Hysteretic resistance spikes in quantum Hall ferromagnets without domains

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We use spin-density-functional theory to study recently reported hysteretic magnetoresistance $\rho_{xx}$ spikes in Mn-based 2D electron gases [Jaroszyński et al. Phys. Rev. Lett. 89, 266802 (2002)]. We find hysteresis loops in our calculated Landau fan diagrams and total energies signaling quantum-Hall ferromagnet phase transitions. Spin-dependent exchange-correlation effects are crucial to stabilize the relevant magnetic phases arising from distinct symmetry-broken excited- and ground-state solutions of the Kohn-Sham equations. Besides hysteretic spikes in $\rho_{xx}$, we predict hysteretic dips in the Hall resistance $\rho_{xy}$. Our theory, without domain walls, satisfactorily explains the recent data.

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Two-dimensional electron gases (2DEGs) under strong magnetic fields exhibit fascinating physical phenomena; the mostly widely known of these being the integer and fractional quantum Hall effects [1]. Spontaneous magnetic order in quantum-Hall systems is yet another interesting possibility. Quantum Hall ferromagnetism arises from the interplay of the Zeeman, Coulomb, and thermal energies within the macroscopically degenerate Landau levels of the 2DEG [2]. Landau level crossings [4] offer a convenient means to probe symmetry-broken quantum-Hall ferromagnetic transitions. At crossings, opposite-spin levels can benefit from Coulomb exchange to form spin-ordered states at low temperatures [2].

Many groups have investigated quantum Hall ferromagnetism in the integer and fractional quantum-Hall regimes by inducing Landau level crossings via tilted magnetic fields, density and level tuning via gate electrodes, hydrostatic pressure [5], and the $s$-$d$ exchange-induced level bowing in Mn-based 2DEGs [6, 7]. These studies [3, 4, 7] find ubiquitous “anomalous” peaks and hysteretic spikes in Shubnikov-de-Haas measurements of the magnetoresistance $\rho_{xx}$. The hysteretic behavior here means that the spikes appear at distinct magnetic fields as the field is swept up and down. In the fractional quantum-Hall regime recent experiments show that these features follow from the hyperfine coupling between electrons and nuclei [8]. In the integer quantum Hall regime, the hysteretic spikes have been suggested to arise from charge transport along long domain-wall loops acting as one-dimensional (“percolating”) channels in the 2DEG near an Ising-like quantum-Hall ferromagnet transition [4]. Though appealing, this description is largely qualitative: no magnetotransport quantities (e.g., $\rho_{xx}$) have been calculated so far accounting for domain walls.

Alternate picture for the hysteretic spikes. In this Letter we apply the Spin Density Functional Theory (SDFT) [10] implemented via the Kohn-Sham (KS) scheme in a Local Spin Density Approximation (LSDA) to determine the electronic structure of a 2DEG, which we then use in a linear response model [11] to explicitly calculate $\rho_{xx}$ and $\rho_{xy}$. For concreteness, we focus on the experiment of Jaroszyński et al. [3] in Mn-based 2DEGs [12]. Interestingly, we find hysteretic behavior in $\rho_{xx}$ and $\rho_{xy}$, Figs. 1(a)-(b), without taking into account domain walls. This behavior follows from our system having two self-consistent KS solutions – for a same set of parameters – with distinct total energies as shown in Figs. 1(c)-(d), see e.g. range $B_{c2}^d < B < B_{c1}^d$. As we discuss later on, these solutions correspond to ground and excited states describing distinct quantum Hall ferromagnetic phases of our interacting 2DEG, and, most importantly, provide a concrete example for a theorem of Perdew and Levy on the existence of excited states from ground-state density.

![Image](https://example.com/image.png)
functionals. These phases comprise differing sets of conducting states contributing to the magnetotransport and hence have distinctive $\rho_{xx}$'s and $\rho_{xy}$'s. The hysteresis then arises because the 2DEG can go through a different sequence of magnetic phases (i.e., the system can become trapped into distinct local minima) as the $B$ field is swept up and then down, e.g., phases I to II in the up sweep at $B \approx B^*_{\perp}$ and phases III to IV in the down sweep at $B \approx B^*_{\parallel}$, Fig. 1(d). We predict hysteretic dips (and peaks) in $\rho_{xy}$ [14] [Fig. 1(a)] and that the spikes shift to opposite directions (Fig. 3) in samples with positive and negative $g$ factors, for increasing tilt angles of $B$.

