Spin splitting of subbands in quasi-one-dimensional electron quantum channels

Chuan-Kui Wang and K.-F. Berggren
Department of Physics and Measurement Technology, Linköping University, S-58183 Linköping, Sweden

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We report on self-consistent calculations of the electronic structure of quantum wires with an in-plane magnetic field parallel to the wire. The spin-polarized density-functional theory of Kohn and Sham is used. The self-consistent results show that exchange interactions cause a large subband splitting whenever the Fermi energy passes the subband threshold energies. Full spin polarization appears at low electron densities. The results are consistent with recent observations of a conductance anomaly in a quantum point contact and its interpretation in terms of spontaneous spin polarization of the lowest subband. On the basis of the present model we conjecture that similar conductance anomalies may appear also in the higher subbands at zero magnetic field. Finite magnetic fields tend to suppress the spin polarization induced by exchange interactions. A diamagnetic shift of the subbands is determined and is in qualitative agreement with observations. [S0163-1829(96)51944-2]

New conductance measurements have been carried out for point contacts (QPC) formed at the interface between GaAs and modulation-doped $Al_xGa_{1-x}As$ with an in-plane magnetic field parallel to the current.[1] The measurements show that g^*, the effective g factor, is larger than the value $g=0.44$ of bulk GaAs when only a few subbands are occupied. Even in the absence of a magnetic field there are indications that spin polarization occurs in the lowest subband in the limit of low electron densities. The experimental evidence is a structure in the conductance G that develops at $G\approx 0.7(2e^2/h)$.

As is well known, the homogeneous three- and two-dimensional electron gases are unstable against spin-polarization at low densities because of the domination of exchange over kinetic energy. Quasi-one-dimensional systems should display a similar behavior. Indeed, Gold and Calmels[2] have shown recently that spin polarization can take place in an infinite, cylindrical quantum wire. In their calculation they assumed one-subband occupancy only and self-consistency was not implemented. In the present communication we show how the inclusion of higher subbands and self-consistency will bring about a more complex picture.

Below we present a self-consistent theoretical calculation of the electronic structure of a quasi-one-dimensional, infinite, straight electron channel with an in-plane magnetic field parallel to the channel. Spontaneous spin polarization is found at low electron densities as expected. However, spin polarization is also predicted when the Fermi level E_F evolves through subband threshold energies on increasing density. The reason is that, as the higher subbands become open, new low-density channels are formed repeatedly. At the same time, enhancement of g^* is clearly seen.

We assume that electrons have a free motion in the x direction along the channel and experience an electric confinement in the y direction by, e.g., negative gate voltages. The z direction is perpendicular to the GaAs-$Al_xGa_{1-x}As$ interface. In the modeling we use the density-functional theory of Kohn and Sham.[3] When an in-plane magnetic field B is applied along the x direction, the effective Schrödinger equation can be expressed as

$$\left(\frac{p_x^2+p_y^2}{2m^*}+\frac{(p_z+eBy)^2}{2m^*}+V_{\rm conf}(y)+V_{\rm conf}(z)+V_H+V_{\rm exch}^{\sigma}+g\mu_B B\sigma\right)\psi^{\sigma}(x,y,z)=E^{\sigma}\psi^{\sigma}(x,y,z) \tag{1}$$

where we use the gauge $\mathbf{A}=(0,0,By)$ and $\sigma=\pm 1/2$ is the spin quantum number. $V_{\rm conf}(y)$ and $V_{\rm conf}(z)$ are the bare confinement potentials in y and z directions, respectively. V_H is the Hartree potential and $V_{\rm exch}^{\sigma}$ is the exchange potential. The last term of the Hamiltonian is the Zeeman term.

Since the confinement in the z direction is much stronger than in the y direction, we assume that only the first subband related to the z direction is occupied, and that the energy spacing is large. Therefore we may use the decoupling approximation,

$$\psi^{\sigma}(x,y,z)\simeq e^{ik_x x}\varphi^{\sigma}(y)\phi_1(z). \tag{2}$$

Inserting Eq. (2) in Eq. (1) and averaging over z we have

$$-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial y^2}\varphi_l^{\sigma}(y)+[V_{\rm conf}(y)+V_H(y)+V_{\rm exch}^{\sigma}(y)+V_B(y)+g\mu_B B\sigma]\varphi_l^{\sigma}(y)=E_l^{\sigma}\varphi_l^{\sigma}(y), \tag{3}$$

