tc,\alpha}(\mathbf{r}) = 2 \sum_{\beta} \frac{\partial}{\partial r_{\beta}} t_{c,\alpha\beta}(\mathbf{r}), \quad (16)$$

where the tensor $t_{c,\alpha\beta}(\mathbf{r})$ is

$$t_{c,\alpha\beta}(\mathbf{r}) = \frac{1}{4} \left[\frac{\partial^2}{\partial r'_{\alpha} \partial r''_{\beta}} + \frac{\partial^2}{\partial r'_{\beta} \partial r''_{\alpha}} \right] [\gamma_s(\mathbf{r}'\mathbf{r}'') - \gamma(\mathbf{r}'\mathbf{r}'')]_{\mathbf{r}'=\mathbf{r}''=\mathbf{r}}. \quad (17)$$

The quantal sources are the density $\rho(\mathbf{r})$,

$$\rho(\mathbf{r}) = \langle \Psi(\mathbf{X}) | \hat{\rho}(\mathbf{r}) | \Psi(\mathbf{X}) \rangle = \langle \Phi\{\phi_i\} | \hat{\rho}(\mathbf{r}) | \Phi\{\phi_i\} \rangle, \quad (18)$$

the pair-correlation function $P(\mathbf{r}\mathbf{r}')$,

$$P(\mathbf{r}\mathbf{r}') = \langle \Psi(\mathbf{X}) | \hat{P}(\mathbf{r}\mathbf{r}') | \Psi(\mathbf{X}) \rangle, \quad (19)$$

and the single-particle $\gamma(\mathbf{r}\mathbf{r}')$ and Dirac $\gamma_s(\mathbf{r}\mathbf{r}')$ density matrices,

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

$$\gamma_s(\mathbf{r}\mathbf{r}') = \langle \Phi\{\phi_i\} | \hat{\gamma}(\mathbf{r}\mathbf{r}') | \Phi\{\phi_i\} \rangle. \quad (21)$$

The corresponding Hermitian or complex sum of Hermitian operators from which these quantal sources are obtained is

$$\hat{\rho}(\mathbf{r}) = \sum_i \delta(\mathbf{r}_i - \mathbf{r}), \quad (22)$$

$$\hat{P}(\mathbf{r}\mathbf{r}') = \sum_{i,j} \delta(\mathbf{r}_i - \mathbf{r}) \delta(\mathbf{r}_j - \mathbf{r}'), \quad (23)$$

$$\hat{\gamma}(\mathbf{r}\mathbf{r}') = \hat{A} + i\hat{B}, \quad (24)$$

$$\hat{A} = \frac{1}{2} \sum_j [\delta(\mathbf{r}_j - \mathbf{r}) T_j(\mathbf{a}) + \delta(\mathbf{r}_j - \mathbf{r}') T_j(-\mathbf{a})], \quad (25)$$

$$\hat{B} = -\frac{i}{2} \sum_j [\delta(\mathbf{r}_j - \mathbf{r}) T_j(\mathbf{a}) - \delta(\mathbf{r}_j - \mathbf{r}') T_j(-\mathbf{a})], \quad (26)$$

where $T_j(\mathbf{a})$ is a translation operator such that $T_j(\mathbf{a}) \psi(\mathbf{r}_1, \dots, \mathbf{r}_j, \dots, \mathbf{r}_N) = \psi(\mathbf{r}_1, \dots, \mathbf{r}_j + \mathbf{a}, \dots, \mathbf{r}_N)$, and $\mathbf{a} = \mathbf{r}' - \mathbf{r}$.

The field $\mathcal{E}_{ee}(\mathbf{r})$ may also be thought of as being due to the quantal source of the pair-correlation density $g(\mathbf{r}\mathbf{r}')$,

$$g(\mathbf{r}\mathbf{r}') = \frac{P(\mathbf{r}\mathbf{r}')}{\rho(\mathbf{r})} = \rho(\mathbf{r}') + \rho_{xc}(\mathbf{r}\mathbf{r}') \quad (27)$$

$$= \rho(\mathbf{r}') + \rho_x(\mathbf{r}\mathbf{r}') + \rho_c(\mathbf{r}\mathbf{r}'), \quad (28)$$

where $\rho_{xc}(\mathbf{r}\mathbf{r}')$, $\rho_x(\mathbf{r}\mathbf{r}')$, and $\rho_c(\mathbf{r}\mathbf{r}')$ are, respectively, the Fermi-Coulomb, Fermi, and Coulomb hole charge

FIG. 1. (Color online) Structure of the ground-state wave function $\Psi(\mathbf{r}\mathbf{r}')$ in the high-correlation regime for $\theta_{\mathbf{r}\mathbf{r}'} = 0^\circ$, where $\theta_{\mathbf{r}\mathbf{r}'}$ is the angle between vector $\mathbf{r}$ and vector $\mathbf{r}'$. Vectors $\mathbf{r}$ and $\mathbf{r}'$ are oriented along either the positive or the negative z axis.

distributions. The latter two are, in turn, defined as

$$\rho_x(\mathbf{r}\mathbf{r}') = -|\gamma_s(\mathbf{r}\mathbf{r}')|^2/2\rho(\mathbf{r}), \quad (29)$$

$$\rho_c(\mathbf{r}\mathbf{r}') = \rho_{xc}(\mathbf{r}\mathbf{r}') - \rho_x(\mathbf{r}\mathbf{r}'). \quad (30)$$

The density $\rho(\mathbf{r})$, Fermi hole $\rho_x(\mathbf{r}\mathbf{r}')$, and Coulomb hole $\rho_c(\mathbf{r}\mathbf{r}')$ then constitute the quantal sources for the Hartree $\mathcal{E}_H(\mathbf{r})$, Pauli $\mathcal{E}_x(\mathbf{r})$, and Coulomb $\mathcal{E}_c(\mathbf{r})$ fields.

III. WIGNER SYSTEM

The system we employ to study the Wigner regime of a nonuniform-electron-density gas is the Hooke's atom [16], for which the external potential in the Hamiltonian of Eq. (2) is

$$\hat{V} = \frac{k}{2} \sum_{i=1}^2 r_i^2, \quad (31)$$

with $k = 3.00891 \times 10^{-4}$. The corresponding *exact* spatial part of the singlet ground-state wave function is derived to be

$$\Psi(\mathbf{r}\mathbf{r}') = N e^{-\omega R^2} e^{-\frac{1}{4}\omega s^2} \left[1 + \frac{s}{2} + \sum_{j=2}^4 a_j \left(s \sqrt{\frac{\omega}{2}} \right)^j \right], \quad (32)$$

where $\mathbf{R} = (\mathbf{r} + \mathbf{r}')/2$, $\mathbf{s} = \mathbf{r} - \mathbf{r}'$, $N = 8.94669 \times 10^{-6}$, $\omega = \sqrt{k} = 1.73462 \times 10^{-2}$, $a_2 = 8.274917$, $a_3 = 4.720056$, and $a_4 = 0.879153$. In Figs 1 and 2 we plot the wave function for $\theta_{\mathbf{r}\mathbf{r}'} = 0^\circ$, where $\theta_{\mathbf{r}\mathbf{r}'}$ is the angle between vector $\mathbf{r}$ and vector $\mathbf{r}'$. Vectors $\mathbf{r}$ and $\mathbf{r}'$ are oriented along either the positive or the negative z axis. As the Hooke's atom is the interacting system, the corresponding wave function $\Psi(\mathbf{r}\mathbf{r}')$ must satisfy the electron-electron coalescence [33,34,42–47]