*Mn-based system. We consider a CdTe quantum well between Cd$_{0.8}$Mg$_{0.2}$Te barriers, with three evenly spaced Cd$_{1-x}$Mn$_x$Te monolayers ("Mn barriers") in the well region [7]. Fig. 1(a) (inset); $x_p$ is the planar concentration of Mn. Adjacent to the barriers lie two symmetric n-doped regions [12]. In an external field $B$, the s-d exchange interaction between the electrons in the well (2DEG) and those of the localized $d$ orbitals of the Mn gives rise to a spin-dependent electron potential

$$
\psi_{e,\sigma}(z; B, T) = \frac{\sigma}{2} N_0 \alpha x(z) \sqrt{\frac{5}{2B/k_B(T + T_0)}},
$$

where $N_0\alpha$ is the s-d exchange constant, $B/2$ is the spin-5/2 Brillouin function, $x(z)$ and $T_0$ are the effective Mn profile and temperature [10], respectively, and $\sigma = \pm 1$ (or $\uparrow, \downarrow$) denotes the electron spin components.

The structural confining potential of the well is assumed to be a harmonic oscillator eigenfunction centered at $z_0 = (n + 1/2)\hbar\omega_c$, where $\omega_c$ is the cyclotron frequency. The total wavefunction is $\psi_{e,\sigma}(z) = \psi_{e,\sigma}^z(z)\psi_{e,\sigma}^y(z)$, where $

$$
\psi_{e,\sigma}^y(z) = \frac{1}{\sqrt{L_y}} \exp(ik_y y) \varphi_n(x) \chi_{\sigma}^z(z),
$$

is the effective mass,

$$
\hbar^2 d \frac{d^2}{dz^2} + v_{e,\sigma}^\text{eff}(z; [n, \eta_k]) \chi_{\sigma}^z(z) = \varepsilon_{\sigma}^{\text{eff}} \chi_{\sigma}^z(z),
$$

where $m$ is the effective mass, $i = 1, 2 \ldots$ the band index, and $v_{e,\sigma}^\text{eff}(z; [n, \eta_k])$ the effective single-particle potential

$$
v_{e,\sigma}^\text{eff}(z; [n, \eta_k]) = v_{e,\sigma}^y(z) + v_{e,\sigma}^z(z) + v_{e,\sigma}^v(z; [n])
$$

$$
+ v_{e,\sigma}^{\text{xc}}(z; [n, \eta_k]),
$$

In Eq. 3 $v_{x}(z) = v_{y}(z) + v_{z}(z)$, $v_{x}^y(z; [n])$ is the Hartree potential, calculated by solving Poisson’s equation, and $v_{e,\sigma}^{\text{xc}}(z; [n, \eta_k])$ is the spin-dependent exchange-correlation (XC) potential [19]. The motion in the $xy$ plane is quantized into Landau levels with energies $\varepsilon_n = (n + 1/2)\hbar\omega_c$, $n = 0, 1, 2 \ldots$ and $\omega_c = eB/m$. The total wavefunction is $\psi_{e,\sigma}(x, y, z) = \psi_{e,\sigma}^x(x) \psi_{e,\sigma}^y(y) \psi_{e,\sigma}^z(z)$, $\varphi_n(x)$ is the $n$-th harmonic oscillator eigenfunction centered at $x_0 = -\hbar k_y/m\omega_c$ and $k_y$ is the electron wave number along the $y$ axis; $L_y$ is a normalizing length. This decoupling of the $z$ and $xy$ motions follows from the uniformity of the total electron density within the $xy$ plane: because each electron can be anywhere within the plane, we use the average total electron density $n(z) = \int f^\sigma_{n, k_y} |\psi_{e,\sigma}^n(x, y, z)|^2 \, dy = \int f^\sigma_{n, k_y} |\psi_{e,\sigma}^n(x, y, z)|^2 \, dy$ in Poisson’s equation, instead of $n(x, y, z)$ [here $f^\sigma_{n, k_y}$ is the Fermi function and $L_x$ is a normalizing length]. This procedure makes the 2DEG uniform thus rendering a separable KS set.

