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Various spin-polarization states beyond the maximum-density droplet: A quantum Monte Carlo study

S. Siljamäki, A. Harju, and R. M. Nieminen
Laboratory of Physics, Helsinki University of Technology, P.O. Box 1100, FIN-02015 HUT, Finland

V. A. Sverdlov
Department of Physics and Astronomy, State University of New York, Stony Brook, New York 11794-3800

P. Hyvönen
Department of Physical Sciences, Theoretical Physics, University of Oulu, P.O. Box 3000, FIN-90401 Oulu, Finland

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Using a variational quantum Monte Carlo method, the effect of Landau-level mixing on the lowest-energy–state diagram of small quantum dots is studied in the magnetic-field range where the density of magnetic flux quanta just exceeds the density of electrons. An accurate analytical many-body wave function is constructed for various angular momentum and spin states in the lowest Landau level, and Landau-level mixing is then introduced using a Jastrow factor. The effect of higher Landau levels is shown to be significant; the transition lines are shifted considerably towards higher values of magnetic field and certain lowest-energy states vanish altogether.

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Quantum dots (QD) are systems containing a number of charge carriers in a nanoscale volume. A two-dimensional semiconductor QD (Ref. 1) can be constructed, e.g., by superimposing a confining potential on two-dimensional electron gas, which can be fabricated into the inversion layer between two different semiconductor materials. In the inversion layer, the confinement perpendicular to the interface can be made so strong that only the lowest-energy eigenstate in that direction has a nonnegligible probability of being occupied. This makes the system genuinely two dimensional, and leads to some physical effects that are absent in higher dimensions: in thermodynamical limit the integer and fractional quantum Hall effects[2] are perhaps the most famous examples.

Experimentally, QD's are observed to have a series of different ground states as the magnetic field is increased.[3] While many properties of the states can be measured, understanding their nature is still one of the major theoretical goals in the field. In a large range of moderately high magnetic field the very stable and fully spin polarized maximum-density–droplet state (MDD) remains the ground state. This many-particle state has an extremely accurate analytical description,[4] and is here used as the starting point to study phase diagrams of possible lowest-energy states in stronger fields.

The variational quantum Monte Carlo (VMC) (Ref. 5) method is used to study the QD system. In this method a trial many-body wave function Ψ with desired properties and with free variational parameters α_i is first constructed, and then the parameters are optimized to converge towards the exact wave function Ψ_0. Using the optimized wave function, the expectation value of an observable $\mathcal{A}$ can be evaluated as the average of the corresponding local quantity $\Psi^{-1}\mathcal{A}\Psi$, e.g., for the Hamiltonian operator $\mathcal{H}$:

$$E_\Psi = \lim_{M\to\infty} \frac{1}{M} \sum_{i=1}^{M} \frac{\mathcal{H}\Psi(\mathbf{R}_i)}{\Psi(\mathbf{R}_i)} = \langle \Psi|\mathcal{H}|\Psi\rangle, \qquad (1)$$

where the N-particle–coordinate configurations $\mathbf{R}_i$ are distributed as $|\Psi|^2$ and generated using the Metropolis algorithm.

The variational principle guarantees that the total energy given by the VMC method, using any trial wave function, is always an upper bound for the true total energy of the quantum state in question. The variance of the local energy $\Psi^{-1}\mathcal{H}\Psi$ diminishes as the trial wave function approaches an eigenstate of the Hamiltonian, and as a result it can be used not only as a measure of the statistical error in E_Ψ, but also as a measure of the difference between calculated and true energies $E_\Psi - E_{\Psi_0}$.

The variational parameters in the trial wave function are optimized by minimizing the total energy. The minimization process itself was done using the stochastic gradient method[6] with analytical expressions for derivatives.[7] The method has proven to be fast in finding a minimum of a function whose values are not exact.

The QD in this study is an N-electron system on a two-dimensional plane, in rotationally symmetric and parabolic potential $V(r) = \frac{1}{2} m^* \omega_0^2 r^2$, and in perpendicular magnetic flux density $\mathbf{B} = B\mathbf{u}_z$. An effective mass m^* is used to describe the effects of the underlying crystal structure, and ω_0 determines the strength of the in-plane confinement. In the symmetric gauge, $\mathbf{A} = \frac{1}{2}\mathbf{B}\times\mathbf{r}$, the effect of the vector potential on the Hamiltonian is to enhance the confinement strength, $\omega_0^2 \to \omega_0^2 + (\omega_c/2)^2 = \omega^2$, where $\omega_c = eB/m^*$ is the effective cyclotron frequency, and to introduce angular-momentum and spin-dependent terms. Switching to the effective harmonic oscillator units ($m^* = \hbar = \omega = e = 1$), the total Hamiltonian operator can be written as

$$\mathcal{H} = \tfrac{1}{2} \sum_{i=1}^{N} \left[-\nabla_i^2 + r_i^2 + \omega_c (l_{z,i} + \gamma^* s_{z,i}) \right] + \sum_{i<j} \frac{C}{r_{ij}}. \qquad (2)$$

Here $l_{z,i}$ and $s_{z,i}$ are the z components of angular-momentum and spin operators for the ith particle, γ^* is defined as $\gamma^* = g^* m^*/m_0$, where g^* is the effective Landé g factor, and C is a dimensionless interaction strength, $C^2 = \text{Hartree} \times m^*/m_0 \epsilon_r^2 \hbar\omega$. In these units $\omega_c = B < 2$.

