Low density spin-polarized transport in 2D semiconductor structures: The enigma of temperature dependent magnetoresistance of Si MOSFETs in an in-plane applied magnetic field

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The temperature dependence of 2D magnetoresistance in an applied in-plane magnetic field is theoretically considered for electrons in Si MOSFETs within the screening theory for long-range charged impurity scattering limited carrier transport. In agreement with recent experimental observations we find an essentially temperature independent magnetoresistance for carrier densities well into the 2D metallic regime due to the field-induced lifting of spin and, perhaps, valley degeneracies. In particular the metallic temperature dependence of the ballistic magnetoresistance is strongly suppressed around the zero-temperature critical magnetic field ($B_c$) for full spin-polarization, with the metallic temperature dependence strongest at $B = 0$, weakest around $B \sim B_s$, and intermediate at $B \gg B_s$

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I. INTRODUCTION

The phenomena of 2D metallic behavior and the associated 2D metal-insulator transition (MIT) comprise a complex set of low-temperature transport behavior of low-density 2D electron (or hole) systems in high-quality (i.e. low-disorder and high-mobility) semiconductor structures. In particular, the 2D resistivity, $\rho(n, T, B)$, shows intriguing and anomalous dependence on carrier density ($n$), temperature ($T$), and applied magnetic field ($B$) parallel to the 2D plane [1,2]. For example, the low temperature $\rho(T)$, in zero applied field, shows remarkably strong “metallic”-like (i.e. $d\rho/dT > 0$ for $n > n_c$) temperature dependence for 2D carrier densities above the so-called critical density ($n_c$) for the 2D MIT whereas, for $n < n_c$, the system exhibits insulating behavior ($d\rho/dT < 0$). The strength of the metallicity (i.e. how strongly $\rho(T)$ increases with $T$ at low temperatures for $n > n_c$) and the actual value of $n_c$ are highly nonuniversal, and depend strongly (and nontrivially) on the material and on the 2D sample quality. The application of an in-plane magnetic field $B$ has several interesting effects on the 2D metallic phase [3–10]: (1) at a fixed low $T$, the system develops a large positive magnetoresistance with $\rho(B)$ increasing very strongly (by as much as a factor of 4) with $B$ up to a maximum field $B_s$; (2) for $B > B_s$, $\rho(B)$ either saturates (or increases slowly with $B$ for $B > B_s$) showing a distinct kink at $B = B_s$; (3) the temperature dependence of resistivity is considerably suppressed in a finite parallel field; (4) for 2D electrons in Si MOSFETs, which is the most extensively studied system in the context of 2D MIT, the external magnetic field at densities close to the critical density (i.e. $n \geq n_c$) seems to drive the system into a strongly insulating phase generating a huge positive magnetoresistance and manifesting the strongly insulating activated temperature dependence typical of the zero-field transport for $n < n_c$

In this paper we restrict ourselves to the highly metallic (“ballistic”) $n > 2n_c$ regime and investigate theoretically the enigmatic temperature dependence of the parallel field magnetoresistance $\rho(B; T)$ of n-Si MOSFETs as described in items (1) –(3) above. The item (4), which arises from the destruction of the 2D effective metallic phase by a large in-plane field in the $n \geq n_c$ regime, is obviously related to the 2D metal-insulator transition itself (or more precisely, its parallel field dependence) and is beyond the scope of the current theory which deals only with the apparent effective 2D metallic phase in the ballistic regime. We include in the theory only resistive carrier scattering by screened effective disorder arising from charged impurity centers randomly distributed at the Si-SiO$_2$ interface with the screening calculated within the finite wave vector self-consistent field random-phase-approximation (RPA) at finite temperatures fully incorporating the carrier spin polarization induced by the applied in-plane magnetic field. In our theory the magnetic field effects enter only through the carrier spin polarization correction. The temperature dependence (at zero field) [11] and the parallel-field dependence (at $T = 0$) [12] of $\rho(T; B)$ have earlier been individually theoretically studied in the literature for Si MOSFETs within the screening theory formalism – our goal here is to combine the two to obtain a full theory for $\rho(T; B)$ in Si MOSFETs including spin-polarization effects on the finite-temperature screening properties.

We emphasize that, although the 2D “metallic” transport properties are anomalous in the presence of a parallel magnetic field in all of the 2D systems studied so far, the 2D Si MOS system is unique in exhibiting a particularly intriguing temperature dependent magnetoresistance $\rho(T, B)$ where $\rho(T)$ for $B > B_s$ and $n \geq 1.5n_c$ seems to be essentially a constant at low temperatures [7,8]. In this paper we propose a simple physically motivated theoretical explanation for the anomalous trans-
port properties of Si MOSFETs in the presence of a strong parallel magnetic field. Our explanation is based on the substantial modification of the effective quenched disorder in the system (arising from the screened background impurity potential) due to the applied parallel field which strongly affects the 2D screening properties. We believe (and show in this paper) that a qualitative understanding of the temperature dependence of \( \rho(T; B) \) can be obtained on the basis of an effective field-dependent disorder.

The applied parallel magnetic field has, in principle, seven distinct (and sometimes, opposing) physical effects on the 2D metallic transport behavior: (1) the magneto-orbital coupling [13] due to the finite thickness of the 2D layer leads to an anisotropically increasing 2D effective mass, consequently giving rise to a positive anisotropic magnetoresistance; (2) the parallel field couples the 2D in-plane dynamics to the dynamics in the confinement direction (perpendicular to the 2D plane) leading to intersubband scattering (i.e. 2D to 3D crossover) induced positive magnetoresistance [13]; (3) the parallel field may effectively “enhance” weak localization “insulating” temperature correction [14] by suppressing various “metallic” contributions (e.g. screening) to the temperature dependent resistivity; (4) the parallel field-induced carrier spin polarization leads to an enhancement of the effective Fermi momentum, \( k_F(B) \), which tends to contribute a negative magnetoresistance through the decrease of the charged impurity scattering matrix elements; (5) the parallel field-induced carrier spin polarization reduces the strength of screening (by as much as a factor of 2) since the electronic density of states decreases from 2 to 1 as the 2D electrons become completely spin-polarized; (6) the parallel field may further suppress screening (by as much as an additional factor of 2) in Si MOSFETs by lifting the valley degeneracy factor (for example, from 2 to 1 if \( \Delta_v > E_F \), \( k_B T \), where \( \Delta_v \) is the valley splitting in the presence of the parallel field); (7) the parallel field induced modification of the electron-electron interaction [15], due to the spin-polarization of the 2D electrons which suppresses the “triplet” interaction channel.

