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Study of the Kinetic Energy Densities of Electrons as Applied to Quantum Dots in a Magnetic Field

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Abstract

There are three expressions for the kinetic energy density $t(\mathbf{r})$ expressed in terms of its quantal source, the single-particle density matrix: $t_A(\mathbf{r})$, the integrand of the kinetic energy expectation value; $t_B(\mathbf{r})$, the trace of the kinetic energy tensor; $t_C(\mathbf{r})$, a virial form in terms of the ‘classical’ kinetic field. These kinetic energy densities are studied by application to ‘artificial atoms’ or quantum dots in a magnetic field in a ground and excited singlet state. A comparison with the densities for natural atoms and molecules in their ground state is made. The near nucleus structure of these densities for natural atoms is explained. We suggest that in theoretical frameworks which employ the kinetic energy density such as molecular fragmentation, density functional theory, and information-entropic theories, one use all three expressions on application to quantum dots, and the virial expression for natural atoms and molecules. New physics could thereby be gleaned.

I. INTRODUCTION

For a localized system of electrons in a conservative electric field, which is a definition of natural and artificial matter – atoms, molecules, solids, two-dimensional ‘artificial atoms’ or quantum dots, quantum wells, metal-oxide semiconductor structures, etc. – the kinetic energy T of the electrons can be expressed in terms of a kinetic energy density $t(\mathbf{r})$:

$$T = \int t(\mathbf{r}) d\mathbf{r}. \quad (1)$$

The kinetic energy T written as above is interesting in that there exist three different expressions for the density $t(\mathbf{r})$ that all lead to the same value of T . The three expressions are all defined in terms of the single-particle density matrix $\gamma(\mathbf{r}\mathbf{r}')$ which can then be thought of as constituting the *nonlocal* (dynamic) quantal source [1, 2] for the kinetic energy density $t(\mathbf{r})$, and hence for the kinetic energy T . A quantal source is defined as the expectation value of a Hermitian operator which then gives rise to a field that is ‘classical’ in the sense that it pervades all space. The interpretation of the density matrix $\gamma(\mathbf{r}\mathbf{r}')$ as a quantal source follows from the fact that it is the expectation of a complex operator whose real and imaginary parts are Hermitian operators [1–4]. In turn it gives rise to the kinetic field as explained below.

The first expression $t_A(\mathbf{r})$ corresponds to rewriting the integrand of the expression for the kinetic energy as the expectation of the kinetic energy operator $\hat{T}$ taken with respect to the many-electron wave function Ψ .

The second expression $t_B(\mathbf{r})$ corresponds to the trace of the kinetic energy tensor $t_{\alpha\beta}(\mathbf{r}; [\gamma])$. Having defined $\gamma(\mathbf{r}\mathbf{r}')$ as being the quantal source, the tensor and hence its trace, can be thought of as being ‘classical’ in definition. This interpretation is substantiated by the fact that for the ground state of natural atoms and molecules [5, 6] (H_2, He_2, LiF, LiH) (i.e. for three-dimensional Coulombically bound electrons), the kinetic energy density $t_B(\mathbf{r})$ is finite and positive throughout space as is the case in classical physics.

The third expression $t_C(\mathbf{r})$, one less familiar, is expressed in virial form [1, 2, 7, 8]. It is in terms of a kinetic field $\mathcal{Z}(\mathbf{r})$ whose quantal source is the density matrix $\gamma(\mathbf{r}\mathbf{r}')$. This definition is arrived at from the ‘Quantal Newtonian’ first law which is the equation of motion for the individual electron in the sea of electrons [1, 2, 7–10]. In this description of Schrödinger theory, the properties of the system can be defined in terms of ‘classical’

fields whose sources are quantum-mechanical expectations of Hermitian operators taken with respect to the wave function Ψ . Thus, for example, electron correlations due to the Pauli exclusion principle and Coulomb repulsion are represented by an electron-interaction field $\mathcal{E}_{ee}(\mathbf{r})$ whose quantal source is the pair-correlation density. The kinetic effects are represented by the kinetic field $\mathcal{Z}(\mathbf{r})$. From the ‘Quantal Newtonian’ first law, the integral virial theorem can be derived and expressed in terms of these various fields [1, 2, 7, 8]. The integrand of the kinetic energy term in the integral virial theorem is thus in virial form. (Unlike the expressions for $t_A(\mathbf{r})$ and $t_B(\mathbf{r})$, the virial expression $t_C(\mathbf{r})$ though employed to determine the kinetic energy, has not been previously studied in itself.)

As a consequence of advances in semiconductor technology, it has been possible to create ‘artificial atoms’ or quantum dots in which the motion of the electrons is restricted to a plane [11–14]. The motion of the electrons is confined to a quantum well in a thin layer of semiconductor (GaAs) sandwiched between two layers of another semiconductor (AlGaAs). The motion of the electrons is restricted by an electrostatic field to create the quantum dot. The electrons can be further confined by a magnetic field perpendicular to the plane of motion. Being housed in a condensed matter system, the mass of the electron is the band effective mass m^* . Further, the electron-interaction potential must be modified by the dielectric constant ϵ of the semiconductor. For GaAs quantum dots, $m^* = 0.067m$, where m is the electron mass, and $\epsilon = 12.4$. Based on both theory and experiment [11, 12], it is accepted that the electrons in such ‘artificial atoms’ are confined by a harmonic potential. Recent work [15, 16] which proves the Schrödinger equation to be self-consistent can also be employed to arrive at this conclusion. As a consequence of these facts, the size of a quantum dot is an order of magnitude greater than that of a natural atom. Thus, there is a lowering of the electron density, and therefore an increase in the effects of electron correlations, *viz.* those arising from the Pauli exclusion principle and Coulomb repulsion. In particular, the contribution to the kinetic energy due to the electron correlations – the correlation-kinetic contribution – is large. Hence, quantum dots are characterized not only by a high electron-interaction energy, but also a high value of the correlation-kinetic energy [17–21]. This has significance for calculations within the context of traditional density functional theory as discussed below. However, although such ‘artificial atoms’ differ in dimensionality, size and binding potential, their electronic properties exhibit structure similar to those of natural atoms [11–24].

The purpose of the paper is to study the three expressions for the kinetic energy density as applied to two-electron quantum dots in a magnetic field [25–30], *i.e.* two-dimensional interacting electronic systems in which the binding potential is harmonic. The calculations are for two different quantum dots, one in a ground and the other in an excited singlet state. Further, these calculations are performed employing *exact* closed-form analytical expressions for the ground and excited state wave functions. Finally, we compare our results with those [5, 6] of three-dimensional Coulomb potential bound natural atoms in their ground state.

