City University of New York (CUNY)

CUNY Academic Works

Publications and Research

CUNY Graduate Center

2018

Kinetic Effects in 2D and 3D Quantum Dots: Comparison between High and Low Electron Correlation Regimes

Marlina Slamet
Sacred Heart University

Viraht Sahni
CUNY Brooklyn College

[How does access to this work benefit you? Let us know!](#)

More information about this work at: https://academicworks.cuny.edu/gc_pubs/507

Discover additional works at: <https://academicworks.cuny.edu>

This work is made publicly available by the City University of New York (CUNY).
Contact: AcademicWorks@cuny.edu

Kinetic effects in 2D and 3D Quantum Dots: Comparison between high and low electron correlation regimes

Marlina Slamet ¹ and Viraht Sahni ²

¹*Sacred Heart University, Fairfield, Connecticut 06825*

²*The Graduate Center of the City University of New York, New York, New York 10016.*

(Dated: August 9, 2018)

Abstract

Kinetic related ground state properties of a two-electron 2D quantum dot in a magnetic field and a 3D quantum dot (Hooke's atom) are compared in the Wigner high (HEC) and low (LEC) electron correlation regimes. The HEC regime corresponds to low densities sufficient for the creation of a Wigner molecule. The LEC regime densities are similar to those of natural atoms and molecules. The results are determined employing exact closed-form analytical solutions of the Schrödinger-Pauli and Schrödinger equations, respectively. The properties studied are the local and nonlocal quantal sources of the density and the single particle density matrix; the kinetic energy density; the kinetic 'force' and its divergence; the kinetic field; and the kinetic energy. The correlation-kinetic energy is obtained by mapping the 2D and 3D quantum dots via quantal density functional theory to systems of noninteracting fermions possessing the same density and physical current density for the former, and the same density for the latter. A key observation is that the structure of the 2D and 3D system properties within a specific electron correlation regime are similar. The quantal compression of the kinetic energy density about the center of the quantum dots in the HEC regime, and the quantal decompression away from the center in the LEC regime is explained via the structure of the kinetic 'force' and of its divergence, as are the values of the kinetic energy. The correlation-kinetic energy constitutes a significant fraction of the total energy in the HEC regime as well as for the 2D quantum dot in the LEC regime. Hence, a reduction in dimensionality too leads to a high correlation-kinetic energy. Any low electron density system thus ought to be characterized by both high electron-interaction energy and a high correlation-kinetic energy relative to the total energy.

I. INTRODUCTION

With the advent of the creation of man-made two-dimensional (2D) ‘artificial atoms’ or quantum dots [1, 2], it is of interest to study the properties of such reduced-dimensionality ‘atoms’. In this work, we investigate quantum dots in both the low- electron-correlation (LEC) (high electron density) regime as well as in the high-electron-correlation (HEC) (low electron density) Wigner regime [3, 4]. By the LEC regime, we mean those of natural atoms and molecules, and not the Gell-Mann–Brueckner [5] very high electron density system defined by the limit in which the Wigner-Seitz radius r_s tends to zero. The HEC regime we consider is such as to be the equivalent [6] to creating a stable Wigner molecule. The LEC regime is characterized, relative to the total energy, by an electron-interaction energy component less than the kinetic energy, and a low value for the correlation-kinetic energy. (The correlation-kinetic energy is the contribution of the electron correlations due to the Pauli exclusion principle and Coulomb repulsion to the kinetic energy [7, 8].) In contrast, the HEC regime is characterized, again relative to the total energy, by an electron-interaction energy greater than the kinetic energy, and a correlation-kinetic energy that constitutes a significant fraction of the total energy [9]. In this work we focus on kinetic effects: the properties of the kinetic energy density, its respective quantal decompression and compression in the two regimes [10], the kinetic ‘force’, the kinetic field, the kinetic energy, and the correlation-kinetic energy.

The motion of electrons in a quantum dot is confined to two dimensions within a quantum well in a thin layer of semiconductor (GaAs) sandwiched between two layers of another semiconductor (AlGaAs). The two-dimensional motion of the electrons is confined by an electrostatic field to create the quantum dot. The size of the quantum dot can be further reduced by application of a magnetic field perpendicular to the plane of motion. A key difference between the artificial and natural atoms is the potential that confines the electrons. Whereas this potential in natural atoms is Coulombic, in quantum dots the confining potential is harmonic. The latter result is arrived at via both experiment [11, 12] and theory [11, 13], with further support for this conclusion being provided by the Generalized Kohn theorem [11, 14–20]. The length and energy scales of a quantum dot also differ from that of natural atoms. As the quantum dot is housed in a semiconductor, its electron mass is the conduction band effective mass m^* . Additionally, the interaction between the electrons

is modified by the dielectric function ϵ of the semiconductor. As a consequence, the size of the quantum dot is an order of magnitude greater than that of natural atoms. Hence, there is a lowering of the electron density with a subsequent increase in the electron correlations effects [11, 12, 21–23] and in particular the correlation-kinetic energy [24, 25] (akin to that of a Wigner system).

We perform our analysis of the kinetic effects within the ‘Quantal Newtonian’ perspective [7] of Schrödinger theory. This is a description of the many-electron system from the viewpoint of the individual electron via the corresponding equation of motion or ‘Quantal Newtonian’ first and second laws. The description is in terms of quantal sources that are expectations of Hermitian operators taken with respect to the wave function, and the corresponding ‘classical’ fields that arise from them. Hence, for example, the kinetic energy T may be expressed in integral virial form in terms of a kinetic field $\mathbf{Z}(\mathbf{r})$. The *nonlocal* quantal source of this field is the single-particle density matrix $\gamma(\mathbf{r}\mathbf{r}')$, which is the expectation value of the density matrix operator $\hat{\gamma}(\mathbf{r}\mathbf{r}')$. The definitions of these and other properties will be provided in the section on Results. We refer the reader to Chapter 2 of [7] for further details of the perspective.

For the property of the correlation-kinetic energy, we map the interacting quantum dot system of electrons via quantal density functional theory (QDFT) [7] to a model S system of noninteracting fermions experiencing the *same* external fields [26], also in their ground state, and possessing the *same basic variables* [26]. This mapping too is in terms of ‘classical’ fields and quantal sources. Thus, the kinetic energy T_s of the model fermions can once again be expressed in integral virial form in terms of a corresponding kinetic field $\mathbf{Z}_s(\mathbf{r})$. The quantal source of the field is the Dirac density matrix $\gamma_s(\mathbf{r}\mathbf{r}')$, the expectation of the density matrix operator $\hat{\gamma}(\mathbf{r}\mathbf{r}')$ taken with respect to the Slater determinant wave function of the model fermions.

(The concept of a basic variable of quantum mechanics stems from the first Hohenberg-Kohn theorem [27]: It is a gauge invariant property, knowledge of which determines the wave functions of the system. Thus, for electrons in an external electrostatic field, the theorem proves that the basic variable is the ground state density $\rho(\mathbf{r})$. The constraint in the proof is that of constant electron number N . In recent work [28] it has been proved that for electrons in an external electrostatic and uniform magnetostatic field, the basic variables are the ground state density $\rho(\mathbf{r})$ and the *physical* current density $\mathbf{j}(\mathbf{r})$. The constraints

in this case are those of constant electron number N , the orbital $\mathbf{L}$ and spin $\mathbf{S}$ angular momentum. Thus, knowledge of the ground state $\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})$ determines the wave functions of the system.)

There is a second component to the paper. This is a comparison of the results of the 2D quantum dot with those [7, 9, 29] of what one might refer to as a 3D quantum dot known more commonly as the Hooke's atom [30–32]. The 3D atom is comprised of two electrons that are also harmonically confined. Thus, we compare the kinetic properties: the kinetic energy, the kinetic energy density and its quantal decompression and compression in the LEC and HEC regimes, and the correlation-kinetic energy, with those of the 2D quantum dot. Once again, to obtain the correlation-kinetic energy, one maps via QDFT the interacting system to one of model noninteracting fermions possessing the same external potential and basic variable which in this case is the ground state density $\rho(\mathbf{r})$.

In Sect. II we describe the 2D quantum dot in a magnetic field, and the 3D quantum dot via their corresponding Hamiltonians. The *exact* closed-form analytical ground state solutions of the resulting Schrödinger-Pauli and Schrödinger equations in both the LEC and HEC regimes are provided. The corresponding Schrödinger equations of the model fermionic systems, and the orbitals reproducing the same basic variables as that of each interacting system are also given. Our results for the kinetic properties of the 2D and 3D quantum dots are described in Sect. III, The definition of each property discussed is provided there. The analytical and semi-analytical expressions for these properties are given in Appendix A. Concluding remarks, and a discussion of how these results are related to traditional Kohn-Sham density functional theory [33] are made in Sect. IV.

II. QUANTUM DOTS IN 2D AND 3D

A. Quantum Dot in 2D in a magnetic field

The Schrödinger-Pauli Hamiltonian $\hat{H}$ for a N -electron quantum dot housed in a semiconductor of dielectric constant ϵ with the electrons confined by an electric field $\mathcal{E}(\mathbf{r}) = -\nabla v(\mathbf{r})/e$, where the scalar potential $v(\mathbf{r}) = \frac{1}{2}m^*\omega_0^2 r^2$ with ω_0 the harmonic frequency, and a magnetic field $\mathcal{B}(\mathbf{r}) = \nabla \times \mathbf{A}(\mathbf{r})$, with $\mathbf{A}(\mathbf{r})$ the vector potential, is

$$\hat{H} = \frac{1}{2m^*} \sum_k (\hat{\mathbf{p}}_k + \frac{e}{c} \mathbf{A}(\mathbf{r}_k))^2 + \frac{1}{2\epsilon} \sum_{k,\ell}' \frac{e^2}{|\mathbf{r}_k - \mathbf{r}_\ell|} + \sum_k v(\mathbf{r}_k) + g^* \mu_B \sum_k \mathcal{B}(\mathbf{r}_k) \cdot \mathbf{s}_k. \quad (1)$$

The various operator terms of the Hamiltonian are the physical kinetic $\hat{T}_A$ (with canonical momentum $\hat{\mathbf{p}}_k = -i\nabla_{\mathbf{r}_k}$), electron-interaction $\hat{U}$, external electrostatic $\hat{V}$, and the magnetic field-spin interaction, with $\mathbf{s}$ the electron spin momentum vector. The band effective mass is m^* ; the corresponding gyromagnetic ratio is g^* ; and $\mu_B = e\hbar/2mc$ the Bohr magneton. The Schrödinger-Pauli equation is

$$\hat{H}\Psi(\mathbf{X}) = E\Psi(\mathbf{X}), \quad (2)$$

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

We consider two two-electron quantum dots [34–37], one in the LEC and the other in the HEC regime. In the symmetric gauge $\mathbf{A}(\mathbf{r}) = \frac{1}{2}\mathbf{B}(\mathbf{r}) \times \mathbf{r}$ and with the magnetic field applied in the z-direction: $\mathbf{B}(\mathbf{r}) = B\mathbf{i}_z$, the corresponding ground state wave functions we employ are given below. As these are singlet states, it is the spatial part of the wave functions that are given.

