Many-body effects on the $\rho_{xx}$ ringlike structures in two-subband wells

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The longitudinal resistivity $\rho_{xx}$ of two-dimensional electron gases formed in wells with two subbands displays ringlike structures when plotted in a density–magnetic-field diagram, due to the crossings of spin-split Landau levels (LLs) from distinct subbands. Using spin density functional theory and linear response, we investigate the shape and spin polarization of these structures as a function of temperature and magnetic-field tilt angle. We find that (i) some of the rings “break” at sufficiently low temperatures due to a quantum Hall ferromagnetic phase transition, thus exhibiting a high degree of spin polarization ($\sim 50\%$) within, consistent with the NMR data of Zhang et al. [Phys. Rev. Lett. 98, 246802 (2007)], and (ii) for increasing tilting angles the interplay between the anticrossings due to inter-LL couplings and the exchange-correlation (XC) effects leads to a collapse of the rings at some critical angle $\theta_c$, in agreement with the data of Guo et al. [Phys. Rev. B 78, 233305 (2008)].

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The fascinating quantum Hall regime hosts a number of fundamental physical phenomena, being also relevant for metrology (standard for resistance) and as an alternate means to precisely determine the fine structure constant. The spectrum of two-dimensional electron gases (2DEGs) in the quantum Hall regime is quantized into highly degenerate Landau levels (LLs) [1]. At opposite-spin LL crossings near the Fermi level, a ferromagnetic instability of the 2DEG may arise thus leading to a quantum Hall ferromagnetic phase. This spontaneous spin polarization of the electrons lowers the repulsive Coulomb energy of the Fermi sea, because electrons with parallel spins avoid each other due the Pauli exclusion principle. Even for vanishingly small Zeeman splittings the exchange-energy gain can stabilize quantum Hall ferromagnetism at low enough temperatures [2–4].

Quantum Hall ferromagnetism has been extensively studied in the quantum Hall regime via magnetotransport measurements [5]. Near LL crossings in tilted magnetic fields $B$, the longitudinal resistivity $\rho_{xx}$ vs $B$ of wells with a singly occupied subband exhibits ubiquitous hysteretic spikes, which signals quantum Hall ferromagnetism [6–8]. In two-subband wells, spin-split LLs from distinct subbands cross even without a tilted $B$ field and can form closed loops [ABCD loop, Fig. 1(a)]. Quite generally, $\rho_{xx}$ is directly related to the energy spectrum near the Fermi level (linear response) and hence the topology in Fig. 1(a) translates into ringlike structures [9,10] in $\rho_{xx}$ when plotted in a density–$B$-field diagram $n_{2D}−B$, Fig. 1(b). Recently Zhang et al. [11] have shown that near opposite-spin LL crossings the rings “break” at low enough temperatures (70 mK). NMR measurements [12] near the broken edge C show a high degree of spin polarization, which points to a ferromagnetic instability of the 2DEG. For tilted $B$ fields some of rings “shrink”, fully collapsing for angles above a critical value [13].

Here we use spin density functional theory (SDFT) [14] together with a linear response model [15] to investigate the shape and spin polarization of the ringlike structures in realistic quantum wells with two subbands at various filling factors $\nu$, as a function of the temperature and tilt

![FIG. 1: (a) Two-subband GaAs well and schematic fan diagram with LL crossings from distinct subbands. The ABCD loop gives rise to ringlike structures in the calculated $n_{2D}−B$ diagram of $\rho_{xx}$ (b) for $\nu = 4$. This ring “breaks” at lower temperatures (c) due to quantum Hall ferromagnetic transitions, thus displaying a high spin polarization within (d) [12]. For increasing $B$ field tilt angles $\theta$, the ring shrinks (i.e., A and C move closer) and fully collapses (A=C) at $\theta_c$ (e), in agreement with the data [13] (cf. empty and solid circles).](https://example.com/fig1.png)
angle \( \theta \) of the B field. We find that exchange-correlation (XC) effects are crucial to quantitatively describe the experiments: in particular (i) the \( \nu = 4 \) ring breakup at low temperatures [Fig. 1(c)] follows from quantum Hall ferromagnetic phase transitions [10 11], Fig. 2. The calculated spin polarization [Fig. 2(d)] within the broken ring reaches 50\%, consistent with NMR data [12]. (ii) The shrinking of the \( \nu = 4 \) ring for increasing \( \theta \) and its full collapse at \( \theta = \theta_c \) [Fig. 1(e)] arises from the interplay between the anticrossings due to the inter-LL couplings and the exchange field, Fig. 3. We note that only rings formed from consecutive LLs, for which inter-LL coupling is operative, collapse for increasing \( \theta \).

