Interaction effects in quantum dots in a vertical magnetic field

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Abstract. The Hartree-Fock approximation has been used to compute the properties of parabolic two-dimensional quantum dots under a perpendicular magnetic field. The addition energies for vertical quantum dots up to $N=20$ electrons is analysed at different strengths of the effective electron-electron interaction. A remarkable agreement between experimental data and results for the addition energy for $N=2,3,4,5$ electrons exhibits an important role of the screening of the effective interaction for interpretation of the ground state transitions in the magnetic field. We suggest a recipe to determine the orbital momenta of the QD ground states. We show that quantum shell structure of quantum dots survives only at small magnetic fields.

1. Introduction
Quantum dots (QDs) attract a considerable experimental and theoretical attention during last decade (cf [1, 2, 3, 4]). In particular, this interest is due to the fact that QDs may provide a natural realization of quantum bit. On the other hand, QDs can be considered as a tiny laboratory allowing direct investigation of fundamental properties of charge and spin correlations at the atomic scale.

Mesoscopic systems such as QDs exhibit many common properties specific to a finite Fermi system. A prominent feature is a regular single–particle motion which can manifest itself in pronounced shell effects. In recent experiments [5, 6] it was found that the energy needed to place an extra electron (addition energy) into a vertical QD at zero magnetic field has characteristic maxima which correspond to the sequence of magic numbers of a two-dimensional harmonic oscillator. If a QD is placed under a perpendicular magnetic field, one observes the orbital momentum and spin oscillations of the ground state of a QD with alteration of the field strength [1]. At certain field range the oscillations disappear and it is believed that the electrons form a finite-size analog of infinite integer quantum Hall liquid (with filling one) [2]. In QDs this fully polarized state is called the maximum density droplet (MDD). Further, for a low enough electron density, Wigner [7] predicted that electrons should localize, creating an ordered spatial structure that breaks the complete translational symmetry of the homogeneous electron gas. According to a general opinion, the Wigner crystallization in QDs, whose localized states are referred to as Wigner molecules, should occur at significantly larger densities than in bulk. This is based on the argument that in QDs potential-energy contributions can easily exceed the kinetic terms and, therefore, electronic motion can be effectively quenched by manipulating the external confinement and/or an applied magnetic field.
The existence of different phases in QDs has become a topical subject in mesoscopic physics [2, 3]. Such studies shed light on various aspects of strongly correlated finite systems, which are different from bulk and can be controlled experimentally. It gives a hope to understand the transition from finite-size effects to a conventional condensed matter picture of a many-body quantum system, as a function of electron-electron interaction and external fields. In fact, the high controllability of QDs creates a remarkable opportunity to study in detail novel strongly correlated phenomena in various experimental setups.

In theoretical studies of QDs the underlying lattice of the semiconductor material is taken into account by using an effective mass for the conduction electrons, and a static dielectric constant, reducing the Coulomb repulsion. For vertical QDs, the resulting confining potential is, to a good approximation, harmonic [1, 5, 6]. Various approaches, based on such approximations, including ab initio calculations such as diffusion or path integral Monte Carlo methods, spin-density functional methods have been applied with some degree of success to analyze the ground state energies of N-electron QD [2]. In many cases, a convenient starting point to treat finite systems is a mean field description like the Hartree-Fock (HF) approach. Self-consistency between the mean field and the single-particle orbitals and total energy minimization are the basic conditions at this level. However, the total energy minimization procedure being of nonlinear nature is still a real challenge for many-body quantum theory.

Recently we developed an efficient, numerically stable HF procedure. In the present communication we compare our results with the state of art calculations [8] for few-electron vertical QDs. The main focus of our report is, however, the analysis of quantum size effects (like shell structure) and transition to the classical limit of localized electronic states in vertical QDs, with the increase of the electron-electron interaction and/or the magnetic field.

