Confinement-induced depletion of the enhanced *g*-factor in quantum wires

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The spin splitting of the electronic subbands in a parabolically confined quantum wire in a strong magnetic field is calculated using the self-consistent Hartree-Fock approximation. The effective *g*-factor and the critical density at which the subbands become almost spin-degenerate are determined. The results are compared with recent experimental data.

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I. INTRODUCTION

At high magnetic field the energy spectrum of noninteracting electrons in electron inversion layers in semiconductor heterostructures consists of Zeeman split, disorder broadened Landau bands. In AlGaAs/GaAs the corresponding Landé *g*-factor can be much larger than the bulk value ($g=-0.44$) and it decreases with increasing electron concentration.[1–3] This is assigned to electron exchange interaction. When the electron density is varied such that the Fermi energy traverses a Landau band, the Zeeman splitting acquires a maximum when only the energetically lower band (with spin $s=\uparrow$) is occupied. Then, the exchange energy of the electrons will dominate, and the occupied band will be shifted to lower energy.

Confining the two-dimensional electron system (2DES) in lateral direction it forms a quasi-1D electron system. The degeneracy of the Landau levels is lifted due to the confinement. Still, the enhancement of the Zeeman splitting is present although the Landau subbands corresponding to the two directions of the spin overlap at high energies. For high electron density ρ, such that the partial densities $\rho_\uparrow \approx \rho_\downarrow$, and there is no spin polarization, the Zeeman splitting is close to the bulk value. However, for densities below some crossover value $\rho < \rho_c$, only the lowest spin polarized subband will be occupied at temperatures close to zero. Due to the alignment of the spins, the exchange interaction will decrease the energy and enhance the Zeeman splitting. Eventually, all of the electrons will only occupy the polarized state. It has been suggested that this is similar to a quantum phase transition.[4] Such effect has been observed in magnetotransport measurements done on GaAs/AlGaAs quantum wires[5] and on narrow silicon inversion channels.[6]

In previous works on the 2DES[1,3] and quantum wires[4,7] the Hartree contribution to the self-energy has been neglected. However, for quantum wires, it has been shown that the Hartree term is very important for quantitatively estimating the energy dispersion and the self-consistent potential.[8] Then, one can expect that this must influence ρ_c and change the *g*-factor. It is indeed not clear whether the *g*-factor enhancement in a quantum wire is similar to a phase transition or must be considered as a simple crossover, even at zero temperature.

In this paper, we address this question by using the self-consistent Hartree-Fock method. We find that the spin independent Hartree term supports the polarizing effect of the exchange interaction and assists to force the system into the polarized state.[11,12]

We compare the results with magnetocapacitance experiments[9] in which ρ_c and the Zeeman splitting have been estimated. Within experimental errors, the Hartree-Fock results can be fitted reasonably well to the experimental data if the interaction is assumed to be exponentially screened. In contrast to the earlier suggestions[4,7] we find a smooth crossover from the polarized to the unpolarized state. Our results indicate that correlation effects beyond mean field are likely to be important for understanding the *g*-factor in nanostructures.

II. THE MODEL

The interacting 2DES in a perpendicular magnetic field, parabolically confined to 1D, is described by the Hamiltonian $H=H_0+H_i$ where

$$H_0^s = \frac{1}{2m}\sum_{i=1}^{N}\left[(\mathbf{p}_i - e\mathbf{A})^2 + \frac{m}{2}\omega_0^2 x_i^2 + \frac{s}{2}g\mu_0 B\right] \qquad (1)$$

with the vector potential $\mathbf{A}=(0,Bx,0)$, the effective mass m, the confinement frequency ω_0, and $s=\pm 1$ the spin directions. We model the interaction $H_i=\Sigma_{i<j}V(\mathbf{r}_i-\mathbf{r}_j)$ with a Yukawa potential $V(r)=V_0\exp(-\kappa r)/r$ with $V_0=e^2/4\pi\epsilon\epsilon_0>0$ and a screening parameter κ, rather than treating the screening within a time-dependent Hartree-Fock calculation.[12] In our model for the interaction, the screening length is independent of the density. To compensate this somewhat artificial form of the screened Coulomb interaction, we define κ empirically from comparison with experimental data.[9] We do not consider edge stripe reconstruction effects which become relevant in wider quantum wires.[13–15]