We develop a theory for \( \rho(T, B, n) \) in Si MOSFETs including the three physical mechanisms [(4) - (6) listed above] which are important for Si MOS systems. We leave out the magneto-orbital effects (items (1) and (2) above) [13] because the magneto-orbital corrections are rather small in Si MOSFETs since the quasi-2D layer width (i.e. the confinement size transverse to the 2D plane) is rather small, making magneto-orbital coupling essentially negligible in Si MOSFETs except at very high parallel fields. We do not consider the weak localization correction since it is straightforward to include it (in an ad hoc fashion) if experimental results warrant such a theoretical adjustment [14]. We also uncritically ignore all electron-electron interaction corrections beyond the screening (i.e. ring diagrams) effects, arguing screening to be the dominant physical mechanism controlling transport limited by Coulomb disorder arising from charged impurity scattering. Interaction effects in the presence of a parallel magnetic field have been considered in the literature [15].

The main physical effect we consider, namely the parallel field induced decrease of the 2D density of states leading to a strong field induced suppression of screening (and hence a strong positive magnetoresistance), has earlier been discussed in the literature [12], primarily in the context of the \( T = 0 \) magnetoresistance itself (whereas our focus is on the temperature dependence of magnetoresistance). We have recently [16] discussed the similarity between the behavior of \( \rho(B; T = 0) \) and \( \rho(T; B = 0) \) in Si MOSFETs [17] as arising from the field-induced or the temperature-induced suppression of screening, leading to qualitatively “similar” parallel-field dependent (at \( T = 0 \)) and temperature-dependent (at \( B = 0 \)) effective disorder in MOSFETs. (As an aside we mention that the situation is quite different in 2D GaAs electron [18] and hole [19] systems where substantial magneto-orbital coupling is present, leading to qualitatively different \( \rho(B) \) and \( \rho(T) \) behaviors.) The goal of the current paper is to develop a theory for \( \rho(T; B) \), the temperature dependence of the 2D magnetoresistivity in Si MOSFETs, particularly at large fields \( B \geq B_s \), where the 2D system is presumably completely spin-polarized. The motivation for our theoretical work comes from the recent experimental work [7] reporting a puzzling absence of any temperature dependence in \( \rho(T; B > B_s) \) of Si MOSFETs in the completely spin-polarized large applied parallel field (\( B > B_s \)) ballistic \( (n > 1.5n_c) \) transport regime. Since the zero-field (i.e., spin unpolarized) 2D transport in these high-quality low-density Si MOSFETs is characterized by strong metallicity, i.e. a strong metallic temperature dependence in \( \rho(T) \), the apparent complete suppression of the metallicity in the spin-polarized system is intriguing and has attracted a great deal of attention. The complete reported absence of any temperature dependence of \( \rho(T; B > B_s) \) in Si MOSFETs [7] also stands in sharp contrast to the corresponding situation [20] in n-Si/SiGe 2D structures, where \( \rho(T; B > B_s) \) shows metallic temperature dependence in the spin-polarized case, albeit with a reduced magnitude of \( d\rho/dT \) in accordance with the screening theory. We discuss these issues in great details in the next four sections of this article. In sec. II we provide the Boltzmann transport theory. In sec. III we give our calculated results. In sec. IV we discuss our results. We conclude our paper in sec. V.

II. THEORY

We use the semiclassical Boltzmann transport theory [11] including only the effect of resistive scattering by random charged impurities at the Si-SiO\(_2\) interface –
at low carrier densities (and at low temperatures where phonon scattering is unimportant) of interest in the 2D MIT problem, transport in high-mobility Si MOSFETs is known to be predominantly (but perhaps not entirely) limited by long-range charged impurity scattering. The density of the random interface charged impurity centers is therefore the only unknown parameter in our model, which sets the overall scale of $\rho(T = 0)$ without affecting the $(T, n, B)$ dependence of resistivity that is of interest in the problem. The bare disorder potential arising from oxide charged impurity centers being long-range Coulombic in nature, the most important physics ingredient (at the zeroth-order) that any transport theory must incorporate is the regularization of the bare long-range Coulombic disorder potential by screening the impurity potential. Within our zeroth-order minimal transport theory, this is precisely what we do by calculating the finite temperature screened effective disorder through the static (finite-temperature and finite-wave vector) RPA screening of the bare long-range Coulombic disorder [11].

We then use the Boltzmann theory to calculate the finite-temperature carrier resistivity limited by scattering due to the effective “regularized” (i.e. screened) impurity disorder. We include in our theory the realistic effects of the \textit{quasi}-2D layer width of Si MOSFETs through the appropriate quantum form factors, and most importantly we include the nonperturbative effect of the parallel magnetic field through the spin polarization of the 2D electron system fully incorporating the physical mechanisms (4) and (5) discussed above [12,16] in Sec. I. (The inclusion of the mechanism (6) in the theory, namely the field-induced lifting of valley degeneracy, i.e. valley polarization, is straightforward by adjusting the valley degeneracy factor $g_v$ in the 2D density of states and is discussed below.)

The formal aspects of the calculation for $\rho(n; T; B)$ in the presence of the parallel magnetic field are essentially the same as those for $\rho(n; T) = 0$ except for the existence of different spin-polarized carrier densities $n_{\pm}$. When the parallel magnetic field is applied to the system the carrier densities $n_{\pm}$ for spin up/down are not equal. Note that the total density $n = n_+ + n_-$ is fixed. The spin-polarized densities themselves are obtained from the relative shifts (i.e. the spin-splitting) in the spin up and down bands introduced by the Zeeman splitting associated with the external applied field $B$. At $T = 0$, one simply has $n_{\pm} = n(1 \pm B/B_s)/2$ for $B \leq B_s$ with $n_+ = n$ and $n_- = 0$ for $B \geq B_s$ (and $n_+ = n_- = n/2$ at $B = 0$), where $B_s$ is the so-called saturation (or the spin-polarization) field, is given by $g \mu_B B_s = 2E_F$ where $g$ is the electron spin $g$-factor and $\mu_B$ the Bohr magneton. For $T \neq 0$, $n_{\pm}$ is determined using the Fermi distribution function in the standard manner. Thus, in the presence of the magnetic field the total conductivity can be expressed as a sum of spin up/down contributions

