Exchange interaction in a quantum wire in a strong magnetic field

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We show that, for a sufficiently high number of electrons per unit length, the lateral confinement in narrow wires restores degeneracies that are lifted by exchange effects in two-dimensional systems in a magnetic field. The results are used to explain some experimental observations where the two-probe conductance of a quantum wire was found to be quantized with step size $2e^2/h$.

The increasingly sophisticated microelectronic fabrication techniques have made it possible to study electronic structures of reduced dimensionality. One- and two-dimensional systems have exhibited a wide range of interesting physical phenomena that have attracted a great deal of interest in the past few years. Ever since the discovery of the quantum Hall effect[1,2] both experimentalists and theorists have paid much attention to understanding the behavior of low-dimensional systems in strong magnetic fields. It has been shown that many of the transport properties of these systems can be explained in terms of edge states propagating along the boundaries of the sample.[3-5] We want to study the role of many-body effects in mesoscopic systems and see how they alter some of the predictions of single-particle theories.

In this paper we calculate the exchange contribution to the energy of the quasi-one-dimensional electron gas in a strong magnetic field, and discuss its importance to the valley and spin splittings of the energy levels. This calculation is motivated by some experimental results that indicate that the two-probe conductance of narrow wires is quantized with step size $2e^2/h$ instead of the usual e^2/h.[6,7] The doubling of the step size can be understood in terms of edge states by assuming that in narrow systems there are two degenerate edge states, due to either valley or spin degeneracy, which are filled simultaneously. In wider systems the degeneracies are lifted and the edge states are filled one after another leading to the ordinary step size e^2/h.[3-5] Recently it has been shown experimentally that in Si wires both valley and spin splittings weaken continuously as the width of the wire is reduced and, in narrow enough wires, the valley splitting vanishes completely.[8] We want to explain these observations by considering the combined effects of the magnetic field, the combining potential, and the exchange interactions, and show that in these systems the valley splitting vanishes above a critical electron density. Similar results are obtained for the spin splitting but with a higher critical density. The suppression of spin polarization by lateral confinement has been indirectly observed in recent experiments,[9] where the Hall conductance of a narrow $GaAs/Al_{1-x}Ga_xAs$ interface exhibited a plateau of $e^2/2h$.

It has been shown earlier that exchange interactions play an important role in both one- and two-dimensional electron systems. Ando and Uemura[10] considered a two-dimensional electron gas in a magnetic field and showed that exchange and correlation effects lead to an oscillating electron g factor that can be considerably larger than the one-particle value $g=2$. Kelly and Falicov, among others,[11-13] studied a two-dimensional electron gas without magnetic field and showed that the degenerate energy valleys are asymmetrically occupied if the electron density is below a critical density, whereas at higher electron concentrations both valleys are filled simultaneously. Gold *et al.*[14,15] considered the role of exchange interactions in parabolically confined quasi-one-dimensional wires without a magnetic field.

We consider a system consisting of two degenerate energy bands (valleys) with electron densities ρ_1 and ρ_2. The total energy of the two-valley system per unit area is given by $E_{\rm tot}=E(\rho_1)+E(\rho_2)$. We minimize the total energy subject to the constraint that the total number of electrons is fixed, $\rho=\rho_1+\rho_2$. It is convenient to express ρ_1 and ρ_2 in terms of the total electron concentration and an asymmetry parameter $\delta\rho$, $\rho_1=\frac{1}{2}\rho+\delta\rho$, and $\rho_2=\frac{1}{2}\rho-\delta\rho$. The energy of a single valley consists of kinetic energy and the exchange and correlation energy. The Coulombic exchange energy per particle is proportional to the inverse of the typical separation between electrons, which scales like $\rho^{1/d}$ where d is the dimensionality of the system. The total kinetic energy of a fermion system is proportional to $\rho^{1+2/d}$ in the absence of the magnetic field, and the total energy of the two-valley system is then given by

$$E_{\rm tot}=A[(\tfrac{1}{2}\rho+\delta\rho)^{1+2/d}+(\tfrac{1}{2}\rho-\delta\rho)^{1+2/d}] - A'[(\tfrac{1}{2}\rho+\delta\rho)^{1+1/d}+(\tfrac{1}{2}\rho-\delta\rho)^{1+1/d}] . \quad (1)$$

For a two-dimensional system in a magnetic field the kinetic energy is quenched (Landau levels) and the coefficient A vanishes. We immediately see that the minimum is obtained for $\delta\rho=\frac{1}{2}\rho$. Hence, in two-dimensional systems, the valley degeneracy is spontaneously broken by the magnetic field. In narrow wires the coefficient A is positive and it is no longer obvious that the valley degeneracy is lifted. Now we want to study that in more detail and introduce a specific model.