The eigenvalues of the noninteracting part H_0

$$\varepsilon_{nk}^s = \hbar\Omega\left(n+\frac{1}{2}\right) + \frac{\hbar^2k^2}{2m(B)} + \frac{s}{2}g\mu B \qquad (2)$$

consist of the discretization energy due to the confinement and the magnetic field, the kinetic energy in the nonconfined *y*-direction, and the Zeeman contribution. Periodic boundary conditions in *y*-direction imply wave numbers $k_j=2\pi j/L_y$ (integer j, wire length L_y). The effective mass $m(B)=m\Omega^2/\omega_0^2$ contains the renormalized frequency Ω

$=\sqrt{\omega_0^2+\omega_B^2}$ ($\omega_B=eB/m$ cyclotron frequency). It diverges in the quantum Hall limit, $B\to\infty$. The corresponding wave functions $\langle x,y|nk\rangle=L_y^{-1/2}\exp(-iky)\chi_n(x-X_k)$ contain the states χ_n of the 1D harmonic oscillator at position $X_k=k\ell^2A$ with the characteristic length $\ell=\sqrt{\hbar/m\Omega}$ and $A=\omega_B/\Omega$.

III. HARTREE-FOCK EQUATIONS AND *g*-FACTOR FOR THE QUANTUM WIRE

The Hartree-Fock equations in Landau representation

$$\sum_{n'k'}\langle nk|(H_0^s+F^s)|n'k'\rangle c_\alpha^s(n'k')=E_\alpha^s c_\alpha^s(nk) \tag{3}$$

determine the expansion coefficients $\langle nk|\alpha s\rangle=c_\alpha^s(nk)$ of the electron states and the eigenenergies E_α^s. The size of the basis in a Landau level is determined by the degeneracy $N_\phi=L_xL_y/2\pi\ell^2$. We use indices i,j,a,b for labeling the basis states. The Fock matrix is

$$F_{ij}^s=\sum_{ab}\rho_{ab}M_{ijab}+\sum_{ab}\rho_{ab}^s M_{ibaj}, \tag{4}$$

with interaction matrix elements

$$M_{ijab}=\int d\mathbf{q}V(q)\langle i|e^{i\mathbf{q}\cdot\mathbf{r}}|j\rangle\langle a|e^{-i\mathbf{q}\cdot\mathbf{r}}|b\rangle \tag{5}$$

and density matrices

$$\rho_{ab}^s=\sum_{\alpha(\mathrm{occ})^s}c_{\alpha(\mathrm{occ})}^{s*}(a)c_{\alpha(\mathrm{occ})}^s(b). \tag{6}$$

Here, α(occ) denotes the label for the occupied states with an energy below the Fermi level, $E_{\alpha(\mathrm{occ})}<\epsilon_\mathrm{F}$.

Furthermore, $\langle i|e^{i\mathbf{q}\mathbf{r}}|j\rangle=\langle nk|e^{iqx}|n',k'\rangle\delta_{q_y,k-k'}$,

$$\langle nk|e^{iqx}|n'k'\rangle=e^{-[|q_A|^2+iq(k+k')A]\ell^2/2}\times\sqrt{\frac{m}{n}}\left(\frac{q_A\ell}{\sqrt{2}}\right)^{m-n}L_n^{m-n}\left(\frac{|q_A|^2\ell^2}{2}\right), \tag{7}$$

with $q_A=iq-\mathrm{sgn}(n-n')(k-k')A$, $n=\mathrm{Min}(n,n')$, $m=\mathrm{Max}(n,n')$, and L_n^{m-n} the associated Laguerre polynomials.

The single particle energies $E_\alpha^s=\epsilon_\alpha^s+\Sigma_\alpha^s$, obtained by solving Eq. (3) self-consistently, contain the self-energy

$$\Sigma_{\alpha s}=\sum_{ij}F_{ij}^s c_\alpha^{s*}(i)c_\alpha^s(j)\equiv\Sigma_\alpha^H+\Sigma_{\alpha s}^F \tag{8}$$

with Hartree and Fock terms, Σ_α^H and $\Sigma_{\alpha s}^F$, respectively.