$$\sigma = \sigma_+ + \sigma_-,$$

where $\sigma_{\pm}$ is the conductivity of the $(\pm)$ spin subband. The total carrier resistivity $\rho$ is defined by $\rho = 1/\sigma$. The conductivities $\sigma_{\pm}$ are given by

$$\sigma_{\pm} = n_{\pm}e^2 \langle \tau_{\pm} \rangle / m,$$

where $m$ is the carrier effective mass, and the energy averaged transport relaxation time $\langle \tau_{\pm} \rangle$ for the $(\pm)$ subbands are given in the Boltzmann theory by

$$\langle \tau_{\pm} \rangle = \int d\varepsilon \tau(\varepsilon) \varepsilon^{-1} \frac{d f_{\pm}(\varepsilon)}{d\varepsilon},$$

where $\tau(\varepsilon)$ is the energy dependent relaxation time, and $f_{\pm}(\varepsilon)$ is the carrier (Fermi) distribution function

$$f_{\pm}(\varepsilon) = \frac{1}{1 + e^{[\varepsilon - \mu_{\pm}(T)]/k_B T}},$$

where $\beta \equiv (k_B T)^{-1}$, and $\mu_{\pm} = \frac{1}{\beta} \ln [-1 + \exp(\beta E_{F\pm})]$ is the chemical potential for the up/down spin state (with Fermi energy $E_{F\pm}$) at finite temperature. The spin-polarized transport can then be calculated within this two-component (spin-up and -down) carrier system (without any spin-flip scattering since the bare impurities are non-magnetic), with the screening of the bare disorder being provided by both spin up and down carriers.

Within the framework of linear transport theory the relaxation time for a carrier with energy $\varepsilon_k$ is given by

$$\frac{1}{\tau(\varepsilon_k)} = \frac{2\pi}{\hbar} \sum_{\alpha, \alpha'} \int_{-\infty}^{\infty} dz N_{\alpha}(z) |u^{(\alpha)}(k - k'; z)|^2 \times (1 - \cos \theta_{kk'}) \delta(\varepsilon_k - \varepsilon_{k'}) \equiv \tau_{\alpha, \alpha'}(\varepsilon_k),$$

where $\theta_{kk'}$ is the scattering angle between wave vectors $k$ and $k'$ and $\varepsilon_k = \hbar^2 k^2/2m$; the screened scattering potential is denoted by $u^{(\alpha)}(q; z)$ with $q \equiv k - k'$ and $z$ is the confinement direction normal to the 2D layer. $N_{\alpha}(z)$ in Eq. (5) is the 3D charged impurity density of the $\alpha$-th kind of charged center. Here we have assumed that the charged centers are distributed completely at random in the Si-SiO$_2$ interface for MOSFETs. The screened impurity potential $u^{(\alpha)}(q; z)$ is given by:

$$u^{(\alpha)}(q; z) = \frac{2\pi Z^{(\alpha)} e^2}{\kappa q \epsilon(q)} F^{(\alpha)}(q; z),$$

where $Z^{(\alpha)}$ is the impurity charge strength, $\kappa$ is the background (static) lattice dielectric constant, and $F_{\gamma}$ is a form factor determined by the location of the impurity and the subband wavefunction $\psi(z)$ defining the 2D
confinement. The finite wave vector dielectric screening function \( \epsilon(q) \) is written in the RPA as

\[
\epsilon(q) = 1 - \frac{2\pi e^2}{\kappa q} f(q) \Pi(q, T),
\]

where \( f(q) \) is the Coulomb form factor arising from the subband wavefunctions \( \psi(z) \). In the strict 2D limit \( f(q) = 1 \). \( \Pi(q, T) \) is the 2D irreducible finite-temperature (and finite wave vector) polarizability function and is given by \( \Pi(q; T) = \Pi_+ (q; T) + \Pi_- (q; T) \), where \( \Pi_\pm (q; T) \) are the polarizabilities of the polarized up/down spin states (±). At finite temperature we have

\[
\Pi_\pm (q; T) = \frac{3}{4} \int_0^\infty d\mu' \frac{\Pi_{0 \pm} (q, \mu')}{\cosh^2 \frac{B}{2} (\mu_\pm - \mu')},
\]

where \( \Pi_{0 \pm} (q, E^F_\pm) \equiv \Pi_{0 \pm} (q) \) is the zero-temperature non-interacting static polarizability, given by

\[
\Pi_{0 \pm} (q) = N_F \left[ 1 - \sqrt{1 - (2k_F / q)^2} \theta(q - 2k_F) \right],
\]

where \( N_F = g_v m / 2\pi \) is the density of states per spin at Fermi energy, and \( k_F = (4\pi n_\pm / g_v)^{1/2} \) is the 2D Fermi wave vector for the spin up/down carriers. Note that \( g_v = 2 \) in the usual bulk 0 Si MOS case is the valley degeneracy, and the spin degeneracy, by definition, is assumed to be lifted by the in-plane field \( B \), the usual unpolarized \( B = 0 \) paramagnetic case being \( k_{F^+} = k_{F^-} \); \( n_+ = n_- = n / 2 \).

We mention that Eqs. (1) - (9) for the finite-temperature carrier transport properties in 2D systems comprise a complex set of multi-dimensional integrals along with the determination of the quasi-2D Coulomb form factors as well as the chemical potential of the system. In the asymptotic regimes of \( T / T_F \ll 1 \) and \( T / T_F \gg 1 \), Eqs. (1) - (7) simplify (as discussed in ref. [11]) giving rise to simple analytic behaviors in \( \rho(T) \sim O(T / T_F) \) for \( T / T_F \ll 1 \) and \( \rho(T) \sim O(T_F / T) \) for \( T / T_F \gg 1 \), but these asymptotic analytic behaviors are of limited experimental relevance since few experimental parameter regimes satisfy the required conditions [11] for the asymptotic behavior. Also, at the lowest experimental temperatures \( \rho(T) \) invariably saturates essentially in all experiments. For arbitrary \( T \) and \( n \) (as well as \( B \)) one must evaluate Eqs. (1) - (7) with sufficient accuracy to obtain \( \rho(T, n, B) \) for 2D systems.

