Correlations and entanglements in a few-electron quantum dot without Zeeman splitting

Ning Yang, Jia-Lin Zhu, Zhengsheng Dai, and Yuquan Wang

Department of Physics, Key Lab of Atomic and Molecular Nanoscience, and Center for Quantum Information, Tsinghua University, Beijing 100084, People’s Republic of China
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We explore the correlations and entanglements of exact-diagonalized few-electron wave functions in a quantum dot without the Zeeman splitting. With the increase of the field, the lowest states with different spins gradually form a narrow band and the electronic states undergo a transition from liquids to rotating Wigner molecules which are accompanied by different characters of charge correlations. For both the liquid and crystal states, the spin conditional probability densities show magnetic couplings between the particles which depend on the particle numbers, the total spins and the angular momenta of the states. The von Neumann entropies show the spin-dependent entanglements between electrons. The regular magnetic-coupling oscillations and converging entanglement entropies emerge in the rotating Wigner molecular states.

I. INTRODUCTION

Driven by the interests in both basic research and technological application, the electronic structures of two-dimensional quantum dots (QDs) have been a topic extensively studied in recent years. The particle number in QDs can be reduced precisely down to a few electrons with highly controllable confinements, interactions and external fields. The specific spin states of electrons and their manipulations by magnetic and electric fields have been proposed for basic qubit schemes for future quantum computation. Therefore, it is important to understand the quantum behaviors of few-electron QDs. Theoretically, the system with appropriate magnetic fields may be viewed as a finite-size precursor of integer and fractional quantum Hall states in two-dimensional electron gas (2DEGs) which can be understood by the Laughlin wave functions in liquid and crystal states, the spin conditional probability densities show magnetic couplings between the particles which depend on the particle numbers, the total spins and the angular momenta of the states. The von Neumann entropies show the spin-dependent entanglements between electrons. The regular magnetic-coupling oscillations and converging entanglement entropies emerge in the rotating Wigner molecular states.

II. MODEL AND FORMULA

The Halmiltonian of a N-electron QD in a perpendicular magnetic field without the Zeeman splitting is written as

\[
H = \sum_{i=1}^{N} \left[ \frac{1}{2m} \left( \hat{P}_i + e\hat{A} \right)^2 + V(r_i) \right] + \sum_{i<j} \frac{e^2}{4\pi \epsilon |\vec{r}_i - \vec{r}_j|},
\]

(1)

The first and second parts of Eq. (1) are respectively the single-particle energies and interaction energies of the electrons. \( \hat{A} \) is the vector potential of the magnetic field. \( m \) and \( \epsilon \) are the effective mass and static dielectric constant which are respectively 0.067\( m_e \) and 12.4 for GaAs. \( V \) is the confinement of the dot.

We use the method of series expansion to get exact eigenstates \( \psi_e(\vec{r}) \) of the single-particles parts of Eq. (1) as a set of single-particle bases. Then in the second quantization scheme the Hamiltonian can be written as

\[
H = \sum_{\alpha} \epsilon_{\alpha} a_{\alpha}^\dagger a_{\alpha} + \frac{1}{2} \sum_{\alpha\neq\beta} g_{\alpha'\beta'\alpha\beta} a_{\alpha'}^\dagger a_{\beta'}^\dagger a_{\beta} a_{\alpha}
\]

(2)

with

\[
g_{\alpha'\beta'\alpha\beta} = \int d\vec{r}_1 d\vec{r}_2 \langle \psi_{\alpha'}(\vec{r}_1)\psi_{\beta'}(\vec{r}_2) | \frac{e^2}{4\pi \epsilon |\vec{r}_1 - \vec{r}_2|} | \psi_{\beta}(\vec{r}_1)\psi_{\alpha}(\vec{r}_2) \rangle
\]

where \( a_{\alpha}^\dagger \) is the creation (annihilation) operator of the single-particle state \( \psi_{\alpha} \), and \( \epsilon_{\alpha} \) is its energy. Then Eq. (2) is diagonalized to obtain the energies and the corresponding wave functions \( \Psi \) of the few-electron states. In the following discussions, the confinement of the dot is parabolic and the strength is 2 meV. It is worthwhile to point out that the series expansion method is applicable not only to the parabolic confinement, but also other confinement forms for which analytic
single-particle bases cannot be obtained. Without spin-orbit coupling, the few-electron states can be the common eigenstates of total angular momentum \( L \), total spin \( S \) and its \( z \)-component \( S_z \). In the paper, we will mark the lowest states with different spins as \( (L,S,S_z) \) for brevity. Of course, the states with same \( L \) and \( S \) but different \( S_z \) are degenerate due to the absence of the Zeeman splitting.