and

$$E^{\sigma}=E_l^{\sigma}+\frac{\hbar k_x^2}{2m^*}. \tag{4}$$

To arrive at this expression we have used $\langle p_z\rangle=0$ because $\phi_1(z)$ is a bound state. The fundamental z-related subband edge is taken as the reference energy. The magnetic field enters through the additional confinement potential

$$V_B(y)=\frac{e^2B^2y^2}{2m^*}. \tag{5}$$

If we let the electrostatic potential be zero at the point $y=y_0$ and perform an integration over x, the Hartree potential can be expressed in the 2D limit as

$$V_H(y) = -\frac{e^2}{4\pi\epsilon_0\epsilon}\int_{-\infty}^{\infty} n(y')dy'\{\ln[(y-y')^2] - \ln[(y_0-y')^2]\}. \quad (6)$$

Here $n(y')$ is defined as

$$n(y') = \sum_{\sigma} n^{\sigma}(y'), \quad (7)$$

where

$$n^{\sigma}(y') = \frac{1}{\pi}\sum_{E_l^{\sigma} \leq E_F}\left(\frac{2m^*}{\hbar}(E_F - E_l^{\sigma})\right)^{1/2} |\varphi_l^{\sigma}(y')|^2 \quad (8)$$

is the electron distribution for all occupied states with spin σ and $\varphi_l^{\sigma}(y')$ is normalized to one. Integration over y' yields the 1D electron density,

$$\sum_{\sigma}\sum_{E_l^{\sigma} \leq E_F}\left(\frac{2m^*}{\hbar}(E_F - E_l^{\sigma})\right)^{1/2} = \pi n_{1d}, \quad (9)$$

which is kept at a given value in the calculations. In the local-density approximation (LDA) the exchange potential energy for a 2DEG is[4]

$$V_{\text{exch}}^{\sigma}(y) = -\frac{e^2}{\epsilon_0\epsilon\pi^{3/2}}[n^{\sigma}(y)]^{1/2}. \quad (10)$$

For a quantum wire defined lithographically by a split gate the bare confinement potential $V_{\text{conf}}(y)$ can, to a good approximation, be represented by the parabolic form,[5]

$$V_{\text{conf}}(y) = \tfrac{1}{2}m^*\omega^2 y^2, \quad (11)$$

where the typical value of $\hbar\omega$ is a few meV.

In our calculation we put $m^* = 0.067m_e$, $\epsilon = 13.1$, which are appropriate values for the GaAs-$Al_xGa_{1-x}As$ interface. Furthermore, we choose $\hbar\omega = 2$ meV and $g = 0.44$ of bulk GaAs. For each given value of n_{1d} we need to find the self-consistent solutions of the effective Schrödinger equation (3) with the subsidiary constraint in Eq. (9). Self-consistency is reached when the Fermi energies E_F in successive iterations are identical within a given numerical accuracy ($\sim 10^{-4}$ meV).

By convention, ‘‘aligned’’ will refer to electrons with spin $\sigma = -\frac{1}{2}$ and ‘‘antialigned’’ to $\sigma = \frac{1}{2}$. Figure 1(a) displays the density dependence of the energy spectra of aligned and antialigned electrons at a constant magnetic field $B = 3$ T.[6] Four features are clear: First, at very low electron densities only the first subband of aligned electrons is occupied, which shows that full spin polarization takes place. This feature seems consistent with the recent measurements[1] indicating the possibility of spin polarization in a QPC at low electron densities. Second, in electron density regimes where the Fermi level crosses a subband threshold energy, the splitting becomes very pronounced. This strong spin splitting is driven by the exchange potential, not by the Zeeman term. In these regions of strong polarization the number of occupied subbands of aligned and antialigned electrons is an odd integer. A similar phenomenon was discussed by Gudmundsson and Pálsson[7] for a strictly 2D circular dot with a perpendicular magnetic field in the quantum Hall regime. Third, at a given density the spin splitting of the occupied states increases with subband index. Fourth, as the number of occupied subbands increases, the spin splitting decreases. This is to be expected as one approaches the 2D limit.