We next put our work in context. In the original work by Bader et al [5, 6], the kinetic energy densities $t_A(\mathbf{r})$ and $t_B(\mathbf{r})$ were employed to determine conditions defining a surface partitioning a molecule such that the kinetic energy of each fragment was unique, and each fragment satisfied the resulting virial theorem. Both $t_A(\mathbf{r})$ and $t_B(\mathbf{r})$ hence led to the same kinetic energy for each fragment. The calculations were performed employing Hartree-Fock theory single-particle orbitals, and hence the quantal source for these kinetic energy densities is the Hartree-Fock theory Dirac density matrix. It would be interesting to study how the virial expression for the kinetic energy density $t_C(\mathbf{r})$ affects the fragmentation of a molecule, and whether for the surfaces thus defined it too would lead to the same value of the kinetic energy for each fragment. We believe the fragmentation of molecules can be defined in a different manner in terms of the kinetic field $\mathbf{Z}(\mathbf{r})$. For the fragmentation of the H_2 molecule in the context of quantal density functional theory, see [2, 31].

An area where the present results will be of value is Kohn-Sham (KS) density functional theory [32]. This is a local effective potential theory [33] in which the electron correlations due to the Pauli exclusion principle, Coulomb repulsion, and correlation-kinetic effects are subsumed in an universal electron-interaction energy functional $E_{ee}^{KS}[\rho]$ of the ground state density $\rho(\mathbf{r})$. The local electron-interaction potential $v_{ee}(\mathbf{r})$ representative of these correlations is the functional derivative $\delta E_{ee}^{KS}[\rho]/\delta\rho(\mathbf{r})$. As the functional $E_{ee}^{KS}[\rho]$ is unknown, it must be approximated. In various meta-generalized gradient approximations (GGA) [34–37], the functional $E_{ee}^{KS}[\rho]$ is expressed in terms of an approximate electron-interaction energy density $\epsilon_{ee}^{\text{approx}}(\mathbf{r})$. This energy density in turn is written in terms of the density $\rho(\mathbf{r})$, the gradient of the density $\nabla\rho(\mathbf{r})$, and to account for correlation-kinetic effects the kinetic energy density $t_B(\mathbf{r})$. The corresponding quantal source for $t_B(\mathbf{r})$ is the KS Dirac density matrix $\gamma_s(\mathbf{r}\mathbf{r}') = \sum_i \phi_i^*(\mathbf{r})\phi_i(\mathbf{r}')$, where the single-particle orbitals $\phi_i(\mathbf{r})$ are those of the corresponding KS differential equation. Thus, $t_B(\mathbf{r}) = \frac{1}{2} \sum_i |\nabla\phi_i(\mathbf{r})|^2$. The meta-GGA functionals

developed are for three-dimensional systems. We suggest the use of the virial expression $t_C(\mathbf{r})$ in such electron-interaction energy functionals. (The kinetic energy density $t_A(\mathbf{r})$ is singular at the nucleus for natural atoms and molecules, and thus is not employed.) However, when such approximate functionals are extended to two-dimensional ‘atoms’, then all three kinetic energy densities $t_A(\mathbf{r})$, $t_B(\mathbf{r})$, and $t_C(\mathbf{r})$ can be employed as explained below.

The kinetic energy density $t_B(\mathbf{r})$ for single particle orbitals is also employed to define the electron localization function (ELF) [38] which helps to identify different chemical bonds. The definition of ELF is again based on the use of single particle orbitals. We propose investigating the use of the virial expression of the kinetic energy density $t_C(\mathbf{r})$ in defining such localization functions.

Yet another area where our work will be of value is one in which information-entropic measures [39–41] are employed within the framework of quantum mechanics to define various properties of systems. For example in the work of Ghosh et al [42, 43], density functional theory is described in terms of a local temperature $T(\mathbf{r})$. This temperature is defined in terms of the kinetic energy density. As the latter is not unique, nor is the local temperature. The nonuniqueness of the kinetic energy density on the local temperature has been investigated [44–46]. For more recent work on the idea of a local temperature see [47, 48]. It would be interesting to learn how the concept of a local temperature is affected by the virial expression $t_C(\mathbf{r})$, and by all three different kinetic energy densities in two dimensions.

The definitions of the kinetic energy densities $t_A(\mathbf{r})$, $t_B(\mathbf{r})$, and $t_C(\mathbf{r})$ in terms of the common quantal source, the single-particle density matrix $\gamma(\mathbf{r}\mathbf{r}')$, are given in Sect. II. The Schrödinger-Pauli equation for a N -electron quantum dot in a magnetic field, and the corresponding analytical wave functions for two-electron quantum dots, one in a ground and the other in a first excited singlet state, are given in Sect. III. In that section, the application to the two quantum dots for the determination and analysis of the structure of the corresponding *nonlocal* (dynamic) quantal source for each state and the various kinetic energy densities, is also described. Closed-form analytical and semi-analytical expressions for the relevant properties are given in the Appendix. In Sect. IV, concluding remarks and a comparison of our results for the two-dimensional quantum dots with those of three-dimensional natural atoms are made. There, the near nucleus structure of all three kinetic energy densities for natural atoms is explained.

II. DEFINITIONS

Consider a system of N electrons in an external conservative electrostatic field $\mathcal{E}(\mathbf{r}) = -\nabla v(\mathbf{r})$. The corresponding Schrödinger equation in atomic units ($e = \hbar = m = 1$) is

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

where the operators are the kinetic $\hat{T} = -\frac{1}{2}\sum_k \nabla_k^2$; electron-interaction potential $\hat{U} = \frac{1}{2}\sum_{k,\ell}' 1/|\mathbf{r}_k - \mathbf{r}_\ell|$; external potential $\hat{V} = \sum_k v(\mathbf{r}_k)$, and where $\{\Psi(\mathbf{X}), E\}$ are the eigenfunctions and eigenvalues, with $\mathbf{X} = \mathbf{x}_1, \dots, \mathbf{x}_N$; $\mathbf{x} = \mathbf{r}\sigma$, and $\mathbf{r}$ and σ the spatial and spin coordinates. The eigenenergies are defined as the expectation value $E = \langle \Psi(\mathbf{X}) | \hat{H} | \Psi(\mathbf{X}) \rangle$.

The quantal source for all kinetic properties, *viz.* the single-particle density matrix is defined [1–4] as the expectation value of the density matrix operator $\hat{\gamma}(\mathbf{r}\mathbf{r}')$:

$$\gamma(\mathbf{r}\mathbf{r}') = \langle \Psi(\mathbf{X}) | \hat{\gamma}(\mathbf{r}\mathbf{r}') | \Psi(\mathbf{X}) \rangle, \quad (3)$$

where

$$\hat{\gamma}(\mathbf{r}\mathbf{r}') = \hat{A} + i\hat{B}, \quad (4)$$

$$\hat{A} = \frac{1}{2} \sum_k \left[\delta(\mathbf{r}_k - \mathbf{r}) T_k(\mathbf{a}) + \delta(\mathbf{r}_k - \mathbf{r}') T_k(-\mathbf{a}) \right], \quad (5)$$

$$\hat{B} = -\frac{i}{2} \sum_k \left[\delta(\mathbf{r}_k - \mathbf{r}) T_k(\mathbf{a}) - \delta(\mathbf{r}_k - \mathbf{r}') T_k(-\mathbf{a}) \right], \quad (6)$$