In the self-consistent Hartree-Fock method the charge distribution in the system is determined by searching for the electronic configuration for which the ground state energy

$$E_\mathrm{g}=\sum_{ab}\rho_{ab}^s(H_{0,ab}^s+F_{ab}^s) \tag{9}$$

is minimized. This implicitly determines the spin polarization

$$\gamma=\frac{\rho_\uparrow-\rho_\downarrow}{\rho_\uparrow+\rho_\downarrow}=\frac{\delta\rho}{\rho} \tag{10}$$

with

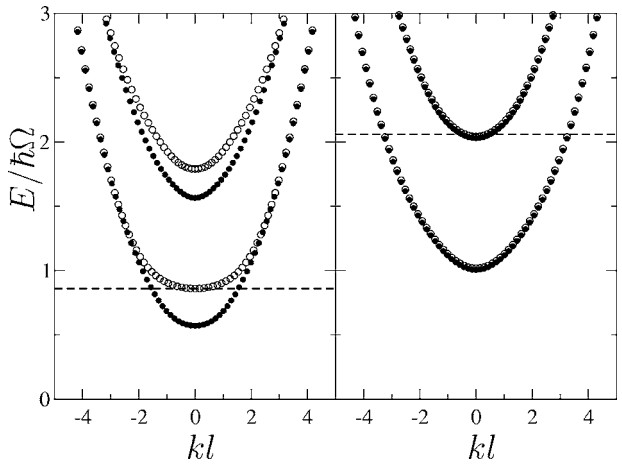

FIG. 1. Hartree-Fock energies of a quantum wire in a magnetic field for the four lowest subbands at densities where the second (spin ↓, left) and third (spin ↑, right) subbands start to be occupied (bullets: $s=\uparrow$, circles: $s=\downarrow$, dashed: Fermi level).

$$\rho_s=\sum_{\alpha(\mathrm{g})}\sum_{nk}|c_\alpha^s(nk)|^2, \tag{11}$$

where α(g) denotes the labels of the occupied states after reaching self-consistency.

The effective *g*-factor is defined by

$$g^*=g(k=0)=g+\frac{\Sigma_{\alpha(k=0)\uparrow}-\Sigma_{\alpha(k=0)\downarrow}}{\mu_0 B}. \tag{12}$$

This coincides with the definition of the optical *g*-factor in Refs. 3, 7, and 12 and, evaluated at the band center $k=0$, maps the quantity obtained in the experiment.[9] The self-consistent numerical solution of the Hartree-Fock equations requires a truncation of the complete othonormal set $|nk\rangle$. This is done by defining a cutoff wave number k_max via $X_{k,\mathrm{max}}=k_\mathrm{max}l^2=L_x$. The integral over q_x in M_{ijab} [Eq. (5)] is approximated by a sum over discrete wave numbers $q_x=2\pi n_x/w$ with $w\gg L_x$ and n_x integer. We have achieved convergence for the integrals, spectra, and the wave functions for $w>50L_x$ and $-w/l<n_x<w/l$. For obtaining the results described in the following we have used $w=100L_x$.

For electron numbers such that the Fermi energy is located in the second Landau level, there are states with low wave numbers at approximately the same energies as states with high wave numbers of the lower Landau levels (Fig. 1). In order to treat these correctly, inter-Landau level interaction matrix elements have to be taken into account. The maximum system size L_x depends then on the number of Landau levels included and the confinement strength. We have estimated $X_{k,\mathrm{max}}$ by using the spectrum of noninteracting electrons. We have done calculations for increasing $L_x>X_{k,\mathrm{max}}$ until the eigenenergies became insensitive to the value of L_x. The system length L_y was used to adjust the size of the basis, independently of L_x, but always $L_y>L_x$.