The most salient aspects of the parallel field induced carrier spin polarization are an enhancement of the 2D Fermi wave vector by a factor of \( \sqrt{2} \) and a suppression of the 2D screening ("Thomas-Fermi") wave vector by a factor of 2 as the unpolarized ("paramagnetic") 2D system becomes completely spin-polarized ("ferromagnetic") with the parallel field increasing from \( B = 0 \) to \( B \geq B_s \) (with \( B_s \) being the full or saturation spin polarization field). In the most naive theoretical level one can write (at \( T = 0 \)) \( \rho \propto (q_{TF} + 2k_F)^{-2} \) in the strong screening limit for scattering by screened charged impurities, leading to

\[
\frac{\rho(B \geq B_s)}{\rho(0)} \leq \left( \frac{q_{TF}(0) + 2k_F(0)}{q_{TF}(B_s) + 2k_F(B_s)} \right)^2.
\]

In the usual range of experimental 2D densities \( q_{TF} \gg 2k_F \) ("strong screening") in Si MOSFETs, and therefore \( \rho(B \geq B_s) / \rho(0) \leq [q_{TF}(0) / q_{TF}(B_s)]^2 \leq 4 \). (As an aside, we note that in the opposite limit of weak screening, \( q_{TF} \ll 2k_F \), which may be approximately the situation in the high-density 2D n-GaAs system, one gets \( \rho(B_s) / \rho(0) \leq 1 / 2 \).) At finite temperatures and with finite wave vector screening \( \rho(B \geq B_s) / \rho(0) \) is expected to be less than 4 in Si MOSFETs as observed experimentally. Note that the 2D strong screening condition, \( q_{TF} \gg 2k_F \), occurs at low carrier densities since \( k_F \propto \sqrt{n} \) and \( q_{TF} \) is independent of density in the lowest order.

The suppression of screening due to the parallel field-induced spin polarization has direct consequences for the temperature dependence of the magnetoresistivity \( \rho(T, B) \) since the temperature dependence of screening gives rise to an effective metallic behavior of \( \rho(T) \) at zero magnetic field [11,16]. In particular, the strength of the metallicity, i.e. how strong the low temperature metallic temperature dependence is, is a function of dimensionless parameter \( (q_{TF} / 2k_F)^2 \sim (4.2/\tilde{n})(g_s g_v)^3 \) in Si MOSFETs where \( \tilde{n} \) is the carrier density measured in the units of \( 10^{11} \text{cm}^{-2} \) and \( g_s, g_v \) are respectively the spin and valley degeneracy factors (with \( g_s = 2 \) and \( g_v = 2 \) being the usual zero-magnetic field spin and valley unpolarized case). As the parallel field increases, \( 0 \leq B \leq B_s \), the 2D carriers become spin-polarized with \( g_v \) decreasing from 2 (for \( B = 0 \)) to 1 (\( B \geq B_s \)), consequently suppressing the metallicity parameter \( (q_{TF} / 2k_F)^2 \) by a factor 8 between \( B = 0 \) and \( B \geq B_s \). This implies that the temperature dependence of the finite field resistivity \( \rho(T, B, n) \) for \( B \geq B_s \) at a particular carrier density \( n_B \) will be approximately (and qualitatively) similar to the corresponding zero-field metallic temperature dependence at a carrier density \( n_0 \) which is roughly 8 times higher: \( n_0 \approx 8n_B \). Since the 2D metallic temperature dependence is strongly suppressed by increasing density, these simple screening considerations immediately suggest a very strong suppression of 2D "metallicity" (i.e. the temperature dependence of 2D resistivity) at high parallel fields. An equivalent physical way of describing this strong screening induced (through the spin-polarization dependence of screening) suppression of the temperature dependence of 2D parallel field magnetoresistivity is to observe that the metallicity parameter in the 2D n-GaAs system (where \( g_v = 1 \) is much smaller, \( (q_{TF} / 2k_F)^2 \sim (0.9/\tilde{n})g_s^2 \), due to the much smaller electronic carrier effective mass in GaAs \( m_{GaAs} = 0.067m_e \) and \( m_{Si} = 0.19m_e \), and therefore in
the presence of a strong parallel field \((B \geq B_s)\) so that 
\(g_s = 1\) the Si MOSFET system at a particular carrier density \(n_{Si}\) has a “metallicity” which is roughly equal to the corresponding zero-field (i.e. \(g_s = 2\)) metallicity in the 2D n-GaAs system at a density \(n_{GaAs} \approx 2n_{Si}\). Since the observed metallic behavior (i.e. the temperature dependence of \(\rho\)) in 2D n-GaAs system is extremely weak except [21] at very low electron densities (below \(10^{10} cm^{-2}\)), the temperature dependence of the magnetoresistivity \(\rho(T, B)\) in Si MOSFETs would thus be strongly suppressed at large parallel fields. We emphasize that the same physical mechanism, namely the suppression of screening due to carrier spin-polarization, leading to the strong positive magnetoresistance \(\rho(B)\) at a fixed low temperature also leads to the strong suppression of the temperature dependence of \(\rho(B, T)\) at a finite parallel field.

\section{III. RESULTS}

In Fig. 1 we show our calculated temperature dependence of n-Si MOS 2D resistivity, \(\rho(T)\), for several carrier densities in the unpolarized zero-field case \((g_s = 2, g_v = 2)\). Fig. 1(a) as well as the high field \((B \gg B_s)\) fully spin polarized case \((g_s = 1, g_v = 2)\), Fig. 1(b).

(All magneto-orbital effects [13] have been ignored in these calculations.) A comparison of Figs. 1(a) and (b) immediately demonstrates the strong suppression of 2D metallicity (i.e. the temperature dependence of \(\rho\)) in the high-field spin-polarized system, particularly at higher \((n > 10^{11} cm^{-2})\) carrier densities. At lower 2D densities, however, our calculated \(\rho(T)\) in the spin-polarized system seems to manifest stronger metallicity than that observed recently by Tsui \textit{et al.} [7] and by Shashkin \textit{et al}. [8] who have measured the temperature dependence of 2D magnetoresistivity in low-density Si MOSFETs, reporting essentially no temperature dependence in the spin polarized Si MOS systems.