The quantum phase transitions we find here are not specific to the \( \nu = 4 \) ring. They are general and should also occur for \( \nu = 6 \) and others, but for distinct ranges of parameters. Other 2DEG systems, e.g., formed in Mn-based wells [10], can also show peculiar ring structures.

System. We consider the structures of Zhang et al. [10 13]: a wide 240 Å GaAs square quantum well with Al\(_{0.3}\)Ga\(_{0.7}\)As barriers and symmetric \( \delta \)-doping (Si) with 240 Å spacers [Fig. 1(a)]. The electron density in the well is controlled by a gate voltage, as in an ideal capacitor [10–13]: a wide 240 Å GaAs square quantum well with based wells [16], can also show peculiar ring structures.

Kohn-Sham problem. The Kohn-Sham implementation of density-functional theory maps the problem of fully interacting electrons onto a non-interacting Schroedinger equation – the KS equation – with electrons in an effective single-particle potential [14]. For magnetic fields \( B \) tilted \( \theta \) with the 2DEG normal, this reads

\[
(H_{||} + H_{\perp\perp} + \delta H_\theta) \psi = \epsilon \psi,
\]

with

\[
H_{||} = \frac{P^2}{2m} + \frac{1}{2} \mu \omega_p^2 (x - x_0)^2,
\]

\[
H_{\perp\perp} = \frac{P^2}{2m} + \frac{1}{2} \mu \omega_p^2 z^2 + \frac{1}{2} g_e \mu_B \sigma z B + v_{eff}(z),
\]

\[
\delta H_\theta = \omega_p z P_z,
\]

where \( m \) (0.067\( m_0 \)) is the effective mass, \( g_e \) \((-0.44)\) the bulk g-factor, \( P_{x,y,z} \) the \( x,y,z \) components of the electron momentum operator, \( \omega_c = eB \cos \theta/m \) the cyclotron frequency, \( \sigma_z = \pm (\cos \theta, \sin \theta) \), \( \omega_p = eB \sin \theta/m \), \( x_0 = -\hbar^2 P_y / \hbar \), \( \hbar^2 = \hbar/eB \cos \theta \) the magnetic length and

\[
v_{eff}(z) = v_c(z) + v_H(z; [n]) + v_{xc}(z; [n], [n]),
\]

\( v_c \) is the structural well potential. The Hartree potential \( v_H(z; [n]) \) is obtained self-consistently from Poisson’s equation. For the XC potential \( v_{xc}(z; [n], [n]) \), we use the PW92 parametrization [18] of the local-spin-density approximation (LSDA) [19]. Here we have approximated the electron density \( n(x, y, z) \) by its average over the \( xy \) plane \( n(z) = n_\uparrow(z) + n_\downarrow(z) \) [8]. This renders both the Hartree and the XC potentials dependent upon only \( z \).

