Ground state energies of quantum dots in high magnetic fields: 
A new approach
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Abstract
We present a new method for calculating ground state properties of quantum dots in high magnetic fields. It takes into account the equilibrium positions of electrons in a Wigner cluster to minimize the interaction energy in the high field limit. Assuming perfect spin alignment the many-body trial function is a single Slater determinant of overlapping oscillator functions from the lowest Landau level centered at and near the classical equilibrium positions. We obtain an analytic expression for the ground state energy and present numerical results for up to \( N = 40 \).

1. Introduction
Quantum dots, often referred to as artificial atoms [1], were intensively studied in recent years both experimentally [2,3] and theoretically [4–18]. A number of different theoretical methods, including, e.g., exact diagonalization [4–7], quantum Monte Carlo (QMC) [8–12], Hartree-Fock [13–15] and density-functional calculations [16–18], were employed for investigating the ground state properties of dots, which are responsible for many of the experimentally observed effects.

In this paper we present a new concept to calculate ground state properties of quantum dots in high magnetic fields, with application to systems with up to 40 electrons. This approach is motivated by the evidence that in high magnetic fields \( B \) quantum dot electrons tend to form a Wigner cluster [8–10]. Therefore, we construct a ground-state many-body variational wave function in the form of a Slater determinant with (overlapping) single-particle wave functions centered at or near equilibrium positions of classical point particles. The classical configurations are calculated either analytically (for \( N \leq 8 \)) or using the Monte Carlo minimization [8,9]. Expectation values of observables can be formulated analytically. Here we present ground state energies for disc-like quantum dots with up to 40 electrons.

2. The model Hamiltonian
We consider a system of \( N \) electrons moving in the plane \( z = 0 \), in the lateral potential \( V(\mathbf{r}) = m^* \omega_0^2 (x^2 + y^2)/2 \), and in the perpendicular magnetic field \( \mathbf{B} = (0, 0, B) \). The Hamiltonian of the system has the form
\[
\hat{H} = \sum_{i=1}^{N} \left[ \frac{\left[ p_i + e A(\mathbf{r}_i) \right]^2}{2m^*} + V(\mathbf{r}_i) \right] + V_C + E_Z, \tag{1}
\]

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where $A(r) = (B/2)(-y, x)$, $V_C$ is the Coulomb energy of electron-electron interaction and $E_Z$ is the Zeeman energy. The solutions of the single-particle problem (Fock and Darwin, [20]) are given by

$$\psi_{n,l}(r, \phi) \propto e^{i l \phi} r^{|l|} e^{-r^2/4L^2} L^{|l|}_n(r^2),$$

where $r^2 = (x^2 + y^2)/\lambda^2$, $\lambda^2 = (\hbar/m^*)[\omega_c^2 + (\omega_c^2/2)]^{-1/2}$, $\omega_c = eB/m^*$ is the cyclotron frequency, $L^{|l|}_n$ are associated Laguerre polynomials, $n \in \mathbb{N}_0$ is the number of nodes, and $l \in \mathbb{Z}$ is the angular momentum quantum number.

3. The new approach

In strong magnetic fields electrons tend to localize around the classical equilibrium positions, and their spins to be aligned along the magnetic field. This tendency suggests to write the trial many-body wave function $\Psi_L$ in the form of a Slater determinant (as has been done in Ref. [21] for a related problem)

$$\Psi_L = \det |\chi^{(L)}_{ij}|/\sqrt{N!}, \quad \chi^{(L)}_{ij} = \psi_{0,-L}(r_i - R_j) \exp \left(-\frac{ie}{2\hbar}(B \times R_j) \cdot r_i \right),$$

(2)

where $\chi^{(L)}_{ij}$ are Fock-Darwin wave functions with an additional phase factor caused by a magnetic translation [22] of the $i$-th electron to the center at $R_j$. The non-negative integer $L$ and the vectors $R_1, \ldots, R_N$ are free parameters of the theory. In general, the single particle wave functions $\chi^{(L)}_{ij}$ are not orthogonal, and the overlap of the neighbor single-particle states needs not to be small.