One possible reason for this weaker experimental temperature dependence of \(\rho(T, B)\) could be that the strong parallel field lifts the valley dependency (i.e., \(g_v = 1\) in the high field situation) as well as the spin degeneracy. The long-standing valley degeneracy problem in Si MOSFETs is poorly understood theoretically except that it is experimentally well-established that the valley degeneracy is typically lifted by a small valley splitting, similar to spin splitting, \(\Delta_v\) of poorly understood theoretical origin. It is also established experimentally that \(\Delta_v\) increases with decreasing carrier density and increasing magnetic field [22]. We speculate that it is possible that at low carrier densities in the presence of the parallel magnetic field the valley degeneracy is lifted \((\Delta_v > E_F)\) so that the Si MOS system becomes a spin and valley polarized system \((g_s = g_v = 1)\) for \(B \gg B_s\). This is not unreasonable since the suppression of screening at large parallel fields would lead to strong many-body enhancement of valley splitting leading perhaps to the lifting of valley degeneracy at low densities and high fields. (Whether the valley degeneracy is indeed lifted in the experimental MOSFETs in the presence of a strong in-plane field \(B \gg B_s\) can only be ascertained experimentally – we are here suggesting only the theoretical possibility.) In Fig. 1(c) we show our calculated high field Si MOS \(\rho(T)\) in the spin and valley polarized situation, to be compared with the spin-polarized (but valley- unpolarized) case in Fig. 1(b) and both spin and valley unpolarized (i.e. \(B = 0\)) case in Fig. 1(a). The spin and valley polarized theoretical results in Fig. 1(c) are remarkably similar to the recent experimental results of Tsui \textit{et al.} [7] – in fact, our results in Fig. 1(c) even reproduce the experimental observation, as noted in ref. [7], of a weak negative (i.e. \(\rho(T)\) decreasing with increasing \(T\)) temperature dependence of \(\rho(T)\) arising from the rather small value of \(\frac{qT_F}{2k_F}\) is...
the full spin and valley polarized situation which leads to a sub-leading negative temperature contribution to $\rho(T)$. In Fig. 2 we compare $\rho(T)$ at different spin and valley degeneracies ($g_s = g_v = 2$; $g_s = 1$, $g_v = 2$; $g_s = g_v = 1$) at different densities, with the observation that our $g_s = g_v = 1$ results are in good agreement with the recent experimental Si MOS data in the high field ($B > B_s$) situation [7,8]. Our speculation of the Si valley degeneracy being lifted ($g_v = 1$), in addition to the spin degeneracy, for $B > B_s$ could be further tested by considering $\rho(B)$ at a fixed temperature, as shown in Fig. 2. At $T = 0$ and in the unrealistic and incorrect strictly 2D limit the lifting of both spin and valley degeneracies will lead to $\rho(B_s)/\rho(0) \to 16$ as $n \to 0$ [Fig. 2(b)]. This will be in direct disagreement with experimental observations where $\rho(B_s)/\rho(0) < 4$ in Si MOS systems.

But, in the realistic quasi-2D systems (and at finite temperatures) we find [Fig. 2(a)] that $\rho(B_s)/\rho(0) < 4$ for $n \geq 2.0 \times 10^{11} \text{cm}^{-2}$. For $n < 2.0 \times 10^{11} \text{cm}^{-2}$, we find $\rho(B_s)/\rho(0) > 4$ in Si MOS systems in the valley polarized situation.

There is, in fact, a qualitative physical explanation [23] for the observed temperature independence of the high-field magnetoresistance in Si MOSFETs, which is generic and universal in nature and does not invoke the ad hoc explanation of the field-induced lifting of the silicon valley degeneracy we propose above as a possibility. This explanation is, however, based on a categorical repudiation of the existing experimental claims [7] that the constancy (i.e. temperature independence) of $\rho(T; B > B_s)$ as a function of temperature at high parallel fields does not in any way indicate a fundamental suppression of “metallicity” (i.e. the metallic temperature dependence) in the fully spin-polarized Si MOSFETs, as has been repeatedly emphasized by several experimental groups in the past [7,8,1]. Instead, the rather generic explanation, recently suggested in ref. [23], is that the observed (essentially) complete suppression of the metallic temperature dependence occurs at fields below the full spin polarization field (at finite temperature) where the 2D system is still partially spin-polarized. In Fig. 3 we show the calculated spin-polarization as a function of the in-plane magnetic field for different temperatures.

![Graph](image)

**FIG. 2.** Calculated $\rho(B_s)/\rho(0)$ as a function of density (a) for quasi-2D system and (b) for pure 2D system. Here, at $B = 0$, $g_s = g_v = 2$. Note at $B = B_s$ the spins are completely polarized. The lines corresponding to $g_s = 1$ (2) indicate that the valley degeneracy is (not) lifted at $B = B_s$.

**FIG. 3.** Spin-polarization $\eta = (n_+ - n_-)/(n_+ + n_-)$ as a function of in-plane magnetic field for $n = 1.5 \times 10^{11} \text{cm}^{-2}$ and for different temperatures $T = 0, 1.0, 2.0, 3.0K$. $B_s$ is the T=0K full spin-polarization field. Note that for $T \neq 0$, full spin-polarization requires $B \approx 2B_s$. 

Increasing temperature induces two competing trends in screening – increased thermal broadening reduces screening and thermal excitation enhances screening by reduc-
ing the net spin polarization. Our theory and the numerical results, of course, include these two mechanisms.