In our calculations we employ effective atomic units: $e^2/\epsilon = m^* = \hbar = 1$. We also assume $c = 1$. (The effective Bohr radius $a_0^* = a_0(m/m^*)$ where m is the mass of the electron. The effective energy unit is $(a.u.)^* = (a.u.)(m^*/m\epsilon^2)$. Typically, for GaAs quantum dots, $\epsilon = 12.4$ and $m^* = 0.067m$.)

Low Electron Correlation Regime

The wave function we employ in this regime is [24]

$$\Psi_{2D}^{\text{LEC}}(\mathbf{r}_1\mathbf{r}_2) = Ae^{-\Omega R^2} e^{-\frac{1}{4}\Omega u^2}(1+u), \quad (3)$$

where $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2$ the center of mass, and $u = |\mathbf{r}_2 - \mathbf{r}_1|$ the relative coordinates; $A = 0.135646$; $\Omega^2 = k_{\text{eff}} = 1$, where k_{eff} is an effective force constant: $k_{\text{eff}} = \omega_0^2 + \omega_L^2$, with $\omega_L = B/2$ is the Larmor frequency.

High Electron Correlation Regime

The wave function we employ in this regime is

$$\Psi_{2D}^{\text{HEC}}(\mathbf{r}_1\mathbf{r}_2) = Be^{-\Omega R^2} e^{-\frac{1}{4}\Omega u^2} \left[1 + u + \sum_{j=2}^4 a_j \left(u \sqrt{\frac{\Omega}{2}} \right)^j \right], \quad (4)$$

where $B = 9.26662 \times 10^{-5}$; $\Omega^2 = k_{\text{eff}} = 5.606370 \times 10^{-4}$; $a_2 = 19.116851$; $a_3 = 13.394665$; $a_4 = 2.914869$. The derivation of this wave function follows from Taut [34].

The Schrödinger equation for the model fermions is

$$\left[\frac{1}{2} \hat{p}_k^2 + \frac{1}{2} k_{\text{eff}} r^2 + v_{\text{ee}}(\mathbf{r}) \right] \phi_k(\mathbf{r}) = \epsilon_k \phi_k(\mathbf{r}); \quad k = 1, 2, \dots, N \quad (5)$$

where the $\phi_k(\mathbf{r}), \epsilon_k$ are the orbitals and eigenvalues. The orbitals $\phi_k(\mathbf{r})$ lead to the same $\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})$ as that of the quantum dot. As the model fermions are also in a ground state, the orbitals $\phi_k(\mathbf{r}) = \sqrt{\rho(\mathbf{r})/2}$. All the many-body effects [7, 26], *viz.* those due to the Pauli exclusion principle, Coulomb repulsion, and correlation-kinetic effects, are incorporated in the *local* electron-interaction potential $v_{\text{ee}}(\mathbf{r})$. The potential $v_{\text{ee}}(\mathbf{r})$ is the work done in a conservative field whose components are separately representative of these correlations [7, 26]. The correlation-kinetic energy T_c is then the difference in the kinetic energies of the interacting and noninteracting fermionic systems. Thus, it could equivalently be defined in integral virial form in terms of the difference between the kinetic fields $\mathcal{Z}(\mathbf{r})$ and $\mathcal{Z}_s(\mathbf{r})$ of the two systems. (The details of the mapping from the interacting system of electrons to those of noninteracting fermions via QDFT are not provided here.)

B. Quantum Dot in 3D

The Hamiltonian for a two-electron quantum dot in 3D (Hooke's atom) in atomic units ($e = \hbar = m = 1$) is

$$\hat{H} = \frac{1}{2} \sum_{k=1}^2 \hat{\mathbf{p}}_k^2 + \sum_{k=1}^2 v(\mathbf{r}_k) + \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}, \quad (6)$$

with the first term being the kinetic energy operator $\hat{T}$, and where the electrons are confined by an electric field $\mathcal{E}(\mathbf{r}) = -\nabla v(\mathbf{r})$, with $v(\mathbf{r}) = \frac{1}{2} \omega^2 r^2$ and ω the harmonic frequency. The corresponding ground state wave functions in the LEC and HEC regimes that we employ are given below.

Low Electron Correlation Regime

The wave function in this regime is [29]

$$\Psi_{3D}^{\text{LEC}}(\mathbf{r}_1\mathbf{r}_2) = Ce^{-\omega R^2} e^{-\frac{1}{4}\omega u^2} \left(1 + \frac{u}{2}\right), \quad (7)$$

with $C = 2.91122 \times 10^{-2}$; $\omega^2 = k = \frac{1}{4}$ and k the force constant.

High Electron Correlation Regime

The wave function in this regime is [9]

$$\Psi_{3D}^{\text{HEC}}(\mathbf{r}_1\mathbf{r}_2) = De^{-\omega R^2} e^{-\frac{1}{4}\omega u^2} \left[1 + \frac{u}{2} + \sum_{j=2}^4 a_j \left(u\sqrt{\frac{\omega}{2}}\right)^j\right], \quad (8)$$

with $D = 8.94669 \times 10^{-2}$; $\omega^2 = k = 3.00891 \times 10^{-4}$; $a_2 = 8.274917$; $a_3 = 4.720056$; $a_4 = 0.879153$.

The corresponding Schrödinger equation for the model fermions possessing the same density $\rho(\mathbf{r})$ is

$$\left[\frac{1}{2}\hat{p}^2 + \frac{1}{2}kr^2 + v_{\text{ee}}(\mathbf{r})\right]\phi_k(\mathbf{r}) = \epsilon_k\phi_k(\mathbf{r}); \quad k = 1, 2, \dots, N \quad (9)$$

where the $\phi_k(\mathbf{r})$, ϵ_k are the orbitals and eigenvalues. The local electron interaction potential $v_{\text{ee}}(\mathbf{r})$ is the work done in a conservative field whose components are separately representative of electron correlations due to the Pauli exclusion principle, Coulomb repulsion, and correlation-kinetic effects. Again, as the model fermions are in their ground state, each orbital $\phi_k(\mathbf{r}) = \sqrt{\rho(\mathbf{r})/2}$. (Once more, the details of the mapping from the interacting to the model system are not provided here.)

As the above 2D and 3D wave functions are exact, they all satisfy the integral form of the electron-electron cusp coalescence condition [8, 38]. The general form of the cusp coalescence condition in D-dimension space for $D \geq 2$ for two particles of masses m_1 and m_2 , and charges Z_1 and Z_2 is

$$\psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) = \psi(\mathbf{r}_2, \mathbf{r}_2, \mathbf{r}_3, \dots, \mathbf{r}_N) \left(1 + \frac{2Z_1Z_2\mu_{12}}{D-1}r_{12}\right) + \mathbf{r}_{12} \cdot \mathbf{C}(\mathbf{r}_2, \mathbf{r}_3, \dots, \mathbf{r}_N), \quad (10)$$

where $\mu = m_1m_2/(m_1 + m_2)$ is the reduced mass, $\mathbf{r}_{12} = \mathbf{r}_1 - \mathbf{r}_2$, $r_{12} = |\mathbf{r}_{12}|$, and $\mathbf{C}$ an undetermined vector.

The results of our calculations are presented in the following section.

III. RESULTS

We discuss our results for the following kinetic effects related properties: (a) the *local* quantal source, the density $\rho(\mathbf{r})$; (b) the *nonlocal* quantal source, the single-particle density matrix $\gamma(\mathbf{r}\mathbf{r}')$; (c) the kinetic energy tensor $t_{\alpha\beta}(\mathbf{r}; \gamma)$ and its trace, the kinetic energy density $t(\mathbf{r})$; (d) the kinetic ‘force’ $z(\mathbf{r})$; the divergence of the kinetic ‘force’ $\nabla \cdot z(\mathbf{r})$; the kinetic energy T ; (e) the *S*-system properties of the *nonlocal* quantal source, the Dirac density matrix $\gamma_s(\mathbf{r}\mathbf{r}')$; kinetic energy tensor $t_{s,\alpha\beta}(\mathbf{r}; \gamma_s)$; kinetic ‘force’ $z_s(\mathbf{r})$; kinetic field $\mathbf{Z}_s(\mathbf{r})$; kinetic energy T_s ; (f) the correlation-kinetic field $\mathbf{Z}_{t_c}(\mathbf{r})$ and correlation-kinetic energy T_c . Analytical and semi-analytical expressions for these properties are given in the Appendix A.

Prior to discussing the results, and in order to distinguish between the HEC and LEC regimes, we present in Table I the values for the total energy $E = \langle \Psi | \hat{H} | \Psi \rangle$, the canonical kinetic energy $T = \langle \Psi | \hat{T} | \Psi \rangle$, and the electron-interaction energy $E_{ee} = \langle \Psi | \hat{U} | \Psi \rangle$ for the quantum dot in a magnetic field and the Hooke’s atom. (The external energy component $E_{\text{ext}} = \int \rho(\mathbf{r}) [\frac{1}{2}k_{\text{eff}}r^2 \text{ or } \frac{1}{2}kr^2] d\mathbf{r}$ and the Hartree energy $E_H = \frac{1}{2} \int \rho(\mathbf{r})\rho(\mathbf{r}') d\mathbf{r}d\mathbf{r}'$ are also quoted.) Observe that in the HEC regime the ratio E_{ee}/E is 46.2% and 43.4% and the ratio T/E is 15.3% and 17.4%, respectively, for the quantum dot and Hooke’s atom. In the LEC regime, the ratio E_{ee}/E is 27.3% and 22.4% whereas the ratio T/E is 29.5% and 33.2%, respectively, for these systems. These results clearly indicate the significant role that electron correlations play in comparison to the kinetic energy in the HEC regime, and of the reverse in the LEC regime.