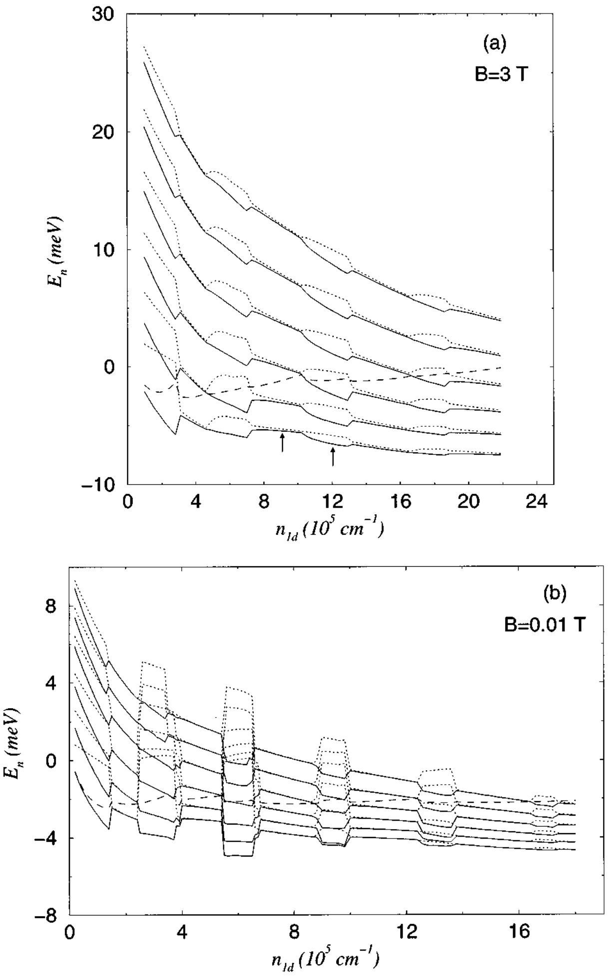

FIG. 1. Sublevels in an infinite, straight quantum wire with a magnetic field parallel to the wire versus the one-dimensional electron density n_{1d}: (a) refers to $B = 3$ T and (b) to $B = 0.01$ T. Dotted lines correspond to antialigned electrons and solid lines to aligned electrons. The dashed line shows the position of the Fermi level E_F. The two arrows in (a) mark the values of n_{1d} for which effective potentials and electron distributions are detailed in Fig. 3.

For comparison we also give the subband energies at a very small value of B. Figure 1(b) shows the results for $B = 0.01$ T. General features are obviously very similar to Fig. 1(a). It is notable, however, that when the Fermi level passes the second and third subband thresholds, *full* spin polarization appears for a range of electron densities. The increase in the polarization at low fields can be understood in the following way. In general, a parabolic confinement favors singlet states.[8] Thus the additional parabolic confinement caused by a magnetic field counteracts the exchange potential that strives for parallel spins. Therefore, reduced spin polarization at increased B is to be expected as shown by Fig. 1(a). However, at low densities, when only one spin-split subband is occupied, this mechanism is not strong enough to make a difference between high and low fields. As a consequence, the state remains fully polarized in both cases as shown by Fig. 1.

For simplicity, let us make the ideal assumption that the system is ballistic. According to Fig. 1(a) one then expects a zero-temperature conductance G that equals $\frac{1}{2},1,\frac{3}{2},2,\frac{5}{2},3,\ldots$ in units of $2e^2/h$. Half-plateaus refer to regions in which exchange interactions give rise to an odd number of occupied subbands. Also at very small (or zero) fields there are regions of strong exchange polarization [Fig. 1(b)]. The conductance is now quite different, however, because the subband filling is not the same as at higher fields. The corresponding conductance is therefore $\frac{1}{2},1,\mathbf{1},2,\mathbf{2},3$, i.e., higher half-values are replaced by integer values ($\frac{3}{2}\rightarrow\mathbf{1},\frac{5}{2}\rightarrow\mathbf{2}$) according to the subband filling in Fig. 1(b). Although there are very narrow regions between strongly polarized and paramagnetic regions, which could exhibit half-plateaus, these regions are likely to be much too narrow to be of experimental relevance.

