Density dependence of critical magnetic fields at the metal-insulator bifurcation in two dimensions

D. J. W. Geldart[1,2,3] and D. Neilson[1,4]
[1]*School of Physics, University of New South Wales, Sydney 2052 Australia*
[2]*Department of Physics, Dalhousie University, Halifax, NS B3H3J5 Canada*
[3]*Laboratoire des Verres, Université de Montpellier II, Montpellier 34095 France*
[4]*Dipartimento di Matematica e Fisica, Università di Camerino, I-62032 Camerino, Italy*
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The density dependence of the critical in-plane magnetic field B_c at the bifurcation of the resistivity of two-dimensional electron systems with low levels of disorder is determined using the spin-polarization dependence of the electron exchange-correlation hole. Recent numerical simulation results for ground-state energies also permit determination of the magnetic field $B_{\rm pol}(n)$ needed to saturate the spin polarization. The resulting picture gives a good account of reported experimental results for B_c as a function of electron density in *p*-type GaAs systems and indicates that the interactions between electrons play a crucial role in the bifurcation phenomenon.

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I. INTRODUCTION

The observations[1] of a bifurcation of the resistivity of high quality low carrier density two-dimensional (2D) electron or hole systems into two branches (metal-like and insulatorlike) at low temperatures has raised several important questions. The intriguing scaling of resistivity with temperature, density, and electric field is suggestive of a continuous phase transition associated with a quantum critical point. Irrespective of whether or not there is a metal-insulator phase transition at zero temperature, the bifurcation observed at finite temperature is itself very striking. There has been considerable discussion about the importance of the electron-electron interactions at low electron densities at which these effects are observed and also of the extent to which the phenomenon might be explained by material-dependent effects. However, the physical origin of the bifurcation remains unclear. A review of the experimental results and of explanations offered has been given by Abrahams *et al.*[2]

The regime of metal-like resistivity, defined by having $\partial\rho(T)/\partial T>0$, occurs for electron or hole densities greater than a critical value $n>n_c$. The critical density depends on the disorder level of the particular sample. Application of even a relatively weak external magnetic field to a sample of density $n>n_c$ can suppress the metallic behavior and drive the sample into the insulating regime $[\partial\rho(T)/\partial T<0]$. The magnetic field at which the resistivity slope is just reduced to zero, $B_c(n)$, is density dependent. The case of a magnetic field B applied parallel to the plane of the 2D sample is particularly revealing in that a parallel field does not cause orbital effects (neglecting effects due to the finite thickness of the 2D layer or complex band structure). The fact that the in-plane magnetic field then couples only to the electron spins via the Zeeman energy indicates that the degree of spin polarization induced by B plays a dominant role.

As the magnetic field is further increased beyond $B_c(n)$, the resistivity at a fixed temperature continues to increase until it saturates at a field $B_{\rm sat}(n)$ at a plateau value.[3–7] The plateau is clearer in the Si samples but a similar change in character occurs in GaAs samples. Shashkin *et al.* suggested that the saturation of the resistivity in 2D electron Si samples coincides with complete polarization of the electron spins in the magnetic field.[5] The saturation fields tended to vanish at a finite density when extrapolated to the zero field limit. This was interpreted as a ferromagnetic instability. A very different scaling analysis of magnetoconductivity data on a Si metal oxide semiconductor field-effect transistor has been given by Vitkalov *et al.*[4] With a suitable empirical definition of a reference saturation field, the magnetic-field-dependent part of the conductivity was found to satisfy a scaling relation to within an accuracy of about 5% over the density and temperature range of the experiment. This suggested a quantum critical point, also possibly due to a transition to a ferromagnetic state. Knowledge of the magnetic field required to achieve complete spin polarization, $B_{\rm pol}(n)$, is an important piece of information for piecing together the magnetic equation of state of the electron system. This is highly relevant for the very low density electron systems that are especially sensitive to magnetic fields.

