Metal-insulator transition in two dimensions: Role of the upper Hubbard band

V. I. Kozub and N. V. Agrinskaya
A. F. Ioffe Institute, 194021 Saint Petersburg, Russia

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To explain the main features of the metal-insulator transition (MIT) in a two-dimensional (2D) electron system, we suggest a simple model, taking into account strongly localized states in the tail of a 2D conductivity band with a specific emphasis on the role of doubly occupied states [the upper Hubbard band (UHB)]. The metallic behavior of the resistance is explained as result of the activation of localized electrons to a conductance band, leading to a suppression of the nonlinear screening of the disorder potential. The magnetoresistance (MR) in the critical region is related to depopulation of double occupied localized states, also leading to a partial suppression of the nonlinear screening. The most informative data are related to a nearly activated temperature dependence of MR in the strongly insulating limit (which can, in particular, be reached from the metallic state in high enough fields). According to our model, this behavior originates in a lowering of the chemical potential in the UHB due to Zeeman splitting. We compare theoretical predictions with the existing experimental data, and demonstrate that the model explains such features of the 2D MIT as the scaling behavior in the critical region, the saturation of the MR and the H/T scaling of the MR in the insulating limit. The quantitative analysis of the MR in strongly insulating limit based on our model leads to values of the g factors in good agreement with the known values in the localized states in the same materials.

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I. INTRODUCTION

The problem of an apparent metal-insulator transition in two-dimensional (2D) structures is still far from being completely understood. Such a transition was observed in different 2D systems, including in particular Si metal-oxide-semiconductor field-effect transitions (MOSFET's) (see, e.g., Refs. 1 and 2) and GaAs-$Al_xGa_{1-x}As$ heterostructures (see, e.g., Refs. 3–5); an extended review of the situation was given in Ref. 6). At the present time two possible scenarios are being discussed. According to the one of them an unusual metallic behavior which apparently contradicts the scaling theory of localization (STL)[7] is a real manifestation of some physical mechanism. According to the second scenario, the metallic conductivity is still expected to be suppressed at low enough temperature, while the behavior observed until now is related to the mechanisms of a more conventional nature such as temperature-dependent disorder[8] or magnetic-field-driven disorder.[9] Despite the various mechanisms proposed, according to the conclusion of Ref. 6, "while each of these is capable of explaining one or another part of experimental observations, none of them provide a comprehensive picture."

The theoretical approaches developed up to now are concentrated mostly on the metallic state, and discussed an effect of disorder and electron-electron interactions on this state; however, to the best of our knowledge, practically no attempts have been made to look at the problem starting from the insulating limit. The role of localized states was discussed to some extent in Refs. 8–11 where the effect of traps in an oxide layer or the interface region of Si MOSFET's was considered. However, these localized states are actually external with respect to the states of a 2D conduction band, and only play the role of additional scattering centers, while we are interested in the states responsible for the 2D transport deep in the insulating limit. In addition, the traps—although no doubt important for Si MOSFET's—can be hardly considered for other systems exhibiting the 2D metal-insulator-transitions (MIT) behavior.

In our opinion, the clue to the problem of the 2D MIT can be related to the magnetoresistance (MR) in the strongly insulating limit (which can, in particular, be reached from an initially metallic state in high enough fields). As is well known, the strong positive MR in a parallel magnetic field, leading to a suppression of the metallic state in the "critical" region, remains one of the puzzles of the 2D MIT. We especially emphasize that a strong positive MR persists deep into the insulating state, and is exhibited by systems which were perfectly insulating at $H=0$.[6] The specific feature of the MR in this regime is the fact that its temperature dependence is close to the Arrhenius law even if for $H=0$ the system exhibits a variable range hopping of Efros-Shklovskii type [such a behavior was observed for Si MOSFET's (Ref. 12) and n-type GaAs heterostructures[13]]. In particular, we believe that a renormalization approach starting from the metallic state (see, e.g., Ref. 14) which could possibly explain the MIT and the suppression of metallic phase by magnetic field, would fail to explain this MR deep in the insulating phase.

As suggested earlier,[15] the activated behavior of the MR in the hopping regime is a signature of the hopping over the states of the upper Hubbard band (UHB), that is, over doubly occupied localized states. Because of on-site spin correlations the Hubbard energy in this case acquires a Zeeman term $g\mu_B H$ (g being the g factor), and this magnetic-field-dependent term is a universal one (at least for $g\mu_B H \gg T$). Based on these facts, we have suggested that the UHB plays an important role in the problem of a 2D MIT.[16] Note that a possible role of the multiply occupied electron states in a 2D MIT was also discussed in Ref. 17.

