

Vortex formation in quantum dots in high magnetic fields

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Abstract

We study electronic structures of two-dimensional quantum dots in high magnetic fields using the density-functional theory (DFT) and the exact diagonalization (ED). With increasing magnetic field, beyond the formation of the totally spin-polarized maximum density droplet (MDD) state, the DFT gives the ground-state total angular momentum as a continuous function with well-defined plateaus. The plateaus agree well with the magic angular momenta of the ED calculation. By constructing a conditional wave function from the Kohn–Sham states we show that vortices enter the quantum dot one-by-one at the transition to the state with the adjacent magic angular momentum. Vortices are also observed outside the high-density region of the quantum dot. These findings are compared to the ED results and we report a significant agreement. We also study interpretations and limitations of the density functional approach in these calculations.

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Quasi-two-dimensional (2D) quantum dots fabricated into semiconductor heterostructures are expected to be basic components in the future nano-electronics [1]. Moreover, they provide a unique playground in physics with a rich diversity of quantum effects among interacting electrons [2]. The reason is especially the strong influence of magnetic fields on the electron states. Already for fields attainable in the laboratory environment the interaction with electrons is of the same order as

the electron–electron interactions. The understanding of experimental findings in quantum dots and the prediction of new phenomena have inspired a huge amount of theoretical and computational work.

Recent developments in the electronic structure theory of 2D quantum dots in magnetic fields have shown a rich variety of phenomena related to vortices [3–6]. These vortices correspond to magnetic field quanta with rotating currents of charge around them and a zero in the wave function at the vortex centre. By going around one vortex the wave function gains a phase change of

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$2\pi n$, where n is the winding number. In the fractional quantum Hall effect (FQHE) the state of the matter is described by Laughlin wave functions which attach vortex zeros at each electron. Electronic structure calculations of charge droplets in quantum dots have predicted the appearance of additional free vortices which cluster near electrons [3,4].

In this paper we perform a detailed study of vortex formation in circularly symmetric 2D quantum dots in a parabolic external confinement $V_c(\mathbf{r}) = \frac{1}{2}m^*\omega_0^2 r^2$. We model the system by an effective-mass Hamiltonian

$$H = \left(\sum_{i=1}^N \frac{(-i\hbar\nabla_i + e\mathbf{A})^2}{2m^*} + V_c(\mathbf{r}_i) \right) + \frac{e^2}{4\pi\epsilon} \sum_{i<j} \frac{1}{r_{ij}}, \quad (1)$$

where N is the number of electrons in the dot, $\mathbf{A}$ is the vector potential of the external perpendicular magnetic field B , m^* the effective electron mass, and ϵ is the dielectric constant of the medium. We use the material parameters of GaAs, $m^*/m_e = 0.067$ and $\epsilon/\epsilon_0 = 12.4$. In high magnetic fields the quantum dot is spin-polarized due to the Zeeman effect and the maximum density droplet state (MDD) is formed [7]. This state is a finite-size precursor of the $\nu = 1$ quantum Hall state. In parabolic external confining potential the state is formed by the lowest-Landau-level (LLL) orbitals with angular momenta $l = 0, -1, \dots, -N + 1$, and the total angular momentum L equals to $-N(N - 1)/2$. For a stronger B , ED has shown ground states to occur only at certain “magic” L values, and L shows a stepwise structure as a function of B [8–10].

We solve for the ground state electronic structure using the spin-density-functional theory (SDFT), the current-density-functional theory (CDFT) [11], and the exact diagonalization method (ED). The density-functional approaches are implemented in the real-space without symmetry restrictions [12]. The main results were calculated using 128×128 grid points but similar results were obtained using larger grids up to 256×256 grid points. High spatial resolution of fine grids is necessary to accurately describe

systems with several vortices inside the quantum dot. The exchange-correlation effects are taken into account using local spin density approximation (LSDA) [13]. In CSDFT we also use local approximation for the vorticity dependence of exchange-correlation energy [14].

The Hamiltonian of the system is rotationally symmetric and therefore the particle density, defined as $|\Psi(\mathbf{r})|^2$, should also be rotationally symmetric. Calculations, however, show that the particle density in the density-functional formalism is *not* necessarily symmetric. In this work we adopt the approach that even if broken symmetry solutions cannot be identified as the true particle density we may use them to find out correlations in the system. Otherwise, the correlations may remain hidden in the one-particle picture of the density functional approach. On the other hand, one should be cautious with the interpretations since it has been shown that the symmetry breaking solutions may be wrong mixtures of the eigenstates of the system and therefore the interpretation of the solution may be unphysical [15]. We therefore emphasize that solutions of the DFT should be used as guidelines and approximations and the final proofs should be done using exact many-body techniques.

We examine the 6-electron quantum dot ($N = 6$). For an easy comparison with the low magnetic field results in Ref. [12] we set the confinement strength to $\omega_0 = 5$ meV. The MDD state is characterized by a relatively constant electron density and currents concentrated at the edge of the dot. The transition to the MDD state occurs at 4.8 T.

The total angular momentum in the SDFT in the beyond-MDD domain is shown in Fig. 1. The curve has plateaus of nearly constant L . The plateau regions are characterized by electron densities with vortex depressions inside the quantum dot and outside the dot in the low-density region. The number of vortices inside the quantum dot increases by one between adjacent plateaus. The plateaus correspond well to the magic angular momenta from the ED calculations. The ED four-vortex configuration has the pentagon or hexagon symmetry which correspond to angular momenta $L = -35$ and -39 , respectively. In the DFT solutions, however, only the $L = -35$ plateau is visible.

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