FIG. 2. (Color online) Same as Fig. 1 but showing only the $r > 0$ and $r' > 0$ quadrant.

condition, which in general is

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) = \Psi(\mathbf{r}_2, \mathbf{r}_2, \mathbf{r}_3, \dots, \mathbf{r}_N) \left(1 + \frac{s}{2} \right) + \mathbf{s} \cdot \mathbf{C}(\mathbf{r}_2, \mathbf{r}_3, \dots, \mathbf{r}_N) + O(s^2), \quad (33)$$

where $\mathbf{C}(\mathbf{r}_2, \mathbf{r}_3, \dots, \mathbf{r}_N)$ is an undetermined vector. Observe the cusp in Figs. 1 and 2 along $\mathbf{r} = \mathbf{r}'$. In Figs 3 and 4, the wave function is drawn for $\theta_{\mathbf{r}\mathbf{r}'} = 90^\circ$, where $\mathbf{r}$ is along the z axis and $\mathbf{r}'$ is in the x - y plane. The azimuthal symmetry is evident in Fig. 3. Also, observe the electron-electron cusp at $\mathbf{r} = \mathbf{r}' = 0$ in Fig. 4.

The mapping of the above interacting system is to a model system of noninteracting fermions also in a ground (singlet) state, but with the same density and hence also in the Wigner

FIG. 3. (Color online) Structure of the ground-state wave function $\Psi(\mathbf{r}\mathbf{r}')$ in the high-correlation regime for $\theta_{\mathbf{r}\mathbf{r}'} = 90^\circ$, where $\theta_{\mathbf{r}\mathbf{r}'}$ is the angle between vector $\mathbf{r}$ and vector $\mathbf{r}'$. Vector $\mathbf{r}$ is along the z axis, whereas vector $\mathbf{r}'$ lies in the x - y plane.

FIG. 4. (Color online) Same as Fig. 3, but showing only the $r > 0$ and $r' > 0$ quadrant.

regime. As such, the wave function $\Phi\{\phi_i\}$ of the latter is a Hartree product of the single-particle orbitals $\phi_i(\mathbf{r})$. It follows from Eq. (18) that the spatial part $\phi_i(\mathbf{r})$ of these orbitals is then

$$\phi_i(\mathbf{r}) = \sqrt{\rho(\mathbf{r})/2}, \quad i = 1, 2, \quad (34)$$

and hence solution of the model system differential equation is not required.

IV. QUANTAL SOURCES

In this section, we present the quantal sources of the density $\rho(\mathbf{r})$, Fermi hole $\rho_x(\mathbf{r}\mathbf{r}')$, Coulomb hole $\rho_c(\mathbf{r}\mathbf{r}')$, single-particle density $\gamma(\mathbf{r}\mathbf{r}')$, and Dirac $\gamma_s(\mathbf{r}\mathbf{r}')$ density matrices.

A. Density $\rho(\mathbf{r})$

In Fig 5(a) we plot the density $\rho(\mathbf{r})$. Observe the “fat attractor” profile characteristic of the Wigner regime: The maximum does not occur at the nucleus but farther away from it in the atom. The radial probability density $r^2\rho(\mathbf{r})$ is plotted in Fig. 5(b). The relative coordinate wave function $\phi(s)$ where

$$\phi(s) = N_s e^{-\frac{1}{4}\omega s^2} \left[1 + \frac{s}{2} + \sum_{j=2}^4 a_j \left(s \sqrt{\frac{\omega}{2}} \right)^j \right], \quad (35)$$

with $N_s = 2.626 \times 10^{-4}$, is plotted in Fig. 6(a), and the corresponding density $|\phi(s)|^2$ in Fig. 6(b). Observe the electron-electron cusp at the origin. The most probable separation is indicated by the arrow.

B. Fermi hole $\rho_x(\mathbf{r}\mathbf{r}')$

Employing the orbitals $\phi_i(\mathbf{r})$ of Eq. (34), the Fermi hole $\rho_x(\mathbf{r}\mathbf{r}')$ defined by Eq. (29) is then

$$\rho_x(\mathbf{r}\mathbf{r}') = -\rho(\mathbf{r}')/2 \quad (36)$$

and, in this case, is independent of electron position. Thus, it is a local (static) charge distribution. The Fermi hole is plotted in Fig 7. Observe that it is spherically symmetric about

FIG. 5. (a) Density $\rho(\mathbf{r})$ and (b) radial probability density $r^2\rho(\mathbf{r})$. The arrow indicates the maximum in the profile.

the nucleus, exhibiting a double-well structure. It satisfies the required constraints:

$$\int \rho_x(\mathbf{r}\mathbf{r}') d\mathbf{r}' = -1, \quad \rho_x(\mathbf{r}\mathbf{r}') \leq 0, \quad \rho_x(\mathbf{r}\mathbf{r}') = -\rho(\mathbf{r})/2. \quad (37)$$

It is worth noting, as might be expected, that the size of the Fermi hole is an order of magnitude larger than that for the low-correlation regime described by the force constant value of

FIG. 6. (a) Relative coordinate wave function $\phi(s)$ and (b) the corresponding density $|\phi(s)|^2$. The arrow indicates the most probable separation.

FIG. 7. Fermi hole charge distribution $\rho_x(\mathbf{r}\mathbf{r}')$.

$k = \frac{1}{4}$ [33,48]. This is a consequence of the wider distribution of the electron density due to the weaker confinement of the electrons.

C. Coulomb holes $\rho_c(\mathbf{r}\mathbf{r}')$

In Figs. 8–10 are plotted a cross section of the nonlocal (dynamic) Coulomb hole $\rho_c(\mathbf{r}\mathbf{r}')$ for electron positions at $r = 0, 1, 2, 10, 20, 40, 100$, and 200 a.u. The electron is on the z axis corresponding to $\theta = 0^\circ$. For the electron at the nucleus [Fig 8(a)], the hole has spherical symmetry. In both Figs. 8(a) and 8(b), the electron-electron coalescence cusp is clearly evident. The nonlocal structure of the Coulomb hole is also evident in Figs. 8(b)–10 for electron positions other than

FIG. 8. Cross section of the Coulomb holes for electron positions at (a) the nucleus at $r = 0$, and (b) at $r = 1$ a.u. The electron is on the z axis, corresponding to $\theta = 0^\circ$. Vector $\mathbf{r}'$ corresponds to a general point in the structure of the Coulomb hole. The $\mathbf{r}' < 0$ structure corresponds to $\theta' = \pi$, $r' > 0$. The $\mathbf{r}' > 0$ structure corresponds to $\theta' = 0^\circ$, $r' > 0$.