Single-particle states of the noninteracting part of the Hamiltonian (2) can be solved analytically for arbitrary magnetic flux density B.[8] As B is increased the states separate to Landau levels with level spacing asymptotically proportional to B, and intra-level energy spacing of states asymptotically proportional to B^{-1}. In the limit of infinite magnetic flux density only the lowest Landau level (LLL) remains occupied. The single-particle wave functions φ_m, that the LLL is composed of, have a particularly simple form:

$$\varphi_m(z) = z^{|m|} \exp(-\tfrac{1}{2}|z|^2), \tag{3}$$

with energies (in units of $\hbar\omega$)

$$E_m = 1 + (1 - \tfrac{1}{2}\omega_c)m. \tag{4}$$

In Eq. (3), z is a complex coordinate in the plane of the electrons: $z = x + iy$, and $m = 0,1,\ldots$ is $l_z/\hbar$.

It is a common approximation to truncate the full Hilbert space to the lowest Landau level only, and ignore the effects of higher Landau levels altogether. For example, exact diagonalization calculations[9] are done within the LLL approximation for $N \gtrsim 4$. The approximation improves with increasing B, since higher Landau levels move farther off in energy, but as will be shown, Landau-level mixing (LLM) can qualitatively alter the behavior of the system even in such regions of B, where the LLL approximation is frequently used.

In this study, the trial wave functions Ψ are of the Jastrow-Slater form. The construction of Ψ begins by creating an LLL-many-particle wave function Ψ_{LLL}, which determines, e.g., the angular momentum and the spin of the state. The LLM is then introduced using two-body correlation functions of Jastrow type.[10] To construct the LLL part of the wave function, the unnormalized maximum-density droplet state Ψ_{MDD} is used as a starting point:

$$\Psi_{\text{MDD}} = \prod_{i<j} (z_j - z_i) \exp\left(-\tfrac{1}{2} \sum_{i=1}^{N} |z_i|^2 \right). \tag{5}$$

In the thermodynamical limit this configuration corresponds to the very stable quantum-Hall state[4] at filling factor $\nu = N/N_\Phi = 1$. For QD's in the LLL approximation, Ψ_{MDD} is the lowest-energy state in a large region around $\nu = L_{\text{MDD}}/L = 1$, where L denotes the total angular momentum, $L = \Sigma l_{z,i}$. The state is composed of consecutive single-particle states of the form of Eq. (3) with $m = 0,\ldots,N-1$, and it has the total angular momentum $L_{\text{MDD}} = \frac{1}{2}N(N-1)$.

In this study only post-MDD states are considered, that is, states that have non-negative additional angular momentum $\Delta M = L - L_{\text{MDD}}$ with respect to the MDD state. Since the parabolic form of the external confinement allows one to perform the elimination of the center-of-mass motion, the spin-up and spin-down degrees of freedom are not independent. Therefore it is assumed that it is favorable for an electron to put zeros of the wave function on the positions of other spin type electrons also. This is equivalent to the requirement that any post-MDD state should contain Ψ_{MDD} as a factor:

$$\Psi_{\text{LLL}} = \Psi_{\text{MDD}} P_{\Delta M}, \tag{6}$$

where $P_{\Delta M}$ is a polynomial of proper symmetry and degree ΔM. Under this assumption, constructing the LLL trial wave function is a matter of choosing the suitable polynomial $P_{\Delta M}$. It must have the correct symmetry, and its degree ΔM gives the additional angular momentum with respect to the MDD state.