(i) *Electron density* $\rho(\mathbf{r})$

The *local* (static) electron density $\rho(\mathbf{r})$ quantal source is defined as the expectation

$$\rho(\mathbf{r}) = \langle \Psi | \hat{\rho}(\mathbf{r}) | \Psi \rangle, \quad (11)$$

where the density operator $\hat{\rho}(\mathbf{r})$ is

$$\hat{\rho}(\mathbf{r}) = \sum_k \delta(\mathbf{r}_k - \mathbf{r}). \quad (12)$$

In Fig. 1 we plot the electron density $\rho(\mathbf{r})$ in the LEC regime in panel (a) and in the HEC regime in panel (b). The symbols 2D and 3D refer, respectively, to the quantum dot in a magnetic field and to the Hooke’s atom. In the LEC regime, the density is a maximum at the center of the atom, whereas in the HEC regime, the density has the ‘fat attractor’ profile

TABLE I: The total E , kinetic T , S -system kinetic T_s , correlation-kinetic T_c , external E_{ext} , Hartree E_H , and electron-interaction E_{ee} energies in atomic units for the ground state of a 2D quantum dot in a magnetic field (with effective force constant k_{eff}), and a 3D Hooke's atom (with force constant k) in the high electron correlation (HEC) and low electron correlation (LEC) regimes.

	Electron Correlation regimes			
	High Correlation (HEC)		Low Correlation (LEC)	
Property	Quantum dot with $\mathbf{B}$ (2D) $k_{\text{eff}} = 5.60637 \times 10^{-4}$	Hooke's atom (3D) $k = 3.00891 \times 10^{-4}$	Quantum dot with $\mathbf{B}$ (2D) $k_{\text{eff}} = 1$	Hooke's atom (3D) $k = \frac{1}{4}$
E	0.142067	0.121424	3.000000	2.000000
T	0.021771	0.021158	0.886199	0.664418
T_s	0.013495	0.015458	0.780987	0.635245
T_c	0.008276	0.005700	0.105212	0.029173
E_{ext}	0.054613	0.047527	1.295400	0.888141
E_{ee}	0.065683	0.052739	0.818401	0.447443
E_H	0.244584	0.151474	1.789832	1.030250
E_{ee}/E	46.2 %	43.4 %	27.3 %	22.4 %
T/E	15.3 %	17.4 %	29.5 %	33.2 %
T_c/T	38.0 %	26.9 %	11.9 %	4.4 %
T_c/E	5.8 %	4.5 %	3.5 %	1.45 %
$(T_c + E_{ee})/E$	52.1 %	48.1 %	30.8 %	23.8 %

[9, 39] with a local minimum at the center and a maximum away from the center with the electrons localized to a shell about it. The two electrons are confined to a ring about the center, and are antipodal *i.e.* on opposite sides. This thus constitutes a two-electron Wigner molecule [6]. (Note that the Hooke's atom densities have been magnified in order to enable a comparison with those of the quantum dot.) Observe that in each regime, the structure of the corresponding densities in 2D and 3D are similar. Thus, confining the electrons harmonically leads to a similar structure of the densities in both 2 and 3 dimensions.

The current density $\mathbf{j}(\mathbf{r})$ is the expectation $\langle \Psi | \hat{\mathbf{j}}(\mathbf{r}) | \Psi \rangle$, where the current density operator

$\hat{\mathbf{j}}(\mathbf{r}) = \hat{\mathbf{j}}_p(\mathbf{r}) + \hat{\mathbf{j}}_d(\mathbf{r})$ with the paramagnetic component being $\hat{\mathbf{j}}_p(\mathbf{r}) = \frac{1}{2} \sum_k [\hat{\mathbf{p}}_k \delta(\mathbf{r}_k - \mathbf{r}) + \delta(\mathbf{r}_k - \mathbf{r}) \hat{\mathbf{p}}_k]$, and the diamagnetic component $\hat{\mathbf{j}}_d = \hat{\rho}(\mathbf{r}) \mathbf{A}(\mathbf{r})$. As the wave functions employed are real, the paramagnetic current density $\mathbf{j}_p(\mathbf{r})$ vanishes, and hence $\mathbf{j}(\mathbf{r}) = \rho(\mathbf{r}) \mathbf{A}(\mathbf{r})$, the diamagnetic current density.

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

The *nonlocal* (dynamic) single-particle density matrix $\gamma(\mathbf{r}\mathbf{r}')$ quantal source is defined as the expectation

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

where the density matrix operator $\hat{\gamma}(\mathbf{r}\mathbf{r}')$ is

$$\hat{\gamma}(\mathbf{r}\mathbf{r}') = \hat{A} + i\hat{B}, \quad (14)$$

$$\hat{A} = \frac{1}{2} \sum_j [\delta(\mathbf{r}_j - \mathbf{r}) T_j(\mathbf{a}) + \delta(\mathbf{r}_j - \mathbf{r}') T_j(-\mathbf{a})], \quad (15)$$

$$\hat{B} = \frac{i}{2} \sum_j [\delta(\mathbf{r}_j - \mathbf{r}) T_j(\mathbf{a}) - \delta(\mathbf{r}_j - \mathbf{r}') T_j(-\mathbf{a})], \quad (16)$$

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

In Figs. 2 and 3 we plot the density matrix $\gamma(\mathbf{r}\mathbf{r}')$ in the HEC regime for the 2D quantum dot. In Fig. 2 the panels (a) and (b) correspond to $(\theta = 0^\circ; \theta' = 0^\circ)$ and $(\theta = 0^\circ; \theta' = 45^\circ)$, respectively, and in Fig. 3 the panels (a) and (b) are for $(\theta = 0^\circ; \theta' = 60^\circ)$ and $(\theta = 0^\circ; \theta' = 90^\circ)$. (The vectors are $\mathbf{r} = (r\theta)$ and $\mathbf{r}' = (r'\theta')$. By changing θ' one changes the vector $\mathbf{r}'$ relative to the vector $\mathbf{r}$.) These figures show the *dynamic* nature of this quantal source: as the vector $\mathbf{r}'$ changes, the structure of this source changes. Another fact evident from these figures, and in particular from that of Fig. 3(b), is that the off-diagonal elements of the density matrix are significant in the HEC regime. (Note that the diagonal matrix elements $\gamma(\mathbf{r}\mathbf{r}) = \rho(\mathbf{r})$. The structure for $\mathbf{r} = \mathbf{r}'$ is that of the density $\rho(\mathbf{r})$ of Fig. 1(b)).

In Fig. 4, we plot $\gamma(\mathbf{r}\mathbf{r}')$ for the 2D quantum dot in the LEC regime. The panels (a) and (b) correspond to $(\theta = 0^\circ; \theta' = 0^\circ)$ and $(\theta = 0^\circ; \theta' = 60^\circ)$, respectively. In this instance, the dynamic nature of the quantal source is not that evident on the scale plotted. What is evident, however, is that in the LEC, the off-diagonal elements of the density matrix are negligible.

(iii) Kinetic energy density $t(\mathbf{r})$ and kinetic energy T

The kinetic energy density $t(\mathbf{r})$ is the trace of the kinetic energy tensor $t_{\alpha\beta}(\mathbf{r}; [\gamma])$:

$$t(\mathbf{r}) = \sum_{\alpha} t_{\alpha\alpha}(\mathbf{r}) \geq 0, \quad (17)$$

where

$$t_{\alpha\beta}(\mathbf{r}; [\gamma]) = \frac{1}{4} \left[\frac{\partial^2}{\partial r'_{\alpha} \partial r''_{\beta}} + \frac{\partial^2}{\partial r'_{\beta} \partial r''_{\alpha}} \right] \gamma(\mathbf{r}'\mathbf{r}'') \Big|_{\mathbf{r}'=\mathbf{r}''=\mathbf{r}}. \quad (18)$$

For both the 2D and 3D systems being considered, the tensor $t_{\alpha\beta}(\mathbf{r}; [\gamma])$ can be written as

$$t_{\alpha\beta}(\mathbf{r}; [\gamma]) = \frac{r_{\alpha} r_{\beta}}{r^2} f(r) + \delta_{\alpha\beta} k(r), \quad (19)$$

where the functions $f(r)$ and $k(r)$ are given in the Appendix A.

The kinetic energy T is then

$$T = \int t(\mathbf{r}) d\mathbf{r}. \quad (20)$$

In Fig. 5 we plot the kinetic energy density $t(\mathbf{r})$ in the LEC and HEC regimes. Observe that in the LEC regime, Fig. 5a, there is a *quantal decompression* of $t(\mathbf{r})$ away from the center of the atom in both the 2D quantum dot and the 3D Hooke's atom. By this we mean that the maximum of $t(\mathbf{r})$ is away from the center of the respective atom. Hence, from the volume (for 3D) or area (for 2D) integral of Eq. (20), it is evident that since in the LEC $t(\mathbf{r})$ is large for large r , the kinetic energy is large. This is also reflected by the ration T/E , where E is the total energy (see Table I). On the other hand, in the HEC regime, Fig. 5b, there is a *quantal compression* of $t(\mathbf{r})$ towards the center of the atom. That is the maximum of $t(\mathbf{r})$ occurs at the center of each atom so that it is large for small r . Again, it follows from Eq. (20) that the corresponding kinetic energies T in both 2D and 3D are small. Once again this is reflected by the ration T/E (see Table I). Note also the similarity in structure of $t(\mathbf{r})$ for both 2D and 3D in the respective LEC and HEC regimes.

We next explain the reason underlying the structure of $t(\mathbf{r})$ shown in Fig. 5.