FIG. 9. Same as Fig. 8, but for electron positions at $r = 2$ and 10 a.u.

at the nucleus. Note the enhancement of the positive part of the Coulomb hole for $\mathbf{r}' < 0$ as the electron is moved farther away from the nucleus in Figs 9 and 10. By $r = 200$ a.u., the hole can be observed to again become spherically symmetric about the nucleus. It also tends towards becoming a more static charge distribution. This is rigorously the structure for asymptotic electron positions. For each electron position, the Coulomb hole satisfies the constraint

$$\int \rho_c(\mathbf{r}\mathbf{r}') d\mathbf{r}' = 0. \quad (38)$$

Although the broad characteristics of these holes are similar to those of the low-correlation case ($k = \frac{1}{4}$) [33,48], there are differences due to the large size of these holes in the high-correlation regime.

FIG. 10. Same as Fig. 8, but for electron positions at $r = 20, 40, 100$, and 200 a.u.

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

The reduced single-particle density matrix $\gamma(\mathbf{r}\mathbf{r}')$ of Eq. (20) for this case is

$$\gamma(\mathbf{r}'\mathbf{r}'') = 2 \int \Psi^*(\mathbf{r}\mathbf{r}')\Psi(\mathbf{r}\mathbf{r}'')d\mathbf{r}. \quad (39)$$

In general the vectors $\mathbf{r}$, $\mathbf{r}'$, and $\mathbf{r}''$ are situated in Cartesian space, which, in the absence of symmetry, implies a 9D computational solution. However, we can considerably reduce the dimensionality of the problem by taking advantage of the symmetry admitted by spherical density systems. This is realized by an orthogonal transformation of the Cartesian coordinate system whereby rotation about its origin places the z axis along the direction of the general $\mathbf{r}$ vector. The remaining vectors $\mathbf{r}'$ and $\mathbf{r}''$ then span an arbitrary plane which we take to be the zx plane. Thus,

$$\begin{aligned} \gamma(\mathbf{r}'\mathbf{r}'') &= 4\pi \int_0^{\pi/2} \int_0^\infty \Psi^*[\mathbf{r}(r_z)\mathbf{r}'(r'\theta')]\Psi \\ &\quad \times [\mathbf{r}(r_z)\mathbf{r}''(r''\theta'')]r_z^2 \sin\theta dr_z d\theta. \end{aligned} \quad (40)$$

We next turn our attention towards construction of a matrix representation of the interacting KED tensor $t_{\alpha\beta}(\mathbf{r})$, a second-rank Cartesian tensor:

$$t_{\alpha\beta}(\mathbf{r}) = \frac{1}{4} \left[\frac{\partial}{\partial r'_\alpha \partial r''_\beta} + \frac{\partial^2}{\partial r'_\beta \partial r''_\alpha} \right] \gamma(\mathbf{r}'\mathbf{r}'') \Big|_{\mathbf{r}'=\mathbf{r}''=\mathbf{r}}. \quad (41)$$

For $\gamma(\mathbf{r}\mathbf{r}')$ of arbitrary symmetry in $\mathbb{R}^3$, the tensor in matrix form is

$$[t_{\alpha\beta}] = \begin{bmatrix} t_{zz} & t_{zy} & t_{zx} \\ t_{yz} & t_{yy} & t_{yx} \\ t_{xz} & t_{xy} & t_{xx} \end{bmatrix}. \quad (42)$$

Since the tensor is symmetric, a computation in full 3D Cartesian space would require six components, i.e., the three diagonal components in addition to the components either above or below the diagonal.

It is far more computationally efficient to transform the components of the KED tensor to a spherical coordinate basis $[t_{\mu\nu}]$ in which the tensor becomes diagonal. In general, this is effected by applying a rotation matrix $\chi[\theta\phi]$ to the $[t_{\alpha\beta}]$, resulting in another second-rank tensor whose components $[t_{\mu\nu}]$ are now indexed in terms of spherical coordinates [49,50],

$$[t_{\mu\nu}] = \chi^T[\theta\phi][t_{\alpha\beta}]\chi[\theta\phi] = \begin{bmatrix} t_{rr} & 0 & 0 \\ 0 & t_{\theta\theta} & 0 \\ 0 & 0 & t_{\phi\phi} \end{bmatrix}, \quad (43)$$

where the rotation matrix

$$\chi[\theta\phi] = \begin{bmatrix} \sin\theta \cos\phi & \cos\theta \cos\phi & -\sin\phi \\ \sin\theta \sin\phi & \cos\theta \sin\phi & \cos\phi \\ \cos\theta & -\sin\theta & 0 \end{bmatrix}. \quad (44)$$

For spherical density systems, the tensor $t_{\alpha\beta}(\mathbf{r})$ transforms as [33,48]

$$t_{\alpha\beta}(\mathbf{r}) = \frac{r_\alpha r_\beta}{r^2} f(r) + \delta_{\alpha\beta} k(r), \quad (45)$$

so that when one applies the rotation matrix $\chi[\theta\phi]$ to $[t_{\alpha\beta}]$ expressed in terms of $f(r)$ and $k(r)$, one obtains

$$[t_{\mu\nu}] = \chi^T[\theta\phi] \begin{bmatrix} \cos^2\theta f(r) + k(r) & 0 & \cos\theta \sin\theta f(r) \\ 0 & k(r) & 0 \\ \cos\theta \sin\theta f(r) & 0 & \sin^2\theta f(r) + k(r) \end{bmatrix} \chi[\theta\phi] \quad (46)$$

$$= \begin{bmatrix} f(r) + k(r) & 0 & 0 \\ 0 & k(r) & 0 \\ 0 & 0 & k(r) \end{bmatrix}, \quad (47)$$

where ϕ has been set to 0 without loss of generality. In arriving at the above expression, the only assumption made is that the density is spherical, i.e., $\rho(\mathbf{r}) = \rho(r)$. In general, then, for spherical density systems, the KED tensor can be cast into purely radial form. Accordingly, the KED is radial: $t(\mathbf{r}) = t(r)$. Note also that the trace of the KED tensor which remains invariant to the orthogonal rotation [49] transforms as $t(r) = f(r) + 3k(r)$. Thus, there must exist a purely radial expression for the kinetic force and field entirely in terms of $f(r)$ and $k(r)$.

The remaining task, therefore, is to find computational expressions for $f(r)$ and $k(r)$ that can be derived from the quantal source $\gamma(\mathbf{r}\mathbf{r}')$. Such expressions not only will supply us with the kinetic and ultimately the correlation-kinetic information but also will be generally applicable to arbitrary spherical N -fermion systems. Before embarking on this task,

however, we first need to reckon with the prohibitively high dimensionality of the tensor in $\mathbb{R}^3$ space.