We consider the Hamiltonian

$$H_0=\frac{1}{2m}\left[-i\hbar\nabla-\frac{e}{c}Bx\hat{z}\right]^2+U(x)\ , \tag{2}$$

where $U(x)$ is an arbitrary confining potential [$\lim_{x\to\pm\infty}U(x)=\infty$]. The eigenstates of H_0 can be written as

$$\psi_{nk}(x,z)=\frac{1}{\sqrt{L}}e^{ikz}\chi_{nk}(x)\ , \tag{3}$$

where n is the band index and k the longitudinal wave vector. To calculate the exchange energy we use the Hartree-Fock approximation and evaluate the diagram in Fig. 1. In evaluating the diagram we have to calculate the Coulombic matrix element $\langle nk,n'k'|V|n'k',nk\rangle$ which can be shown to give

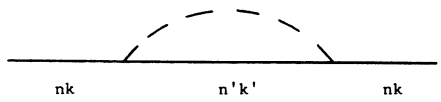

FIG. 1. Exchange diagram.

$$V_{12,21}=\frac{1}{L}\int_{-\infty}^{+\infty}\frac{dq}{2\pi}V(\tilde{q})|\langle kn|e^{iqx}|k'n'\rangle|^2\ , \tag{4}$$

where $\tilde{q}=q\hat{e}_x+(k-k')\hat{e}_z$ and $V(q)$ is the Coulomb potential $V(q)=2\pi(e^2/q)$ and $|nk\rangle$ denotes the transverse wave function χ_{nk}. At zero temperature the nth band is filled for wave vectors $|\mathbf{k}|<k_F(n)$. We can now insert the appropriate Green's functions from Fig. 1 and evaluate the exchange diagram, which yields for the exchange energy for one particle

$$\varepsilon_{\rm exc}(n,k)=-e^2\sum_{n'}\int_{-k_F(n')}^{k_F(n')}\frac{dk'}{2\pi}\int_{-\infty}^{+\infty}dq[(k-k')^2+q^2]^{-(1/2)}|\langle nk|e^{iqx}|n'k'\rangle|^2\ . \tag{5}$$

We still have not specified the confining potential $U(x)$. From now on we will consider a parabolic confining potential,

$$U(x)=\tfrac{1}{2}m\omega_p^2x^2\ . \tag{6}$$

The advantage of a parabolic potential is that we know the eigenstates $|nk\rangle$ and can evaluate the matrix element in (5). However, we should point out that the parabolic potential has a special feature. The states $|nk\rangle$ are harmonic oscillator eigenstates with an energy that increases with increasing k. The width of the state $|nk\rangle$ is independent of k and the states are equidistant in x, so the width of the wire is linearly proportional to number of filled k states (in a given band), $W=2k_Fl^2-l$. The number of filled k states is determined by the total number of electrons in the system, $k_F=\pi N/L$ (neglecting spin), so the areal density of electrons is given by $\rho=(1/\pi)k_F/(2k_Fl^2+1)$, which is almost constant for large enough k_F. Hence, the wire expands if the total number of electrons is increased and the areal density of electrons remains almost unchanged. The actual confining potential in real physical systems is likely to be somewhere between a parabolic and a square-well potential. Nevertheless, the parabolic potential will serve as a useful example to illustrate the general principle of suppression of the spontaneous degeneracy splitting due to lateral confinement.

For a parabolic confining potential the matrix element $\langle nk|e^{iqx}|n'k'\rangle$ can be evaluated in the same way as in the two-dimensional case giving[8]

$$|\langle nk|e^{iqx}|n'k'\rangle|^2=\frac{m'!}{m!}(\tfrac{1}{2}l^2\tilde{q}^2)^{m-m'}[L_{m'}^{m-m'}(\tfrac{1}{2}l^2\tilde{q}^2)]^2e^{-(1/2)l^2\tilde{q}^2}\ , \tag{7}$$

where $m=\max(n,n')$ and $m'=\min(n,n')$ and l is the effective magnetic length

$$l^2=l_B^2\frac{\omega_c^2}{\omega_c^2+\omega_p^2}\ . \tag{8}$$

We substitute into expression (5) and find the exchange contribution to the single-particle energies in a parabolically confined wire,