Perpendicular B field. For \( \theta = 0^\circ \), \( \omega_p = 0 \Rightarrow \delta H_\theta = 0 \), the KS equation (1) is separable in the \( xy \) and \( z \) variables and has eigenfunctions \( \psi_{i,n,k_z}(x, y, z) = \frac{1}{\sqrt{\pi \hbar^2}} \exp(ik_y y) \varphi_n(x) \chi_z^\sigma(z) \) (Landau gauge), with \( \varphi_n(x) \) being the \( n \)th harmonic-oscillator eigenfunction centered at \( x_0 = -\hbar k_y / m \omega_c \) and \( k_y \) the electron wave number along the \( y \) axis: \( L_y \) is a normalizing length. The KS eigenenergies are \( \epsilon_{i,n}^\sigma = \epsilon_n + \hbar \omega_c (n+1/2) \) (Landau fan diagram), with \( \epsilon_n = (n+1/2) \hbar \omega_c \). As \( n \) increases, the LL energies (degeneracy \( n_B = eB / \hbar \) and \( \epsilon_{n+1}^\sigma - \epsilon_n^\sigma \) the quantized levels obeying \( H_{\perp\perp}^\sigma \chi_z^\sigma = \epsilon_{n+1}^\sigma \chi_z^\sigma \), \( i = 0, 1, \ldots \), with a self-consistently calculated chemical potential \( \mu \).

Tilted B field. For \( \theta > 0^\circ \) the KS equation (1) is not separable because \( \delta H_\theta \sim \sin \theta \omega_p \neq 0 \). However, since \( \delta H_\theta \ll H_0 = H_{||} + H_{\perp\perp} \) and only couples consecutive LLs from distinct subbands, we can obtain the KS solutions \( \psi(x, y, z; \theta) \) as an expansion in terms of the eigenfunctions \( \varphi_{i,n,k_z}(x, y, z; \theta) \) of \( H_0 \). We perform this expansion at every iteration of our self-consistent scheme. We obtain good results by truncating the expansion for energies greater than \( \mu + k_B T \). This LL coupling leads to anticrossings of the KS energies for equal-spin LLs, which ultimately make the ring shrink for tilted fields, Fig. 3.

Linear-response \( \rho_{xx} \). By assuming that the KS eigenvalues \( \epsilon_{i,n}^\sigma \) represent the eigenenergies of the actual (Fermi-liquid) quasi-particles in our 2DEG, we use them in a Kubo-type formula [15] to calculate the conductivity tensor \( \sigma \). For instance, within the self-consistent Born-approximation with short-range scatterers [15] \( \sigma_{xx} = \frac{e^2}{\hbar} \int_{-\infty}^{\infty} \left( -\frac{\partial f(e)}{\partial e} \right) \sum_{i,n,\sigma} \left( n + \frac{1}{2} \right) \exp \left[ -\frac{(\epsilon_{i,n}^\sigma - \epsilon_{i,n})^2}{2 \Gamma_{\text{ext}}} \right] \, de \), \( \Gamma_{\text{ext}} \) denotes the width of the extended-state region within the broadened density of states and \( f(e) \) the Fermi function. We obtain the resistivity from \( \rho = -\sigma^{-1} \).

Spin-polarized rings. Figures 1(b) and 1(c) show our calculated \( n_{2D} - B \) diagram of \( \rho_{xx} \) for two different temperatures \( T = 340 \text{ mK} \) and \( T = 70 \text{ mK} \), respectively, near the \( \nu = 4 \) ring. Similarly to the experiment of Ref. [11], we find that the \( \nu = 4 \) ring “breaks” at the opposite spin LL crossings (points \( A \) and \( C \)) at lower temperatures [20], Fig. 1(c). Figure 1(d) shows the corresponding \( n_{2D} - B \) diagram of the spin-polarization \( \xi \). For \( T = 340 \text{ mK} \) the spin polarization of the \( \nu = 4 \) ring (not shown), though high, varies smoothly at the opposite spin crossings. We note that the high spin polarization \( \xi \) within the ring points to quantum Hall ferromagnetism, being also consistent with resistively-detected NMR data available [12], however, we contend that the high \( \xi \) and the discontinuities
of $\rho_{xx}$ at the crossings A and C [Fig. 1(c)] constitute the signature for the quantum Hall ferromagnetic instability.