The polynomial $P_{\Delta M}$ is constructed as follows: One starts from the product

$$P^0_{\Delta M} = \prod_{i=1}^{\Delta M} \tilde{z}_i, \tag{7}$$

where the coordinate transformation $\tilde{z}_i = z_i - 1/N \Sigma_j z_j$ has been applied to remove the center-of-mass motion. This fixes the additional angular momentum ΔM of the trial state. Correct symmetry is now built in using the Young symmetrization operator[11] $\mathcal{Y}_\chi$:

$$\Psi_{\text{LLL}} = \mathcal{Y}_\chi(\Psi_{\text{MDD}} P^0_{\Delta M}) = \Psi_{\text{MDD}} \mathcal{Y}'_\chi P^0_{\Delta M}, \tag{8}$$

where $\mathcal{Y}'_\chi P^0_{\Delta M}$ is $P_{\Delta M}$ above. The parameter χ is the number of inverted spins with respect to a fully spin-polarized state, and it determines the shape of the Young tableau corresponding to $\mathcal{Y}_\chi$. Because an antisymmetric factor Ψ_{MDD} was taken out of $\mathcal{Y}_\chi$, the directions of symmetrization and antisymmetrization are interchanged in $\mathcal{Y}'_\chi$. By fixing the spin and angular momentum through parameters ΔM and χ, the LLL part of the trial wave function is determined completely, i.e., it has no variational parameters. This family of trial wave functions covers most spin configurations in the region $\Delta M = 0,\ldots,N$. For example, for seven electrons there are only three states (out of 23 nondegenerate states) that are unavailable: $S = 1/2$ at $L = 27$, and $S = 3/2$ and $S = 1/2$ at $L = 28$. These inaccessible configurations are not expected to be lowest-energy states, based on exact diagonalization results.[12] For states with $2S = |N - 2\Delta M|$, the LLL construction above results in wave functions that are very similar to skyrmion states.[13]

After the lengthy construction of the LLL part, the LLM part is simply multiplied into the trial wave function as a two-body correlation function of Jastrow type,

$$J(\{r_{ij}\}_{i<j}) = \prod_{i<j} \exp\left(\frac{\beta_{ij} r_{ij}}{1 + \alpha_{ij} r_{ij}} \right). \tag{9}$$

The total wave function is then

$$\Psi = \Psi_{\text{LLL}} J. \tag{10}$$

This form of the correlation factor leaves the spin and angular-momentum properties of Ψ intact. The Jastrow factor has two adjustable parameters: $\alpha_{ij} = \alpha_{\uparrow\uparrow}$ for parallel spins and $\alpha_{ij} = \alpha_{\uparrow\downarrow}$ for antiparallel spins. For each trial state, these parameters are functions of B, and have to be optimized separately for each magnetic-field value. Constants β_{ij} are

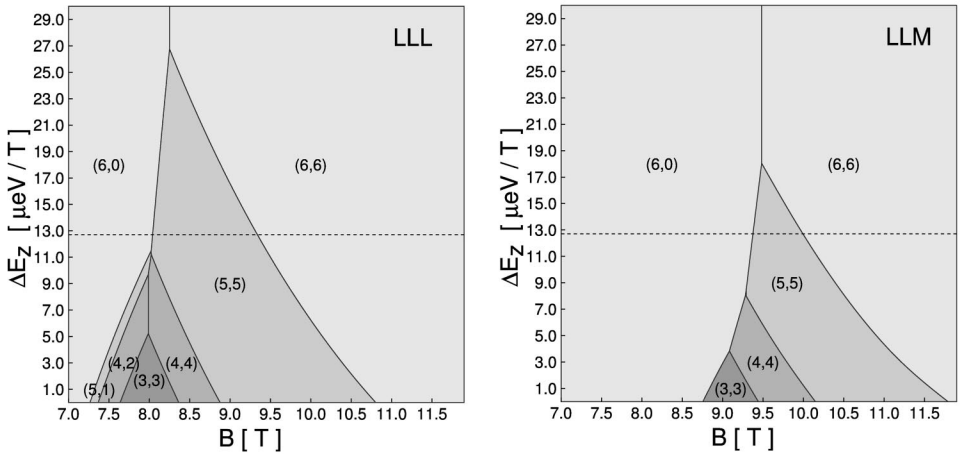

FIG. 1. Phase diagrams for six electrons in the lowest Landau-level approximation (left panel) and with Landau-level mixing (right panel). The labeling of the states is $N_\uparrow, \Delta M$, where $N_\uparrow$ is the number of spin-up electrons and ΔM is the additional angular momentum ($L_{\mathrm{MDD}}=15$ for six electrons). The vertical axis is the strength of the Zeeman coupling per spin, $\Delta E_z=\left|\frac{1}{2}\mu_B g^*\right|$, the value of which in GaAs (12.7 μeV/T) is marked by dashed lines in the figures. Other parameters were $m^*/m_0=0.067$, $\hbar\omega_0=5$ meV, and $\epsilon_r=12.4$. The relative interaction strength C varies from 1.23 ($B=7$ T) to 1.01 ($B=12$ T).

determined by cusp conditions.[14] The form of Eq. (10) has proven very efficient in capturing the Landau-level mixing; in small systems as much 98% of the correlation energy can be recovered.[15]

Results for two systems $N=6$ and $N=7$ are presented in this paper. In order to test the accuracy of the LLL construction an exact diagonalization calculation[12] was performed for seven electrons at $B=5$ T. This showed that for all possible LLL lowest-energy states the error in total energy is very small, at most 0.065%. In the case of the LLM wave function, no such diagonalizations are currently available.