2. The Model
We consider a system of $N$ interacting electrons whose motion is restricted to the $xy$ plane by a circular parabolic potential. The system is also subject to an external magnetic field applied in the vertical direction ($z$). The full Hamiltonian thus reads

$$H = \sum_{i=1}^{N} \left[ \frac{1}{2m} \left( \mathbf{p} - \frac{e}{c} \mathbf{A} \right)^2 + \frac{1}{2} m \omega_0^2 r_i^2 \right] + \frac{\kappa}{2} \sum_{i>j=1}^{N} r_{ij}^2 + g^* \mu_B B S_z .$$

Here, $m$, $\kappa (= \epsilon_r)$ and $g^*$ are the electron’s effective mass, the dielectric constant and the effective gyromagnetic factor, respectively, and we have used planar polar coordinates ($r^2 = x^2 + y^2$). The two contributions within the square brackets are, respectively, the generalized kinetic energy in terms of the vector potential $\mathbf{A}$, and the external confinement. Within the so-called symmetric gauge one has $\mathbf{A}(x, y) = B/2(-y, x)$. The next contribution is the Coulomb interaction and, finally, the last term is the Zeeman energy involving the total spin operator $S_z$ and the universal Bohr’s magneton $\mu_B = |e|\hbar/2mc$.

In the chosen gauge the magnetic field contributions can be recast into the form of an effective parabolic confinement of frequency $\Omega = \sqrt{\omega_0^2 + \omega_c^2}/4$, where $\omega_c = |e|B/mc$ is the cyclotron frequency, and an addition orbital-momentum-dependent term $(\hbar \omega_c/2)\ell_z$ (cf [4]). By introducing the length $\ell_\Omega = \sqrt{\hbar/(m\Omega)}$ and the energy $E_0 = \hbar\Omega$ units we can rewrite Hamiltonian (1) in terms of only two adimensional parameters: $R_{mp} = \epsilon^2/(\kappa \ell_\Omega)\hbar\Omega$ and $W_{mp} = \omega_c/\Omega$, -- the magneto-parabolic units (mpu) [9]. In the absence of a magnetic field $R_{mp}$ coincides with the so-called Wigner parameter $R_W$ (cf [3]). Note also that $W_{mp}$ has a maximal value $W_{mp} = 2$ that corresponds to a zero confinement $\omega_0 = 0$ or an infinite magnetic field. Within the mpu
system the Hamiltonian reads

$$\mathcal{H} = \frac{H}{\hbar \Omega} = \sum_{i=1}^{N} \left[ -\frac{1}{2} \nabla^2 + \frac{1}{2} r^2 + \frac{W_{mp}}{2} \ell_i^2 \right] + R_{mp} \sum_{i>j=1}^{N} \frac{1}{r_{ij}} + \frac{g^* m^*}{2} W_{mp} S_z,$$

where \( m^* = m/m_e \) is the adimensional ratio of effective to bare electron mass, and \( r \rightarrow r/\ell \). The passage from the mpu system, with a given \( R_{mp} \) and \( W_{mp} \), to physical units requires the knowledge of the effective mass \( m \) and the dielectric constant \( \kappa \). More specifically, with fixed \( m \) and \( \kappa \) one can invert \( R_{mp} \) and \( W_{mp} \) for the effective confinement \( \Omega \) and cyclotron \( \omega_c \) frequencies or, equivalently, for the external confinement \( \omega_0 \) and the magnetic field \( B \). In terms of these results the physical values of the energy (\( h\Omega \)) and length (\( \ell_\Omega \)) units are readily found (see Fig.1 in [9]). The \( R_{mp} \) parameter is a measure of the relative importance of electron-electron interaction to confinement potential strength. It is used usually as a measure to define the different phases in QDs and, in particular, a formation of Wigner molecules [3, 9]. Note that we use the effective electron-electron interaction, where the parameter \( R_{mp} \) is associated with the effective charge (a screening parameter). Such a form can be justified due to, for example, the QD thickness [10].

Introducing the basis of oscillator and spin states that diagonalizes the first term in Eq. (2), \( \{ |a\eta \rangle; a = 1, \ldots, N; \eta = \uparrow, \downarrow \} \), where \( a \) labels the orbital part and \( \eta \) the spin, an arbitrary single-particle orbital \( |i\rangle \) is expanded as \( |i\rangle = \sum_{a\eta} \beta_{a\eta}^i |a\eta\rangle \). The oscillator (Fock-Darwin) states \( |a\rangle \) are characterized by radial \( (n_a) \) and orbital momentum \( (m_a) \) quantum numbers (cf [4]). In our calculations ground states are eigenstates of the \( S_z \) and of the \( \hat{l}_z \) operators. In the chosen basis, the HF equations are written as a system of nonlinear eigenvalue equations for the matrix of \( B \) coefficients.