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

The kinetic energy density $t_A(\mathbf{r})$ whereby the integrand of the kinetic energy expectation value $T = \langle \Psi(\mathbf{X}) | \hat{T} | \Psi(\mathbf{X}) \rangle$ can be expressed in terms of $\gamma(\mathbf{r}\mathbf{r}')$ is

$$t_A(\mathbf{r}) = -\frac{1}{2} \nabla_{\mathbf{r}}^2 \gamma(\mathbf{r}\mathbf{r}') \Big|_{\mathbf{r}'=\mathbf{r}}. \quad (7)$$

The kinetic energy tensor $t_{\alpha\beta}(\mathbf{r}; [\gamma])$ also depends on the density matrix $\gamma(\mathbf{r}\mathbf{r}')$. The tensor is defined as

$$t_{\alpha\beta}(\mathbf{r}; [\gamma]) = \frac{1}{4} \left[\frac{\partial^2}{\partial r'_\alpha \partial r''_\beta} + \frac{\partial^2}{\partial r'_\beta \partial r''_\alpha} \right] \gamma(\mathbf{r}'\mathbf{r}'') \Big|_{\mathbf{r}'=\mathbf{r}''=\mathbf{r}}. \quad (8)$$

The kinetic energy density $t_B(\mathbf{r})$ is the trace of the tensor so that

$$t_B(\mathbf{r}) = \sum_\alpha t_{\alpha\alpha}(\mathbf{r}) = \frac{1}{2} \nabla_{\mathbf{r}'} \cdot \nabla_{\mathbf{r}''} \gamma(\mathbf{r}'\mathbf{r}'') \Big|_{\mathbf{r}'=\mathbf{r}''=\mathbf{r}}. \quad (9)$$

The kinetic energy densities $t_A(\mathbf{r})$ and $t_B(\mathbf{r})$ are related via

$$t_A(\mathbf{r}) - t_B(\mathbf{r}) = -\frac{1}{4}\nabla^2\rho(\mathbf{r}), \quad (10)$$

where $\rho(\mathbf{r})$, the electron density, is the expectation value of the density operator $\hat{\rho}(\mathbf{r})$:

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

where

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

The kinetic energy density $t_C(\mathbf{r})$ written in virial form is

$$t_C(\mathbf{r}) = -\frac{1}{2}\rho(\mathbf{r})\mathbf{r} \cdot \mathbf{Z}(\mathbf{r}; [\gamma]), \quad (13)$$

where the kinetic field $\mathbf{Z}(\mathbf{r}; [\gamma])$ experienced by each electron is defined in terms of the kinetic ‘force’ $\mathbf{z}(\mathbf{r}; [\gamma])$ as (‘force’/charge):

$$\mathbf{Z}(\mathbf{r}; [\gamma]) = \frac{\mathbf{z}(\mathbf{r}; [\gamma])}{\rho(\mathbf{r})}. \quad (14)$$

In turn, the components $z_\alpha(\mathbf{r})$ of the kinetic ‘force’ are defined in terms of the kinetic-energy-tensor $t_{\alpha\beta}(\mathbf{r}; [\gamma])$ as

$$z_\alpha(\mathbf{r}) = 2 \sum_\beta \frac{\partial}{\partial r_\beta} t_{\alpha\beta}(\mathbf{r}; [\gamma]). \quad (15)$$

It is important to note that the tensor $t_{\alpha\beta}(\mathbf{r}; [\gamma])$, and hence the kinetic ‘force’ $\mathbf{z}(\mathbf{r}; [\gamma])$ and field $\mathbf{Z}(\mathbf{r})$, depend on both the diagonal and off-diagonal elements of the density matrix $\gamma(\mathbf{r}\mathbf{r}')$. In general, the kinetic field $\mathbf{Z}(\mathbf{r}; [\gamma])$ is not conservative, i.e., $\nabla \times \mathbf{Z}(\mathbf{r}) \neq 0$. However, for the determination of the kinetic energy T via Eq. (1), it is irrelevant whether or not the field is conservative.

For purposes of completeness we note that the expression $t_C(\mathbf{r})$ follows from the ‘Quantal Newtonian’ first law [1]. Briefly, according to the law, the sum of the external field $\mathcal{F}^{\text{ext}}(\mathbf{r}) = \mathcal{E}(\mathbf{r})$ and internal field $\mathcal{F}^{\text{int}}(\mathbf{r})$ experienced by each electron vanishes: $\mathcal{F}^{\text{ext}}(\mathbf{r}) + \mathcal{F}^{\text{int}}(\mathbf{r}) = 0$. The internal field $\mathcal{F}^{\text{int}}(\mathbf{r})$ is the sum of an electron interaction field $\mathcal{E}_{\text{ee}}(\mathbf{r})$ representative of electron correlations due to the Pauli exclusion principle and Coulomb repulsion, a differential density field $\mathcal{D}(\mathbf{r})$ representative of the density, and the kinetic field $\mathbf{Z}(\mathbf{r})$ of Eq. (14). Thus, $\mathcal{F}^{\text{int}}(\mathbf{r}) = \mathcal{E}_{\text{ee}}(\mathbf{r}) - \mathcal{D}(\mathbf{r}) - \mathbf{Z}(\mathbf{r})$,

where $\mathcal{E}_{ee}(\mathbf{r}) = \mathbf{e}_{ee}(\mathbf{r})/\rho(\mathbf{r})$ and $\mathcal{D}(\mathbf{r}) = \mathbf{d}(\mathbf{r})/\rho(\mathbf{r})$. The electron-interaction ‘force’ is obtained from its quantal source the pair-correlation function $P(\mathbf{r}\mathbf{r}')$ via Coulomb’s law: $\mathbf{e}_{ee}(\mathbf{r}) = \int [P(\mathbf{r}\mathbf{r}')(\mathbf{r} - \mathbf{r}')/|\mathbf{r} - \mathbf{r}'|^3] d\mathbf{r}'$, where $P(\mathbf{r}\mathbf{r}') = \langle \Psi(\mathbf{X}) | \hat{P}(\mathbf{r}\mathbf{r}') | \Psi(\mathbf{X}) \rangle$, and the pair-correlation operator $\hat{P}(\mathbf{r}\mathbf{r}') = \sum'_{k,\ell} \delta(\mathbf{r}_k - \mathbf{r}) \delta(\mathbf{r}_\ell - \mathbf{r}')$. The differential density ‘force’ $\mathbf{d}(\mathbf{r}) = -\frac{1}{4} \nabla \nabla^2 \rho(\mathbf{r})$ with $\rho(\mathbf{r})$ the quantal source. From the ‘Quantal Newtonian’ first law, the integral virial theorem can be expressed [1, 2, 7, 8] in terms of the various fields as

$$\int \rho(\mathbf{r}) \mathbf{r} \cdot \mathcal{F}^{\text{ext}}(\mathbf{r}) + E_{ee} + 2T = 0. \quad (16)$$

Here the electron-interaction energy $E_{ee} = \langle \Psi(\mathbf{X}) | \hat{U} | \Psi(\mathbf{X}) \rangle$ may be written in terms of the electron-interaction field $\mathcal{E}_{ee}(\mathbf{r})$ as

$$E_{ee} = \int \rho(\mathbf{r}) \mathbf{r} \cdot \mathcal{E}_{ee}(\mathbf{r}) d\mathbf{r}. \quad (17)$$

In turn the kinetic energy T is expressed in terms of the kinetic field $\mathcal{Z}(\mathbf{r})$ as

$$T = -\frac{1}{2} \int \rho(\mathbf{r}) \mathbf{r} \cdot \mathcal{Z}(\mathbf{r}) d\mathbf{r}. \quad (18)$$

The virial expression for $t_C(\mathbf{r})$ is then evident.