In what follows we propose a model which starts from the localized limit of a 2D MIT rather than from the metallic

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one, and thus is concentrated mainly on the "insulating" and "critical" regimes. We believe that in systems exhibiting a 2D MIT there exists a tail of strongly localized states below the bottom of the 2D conductance band, with localization lengths a smaller than predicted by the scaling theory of localization starting from the metallic regime.[7] The localization length a for these deep states is expected to increase with an increase of energy, exhibiting a critical divergency. The divergency has a cutoff imposed by the STL at some threshold energy. The highest of these states, according to the predictions by Kamimura,[18] are the doubly occupied ones. That is, the energy dependence of the Hubbard energy leads to the formation of a peak of the UHB close to the bottom of the conductance band.[18] The metallic behavior of the resistance in our model is related (as in the model of Ref. 8) to temperature-dependent disorder. In our case this disorder originates due to the activation of electrons from strongly localized states to the conductance band, which leads to a partial undressing of the disordered potential. The MR in the metallic regime is expected to be due to a redistribution of electrons between different doubly and singly occupied states (driven by the Zeeman addition to the energy of doubly occupied states), which also leads to a partial suppression of the screening of the disorder potential. (Similar concepts were suggested in Refs. 11 and 9, where the depopulation of filled traps to delocalized states due to an increase of energy of the traps in magnetic field was considered). This simple model is shown to explain—at least qualitatively—most of the features of the observed 2D MIT (including the scaling of the resistance in the critical region, H/T scaling of the MR in the insulating limit, and saturation of the MR at large H). Based on the fact that in the strongly insulating limit the values of the g factor are not expected to be renormalized by Fermi-liquid effects, we have compared some existing MR data with the predictions of our model. A good agreement between g factors extracted according to our predictions and their known values gives strong support to our model.

II. FORMULATION OF THE MODEL

We *assume* that the 2D conductance band has a tail of strongly localized states originating due to the localization of carriers in the potential relief imposed by the disorder. We believe that the localization length for these states behaves as

$$a \propto (\varepsilon_m - \varepsilon)^{-\nu}, \tag{1}$$

where ε_m is some energy which for three dimensions would correspond to the mobility edge, while ν is an index of the localization length.

Actually the STL, for two dimensions, predicts the absence of any mobility edge, and allows only some threshold values of conductance separating regimes of weak and strong localization. The localization length is expected to be exponentially dependent on the value of the conductance in the weakly localized regime, and to decrease when the conductance tends toward the critical value mentioned above. Thus one may expect that for a given degree of disorder there is some minimal value of the localization length $\tilde{a}$ available in the STL (of the order of the mean free path).

In our model we will assume that the localization lengths of the strongly localized states described by Eq. (1) are *smaller* than $\tilde{a}$. This assumption corresponds to a cutoff of the divergency on the right-hand side of Eq. (1) at some

$$\varepsilon = \tilde{\varepsilon}_m < \varepsilon_m,$$

while for higher energies the situation can be controlled by the STL. In other words, at $\tilde{\varepsilon}_m$ we have a crossover from strongly localized states, described by Eq. (1), to the states described by the STL.

In what follows we will also assume that the difference $\varepsilon_m - \tilde{\varepsilon}_m$ is small with respect to the characteristic energy scales, and can be neglected (the corresponding criterion is given in Appendix A). Keeping these considerations in mind, we will still use the term "mobility edge" for the energy ε_m.

As is known, systems exhibiting a 2D MIT are characterized by strong electron-electron interactions. In our model we will directly take into account the intrastate electron-electron interactions, which were shown in Ref. 18 to be most important. Following the concepts of Kamimura,[18] we take into account the energy dependence of the Hubbard energy U,

$$U \simeq \frac{e^2}{\kappa a}, \tag{2}$$

where a is the energy-dependent localization length and κ is the dielectric constant. While for in three dimensions κ is known to be strongly dependent on the localization length (through the wave-vector dependence) there are arguments allowing to assume that for two dimensions the value of κ is nearly independent of a and close to its bulk value. These arguments were given in Ref. 20, where the exponent in the relation $\kappa \propto a^{\alpha_2}$ was estimated to be $\alpha_2 < 0.2$. However, we still consider a possibility of $\alpha_2 \neq 0$, and thus we have

$$U \propto (\varepsilon_m - \varepsilon)^u, \tag{3}$$

where $u > \nu$.

