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 study also interpretations and limitations of the density functional approach in these calculations.

Key words: quantum dot, vortex, charge-density-wave, current-density-functional method, exact diagonalization

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Quasi-two-dimensional (2D) quantum dots fabricated into semiconductor heterostructures are expected to be basic components in the future nanoelectronics [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 [3,4,5,6]. These vortices correspond to magnetic field quanta with rotating currents of charge around them and a zero in the wave function at the vortex centres. By going around one vortex the wave function gains a phase change of $2\pi n$, 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 a circulary symmetric 2D quantum dots in a parabolic external confinement $V_c(r) = \frac{1}{2}m^*\omega_0^2 r^2$. The model the system by an effective-mass Hamiltonian

$$H = \sum_{i=1}^{N} \left( -\frac{i\hbar}{2m^*} \nabla_i + eA_i \right)^2 + V_c(r_i) + \frac{e^2}{4\pi\epsilon} \sum_{i<j} \frac{1}{r_{ij}}.$$

(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 \( \epsilon \) 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 \( l = 0, -1, \ldots, -N + 1 \), 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 \( B \) [8,9,10].

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 \( 128 \times 128 \) grid points but similar results were obtained using larger grids up to \( 256 \times 256 \) 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 approximations for the spin densities and the vorticity in the 2D electron gas [13,14].

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 maximum density droplet (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. In the ED four-vortex configuration has the pentagon or hexagon symmetry which correspond to angular momenta \( L = -35 \) and \( L = -39 \), respectively. In the DFT solutions, however, only the \( L = -35 \) plateau is visible.

In the density-functional solutions vortices appear as static holes which break the rotational symmetry of the particle density. The wave function must vanish at the vortex position in order to keep the kinetic energy finite. In the beyond MDD-domain there are also
charge-density-wave (CDW)-like solutions with fractional \( L \) values in the transition regions between the adjacent magic angular momentum values. For example, solutions from \( B \approx 8.3 \) T to \( B \approx 11 \) T have 6 density maxima at the edge of the dot and a minimum at the dot center (see Fig. 2).

We do a detailed analysis of the vortex solutions in the SDFT by constructing a conditional wave function of the Kohn-Sham states. We do it iteratively by fixing \( N-1 \) electrons to positions \( \{r_i^0\}_{i=2}^N \) and then calculate a determinant of the \( N \) occupied Kohn-Sham states \( \phi_1, ..., \phi_N \)

\[
\Phi_{KS}(r) = \begin{vmatrix}
\phi_1(r) & \phi_2(r) & ... & \phi_N(r) \\
\phi_1(r_2^0) & \phi_2(r_2^0) & ... & \phi_N(r_2^0) \\
. & . & . & . \\
\phi_1(r_N^0) & \phi_2(r_N^0) & ... & \phi_N(r_N^0)
\end{vmatrix}. \tag{2}
\]

The electron positions are moved until the total probability of the \( \Phi_{KS} \) obtains a maximum value. Strictly speaking \( \Phi_{KS}(r) \) constructed in this way is only an auxiliar function which emulates the true conditional many-body wave function \([3]\) which is unknown in the density functional approach.

\( \Phi_{KS}(r) \) for the MDD-state correctly assigns one vortex for each electron. The evolution of this state as the magnetic field is increased is shown in Fig. 3. It depicts a vortex hole entering the quantum dot as the magnetic field is increased. The CDW solutions can be analyzed further by projecting the Kohn-Sham states on the Fock-Darwin states \([2]\) and comparing the results with those from the exact diagonalization (Fig. 2). From this data we can conclude that the charge-density-wave originates from the combinations of the \( L = -15 \) and \( L = -21 \) states. The mixture of these two states result in a density with six peaks in a form of a hexagon. The linear behaviours between plateaus can be thought to be unphysical since the exact ground state jumps directly from the MDD to \( L = -21 \). However the DFT gives the same qualitative picture than the ED where the (excited state) solutions between \( L = -15 \) and \( -21 \) show a vortex-hole moving from the outer edge toward the center \([16]\). The other CDW-regions show similar solutions, transport of one additional vortex-hole to the center of the dot.

The triple-vortex solution at \( B = 15.5 \) T is shown in Fig. 4. The DFT localizes the vortices in the electron density. The conditional wave function shows vortices at exactly these positions. External vortices appear both in the conditional wave function and in the logarithmic plot of the electron density (not shown).

Fig. 2. Charge-density-wave (CDW) solution in a six-electron quantum dot at 9.7 T. The total angular momentum \( L \approx -18.230 \). Left panel: the electron density. Right panel: the projections of the angular momentum to Fock-Darwin states for the CDW solution (black bars) are compared to the \( L = -18 \) solution from the exact diagonalization method (grey bars).

Fig. 3. Conditional wave function from the Kohn-Sham states \( \Phi_{KS}(r) \) for the MDD-state, two charge-density-wave states, and a single-vortex state. The contour plots are logarithmic conditional electron densities, the shadowings show the phases of the wave-function, and the crosses mark the most probable electron positions. At the lines where shadowing changes from the darkest grey to the lightest grey the phase changes by \( 2\pi \).

MDD, \( L = -15 \)  \hspace{2cm}  CDW, \( L \approx -16.103 \)

CDW, \( L \approx -17.258 \)  \hspace{2cm}  Single-vortex, \( L = -21 \)
The comparison with the ED results for $L = -30$ in Ref. [3] shows that the conditional DFT wave function given by Eq. (2) correctly predicts the existence of three vortices of winding number one inside the ring of the fixed electrons. In the ED the vortices start to cluster around the fixed electrons for larger angular momenta [3,4]. The conditional DFT wavefunction (2) predicts the right amount of vortices inside the quantum dot but fails to predict the clustering of vortices. This can be seen by comparing the ED and DFT results for the $L = -45$ case in Fig. 5. Therefore the $L = -45$ state can be identified as a finite size precursor of the $\nu = 1/3$ FQHE state only in the ED.

To conclude, we have studied vortex formation in parabolically confined quantum dots and found that both the DFT and the ED predict the existence of solutions with free vortices moving between the electrons. We have analysed the structure of these solutions using conditional wave functions and we found that the DFT gives qualitatively right results but is unable to predict the clustering of vortices near the electrons. We hope that these results will encourage further analysis of vortex solutions e.g. in systems of large electron number and low symmetry [17].

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