Having got the eigenstates of Eq. (2), we can evaluate the charge and spin correlations by the conditional probability densities (CPDs)

\[
P(r, r') = \frac{1}{2} \langle \Psi | \sum_{\alpha \beta} \delta(\vec{r} - \vec{r}') \delta(\vec{r} - \vec{r}') a_{\alpha}^{\dagger} a_{\beta} a_{\beta} a_{\alpha} | \Psi \rangle (3)
\]

and

\[
P(r, r'; \sigma, \sigma') = \frac{1}{2} \langle \Psi | \sum_{\alpha \beta} \delta(\vec{r} - \vec{r}') \delta(\vec{r} - \vec{r}') \delta(\sigma - \sigma') \delta(\sigma' - \sigma') a_{\alpha}^{\dagger} a_{\beta} a_{\beta} a_{\alpha} | \Psi \rangle. \tag{4}
\]

In this paper, we also investigate the behaviors of entanglements of the few-electron electronic states. It has been demonstrated that the von Neumann entropy \( S = -\text{tr}[\rho^f \ln \rho^f] \) can be used for quantifying the entanglements between particles. \( \rho^f \) is the single-particle reduced density matrix. Although in multiparticle case it is not convinced how to quantify all the entanglement properties of an identical-particle state, the von Neumann entropy can still give the entanglement information between one particle and the other part of the system. In the following discussions, we employ a modified form of the von Neumann entropy as

\[
S = -\text{tr}[\rho^f \ln \rho^f] - \ln N \tag{5}
\]

where \( N \) is the particle number of the system. With such modification, the entropy due to the indistinguishability of the particles is subtracted. And the lower limit values of entropies for the system with different particle number are all equal to zero, which corresponds to the unentangled states.

### III. RESULTS AND DISCUSSION

#### A. Energy level structures

The energy spectra of four- and five-electron QDs in magnetic fields are shown in Fig. 1. For clarity, \( N \) times of the energy of the first Landau level have been subtracted from the total energy. In smaller fields, the states with different spins are clearly separated. The full-polarized ground state corresponding to filling factor \( \nu = 1 \), namely the maximum density droplet (MDD), has lower energy in a long range of magnetic field. Without the Zeeman splitting, the states with lower spin can become the ground states even in strong magnetic fields. The ground states in the magnetic fields corresponding to fractional filling factors (1/3, 1/5, etc.) are still full-polarized. In the magnetic fields where the flux deviates from the values of fractional filling factors by \( \pm \phi_0 \) (\( \phi_0 \) is the quantum of magnetic flux) the ground states will be the ones with lowest total spin. Such situation is same as that in 2DEGs with spin degree of freedom. In strong fields, the electrons form the RWMs. With the decreased overlapping of electrons, the exchange energies of different spin states are depressed totally. Then the states with different total spins are almost degenerate and form a narrow band.

With the increase of the field, there are angular momentum transitions for the ground states. The allowable angular momenta are so called magic numbers. With the Zeeman splitting, the angular momentum transition of the four- and five-electron ground states in magnetic fields has the period as the particle number \( N \). Including the spin degree of freedom, the angular momentum transition of ground states with the increase of the field is almost continuous. However, for the...
lowest states with different total spins, the angular momentum transitions indeed have some rules. In strong magnetic fields where the electron are well localized, such rules can be obtained from the theory of electron molecules. For example, the lowest four-electron states with $S=0$ must be the ones with angular momenta $|L|=4n$ or $4n+2$, the lowest states with $S=1$ must be the ones with $|L|=4n$ or $4n+1$. For five electrons, it can be obtained from our studies that the angular momenta of lowest states with $S=0.5$ can be the continuous integers, the lowest states with $S=1.5$ must be the ones with $L=5n$, where $n$ is an integer. In both cases, the transitions for full-polarized states still have a period of particle number $N$.

In small magnetic fields where the electronic states are still liquid-like ones, the transition rules of angular momenta described above are not exact. The states with some angular momenta coincide with the rules do not appear as the lowest states. For example, for the five-electron case with $S=0.5$, the angular momenta can be arbitrary integers in strong fields, but the states with $|L|=2,3,6,9,10,11,14,17,18,20,22,23,25,29$ do not appear as the lowest states. Examining the results obtained by exact diagonalization carefully, it can be found that such deletion for four- (five-) electron states disappears when the filling factor $v<1/2\,1/3$. The different angular momentum transition patterns just reflect the transition of the electronic states from the liquid to crystal ones with the increase of the field. We also illustrate the angular momentum transition pattern for the lowest states with different spins in Fig. 3. It can be seen in both Fig. 1 and Fig. 2 that the angular momentum transitions become regular in strong fields, as discussed above.

**B. Spin correlations and magnetic couplings**

Within the liquid-crystal transition, the correlations between electrons of the lowest states change from the short-range liquid to long-range crystal ones. In the third row of Fig. 2, we show some examples of the two kinds of correlations. It can be seen in the plot that the CPDs of the four-electron state (-4,0,0) and five-electron state (-8,0,5,0.5) are liquid-like. In strong magnetic fields, the states with larger angular momenta exhibit crystal-like correlations, which are the characters of the RWMs.