We assume that the KS eigenvalues

$$
\varepsilon_{\sigma}^{\text{eff}}(B) = \varepsilon_{\sigma}^z(B) + \left( n + \frac{1}{2} \right) \hbar\omega_c + \frac{\sigma}{2} g\mu_B B,
$$

where $g\mu_B B\sigma_z/2$ is the ordinary Zeeman term ($g$: effective Landé factor), describe the actual electronic structure of our 2DEG. This assumption is, in principle, unjustified within DFT: the individual KS orbitals represent states of a fictitious non-interacting electron gas in an effective potential, Eqs. 2 and 4. With this assumption, however, we satisfactorily explain observed hysteretic phenomena in 2DEGs [12].

*System parameters. In our simulations we use (see Ref. 7): $m/m_0 = 0.099$, dielectric constant $\epsilon/\epsilon_0 = 10$, $g = -1.67$, $N_0\alpha = 220$ meV, quantum-well width $L = 100$ Å, spacing width $L_z = 200$ Å, $\nu_{SD} = 2.97 \times 10^{11}$ cm$^{-2}$, number of Mn monolayers $N_b = 3$, $x_p = 0.115$, $v_0 = 248.1$ meV, $v_1 = 1183.5$ meV, $T_0 = 0.47$ K, and assume a diffusion length $\ell \sim 4.67$ Å for the Mn profile.

Figures 1 and 2 show our theoretical results for $\rho_{xx}$, $\rho_{xy}$ 1(a)-(b), total energy $E$ 1(c)-(d), Landau level fan diagram 2(a), spin-resolved electron densities $n_{\sigma}^\text{cf}(2, b)$, and spin-polarization $\zeta$ 2(c). Remarkably, all of these quantities show abrupt hysteretic changes near 5.8 T as the $B$ field is swept up and down. The discontinuous nature of these features follows from the 2DEG undergoing (quantum) phase transitions in which its degree of spin-polarization $\zeta$ suddenly changes, 2(b)-(c), e.g., in the down sweep the 2DEG becomes highly spin-polarized near 5.8 T 2(c): a quantum Hall ferromagnetic phase transition takes place. Our calculated fan diagram 2(a) and total energy 1(d) corroborate this scenario: the opposite-spin levels $\varepsilon_{1,0}^\uparrow, \varepsilon_{1,1}^\downarrow$ suddenly cross near $\mu$ thus lowering the total energy $E$ [see III to IV discontinuity in 1(d)]. This is similar to the Giuliani-Quinn instability where the 1st-order transition is due to the gain of exchange energy in the ferromagnetic state [2]. Our calculation also includes correlation which somewhat reduces the exchange effects. The role of the s-d exchange [Eq. 1] in our system is to cause “level bowing” ($B < 2$ T) thus inducing opposite-spin Landau level crossings, see e.g. crossings for $B < 4$ T in 2(a). When crossings occur near $\mu$, spin-dependent XC effects may induce phase transi-
Hysteresis arises in our SDFT calculation.

The absolute minima represent the ground states, and the extrema lying above the minimum represent a subset of the excited states.” These authors have also proved that some of the self-consistent solutions of the KS equations extremize $E_i[n]$; provided that these solutions obey ground-state Fermi statistics (\textit{aufbau} principle) with a single chemical potential — this is a necessary and sufficient condition.

Our simulations show that for a certain window of magnetic field \textit{e.g.}, $B_{c1}^d < B < B_{c1}^u$ in Fig. 1(d)\textit{]} the KS equations have indeed two self-consistent solutions — both satisfying the necessary and sufficient condition above. At each $B$ in this range, one of these two solutions is stable (true minimum, ground state) and the other metastable (local minimum, excited state). In practice, these two states (phases) are separated by an energy barrier \textit{23} which may trap the system in the metastable states during the up==down $B$ sweeps thus giving rise to hysteretic loops, Figs. 1 and 2.