The measurements in Ref. 1 were made for a QPC which is normally modeled with a saddle potential. This type of constriction is obviously different from our model system and one should be cautious in using our model to interpret the experimental data. On the basis of our calculations we conjecture, however, that full spin polarization can occur in the narrow region of the saddle potential, i.e., the system becomes locally polarized under certain conditions. Consider the case when only a few electrons reside in the saddle region ($G\leqslant 2e^2/h$) and let the field be zero. When polarization sets in spontaneously as density is decreased by sweeping the gate voltage, the effective transmission barrier suddenly becomes different for the two spin directions. The spin-aligned electrons occupying the lowest spin-split subband will conduct current via propagating states in a normal way, while electrons with opposite spins now have to tunnel from source to drain. Thus, when spin polarization occurs at low densities one should expect an anomaly in the conductance. The critical value of the conductance should be equal to or larger than e^2/h, but the exact value may be device dependent. The discussion so far is in line with the interpretation in Ref. 1. Our calculations suggest, however, that conductance anomalies could be observed also in the higher subbands. Above we argued that the spin polarization associated with these subbands cannot be observed in conductance measurements for very long channels. The situation is different for a short constriction like a QPC because of the tunneling mechanism discussed above.

At higher fields the exchange interactions induce an odd number of occupied states in the infinite channel as shown in Fig. 1(a) and half-plateaus are expected as mentioned above. In the case of a QPC, however, the possibility of tunneling brings about a new feature. This is because the spin splitting becomes less with increasing density. Hence, at a constant magnetic field the half-plateaus would narrow and eventually vanish in the limit of many occupied subbands. This behavior is clearly seen in the measured conductance data in Fig. 1 of Ref. 1.

If we interpret the splitting of the subbands as a normal Zeeman spin splitting, $g^*\mu_B B$, with an effective g factor, Fig. 2 shows the variation of g^* for the first subband in Fig. 1(a). The quantity g^* clearly takes peak values whenever the

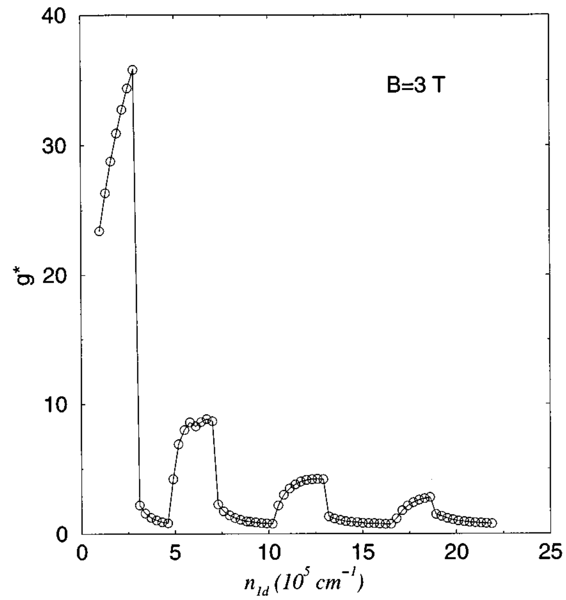

FIG. 2. Effective g factor as a function of electron density n_{1d} for the lowest spin-split subband at $B=3$ T.

number of occupied subbands is an odd integer. The maxima in g^* become lower with increasing density. The average density dependence of g^* is consistent with the measurements in Ref. 1. However, theoretical values are too large. In addition, experiments do not appear to show any structure in g^*, although the resolution appears too limited to draw definite conclusions. In a QPC the exchange polarization takes place only locally and is constrained by the surrounding unpolarized 2D reservoirs. Perhaps it is then natural to expect lower values for g^*.

Effective potentials for different spins and corresponding electron distributions at $n_{1d}=9\times10^5$ cm^{-1} and $n_{1d}=12\times10^5$ cm^{-1} are shown in Fig. 3. The self-consistent results demonstrate that the effective potentials can approximatively be taken as truncated parabolas in agreement with previous simulations.[5] The effect of the magnetic field is to make the well narrower, thereby shifting the sublevels upwards. We have calculated this shift for the lowest level as a function of magnetic field. The self-consistent result is shown in Fig. 4 for $n_{1d}=1\times10^5$ cm^{-1}, where only the lowest subband of the aligned electrons is occupied. The diamagnetic shift causes the transconductance peaks to move to more positive gate voltages. This is consistent with measurements.[1]