Figure 1 shows results for a six-electron QD, and corresponding data for seven electrons are shown in Fig. 2. Both systems use GaAs parameters: $m_{\mathrm{rel}}=0.067$, $g^*=-0.44$, and $\epsilon_r=13.0$ for $N=7$ as in Ref. 12, but 12.4 for $N=6$ as in Ref. 16.

The figures show magnetic flux density vs Zeeman coupling strength $\Delta E_z=\left|\frac{1}{2}\mu_B g^*\right|$. Generally, with increasing Zeeman coupling strength the degree of spin polarization increases, and above some critical value ΔE_z^* the system remains spin-polarized at all values of B in the post-MDD region. In the LLL approximation, this happens at $\Delta E_z^*=26.5$ μeV/T for $N=6$, and at 34.5 μeV/T for $N=7$. Lowering the Zeeman coupling strength allows other total-spin values, and with $\Delta E_z=0$ the system goes through all possible spin configurations. The lowest-energy states are the skyrmionic states as discussed above.

The effect of the Landau-level mixing can be seen on the right-hand panels. Quantitatively, the transition lines are shifted towards higher fields and lower Zeeman couplings. In the case $N=6$, half of the lowest-energy states even vanish completely when the LLM is taken into account.

The shift towards higher B means that in the LLM case the states are more stable against radial expansion as B is increased. (ΔM increases as one moves to the right in the figures.) This should be compared with Ref. 17, where similar results have been obtained within the LLL approximation, by assuming the QD to have finite thickness. Both effects are results of the expansion of the basis set of the Hilbert space, but in our case the system still remains two dimensional. The vanishing of some lowest-energy states can be explained by noting that the two-body correlation factor has strongest ef-

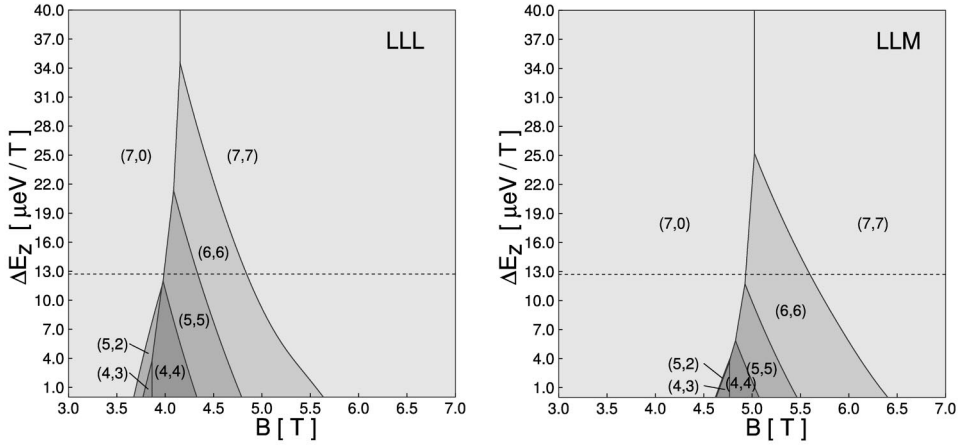

FIG. 2. Phase diagrams for seven electrons. In this case $L_{\mathrm{MDD}}=21$, and the value $\epsilon_r=13.0$ was used to compare with our exact diagonalization calculation. The relative interaction strength C varies from 1.38 ($B=3$ T) to 1.17 ($B=7.0$ T).

fect on the states that are most compact (i.e., have the lowest angular momenta). For the MDD state, the gain in energy is largest, and it can completely block some neighboring states whose energy is only slightly lower in the LLL approximation.

The value of ΔE_z (corresponding to $g^*=-0.44$) for GaAs is 12.7 μeV/T. This is a maximum value (within approximations and assumptions used) that can only be lowered, using tilted field experiments. Since the value is much lower than ΔE_z^*, it should be possible to encounter partially spin-polarized post-MDD states in experiments, even without tilting the magnetic field.

In summary, simple trial wave functions for partially and fully spin-polarized QD systems have been constructed. The wave functions were shown to produce excellent total energies, and provide an accurate estimate of Landau-level mixing.

We demonstrate that the LLM, which is almost always neglected in previous studies, is able to suppress the existence of certain lowest-energy states with small amount of additional angular momentum (compared to N). Furthermore, a strong shift of transition points towards higher magnetic fields due to the LLM is observed. Another important result is that despite the LLM, partially spin-polarized states can exist in the post-MDD region with realistic Zeeman coupling strengths. The most visible of these states is likely to have a single spin flipped and angular momentum equal to $L_{\mathrm{MDD}}+N-1$.

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