3. Shell structure and classical limit

The most simple theoretical approach to analyse the experimental data from transport studies of correlated QD states is to calculate the addition energy

$$E_{\text{add}}(N) = E_{N+1} - 2E_N + E_{N-1},$$

where \( E_N \) is the energy of the an N-electron dot state [1]. The energy \( E_{\text{add}}(N) \) is proportional to the difference between the gate voltages for two successive current peaks in transport experiments.

Recently Maksym et al [8] developed a model of a vertical QD and reproduced quite well experimental addition energies for \( N = 2, 3, 4 \). Although the three-dimensional nature of QDs is accounted for, the real calculations are based on the two-dimensional parabolic potential. The authors constructed the effective two-dimensional electron-electron interaction (the screened Coulomb interaction) which does not depend on the magnetic field. They diagonalized the model Hamiltonian in the many-electron basis consisted of Slater determinants. To compare with the results [8], we have used the following parameters for InGaAs QDs: \( h\omega_0 = 4.5 \text{ meV} \), \( m^* = 0.0653 \), dielectric constant \( \varepsilon_r = 12.7 \). These values provide for the strength of the bare Coulomb interaction the following estimation: \( R_{mp}(\omega_c = 0) \equiv R_W \approx 1.56 \). Since we use the effective two-dimensional interaction, the effective value \( R_W = 0.78 \) was taken to reproduce the available experimental data. Our calculations demonstrate a good agreement with the experimental data as well as with the theoretical results obtained in [8].

For \( N=2 \), we found that the singlet \( (L_z, S_z) = (0,0) \) state is replaced by fully polarized triplet \( (-1,1) \) state (MDD phase) at \( B_{HF} = 3.8 \text{ T} \) (\( L_z \) and \( S_z \) are the quantum numbers of the z-component of the total orbital momentum and of the total spin, respectively). The experimental transition takes place at \( B_{\text{exp}} = 4.2 \text{ T} \), while the theoretical calculations of Maksym et al [8] give \( B_{\text{theor}} = 3.8 \text{ T} \).
For $N = 3$ our calculations predict the state $(-1, 1/2)$ to be the lowest state until $B_{HF} = 4.72$ T. Two electrons occupy the lowest available states with $m = 0$ but with different $S_z = \pm 1/2$ quantum numbers. The next available state is characterized by $m = -1$, and the largest possible value for this configuration has $S_z = 1/2$. At $B_{HF} = 4.72$ T we obtain the onset of the MDD phase $(-3, 3/2)$.

At small magnetic field $B_{HF} < 0.46$ T, for $N = 4$ we obtain the ground state $(0, 1)$. A partially polarized state is favourable due to the HF exchange term which supports the configuration with two aligned spins. At $B_{HF} = 0.46$ T ($B_{exp} = 0.33$ T, $B_{theor} = 0.3$ T) the magnetic field overcomes the exchange contribution and we obtain $(-2, 0)$ state. This state persists till $B_{HF} < 4.42$ T. At $B_{HF} = 4.42$ T ($B_{exp} = 4.06$ T, $B_{theor} = 4.0$ T) the magnetic field polarizes the system partially, and, with the aid of the exchange term, the HF calculations produce the ground state $(-3, 1)$. At $B_{HF} \geq 5.33$ T we obtain the onset of the MDD phase $(-6, 2)$. At $B_{HF} = 14.31$ T the MDD state is replaced by the ground state $(-10, 2)$.

We reproduce a double peak structure for $N=3$ and $N=4$ around 4-6 T. The spike observed for $N = 3$ at $B_{HF} = 3.8$ T is due to the transition to the MDD phase in two-electron system (see also Eq.(3)). The following dip is caused by the transition $(-1, 1/2)$ to $(-3, 3/2)$ in $N = 3$, while the transition from $(-2, 0)$ to $(-3, 1)$ in $N = 4$ changes only the slope of the former transition. The next spike observed for $N = 3$ at $B_{HF} = 5.33$ T is due to the transition $(-3, 1) \rightarrow (-6, 2)$ in $N = 4$. The large peak at $B_{HF} = 1.3$ T for $N = 4$ is due to the ground state transition $(-1, 1/2) \rightarrow (-4, 1/2)$ in $N = 5$ (not shown). The next transition in $N = 5$: $(-4, 1/2) \rightarrow (-6, 3/2)$ at $B_{HF} = 4.80$ T, has a little effect. However, the transition to the MDD phase $(-6, 3/2) \rightarrow (-10, 5/2)$ in $N = 5$ is responsible for the small spike in the addition energy of $N = 4$ at $B_{HF} = 5.87$ T.