However, Pudalov *et al.*[8] have recently questioned this interpretation of $B_{\rm sat}(n)$. They consider a direct determination of $B_{\rm pol}(n)$ expressed as

$$B_{\rm pol}(n)=\pi\hbar^2 n/[m^* g^* \mu_B], \tag{1}$$

where the g factor g^* and mass m^*, renormalized by Coulomb interactions, were determined in a series of experiments on Si samples and are sample independent. The valley degeneracy $g_v=2$ has been taken into account in Eq. (1). No ferromagnetic instability was found over their range of density, which included the bifurcation. The saturation magnetic fields were also obtained and studied carefully as a function of the cool-down rate of the samples. Two very important facts emerged. First, $B_{\rm sat}(n)$ was found to depend on the cool-down rate although the dependence was weak for the slowest cool-down rates and results were then quite reproducible. Second, $B_{\rm sat}(n)$ as determined from the slow cool-down experiments was consistently larger, especially at the

lower densities, than the measured polarization fields $B_{\rm pol}(n)$ as expressed by Eq. (1). This suggested that the saturation of the magnetoresistance may not be due entirely to the spin polarization of itinerant electrons.

It is clear that an independent determination of $B_{\rm pol}(n)$ would be very helpful in other low carrier density and high mobility systems for which experimental data for $B_{\rm sat}(n)$ are available. The saturation magnetic fields $B_{\rm sat}(n)$ have been measured for *p*-type GaAs systems.[6,7] The critical fields $B_c(n)$ have also been measured. However, the required Landau parameters have not yet been measured. In addition, the prospects for accurate calculation of the Landau parameters from first principles are not good because of the strong Coulomb interaction effects at low density.

Regarding the role of the electron-electron interactions, we present a theoretical procedure which leads to a physical picture of the bifurcation and makes clear the importance of electron-electron interactions in the development of the bifurcation. A procedure is described for the determination of the field and density dependence of the polarization and the density dependence of the spin-polarization saturation field. Published numerical data then give $B_{\rm pol}(n)$ and $B_c(n)$ for strongly interacting electron systems provided the disorder is weak. At very low electron densities the effect of finite temperature is taken into account. This picture gives a good description of the critical and saturation fields in *p*-type GaAs and is also consistent with results on Si systems. Here we will primarily focus on analyzing results for *p*-type GaAs.

II. GROUND-STATE SPIN PROPERTIES

Reliable numerical data are available for the ground-state properties of defect-free 2D electron systems. It is known from quantum Monte Carlo (QMC) calculations of the ground-state energy that the pure electron system undergoes a first-order transition from a liquid state to an electron solid (Wigner crystal) at an extremely low density[9–11] corresponding to $r_s=37\pm5$, where r_s is the average electron spacing measured in units of effective Bohr radii a_B^*. For *p*-type GaAs $a_B^*=2.2\times10^{-7}$ cm. Results for a disordered electron system are sparse. It has been suggested that the effect of disorder is to shift the liquid to solid transition to higher density.[12] There are also QMC results for spin-polarized systems.[10,13] These results suggest that the ground state of the homogeneous electron fluid may become fully spin-polarized just prior to the liquid-solid transition. No evidence for ground states of partial spin polarization has been given. Comparable results have been obtained by a recent semianalytical procedure based on hypernetted chain methods (including bridge corrections) with some numerical input from a previous QMC calculation of the correlation energy of the unpolarized ground state.[14] The resulting ground-state energies for the unpolarized and polarized systems are in good agreement with diffusion QMC results.

We use the most recent diffusion QMC data for the ground-state energy of the defect-free electron system as a function of *n*, the number of electrons per unit area *A*, and of $\zeta=(n_\downarrow-n_\uparrow)/n$, the spin polarization.[13] With these data we now determine ζ as a function of *n* and the in-plane magnetic field *B*, and also the field $B=B_{\rm pol}(n)$ required to fully polarize the electron spins ($\zeta=1$).