$$\begin{aligned}\varepsilon_{\rm exc}(n,k)=-e^2\int_{-\infty}^{+\infty}dq\Bigg\{&\sum_{n'=0}^{n}\frac{n'!}{n!}\int_{k-k_F(n')}^{k+k_F(n')}\frac{dk'}{2\pi}\frac{e^{-(1/2)l^2(k'^2+q^2)}}{\sqrt{k'^2+q^2}}\left[\frac{l^2}{2}(k'^2+q^2)\right]^{n-n'}\left[L_{n'}^{n-n'}\left[\frac{l^2}{2}(k'^2+q^2)\right]\right]^2\\&+\sum_{n'=n+1}\frac{n!}{n'!}\int_{k-k_F(n')}^{k+k_F(n')}\frac{dk'}{2\pi}\frac{e^{(-1/2)l^2(k'^2+q^2)}}{\sqrt{k'^2+q^2}}\left[\frac{l^2}{2}(k'^2+q^2)\right]^{n'-n}\\&\times\left[L_n^{n'-n}\left[\frac{l^2}{2}(k'^2+q^2)\right]\right]^2\Bigg\}\ .\end{aligned} \tag{9}$$

If only one band is occupied the result assumes a particularly simple form

$$\varepsilon_{\rm exc}(0,k)=-\frac{e^2}{l}\int_{(k-k_F)l}^{(k+k_F)l}\frac{dk'}{2\pi}\int_{-\infty}^{+\infty}(k'^2+q^2)^{-(1/2)}e^{-(1/2)(k'^2+q^2)}\,. \tag{10}$$

For an extended two-dimensional system the corresponding result is

$$\varepsilon_{\rm exc}=-\left[\frac{\pi}{2}\right]^{1/2}\frac{e^2}{l}\,. \tag{11}$$

In the remainder of this paper we will concentrate for simplicity on one-band results only. We believe that multiband results are qualitatively similar.

For a parabolic confining potential it is not convenient to express the total energy in terms of the areal density for reasons discussed above. More useful quantities are the linear density $n=N/L$ that is directly proportional to the Fermi wave vector, and the linear density asymmetry ν between the valleys. The kinetic energy per unit length of the wire for one valley is given by

$$E_{\rm kin}(n)=\frac{\omega_p^2}{\omega_c^2+\omega_p^2}\frac{\pi^2\hbar^2}{6m}n^3+\frac{\hbar}{2}\left[\omega_c^2+\omega_p^2\right]^{1/2}n \tag{12}$$

and the exchange energy per unit length is obtained by integrating (10). The integration can be easily carried out and yields

$$E_{\rm exc}(n)=-n\left[\frac{\pi}{8}\right]^{1/2}\frac{e^2}{l}+\frac{e^2}{2\pi^2l^2}[1-g(2\pi nl)]\,, \tag{13}$$

$$g(\alpha)=\int_1^\infty\frac{dt}{t^2}\arccos\left[\frac{1}{t}\right]e^{-(1/2)\alpha^2t^2}\,. \tag{14}$$

The integral converges quite rapidly and it can be evaluated numerically. The total energy of a parabolically confined wire is the sum of the energies of the two valleys, $E_{\rm tot}(n)=E(\frac{1}{2}n+\nu)+E(\frac{1}{2}n-\nu)$. It is shown in Fig. 2 as a function of the asymmetry ν for a fixed magnetic field and confining potential. Depending on the total number of electrons, the magnetic field and the parameter ω_p, the total energy has its minimum either at $\nu=0$ (symmetric occupation) or $\nu=\frac{1}{2}n$ (completely asymmetric occupation). The critical linear electron density n_v in Si using effective mass $m_{\rm eff}=0.19$ and dielectric constant $\epsilon=12.0$ is plotted as a function of ω_p for a number of different magnetic fields in Fig. 3. The curve