In Fig. 4 we show the calculated polarizabilities, $\Pi(q,T)/N_{F0}$ ($N_{F0} = 2N_F = g_v m/2\pi$), for different in-plane magnetic fields: (a) for $B = 0$ and $B = 2B_s$, and (b) for $B = B_s$. At $B = 0$ (i.e., the system is unpolarized and $n_+ = n_-$), the decrease of the screening function (i.e. $\Pi$) with increasing temperature at $q = 2k_{F0}$ ($k_{F0} = \sqrt{2\pi n/g_v}$) gives rise to increasing resistivity as the temperature increases. Most of the temperature dependence of the resistivity at low temperature regime comes from the suppression of screening at $q = 2k_{F0}$. The reduction of screening near $q = 2k_{F0}$ determines the strength of metallicity at $B = 0$. At $B = 2B_s$ (i.e., the system is completely polarized and $n_+ = n$ at $T = 0$), we find a very similar behavior of the screening function, but the rate of the change of screening at $q = 2k_{F+}$ ($k_{F+} = \sqrt{4\pi n/g_v}$) is reduced by about a factor of four compared to the $B = 0$ case in the same temperature range. Thus, we expect that the temperature dependence of $\rho(T)$ at $B = 0$ is roughly a factor of 4 stronger than that at $B = 2B_s$. At $B = 2B_s$ the population of the minority band due to the thermal excitation is negligible in the given temperature range. In Fig. 4(b) we show the polarizability function at $B = B_s$. As the temperature increases the screening function decreases at $q = 2k_{F+}$ for $B = B_s$, but due to the occupation of the minority band we also find an enhancement of the screening function near $q = 2k_{F+}$ ($k_{F+} = \sqrt{4\pi n/g_v} < k_{F0}$). Thus, the enhancement of the screening function near $2q_{k_{F+}}$ with increasing of the minority spin carrier density and the reduction of screening near $q = 2k_{F+}$ by thermal broadening give rise to weak temperature dependence in $\rho$ around $B \approx B_s$.

It is, in principle, possible for these two competing mechanisms to almost completely cancel each other, close to $B \approx B_s$. In Fig. 5 we show our numerical results for both situations of the valley degeneracy being affected (and unaffected) by the parallel field. Obviously the temperature independence of $\rho(T)$ around $B \approx B_s$ is more prominent in the situation where the valley degeneracy (as well as the spin degeneracy) is lifted by the external magnetic field. We emphasize that these competing temperature induced trends in screening in the presence of a finite spin-polarizing parallel magnetic field (i.e. the direct suppression of screening by increasing temperature and the indirect enhancement of screening by the temperature induced decrease of effective spin-polarization) is a generic phenomenon, and is therefore present in all 2D carrier systems. In particular, these competing mechanisms could be the underlying cause for the occurrence of the so-called parallel field-induced 2D metal-insulator
transition, which has been widely discussed in the context of hole transport in high-mobility 2D p-GaAs structures. It may, therefore, be possible that the peculiar temperature independence of 2D resistivity around \( B \sim B_s \) observed in n-Si MOSFETs arises from both the parallel field induced lifting of valley degeneracy as well as the competing mechanisms discussed above (since valley degeneracy is the only physical mechanism that distinguishes the Si MOS system from all the other 2D semiconductor systems).

It is important to emphasize that our finding (see Fig. 5) of the temperature dependence of \( \rho(T, B) \) being the weakest below the full-spin-polarization field (at finite temperature), i.e. for \( B \approx B_s \), and the strongest for \( B = 0 \) with the fully spin-polarized system \( (B \gg B_s) \) having an intermediate behavior, as observed experimentally in ref. [23], is valid independent of whether the Si valley degeneracy is lifted by the applied magnetic field or not. This is a generic result which is always true in all 2D systems independent of the number of valleys: The temperature dependence of \( \rho(T, B) \) is always the weakest for \( B \approx B_s \) due to the competition between the thermal excitation between spin up/down bands and the thermal suppression of screening. This is obvious from Fig. 5 where the temperature dependence of \( \rho(T, B) \) is the weakest around \( B \sim B_s \) both in Fig. 5(a) and in Fig. 5(b) with the assumed valley degeneracy being 2 and 1 respectively. As we have emphasized above, the additional assumption of a magnetic field induced lifting of the valley degeneracy makes \( \rho(T) \) almost a constant, completely independent of temperature, in quantitative agreement with the data of Tsui \textit{et al.} [7]. Whether this actually happens or not can only be decided experimentally [22]. We should, however, emphasize that even if the valley splitting \( \Delta_v \) is small (e.g. \( \Delta_v < 2E_F \) so that the valley degeneracy is not completely lifted), a partial lifting of valley degeneracy \( (\Delta_v \neq 0) \) will certainly contribute to the physics being proposed here. For a partial lifting of the valley degeneracy, our calculated temperature dependence of \( \rho(T) \) will be intermediate between that shown in Figs. 1(b) and 1(c) or Figs. 5(a) and 5(b) as the case may be. In particular, a finite valley splitting will lead to the same competing thermal trends in \( \rho(T) \) as discussed above and by Shashkin \textit{et al.} [23] for the spin splitting, producing an additional suppression of \( \rho(T) \) bringing our theoretical results to better quantitative agreement to the Tsui \textit{et al.} [7] data.

**IV. DISCUSSION**

We have shown in this paper that the enigmatic temperature dependence of the parallel field magnetoresistance, \( \rho(T, B) \), in 2D Si MOSFETs can be qualitatively and semiquantitatively well explained by the screening theory, assuming charged impurity scattering to be the dominant low-temperature resistive scattering mechanism. Our screening theory based explanation, in fact, becomes quantitatively accurate if we assume that the valley degeneracy is lifted by the external magnetic field in the same manner as the spin degeneracy. The fully spin- and valley-polarized Si MOS system at high field has a factor of 4 lower density of states than the corresponding zero-field spin- and valley-unpolarized system, leading consequently to substantially weaker screening with the corresponding strong suppression in the temperature dependence of the resistivity. We show that, independent of the valley degeneracy question, the weakest temperature dependence in the resistivity happens \textit{not} at \( B \gg B_s \) (where the carriers are essentially completely spin-polarized), but at \( B \leq B_s \), just below the \( T = 0 \) full spin-polarization field, where the system is almost, but not quite, fully spin-polarized. Thus, the metallicity (i.e. the magnitude of \( dp/dT \)) is the strongest for \( B = 0 \) and the weakest for \( B \leq B_s \), with the fully spin-polarized \( (B \gg B_s) \) situation being intermediate. This specific prediction of the screening theory is in good agreement with experimental observations both in n-Si MOSFETs [23] and in n-Si/SiGe [20] 2D systems. The key feature of our theory is a realistic and quantitatively accurate description of 2D screening taking into account finite temperature and finite spin-polarization effects on an equal (and non-perturbative) footing. The important ingredient of physics leading to the strong suppression of metallic temperature dependence of \( \rho(T, B \approx B_s) \) in our theory is a competition between two physical mechanisms: Thermal excitation of reversed spin quasiparticles leading to enhanced screening with increasing temperature for \( B \leq B_s \) and the direct thermal suppression of screening by the majority spin carriers. We note that this competition would always lead to a strong suppression in the temperature dependence of \( \rho(T) \) around \( B \leq B_s \), independent of the member of valleys involved in the 2D system. It is also important to emphasize that for \( B > B_s \) (and at not too low carrier densities) our theory predicts a negative magnetoresistance with monotonically decreasing \( \rho(B) \) with increasing \( B \) due to the Coulomb matrix element effect arising from an increasing effective \( k_F(B) \) in the system. This also leads to the suppression of metallic temperature dependence at high fields.