We next develop a new high-symmetry KED tensor $\tau_{\alpha\beta}$ in $\mathbb{R}^2$ space. Recall that the geometry in which $\gamma(\mathbf{r}\mathbf{r}')$ was computed maintained the $\mathbf{r}'$ and $\mathbf{r}''$ vectors entirely in the zx plane. Consequently all the derivatives applied against it must also exist in the zx plane. The tensor components thus obtained must therefore belong entirely to a 2D space. This admits the definition of a new high-symmetry second-rank symmetric tensor in $\mathbb{R}^2$ which we denote $\tau_{\alpha\beta}$, where $\alpha, \beta \in \{x, z\}$ and generally applicable to N -fermion systems with spherically symmetric densities

$$\tau_{\alpha\beta} = \begin{bmatrix} \tau_{zz} & \tau_{zx} \\ \tau_{xz} & \tau_{xx} \end{bmatrix}, \quad (48)$$

where its four components are expressed in terms of $\gamma(\mathbf{r}\mathbf{r}')$ as

$$\tau_{zz} = \frac{1}{2} \left(A \cos^2 \theta - B \frac{2}{r} \cos \theta \sin \theta + C \frac{\sin^2 \theta}{r^2} \right), \quad (49)$$

$$\tau_{xx} = \frac{1}{2} \left(A \sin^2 \theta + B \frac{2}{r} \cos \theta \sin \theta + C \frac{\cos^2 \theta}{r^2} \right), \quad (50)$$

$$\begin{aligned} \tau_{zx} &= \tau_{xz} \\ &= \frac{1}{2} \left(A \cos \theta \sin \theta + B \frac{\cos^2 \theta - \sin^2 \theta}{r} - C \frac{\sin \theta \cos \theta}{r^2} \right), \end{aligned} \quad (51)$$

such that A , B , and C represent the sphericalized single-particle density matrix,

$$A = \frac{1}{4\pi} \int \gamma_{r'r''}(r\theta) d\Omega, \quad (52)$$

$$B = \frac{1}{4\pi} \int \gamma_{r'\theta''}(r\theta) d\Omega, \quad (53)$$

$$C = \frac{1}{4\pi} \int \gamma_{\theta'\theta''}(r\theta) d\Omega, \quad (54)$$

where

$$\gamma_{r'r''}(r\theta) = \left. \frac{\partial}{\partial r''} \left(\frac{\partial}{\partial r'} \gamma(r'\theta', r''\theta'') \right) \right|_{\substack{r'=r''=r \\ \theta'=\theta''=\theta}}, \quad (55)$$

$$\gamma_{r'\theta''}(r\theta) = \left. \frac{\partial}{\partial \theta''} \left(\frac{\partial}{\partial r'} \gamma(r'\theta', r''\theta'') \right) \right|_{\substack{r'=r''=r \\ \theta'=\theta''=\theta}}, \quad (56)$$

$$\gamma_{\theta'\theta''}(r\theta) = \left. \frac{\partial}{\partial \theta''} \left(\frac{\partial}{\partial \theta'} \gamma(r'\theta', r''\theta'') \right) \right|_{\substack{r'=r''=r \\ \theta'=\theta''=\theta}}. \quad (57)$$

By analogy to the transformation of the tensor in $\mathbb{R}^3$ space, we can also transform the $[\tau_{\alpha\beta}]$ matrix representation from a Cartesian basis to a computationally efficient orthonormal eigenvector basis. We accomplish this by invoking a Euler rotation matrix which rotates the Cartesian coordinate system by an angle θ about the y axis so that the z axis becomes coincident with the position vector $\mathbf{r}$ in the zx plane. As $[\tau_{\alpha\beta}]$ is real and symmetric, the new high-symmetry tensor in the transformed polar eigenvector basis denoted $[\tau_{\mu\nu}]$, where $\mu\nu \in \{r, \theta\}$, becomes diagonal,

$$[\tau_{\mu\nu}] = \Theta_y^T[\theta] \begin{bmatrix} \tau_{zz} & \tau_{zx} \\ \tau_{xz} & \tau_{xx} \end{bmatrix} \Theta_y[\theta] \quad (58)$$

$$= \begin{bmatrix} \tau_{rr} & 0 \\ 0 & \tau_{\theta\theta} \end{bmatrix}, \quad (59)$$

where the rotation matrix is

$$\Theta_y[\theta] = \begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix}. \quad (60)$$

Upon applying the rotation matrix to the Cartesian components of the tensor $\tau_{\alpha\beta}$ of Eq. (48), and recognizing the fact that $[\tau_{\mu\nu}]$ is of the form of Eq. (59), we obtain the components of the $\mathbb{R}^2$

FIG. 11. (Color online) Surface contour of the derivative function $\gamma_{r'r''}(r\theta)$ of Eq. (55).

kinetic energy tensor $[\tau_{\mu\nu}]$ in a polar basis to be

$$\tau_{rr} = \frac{1}{8\pi} \int \gamma_{r'r''}(r\theta) d\Omega, \quad (61)$$

$$\tau_{\theta\theta} = \frac{1}{8\pi r^2} \int \gamma_{\theta'\theta''}(r\theta) d\Omega, \quad (62)$$

with $\gamma_{r'r''}(r\theta)$, $\gamma_{\theta'\theta''}(r\theta)$ defined by Eqs. (55) and (57) respectively. The interacting system KED is then

$$t(\mathbf{r}) = t(r) = \sum_u \tau_{uu} = \tau_{rr} + \tau_{\theta\theta}, \quad (63)$$

and the kinetic energy

$$\begin{aligned} T &= \int t(\mathbf{r}) d\mathbf{r} \\ &= \pi \int_0^\infty \int_0^\pi \left[\gamma_{r'r''}(r\theta) + \frac{\gamma_{\theta'\theta''}(r\theta)}{r^2} \right] r^2 \sin \theta dr d\theta. \end{aligned} \quad (64)$$

The quantities $\gamma_{r'r''}(r\theta)$ and $\gamma_{\theta'\theta''}(r\theta)$ are thus intrinsic to the determination of the KED, the kinetic energy, the kinetic field, and hence the correlation-kinetic field and energy. In Figs 11 and 12 are plotted the surface contours of the derivatives $\gamma_{r'r''}(r\theta)$ and $\gamma_{\theta'\theta''}(r\theta)$.

Finally, we derive new expressions for the functions $f(r)$ and $k(r)$ of the interacting system KED tensor $t_{\mu\nu}$ in a spherical basis of Eq. (47). We accomplish this by comparing the new high-symmetry $\tau_{\mu\nu}$ tensor with that of $t_{\mu\nu}$. Recall that in order to obtain the $\tau_{\mu\nu}$ representation, the z axis of the Cartesian coordinate system in the $\tau_{\alpha\beta}$ representation is brought into alignment with the radial basis vector of the polar coordinate basis. The $\mathbf{r}$ vector of $\tau_{rr}(\mathbf{r})$ defined in $\mathbb{R}^2$ is thus geometrically identical to the $\mathbf{r}$ vector of $t_{rr}(\mathbf{r})$ defined in $\mathbb{R}^3$. Thus we conclude that τ_{rr} also transforms as $f(r) + k(r)$. Accordingly, we know that $\tau_{\theta\theta}$ must transform as $2k(r)$. The spherical average over $\gamma_{\theta'\theta''}(r\theta)$ in the 2D $(r\theta)$ plane thus recovers the total angular contribution to the KED in a 3D $(r\theta\phi)$ spherical space, i.e., $\tau_{\theta\theta} = t_{\theta\theta} + t_{\phi\phi}$. Summarizing the above

FIG. 12. (Color online) Surface contour of the derivative function $\gamma_{\theta'\theta''}(r\theta)$ of Eq. (57).

we have

$$\tau_{rr} = f(r) + k(r), \quad (65)$$

$$\tau_{\theta\theta} = 2k(r). \quad (66)$$

This admits the following new computational expressions for $f(r)$ and $k(r)$ using the new $\tau_{\mu\nu}$ high-symmetry $\mathbb{R}^2$ formulation:

$$k(r) = \frac{\tau_{\theta\theta}}{2} = \frac{1}{16\pi r^2} \int \gamma_{\theta'\theta''}(r\theta) d\Omega, \quad (67)$$

$$f(r) = \tau_{rr} - \frac{\tau_{\theta\theta}}{2} = \tau_{rr} - k(r) \quad (68)$$

$$= \frac{1}{8\pi} \int \left[\gamma_{r'r''}(r\theta) - \frac{\gamma_{\theta'\theta''}(r\theta)}{2r^2} \right] d\Omega. \quad (69)$$

These expressions are generally applicable to arbitrary spherical N -fermion systems. The functions $f(r)$, $k(r)$, and $t(r) = f(r) + 3k(r)$ are plotted in Figs 13, 14, and 15, respectively. The appearance of a node in $f(r)$ is a quantal signature reflecting the fat attractor topology of the density $\rho(r)$. There

FIG. 13. Function $f(r)$ of the diagonal matrix element of the kinetic energy density tensor $t_{\mu\nu}$ of Eq. (47).