The ground-state energy in the presence of quenched disorder due to nonmagnetic impurities and with in-plane magnetic field *B* is, in the sense of spin density functional theory, given by

$$E[n_\uparrow,n_\downarrow;B]=E^{\rm dis}[n]+E^{\rm el}[n_\uparrow,n_\downarrow]+E^Z, \tag{2}$$

where

$$E^{\rm dis}[n]=\int d^2r V^{\rm dis}(r)n(r), \tag{3}$$

provided the disorder can be described by a spin-independent one-body potential $V^{\rm dis}(r)$. The density of electrons of spin σ is $n_\sigma=N_\sigma/A$ where $N_\sigma=\int d^2r n_\sigma(r)$. The second term in Eq. (2) is the sum of the kinetic and Coulomb interaction energies intrinsic to the electron system and the third term is the usual Zeeman energy with g_0 the bare *g* factor

$$E^Z=\int d^2r(g_0\mu_B/2)[n_\uparrow(r)-n_\downarrow(r)]B. \tag{4}$$

Numerical data are available only for pure systems but the net effect of a perturbing potential on the energies $E[n_\uparrow,n_\downarrow;B]$ should be small if we assume the level of disorder is sufficiently low. Then pure system densities can be used in the sense of a variational principle to give good first approximations to $E^{\rm el}[n_\uparrow,n_\downarrow]$ and $dE^{\rm el}/d\zeta$. For applied field $B<B_{\rm pol}(n)$ the polarization $\zeta(B)$ is obtained by minimizing Eq. (2) with respect to ζ. The ζ derivative at fixed *n* of $E^{\rm dis}[n]$ is zero so we obtain

$$\left.\frac{\partial\epsilon(n,\zeta)}{\partial\zeta}\right|_n-\frac{g_0\mu_B}{2}B=0, \tag{5}$$

where $\epsilon(n,\zeta)=E^{el}[n_\uparrow,n_\downarrow]/N$. The solution of Eq. (5) gives the induced polarization $\zeta(B)$ for the given magnetic field *B*. The saturation field $B=B_{\rm pol}$ occurs when the polarization obtained from Eq. (5) reaches unity, that is,

$$g_0B_{\rm pol}(n)=\frac{2}{\mu_B}\left.\frac{\partial\epsilon(n,\zeta)}{\partial\zeta}\right|_n \tag{6}$$

at $\zeta=1$.

The derivative in Eq. (6) is obtained from fits to diffusion QMC data given in Ref. 13. The resulting $g_0B_{\rm pol}(n)$ for the ground state of a weakly disordered 2D electron system is shown as the dashed line in Fig. 1. However, at the lower electron densities, the energy scale of the $T=0$ polarization field becomes less than or comparable to thermal energies in the typical temperature range of the experiments, $0.1\lesssim T\lesssim2$ K. The thermal disordering influence of finite temperature opposes the spin ordering induced by the applied magnetic field. The magnetic field required at finite temperature to produce a given polarization is then greater than the corresponding $T=0$ value. We account for the effect of finite temperature by the empirical form

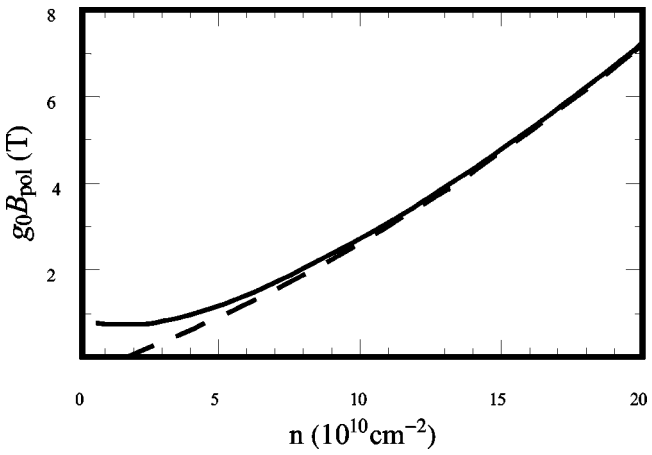

FIG. 1. $B_{\mathrm{pol}}(n)$ needed to saturate the spin polarization as a function of density for p-type GaAs at temperature $T_0=0.5$ K. Dashed line is $B_{\mathrm{pol}}(n)$ at zero temperature.