Besides the angular momentum and charge correlation transitions, there are also different spin correlations. We inspect the spin correlations by examining the spin CPDs to find electrons with a certain spin when a spin-up electron is fixed. We found that the spin correlations can reveal the magnetic couplings between electrons in non- and partial-polarized states with minimum $S_z$. We illustrate some spin CPDs in the first two rows of Fig. 2. It can be seen that when a spin-up electron is fixed at the position indicated by the white dot, the spin-up and spin-down electrons in the state (-16,0,0) will be probably at the neighbor and opposite positions, respectively. Such CPDs just reveal the existence of ferromagnetic couplings between electrons. For the state (-16,1,0), the CPDs shown in the figure are just contrary to that for (-16,0,0) and reveal the anti-ferromagnetic couplings. For the five-electron state (-35,0,5,0.5), the spin CPDs show that neither the spin-up nor the spin-down electrons have preferable positions when a spin-up electron is fixed. Then we cannot expect any specific magnetic coupling for it.

We have found that other states also exhibit respective couplings even if the angular momenta are so small that the states are still liquid ones. As shown in Fig. 2, the CPDs for the state (-4,0,0) and (-8,0,5,0.5) also reveal the ferromagnetic couplings between electrons. Although the electrons are no longer well localized, the spin-up electrons are closer to the fixed electron than the spin-down ones.

It should be pointed out that, strictly speaking, the four-electron states can perform the ferromagnetic and anti-ferromagnetic couplings. For five-electron states, only ferromagnetic coupling along with the ferromagnetic coupling exist because of the unequal electron numbers with two species of spins. One example of CPDs showing the ferrimagnetic coupling are presented in the inset of Fig. 2b. And full-polarized states cannot exhibit any specific magnetic coupling.

In the previous discussions, we have shown that the spin CPDs can reveal the magnetic couplings in the lowest states with different spins although the correlations are quite different for the liquid and crystal ones. Then we can iden-
The states with have their own magnetic coupling rules as shown in Fig. 3. where \( n \) \( |S| = 0 \) ferromagnetic (anti-ferromagnetic). The couplings for the states with \( S = 1 \) are just contrary to that with \( S = 0.5 \). In any case, the oscillation with respect to the momenta performs a period of particle number \( N \). A special feature of the five-electron case is that the states with \( S = 0.5 \) and \( |L| = 5n \) have no specific magnetic coupling, as the example \((-35,0.5,0.5)\) in Fig. 2. Such systematic vanish of the magnetic coupling is absent in the four-electron case.

In small fields, the oscillations are no longer regular. This is because that the angular momentum transition pattern in small fields is different from that in strong fields. The vanishing states with some angular momenta cause the irregularity of the oscillation.

**C. Entanglement**

![Image](https://via.placeholder.com/150)

**FIG. 4:** (Color online) Entanglement entropies of the lowest states of four (a) and five (b) electrons with different spins. A term \( \log N \) has been subtracted. \( \times \), \( \bullet \) and \( \square \) correspond to the states with non-, partial to full-polarized spins, respectively.

In this subsection, we investigate the features of entanglements in the liquid-crystal transition. The von Neumann entropy is used for the quantification of the extent of the entanglement. According to Eq. (5), the entanglement entropies of different spin states as functions of the magnetic field are given in Fig. 4.

A feature of the entanglements in QD is that the entropies of the states with same \( L \) and \( S \) but different \( S_z \) are unequal although their energies are same when the Zeeman splitting is ignored. The differences corresponding to different \( S_z \) are
approximately constant in strong magnetic fields. Especially for a state with maximum $S_z$, where the entropy owing to the spin components is totally eliminated, its entropy should differ from that of the state with minimum $S_z$ by one, which is revealed by our calculation. Without the Zeeman splitting, the energies of the states with same $L$ but different $S$ in strong magnetic fields are nearly degenerate. In Fig[4] the entropies of such states with same $S_z$ also converge and increase monotonously. Such convergence of the entanglements is also a character of RWMs.

For the liquid states in lower magnetic fields where the interaction energies vary in different spin states, the variations of entanglements are not monotonous any more. The states with different $S$ have their own minimal values in respective fields. The state corresponding to the MDD with maximum $S_z$ has the global minimum entanglement entropy, i.e. the minimum correlation. In 2DEGs, the Laughlin wave function with filling factor $\nu = 1$ is unentangled. Similarly, in few-electron QDs, the entanglement entropies of the MDD states are also very close to zero.

### IV. SUMMARY

To conclude, we have investigated the liquid-crystal transitions in the few-electron quantum dot without the Zeeman splitting. The spin degree of freedom brings various characters to the transition. The energy level structures in the range of liquid and crystal phase are quite different. In strong magnetic fields, different spin states with specific angular momentum transition rules form a narrow band which is the character of the rotating Wigner molecular states. In small fields, such rules are no longer strictly obeyed by the liquid-like states. For both the liquid- and crystal-like states with the lowest $S_z$, there are magnetic couplings between electrons although the spin CPDs are quite different. The species of the couplings depend on the particle numbers, the total spins and the angular momenta of the states. In the RWMs, the magnetic couplings oscillate regularly with respect to the field. The entanglement entropies which do not depend on the total spins of the states increase monotonously. The entropy differences due to the different $S_z$ are approximately constant. In the liquid states, the oscillations of the magnetic couplings are irregular and the variations of the entanglements are not monotonous. The studies imply that the extent works on QDs with different Zeeman splittings and other spin-related terms will be important for understanding and controlling the quantum states of few electrons in the future.

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