Although the agreement is good in general till $B_{exp} \leq 6$ T, there are some discrepancies at high magnetic field for $N = 4$ case (see Fig.1). Similar problem appears in more sophisticated calculations of Maksym et al [8]. The analysis of finite-thickness effect in two-electron QDs...
reveals a magnetic-field dependence of the screening of the effective interaction [10]. The stronger is the magnetic field the lesser is expected the screening effect in QDs. Indeed, we reproduce the decrease and the increase of the addition energies for $N=3$ and $N=4$, respectively, at $B \geq 7\, \text{T}$ with the effective value $R_W = 1.5$. However, the positions of the transitions are slightly higher in the energy scale. One of the possible reasons for this discrepancy is the change of the effective confining potential (the parabolic confinement frequency) at high magnetic field. It appears from our calculations that there is a visible suppression of the electron-electron interaction in the observed experimental data. Indeed, the experimental evidence [6] is that the QD has a high degree of a circular symmetry. We can conclude that for this device the confining potential dominates in the electron dynamics.

The origin of magic values of the orbital momenta which occur after the onset of the MDD phase for $N=4$ ($L_z = 6, 10, 14, \ldots$) can be understood from the symmetry properties of the total wave function of a few-electron QD. The classical minimum-energy configuration of a few point charges in a parabolic potential is highly symmetric [14]. Such configurations takes place if $N$ point charges create equidistant nodes on the ring, with the angle $\alpha = 2\pi/N$. It is reasonable to suppose that a quantum ground state is localized around the equilibrium classical state (see below). However, we have to take into account that the total wave function should be antisymmetric. Note that the rotation on the angle $\alpha$ is equivalent to a cyclic permutation of the particle coordinates on the ring. Since the spatial part of the total wave function $\Phi_r$ is the eigenstate of $L_z$ operator, one can require the fulfillment of the following symmetry condition

$$R_z(\alpha)\Phi_r = \exp(i\frac{2\pi}{N}L_z)\Phi_r \equiv P_p\Phi_r = \varepsilon\Phi_r$$  \hspace{1cm} (4)

Here $\varepsilon = \pm$ is the parity of the permutation for $N$ point charges located on the ring. If the permutation is odd, then $\exp(i\frac{2\pi}{N}L_z)\Phi_r = -\Phi_r$, and the total orbital momentum takes values $L_z = N(2k + 1)/2$ ($k = 1, 2, \ldots$). If the permutation is even, one has $\exp(i\frac{2\pi}{N}L_z)\Phi_r = \Phi_r$. As a result, the lowest quantum states carry the magic orbital momenta $L_z = Nk$ ($k = 1, 2, \ldots$) (see also [15]). We recall, however, that the classical configuration ($R_W \gg 1$) can contain a few rings (see Fig.2). In this case the magic numbers can be determined by the number of electrons in
the external or in the internal rings starting from the orbital momentum $L^{(MDD)}_z$ of the MDD phase. For nonzero magnetic field this number must obey also the condition Eq.(6) (see below). Although for different strengths $R_W$ the HF results provide different sequence of the total orbital momentum for the ground states, we found that these sequences are subject to this rule at a nonzero magnetic field.

The total energy for the Hamiltonian (1) can be written in the following form

$$E_N = \left\langle \sum_{i=1}^N \left( \frac{p_x^2 + p_y^2}{2m} + \frac{m}{2}(\omega_0^2 + \omega_L^2) r_i^2 + \omega_L \ell_i \right) \right\rangle + \langle V_C + g^* \mu_B B S_z \rangle, \quad (5)$$

where $\omega_L = \omega_c/2$ and $\langle \ldots \rangle$ means a mean field value. For a nonzero magnetic field we have a sequence of different energies for a fixed value of the total orbital momentum $L_z$. In virtue of Hellman-Feynman theorem, we obtain for the lowest equilibrium state for a fixed value of the the total orbital momentum $L_z$ at a given magnetic field

$$\frac{\partial E_N}{\partial \omega_L} \bigg|_{L_z=L} = 0 \quad \Rightarrow \quad L_z = \left\langle \sum_{i=1}^N \ell_i \right\rangle = -m \omega_L \left\langle \sum_{i=1}^N r_i^2 \right\rangle = -\omega_L \Im \quad (6)$$