We have assumed that convergence of the self-consistent Hartree-Fock procedure was achieved when $\Delta\rho/\rho<10^{-7}$ with $\Delta\rho$ the difference between the densities $\rho=\rho^\uparrow+\rho^\downarrow$ corresponding to successive interations. In all of the results

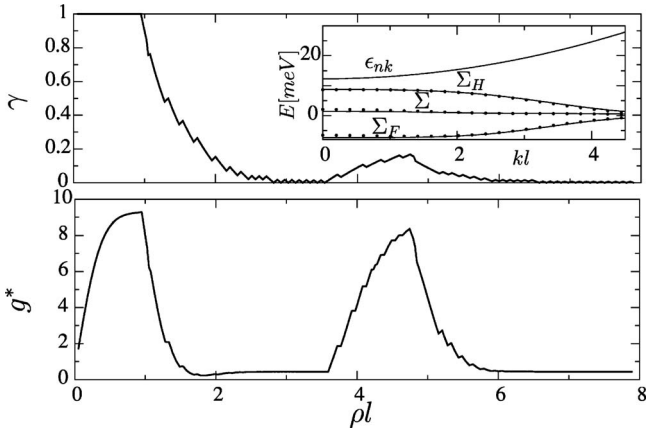

FIG. 2. Spin polarization γ (top) and effective g-factor g^* (bottom) as functions of the density ρ obtained from the self-consistent Hartree-Fock method taking into account the three lowest Landau bands (parameters: $B=14$ T, $\hbar\omega_0=6$ meV, $\rho_c=1.1/l$ in the lowest subband, screening parameter $\kappa=2/l$). Inset: Energy $\epsilon(k)$ (dashed) in the noninteracting limit; self-energies Σ, Σ^F (Fock), and Σ^H (Hartree) at ρ_c, respectively, as functions of the wave number kl; solid: perturbative, bullets: self-consistent results.

shown below, the electronic energies have converged within a relative error of 10^{-3}. Due to the translational invariance in the y direction k is a good quantum number for the Hartree-Fock states.

IV. RESULTS

Figure 1 shows the energy dispersions of the four lowest subbands for different electron numbers. The dispersions keep a more or less parabolic shape similar to the noninteracting system. If the electron density is small such that only energy levels in the lowest subband (spin $\uparrow$) are occupied, the Zeeman splitting is large. With increasing density the second subband (spin $\downarrow$) becomes occupied. Then, the Zeeman splitting decreases until it reaches the bulk value. This is periodically repeated when higher spin subbands are occupied.

In order to identify the roles of the Hartree and the Fock parts of the self-energy, we consider the lowest subband ($n=0,\uparrow$). In a strong magnetic field, both Fock and Hartree terms depend on the wave number. The Hartree energy is of the same order as the Fock energy, but of opposite sign. The total interaction energy Σ is then much smaller than the absolute values of Σ^H and Σ^F. The latter are comparable to the kinetic energy ϵ_k (Fig. 2). This suggests that for determining the crossover density one can replace the self-consistent Hartree-Fock approximation by lowest-order perturbation theory.[4] The result for the lowest subband is

$$\Sigma_k^H = \frac{2V_0}{\sqrt{2}l}\sum_s \int_{Q_-}^{Q_+} dk' \int dq \frac{e^{-[q^2 - iAqk']}}{\sqrt{q^2+q_\kappa^2}}, \tag{13}$$

$$\Sigma_{ks}^F = -\frac{V_0}{\pi\sqrt{2}l}\int_{Q_-}^{Q_+} dk' e^{-[(2A^2-1)k'^2 - q_\kappa^2]/2} K_0[(k'^2+q_\kappa^2)/2], \tag{14}$$

where $Q_\pm = l(k \pm k_{Fs})/\sqrt{2}$, $q_\kappa = \kappa l/\sqrt{2}$, and $K_0(z)$ is a modified Bessel function.