FIG. 14. Function $k(r)$ of the diagonal matrix element of the kinetic energy density tensor $t_{\mu\nu}$ of Eq. (47).

is no such node in the low-correlation regime [33,48]. The impact of the large negative oscillation on the kinetic force results in a substantial reduction in the ratio of the kinetic T to the total E energy. Moreover, since the derivative contributions are both positive definite,

$$\gamma_{r'r''}(r\theta) \geq 0, \quad \gamma_{\theta'\theta''}(r\theta) \geq 0, \quad (70)$$

this implies strong angular kinetic contributions within the critical sphere in the Wigner regime of the Hooke's atom. The function $k(r)$ reflects angular contributions to the kinetic energy, as it relies only on the angular derivatives of $\gamma(\mathbf{r}\mathbf{r}')$. In contrast to the low-correlation regime for which $k(r) \ll f(r)$, our results reveal $k(r) \sim f(r)$. This is a direct indication of angular kinetic energy contributions in the Wigner regime. More significantly, the newfound prominence of $k(r)$ catapults the correlation-kinetic energy T_c -to-kinetic energy T ratio to a high level.

E. Dirac density matrix $\gamma_s(\mathbf{r}\mathbf{r}')$

The quantal source for the kinetic field of the model fermion system is the Dirac density matrix $\gamma_s(\mathbf{r}\mathbf{r}')$. From Eqs. (21)

FIG. 15. Kinetic energy densities for the interacting $t(r) = f(r) + 3k(r)$ and model noninteracting $t_s(r) = h(r)$ systems.

FIG. 16. The function $h(r)$, which corresponds to the kinetic energy density $t_s(r)$ of the model noninteracting system.

and (34), it follows that

$$\gamma_s(\mathbf{r}\mathbf{r}') = \sqrt{\rho(\mathbf{r})}\sqrt{\rho(\mathbf{r}')} \quad (71)$$

The corresponding KED tensor, a second-rank Cartesian tensor, is defined as

$$t_{s,\alpha\beta}(\mathbf{r}) = \frac{1}{4} \left[\frac{\partial^2}{\partial r'_\alpha \partial r''_\beta} + \frac{\partial^2}{\partial r'_\beta \partial r''_\alpha} \right] \gamma_s(\mathbf{r}'\mathbf{r}'') \Big|_{\mathbf{r}'=\mathbf{r}''=\mathbf{r}}. \quad (72)$$

For spherical density systems, ϕ becomes arbitrary, and we set it to 0. The KED in matrix form is then

$$[t_{s,\alpha\beta}] = \begin{bmatrix} t_{s,zz} & 0 & t_{s,zx} \\ 0 & 0 & 0 \\ t_{s,xz} & 0 & t_{s,xx} \end{bmatrix}. \quad (73)$$

For the $\gamma_s(\mathbf{r}\mathbf{r}')$ of Eq. (71) each nonvanishing component transforms as [33,48]

$$t_{s,\alpha\beta}(\mathbf{r}) = \frac{r_\alpha r_\beta}{r^2} h(r), \quad h(r) = \frac{1}{8\rho(r)} \left(\frac{\partial \rho(r)}{\partial r} \right)^2. \quad (74)$$

The KED is then

$$t_s(\mathbf{r}) = t_s(r) = \sum_\alpha t_{s,\alpha\alpha}(r) = h(r). \quad (75)$$

The function $h(r)$ is plotted in Figs. 15 and 16. As demanded by the local minimum in $\rho(\mathbf{r})$, a weak oscillatory structure is clearly visible near the nucleus, reflecting the fat attractor quantum topology. The model system kinetic energy is then

$$T_s = 4\pi \int_0^\infty h(r) r^2 dr. \quad (76)$$

The magnitude of correlation-kinetic effects can be gauged from Fig. 15 by noting the separation between $t(r)$ and $t_s(r)$. Clearly, we see that the correlation kinetic energy is substantial.

V. FIELDS

From the quantal sources described in the previous section, we determine the corresponding fields.

FIG. 17. The Hartree field $\mathcal{E}_H(\mathbf{r})$. The function $2/r^2$ is also drawn.

A. Hartree $\mathcal{E}_H(\mathbf{r})$, Pauli $\mathcal{E}_x(\mathbf{r})$, and Coulomb $\mathcal{E}_c(\mathbf{r})$ fields

The Hartree $\mathcal{E}_H(\mathbf{r})$, Pauli $\mathcal{E}_x(\mathbf{r})$, and Coulomb $\mathcal{E}_c(\mathbf{r})$ fields are obtained via Coulomb law from their respective quantal sources: the density $\rho(\mathbf{r})$, Fermi hole $\rho_x(\mathbf{r}\mathbf{r}')$, and Coulomb holes $\rho_c(\mathbf{r}\mathbf{r}')$. Thus,

$$\mathcal{E}_H(\mathbf{r}) = \int \frac{\rho(\mathbf{r}')(\mathbf{r} - \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|^3} d\mathbf{r}', \quad (77)$$

$$\mathcal{E}_x(\mathbf{r}) = \int \frac{\rho_x(\mathbf{r}\mathbf{r}')(\mathbf{r} - \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|^3} d\mathbf{r}', \quad (78)$$

$$\mathcal{E}_c(\mathbf{r}) = \int \frac{\rho_c(\mathbf{r}\mathbf{r}')(\mathbf{r} - \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|^3} d\mathbf{r}'. \quad (79)$$

The fields $\mathcal{E}_H(\mathbf{r})$, $\mathcal{E}_x(\mathbf{r})$, and $\mathcal{E}_c(\mathbf{r})$ are plotted in Figs. 17, 18, and 19, respectively. These structures are predictable based on the structure of the corresponding quantal sources. For example, since $\rho(\mathbf{r})$ and $\rho_x(\mathbf{r}\mathbf{r}')$ are spherically symmetric about the nucleus, the fields $\mathcal{E}_H(\mathbf{r})$ and $\mathcal{E}_x(\mathbf{r})$ vanish at the origin, as they must. As the total charge of the density $\rho(\mathbf{r})$ is 2 a.u., and that of the Fermi hole $\rho_x(\mathbf{r}\mathbf{r}')$ is -1 a.u., and because in this case both charge distributions are static, the asymptotic structures of these fields in the classically forbidden region

FIG. 18. The Pauli field $\mathcal{E}_x(\mathbf{r})$. The function $-1/r^2$ is also drawn.