Using the trial wave functions $\Psi_L$ we analytically calculate expectation values of the energy and the density of electrons. The energy is minimized with respect to the variational parameters $L$ and $R_1, \ldots, R_N$.

4. Results

Figure 1 shows the calculated ground state energy of a system of 3–10 electrons, together with reference data from Ref. [8], obtained by the QMC method. The small numbers 0 and 1 over the dotted lines indicate that, starting from the corresponding points the trial wave functions $\Psi_{L=0}$ or $\Psi_{L=1}$ gave the lowest energy. The parameters $R_i$ were chosen according to classical equilibrium configurations and were not varied in Figure 1.

As seen from the Figure, our results are very close to (and sometimes even lower than) the QMC results at $\omega_c/\omega_0 \gtrsim 2$. In this range typical relative deviations of the total energy are 2% and less. Optimizing the parameters $R_i$ we could get even better agreement with the QMC results in the range $0.6 \lesssim \omega_c/\omega_0 \lesssim 2.4$ (the optimized radius of electron shells is up to 20% larger at small magnetic fields than the classical radius). The accuracy of our results shows a tendency to increase with larger $B$ and/or $N$. At the upper range of the magnetic field the relative deviation is about 1% for $N \leq 6$ and even less for higher $N$. This remarkably good agreement and its tendency to become even better with increasing electron number demonstrates the capability of the new method and is promise for obtaining reliable results for even higher electron numbers.

Figure 2 gives calculated ground state energies $E_N$ in the range of up to $N = 40$, for which suitable exact reference values were not available. With increasing magnetic field we find a.
Figure 1. Calculated expectation values for the ground state energy (dotted) of \( N = 3 - 10 \) electrons. Bold numbers designate the number of electrons, \( \omega = (\omega_0^2 + \omega_c^2/4)^{1/2} \). Full curves show the QMC results from Ref. [8]. For this plot we have chosen \( l_0/a_B = 1.91 \), where \( l_0^2 = \hbar/m^*\omega_0 \) and \( a_B \) is the effective Bohr radius. The Zeeman energy with effective g-factor \( g^* = -0.44 \) was taken into account.

Figure 2. Calculated ground state energies for 10–40 electrons (dotted curves). The horizontal dashed lines indicate the value of classical ground state energy \( E_{\text{class}}^{N/\hbar\omega_0} \). The meaning of the numbers in the plot and the parameter \( l_0/a_B \) are as in figure 1, except \( g^* = 0 \) here.

clear convergence of \( E_N - N\hbar\omega \) towards \( E_N^{\text{class}} \), so that we can write

\[
E_N = E_N^{\text{class}} + N\hbar\sqrt{\omega_0^2 + (\omega_c/2)^2} + \delta E_N. \tag{3}
\]

The correction \( \delta E_N \) is positive, tends to zero at \( B \to \infty \), and for \( 10 \leq N \leq 40 \) it is smaller than 2% at \( \omega_c/\omega_0 > 6 \) and smaller than 0.6% at \( \omega_c/\omega_0 > 18 \). Equation (3) refines the rigorous
mathematical result by Yngvason \[23\] and has a transparent physical meaning: The quantum mechanical ground state energy of the dot is a sum of the classical potential energy, the quantum mechanical kinetic energy, and the small rest energy $\delta E_N$, which decreases with $B$.

5. Conclusion

We have presented a new method to calculate ground state expectation values for parabolic quantum dots in (high) magnetic fields. The results were obtained by evaluating the expectation value, for which we found an analytical expression using a specially designed trial wave function. It takes into account the classical equilibrium positions of the electrons and has the correct symmetry for a fermion system with fully polarized spins. In the high magnetic field regime our results compare favourably with QMC data, but are much less demanding in computer time. Therefore, an extension to higher electron numbers becomes possible as we demonstrate by showing results for up to 40 electrons. We put forward a simple interpretation of our results for the ground state energy, Eq. (3), and gave the upper estimate for the rest energy term $\delta E_N$ in the studied range of $N$ and the magnetic field.

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