Since the moment of inertia $\Im \sim R_W^{2/3}$, one obtains an estimation for the optimal sequence of values of the ground state orbital momentum $L_z$ at different values of the magnetic field ($\omega_L$) and for different values of the Wigner parameter $R_W$ ($\Im$) (see Fig.2).

**Figure 3.** The addition energy $E_{add}$ as a function of the magnetic field $B$ and the strength parameter $R_W$. The values of $E_{add}$ at different values of the magnetic field: $\cdots$ line connects the maxima $\bullet$ for $B = 0$ T; $\cdots$ line connects the maxima $\triangledown$ for $B = 2$ T; $\cdots$ line connects the maxima $\blacksquare$ for $B = 15$ T; a thick line displays the classical limit.
While the electron-electron interaction is important for the explanation of spin and orbital ground-state oscillations of QDs in the magnetic field (cf [11]), for small number of electrons the confinement energy may become prevalent over the Coulomb energy [12], indeed. To investigate the evolution of the shell structure, we calculate the addition energy for the QD up to $N=20$ electrons at different values of the strength parameter $R_W$ and the magnetic field $B$ (see Fig.3). At $R_W = 0$ (noninteracting case) one observes a strong shell structure effects for $B = 0$ and 2 T. For $B = 0$ T the magic numbers (including spin) turn out to be the usual sequence of the two-dimensional isotropic oscillator, that is 2, 6, 12, 20 [5, 6]. For $B = 2$ T we find new shells as if the confining potential were be a deformed harmonic oscillator without a magnetic field. The magic numbers are 2, 4, 8, 12, 18. In this case shell structure occurs whenever the ratio of the two eigenmodes of the Hamiltonian (1) (without the Zeeman term) $\Omega_{\pm} = \Omega \pm \omega_c/2$ is a rational number with a small numerator and denominator [13]. With the increase of the interaction strength $R_W = 0.8$ the shell structure survives only without the magnetic field. The magnetic field compresses the energy gaps between energy levels forming the Hall liquid. At relatively large $R_W = 5$ one observes the onset of the classical limit (Thomson model) [14]. We recall that the classical limit can be reached also at a high magnetic field but a relatively small $R_W$. In the classical limit, the total energy for one-ring equilibrium configuration is

$$E^c_N = (3/8) (2R_W S_N)^{2/3} N \hbar \omega_0, \quad S_N = \sum_{j=1}^{N-1} \frac{1}{\sin \frac{\pi}{N} j}. \quad (7)$$

While the quantum shell structure diminishes, one observes the onset of the classical shell structure (see Fig.3) due to an optimal packing of electrons in various two-dimensional rings with $R_W \gg 1$. In the classical limit one has, for example, the following sequences of rings: $N = 6 \Rightarrow (1, 5),..., N = 10 \Rightarrow (2, 8),..., N = 20 \Rightarrow (1, 7, 12)$ [14].

4. Summary
We developed an efficient, numerically stable HF procedure and compare our results with available experimental and theoretical results [8]. We found that, in order to reproduce the experimental data, the screening of the effective electron-electron interaction in the HF approach should be decreased with the increase of the magnetic field. Based on our procedure, we have shown that the effective interaction gives rise to dynamical symmetries of $N$-electron QDs ($N \leq 20$). These symmetries manifest themselves as near-degeneracies in the quantum spectrum and produce maxima in the addition spectra for specific electron numbers at specific values of the magnetic field. Varying the effective strength parameter $R_W$ and the strength of the magnetic field we discuss the evolution of the localized states, formed in the ground state, from $N = 2$ to $N = 20$ electrons. The increase of the magnetic field strength and/or the effective electron-electron interaction strength diminishes the quantum shell structure and gives rise to the classical shell structure produced by an optimal packing of electrons in two-dimensional QDs. We propose a transparent recipe to determine the ground state orbital momenta at arbitrary values of the magnetic field and the strength of the effective Coulomb interaction.

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