FIG. 19. The Coulomb field $\mathcal{E}_c(\mathbf{r})$. The function $-\delta/r^4$, where $\delta = 461.1960$, is also drawn.

must be

$$\mathcal{E}_H(\mathbf{r}) \underset{r \rightarrow \infty}{\sim} \frac{2}{r^2}, \quad (80)$$

$$\mathcal{E}_x(\mathbf{r}) \underset{r \rightarrow \infty}{\sim} -\frac{1}{r^2}. \quad (81)$$

For an electron at the nucleus, the Coulomb hole is spherically symmetric about it [see Fig. 8(a)]. Thus, the Coulomb field $\mathcal{E}_c(\mathbf{r})$ vanishes at the origin. The Coulomb holes are both positive and negative, and this is reflected in the structure of the field. In prior work [33,48], it has been proved analytically that, in general, the asymptotic structure of $\mathcal{E}_c(\mathbf{r})$ for the Hooke's atom decays as

$$\mathcal{E}_c(\mathbf{r}) \underset{r \rightarrow \infty}{\sim} -\frac{\delta}{r^4}. \quad (82)$$

In the present example $\delta = 461.1960$. This asymptotic structure is clearly evident in Fig. 19.

The structures of the fields $\mathcal{E}_H(\mathbf{r})$, $\mathcal{E}_x(\mathbf{r})$, and $\mathcal{E}_c(\mathbf{r})$ in the Wigner regime are entirely similar to those of the low-correlation case of $k = \frac{1}{4}$ [33,48] but, of course, spread over a much wider range of configuration space.

B. Correlation-kinetic field $\mathcal{Z}_{tc}(\mathbf{r})$

The α Cartesian component of the kinetic “force” for an N -fermion system is given by the expression

$$z_\alpha(\mathbf{r}) = 2 \sum_\beta \frac{\partial t_{\alpha\beta}(\mathbf{r})}{\partial r_\beta}. \quad (83)$$

For spherically symmetric systems, the kinetic force must be along the radial direction, which we take to be the z axis. The kinetic force $z(r)$ can therefore be derived entirely from its z subcomponent according to the expression

$$z(r) = z_z(r) = 2 \sum_\beta \frac{\partial t_{z\beta}(\mathbf{r})}{\partial r_\beta} \quad (84)$$

$$= 2 \left[\frac{\partial}{\partial r_z} \left(\frac{r_z^2 f(r) + k(r)}{r^2} \right) + \frac{\partial}{\partial r_x} \left(\frac{r_z r_x f(r) + k(r)}{r^2} \right) \right], \quad (85)$$

FIG. 20. The kinetic “force” $z(\mathbf{r})$ for the interacting system.

where ϕ has been set to 0, as it is arbitrary for spherical density systems. After some algebra, it can be shown that

$$z(r) = \frac{4f(r)}{r} + 2 \frac{\partial}{\partial r} [f(r) + k(r)]. \quad (86)$$

This is a new expression that significantly lowers the computational burden because it only requires a single derivative applied against radial quantities already computed. The kinetic force $z(r)$ is plotted in Fig. 20. This structure differs significantly from that of the low-correlation regime ($k = \frac{1}{4}$) in that it has a large negative component about the nucleus. Asymptotically, the structures are similar. The negative component of the force is critical to the understanding of the “quantal compression” of the KED $t(r)$ at and about the nucleus (see Fig. 15), discussed later. However, at this juncture, and to make the later explanation clearer, we plot in Fig. 21 the divergence of the kinetic force given by the expression

$$\nabla \cdot \mathbf{z}(\mathbf{r}) = \frac{4f(r)}{r^2} + \frac{8}{r} \frac{\partial f(r)}{\partial r} + \frac{4}{r} \frac{\partial k(r)}{\partial r} + 2 \frac{\partial^2 (f(r) + k(r))}{\partial r^2}. \quad (87)$$

The interacting system kinetic field $\mathcal{Z}(\mathbf{r})$ is then

$$\mathcal{Z}(\mathbf{r}) = \frac{z(r)}{\rho(r)} \quad (88)$$

and is plotted in Fig. 22.

FIG. 21. Divergence of the kinetic “force” for the interacting system.

FIG. 22. Kinetic fields for the interacting $\mathcal{Z}(\mathbf{r})$ and model noninteracting fermion $\mathcal{Z}_s(\mathbf{r})$ systems.

The noninteracting system kinetic force is defined as

$$z_{s,\alpha}(\mathbf{r}) = 2 \sum_{\beta} \frac{\partial t_{s,\alpha\beta}(\mathbf{r})}{\partial r_{\beta}}. \quad (89)$$

Following the procedure above for the interacting system, the kinetic force can be derived from its z subcomponent as

$$z_s(r) = z_{s,z}(r) = 2 \sum_{\beta} \frac{\partial t_{s,z\beta}(r)}{\partial r_{\beta}} = 2 \left[\frac{\partial}{\partial r_z} t_{s,zz} + \frac{\partial}{\partial r_x} t_{s,zx} \right] \quad (90)$$

$$= 2 \left[\frac{\partial}{\partial r_z} \left(\frac{r_z^2}{r^2} h(r) \right) + \frac{\partial}{\partial r_x} \left(\frac{r_z r_x}{r^2} h(r) \right) \right]. \quad (91)$$

Upon taking the derivation to conclusion, one obtains

$$z_s(r) = \frac{4h(r)}{r} + 2 \frac{\partial h(r)}{\partial r}. \quad (92)$$

The corresponding field is

$$\mathcal{Z}_s(r) = \frac{z_s(r)}{\rho(r)}. \quad (93)$$

The force $z_s(r)$ and field $\mathcal{Z}_s(r)$ are given in Figs. 23 and 22, respectively. Note that since $h(r)$ is in terms of the density, the force and field are determined directly from it.

FIG. 23. The kinetic “force” $z_s(r)$ for the noninteracting system.

FIG. 24. The correlation-kinetic field $\mathcal{Z}_{tc}(\mathbf{r})$.

The correlation-kinetic field is then the difference

$$\mathcal{Z}_{tc}(r) = \mathcal{Z}_s(r) - \mathcal{Z}(r) \quad (94)$$

$$= 4 \frac{[h(r) - f(r)]}{r\rho(r)} + \frac{2}{\rho(r)} \frac{\partial}{\partial r} [h(r) - (f(r) + k(r))], \quad (95)$$

and it is plotted in Fig. 24. Observe the cancellation of the fields $\mathcal{Z}_s(r)$ and $\mathcal{Z}(r)$ asymptotically in Fig. 22, which leads to the positive $\mathcal{Z}_{tc}(r)$ field and, consequently, to a positive value for the correlation-kinetic energy T_c . This is similar to the case of low correlations ($k = \frac{1}{4}$ [33,48]). (If the mapping from the ground state of the interacting system were to the model system in, say, the first excited singlet state, then there would be a negative component to $\mathcal{Z}_{tc}(\mathbf{r})$, leading to a negative value for T_c [34,51].)