We note that all of the above different expressions for the kinetic energy density are equally valid for the case of a time-dependent conservative external field $\mathcal{E}(\mathbf{r}t) = -\nabla v(\mathbf{r}t)$, as well as in the added presence of an electromagnetic field $\mathcal{B}(\mathbf{r}t) = \nabla \times \mathcal{A}(\mathbf{r}t)$, $\mathbf{E}(\mathbf{r}t) = -\nabla \Phi(\mathbf{r}t) - \partial \mathcal{A}(\mathbf{r}t)/\partial t$, with $\{v(\mathbf{r}t), \Phi(\mathbf{r}t)\}$ scalar and $\mathcal{A}(\mathbf{r}t)$ vector potentials. The time-dependent expression for the virial form $t_C(\mathbf{r}t)$ follows from the corresponding ‘Quantal Newtonian’ second law [1, 33, 49–51].

III. APPLICATION TO QUANTUM DOTS IN A MAGNETIC FIELD

We next study the expressions for the kinetic energy densities as applied to quantum dots in a magnetic field, one in a ground and the other in the first excited singlet state.

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 m^* the band effective mass, and a magnetic field $\mathcal{B}(\mathbf{r}) = \nabla \times \mathcal{A}(\mathbf{r})$, with $\mathcal{A}(\mathbf{r})$ the vector

potential, is

$$\hat{H} = \frac{1}{2m^*} \sum_k (\mathbf{p}_k + \frac{e}{c} \mathcal{A}(\mathbf{r}_k))^2 + \frac{1}{2\epsilon} \sum_{k,\ell}' \frac{e^2}{|\mathbf{r}_k - \mathbf{r}_\ell|} + \sum_k v(\mathbf{r}_k) + g^* \mu_B \sum_k \mathcal{B}(\mathbf{r}_k) \cdot \mathbf{s}_k. \quad (19)$$

The various terms of the Hamiltonian are the physical kinetic T_A (with canonical momentum $\mathbf{p}_k = i\hbar \nabla_{\mathbf{r}_k}$), electron-interaction $\hat{U}$, external potential $\hat{V}$, and magnetic field-spin interaction, with $\mathbf{s}$ the electron spin momentum vector. Here g^* is the gyromagnetic ratio, and $\mu_B = e\hbar/2mc$ the Bohr magneton, and c the velocity of light. The Schrödinger-Pauli equation is $\hat{H}\Psi(\mathbf{X}) = E\Psi(\mathbf{X})$, where $\{\Psi(\mathbf{X}), E\}$ are the eigenvalues and eigenenergies, respectively; $\mathbf{X} = \mathbf{x}, \dots, \mathbf{x}_N$; $\mathbf{x} = \mathbf{r}\sigma$; $\mathbf{r}\sigma$ the spatial and spin coordinates of each electron.

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 electron mass. The effective energy unit is $(a.u.)^* = (a.u.)(m^*/m\epsilon^2)$.

Wave Functions

We next present the exact analytical wave functions for two-electron quantum dots, one in a ground and the other in the first excited singlet state.

In the symmetric gauge $\mathcal{A}(\mathbf{r}) = \frac{1}{2}\mathcal{B}(\mathbf{r}) \times \mathbf{r}$ with the magnetic field applied in the z -direction: $\mathcal{B}(\mathbf{r}) = \mathcal{B}\mathbf{i}_z$, the electrons experience an effective harmonic force constant $k_{\text{eff}} = \omega_0^2 + \omega_L^2$, with $\omega_L = B/2$ the Larmor frequency. For a two-electron quantum dot in a ground state, the spatial part of the wave function is [17]

$$\Psi_0(\mathbf{r}_1\mathbf{r}_2) = C_0 e^{-\Omega(R^2 + \frac{1}{4}u^2)}(1 + u), \quad (20)$$

where $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2$, $u = |\mathbf{r}_1 - \mathbf{r}_2|$, $\Omega = \sqrt{k_{\text{eff}}}$, $k_{\text{eff}} = 1$, $C_0 = \Omega^{3/2}/\pi[2 + \Omega + \sqrt{2\pi\Omega}] = 0.135646$. The ground state energy is $E_0 = 3.000000$ a.u. The corresponding kinetic energy is $T_0 = 0.886199$ a.u.

For a two-electron quantum dot in the lowest excited singlet state, the spatial part of the wave function is [20]

$$\Psi_1(\mathbf{r}_1\mathbf{r}_2) = C_1 e^{-\Omega(R^2 + \frac{1}{4}u^2)} \left[1 + u + \left(\frac{\Omega}{4} - 0.436815 \right) u^2 + \left(\frac{\Omega}{4} - 0.353786 \right) u^3 \right], \quad (21)$$

with $\Omega = \sqrt{k_{\text{eff}}}$, $k_{\text{eff}} = 0.471716$, $C_1 = 0.108563$. The excited state energy is $E_1 = 3.434076$ a.u. The corresponding kinetic energy is $T_1 = 1.266683$ a.u.

As the binding potential of the electrons is harmonic, the above wave functions are finite at the center of each quantum dot. As these wave functions are exact, they satisfy the electron-electron coalescence condition for dimensions $D = 2$. The $D \geq 2$ dimensional structure of the wave function for the coalescence of two particles of masses m_1, m_2 , and charge Z_1, Z_2 is [2, 52]

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) = \Psi(\mathbf{r}_2, \mathbf{r}_2, \mathbf{r}_3, \dots, \mathbf{r}_N) \left(1 + \frac{2Z_1 Z_2 \mu_{12}}{D-1} r_{12} \right) + \mathbf{r}_{12} \cdot \mathbf{C}(\mathbf{r}_2, \mathbf{r}_3, \dots, \mathbf{r}_N), \quad (22)$$

where μ_{12} is the reduced mass, $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$, and $\mathbf{C}$ an unknown vector. It is important to note that since the spatial part of the wave function is symmetric, the coalescence condition is a *cusp* coalescence condition. (See [17, 20] for figures exhibiting this cusp for these singlet states. For the first excited triplet state, the spatial part of the wave function is antisymmetric giving rise to a *node* electron-electron coalescence condition [53].)

The expressions for the density $\rho(\mathbf{r})$, the single-particle density matrix $\gamma(\mathbf{r}\mathbf{r}')$, and the kinetic ‘force’ $\mathbf{z}(\mathbf{r})$ as obtained from the above wave functions are given in the Appendix.

