Magnetic-field-induced binding of few-electron systems in shallow quantum dots

B. Szafran, S. Bednarek
Faculty of Physics and Applied Computer Science,
AGH University of Science and Technology, PL-30059 Kraków, Poland

F.M. Peeters
Departement Fysica, Universiteit Antwerpen, Groenenborgerlaan 171, B-2020 Antwerpen, Belgium
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Binding of few-electron systems in two-dimensional potential cavities in the presence of an external magnetic field is studied with the exact diagonalization approach. We demonstrate that for shallow cavities the few-electron system becomes bound only under the application of a strong magnetic field. The critical value of the depth of the cavity allowing the formation of a bound state decreases with magnetic field in a non-smooth fashion, due to the increasing angular momentum of the first bound state. In the high magnetic field limit the binding energies and the critical values for the depth of the potential cavity allowing the formation of a bound state tend to the classical values.

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Quantum dots (QDs) formed by weak confinement potentials are susceptible to perturbations by external charge defects and interface roughness. The spectra of disordered QDs exhibit complex behavior in an external magnetic field including pairing and bunching of the charging lines, indicating the formation of multiple charged puddles in local potential minima inside the large QD area. In the quantum Hall effect disorder is held responsible for the formation of localized electron reservoirs that allows for the pinning of the Fermi level between the Landau levels. Coulomb blockade of charge confined within these tiny reservoirs in quantum Hall systems have recently been demonstrated through scanning probe measurements. In this paper we consider electrons localized in a nanometer-size reservoir created by a potential fluctuation. The purpose of the present work is to determine the role of the magnetic field in the formation of bound few-electron states.

The present study is related to the problem of the existence of bound excited states of the negative hydrogen ion $H^-$ or charged donor center $D^-$ in a semiconductor. In the absence of a magnetic field the $H^-$ has only one bound state, but an infinite number of weakly bound and arbitrarily extended excited states appears in weak magnetic field ($B \to 0^+$) due to the interplay of the magnetic field induced localization and the attractive force exerted on the extra electron by the neutral atom $H$, or donor $D^0$. This force results from the electrostatic potential of $D^0$ which is attractive everywhere. In two-dimensional quantum wells the $D^0$ potential for the extra electron is repulsive at large distances which prevents the formation of extended excited bound states in the weak magnetic field limit. For off-center $D^-$ in quantum wells magnetic field induces angular momentum transitions are found, well-known from the theory of QDs. States with angular momenta $L > 4$ cease to be bound which results in magnetic field induced $D^-$ evaporation.

In the symmetric gauge the Hamiltonian of the electron in the magnetic field $(0, 0, B)$ contains a diamagnetic term $V_d(x, y) = m\omega_c^2(x^2 + y^2)/8$ similar to the two-dimensional harmonic oscillator potential with the cyclotron frequency $\omega_c = eB/m$. Due to the parabolic form of $V_d$ one often assumes that a strong magnetic field overcomes the Coulomb repulsion between the electrons and makes them orbit around the center of mass even in the absence of an external confinement potential. Below we demonstrate, that although indeed the magnetic field facilitates the binding of few-electron states, even in the $B \to \infty$ limit a finite external potential is necessary to stabilize the system. Moreover, we show that the potential parameters stabilizing the system in the $B \to \infty$ limit can be determined using classical physics.

For the purpose of the present study we need a confinement model realistic enough to account for the unbound states. We choose the QD model of a shallow two-dimensional Gaussian well. The Gaussian potential is not only the simplest choice but is also realized in vertical QDs with small gates. The discussed physics is not limited to a Gaussian potential and is independent of the specific choice of the confinement provided that it has a finite size and depth. A weak magnetic field induces an infinite number of single-electron states weakly bound in the cavity. On the other hand the binding of extended two-electron states at weak magnetic fields is excluded since the second electron outside the cavity perceives only the Coulomb repulsion of the electron bound in it. In this paper we look for the effect of the magnetic field that overcomes the Coulomb blockade and allows binding of additional electrons in the cavity. This effect can, for example, be used to entangle spins of the electrons localized in the cavity and the unbound electrons.