In conclusion, using the density-functional theory, we have solved the Kohn-Sham equation self-consistently for an infinite, quasi-one-dimensional electron channel with an in-plane magnetic field parallel to the channel. When the Fermi energy moves across subband threshold energies, exchange interactions cause significant splittings of the subbands of aligned and antialigned electrons. We have also found an enhancement of the effective g factor as a consequence of the electron-electron interactions. Usually phenomena of this kind tend to be exaggerated in the exchange-only approximation. The correlation energy, on the other hand, tends to reduce the imbalance of aligned and antialigned electrons, i.e., the splitting of the subbands. One may ask whether elec-

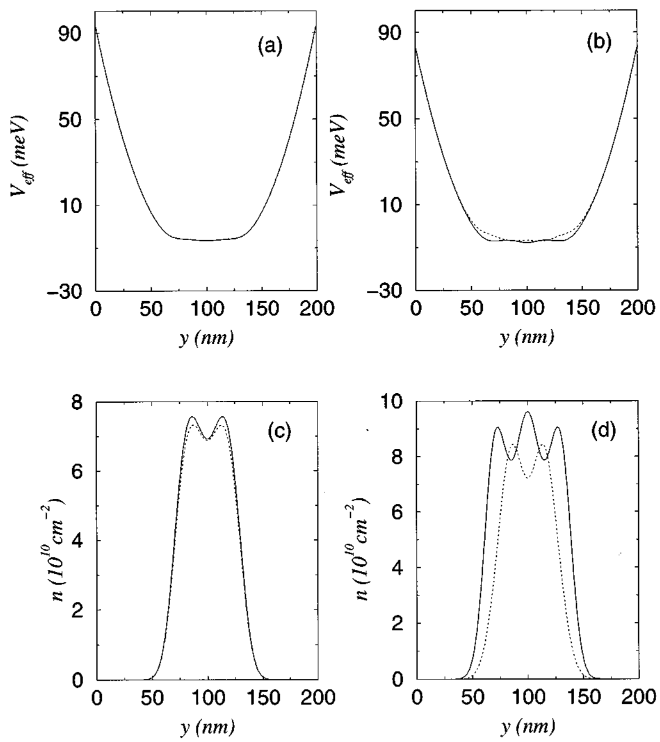

FIG. 3. Curves in (a) and (b) show effective potentials and (c) and (d) corresponding electron distributions for $B=3$ T at $n_{1d}=9\times10^5$ cm^{-2} and 12×10^5 cm^{-2}, respectively [cf. Fig. 1(a)]. Dotted curves are for antialigned electrons and solid curves for aligned electrons.

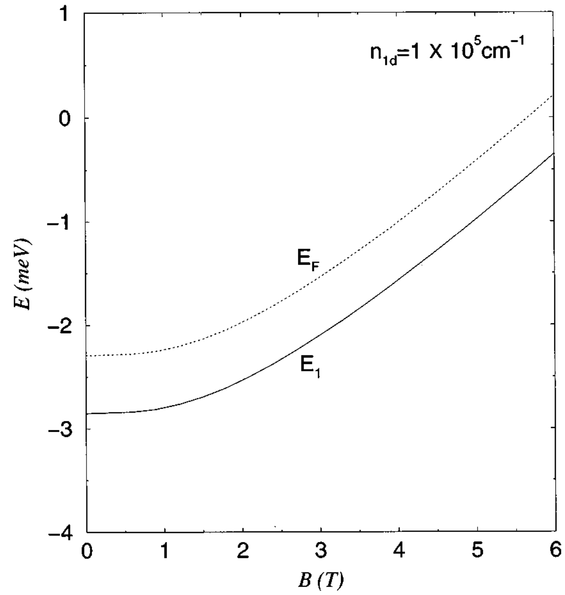

FIG. 4. Diamagnetic shifting of the first subband threshold energy for aligned electrons and the Fermi level as functions of magnetic field at $n_{1d}=1\times10^5$ cm^{-1}.

tron correlation is so important that could it make our findings invalid. To test this point we have included Jonson's 2D correlation potential[9] in the Kohn-Sham equation, Eq. (1). The results show that the correlation energy is much smaller than the exchange energy and is almost a constant in the region occupied by the electrons. The Jonson potential refers to unpolarized systems only. Also Mahan's correlation potential[10] for a fully spin-polarized 2DEG is much too small to bring about any change of physical significance. We therefore conclude that correlation effects are not important in the present case.

Our model for an infinite, straight quantum wire is obviously an oversimplification of a real QPC used in experiments. In spite of this, qualitative agreement with measurements has been reached. The present model should be improved, however, taking the proper geometry of a QPC into account.

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