\textbf{Magneto-transport.} We obtain the longitudinal and Hall resistances from the conductivity tensor ($\rho = \sigma^{-1}$), calculated within the self-consistent Born-approximation model of Ando and Uemura \textit{11}. For short-range scatterers, $\sigma_{xx} = \frac{4e^2}{h^2} \int_{-\infty}^{\infty} \left( -\frac{\partial f}{\partial \varepsilon} \right) \sum_{i, n, \sigma_z} \left( n + \frac{3}{2} \right) \exp \left[ -\left( \frac{\varepsilon - \varepsilon_{\text{ext}}}{\Gamma_{\text{ext}}} \right)^2 \right] d\varepsilon$

and $\sigma_{xy} = en_2D/B + \Delta \sigma_{xy}$; $\Delta \sigma_{xy}$ is a small correction \textit{11}. We model the extended Landau states by a gaussian $g_{\text{ext}}(\varepsilon)$ of width $\Gamma_{\text{ext}} = 0.25$ meV \textit{24}.

\textbf{Hysteretic resistance spikes and dips.} The ordinary $\rho_{xx}$ peaks in Fig. 1(a), \textit{e.g.}, at 2.5, 3.1, and 5 T, are due to subsequent single Landau levels crossing the chemical potential $\mu$ and appear between plateaus in $\rho_{xy}$. Though involving the crossing of two opposite-spin levels at $\mu$, the $\rho_{xx}$ spike at $B \sim 5.8$ T has the same physical origin as the ordinary peaks: electrons in partially filled crossings are susceptible to scattering (“dissipation”) which increases $\rho_{xx}$. This spike, however, corresponds to a dip in a plateau of $\rho_{xy}$: as the two Landau levels cross near $\mu$, the number of conducting channels $n_c$ “fluctuates” thus making $\rho_{xx}$ dip $\left( \Delta n_c > 0 \right)$ [or peak $\left( \Delta n_c < 0 \right)$] toward an adjacent plateau consistent with $n_c$. Whether $\rho_{xy}$ dips or peaks and whether the spikes and dips are stronger in the up or down sweeps depend on the details of the crossings at $\mu$. Fig. 2(a) — these features are, however, hysteretic as $n_c$ differs in the up and down $B$ sweeps. For increasing tilt angles $\theta$, Fig. 3, the hysteretic spike shifts to lower fields while the ordinary Shubnikov-de-Haas maxima do not. Figure 3 uniquely identifies ordinary (single Landau levels crossing $\mu$) and “anomalous peaks” (two Landau levels crossing $\mu$) in $\rho_{xx}$.\n
\textbf{Hysteresis \& critical temperature.} Figure 4(a) shows
The asymmetric shape of our hysteretic loops [Figs. 1(b)-(d)] the hysteresis in the Tal value 1.3 K [7]. The amplitude of the spike is also hysteretic, Fig. 4(b). Here, however, only the up-sweep behavior agrees with the data [6].

Further comparison with experiments. We also reproduce the non-hysteretic $\rho_{xx}$ peak at $\sim 3.2$ T (single level crossing $\mu$) seen in [6]. We find that the peak at $\sim 2.8$ T [6] arises from two levels crossing $\mu$ and predict that it shifts upward (as opposed to Fig. 3 here) as $\theta$ increases because $g > 0$ in [6] while $g < 0$ in [6]. However, we do not find any hysteretic behavior here. Essentially, the non-integral filling factors near the opposite-spin level crossings in [6] (as opposed to [7]) result in exchange energy gains not enough to induce phase transitions.

Final remarks. (i) Quenched-disorder-induced domains – not domains arising in metastable states [8, 23] – can lead to transport anisotropies in 2DEGs [6, 27]. (ii) The relevance of the hyperfine coupling to the hysteretic phenomena has been recognized experimentally only in the fractional quantum Hall regime. We account for disorder effects only via the broadening of the Landau levels and neglect the hyperfine coupling and domains altogether. Our successful description of hysteretic (quantum Hall) ferromagnetic phenomena in 2DEGs highlights the power of DFT in a non-conventional application.

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