(iv) Kinetic 'force' $\mathbf{z}(\mathbf{r})$, kinetic field $\mathbf{Z}(\mathbf{r})$, and kinetic energy T

The concept of the kinetic 'force' $\mathbf{z}(\mathbf{r})$ stems from the 'Quantal Newtonian' first law [7] (for the stationary state case). The quantal source for the kinetic 'force' is the *nonlocal* single particle density matrix $\gamma(\mathbf{r}\mathbf{r}')$. Accordingly, the 'force' is defined as

$$z_{\alpha}(\mathbf{r}) = 2 \sum_{\beta} \frac{\partial}{\partial r_{\beta}} t_{\alpha\beta}(\mathbf{r}; [\gamma]). \quad (21)$$

(Note that the kinetic ‘force’ depends on both the diagonal and off-diagonal elements of the kinetic energy tensor $t_{\alpha\beta}(\mathbf{r}; [\gamma])$. In contrast the kinetic energy density $t(\mathbf{r})$ is simply its trace.) The kinetic field $\mathbf{Z}(\mathbf{r})$ (‘force’/charge) in turn is defined as

$$\mathbf{Z}(\mathbf{r}) = \mathbf{z}(\mathbf{r})/\rho(\mathbf{r}). \quad (22)$$

Again, it follows from the ‘Quantal Newtonian’ first law that the kinetic energy T can be written in integral virial form [5] in terms of the kinetic field $\mathbf{Z}(\mathbf{r})$ or the kinetic ‘force’ $\mathbf{z}(\mathbf{r})$ as

$$T = -\frac{1}{2} \int \rho(\mathbf{r}) \mathbf{r} \cdot \mathbf{Z}(\mathbf{r}) d\mathbf{r} = -\frac{1}{2} \int \mathbf{r} \cdot \mathbf{z}(\mathbf{r}) d\mathbf{r}. \quad (23)$$

In Fig. 6 we plot the kinetic ‘force’ $\mathbf{z}(\mathbf{r})$ for the 2D and 3D systems in the LEC and HEC regimes. The first observation is that once again the 2D and 3D systems in the LEC and HEC regimes, respectively, are similar. Due to the fact that the density $\rho(\mathbf{r})$ surrounding the center of the atom ($0 < r < 1$) in the LEC regime (see Fig. 1a) has its maximum at the center of the atom, the kinetic ‘force’ $\mathbf{z}(\mathbf{r})$ (see Fig. 6a) is initially positive for both the 2D and 3D systems. Beyond this region, the structure is negative. In contrast, in the HEC regime, the density $\rho(\mathbf{r})$ is less than the maximum value in the region about the center ($0 < r < 5$) (see Fig. 1b), so that the ‘force’ $\mathbf{z}(r)$ (see Fig. 6b) for both the 2D and 3D systems is negative in this range. Beyond this range, the ‘force’ $\mathbf{z}(\mathbf{r})$ is initially positive and then becomes negative again.

In Fig. 7 we plot the divergence of the ‘force’ $\mathbf{z}(\mathbf{r})$, *i. e.* $\nabla \cdot \mathbf{z}(\mathbf{r})$. In the LEC regime (see Fig. 7a), the divergence is positive in the near range surrounding the atom for both the 2D and 3D systems. This means there is a net flow of kinetic ‘force’ *away* from the interior of the atom leading thereby to a maximum of the kinetic energy density $t(\mathbf{r})$ in a region away from the center (see Fig. 5a). This explains the quantal decompression of the $t(\mathbf{r})$ in the LEC regime. On the other hand, in the near region surrounding the atom in the HEC regime, the divergence of the kinetic ‘force’ is negative. This implies that there is a net flow of kinetic ‘force’ *towards* the center of the atom. This leads to a global extremum of $t(\mathbf{r})$ at the center of the atom (see Fig. 5b) corresponding to the quantal compression of $t(\mathbf{r})$. The understanding of the remaining structure of the kinetic energy density $t(\mathbf{r})$ in both the LEC and HEC regimes follows as above from that of the ‘force’ $\mathbf{z}(\mathbf{r})$ and its divergence.

The values of the kinetic energy T as obtained from Eq. (23) via the kinetic ‘force’ $\mathbf{z}(\mathbf{r})$ or the field $\mathbf{Z}(\mathbf{r})$ are, of course, the same as noted above and in Table I.

(v) *S*-system Properties

In the mapping to the model system of noninteracting fermions possessing the same density $\rho(\mathbf{r})$, the quantal source for all the *S*-system kinetic properties is the Dirac density matrix $\gamma_s(\mathbf{r}\mathbf{r}')$ which is defined in terms of the Slater determinant wave function $\Phi\{\phi_k\}$ as the expectation

$$\gamma_s(\mathbf{r}\mathbf{r}') = \langle \Phi\{\phi_k\} | \hat{\gamma}(\mathbf{r}\mathbf{r}') | \Phi\{\phi_k\} \rangle. \quad (24)$$

The kinetic energy tensor $t_{s,\alpha\beta}(\mathbf{r}; [\gamma_s])$, kinetic ‘force’ $\mathbf{z}_s(\mathbf{r})$, and the kinetic field $\mathbf{Z}_s(\mathbf{r})$ are all defined as for the interacting system but with $\gamma_s(\mathbf{r}\mathbf{r}')$ as the quantal source. The kinetic energy T_s in terms of the kinetic ‘force’ and field is thus [7]

$$T_s = -\frac{1}{2} \int \rho(\mathbf{r}) \mathbf{r} \cdot \mathbf{Z}_s(\mathbf{r}) d\mathbf{r} = -\frac{1}{2} \int \mathbf{r} \cdot \mathbf{z}_s(\mathbf{r}) d\mathbf{r}. \quad (25)$$

The *S*-system kinetic ‘force’ $\mathbf{z}_s(\mathbf{r})$ for the 2D quantum dot and the 3D Hooke’s atom in the LEC and HEC regimes is plotted in Fig 8 panels (a) and (b), respectively. Once again, observe that the structure in 2D and 3D in each correlation regime is similar. Observe, that in the LEC regime, a comparison of Figs. 8a to Fig. 6a shows that the noninteracting and interacting system ‘forces’ $\mathbf{z}_s(\mathbf{r})$ and $\mathbf{z}(\mathbf{r})$, respectively, are similar in both structure and magnitude. Hence, their difference is small, and as a consequence so is the correlation-kinetic energy in comparison with the total energy. (See subsection (vi) below). In the HEC regime, Fig. 8b, there is more structure than that in the LEC regime to the kinetic ‘force’ $\mathbf{z}_s(\mathbf{r})$ as is the case for the interacting system ‘force’ $\mathbf{z}(\mathbf{r})$ (Fig. 6b). However, the noninteracting and interacting ‘forces’ differ significantly. A consequence of this difference is that the correlation-kinetic energy is large in comparison with the total energy. (See subsection (vi) below.)

The corresponding values for the kinetic energy T_s are given in Table I.

(vi) *Correlation-Kinetic field $\mathbf{Z}_{t_c}(\mathbf{r})$ and energy T_c*

The correlation-kinetic field $\mathbf{Z}_{t_c}(\mathbf{r})$ is defined as the difference

$$\mathbf{Z}_{t_c}(\mathbf{r}) = \mathbf{Z}_s(\mathbf{r}) - \mathbf{Z}(\mathbf{r}), \quad (26)$$

and the correlation-kinetic energy in integral virial form as [7]

$$T_c = \frac{1}{2} \int \rho(\mathbf{r}) \mathbf{r} \cdot \mathbf{Z}_{t_c}(\mathbf{r}) d\mathbf{r}. \quad (27)$$

The correlation-kinetic field $\mathcal{Z}_{t_c}(\mathbf{r})$ is plotted in Fig. 9. Observe that in both the LEC and HEC regimes, and for both the 2D and 3D cases, the field $\mathcal{Z}_{t_c}(\mathbf{r})$ is positive. Hence, the correlation-kinetic energy T_c is positive (see Table I).

The results of Table I show that in the HEC regime, the correlation component of the kinetic energy T_c is a significant fraction of the total kinetic energy T : the ratio T_c/T is 27% and 38%, respectively, for the 3D Hooke's atom and 2D quantum dot. Thus, the correlation-kinetic energy T_c constitutes a significant fraction of the total energy: T_c/E is 4.5% and 5.8%, respectively, for the 3D and 2D cases. In the LEC regime, the correlation-kinetic energy is a smaller fraction of the kinetic energy: T_c/T is 4.4% and 11.9% for the 3D and 2D cases, respectively. Thus, it constitutes a smaller fraction of the total energy too. Note, however, that due to the reduced dimensionality of the 2D quantum dot, correlation-kinetic effects are nonetheless significant in both the HEC and LEC regimes.

IV. CONCLUDING REMARKS

In this work we have studied kinetic related properties for the two-electron 2D quantum dot in a magnetic field, and the two-electron 3D quantum dot (Hooke's atom) in the low (LEC) and high (HEC) electron correlation regimes. Beginning with the *local* and *nonlocal* quantal sources of the electron density $\rho(\mathbf{r})$ and the single-particle density matrix $\gamma(\mathbf{r}\mathbf{r}')$, respectively, the kinetic properties considered are the kinetic energy tensor $t_{\alpha\beta}(\mathbf{r}; \gamma)$; its trace the kinetic energy density $t(\mathbf{r})$; the kinetic 'force' $\mathbf{z}(\mathbf{r})$; the divergence of the kinetic 'force' $\nabla \cdot \mathbf{z}(\mathbf{r})$; the kinetic field $\mathcal{Z}(\mathbf{r})$; and the kinetic energy T . In order to obtain the correlation contribution to the kinetic energy - the correlation-kinetic energy T_c - the interacting-electron quantum dots are then mapped via quantal density functional theory [7] to model systems of *noninteracting* fermions possessing the same density $\rho(\mathbf{r})$ and physical current density $\mathbf{j}(\mathbf{r})$ for the 2D quantum dot, and the same density $\rho(\mathbf{r})$ for Hooke's atom. The corresponding *S*-system kinetic properties obtained are the *nonlocal* quantal source, *viz.* the Dirac density matrix $\gamma_s(\mathbf{r}, \mathbf{r}')$, the kinetic energy tensor $t_{s,\alpha\beta}(\mathbf{r}; \gamma_s)$; the kinetic 'force' $\mathbf{z}_s(\mathbf{r})$; the kinetic field $\mathcal{Z}_s(\mathbf{r})$; and the kinetic energy T_s .

Our main conclusions with regard to the above properties are the following:

- (a) In spite of the fact that the electrons are confined to a plane for the quantum dot in a magnetic field, and those of the Hooke's atom allowed to move in three-dimensional

configuration space, the structure of the properties – for these different dimensional systems are *similar* within a specific electron correlation regime – either the LEC or HEC. However, the structure of the properties within the LEC and HEC regimes differ.