Quantal Sources

We begin our analysis with a study of the quantal source of the density matrix $\gamma(\mathbf{r}\mathbf{r}')$. In Fig. 1 we plot $\gamma(\mathbf{r}\mathbf{r}')$ for the ground state as the electron positions $\mathbf{r}$ and $\mathbf{r}'$ change for (a) $\theta = 0^\circ$, $\theta' = 0^\circ$ and (b) $\theta = 0^\circ$, $\theta' = 90^\circ$. The figures in the two panels differ, but the nonlocal (dynamic) nature of the source is not evident on this scale. The nonlocal structure of $\gamma(\mathbf{r}\mathbf{r}')$ is quite evident for the excited state (Fig. 2) in which the different panels correspond to (a) $\theta = 0^\circ$, $\theta' = 0^\circ$, (b) $\theta = 0^\circ$, $\theta' = 60^\circ$, (c) $\theta = 0^\circ$, $\theta' = 90^\circ$. In particular, note the change in the structure of the shoulder. Observe the existence of the nodes of $\gamma(\mathbf{r}\mathbf{r}')$, a consequence of the node in the excited state wave function $\Psi_1(\mathbf{r}_1\mathbf{r}_2)$. In each panel of Fig. 2, shell structure is also clearly evident. The density matrix $\gamma(\mathbf{r}\mathbf{r}')$ for each state is also finite at the center of the ‘atom’ irrespective of the direction in which the center is approached. The diagonal matrix element $\gamma(\mathbf{r}\mathbf{r})$ is the density $\rho(\mathbf{r})$ which is plotted in Fig. 3. Once again the density $\rho(\mathbf{r})$ for both the ground and excited states are finite at the center of the dot. In neither case do they exhibit a cusp there. Shell structure is clearly evident in the density plot for the excited state.

Kinetic Forces

The kinetic ‘force’ $\mathbf{z}(\mathbf{r})$ for the two states is plotted in Fig. 4. Observe that each ‘force’ vanishes at the center of the quantum dot. The ‘forces’ also vanish asymptotically in the classically forbidden region. The asymptotic structures of the ‘forces’ in these regions follow from those of Eqs. (A12) and (A24) of $\mathbf{z}(\mathbf{r})$ for the ground and excited state, respectively.

Ground State

$$z(r) \underset{r \rightarrow 0}{\sim} 2\pi C_0^2 \left[\left(4 + \frac{15}{4}\sqrt{\pi} \right) r^3 - \left(\frac{17}{3} - \frac{49}{8}\sqrt{\pi} \right) r^5 \right], \quad (23)$$

$$z(r) \underset{r \rightarrow \infty}{\sim} 2\pi C_0^2 e^{-r^2} \left(-2r^5 - 4r^3 + 5r^3 + 11r^2 - 2r - \frac{33}{8} + \frac{2}{r} - \frac{15}{33r^2} + \frac{6}{r^3} \right). \quad (24)$$

Excited Singlet State

$$z(r) \underset{r \rightarrow 0}{\sim} 0.703r - r^3 + 0.459r^5 + \dots, \quad (25)$$

$$z(r) \underset{r \rightarrow \infty}{\sim} e^{-\Omega r^2} \left(-0.0417r^5 - 0.346r^4 - 0.215r^3 + 0.332r^2 + 0.202r - 0.0772 + \frac{0.216}{r} + \frac{0.0343}{r^2} - \frac{0.0650}{r^4} + \dots \right) \quad (26)$$

with $\Omega = 0.686816$.

Further, as might be expected, shell structure is exhibited by the kinetic ‘force’ for the excited state.

Kinetic Energy Densities

Finally, in Fig. 5 we plot the three kinetic energy densities $t_A(\mathbf{r})$, $t_B(\mathbf{r})$, and $t_C(\mathbf{r})$ for (a) the ground state, and (b) the excited state. It is evident that for each state, the three functions differ. They, however, lead to the same value for the kinetic energy T for each state.

For each state, the kinetic energy density $t_B(\mathbf{r})$ is ‘classical’ in the sense that it is positive throughout space. It is also finite at the center. Also observe that there is a quantal decompression of $t_B(\mathbf{r})$ away from the center of the quantum dot. In other words the

maximum of $t_B(\mathbf{r})$ occurs away from the origin. This structure can be explained [19, 21] via the ‘classical’ kinetic ‘force’ $\mathbf{z}(\mathbf{r})$ via its divergence. (The present choice of quantum dots corresponds to the low electron correlation regime in which the kinetic energy T is greater than the electron-interaction energy E_{ee} relative to the total energy E . In the Wigner high electron correlation regime where E_{ee} is greater than T relative to the total energy E , there is a quantal compression of $t_B(\mathbf{r})$ so that its maximum occurs at the center of the quantum dot.) A close examination of the functions $t_A(\mathbf{r})$ and $t_B(\mathbf{r})$ for the excited state in Fig. 5b shows that they both exhibit shell structure.

The kinetic energy density $t_A(\mathbf{r})$ is finite at the nucleus for both states. (This result is in sharp contrast to the case of the Coulomb binding potential, to be discussed below, for which this function is singular at the nucleus.) The function $t_A(\mathbf{r})$ is also quantum-mechanical in nature in that it is both positive and negative, and exhibits shell structure for the excited state.

The structure of $t_C(\mathbf{r})$ follows (with a negative sign) that of the kinetic ‘force’ of Fig. 4. As such it vanishes at the center of the quantum dot for each state. It is quantum-mechanical being both positive and negative. Its oscillations are however greater in magnitude than that of $t_A(\mathbf{r})$ because of the dot product $\mathbf{r} \cdot \mathbf{z}(\mathbf{r})$. Once again, shell structure is clearly exhibited by $t_C(\mathbf{r})$ for the excited state.

IV. CONCLUDING REMARKS

In this work we have studied two well-known expressions $t_A(\mathbf{r}), t_B(\mathbf{r})$ and a more recent virial expression $t_C(\mathbf{r})$ for the kinetic energy density $t(\mathbf{r})$ of electrons in an external binding field. The application is to 2D quantum dots in a magnetic field for which the corresponding binding potential is harmonic. Two different two-electron quantum dots, one in a ground and the other in a first excited singlet state are considered. It is shown that for each state the three functions differ. Importantly, all three kinetic energy densities for both states are *finite* throughout space. Thus we learn that the three quantum-mechanical expressions for the kinetic energy density lead to three different functions each of which integrates to the same kinetic energy T . *A priori* this is a plausible result because the three expressions differ: $t_A(\mathbf{r})$ and $t_B(\mathbf{r})$ depend on the Laplacian and double-gradient operators, respectively, with the expression for $t_C(\mathbf{r})$ involving yet an additional derivative.

In prior work [5, 6] on application to 3D systems in the ground state with a Coulomb binding potential, it was shown that the function $t_B(\mathbf{r})$ was finite at the nucleus, and ‘classical’ in the sense of being positive throughout space, vanishing asymptotically in the classically forbidden region. This is precisely the same behavior observed in our 2D calculations for harmonically bound electrons for both a ground and excited state. This then demonstrates a similarity between the natural and artificial systems.