In 2DES the Hartree term is often neglected. It is argued that it yields only a constant shift of the energy scale.[1,3] Intuitively, one would neglect it also for the quasi-1DES.[4,7,10] However, for a quantum wire in a strong magnetic field the wave number is associated with a transversal position $X = kl^2$. At zero temperature, in the totally polarized state, $\rho_\uparrow = \rho$ and $\rho_\downarrow = 0$, when only the lowest subbands are occupied with electrons, additional electrons will occupy states with wave numbers near the Fermi wave number $k_{F\uparrow} = \pi\rho_\uparrow$. These have to be added near the edge of the wire, $|x_{F\uparrow}| = k_{F\uparrow} l^2$ (Fig. 1) thus minimizing the electrostatic repulsion. However, if the spin-$\downarrow$ subband starts to become occupied, additional electrons would be added at smaller wave numbers in the center of the wire, near the minimum of $E_\downarrow(k)$ where the electron density is large. This would lead to a strongly repulsive energy contribution. Thus it is energetically favorable to continue with the occupation of the states near the edges in the lowest subband before occupying the states in the second subband. The crossover density ρ_c is increased and it is due to the avoided Hartree energy—*supporting, not compensating* the Fock energy—that the system remains in the totally polarized state.

Figure 2 shows results for the Zeeman splitting averaged over the wave number as a function of the mean electron density ρ. In a given Landau level, g^* increases with increasing density until the upper spin subband starts to become occupied. Then, at crossover density ρ_c, $g^*(\rho)$ starts to decrease. The oscillating behavior of g^* is accompanied by oscillations in the spin polarization γ. For $\gamma \approx 0$, $g^* \approx g$. In the lowest subband, the crossover density ρ_c, at which the g-factor starts to decrease, agrees within 10% with the result obtained in lowest order perturbation theory. Taking into account the Hartree term, the crossover to the bulk value is smooth, in contrast to the case when only the Fock term is considered.[4] This is consistent with a recent theory taking edge state correlations into account.[12] It was found in that theory that the collapse of the g-factor can be understood in two scenarios, the first without any, the second with strong redistribution of charges, making the inclusion of the Hartree term essential.

The influence of the screening length on ρ_c is shown in Fig. 3. The crossover density decreases with increasing κ. As expected, the self-energy decreases with decreasing interaction range. For comparison with experiment we assume $\kappa = 2/l$. This turns out to reproduce the experimental findings reasonably well.

V. COMPARISON WITH EXPERIMENTAL RESULTS

The crossover density in the lowest subband as a function of the confinement energy has been determined from measurements of the capacitance of a quantum wire in a strong

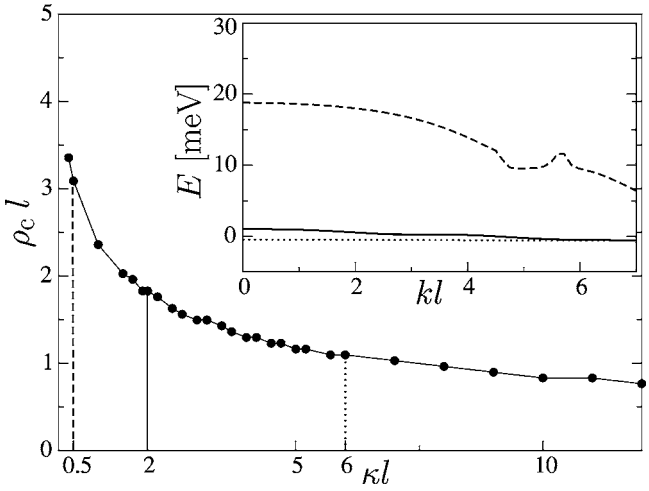

FIG. 3. Crossover density as a function of the screening length κ^{-1}. Data points: self-consistent Hartree-Fock approximation with $B=14$ T, $\hbar\omega_0=6$ meV in the lowest subband; wire width 16 l and wire length 50 l. Inset: self-energy with $\kappa=0.5/l$ (dashed), $\kappa=2.0/l$ (full), and $\kappa=6.0/l$ (dotted).