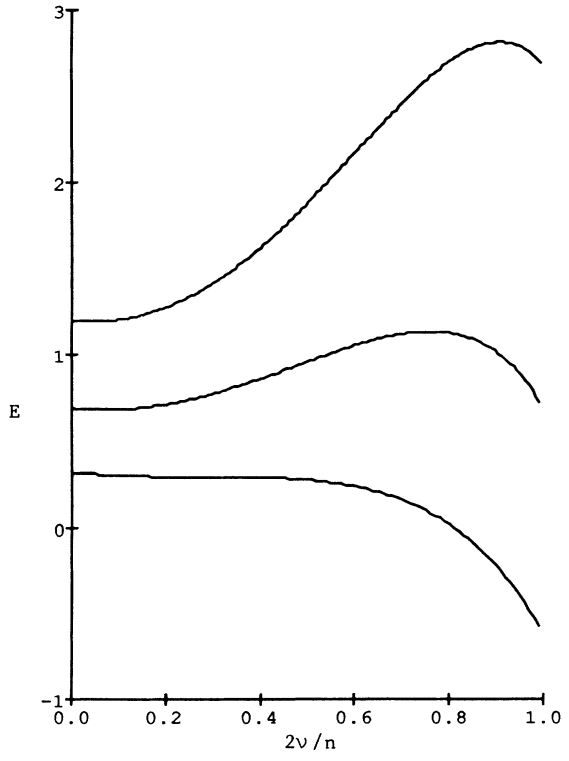

FIG. 2. Total energy of a two-valley system in arbitrary units as a function of $2\nu/n$, the relative occupation asymmetry of the valleys. The magnetic field is $B=1$ T and the total number of electrons per unit length $n=2$, 2.5, and 3 in units of $(\sqrt{2}/\pi)l_B^{-1}$. The frequency unit is chosen so that the cyclotron frequency at 1 T equals 1. In these units the parameter $\omega_p=1$.

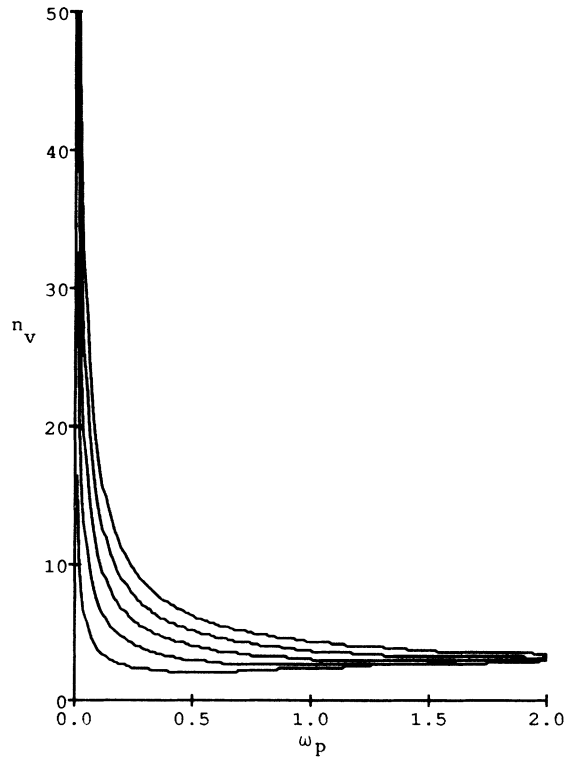

FIG. 3. Critical linear density for valley splitting in Si as a function of ω_p, the steepness of the confining potential. The curves were calculated for $B=0.5$, 1.0, 1.5, 2.0, and 2.5 T (from bottom to top).

$n = n_v(B,\omega_p)$ can be regarded as a phase boundary between an ordered nonsymmetric phase for $n < n_v$ and a disordered phase for $n > n_v$. The roughness of the phase boundaries in Figs. 3–5 is due to the finite n resolution of the calculation and has no physical significance.

To study spin splitting in materials which do not have degenerate energy valleys, we include a Zeeman term $\sigma_z q \mu_B B n$ in Eq. (12). This term favors spin-polarized configurations so the critical density n_s, below which only one spin state is occupied, is higher than the critical density for symmetric valley occupation n_v. Even at linear densities above n_s there is residual paramagnetic polarization but in narrow wires it is quite insignificant. Alternatively we can say that the spin splitting prevails in narrower wires than the valley splitting. The critical linear density n_s for the effective mass $m_{\text{eff}}=0.19$ and dielectric constant $\epsilon=12.0$ is shown in Fig. 4 as a function of the parameter ω_p for a number of different magnetic fields and for the electron g factor $g=2.0$. The difference between n_v and n_s is not very large, so we expect that the step size is $2e^2/h$ even in materials like GaAs where there is no valley degeneracy. In materials which have degenerate energy valleys like Si, the situation for spin polarization is somewhat different. In them the kinetic energy can be further lowered by distributing the electrons in four energy levels. This increases the critical linear density above which the wire is no longer spin polarized. In Fig. 5 we plot the critical linear density n_s for a two-valley material using the same parameters as above.