Hamiltonian of a single electron with the magnetic
field \((0,0,B)\) perpendicular to the plane of confinement reads (symmetric gauge), \(H = -\hbar^2 \nabla^2 / 2m + V_d(x,y) - \frac{\mu B}{2\hbar} (x\partial / \partial y - y\partial / \partial x) + V(x,y)\), where \(m\) stands for the effective band mass (GaAs material parameters are used) and \(V(x,y) = -V_0 \exp(-(x^2 + y^2)/R^2)\) is the potential well of depth \(V_0\) and radius \(R\) (for the numerical calculations we take \(R = 50\) nm). In the absence of the confinement \((V = 0)\) the diamagnetic term \(V_d(x,y)\) induces localization of the single-electron wave functions, but by itself it can not keep several electrons together, since the Hamiltonian eigenstates can be localized anywhere. In particular the lowest Landau level (LLL) eigenfunction (with eigenenergy \(E_{LLL} = \hbar \omega_c/2\)) can be put in the form \(\Psi_{LLL}^{(X,Y)}(x,y) = (\alpha/2\pi)^{1/2} \exp(-\alpha/4)((x-X)^2 + (y-Y)^2) + \alpha B/2m(xY - yX)\), where \((X,Y)\) is the arbitrary center of the Landau orbit and \(\alpha = eB/\hbar\).

![Diagram](image)

**FIG. 1**: (color online) Binding energy of two-electron system vs potential well depth for \(B = 0\) and \(5T\). Solid lines were calculated using the multicenter basis (the inset shows the choice of centers, \(d\) is a variational parameter) and the dashed lines with the finite-difference scheme. Arrow indicates where the ground state angular momentum \(L\) changes.

We studied the dissociation of the two-electron confined system using the multicenter configuration interaction approach \(17\), tailored in a way to account for both the bound and unbound states of the two-electron system. The single-electron states were obtained in the basis of the \(\Psi_{LLL}^{(X,Y)}\) wave functions \(17\) in which the positions of the centers \((X,Y)\) as well as exponents \(\alpha\) are treated as variational parameters. The basis generates also the excited Landau levels and allows for a precise solution of the few-electron Schrödinger equation \(17\). We put 15 centers inside the dot (see: inset to Fig. 1) and a single center localized far away from the dot (at a distance of \(l = 2\) cm). The method ejects an electron from the dot into the LLL localized around the distant center when the two-electron dot-confined system is not bound. For the unbound \(N\) electron states the binding energy \(E_B(N) = E_N - (E_{N-1} + E_{LLL})\) is not negative. Note, that the binding energy is the chemical potential \(\mu_N = E_N - E_{N-1}\) of the \(N\)-electron system determining the single-electron charging of the QD devices calculated with respect to the LLL \(E_B(B) = \mu_N - E_{LLL}\).

The calculated binding energies are plotted in Fig. 1 by the thick solid lines as function of the depth of the well. For \(B = 0\) the two-electron system becomes bound in the \(L = 0\) state near \(V_0 = 5.75\) meV. For \(5T\) binding appears for a shallower well with \(V_0 = 4.2\) meV, and the first bound state has \(L = 4\).

To verify these results, we used an alternative approach \(18\) using single-electron wave functions diagonalized numerically on a finite-difference mesh. The method \(18\) allows for an exact description of states localized in a circular potential of arbitrary profile, but does not account for the delocalized LLL’s since the calculations are performed within a box of finite size. The results are shown by the dashed lines in Fig. 1 and agree very well with our previous approach. Above the dissociation threshold \(E_B = 0\) the dashed lines become positive due to the absence of the distant LLL in the basis \(18\). The critical \(V_0\) value is well reproduced. For \(B = 0\ T\), the finite difference approach works better than the multicenter basis (see Fig. 1), because it better describes the tails of the wave functions for weakly bound states, which in the absence of a magnetic field can be arbitrarily long. In the following we give the results as obtained with the finite difference method \(18\).

![Diagram](image)

**FIG. 2**: (color online) Binding energy of the two-electron system vs the \(B\) for depth of the potential from \(V_0 = 7\) meV (lowest curve) to 4.18 meV (highest curve). Horizontal dashed lines show the binding energies of the classical system. The energy cusps due to the angular momentum transition are linked by the thin solid lines. The dotted curve shows the binding energy of the state with \(L = 3\) for \(V_0 = 5.4\) meV.