$$B_{\mathrm{pol}}(n,T_0)=[B_{\mathrm{pol}}(n,T=0)^2+T_0^2]^{1/2}, \tag{7}$$

where T_0 is proportional to the electron temperature. The correction is important when $g_0\mu_B B_{\mathrm{pol}}(n,T=0) \lesssim k_B T$. Figure 1 shows the dependence of $B_{\mathrm{pol}}(n,T_0)$ on density for $T_0=0.5$ K.

The density at which any spin-dependent ordered state appears in a given experimental sample can vary with the level of disorder but the slope of $B_{\mathrm{pol}}(n)$ and its overall magnitude should be sample independent except very close to such a transition. The transition in the disordered system need not be of first order even though it may be in the pure defect-free system. In the case of finite temperature thermally driven phase transitions it is known that the presence of disorder can cause a first-order phase transition to become continuous.[15,16] This should also apply to a ground-state phase transition in disordered electron systems. This is consistent with the observed scaling behavior with respect to electric field, temperature, and density in the 2D systems that have been studied experimentally.[1,2]

III. PROPOSED MECHANISM AT BIFURCATION

We now consider the density dependence of the critical magnetic field $B_{\mathrm{crit}}(n)$ at the bifurcation. This requires a physical picture of how spin polarization affects conduction near the bifurcation. One of the dramatic features of low density electron systems is the development around each electron of a large exchange-correlation hole, generated by the strong Coulomb interactions, including a region from which all other electrons are excluded. This area of strong exclusion acts effectively like a repulsive hard core, and increasing its size significantly is expected to influence the mobility of the charge carriers. It is known from QMC data that the size of this total exclusion region, relative to the average area per particle, increases when the density is decreased or when the spin polarization is increased.[9,10]

An insulator is characterized by low energy many-electron wave functions in configuration space that are sums of essentially disjoint pieces with very small overlap between them.[17] Conduction in the insulating regime is then well described by a hopping picture. On the other hand, the metallic state exhibits a strong overlap of wave functions, and the picture of transport by itinerant carriers is then correct. The bifurcation is a finite temperature smooth transition between the two regimes. In the presence of disorder, transport in the metallic regime will be hindered by any expansion of the exchange correlation hole.

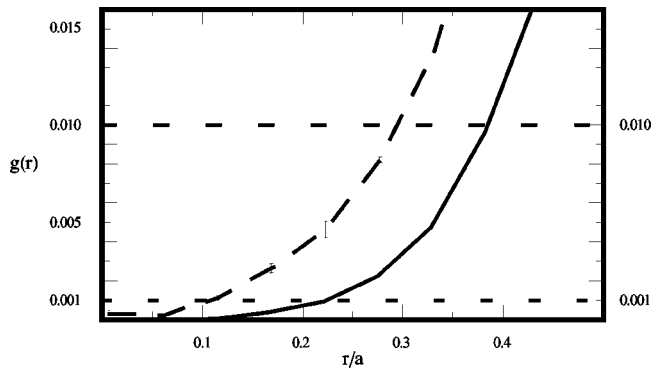

FIG. 2. Pair correlation function $g(r)$ with error bars for small r/a at $r_s=10$ for the unpolarized (dashed line) and fully spin-polarized cases (solid line), from Ref. 10. a is the interparticle spacing.