To better understand the origin of this phase transition it is useful to study the dependence of E_{exc} on the electron density n and make a connection to the qualitative arguments presented earlier. The exchange contribution to the total energy of a single valley as a function of the linear density n is shown in Fig. 6. We can derive approximate expressions for the exchange energy for both low and high linear densities. The crossover density n_0 is given by $2\pi n_0 l = 1$ corresponding to a wire of width $2l$. In the high-density regime $n > n_0$ the exchange energy per unit length is linear in n,

$$E_{\text{exc}}(n) = \frac{e^2}{2\pi^2 l^2} - n\left[\frac{\pi}{8}\right]^{1/2}\frac{e^2}{l}\ , \tag{15}$$

and at low densities we find a more complicated behavior

$$E_{\text{exc}}(n) = e^2 n^2 \ln(2\pi l n) - \frac{e^2}{2}(\pi + 1 + \ln 2 - \gamma + C)n^2\ , \tag{16}$$

where C is the constant

$$C = \sum_{k=1}^{\infty} \frac{(2k)!}{2^{2k}(k!)^2 k(2k+1)} \tag{17}$$

$$\approx 0.244\,702 \tag{18}$$

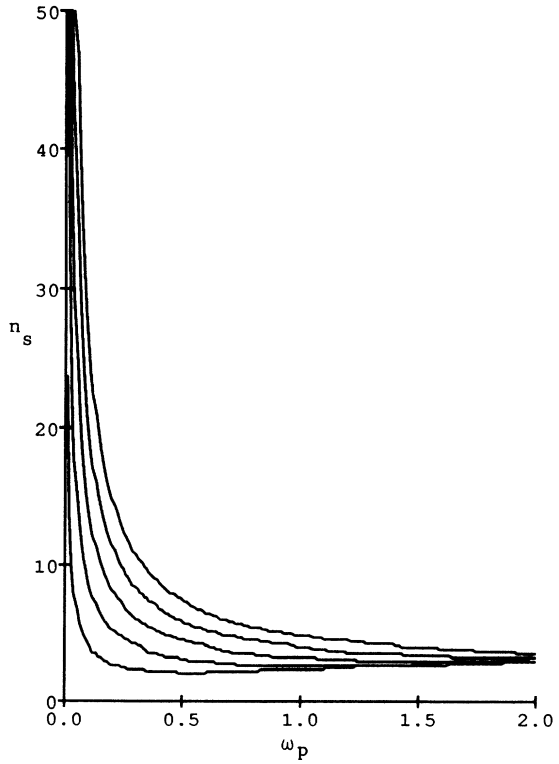

FIG. 4. Critical density for spin polarization as a function of the steepness of the potential for a siliconlike material with no degenerate energy valleys. Magnetic fields are the same as in Fig. 3.

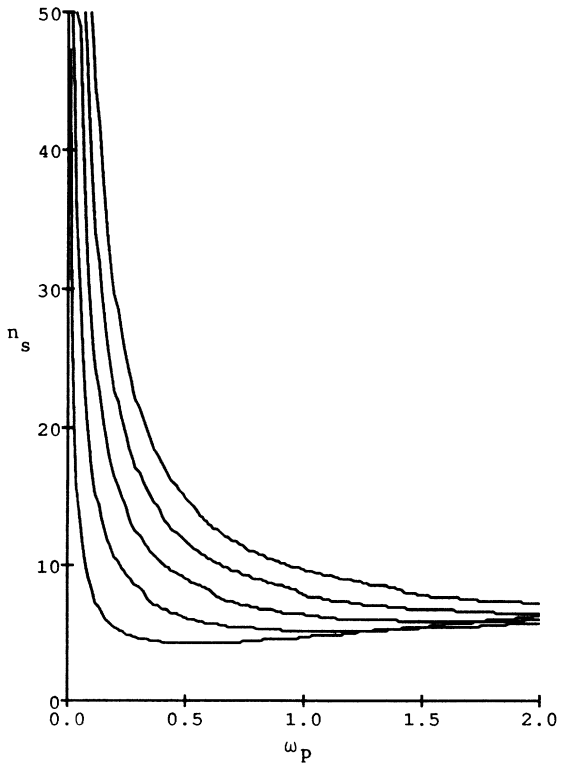

FIG. 5. Critical density for spin polarization for Si as a function of ω_p. Magnetic fields are the same as in Figs. 3 and 4.