VI. POTENTIALS AND ENERGIES

As the quantal source of the Hartree field $\mathcal{E}_H(\mathbf{r})$ is the static charge of the density $\rho(\mathbf{r})$, it is conservative. In this example, the Pauli $\mathcal{E}_x(\mathbf{r})$, Coulomb $\mathcal{E}_c(\mathbf{r})$, and correlation-kinetic $\mathcal{Z}_{tc}(\mathbf{r})$ fields are also each conservative. Thus, the corresponding works done in these fields are each separately path independent. Hence, the Hartree $W_H(\mathbf{r})$, Pauli $W_x(\mathbf{r})$, Coulomb $W_c(\mathbf{r})$, and correlation-kinetic $W_{tc}(\mathbf{r})$ potentials are given by

$$W_H(\mathbf{r}) = - \int_{\infty}^{\mathbf{r}} \mathcal{E}_H(\mathbf{r}') \cdot d\ell', \quad (96)$$

$$W_x(\mathbf{r}) = - \int_{\infty}^{\mathbf{r}} \mathcal{E}_x(\mathbf{r}') \cdot d\ell', \quad (97)$$

$$W_c(\mathbf{r}) = - \int_{\infty}^{\mathbf{r}} \mathcal{E}_c(\mathbf{r}') \cdot d\ell', \quad (98)$$

$$W_{tc}(\mathbf{r}) = - \int_{\infty}^{\mathbf{r}} \mathcal{Z}_{tc}(\mathbf{r}') \cdot d\ell'. \quad (99)$$

The asymptotic structure of these potentials in the classically forbidden region follows from the corresponding fields. The potentials $W_H(\mathbf{r})$, $W_x(\mathbf{r})$, $W_c(\mathbf{r})$, and $W_{tc}(\mathbf{r})$ are, respectively, plotted in Figs. 25, 26, 27, and 28. The potentials $W_H(\mathbf{r})$ and $W_x(\mathbf{r})$, are of the same order of magnitude and opposite in sign,

FIG. 25. The Hartree potential $W_H(\mathbf{r})$. The function $\frac{2}{r}$ is also drawn.

as are the potentials $W_c(\mathbf{r})$ and $W_{tc}(\mathbf{r})$, the latter pair being an order of magnitude smaller. The sum of these potentials [see Eq. (7)] is $v_{ee}(\mathbf{r})$, the local electron-interaction potential of the model fermions that reproduces the density $\rho(\mathbf{r})$ of the interacting system. The potential $v_{ee}(\mathbf{r})$ is plotted in Fig. 29 and has the asymptotic structure of $\frac{1}{r}$.

The Hartree E_H , Pauli E_x , and Coulomb E_c components of the electron-interaction energy E_{ee} [see Eq. (8)] in integral virial form in terms of the respective fields are

$$E_H = \int \rho(\mathbf{r}) \mathbf{r} \cdot \mathcal{E}_H(\mathbf{r}) d\mathbf{r}, \quad (100)$$

$$E_x = \int \rho(\mathbf{r}) \mathbf{r} \cdot \mathcal{E}_x(\mathbf{r}) d\mathbf{r}, \quad (101)$$

$$E_c = \int \rho(\mathbf{r}) \mathbf{r} \cdot \mathcal{E}_c(\mathbf{r}) d\mathbf{r}. \quad (102)$$

The correlation-kinetic energy T_c is given by Eq. (9). The total energy E and its various components are listed in Table I. The eigenvalue ϵ of the model system is the negative of the ionization potential, $I = E^{N-1} - E$ [33,52–56].

VII. ANALYSIS OF RESULTS

For the discussion in this section, the reader is referred to Table I.

FIG. 26. The Pauli potential $W_x(\mathbf{r})$. The function $-\frac{1}{r}$ is also drawn.

FIG. 27. The Coulomb potential $W_c(\mathbf{r})$. The function $-\frac{\eta}{r^3}$, where $\eta = 153.7320$, is also drawn.

The Wigner high electron correlation regime is characterized by a low electron density and an electron-interaction energy E_{ee} greater than the kinetic energy T . The reverse is the case for the low-correlation regime. The ratio E_{ee}/T for the high- and low-correlation regimes is 249.3% and 67.3%, respectively. In a comparison with the total energy E , the ratio E_{ee}/E is 43.4% and 22.4%, respectively. In fact, this trend in the difference is reflected in each component of E_{ee} , i.e., in the ratios E_H/E , E_x/E , and E_c/E .

What we have discovered via QDFT is that, in the Wigner regime, not only is the electron-interaction energy E_{ee} very significant, but so is the contribution of electron correlations to the kinetic energy, viz., the correlation-kinetic energy T_c . Thus, the ratio T_c/T in the Wigner regime is 26.9%, as opposed to 4.4% for the low-correlation case. The correlation-kinetic energy T_c thus constitutes a significant fraction of the total energy E : the ratio T_c/E is 4.5% in the Wigner regime, whereas it is only 1.45% in the low-correlation case. The total contribution of electron correlations to the energy E is $(T_c + E_{ee})$. The ratio $(T_c + E_{ee})/E$ is 48% for the Wigner and 24% for the low-correlation regime. Thus, we propose that, in addition to a high electron-interaction energy value, the Wigner regime also be characterized by a high correlation-kinetic energy.

The result for the eigenvalue ϵ of the model system of noninteracting fermions is also interesting. This eigenvalue,

FIG. 28. The correlation-kinetic potential $W_{tc}(\mathbf{r})$.

FIG. 29. The local electron-interaction potential $v_{ee}(\mathbf{r})$ of the model fermions.

being the highest occupied eigenvalue, has the physical interpretation of being equal to the negative of the ionization potential [52–56]. Even though the electrons are more weakly bound to the nucleus in the Wigner regime, the ratio of this eigenvalue ϵ to the total energy E is 78.6%, whereas for the low-correlation case it is 62.5%. Thus, in the Wigner regime, the removal energy relative to the total energy is also greater than in the low-electron-correlation case.

Yet another interesting and new result observed is that the ratio of the kinetic T to the total energy E is reduced from

TABLE I. Total E , kinetic T , correlation-kinetic T_c , noninteracting kinetic T_s , external E_{ext} , Hartree E_H , Pauli E_x , Coulomb E_c , and electron-interaction E_{ee} energies and noninteracting system eigenvalue ϵ in atomic units for the low-correlation ($k = \frac{1}{4}$) [33,48] and high-correlation ($k \approx 3.00891 \times 10^{-4}$) regimes. The ratio $E_{\text{xc}}^{\text{KS}}[\rho]/T_s$, where $E_{\text{xc}}^{\text{KS}}[\rho]$ is the Kohn-Sham theory “exchange-correlation” energy, is also listed.