The area of the total exclusion region provides a good measure of the effect of strong electron-electron interactions in the exchange-correlation hole. We propose that the bifurcation at a critical density n_c in a given sample corresponds to a critical size of the total exclusion region. Information on the size of the exchange-correlation hole and its dependence on the electron density and spin polarization is obtainable from the published QMC data on pair correlation functions. The pair correlation function, $g(\mathbf{r},\mathbf{r}')$, is the probability of finding a second electron at the point $\mathbf{r}$ in the sample when an initial electron is known to be located at $\mathbf{r}'$. Complete details of the inhomogeneous system are not required and it is sufficient to average the pair correlation function over the random distribution of the impurities. This restores translational invariance so that $[g(\mathbf{r},\mathbf{r}')]_{av}=\bar{g}(|\mathbf{r}-\mathbf{r}'|)$. Information in disordered systems is sparse but a great deal is known about the pair correlation functions of the corresponding pure system ground states.[10] The pure system data are relevant because the total exclusion area is strictly a short distance property. Its maximum radius is about 20% of the average interparticle separation over the density range of the experiments we consider. We expect the averaged pair correlation function $\bar{g}(r)$ of a weakly disordered system to exhibit the same exchange-correlation structure on this small distance scale.

Figure 2 for the pair correlation function[9,10] at $r_s=10$ clearly shows the significant region of practically zero electron density surrounding each electron, which is generated by the strong electron-electron interactions at this quite low density. The error bars are from Ref. 10. The exclusion effect of the exchange-correlation hole is larger for spin-polarized electrons because of the additional exchange acting between

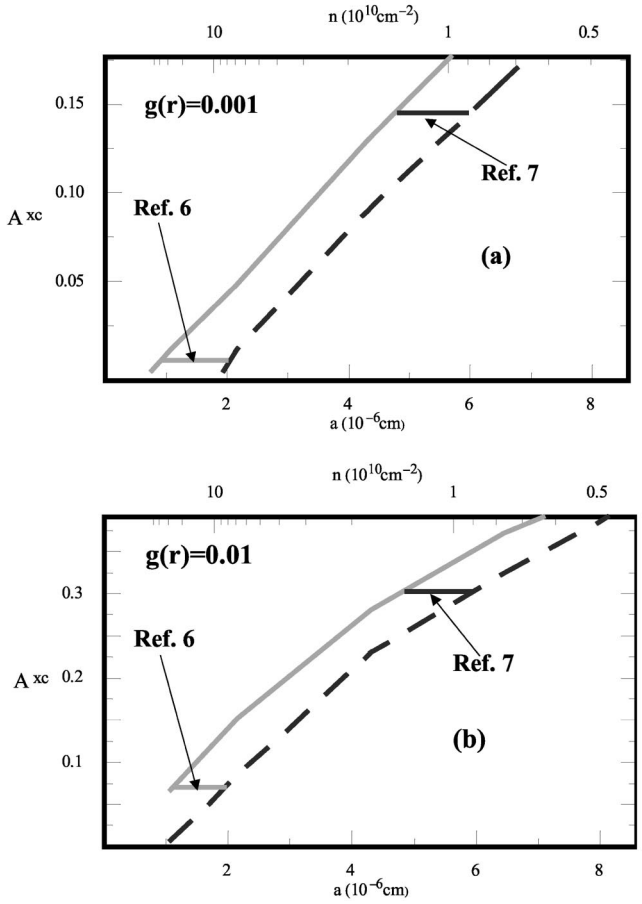

FIG. 3. Exchange correlation relative totally excluded area A^{xc} (scaled to the average area per electron) as a function of the interparticle spacing a. Unpolarized system: dashed line. Fully polarized system: solid line. (a) $g(r_{\mathrm{xc}})=0.001$. (b) $g(r_{\mathrm{xc}})=0.01$. Horizontal lines show constant A_c^{xc} for Refs. 6 and 7 (see discussion in text).

the spin-aligned electrons. As the electron density is increased, the influence of electron-electron interactions decreases relative to the kinetic energy. This causes the relative area of the total electron exclusion region to shrink.