Our finding of the qualitative agreement between the screening theory and the experimentally observed \( \rho(T; B) \) in Si MOSFETs is of considerable importance. Much has been made in the literature of the claimed nonmetallic (i.e. temperature independence or even insulating) behavior of 2D magnetoresistance in Si MOSFETs at high \( (B \geq B_s) \) parallel fields. In particular, interaction-based theories [15] of 2D metallicity have been claimed [1] to provide the definitive explanation for 2D metallicity in Si MOSFETs because the interaction theory predicts the fully spin and valley-polarized 2D system to have an insulating (with \( \rho \propto 1/T \)) temperature dependence,
and it has been categorically asserted that the screening theory cannot possibly be qualitatively correct [24] since it predicts a (weak) metallic behavior in the fully spin-polarized ballistic regime. We have shown in this work that the screening theory is, in fact, in good qualitative (and even quantitative, if we allow the possibility of valley degeneracy lifting) agreement with the most recent Si MOS experimental data [7,23] in the presence of a parallel magnetic field, and in particular, consistent with our theoretical predictions, the strongest suppression of the metallic temperature dependence of resistivity happens for \( B \leq B_s \) where the 2D system is almost, but not quite, fully spin polarized. Thus, \( \rho(T, B) \) manifests the strongest metallicity at \( B = 0 \) (when the system is unpolarized) the weakest at \( B \approx B_s \) (when the system is almost polarized), and intermediate at \( B \gg B_s \) (when the system is fully polarized) both in the screening theory and in the experiment. Exactly the same behavior has also been seen recently by two experimental groups [20] in 2D n-Si/SiGe electron systems which we have theoretically explained [25] recently using the screening theory. Thus, the parallel field induced suppression of metallic temperature dependence in the ballistic regime is now theoretically understood (at least qualitatively) for both n-Si MOS and n-Si/SiGe 2D electron systems, and the early experimental discrepancies between these two systems have now been resolved [23] with both systems agreeing reasonably with the screening theory predictions in the ballistic regime.

There are various proposed non-Fermi liquid scenarios for the 2D metallicity which depend crucially on important distinctions between the spin polarized \( (B > B_s) \) and the unpolarized \( (B = 0) \) transport regimes. At least one of these non-Fermi liquid scenarios, based on a speculative coexistence between 2D Wigner crystal and electron liquid phases [26] is apparently invalidated by the observed weak metallicity in the spin-polarized Si MOSFETs, since the theory [26] specifically predicts absolutely no temperature dependence in \( \rho(T; B \gg B_s) \) in the spin-polarized phase in direct contradiction with the recent experimental results. [20,23]

We briefly discuss the role of interaction in our screening theory, touching upon the closely related (and important) question of why the Boltzmann-RPA screening theory seems to provide a good description of the 2D transport properties at low carrier densities where the dimensionless interaction parameter \( r_s \approx n^{-1/2} \) in 2D, defined as the ratio of the average Coulomb energy to the Fermi energy at \( T = 0 \), is larger than one (in Si-based 2D systems of interest in this paper, \( r_s \sim 6 \) in the experimentally relevant carrier density range of \( n \sim 10^{11} \text{cm}^{-2} \)). We believe that one possible reason for the success of the RPA screening theory is that the dominant contribution to the 2D resistivity arises from charged impurity scattering, and RPA-Boltzmann theory does an excellent job of regularizing the associated Coulomb disorder through the self-consistent screening model. The 2D transport problem is, in fact, semiclassical since the temperature, expressed in units of the Fermi temperature, is not necessarily small (often \( T/T_F \sim O(1) \)), again making finite temperature RPA an excellent approximation. It is important to emphasize that at a fixed finite temperature \( T \), decreasing 2D density increases both \( r_s \) and \( T/T_F \) (since \( T_F \propto n \)), and the finite-temperature interaction parameter, e.g. \( r_s/(T/T_F) \sim \sqrt{n} \), actually decreases with decreasing density! Therefore, it is not obvious at all that finite temperature 2D transport behavior increasingly becomes strong-coupling like as electron density is decreased at a fixed temperature since the low-density \( (r_s \to \infty) \) limit is also at the same time the classical infinite temperature \( (T/T_F \to \infty) \) limit. Under these circumstances, the semiclassical RPA-Boltzmann finite temperature theory may, in fact, become increasingly more valid as the carrier density is reduced, particularly since the carrier temperature can often not be reduced below 100 mK due to electron heating effects. This finite-temperature aspect of the low-density 2D transport problem, which has not been adequately emphasized in the literature, may very well be playing an important role in making RPA a particularly good approximation in the 2D MIT phenomena.

We note that RPA-based many-body theories also seem to describe reasonably well [27,28] the experimental behaviors of finite-temperature, dilute 2D carrier systems with respect to collective mode dispersion [29] and inter-layer drag measurements [30]. This finite-temperature (actually high-temperature) aspect of this problem most likely also invalidates any possible relevance of Wigner crystallization to the physics of 2D MIT phenomena – a Wigner crystal would thermally melt [27,31] at the “relatively” high temperatures (i.e. \( T/T_F \sim O(1) \)) at which the low density 2D transport experiments are typically carried out. It needs to be emphasized that the asymptotic low-temperature behavior of \( \rho(T) \) is essentially never observed in 2D transport experiments since the experimental \( \rho(T) \) always saturates at the lowest measurement temperatures (often for \( T \leq 100\text{mK} \)) indicating that the electrons may not be cooling down to the \( T/T_F \ll 1 \) regime. In this intermediate to high temperature regime our screening theory, which is non-perturbative in temperature, may very well be the qualitatively correct approximate theory. Understanding the true asymptotic temperature dependence of \( \rho(T) \) in the \( T/T_F \ll 1 \) regime, where interaction effects must be important in a low-density strong-coupling electron system, remains an important open experimental and theoretical challenge.