The two-electron binding energy as function of the magnetic field is plotted in Fig. 2 for various depths of the dot. The two electrons are bound for any \(B\) when \(V_0 = 6\) meV, or more. The bound ground state undergoes interaction-induced angular momentum transitions \(11\). The interaction energy increases with increasing magnetic field till it reaches a value at which the transi-
tion to a more weakly localized state of lower interaction energy is more favorable. At high magnetic fields the angular momentum transitions [11] keep the size of the system close to the size of its classical counterpart [19]. The angular momentum transitions are associated with the ground-state spin oscillations. States with even $L$ correspond to spin singlets ($S = 0$), and those with odd $L$ to spin triplets ($S = 1$).

For $V_0 = 5.4$ meV bound states appear only in the presence of an external magnetic field (see Fig. 2). Notice that, for shallower QDs the first bound state has non-zero $L$. We found that states of specific $L$ are bound only within a finite interval of the magnetic field (see the binding energy for $L = 3$ at $V_0 = 5.4$ meV plotted by the dashed line).

The horizontal dashed lines in Fig. 2 show the values of the binding energies obtained for classical point charges [13, 20], via minimization of the two-electron potential energy $E_B^{\text{class}} = \frac{e^2}{4\pi\epsilon_0 w} - 2V(w/2, 0)$ with respect to the interelectron distance $w$. The quantum binding energies tend to the classical values at high $B$. This is shown clearly when we plot the difference between the quantum and classical values as function of the inverse of the magnetic field (see Fig. 3). We conclude that the binding energy tend as $1/B$ to the classical value in the limit of high magnetic fields [21]. The classical character of the binding is due to the point localization of the single-electron LLL wave functions in the high magnetic field.

The cusps of the three-electron binding energy are due to both the $N = 3$ and $N = 2$ angular momentum transitions (cf. Fig. 4). The $1/B$ convergence of the binding energy to the classical limit is also found for three electrons (see Fig. 5).

Fig. 6 shows the 'phase diagram' for the maximum number of bound electrons as function of the well depth and the magnetic field. The thin lines joining the cusps of the phase diagram boundaries corresponding to $N = 2$ angular momentum transitions. The cusps related to the $N = 3$ angular-momentum transitions are marked with arrows. Dashed lines show the depth of the potential well which allows binding of the second and third classical electron [20]. In Fig. 7 we plot the phase diagram as function of $1/B$ to demonstrate the convergence of the phase boundaries to the classical result at infinite magnetic field.

In an external magnetic field the diamagnetic effect increases faster the free-electron LLL than the energies of the states localized in the cavity. This leads to the energy shift of the ionization threshold observed in a magnetic field. According to our results the magnetic field induces the formation of bound electron states in QDs. Such a formation was actually observed in single-electron charg-

![FIG. 3: (color online) Binding energy of the two-electron system vs the inverse of the magnetic field for three values of the potential depth. Horizontal dashed lines show the binding energies of the classical system. The energy cusps corresponding to the angular momentum transitions in the three- (two-) electron ground state are linked by thin solid (dotted) lines. The numbers below the lowest curve list $L$ for $N = 3$.](image1)

![FIG. 4: (color online) Binding energy of the three-electron system vs the magnetic field for three values of the potential depth. Horizontal dashed lines show the binding energies of the classical system. The energy cusps corresponding to the angular momentum transitions in the three- (two-) electron ground state are linked by thin solid (dotted) lines. The numbers below the lowest curve list $L$ for $N = 3$.](image2)

![FIG. 5: (color online) Same as Fig. 3 but for $N = 3$. The thin dashed straight lines are given by $6.6/B$, $5.4/B$ and $4.1/B$.](image3)
One needs a cavity which at gas charging (like the one of Fig. 3 Ref. [22]). The shape of the confinement potential is exactly Gaussian for a thin dashed straight lines are given by $V_N^{\text{class}} + A_N/B$, with $V_2^{\text{class}} = 4.073 \text{ meV}$, $V_3^{\text{class}} = 8.245 \text{ meV}$, $A_2 = 0.7$, $A_3 = 5$. The discussed effect can be used to entangle electron spins [14]. One needs a cavity which at $B = 0$ binds only a single electron. The second electron is bound by the field and one can arrange for the bound state to have zero spin (even $L$). After the magnetic field is switched off the second electron will become unbound and is repelled by the dot and thus goes with its spin state entangled with the localized electron.

In summary, we have shown that a strong magnetic field induces the formation of bound few-electron states in potential cavities that are deep enough to bind the classical point electrons.

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