IV. RESULTS

For a quantitative discussion of the exchange-correlation hole, we consider an effective radius of the excluded area as determined by the condition either $g(r)\leqslant 0.001$ or $g(r)\leqslant 0.01$ for $r\leqslant r^{\mathrm{xc}}$ (see Fig. 2). The radius r^{xc} is determined as a function of density n from the published data. Figure 3 shows the corresponding relative excluded area, $A^{\mathrm{xc}}=[\pi(r^{\mathrm{xc}})^2/\pi a^2]$ scaled relative to the average area per electron (dimensionless units). Results are shown for $g(r^{\mathrm{xc}})=0.001$ and $g(r^{\mathrm{xc}})=0.01$. Our quantitative conclusions are independent of which of these criteria is selected. Figure 3 gives $A^{\mathrm{xc}}(a)$ as a function of a for the unpolarized and fully polarized systems (dashed and solid lines, respectively), and we use this to determine the critical field $B_c(n)$ as a function of density. As the magnetic field increases, the spin polarization and consequently the size of the exchange-correlation hole increase.

Our proposal is that the change in character of the mobility for a given sample occurs at a critical value for the relative area of total exclusion (relative to the average area per particle). An unpolarized sample in zero field at its critical density n_c is represented by a point on the lower unpolarized curve (dashed line) at $n=n_c$. This point specifies the critical excluded area A_c^{xc} for that sample. Our condition for suppression of the metalliclike character of $\rho(T)$ as a function of density is the critical line $A^{\mathrm{xc}}(a,\zeta)=A_c^{\mathrm{xc}}=\mathrm{const}$. This is a line drawn in Fig. 3 horizontally from the point $n=n_c$ on the unpolarized curve across to the polarized curve. The polarization $0\leqslant\zeta(B)\leqslant 1$ and hence the critical magnetic field $0\leqslant B_c\leqslant B_{\mathrm{pol}}$ increase as we travel along this line. This condition can be expressed as

$$0=\delta A_c^{\mathrm{xc}}(a,\zeta)=\left(\frac{\partial A_c^{\mathrm{xc}}}{\partial a}\right)_{\zeta}\delta a+\left(\frac{\partial A_c^{\mathrm{xc}}}{\partial \zeta}\right)_{a}\delta\zeta. \tag{8}$$

For example, suppose in Fig. 3 we start from some critical density $n=n_c$ on the lower unpolarized curve at A_c^{xc}. If we increase the density to $n=n_c+\delta n$, then the dashed line $A^{\mathrm{xc}}(a)$ for the unpolarized system drops below the critical value A_c^{xc} for the bifurcation and the resistivity is metalliclike. For density fixed at $n=n_c+\delta n$ we can return $A^{\mathrm{xc}}(a,\zeta)$ back up to the critical A_c^{xc} value by increasing the polarization $\zeta(B)$. The critical magnetic field $B_c(n)$ produces precisely the polarization $\zeta(B)$ needed to intersect with the horizontal line at $n=n_c+\delta n$. Thus as the magnetic field is increased the bifurcation moves to higher density. Since A_c^{xc} is constant this corresponds to moving left along a horizontal line shown in Fig. 3. $\zeta(B)$ reaches unity at $B=B_{\mathrm{pol}}$ at which point we arrive at the solid line $A^{\mathrm{xc}}(a)$ for the fully polarized system.

From Eq. (8) we deduce that the polarization $\zeta(a)$ as a function of a along the critical line is given by

$$\zeta(a)=\int_0^a da(d\zeta/da) \tag{9}$$

with

$$\frac{\delta\zeta}{\delta a}=\frac{(\partial A_c^{\mathrm{xc}}/\partial a)_{\zeta}}{(\partial A_c^{\mathrm{xc}}/\partial\zeta)_a}. \tag{10}$$