(b) A consequence of this is that irrespective of dimensionality, there is a quantal decompression of the kinetic energy density $t(\mathbf{r})$ in the LEC regime with a maximum for $t(\mathbf{r})$ occurring away from the center of the atom (Fig. 5). In contrast there is a quantal compression of $t(\mathbf{r})$ in the HEC regime with the maximum occurring at the center of the atom (Fig. 5). The quantal decompression and compression in the two regimes, respectively, are explained via the divergence of the kinetic ‘force’ $\mathbf{z}(\mathbf{r})$. This shows that there is a net flow of kinetic ‘force’ away from the interior of the atom in the LEC regime, whereas there is a net flow of kinetic ‘force’ towards the center of the atom in the HEC regime.

(c) The quantal compression of the kinetic energy density $t(\mathbf{r})$ in the HEC regime then explains why the kinetic energy T as a fraction of the total energy E is small in comparison to that of the electron-interaction energy E_{ee} (Table I). In contrast, the quantal decompression of $t(\mathbf{r})$ in the LEC regime leads to a kinetic energy T greater than that of the electron-interaction energy E_{ee} relative to the total energy E .

(d) Finally, in the HEC regime, the correlation-kinetic energy T_c constitutes a large fraction of the kinetic energy T . As a consequence, the contribution to the energy due to electron correlations ($T_c + E_{ee}$) constitutes about 50% of the total energy (Table I). It is interesting to note that in the LEC regime, due to the reduction in dimensionality of the 2D quantum dot, the correlation-kinetic energy T_c is once again a significant part of the kinetic energy T (Table I). (This is the case for both the ground state result quoted in Table I as well as for the excited state of the quantum dot [25].) Hence, in this case ($T_c + E_{ee}$) is about a third of the total energy E (Table I). For the 3D Hooke’s atom in the LEC regime, the correlation-kinetic energy T_c is small as expected for this regime. (This is of course the case for all atoms and molecules in their ground state.) These results for the correlation-kinetic energy T_c confirm our prior conclusion [9, 10] that the Wigner HEC low density systems ought to be characterized not only by a high electron-interaction energy E_{ee} relative to the total energy E , but also by a high value of the correlation-kinetic energy T_c .

In our recent work [25], we have studied the first excited singlet state of a two-electron quantum dot in a magnetic field in the LEC regime. As is the case for the ground state of the quantum dot in this regime [24] (Table I), a key result was once again a high value

for the correlation-kinetic energy relative to the total energy. Hence, a high value for the correlation-kinetic energy is a characteristic of this lower-dimensional artificial atom. We are presently investigating the quantum dot in a magnetic field in its lowest excited triplet state.

We conclude by noting that our results are also related to the many-body energy functional of Kohn-Sham (KS) density functional theory [33]. In KS theory, the many body effects due to the Pauli exclusion principle, Coulomb repulsion, and correlation-kinetic effects are all incorporated in the unknown electron-interaction energy functional $E_{ee}^{KS}[\rho]$ of the density $\rho(\mathbf{r})$. The corresponding electron-interaction potential $v_{ee}(\mathbf{r})$ of Eqs. (5) and (9) is then the functional derivative of this energy functional. For the examples of the quantum dots discussed in our work, the values for the KS electron-interaction energy functional $E_{ee}^{KS}[\rho]$ correspond to $(E_{ee} + T_c)$ of Table I. As our results are exact, so are the corresponding values of the functional $E_{ee}^{KS}[\rho]$. For general remarks on the construction of such functionals we refer the reader to [40], and for recent work within KS theory on the HEC regime to [41].

APPENDIX A: KINETIC EFFECTS RELATED EXPRESSIONS FOR THE (2D) 2-ELECTRON QUANTUM DOT IN A MAGNETIC FIELD, AND THE (3D) 2-ELECTRON HOOKE'S ATOM.

The expressions for the properties in the low electron correlation (LEC) and high electron correlation (HEC) regimes are given.

Electron density $\rho(\mathbf{r})$

Quantum Dot + B (2D)

LEC regime

$$\rho(\mathbf{r}) = 2\pi N^2 e^{-r^2} \left\{ \sqrt{\pi} e^{-r^2/2} \left[(1 + r^2) I_0(r^2/2) + r^2 I_1(r^2/2) \right] + 2 + r^2 \right\} \quad (\text{A1})$$

where $N = 0.135646$ and $I_0(x)$ and $I_1(x)$ are the zeroth- and first-order modified Bessel functions [42].

HEC regime

$$\begin{aligned} \rho(\mathbf{r}) = & \pi N^2 \left\{ \frac{2}{\Omega^5} e^{-\Omega r^2} (K_1 + L_1 r^2 + M_1 r^4 + N_1 r^6 + O_1 r^8) \right. \\ & + \frac{\sqrt{\pi\Omega}}{4\Omega^5} e^{-\frac{3}{2}\Omega r^2} (K_2 + L_2 r^2 + M_2 r^4 + N_2 r^6 + O_2 r^8) I_0(\Omega r^2/2) \\ & \left. + \frac{\sqrt{\pi\Omega}}{2\Omega^4} e^{-\frac{3}{2}\Omega r^2} r^2 (K_3 + L_3 r^2 + M_3 r^4 + N_3 r^6) I_1(\Omega r^2/2) \right\}, \end{aligned} \quad (\text{A2})$$

where

$$\begin{aligned}
N &= 9.26662 \times 10^{-5}, \quad \Omega = 2.36778 \times 10^{-2}, \\
K_1 &= 24C^2 + (6B^2 + 12AC)\Omega + (2A^2 + 4B + 4C)\Omega^2 + (1 + 2A)\Omega^3, \\
L_1 &= 96C^2\Omega + (18B^2 + 36AC)\Omega^2 + (4A^2 + 8B + 8C)\Omega^3 + (1 + 2A)\Omega^4, \\
M_1 &= 72C^2\Omega^2 + (9B^2 + 18AC)\Omega^3 + (A^2 + 2B + 2C)\Omega^4, \\
N_1 &= 16C^2\Omega^3 + (B^2 + 2AC)\Omega^4, \\
O_1 &= C^2\Omega^8, \\
K_2 &= 105BC + 30(AB + C)\Omega + 12(A + B)\Omega^2 + 8\Omega^3, \\
L_2 &= 420BC\Omega + 90(AB + C)\Omega^2 + 24(A + B)\Omega^3 + 8\Omega^4, \\
M_2 &= 376BC\Omega^2 + 56(AB + C)\Omega^3 + 8(A + B)\Omega^4, \\
N_2 &= 104BC\Omega^3 + 8(AB + C)\Omega^4, \\
O_2 &= 8BC^2\Omega^4, \\
K_3 &= 88BC + 23(AB + C)\Omega + 8(A + B)\Omega^2 + 4\Omega^3, \\
L_3 &= 142BC\Omega + 24(AB + C)\Omega^2 + 4(A + B)\Omega^3, \\
M_3 &= 48BC\Omega^2 + 4(AB + C)\Omega^3, \\
N_3 &= 4BC\Omega^3, \\
A &= 0.226322, \quad B = 1.72543 \times 10^{-2}, \quad C = 4.08546 \times 10^{-4}, \tag{A3}
\end{aligned}$$

and $I_0(x)$ and $I_1(x)$ are the zeroth- and first-order modified Bessel functions [42].

Hooke's Atom (3D)

LEC regime

$$\rho(\mathbf{r}) = \frac{\pi\sqrt{2\pi}N^2}{r} e^{-r^2/2} \left[7r + r^3 + \frac{8}{\sqrt{2\pi}} r e^{-r^2/2} + 4(1 + r^2) \operatorname{erf}(r/\sqrt{2}) \right] \tag{A4}$$

where $N = 0.0291122$ and $\operatorname{erf}(x)$ is the error function [42].

HEC regime

$$\rho(\mathbf{r}) = \frac{\pi N^2}{8} \left\{ \frac{e^{-2\omega r^2}}{\omega^{19/2}} (K_4 + L_4 r^2 + M_4 r^4 + N_4 r^6) + \frac{e^{-\omega r^2}}{\omega^{19/2}} (K_5 + L_5 r^2 + M_5 r^4 + N_5 r^6 + O_5 r^8) + \frac{2\sqrt{\pi}}{r\omega^{11/2}} (K_6 + L_6 r^2 + M_6 r^4 + N_6 r^6 + O_6 r^8) \operatorname{erf}(r\sqrt{\omega}) \right\}, \quad (\text{A5})$$

where

$$\begin{aligned} N &= 8.94669 \times 10^{-2}, \quad \omega = 1.73462 \times 10^{-2}, \\ K_4 &= 1116BC\omega^{9/2} + (264AB + 132C)\omega^{11/2} + (40A + 80B)\omega^{13/2} + 16\omega^{15/2}, \\ L_4 &= 1480BC\omega^{11/2} + (224AB + 112C)\omega^{13/2} + (16A + 32B)\omega^{15/2}, \\ M_4 &= 432BC\omega^{13/2} + (32AB + 16C)\omega^{15/2}, \\ N_4 &= 32BC\omega^{15/2}, \\ K_5 &= \sqrt{\pi} \left[945C^2\omega^4 + (210B^2 + 420AC)\omega^5 + 60(A^2 + B + 2C)\omega^6 + (6 + 48A)\omega^7 + 16\omega^8 \right], \\ L_5 &= \sqrt{\pi} \left[2520C^2\omega^5 + (420B^2 + 840AC)\omega^6 + 80(A^2 + B + 2C)\omega^7 + (4 + 32A)\omega^8 \right], \\ M_5 &= \sqrt{\pi} \left[1512C^2\omega^6 + (168B^2 + 336AC)\omega^7 + 16(A^2 + B + 2C)\omega^8 \right], \\ N_5 &= \sqrt{\pi} \left[288C^2\omega^7 + (16B^2 + 32AC)\omega^8 \right], \\ O_5 &= 16C^2\sqrt{\pi}\omega^8, \\ K_6 &= 105BC + (30AB + 15C)\omega + (6A + 12B)\omega^2 + 4\omega^3, \\ L_6 &= 840BC\omega + (180AB + 90C)\omega^2 + (24A + 48B)\omega^3 + 8\omega^4, \\ M_6 &= 840BC\omega^2 + (120AB + 60C)\omega^3 + (8A + 16B)\omega^4, \\ N_6 &= 224BC\omega^3 + (16AB + 8C)\omega^4, \\ O_6 &= 16BC\omega^4, \\ A &= 7.17692 \times 10^{-2}, \quad B = 3.81249 \times 10^{-3}, \quad C = 6.61322 \times 10^{-5}, \end{aligned} \quad (\text{A6})$$

and $\operatorname{erf}(x)$ is the error function [42].