The contrast between the low and high temperature results is more clearly seen in Fig. 2 which shows $\rho_{xx}$ for $n_{2D} = 7.3 \times 10^{11} \text{ cm}^{-2}$ at 340 mK and 70 mK. The spike near $B = 7.6$ T [see arrow in Fig. 2(a)] comes from the left edge of the $\nu = 4$ ring (point A in Fig. 1) and is suppressed at $T = 70$ mK. The Landau fan diagrams for both temperatures differ substantially only around this region [see arrows in Figs. 2(b)-(c)]. At $T = 70$ mK the diagram shows an abrupt transition and the chemical potential $\mu$ jumps to the spin-down state of the lower subband, thus suppressing the $\rho_{xx}$ spike. Note also the exchange enhancement of the spin splittings in Fig. 2(b)-(c) when $\mu$ lies essentially between the spin-split LLs.

A relevant parameter in our simulations is the LL broadening $\Gamma$. For short-range scatterers, the electron mobility $\mu_e$ and the LL broadening are related by $\Gamma = \Gamma_0 \sqrt{B/\mu_e}$ [21], with $\Gamma_0 = (2/\pi)^{1/2} e^2/\hbar m_e$. We use $\Gamma_{70} = 0.130\sqrt{B}$ meV and $\Gamma_{340} = 0.150\sqrt{B}$ meV to simulate the ring structures at $T = 70$ mK and 340 mK, respectively [see Figs. 1(b)-(c)] [22]. Note that the temperature-dependent $\Gamma_0$ differs from the one determined from the zero voltage $\mu_e$, $\Gamma = 0.210\sqrt{B}$ meV. A strong dependence of $\mu_e$ on the gate voltage (or density) is reported in [23] for parabolic two-subband wells, which also show

\[ \frac{1}{\rho_{xx}} = \frac{1}{\rho_{xx}}^{(c)} + \frac{1}{\rho_{xx}}^{(cb)} - \rho_0 \rho_i \sum \frac{1}{\rho_{xx}^{(c)}} \left( \frac{1}{\rho_{xx}^{(cb)}} - \rho_0 \rho_i \right) \]

\[ \rho_0 \rho_i \sum \frac{1}{\rho_{xx}^{(c)}} \]
\(\rho_{xx}\) for a non-interacting model and find ring breakups near D & B. However, the actual ring breakups near D & B at \(\theta = 0^\circ\) could also be related to the derivative discontinuity of the XC functionals \[27\], which is absent in local (LSDA) and semi-local (e.g., generalized gradient approximations) functionals \[28, 29\]. This discontinuity appears as a jump in \(n_{2D}\) at the threshold for the second subband occupation at \(B = 0\) \[30\]. The results of Ref. \[30\] suggest that orbital functionals (e.g., exact-exchange) \[27\] may give rise to phase transitions at the crossings B & D. Clearly more work is needed here. A Hartree-Fock analysis in model bilayer systems \[4\] suggests that quantum Hall ferromagnetic instabilities can occur at same-spin pseudospin LL crossings \[4\].

Summary. We have combined SDFT and linear response to investigate magnetotransport in 2DEGs formed in two-subband wells \[11–13\]. Our calculated \(n_{2D} - B\) maps of \(\rho_{xx}\) show ringlike structures. At low temperatures the \(\nu = 4\) ring breaks due to quantum Hall ferromagnetic phase transitions. The \(n_{2D} - B\) diagram of the 2DEG spin polarization \(\xi\) shows the ring to be \(\sim 50\%\) spin polarized. For tilted B fields, the \(\nu = 4\) ring shrinks and fully collapses at a critical angle \(\theta_c \approx 6^\circ\), in excellent agreement with the data \[13\]. The interplay between the equal-spin LL anti-crossings and the XC effects are crucial here. A direct experimental evidence of our prediction of a high \(\xi\) in the ring is still lacking; the resistivity-detected NMR data of Ref. \[12\] only shows signals near point C. We hope our work stimulates further investigations in the literature.

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