We apply Eqs. (9) and (10) to data from experiments reporting a dependence of the density on an in-plane magnetic field at the metal-insulator bifurcation in p-type GaAs samples.[6,7] The derivatives on the right hand side of Eq. (10) are obtained numerically from data in Ref. 10, and the resulting $\delta\zeta/\delta a$ determines $\zeta(a)$ by Eq. (9). We take an effective hole band mass to free electron mass ratio $m_h^*/m_e=0.3$ and dielectric constant $\kappa=12.5$. The critical hole density, n_c, at which the resistivity bifurcates into two distinct branches in zero magnetic field is sample dependent. In a parallel magnetic field, Hamilton *et al.*[6] reported a shift in the critical density from density $n=7.5\times10^{10}$ cm^{-2} at $B=0$ to 12.4×10^{10} cm^{-2} for $B=0.6$ T. Yoon *et al.*,[7] working at lower hole densities, found a critical density that increased

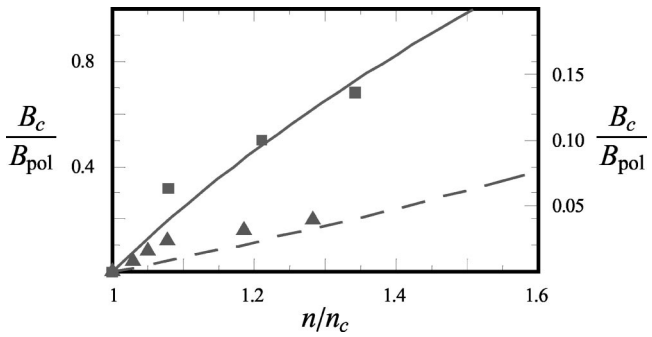

FIG. 4. Critical magnetic field B_c as a function of the hole density n at the bifurcation of the resistivity. n_c is the critical density at zero magnetic field. $B_{\rm pol} \equiv B_{\rm pol}(n_c)$ is given by Eq. (7). The triangles and dashed line are the experimental data and our calculated dependence, respectively, for Ref. 6. The squares and solid line are the corresponding quantities for Ref. 7. Vertical scales on the right and left axes are $B_c/B_{\rm pol}$ for Refs. 6 and 7, respectively.

from $n=0.9\times10^{10}$ cm^{-2} at $B=0$ to 4.2×10^{10} cm^{-2} as the magnetic field increased up to $B=7.5$ T. Data in Ref. 7 for $B>4$ T may be associated with an independent high field phenomenon and for this reason we do not include it in our analysis.

The horizontal lines shown in Fig. 3 correspond to Refs. 6 and 7. The critical $A_c^{\rm xc}$ is determined by the value of the unpolarized curve at $n=7.5\times10^{10}$ cm^{-2} and $n=0.9\times10^{10}$ cm^{-2}, for Refs. 6 and 7, respectively. The polarization $\zeta(B)$ increases from $\zeta=0$ to $\zeta=1$ as we move along the horizontal line. The dependence of $\zeta(B)$ on magnetic field is given by Eqs. (5) and (6).

The resulting dependence of the critical magnetic field B_c on the hole density n at the bifurcation of the resistivity is shown in Fig. 4. The density is scaled to n_c, the critical density at $B=0$, and the magnetic field is scaled to $B_{\rm pol} \equiv B_{\rm pol}(n_c)$, given by Eq. (7). The points are the experimental data and the lines show the theoretical dependence. The g factor in GaAs is very sensitive to the sample and we have taken it as a fixed parameter for each experiment, $g_0=0.2$ for Ref. 6 and $g_0=0.4$ for Ref. 7. The value of $B_{\rm pol}$ is an independent prediction of the magnetic field strength for full polarization in this material.

V. CONCLUSIONS

In conclusion, we have given a physical picture for the bifurcation of the resistivity of 2D systems at low carrier densities and with low levels of disorder. We propose that the critical density at the bifurcation in a particular sample corresponds to a critical size of the total exclusion region in the exchange correlation hole. This supports the importance of the role of electron-electron interactions in driving the bifurcation. The effect of an in-plane magnetic field is interpreted in terms of the dependence of the size of the exchange-correlation hole on spin polarization. The critical field $B_c(n)$ at the bifurcation can then be determined from published QMC numerical data for pair correlation functions and ground-state energies. The resulting picture gives a good account of experimental results for $B_c(n)$.

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