We can speculate on the possibility of incorporating interaction effects into our screening theory of 2D transport. The 2D resistivity, \( \rho(n, T, B) \), depends on density, temperature, and the applied magnetic field, which may...
be expressed in the dimensionless units to write
\[ \rho(n, T, B) = \rho(q_{TF}/2k_F, T/T_F, \Delta_s/T_F), \]
where \( \Delta_s = g \mu_B B \) is the spin splitting induced by the external magnetic field. We note that \( q_{TF}/2k_F \propto m; T/T_F \propto m; \) and \( \Delta_s/T_F \propto gm \propto \chi \) where \( m, g, \) and \( \chi \) are respectively the 2D effective mass, Lande \( g \)-factor, and spin susceptibility. In the RPA theory, interaction effects are ignored in the effective mass and the \( g \)-factor, and therefore, the noninteracting effective mass and the susceptibility are used in calculating the resistivity. In the spirit of the Landau Fermi liquid theory, we could crudely incorporate interaction effects in the theory by using the quasiparticle effective mass \( (m^*) \) and the quasiparticle spin susceptibility \( (\chi^*) \) or equivalently the quasiparticle \( g \)-factor \( (g^*) \) in the effective RPA calculation. A rigorous justification for such a Fermi liquid renormalization of the effective mass and \( g \)-factor in the RPA-Boltzmann transport theory is unavailable, and indeed all our numerical results utilize the non-interacting band mass and \( g \)-factor in the Boltzmann-RPA calculations, but we speculate that such a physically motivated approximation (i.e. \( m^* \) and \( g^* \) replacing \( m \) and \( g \)) to incorporate interaction effects may be quite reasonable since the observed or measured quantities are actually \( m^* \) and \( g^* \) (and \( \chi^* = m^* g^* \)) and not the bare quantities \( (m \) and \( g) \). It is interesting to point out that such an \textit{ad hoc} approximation scheme incorporating interaction effects (by using \( m^* \) and \( g^* \) in the Boltzmann-RPA transport theory) does considerably improve the quantitative agreement between theory and experiment. In particular, the interacting susceptibility \( \chi^* \) is renormalized \cite{32} by a factor of 3 (i.e. \( \chi^*/\chi \sim 3 \)) at \( n \sim 10^{11} \text{cm}^{-2} \) in Si MOSFETs leading to the theoretical spin-polarization saturation magnetic field \( B_s \) \( (\sim 3 - 4T) \) being in good agreement with the experimental data. Similarly, the use of the quasiparticle effective mass \( m^* \sim 3m \) at low densities considerably increases the effective values of \( q_{TF}/2k_F \) and \( T/T_F \) (where “starred” quantities use \( m^* \) rather than \( m \)), again bringing theory and experiment in good quantitative agreement. Whether such an \textit{ad hoc} “improvement” of the theory using quasiparticle rather than bare Fermi liquid parameters can be rigorously theoretically justified or not remains an important open question for the future. We note, however, that the screening theory obtains semi-quantitative and qualitative agreement with the existing 2D transport data even without any such “renormalization”.

Finally, we note that there still seems to be some quantitative difference in the observed experimental temperature dependence of \( \rho(T; B) \) between Si MOS \cite{7,8} and Si/SiGe \cite{20} 2D electron systems. For example, in the Si MOS system \( \rho(B) \) is enhanced approximately by a factor of three at low temperatures as \( B \) increases from zero to \( B_s \) whereas in the Si/SiGe system \( \rho(B) \) the enhancement factor is only almost 1.8. This difference arises (at least partially) from the difference in the charged impurity distribution in the two systems — in the Si/SiGe 2D electron system the dominant scattering is from remote dopants and background impurities \cite{25} whereas in Si MOS system the scattering is mostly by interface charged impurities and interface roughness. In addition, the finite magnetic field behavior in these two Si-based 2D systems may also differ by virtue of the valley degeneracy being lifted in the Si MOS system, but \textit{not} in the Si/SiGe system. Such a non-universal lifting of the valley degeneracy is certainly possible since it is well-known that the Si valley degeneracy near an interface depends critically on the microscopic details of the interface, and it is entirely possible for the valley degeneracy to be lifted in the Si MOS system, but \textit{not} to be lifted in the Si/SiGe system since the latter system has a much better atomically smooth epitaxial interface. In fact, the non-universal lifting of valley degeneracy may apply even to different Si MOS 2D systems, and could provide one possible underlying reason for the observed difference \cite{7,8} in the temperature dependence of \( \rho(T; B \geq B_s) \) in Si MOS data from different groups. Whether such a non-universal parallel field-induced electron valley degeneracy lifting actually happens in reality can only be decided experimentally; we are only suggesting here the theoretical possibility based on our analysis of the experimental transport properties of \( \rho(T; B) \).

V. CONCLUSION

In conclusion, we consider theoretically the parallel magnetic field induced suppression of the screening of long range bare Coulomb disorder in Si MOSFETs, showing that the experimentally observed strong suppression of 2D metallicity in the temperature dependence of the magnetoresistance can be qualitatively and semi-quantitatively understood as arising from spin (and perhaps even valley) polarization induced reduction in carrier screening, leading to stronger parallel field-dependent effective disorder in the system. The competing mechanism of direct thermal reduction of screening and indirect enhancement of screening through the thermal suppression of spin polarization may also be playing an important quantitative role in the temperature dependence of \( \rho(T; B \sim B_s) \). Our theory, as presented in the current work and in our recent work \cite{25} on the 2D Si/SiGe electron system along with the recent experimental work \cite{20,23}, may resolve the earlier discussed qualitative disagreement between Si MOS and Si/SiGe 2D systems, establishing the same qualitative behavior in all 2D Si systems. More work is still needed to precisely understand interaction effects on 2D transport by going beyond the physically motivated screening theory of our work.

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The spin-polarized 2D system in the ballistic limit does not manifest a metallic-like behavior independent of screening. Predicting metallic-like $\rho(T)$ for both spin-polarized and unpolarized states, which is in disagreement with experiments." Our current theoretical work and recent experimental results presented in refs. [20] and [23] clearly show this criticism of the screening theory is unwarranted and is, in fact, incorrect. The spin-polarized 2D system in the ballistic limit does manifest a metallic-like $\rho(T)$, albeit with a weaker temperature dependence in qualitative agreement with the screening theory.

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