For both the Coulomb (3D) and harmonic (2D) binding potentials, the structure of the function $t_A(\mathbf{r})$ is again similar, but quantum-mechanical in nature being both positive and negative. There is one significant difference, however, in that for a Coulomb binding potential in 3D, the function $t_A(\mathbf{r})$ for the ground state is singular at the nucleus. For harmonic binding in 2D it is finite at the center of the quantum dot for both the ground and excited states. This constitutes a fundamental difference between the natural and artificial systems.

For completeness, we explain the near nucleus structure of the three functions $t_A(\mathbf{r})$, $t_B(\mathbf{r})$, and $t_C(\mathbf{r})$ for natural atoms in their ground state, *i.e.* 3D systems with a Coulomb binding potential.

For an N electron system, and for small r , the wave function $\Psi(X)$, density $\rho(\mathbf{r})$, the kinetic energy density $t_B(\mathbf{r})$, and the kinetic ‘force’ $\mathbf{z}(\mathbf{r})$ may be written as [54] (in particular see Chapter 8 of [2]; for earlier work see [5, 6, 55–60]):

$$\begin{aligned}\Psi(\mathbf{r}\mathbf{X}^{N-1}) &= \Psi(0\mathbf{X}^{N-1}) + a(\mathbf{X}^{N-1})r + b(\mathbf{X}^{N-1})r^2 + \dots \\ &+ \sum_{m=-1}^1 \left[a_{1m}(\mathbf{X}^{N-1})r + b_{1m}(\mathbf{X}^{N-1}) \right] Y_{1m}(\theta\phi) + \dots \\ &+ \sum_{m=-2}^2 b_{2m}(\mathbf{X}^{N-1})r Y_{2m}(\theta\phi) + \dots,\end{aligned}\tag{27}$$

$$\begin{aligned}\rho(\mathbf{r}) &= \rho(0) \left\{ 1 - 2Zr + \frac{2}{3\rho(0)} [Z^2\rho(0) + t_B(0)]r^2 \right\} \\ &+ \frac{2}{3}r^2 D + O(r^3),\end{aligned}\tag{28}$$

$$t_B(0) = \frac{1}{2} [Z^2\rho(0) + F],\tag{29}$$

$$\mathbf{z}(\mathbf{r}) = 2Z^2\rho(0) \frac{\mathbf{r}}{r^2} \left(1 + \frac{2Zr}{3} \right) - \frac{4}{3}Z [2t_B(0) + 3D] \frac{\mathbf{r}}{r} + O(r)\tag{30}$$

where

$$D = 3N \int d\mathbf{X}^{N-1} \Psi^*(0\mathbf{X}^{N-1}) b(\mathbf{X}^{N-1}), \quad (31)$$

$$F = 3N \int d\mathbf{X}^{N-1} \frac{1}{4\pi} |a_{1m}(\mathbf{X}^{N-1})|^2, \quad (32)$$

$\mathbf{X}^{N-1} = \sigma, \mathbf{x}_2, \dots, \mathbf{x}_N$; $d\mathbf{X}^{N-1} = \sum_{\sigma} \int d\mathbf{x}_2, \dots, d\mathbf{x}_N$; Z is the nuclear charge, and Y_{lm} the spherical harmonic.

From the above near nucleus asymptotic expressions, observe that the wave function $\Psi(\mathbf{X})$, and hence the single-particle density matrix $\gamma(\mathbf{r}\mathbf{r}')$, the density $\rho(\mathbf{r})$, and the ‘classical’ kinetic energy density $t_B(\mathbf{r})$ are all finite at the nucleus. From Eq. (28) for $\rho(\mathbf{r})$, it is evident that the singularity in the function $t_A(\mathbf{r})$ at the nucleus is due to the $\frac{1}{4}\nabla^2\rho(\mathbf{r})$ term (see Eq. (10)). It is also evident from Eq. (30) for the kinetic ‘force’ $\mathbf{z}(\mathbf{r})$, that the virial expression $t_C(\mathbf{r}) = -\frac{1}{2}\mathbf{r} \cdot \mathbf{z}(\mathbf{r})$ is *finite* at the nucleus of natural atoms. This too is a difference between the natural and artificial atoms. In the latter, the ‘force’ $\mathbf{z}(\mathbf{r})$ and hence $t_C(\mathbf{r})$ vanishes at the center of the quantum dot (see Figs. 4 and 5).

As a consequence of the present study, it is evident that all three expressions for the kinetic energy density $t_A(\mathbf{r})$, $t_B(\mathbf{r})$, and $t_C(\mathbf{r})$ can be employed in any theoretical framework as applied to 2D and 3D (Hooke’s atom) [1, 61] quantum dots, or Hooke’s species [2, 62], i.e. electronic systems with a harmonic binding potential. (For experimentally obtained spherical 3D quantum dots, see [63, 64].) The use of each kinetic energy density expression could lead to different physics. For 3D Coulombically bound systems, we suggest that in addition to the commonly used $t_B(\mathbf{r})$ obtained as the trace of the kinetic energy tensor $t_{\alpha\beta}(\mathbf{r})$, the virial expression $t_C(\mathbf{r})$ now can also be employed in its single-particle representation in which the quantal source is the Dirac density matrix. The expression for $t_C(\mathbf{r})$ depends on the kinetic field $\mathbf{Z}(\mathbf{r})$ or ‘force’ $\mathbf{z}(\mathbf{r})$, both fundamental properties of the system as described via the ‘Quantal Newtonian’ first law. As such we believe much can be learned. In our work [19, 21] on 2D and 3D quantum dots, we have employed the kinetic ‘force’ $\mathbf{z}(\mathbf{r})$ to explain the structure of $t_B(\mathbf{r})$ of quantum dots. In the low-electron correlation regime, (as in the present work), there is a quantal decompression of $t_B(\mathbf{r})$ away from the center of the quantum dot. In the high-electron correlation or Wigner regime, there is a compression of $t_B(\mathbf{r})$ towards the center. The structure of $t_B(\mathbf{r})$ is explained via the divergence of the corresponding kinetic ‘force’ $\mathbf{z}(\mathbf{r})$ which too is obtained from the tensor $t_{\alpha\beta}(\mathbf{r})$ but via both its diagonal and off-diagonal elements. This in turn provides a rigorous explanation of why

the kinetic energy T relative to the total energy E is large for the former and small for the latter.

APPENDIX A: ANALYTICAL EXPRESSIONS FOR KINETIC RELATED PROPERTIES OF A QUANTUM DOT IN A MAGNETIC FIELD: GROUND AND FIRST EXCITED SINGLET STATE

In this Appendix we provide the expressions for the density $\rho(\mathbf{r})$, the single-particle density matrix $\gamma(\mathbf{r}\mathbf{r}')$, the kinetic energy tensor $t_{\alpha\beta}(\mathbf{r};\gamma)$, the kinetic ‘force’ component $z_{\alpha}(\mathbf{r};\gamma)$, and the kinetic energy T for two quantum dots, one in a ground state and the other in its first excited singlet state.