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

Quantum Dot + B (2D)
LEC regime

$$\gamma(\mathbf{r}\mathbf{r}') = 2N^2 e^{-(r^2+r'^2)/2} \int e^{-y^2} [1 + |\mathbf{y} - \mathbf{r}|] [1 + |\mathbf{y} - \mathbf{r}'|] d\mathbf{y}, \quad (\text{A7})$$

where the constant N is given below Eq. (A1).

HEC regime

$$\gamma(\mathbf{r}\mathbf{r}') = 2 N^2 e^{-\Omega(r^2+r'^2)/2} \int e^{-\Omega y^2} \left[1 + |\mathbf{y} - \mathbf{r}| + A|\mathbf{y} - \mathbf{r}|^2 + B|\mathbf{y} - \mathbf{r}|^3 + C|\mathbf{y} - \mathbf{r}|^4 \right] \\ \left[1 + |\mathbf{y} - \mathbf{r}'| + A|\mathbf{y} - \mathbf{r}'|^2 + B|\mathbf{y} - \mathbf{r}'|^3 + C|\mathbf{y} - \mathbf{r}'|^4 \right] d\mathbf{y}, \quad (\text{A8})$$

where the constants N, Ω, A, B and C are given in Eq. (A3).

Hooke's Atom (3D)
LEC regime

$$\gamma(\mathbf{r}\mathbf{r}') = 2N^2 e^{-(r^2+r'^2)/4} \int e^{-y^2/2} \left[1 + \frac{|\mathbf{y} - \mathbf{r}|}{2} \right] \left[1 + \frac{|\mathbf{y} - \mathbf{r}'|}{2} \right] d\mathbf{y}, \quad (\text{A9})$$

where the constant N is given below Eq. (A4).

HEC regime

$$\gamma(\mathbf{r}\mathbf{r}') = 2 N^2 e^{-\omega(r^2+r'^2)/2} \int e^{-\omega y^2} \left[1 + \frac{|\mathbf{y} - \mathbf{r}|}{2} + A|\mathbf{y} - \mathbf{r}|^2 + B|\mathbf{y} - \mathbf{r}|^3 + C|\mathbf{y} - \mathbf{r}|^4 \right] \\ \left[1 + \frac{|\mathbf{y} - \mathbf{r}'|}{2} + A|\mathbf{y} - \mathbf{r}'|^2 + B|\mathbf{y} - \mathbf{r}'|^3 + C|\mathbf{y} - \mathbf{r}'|^4 \right] d\mathbf{y}, \quad (\text{A10})$$

where the constants N, ω, A, B and C are given in Eq. (A6).

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

For any system with electron density $\rho(\mathbf{r})$, the Dirac density matrix is calculated as

$$\gamma_s(\mathbf{r}\mathbf{r}') = \sqrt{\rho(\mathbf{r}) \rho(\mathbf{r}')}.$$
 (A11)

Kinetic energy tensor $t_{\alpha\beta}[\mathbf{r}; \gamma]$
Quantum Dot + B (2D)
LEC regime

$$t_{\alpha\beta}[\mathbf{r}; \gamma] = \frac{r_\alpha r_\beta}{r^2} f(r) + \delta_{\alpha\beta} k(r),$$
 (A12)

where

$$\begin{aligned} f(r) = & \pi N^2 e^{-r^2} \left\{ r^4 + 1 - \frac{1 - e^{-r^2}}{r^2} + \sqrt{\pi} e^{-r^2/2} \right. \\ & \times \left. \left[r^4 I_0(r^2/2) + (r^4 - r^2) I_1(r^2/2) \right] \right\}, \end{aligned}$$
 (A13)

$$k(r) = \pi N^2 e^{-r^2} \frac{(1 - e^{-r^2})}{2r^2},$$
 (A14)

where N is given below Eq. (A1), $I_0(x)$ and $I_1(x)$ are the zeroth- and first-order modified Bessel functions [42].

HEC regime

$$t_{\alpha\beta}[\mathbf{r}; \gamma] = \frac{r_\alpha r_\beta}{r^2} f(r) + \delta_{\alpha\beta} k(r),$$
 (A15)

where

$$f(r) = \pi N^2 e^{-2\Omega r^2} \left[\frac{r}{\Omega} \frac{\partial f_1(r)}{\partial r} - 2r \frac{\partial f_2(r)}{\partial r} \right] + \frac{\Omega^2}{2} r^2 \rho(r),$$
 (A16)

$$k(r) = \frac{\pi N^2}{\Omega} e^{-2\Omega r^2} f_1(r),$$
 (A17)

$$\begin{aligned}
f_1(r) = & \frac{1}{2r^2\Omega^3} \left\{ -\Omega^2 + e^{\Omega r^2} \left[\Omega^2 + 16C^2\Omega^2 r^6 + r^2 \left(96C^2 + \{18B^2 + 32AC\}\Omega + \{4A^2 \right. \right. \right. \\
& + \left. \left. 6B\}\Omega^2 \right) + r^4 \left(96C^2\Omega + \{9B^2 + 16AC\}\Omega^2 \right) \right] + e^{\Omega r^2/2} \sqrt{\pi\Omega} r^2 \left[\left(45BC + \right. \right. \\
& \left. \left. \{9AB + 6C\}\Omega + 2A\Omega^2 + 12BC\Omega^2 r^4 + r^2 \{54BC\Omega + (6AB + 4C)\Omega^2\} \right) \right. \\
& \times I_0(\Omega r^2/2) + \left(9BC + \{3AB + 2C\}\Omega + 2A\Omega^2 + 12BC\Omega^2 r^4 + r^2 \{42BC\Omega \right. \\
& + \left. (6AB + 4C)\Omega^2\} \right) I_1(\Omega r^2/2) \left. \right] \Big\}, \tag{A18}
\end{aligned}$$

$$\begin{aligned}
f_2(r) = & \frac{e^{\Omega r^2/2}}{16\Omega^4} \left\{ 8 e^{\Omega r^2/2} \left[24C^2 + \left(6B^2 + 12AC \right) \Omega + \left(2A^2 + 4B + 4C \right) \Omega^2 \right. \right. \\
& + \left(1 + 2A \right) \Omega^3 + 4C^2\Omega^3 r^6 + r^4 \left(36C^2\Omega^2 + 3\{B^2 + 2AC\}\Omega^3 \right) \\
& + \left. r^2 \left(72C^2\Omega + 12\{B^2 + 2AC\}\Omega^2 + 2\{A^2 + 2(B + C)\}\Omega^3 \right) \right] \\
& + \sqrt{\pi\Omega} \left[\left(105BC + 30\{AB + C\}\Omega + 12\{A + B\}\Omega^2 + 8\Omega^3 + 28BC\Omega^3 r^6 \right. \right. \\
& + \left. r^2 \{315BC\Omega + 60(AB + C)\Omega^2 + 12(A + B)\Omega^3\} + r^4 \{196BC\Omega^2 \right. \\
& + \left. 20(AB + C)\Omega^3\} \right) I_0(\Omega r^2/2) + \left(28BC\Omega^3 r^6 + \{161BC + 40(AB + C)\Omega \right. \\
& + \left. 12(A + B)\Omega^2\}\Omega r^2 + \{168BC\Omega + 20(AB + C)\Omega^2\}\Omega r^4 \right) I_1(\Omega r^2/2) \left. \right] \Big\}, \tag{A19}
\end{aligned}$$

where $\rho(r)$ is given in Eq. (A2), and the constants N, Ω, A, B and C are given in Eq. (A3).

Hooke's Atom (3D)

LEC regime

$$t_{\alpha\beta}[\mathbf{r}; \gamma] = \frac{r_\alpha r_\beta}{r^2} f(r) + \delta_{\alpha\beta} k(r), \tag{A20}$$

where

$$\begin{aligned}
f(r) = & \frac{1}{8} \left\{ r^2 \rho(r) - \frac{4\pi N^2}{r^3} e^{-r^2/2} \left[\sqrt{2\pi} r^5 \right. \right. \\
& - 2\sqrt{2\pi} r^2 (1 - r^2) \operatorname{erf}(r/\sqrt{2}) + 4r^3 e^{-r^2/2} \\
& \left. \left. - 6\sqrt{\pi} \operatorname{daw}(r/\sqrt{2}) - \sqrt{2\pi} r(r^2 - 3) \right] \right\}, \tag{A21}
\end{aligned}$$

$$k(r) = \frac{(\sqrt{2\pi})^3 N^2}{4 r^3} [r - \sqrt{2} \operatorname{daw}(r/\sqrt{2})] e^{-r^2/2}, \quad (\text{A22})$$

where $\rho(r)$ and N are given in and below Eq. (A4), respectively; $\operatorname{erf}(x)$ and $\operatorname{daw}(x)$ are error function and Dawson's integral, respectively [42].