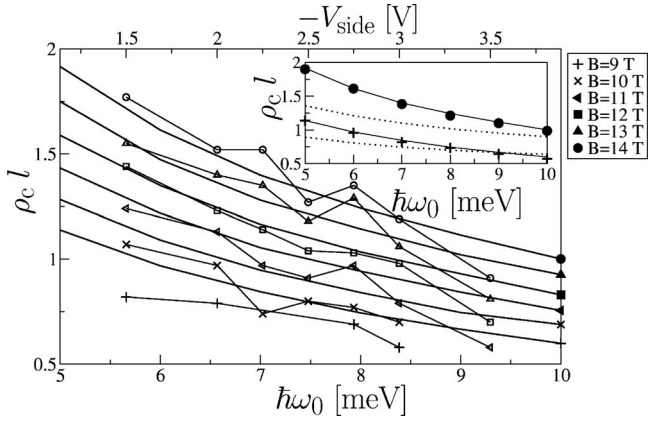

FIG. 4. Crossover density ρ_c at magnetic fields as indicated as a function of the confinement energy $\hbar\omega_p$. Full lines: Hartree-Fock results with screening length $l/2$; open symbols: experimental data of Ref. 9 corresponding to side gate voltages $V_{\rm side}$ from -1.5 to -4 V. Inset: results for $B=9$ T and $B=14$ T obtained self-consistently (dots), and perturbatively (full lines) compared with the results obtained by neglecting the Hartree term (dashed).

magnetic field.[9] It has been found that the crossover density increases with increasing magnetic field (Fig. 4) and with decreasing the voltage applied to a side gate, $V_{\rm side}$. For estimating the confinement energy $\omega_{\rm exp}$ a parabolic confinement has been assumed. By varying the side-gate voltage from -1.5 to -3.5 V $\hbar\omega_{\rm exp}$ increases from 4.8 ± 0.5 to 6.6 ± 0.7 meV.

The potential, which corresponds to the experimentally determined confinement energy $\hbar\omega_{\rm exp}$, is composed of the parabolic external confinement potential $\hbar\omega_0$ tuned by $V_{\rm side}$ and of the screening potential due to the charge density of the electrons in the wire. The confinement energy $\hbar\omega_0$ in general will be larger than the experimentally determined $\hbar\omega_{\rm exp}$. We assume that the external confining potential dominates such that $\hbar\omega_0 \approx \hbar\omega_{\rm exp}$. It is difficult to obtain the confinement energy from experimental data with high accuracy.[9] We therefore choose a mapping of the measured side gate voltage to the corresponding confinement energy (see Fig. 4), which fits our calculations reasonably well to the experimental data and is consistent with the confinement estimates of Ref. 9 With the screening length $1/\kappa=l/2$ the calculated crossover density ρ_c fits the decrease of experimental data with increasing confinement energy qualitatively (Fig. 4). Neglecting the Hartree term,[4] the dependence of ρ_c on the confinement is considerably weaker even if the screening length is assumed to be ∞ and thus the exchange-enhanced critical density is maximized (Fig. 4 inset).

However, our model does not reproduce the experimental data at very small side gate voltages, $|V_{side}| \leqslant 1$ V. We believe that in this regime the external potential of the wire is modified by impurities and thus cannot be described by a parabolic potential. Also there are quantitative discrepancies between experimental data and the self-consistent theory at smaller magnetic field strength ($B=9$ T). Given the relatively large experimental errors, we did not try to get a better fit. In summary, we confirm the experimentally observed trends, namely that by increasing the confinement energy, i.e., decreasing the effective wire width, and decreasing the magnetic field strength, the crossover density for the enhancement of the Zeemann splitting is depleted considerably.

VI. CONCLUSIONS

In summary, we have calculated the Zeeman splitting of the subbands in a quasi-1D quantum wire in a strong magnetic field by using the self-consistent Hartree-Fock approximation to electrons interacting via a screened Coulomb interaction. We have found that Hartree and Fock parts of the self-energy are of the same order but of opposite sign such that the total self-energy becomes small. We have quantitatively determined the effective g-factor and the spin polarization. When γ vanishes g^* is close to the bulk value while it is strongly enhanced if the spin polarization is close to one. Our results imply that the Hartree term cannot be neglected for the enhancement of the g-factor in quantum wires. Especially, it appears that it plays a crucial role in determining the crossover density quantitatively. By comparing calculated crossover densities with experimental data we have found the dependence on the confinement energy can be reproduced within experimental uncertainties for not too small side gate voltages if the screening length is assumed to be about half of the magnetic length. Since the screening can be viewed as being due to correlations, our results imply that these cannot be neglected for understanding the g-factor enhancement in quantum wires.

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