Density Profiles, Energy, and Oscillation Strength of a Quantum Dot in Two Dimensions with a Harmonic Oscillator External Potential using an Orbital-free Energy Functional Based on Thomas–Fermi Theory

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Abstrak

This research aims i) to determine the density profile and calculate the ground state energy of a quantum dot in two dimensions (2D) with a harmonic oscillator potential using orbital-free density functional theory, and ii) to understand the effect of the harmonic oscillator potential strength on the electron density profiles in the quantum dot. This study determines the total energy functional of the quantum dot that is a functional of the density that depends only on spatial variables. The total energy functional consists of three terms. The first term is the kinetic energy functional, which is the Thomas–Fermi approximation in this case. The second term is the external potential. The harmonic oscillator potential is used in this study. The last term is the electron–electron interactions described by the Coulomb interaction. The functional is formally solved to obtain the electron density as a function of spatial variables. This equation cannot be solved analytically, and thus a numerical method is used to determine the profile of the electron density. Using the electron density profiles, the ground state energy of the quantum dot in 2D can be calculated. The ground state energies obtained are 2.464, 22.26, 90.1957, 252.437, and 496.658 au for 2, 6, 12, 20, and 56 electrons, respectively. The highest electron density is localized close to the middle of the quantum dot. The density profiles decrease with the increasing distance, and the lowest density is at the edge of the quantum dot. Generally, increasing the harmonic oscillator potential strength reduces the density profiles around the center of the quantum dot.