HEC regime

$$t_{\alpha\beta}[\mathbf{r}; \gamma] = \frac{r_\alpha r_\beta}{r^2} f(r) + \delta_{\alpha\beta} k(r), \quad (\text{A23})$$

where

$$f(r) = \pi N^2 e^{-2\omega r^2} \left\{ \left[\frac{\partial^2 f_1(r)}{\partial r^2} - \frac{1}{r} \frac{\partial f_1(r)}{\partial r} \right] / (2\omega^2) - 2 r \frac{\partial f_2(r)}{\partial r} \right\} + \frac{\omega^2}{2} r^2 \rho(r), \quad (\text{A24})$$

$$k(r) = \frac{\pi N^2}{2 \omega^2} e^{-2\omega r^2} \left(\frac{1}{r} \right) \frac{\partial f_1(r)}{\partial r}, \quad (\text{A25})$$

$$\begin{aligned} f_1(r) = & \frac{1}{r \omega^4} \left\{ \sqrt{\omega} r e^{\omega r^2} \left[3.54491 A^2 \omega^2 + AC\omega \left(21.2694 + 14.1796 \omega r^2 \right) \right. \right. \\ & + C^2 \left(53.1736 + \omega r^2 \{ 70.8982 + 14.1796 \omega r^2 \} \right) \Big] \\ & + \omega r \left[\omega \left(2.22045 \times 10^{-16} \omega \{ A + C r^2 \} + 2C \right) \right. \\ & + B\sqrt{\omega} e^{\omega r^2} \left(2.65868 \omega + B \{ 11.9641 + 7.97604 \omega r^2 \} \right) \\ & + B \left(\omega A \{ 6 + 4.44089 \times 10^{-16} \omega r^2 \} + C \{ 30 + \omega r^2 (12 \right. \\ & + 8.88178 \times 10^{-16} \omega r^2) \} \Big] + \sqrt{\omega} e^{\omega r^2} \left[\omega \left(1.77245 A \omega \right. \right. \\ & + C \{ 1.77245 + 3.54491 \omega r^2 \} \Big) + B \left(A \omega \{ 5.31736 + 10.6347 \omega r^2 \} \right. \\ & + C \{ 15.9521 + \omega r^2 (63.8083 + 21.2694 \omega r^2) \} \Big] \operatorname{erf}(\sqrt{\omega} r) \\ & + \left[- 5.03762 \times 10^{-14} C^2 + 1.57426 \times 10^{-15} B^2 \omega \right. \\ & \left. \left. + 0.392699 \omega^3 \right] \frac{2}{\sqrt{\pi}} e^{\omega r^2} \operatorname{daw}(\sqrt{\omega} r), \right. \end{aligned} \quad (\text{A26})$$

$$\begin{aligned}
f_2(r) = & \frac{1}{r \omega^{9/2}} \left\{ r \left[e^{\omega r^2} \left(46.5269C^2 + 9.97005B^2\omega + C\{19.9401A + 93.0538Cr^2\}\omega \right. \right. \right. \\
& + \{2.65868A^2 + 5.31736C + 26.5868ACr^2 + 37.2215C^2r^4 + B(2.65868 \\
& + 13.2934Br^2)\}\omega^2 + \{0.221557 + 1.77245A + (1.77245A^2 + 1.77245B \\
& + 3.54491C)r^2 + (2.65868B^2 + 5.31736AC)r^4 + 3.54491C^2r^6\}\omega^3 \Big) \\
& + \sqrt{\omega} \left(\omega\{3.125C + 0.75A\omega + 1.25Cr^2\omega\} + B\{28.875C + 6.25A\omega \right. \\
& + 24.5C\omega r^2 + (1.5 + 2.5Ar^2 + 3.5Cr^4)\omega^2 \Big) \Big] + e^{\omega r^2} \left[11.6317BC \right. \\
& + \left(3.32335AB + C\{1.66168 + 69.7904Br^2\} \right) \omega + \left(1.32934B + 6.6467Cr^2 \right. \\
& + 46.5269BCr^4 + A\{0.66467 + 13.2934Br^2\} \Big) \omega^2 + \left(0.443113 \right. \\
& + r^2\{2.65868B + 2.21557Cr^2 + 6.20359BCr^4 + A(1.32934 \\
& + 4.43113Br^2)\} \Big) \omega^3 \Big] erf(\sqrt{\omega} r) \Big\}, \tag{A27}
\end{aligned}$$

where $\rho(r)$ is given in Eq. (A5) and the constants N, ω, A, B and C are given in Eq.(A6), $erf(x)$ and $daw(x)$ are the error function and the Dawson's integral, respectively [42].

S-system Kinetic energy tensor $t_{s,\alpha\beta}[\mathbf{r}; \gamma_s]$

$$t_{s,\alpha\beta}[\mathbf{r}; \gamma_s] = \frac{r_\alpha r_\beta}{8r^2 \rho(r)} \left(\frac{\partial \rho(r)}{\partial r} \right)^2. \tag{A28}$$

Kinetic ‘force’ $\mathbf{z}[\mathbf{r}; \gamma]$

For 2D cases, the components of kinetic force are calculated as

$$z_\alpha[\mathbf{r}; \gamma] = \frac{2 r_\alpha}{r} \left\{ \frac{\partial[f(r) + k(r)]}{\partial r} + \frac{f(r)}{r} \right\}, \tag{A29}$$

where the functions $f(r)$ and $k(r)$ for 2D-LEC case are given in Eq. (A13) and (A14), respectively, and for 2D-HEC case in Eq. (A16) and (A17), respectively.

For 3D cases, the components of kinetic force are calculated as

$$z_\alpha[\mathbf{r}; \gamma] = \frac{2 r_\alpha}{r} \left\{ \frac{\partial[f(r) + k(r)]}{\partial r} + \frac{2 f(r)}{r} \right\}, \tag{A30}$$

where the functions $f(r)$ and $k(r)$ for 3D-LEC case are given in Eq. (A21) and (A22), respectively, and for 3D-HEC case in Eq. (A24) and (A25), respectively.

S-system Kinetic ‘force’ $\mathbf{z}_s[\mathbf{r}; \gamma_s]$

For 2D cases, the components of s-system kinetic force are calculated as

$$\begin{aligned} z_{s,\alpha}[\mathbf{r}; \gamma_s] &= 2 \sum_{\beta=1}^2 \nabla_{\beta} t_{s,\alpha\beta}[\mathbf{r}; \gamma_s] \\ &= \frac{r_{\alpha}}{2r\rho(r)} \frac{\partial \rho(r)}{\partial r} \left[-\frac{1}{2\rho(r)} \left(\frac{\partial \rho(r)}{\partial r} \right)^2 + \frac{\partial^2 \rho(r)}{\partial r^2} + \frac{1}{2r} \frac{\partial \rho(r)}{\partial r} \right], \end{aligned} \quad (\text{A31})$$

where $\rho(r)$ for 2D-LEC and 2D-HEC cases are given in Eq. (A1) and (A2), respectively.

For 3D cases, the components of s-system kinetic force are calculated as

$$\begin{aligned} z_{s,\alpha}[\mathbf{r}; \gamma_s] &= 2 \sum_{\beta=1}^3 \nabla_{\beta} t_{s,\alpha\beta}[\mathbf{r}; \gamma_s] \\ &= \frac{r_{\alpha}}{2r\rho(r)} \frac{\partial \rho(r)}{\partial r} \left[-\frac{1}{2\rho(r)} \left(\frac{\partial \rho(r)}{\partial r} \right)^2 + \frac{\partial^2 \rho(r)}{\partial r^2} + \frac{1}{r} \frac{\partial \rho(r)}{\partial r} \right], \end{aligned} \quad (\text{A32})$$

where $\rho(r)$ for 3D-LEC and 3D-HEC cases are given in Eq. (A4) and (A5), respectively.

Divergence of Kinetic force $\nabla \cdot \mathbf{z}(\mathbf{r})$

For 2D cases, the Divergence of Kinetic force is calculated as

$$\nabla \cdot \mathbf{z}(r) = \frac{z(r)}{r} + \frac{\partial z(r)}{\partial r}, \quad (\text{A33})$$

where the components of $\mathbf{z}(\mathbf{r})$ for 2D cases is given in (A29).

For 3D cases, the Divergence of Kinetic force is calculated as

$$\nabla \cdot \mathbf{z}(r) = \frac{2 z(r)}{r} + \frac{\partial z(r)}{\partial r}, \quad (\text{A34})$$

where the components of $\mathbf{z}(\mathbf{r})$ for 3D cases is given in (A30).

Kinetic energy T

$$T = (-) \int \int \Psi^*(\mathbf{r}\mathbf{R}) \left(\nabla_r^2 + \frac{1}{4} \nabla_R^2 \right) \Psi(\mathbf{r}\mathbf{R}) \, d\mathbf{r} \, d\mathbf{R} \quad (\text{A35})$$

Quantum Dot + B (2D)

LEC regime

$$T = 2 \pi^2 N^2 \left(\frac{3}{2} + \frac{3}{8} \sqrt{2\pi} \right) = 0.886199 \, a.u., \quad (\text{A36})$$

where the constant N is given below Eq.(A1).

HEC regime

$$\begin{aligned} T = & -\frac{\pi^2 N^2}{4\Omega} \left\{ -\frac{1}{\Omega^4} \left[1536C^2 + 405BC\sqrt{2\pi\Omega} + 64 \left(3B^2 + 5AC \right) \Omega \right. \right. \\ & + 3 \left(19AB + 11C \right) \sqrt{2\pi} \Omega^{3/2} + 16 \left(2A^2 + 3B \right) \Omega^2 + \left(11A + 3B \right) \sqrt{2\pi} \Omega^{5/2} \\ & \left. \left. + 8 \left(1 + A \right) \Omega^3 + 3\sqrt{2\pi} \Omega^{7/2} + 4\Omega^4 \right] \right\} \\ = & 0.0217711 a.u., \end{aligned} \quad (\text{A37})$$

where the constants N, Ω, A, B and C are given in Eq.(A3).

Hooke's Atom (3D)

LEC regime

$$T = \pi^2 N^2 \left(14\pi + 20\sqrt{\pi} \right) = 0.664418 \, a.u., \quad (\text{A38})$$

where the constant N is given below Eq.(A4).

HEC regime

$$\begin{aligned} T &= \frac{\pi^{5/2} N^2}{2\sqrt{2} \omega^6} \left\{ 2\sqrt{\omega} \left[\omega \left(88C + 5\omega\{4A + \omega\} \right) + 24B \left(80C + \omega\{10A + \omega\} \right) \right] \right. \\ &\quad + \sqrt{2} \pi \left[2415C^2 + 30C\omega \left(16A + \omega \right) \right. \\ &\quad \left. \left. + \omega \left(270B^2 + 39A^2\omega + 33B\omega + \omega^2\{2 + 12A + 3\omega\} \right) \right] \right\} \\ &= 0.0211576 \text{ a.u.}, \end{aligned} \tag{A39}$$

where the constants N, ω, A, B and C are given in Eq.(A6).