Employing the wave function of Eq. (20), the ground state properties of the quantum dots (in effective atomic units) are as follows:

Ground State ($k_{\text{eff}} = 1$)

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

$$\rho(\mathbf{r}) = 2\pi C_0^2 e^{-r^2} \left\{ \sqrt{\pi} e^{-\frac{1}{2}r^2} \left[(1+r^2) I_0\left(\frac{1}{2}r^2\right) + r^2 I_1\left(\frac{1}{2}r^2\right) \right] + (2+r^2) \right\}, \quad (\text{A1})$$

with $C_0^2 = 1/\pi^2(3 + \sqrt{2\pi}) = 0.135646$, and where $I_0(x)$ and $I_1(x)$ are the zeroth- and first-order modified Bessel functions $I_{\nu}(x)$ [65] with

$$I_{\nu}(x) = \sum_{n=0}^{\infty} \frac{1}{n! \Gamma(n + \nu + 1)} \left(\frac{1}{2}x \right)^{2n+\nu} \quad (\text{A2})$$

and $\Gamma(x)$ the Gamma function [65]. The asymptotic structure of $\rho(r)$ near the nucleus is

$$\rho(r) \underset{r \rightarrow 0}{\sim} \frac{2}{\pi(3 + \sqrt{2\pi})} \left\{ 2 + \sqrt{\pi} - \left(1 + \frac{1}{2}\sqrt{\pi}\right)r^2 - \frac{1}{16}\sqrt{\pi}r^4 + \dots \right\}, \quad (\text{A3})$$

with

$$\rho(0) = 0.436132 \text{ a.u.} \quad (\text{A4})$$

Employing the asymptotic behavior of the Bessel functions:

$$I_0(z) \underset{r \rightarrow \infty}{\sim} \frac{e^z}{\sqrt{2\pi z}} \sum_{n=0}^{\infty} \frac{(-1)^n}{(2z)^n} \frac{\Gamma(n + \frac{1}{2})}{n! \Gamma(-n + \frac{1}{2})} + \frac{e^{-z}}{\sqrt{2\pi z}} \sum_{n=0}^{\infty} \frac{i}{(2z)^n} \frac{\Gamma(n + \frac{1}{2})}{n! \Gamma(-n + \frac{1}{2})}, \quad (\text{A5})$$

and

$$I_1(z) \underset{r \rightarrow \infty}{\sim} \frac{e^z}{\sqrt{2\pi z}} \sum_{n=0}^{\infty} \frac{(-1)^n}{(2z)^n} \frac{\Gamma(n + \frac{3}{2})}{n! \Gamma(-n + \frac{3}{2})} - \frac{e^{-z}}{\sqrt{2\pi z}} \sum_{n=0}^{\infty} \frac{i}{(2z)^n} \frac{\Gamma(n + \frac{3}{2})}{n! \Gamma(-n + \frac{3}{2})}, \quad (\text{A6})$$

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

$$\rho(r) \underset{r \rightarrow \infty}{\sim} \frac{2}{\pi(3 + \sqrt{2\pi})} e^{-r^2} \left\{ r^2 + 2r + 2 + \frac{1}{2r} + \frac{1}{16r^3} + \dots \right\}. \quad (\text{A7})$$

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

$$\gamma(\mathbf{r}\mathbf{r}') = 2C_0^2 e^{-\frac{1}{2}(r^2 + r'^2)} \int (1 + |\mathbf{r} - \mathbf{y}|)(1 + |\mathbf{r}' - \mathbf{y}|) d\mathbf{y}. \quad (\text{A8})$$

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

$$t_{\alpha\beta}(\mathbf{r}; \gamma) = \frac{r_\alpha r_\beta}{r^2} f(r) + \delta_{\alpha\beta} k(r), \quad (\text{A9})$$

where

$$f(r) = \pi C_0^2 e^{-r^2} \left\{ r^4 + 1 - \frac{1 - e^{-r^2}}{r^2} + \sqrt{\pi} e^{-r^2/2} \left[r^4 I_0\left(\frac{1}{2}r^2\right) + (r^4 - r^2) I_1\left(\frac{1}{2}r^2\right) \right] \right\}, \quad (\text{A10})$$

and

$$k(r) = \pi C_0^2 e^{-r^2} \frac{(1 - e^{-r^2})}{2r^2}. \quad (\text{A11})$$

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

$$\begin{aligned} z_\alpha(\mathbf{r}; [\gamma]) &= 2 \sum_{\beta} \nabla_{\beta} t_{\alpha\beta}(\mathbf{r}; [\gamma]) = \frac{2r_\alpha}{r} \left[\frac{\partial(f(r) + k(r))}{\partial r} + \frac{f(r)}{r} \right] \\ &= \frac{2\pi C_0^2 r_\alpha}{r} e^{-r^2} \left\{ [-2r^5 + 5r^3 - 2r + \frac{2(1 - e^{-r^2})}{r}] \right. \\ &\quad \left. + \sqrt{\pi} e^{-r^2/2} [(-2r^5 + 4r^3) I_0\left(\frac{r^2}{2}\right) + (-2r^5 + 6r^3 - r) I_1\left(\frac{r^2}{2}\right)] \right\}. \end{aligned} \quad (\text{A12})$$

5. Kinetic Energy T

$$T = 2\pi^2 C_0^2 \left[\frac{3}{2} + \frac{3}{8} \sqrt{2\pi} \right] = 0.886199 \text{ a.u.} \quad (\text{A13})$$

Employing the wave function of Eq. (21), the properties of the quantum dot in its first excited singlet state are as follows:

First Excited Singlet State ($k_{\text{eff}} = 0.471716$)

1. Electron density $\rho_1(\mathbf{r})$

$$\begin{aligned} \rho_1(r) = \frac{C_1^2}{2\Omega^4} & \left\{ 4\pi e^{-\Omega r^2} (K_1 + L_1 r^2 + M_1 r^4 + N_1 r^6) + \right. \\ \pi \sqrt{\pi \Omega} e^{-\frac{3}{2}\Omega r^2} & \left[K_2 + L_2 r^2 + M_2 r^4 + N_2 r^6 \right] I_0(\Omega r^2/2) + \\ & \left. (L_3 r^2 + M_3 r^4 + N_3 r^6) I_1(\Omega r^2/2) \right\}, \end{aligned} \quad (\text{A14})$$

where

$$\begin{aligned}
C_1 &= 0.1085631994, \\
\Omega &= \frac{2}{2.91199} = 0.686816, \\
K_1 &= 6B^2 + (2A^2 + 4B) \Omega + (1 + 2A) \Omega^2 + \Omega^3, \\
L_1 &= 18 B^2 \Omega + 4(A^2 + 2B) \Omega^2 + (1 + 2A) \Omega^3, \\
M_1 &= 9 B^2 \Omega^2 + (A^2 + 2B) \Omega^3, \\
N_1 &= B^2 \Omega^3, \\
K_2 &= 15AB + 6(A + B) \Omega + 4 \Omega^2, \\
L_2 &= 45AB \Omega + 12(A + B) \Omega^2 + 4 \Omega^3, \\
M_2 &= 28AB \Omega^2 + 4(A + B) \Omega^3, \\
N_2 &= 4AB \Omega^3, \\
L_3 &= 23AB \Omega + 8(A + B) \Omega^2 + 4 \Omega^3, \\
M_3 &= 24AB \Omega^2 + 4(A + B) \Omega^3, \\
N_3 &= 4AB \Omega^3, \\
A &= \frac{1}{4}(1 + \Omega - 2 \epsilon_r) = -0.2651111137, \\
B &= \frac{1}{9} \left(\frac{1}{4} - \frac{5\epsilon_r}{2} + \frac{9}{4} \Omega \right) = -0.1820822248, \\
\epsilon_r &= 1.37363
\end{aligned} \tag{A15}$$

and $I_0(x)$ and $I_1(x)$ are the zeroth- and first-order modified Bessel functions [65].