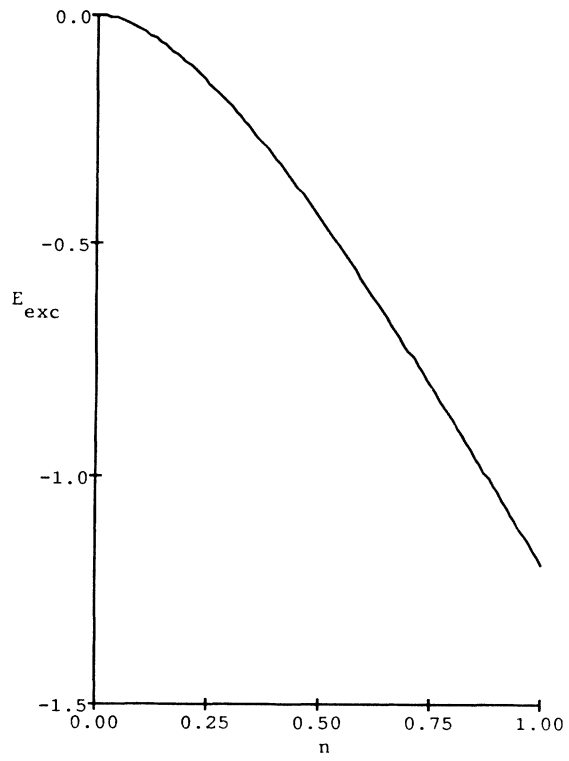

FIG. 6. The total exchange energy for one valley as a function of the linear density in units of e^2/l_B^2. The magnetic field $B=1$ T and $\omega_p=1$.

and γ is Euler's constant. This result can be obtained by expanding the arccos function in (14) in a power series and integrating it termwise.[16] The divergent logarithmic term is then given by the exponential integral $\mathrm{Ei}(-\frac{1}{2}\alpha^2)$, which also gives rise to some of the coefficients of n^2.

For $n<n_0$ the width of the wire is determined by the width of one eigenstate and the areal density of electrons scales as n. The exchange energy per particle increases approximately linearly with n,

$$\varepsilon_{\mathrm{exc}}(n)=-Bn+B'n\ln n \tag{19}$$

corresponding to $d=1$ in (1) and in agreement with Eq. (10). The logarithmic contribution in (19) is due to a divergence at low momentum transfer and is a consequence of the long range of the unscreened Coulomb interaction. For n larger than n_0 the areal density of electrons stays constant, and the exchange energy per particle has a constant value $-\sqrt{\pi/8}e^2/l$. The analytic expression (15) can be used to determine the phase boundary between the symmetric and antisymmetric occupation of energy valleys. We find the critical linear density n_v

$$n_v l_B=\left[\frac{4e^2 m l_B}{\pi^4\hbar^2}\right]^{1/3}\left[\frac{\omega_c^2+\omega_p^2}{\omega_c\omega_p}\right]^{2/3}. \tag{20}$$

This expression agrees well with the numerical results in Fig. 3. The corresponding result can be derived for spin splitting as well but the final expression is more complicated due to the Zeeman term that is linear in n.

Experimental results by Kastner *et al.*[7] show that the two-probe conductance of a narrow Si wire is quantized with step size $2e^2/h$. This corresponds to filling two valleys simultaneously (symmetric phase with respect to the valley splitting). The valleys give rise to one-edge state each, and both of them contribute to the conductance by a factor e^2/h. The spin degeneracy is lifted in the wire, but we expect that in low magnetic fields and narrow wires the step size becomes $4e^2/h$.