S-system Kinetic Energy T_s

For any system with density $\rho(r)$, the non-interacting kinetic energy is calculated as

$$\begin{aligned} T_s &= \int \left(\text{Trace of } t_{s,\alpha\beta}[\mathbf{r}; \gamma_s] \right) d\mathbf{r} \\ &= \int \frac{1}{8\rho(r)} \left(\frac{\partial \rho(r)}{\partial r} \right)^2 d\mathbf{r}. \end{aligned} \tag{A40}$$

-
- [1] R. C. Ashoori, H. L. Stormer, J. S. Weiner, L. N. Pfeiffer, S. J. Pearton, K. W. Baldwin, K. W. West, Single-electron capacitance spectroscopy of discrete quantum levels, *Phys. Rev. Lett.* **68** (1992) 3088-3091.
- [2] R. C. Ashoori, Electrons in artificial atoms, *Nature* **379** (1996) 413-419.
- [3] E. Wigner, On the interaction of electrons in metals, *Phys. Rev.* **46** (1934) 1002.
- [4] E. Wigner, Effects of the electron interaction on the energy levels of electrons in metals, *Trans. Faraday Soc.* **34** (1938) 678-685.
- [5] M. Gell-Mann and K.A. Brueckner, Correlation energy of an electron gas at high density, *Phys. Rev.* **106** (1957) 364-368.
- [6] M. Taut and M. Eschrig, Exact solutions for a two-electron quantum dot model in a magnetic field and application to more complex systems, *Z. Phys. Chem.* **224** (2010) 631-649.
- [7] V. Sahni, *Quantal Density Functional Theory*, second ed., Springer-Verlag, Berlin, Heidelberg, 2016.
- [8] V. Sahni, *Quantal Density Functional Theory II: Approximation Methods and Applications*, Springer-Verlag, Berlin, Heidelberg, 2010.
- [9] D. Achan, L. Massa, V. Sahni, Wigner high electron correlation regime in nonuniform density systems: a quantal density functional theory, *Phys. Rev. A* **90** (2014) 022502.
- [10] D. Achan, L. Massa, V. Sahni, Wigner high electron correlation regime in nonuniform electron density systems: kinetic and correlation-kinetic aspects, *Comp. Theor. Chem.* **1035** (2014) 14.
- [11] S. M. Reimann, M. Manninen, Electronic structure of quantum dots, *Rev. Mod. Phys.* **74** (2002) 1283-1342.
- [12] H. Saarikoski, S. M. Reimann, A. Harju, M. Manninen, Vortices in quantum droplets: analogies between boson and fermion systems, *Rev. Mod. Phys.* **82**, (2010) 2785.
- [13] A. Kumar, S. E. Laux, F. Stern, Electron states in a GaAs quantum dot in a magnetic field, *Phys. Rev. B* **42** (1990) 5166-5175.
- [14] H. M. Zhu, J. W. Chen, X.-Y. Pan, V. Sahni, Wave function for harmonically confined electrons in time-dependent electric and magnetostatic fields, *J. Chem. Phys.* **140** (2014) 024318.
- [15] W. Kohn, Cyclotron resonance and de Haas-van Alphen oscillations of an interacting electron gas, *Phys. Rev.* **123** (1961) 1242.

- [16] L. Brey, N. F. Johnson, B. I. Halperin, Optical and magneto-optical absorption in parabolic quantum wells, *Phys. Rev. B* 40 (1989) 10647-10649.
- [17] S. K. Kip, Magneto-optical absorption by electrons in the presence of parabolic confinement potentials, *Phys. Rev. B* 43 (1991) 1707-1718.
- [18] P. A. Maksym, T. Chakraborty, Quantum dots in a magnetic field: role of electron-electron interactions, *Phys. Rev. Lett.* 65 (1990) 108-111.
- [19] F. M. Peters, Magneto-optics in parabolic quantum dots, *Phys. Rev. B* 42 (1990) 1486-1487.
- [20] J. Dobson, Harmonic potential theorem: implications for approximate many-body theories, *Phys. Rev. Lett.* 73 (1994) 2244-2247.
- [21] T. M. Henderson, K. Runge, R. J. Bartlett, Electron correlation in artificial atoms, *Chem. Phys. Lett.* 337 (2001) 138-142.
- [22] T. M. Henderson, K. Runge, R. J. Bartlett, Excited states in artificial atoms via the equation of motion coupled cluster theory, *Phys. Rev. B* 67 (2003) 045320.
- [23] F. Pederiva, C. J. Umrigar, E. Lipparini, Monte Carlo study of circular quantum dots, *Phys. Rev. B* 62 (2000) 8120.
- [24] T. Yang, X.-Y. Pan, V. Sahni, Quantal density functional theory in the presence of a magnetic field, *Phys. Rev. A* 83 (2011) 042518.
- [25] M. Slamet, V. Sahni, Electron correlations in an excited state of a quantum dot in a magnetic field, *Comp. Theor. Chem.* 1114 (2017) 125-139.
- [26] V. Sahni, X.-Y. Pan, T. Yang, Electron correlations in local effective potential theory, *Computation* 4 (2016) 30.
- [27] P. Hohenberg, W. Kohn, Inhomogeneous electron gas, *Phys. Rev.* 136 (1964) B864-B871.
- [28] X.-Y. Pan and V. Sahni, Hohenberg-Kohn theorems in electrostatic and uniform magnetostatic fields, *J. Chem. Phys.* 143 (2015) 174105.
- [29] Z. Qian, V. Sahni, Physics of transformation from Schrödinger theory to Kohn-Sham density-functional theory: Application to an exactly solvable model, *Phys. Rev. A* 57 (1998) 2527.
- [30] M. Taut, Two electrons in an external oscillator potential : particular analytical solutions of a Coulomb correlation problem, *Phys. Rev. A* 48 (1993) 3561.
- [31] S. Kais, D. R. Herschbach, R. D. Levine, Dimensional scaling as a symmetry operation, *J. Chem. Phys.* 91 (1989) 7791.
- [32] N. R. Kestner, O. Sinanoglu, Study of electron correlation in helium-like systems using an

- exactly solvable model, Phys. Rev. 128 (1962) 2687.
- [33] W. Kohn, L. J. Sham, Self-consistent equations including exchange and correlation effects, Phys. Rev. 140, (1965) A1133-A1138.
 - [34] M. Taut, Two electrons in a homogeneous magnetic field; particular analytical solutions, J. Phys. A 27 (1994) 1945-1055.
 - [35] M. Taut, Corrigenda: Two electrons in a homogeneous magnetic field; particular analytical solutions, J. Phys. A 27 (1994) 4723-4724.
 - [36] M. Dineykhon, R. C. Nazmitdinov, Two electron quantum dot in a magnetic field: analytical results, Phys. Rev. B 55 (1997) 13707-13714.
 - [37] J. L. Zhu, Z.-Q. Li, J.-Z. Yu, K. Ohno, Y. Kawazoe, Size and shape effects of quantum dots on two-electron spectra, Phys. Rev. B 55 (1997) 15819-15823.
 - [38] X.-Y. Pan, V. Sahni, Integral coalescence conditions in $D \geq 2$, dimension space, J. Chem. Phys. 119 (2003) 7083.
 - [39] J. Ciolowski, K. Pernal, The ground state of Harmonium, J. Chem. Phys. 113 (2000) 8434-8443.
 - [40] A. Ruzsinsky, J. P. Perdew, Twelve outstanding problems in ground state density functional theory: a bouquet of puzzles, Comp. Theor. Chem. 963 (2011) 2-6.
 - [41] F. Malet, P. Gori-Giorgi, Strong correlation in Kohn-Sham density functional theory, Phys. Rev. Lett. 109 (2012), 246402 1-6.
 - [42] J. Spanier, K.B. Oldham, An Atlas of Functions, Hemisphere Publishing Corp., New York (1987).

FIG. 1: Electron density $\rho(\mathbf{r})$ in (a) the LEC (low electron correlation) regime and (b) in the HEC (high electron correlation) regime. The symbols 2D and 3D refer, respectively, to the quantum dot in a magnetic field and to the Hooke's atom.

FIG. 2: Single-particle density matrix $\gamma(\mathbf{r}\mathbf{r}')$ in the HEC regime for the 2D quantum dot. In (a) the angle of vector $\mathbf{r}$ and $\mathbf{r}'$, respectively, are $\theta = 0^\circ$ and $\theta' = 0^\circ$. The vectors $\mathbf{r}$ and $\mathbf{r}'$ are oriented along the positive and negative x -axis. (b) The same as in panel (a) but with $\theta' = 45^\circ$. Vector $\mathbf{r}$ is along the $\pm x$ -axis, and vector $\mathbf{r}'$ is at 45° from the $\pm x$ -axis.

FIG. 3: (a) The same as in Fig. 2 but for $\theta' = 60^\circ$. Vector $\mathbf{r}$ is along the $\pm x$ -axis, and vector $\mathbf{r}'$ is at 60° from the $\pm x$ -axis. (b) The same as in Fig. 2 but for $\theta' = 90^\circ$. Vector $\mathbf{r}$ is along the $\pm x$ -axis, and vector $\mathbf{r}'$ is at 90° from the $\pm x$ -axis.

FIG. 4: Single-particle density matrix $\gamma(\mathbf{r}\mathbf{r}')$ in the LEC regime for the 2D quantum dot. In (a) the angle of vector $\mathbf{r}$ and $\mathbf{r}'$, respectively, are $\theta = 0^\circ$ and $\theta' = 0^\circ$. The vectors $\mathbf{r}$ and $\mathbf{r}'$ are oriented along the positive and negative x -axis. (b) The same as in panel (a) but with $\theta' = 60^\circ$. Vector $\mathbf{r}$ is along the $\pm x$ -axis, and vector $\mathbf{r}'$ is at 60° from the $\pm x$ -axis.

FIG. 5: Kinetic energy density $t(\mathbf{r})$ in (a) the LEC regime and (b) in the HEC regime. The symbols 2D and 3D refer, respectively, to the quantum dot in a magnetic field and to the Hooke's atom.

FIG. 6: Kinetic ‘force’ $\mathbf{z}(\mathbf{r})$ in (a) the LEC regime and (b) in the HEC regime. The symbols 2D and 3D refer, respectively, to the quantum dot in a magnetic field and to the Hooke’s atom.

FIG. 7: Divergence of the kinetic 'force' $\nabla \cdot \mathbf{z}(\mathbf{r})$ in (a) the LEC regime and (b) in the HEC regime. The symbols 2D and 3D refer, respectively, to the quantum dot in a magnetic field and to the Hooke's atom.

FIG. 8: S-system kinetic ‘force’ $\mathbf{z}_s(\mathbf{r})$ in (a) the LEC regime and (b) in the HEC regime. The symbols 2D and 3D refer, respectively, to the quantum dot in a magnetic field and to the Hooke’s atom.

FIG. 9: The correlation-kinetic field $\mathcal{Z}_{t_c}(r)$ in (a) the LEC regime and (b) in the HEC regime. The symbols 2D and 3D refer, respectively, to the quantum dot in a magnetic field and to the Hooke's atom.