The asymptotic structure of $\rho_1(\mathbf{r})$ near the center of the quantum dot, and in the classically forbidden region, respectively, are as follows:

$$\rho_1(r) \underset{r \rightarrow 0}{\sim} 0.207 - 0.141 r^2 + 0.0753 r^4 + \dots, \tag{A16}$$

with $\rho_1(0) = 0.207299$ *a.u.*,

$$\begin{aligned}
\rho_1(r) \underset{r \rightarrow \infty}{\sim} e^{-\Omega r^2} & \left(-0.00171 r^3 + 0.00252 r^2 + 0.0549 r + \right. \\
& \left. 0.113 + \frac{0.0398}{r} + \frac{0.00902}{r^3} + \dots \right).
\end{aligned} \tag{A17}$$

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

$$\begin{aligned}
\gamma(\mathbf{r}\mathbf{r}') &= 2 C_1^2 e^{-\Omega(r^2+r'^2)/2} \int e^{-\Omega y^2} \left[1 + |\mathbf{y} - \mathbf{r}| + A|\mathbf{y} - \mathbf{r}|^2 + \right. \\
& \left. B|\mathbf{y} - \mathbf{r}|^3 \right] \left[1 + |\mathbf{y} - \mathbf{r}'| + A|\mathbf{y} - \mathbf{r}'|^2 + B|\mathbf{y} - \mathbf{r}'|^3 \right] d\mathbf{y},
\end{aligned} \tag{A18}$$

where the constants C_1, Ω, A and B are given in Eq. (A15).

3. Kinetic energy tensor $t_{\alpha\beta}[\mathbf{r}; \gamma]$

$$t_{\alpha\beta}[\mathbf{r}; \gamma] = \frac{r_\alpha r_\beta}{r^2} f(r) + \delta_{\alpha\beta} k(r), \quad (\text{A19})$$

where

$$f(r) = \pi C_1^2 e^{-2\Omega r^2} \left[\frac{r}{\Omega} \frac{\partial f_1(r)}{\partial r} - 2 r \frac{\partial f_2(r)}{\partial r} \right] + \frac{\Omega^2}{2} r^2 \rho_1(r), \quad (\text{A20})$$

$$k(r) = \frac{\pi C_1^2}{\Omega} e^{-2\Omega r^2} f_1(r), \quad (\text{A21})$$

$$\begin{aligned} f_1(r) = \frac{1}{2\Omega^2 r^2} \left\{ -\Omega + e^{\Omega r^2} \left[\Omega + (4\Omega A^2 + 6\Omega B + 18A^2 + 9\Omega B^2 r^2) r^2 \right] + \right. \\ \left. A\sqrt{\pi\Omega} r^2 e^{\Omega r^2/2} \left[(2\Omega + 9B + 6\Omega B r^2) I_0(\Omega r^2/2) + \right. \right. \\ \left. \left. (2\Omega + 3B + 6\Omega B r^2) I_1(\Omega r^2/2) \right] \right\}, \end{aligned} \quad (\text{A22})$$

$$\begin{aligned} f_2(r) = \frac{e^{\Omega r^2/2}}{8\Omega^3} \left\{ 4e^{\Omega r^2/2} \left[(6B^2 + 2A^2\Omega + 4B\Omega + \Omega^2 + 2A\Omega^2) + \right. \right. \\ \left. (12B^2\Omega + 2A^2\Omega^2 + 4B\Omega^2) r^2 + 3B^2\Omega^2 r^4 \right] + \sqrt{\pi\Omega} \\ \left[\left(15AB + 6A\Omega + 6B\Omega + 4\Omega^2 + (30AB\Omega + 6(A+B) \right. \right. \\ \left. \left. \Omega^2) r^2 + 10AB\Omega^2 r^4 \right) I_0(\Omega r^2/2) + \left(2\Omega(10AB + \right. \right. \\ \left. \left. 3A\Omega + 3B\Omega)r^2 + 10AB\Omega^2 r^4 \right) I_1(\Omega r^2/2) \right] \right\}, \end{aligned} \quad (\text{A23})$$

where the constants C_{01}, Ω, A and B are given in Eq. (A15).

4. Kinetic ‘force’ $z_\alpha[\mathbf{r}; \gamma]$

$$z_\alpha[\mathbf{r}; \gamma] = \frac{2 r_\alpha}{r} \left\{ \frac{\partial[f(r) + k(r)]}{\partial r} + \frac{f(r)}{r} \right\}, \quad (\text{A24})$$

where the functions $f(r)$ and $k(r)$ are given in Eq. (A20) and (A21), respectively.

5. Kinetic Energy T

$$\begin{aligned} &= \frac{\pi^2 C_1^2}{4\Omega^4} \left(16\Omega (2A^2 + 3B) + \sqrt{2\pi} \Omega^{3/2} (11A + 3B) + 57\sqrt{2\pi\Omega} AB \right. \\ &\quad \left. + 8(A+1)\Omega^2 + 3\sqrt{2\pi}\Omega^{5/2} + 4\Omega^3 + 192B^2 \right) \\ &= 1.266683 \text{ a.u.}, \end{aligned} \quad (\text{A25})$$

where the constants C_1, Ω, A and B are given in Eq. (A15).

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FIG. 1: The single-particle density matrix $\gamma(\mathbf{r}\mathbf{r}')$ for the ground state of the quantum dot in a magnetic field. The panels correspond to (a) $\theta = 0^\circ, \theta' = 0^\circ$; (b) $\theta = 0^\circ, \theta' = 90^\circ$.

FIG. 2: The single-particle density matrix $\gamma(\mathbf{r}\mathbf{r}')$ for the first excited singlet state of the quantum dot in a magnetic field. The panels correspond to (a) $\theta = 0^\circ, \theta' = 0^\circ$; (b) $\theta = 0^\circ, \theta' = 60^\circ$; (c) $\theta = 0^\circ, \theta' = 90^\circ$.

FIG. 3: The electron density $\rho(\mathbf{r})$ for the two quantum dots in a magnetic field, one in a ground state and the other in a first excited singlet state.

FIG. 4: The kinetic ‘force’ $z(\mathbf{r})$ for the quantum dots in a magnetic field in a ground and first excited singlet state.

FIG. 5: The kinetic energy densities $t_A(\mathbf{r})$, $t_B(\mathbf{r})$, $t_C(\mathbf{r})$ for the quantum dots in a magnetic field. Panels: (a) ground state; (b) first excited singlet state.