Property	$k = \frac{1}{4}$	$k \approx 3.00891 \times 10^{-4}$
E	2.000 000	0.121 423 5
E_{ee}	0.447 443	0.052 739
T	0.664 418	0.021 158
E_{ee}/T	67.3%	249.3%
T_c	0.029 173	0.005 700
T_s	0.635 245	0.015 457
E_{ext}	0.888 141	0.047 527
E_H	1.030 250	0.151 474
E_x	−0.515 125	−0.075 735
E_c	−0.067 682	−0.022 998
ϵ	1.250 000	0.095 404
E_{ee}/E	22.4%	43.4%
E_H/E	51.5%	124.7%
E_x/E	25.8%	62.4%
E_c/E	3.4%	18.9%
ϵ/E	62.5%	78.6%
T/E	33.2%	17.4%
T_c/T	4.4%	26.9%
T_c/E	1.45%	4.5%
$(T_c + E_{ee})/E$	24%	48%
$E_{\text{xc}}^{\text{KS}}[\rho]/T_s$	−0.871 528	−6.018 956

33.2% in the low-correlation case to 17.4% in the Wigner regime. The reason for this is the difference in structure of the corresponding kinetic energy densities $t(r)$. In the Wigner regime, there is a “quantal compression” of the kinetic energy density $t(r)$ towards the nucleus, whereas there is a “quantal decompression” of $t(r)$ away from the nucleus for the low-correlation case (see Figs. 15 and 5 of [38] for a comparison). The explanation of the quantal compression or decompression lies in the structure of the corresponding kinetic “forces” $\mathbf{z}(\mathbf{r})$. In the Wigner regime (Fig. 20) the force $\mathbf{z}(\mathbf{r})$ is negative in the region surrounding the nucleus. The divergence of $\mathbf{z}(\mathbf{r})$ is also negative in this region (see Fig. 21). This means that there is a net flow of kinetic force directed towards the interior of any infinitesimal spherical volume in the proximate vicinity surrounding the nucleus. There is thus a quantal compression of the kinetic energy density, with a global extremum occurring at the nucleus. Farther out from this region, the divergence is positive, resulting in a depletion of the kinetic force vector from this region, leading to a decrease in $t(r)$. Still farther out, the divergence is again negative, giving rise to a weaker quantal compression in this region. The quantal compression of $t(r)$ near the nucleus explains why the kinetic energy contribution, and hence why the ratio T/E , in the Wigner regime is small. For small values of r , the kinetic energy density $t(r)$ is large, and thus in a volume integral to obtain the kinetic energy T , the contribution from this region is diminished. In the low-correlation case, there is a quantal decompression of the force vector $\mathbf{z}(\mathbf{r})$ so that the maximum of the kinetic energy density $t(r)$ occurs farther away from the nucleus, leading to a greater T/E ratio.

Finally, the relationship between KS theory and QDFT can be used to further characterize the distinction between the Wigner and the low-correlation regimes. This is via the ratio of the KS theory “exchange-correlation” energy functional $E_{\text{xc}}^{\text{KS}}[\rho]$ to the noninteracting system kinetic energy T_s . In terms of the QDFT-determined properties, the energy functional $E_{\text{xc}}^{\text{KS}}[\rho]$ is defined as $E_{\text{xc}}^{\text{KS}}[\rho] = E_{ee} - E_H + T_c$. The ratio $E_{\text{xc}}^{\text{KS}}[\rho]/T_s$ is also listed in Table I. Observe that the value of the ratio in the Wigner regime is an order of magnitude greater than that in the low-correlation case. For completeness, we note that the corresponding KS “exchange-correlation” potential, which is the functional derivative, $v_{\text{xc}}(r) = \delta E_{\text{xc}}^{\text{KS}}[\rho]/\delta \rho(r) = W_x(r) + W_c(r) + W_t(r)$. In the present example, the KS “correlation” energy functional $E_c^{\text{KS}}[\rho] = E_c + T_c$, and the corresponding potential $v_c(r) = \delta E_c^{\text{KS}}[\rho]/\delta \rho(r) = W_c(r) + W_t(r)$. The local electron-interaction potential $v_{ee}(r)$ of KS theory is, of course, the same as given in Fig. 29 derived via QDFT.

VIII. CONCLUDING REMARKS

We have studied via QDFT the Wigner regime of a nonuniform-electron-density system as described by the Hooke’s atom. Although our calculations are performed for a specific low electron density in this regime, we conjecture that our conclusions are equally applicable to other Wigner low-electron-density systems. As expected, in comparison to the low-electron-correlation regime, the electron-interaction energy E_{ee} as a fraction of the total energy E is much greater than that of the kinetic energy T . So are the individual Hartree E_H , Pauli E_x , and Coulomb E_c components relative to the total

energy E . Additionally, so is the ionization potential I when taken as a fraction of the energy E . But possibly the most unexpected of conclusions was that the correlation-kinetic energy T_c as a ratio of either the electron-interaction E_{ee} or the total energy E is also high in comparison to the low-correlation case. And as the density is further diminished, all these ratios become even more pronounced relative to the low-correlation systems. In the limit of very low density ($k \rightarrow 0$) or, in KS terms, in the limit of the coupling constant $\lambda \rightarrow \infty$, the correlation-kinetic energy T_c becomes the zero-point energy of the electrons. The total contribution of electron correlations to the energy is thus $E_{ee} + T_c$. The correlation-kinetic energy T_c must then also be employed to characterize the Wigner regime. As noted in Sec. I, Wigner, in his original papers on the uniform electron gas, did explicitly consider the zero-point motion of the electrons. For nonuniform electron gas systems, it is the correlation-kinetic energy T_c that is of significance.

A priori, there was no way of knowing that the ratio T_c/E would be high in comparison to that in the low-correlation case. After all, why should this ratio be different in the Wigner regime? As a result of our calculations, we now understand that this is a consequence of the “quantal compression” of the KED at and about the nucleus. In contrast, in low-correlation systems, there is a “quantal decompression” of the KED away from the nucleus, thereby leading to a low value of the T_c/E ratio. In both the high- and the low-correlation cases, the corresponding KED $t_s(r)$ of the noninteracting system is small at and about the nucleus. For larger values of the radial coordinate, the interacting $t(r)$ and noninteracting $t_s(r)$ KEDs are the same. The difference between the KEDs $t(r)$ and $t_s(r)$ leads to the correlation-kinetic energy T_c . (See Figs. 15 and 5 of [38] for a comparison.) Thus, the ratio of T_c/E and T_c/T is greater in the Wigner regime because of the compression of the KED $t(r)$. The concepts of quantal compression and quantal decompression, arrived at by the field perspective of

QDFT, are new. *A posteriori*, we suggest that a high E_{ee}/E ratio implies a high T_c/E ratio. Another way to conclude this is via the kinetic energy quantal sources. A strong interaction energy implies that the difference between the nonidempotent density matrix and the idempotent Dirac density matrix is large so that the correlation-kinetic energy is a significant part of the total electron-interaction energy.

Correlation-kinetic effects also become more significant as the dimensionality of the system is reduced. This fact was observed in a similar QDFT analysis [57] of the low-correlation two-dimensional quantum dot as described by the Hooke’s atom in a magnetostatic field [58,59]. We thus expect these effects to be even more pronounced for a quantum dot with a density in the Wigner regime. Such an analysis is in progress. For corresponding experimental work, see [60–62].

Finally, we have employed the QDFT analysis to obtain exact values for the KS theory “exchange-correlation” and “correlation” energy functionals of the density and of their respective functional derivatives. As noted previously, there is, at present, considerable interest in the development of new approximate KS theory “exchange-correlation” energy functionals applicable to the low-density Wigner regime. We surmise that the failure in this regime of existing functionals designed specifically for the low-correlation systems for which correlation-kinetic effects are small is probably due to not accounting for the significance of these effects in the high-correlation regime. As such, we believe that our exact results and conclusions should prove beneficial in the construction and testing of the new functionals.

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