We note that Kastner *et al.* have suggested that the first two steps are due to orbital effects, whereas we are now suggesting that every second step is due to a spin. This can be checked by introducing an additional magnetic field parallel to the plane of the interface. Orbital states are not affected by parallel fields and if the plateaus are due to orbital effects, the locations of the steps (measured by the gate voltage V_G) are independent of the parallel field. However, the Zeeman energy is given by the total magnetic fields, and the locations of conductance steps due to spin reversal will change. If the wire was completely free of disorder, the conductance steps would occur when the chemical potential in the wire passes through the minimum of a subband. However, because of disorder, the states near the center of the wire are scattered back, and the conductance step is observed only when the linear density on the subband exceeds n_c, which is determined by the scattering potential in the wire. The first conductance step occurs when only one spin state is filled, and its location is independent of the parallel field. The second step will move as a result of the parallel field. We assume that n_c is large enough so that the exchange energy is given by the large n expression (15). For a fixed total linear density n we can then find the linear densities in the two-spin states by minimizing

$$E_{\mathrm{tot}}=\frac{\omega_p^2}{\omega_c^2+\omega_p^2}\frac{\pi^2\hbar^2}{6m}\left[\left[\frac{n}{2}+\nu\right]^3+\left[\frac{n}{2}-\nu\right]^3\right]-\tfrac{1}{2}g\mu_B B\left[\left[\frac{n}{2}+\nu\right]-\left[\frac{n}{2}-\nu\right]\right] \tag{21}$$

with respect to the asymmetry parameter ν. The total exchange energy in the large n approximation is independent of ν and need not be taken into account in the above expression. From the condition that the linear density on the spin reversed subband $\frac{1}{2}n-\nu$ equals n_c, we find that the second conductance step moves to a higher gate voltage as a function of $B/B_\perp$,

$$V_{G2}=C\left[n_c+\left[n_c^2+\frac{\omega_c^2+\omega_p^2}{\omega_p^2}\frac{2gm\mu_B B_\perp}{\pi^2\hbar^2}\frac{B}{B_\perp}\right]^{1/2}\right], \tag{22}$$

where C is the capacitance per unit length of the wire. The third conductance step, which corresponds to an edge state on a higher subband, shifts downward as a function of $B/B_\perp$. The exact form of this shift depends on exchange interaction on the second subband, which we have not calculated.

In their paper Mottahedeh *et al.* report experimental

observation of the weakening of both valley and spin splittings in Si wires as the width of the wire is reduced. The results are in qualitative agreement with our theoretical work. Unfortunately, in the parabolic model we used, the critical width for the disappearance of the valley splitting depends directly on the stiffness of the confining potential, so that a quantitative comparison with experiment is not possible.

In conclusion, we have shown that in the Hartree-Fock approximation the many-body effects break the valley degeneracy at low electron densities. At densities exceeding the critical density n_v the extra cost of increased kinetic energy outweighs the gain due to exchange interactions and the different valleys are occupied symmetrically. The critical linear density n_s above which both spin states are occupied is higher than n_v due to the Zeeman term, and in materials with valley degeneracy n_s is considerably higher because of the lower kinetic energy due to higher symmetry. The results are at least in qualitative agreement with experimental findings and we proposed a new experiment to allow for a more quantitative comparison.

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[1]K. von Klitzing, G. Dorda, and M. Pepper, Phys. Rev. Lett. **45**, 494 (1980).
[2]D. C. Tsui, H. L. Störmer, and A. C. Gossard, Phys. Rev. Lett. **48**, 1559 (1982).
[3]B. I. Halperin, Phys. Rev. B **25**, 2185 (1982).
[4]P. Streda, J. Kucera, and A. H. MacDonald, Phys. Rev. Lett. **59**, 1973 (1987).
[5]M. Büttiker, Phys. Rev. Lett. **57**, 1761 (1986); M. Büttiker, IBM J. Res. Develop **32**, 317 (1988).
[6]A. B. Fowler, A. Hartstein, and R. A. Webb, Physica B+C **117&118B**, 661 (1983).
[7]M. A. Kastner *et al.*, Phys. Rev. Lett. **60**, 2535 (1988).
[8]R. Mottahedeh *et al.*, Solid State Commun. **72**, 1065 (1989).
[9]G. Timp *et al.*, Phys. Rev. Lett. **63**, 2268 (1989).
[10]T. Ando and Y. Uemura, J. Phys. Soc. Jpn. **37**, 1044 (1974).
[11]M. J. Kelly and L. M. Falicov, Phys. Rev. B **15**, 1974 (1977).
[12]W. L. Bloss and L. J. Sham, Phys. Rev. Lett. **43**, 1529 (1979).
[13]W. L. Bloss *et al.*, J. Phys. Soc. Jpn. **49**, 963 (1980).
[14]A. Gold and A. Ghazali, Phys. Rev. B **41**, 8318 (1990).
[15]S. Olszewski, Z. Phys. B **45**, 297 (1982).
[16]I. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals, Series and Products* (Academic, Orlando, FL, 1980), p. 310.