As is shown in Appendix A, the energy dependence of the Hubbard energy has significant consequences for the form of the upper Hubbard band. That is, for strong electron-electron repulsion this band is peaked at some $\varepsilon_{-,c}$ close to ε_m.[18] The peak is characterized by a steep decrease of the density of states (DOS) for $\varepsilon < \varepsilon_{-,c}$ (see Fig. 1) which with reasonable assumptions can be shown (see Appendix A) to obey the Gaussian law.

$$g_- = g_{-,c} \exp - \left(\frac{\varepsilon_c - \varepsilon}{\varepsilon_1} \right)^2. \tag{4}$$

For $\mu = \varepsilon_m$, that is, at the point of the metal-insulator transition (in the sense of strong localization), all the states below the "mobility edge" (except possibly the states deep in the band tail) are doubly occupied. This fact, and the presence of a peaked DOS of the D^- band below ε_m, allow one to conclude that the metal-insulator transition takes place in the D^- band, and that its presence significantly affects the features of the transition.

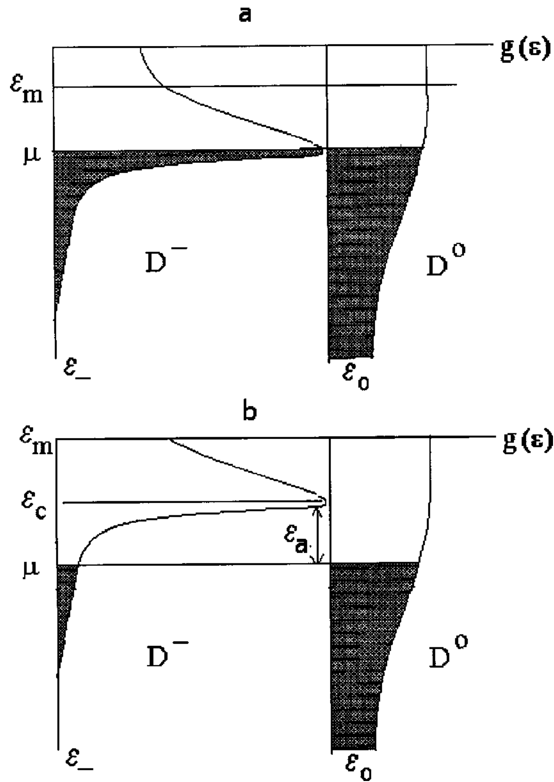

FIG. 1. (a) The structure of the subbands of doubly-occupied (left) and singly-occupied (right) localized states for an electron occupation corresponding to the insulating limit in the absence of a magnetic field. The hopping conductivity is controlled by the states of the D^- band. (b)The occupation of the subbands depicted in (a) for a high magnetic field. Hopping is dominated by activation to the peak of the D^- band ($\varepsilon_a = \varepsilon_c - \mu$).

We would like to note that the D^- states in our case, strictly speaking, are different from the ''standard'' impurity D^- states which are similar to negative hydrogen ions. In the latter case the two electrons are in the field of a single positive elementary charge. For ''tail states'' this is not the case, since the electrons are considered to be localized in the potential wells created by the charge density outside of the 2D sheet, like the charges of interface traps in the case of silicon MOSFET's or spatial charge fluctuation as in GaAS-Al$_x$Ga$_{1-x}$As heterostructures. In this case the localization centers are by no means of Coulomb nature. Thus the double occupation of some localized state is not equivalent to a negatively charged Coulomb center as well as a singly occupied state is not similar to a neutral center. (Nevertheless, for simplicity we will still use the notations D^0 and D^- for singly and doubly occupied states). As mentioned above, the occupation of localized states by single electrons or by electron pairs for an external ''probe'' particle is reduced to the effect of a nonlinear screening of the initial disorder potential.

As for the rest of the electron-electron interactions, we believe that the latter can be taken into account as nonlinear screenings of the initial disordered potential by electrons filling these states, with account taken of electron-electron correlations. As a result, the form of the band tail and the position of the ''mobility edge'' are expected to depend on the electron concentration n. For small variations of the electron density δn, linearizing the dependence in question one obtains

$$\delta\varepsilon_m = -\gamma\delta n. \tag{5}$$

Thus both the chemical potential and the ''mobility edge'' are expected to be sensitive to n, and one has

$$\delta(\varepsilon_m - \mu) = -(\gamma + g_t^{-1})\delta n, \tag{6}$$

where g_t is some total density of states at $\varepsilon = \varepsilon_m$. The critical value of $n = n_c$ corresponds to $\mu(n) = \varepsilon_m(n)$.

While the occupation of the localized states corresponds to a nonlinear screening of the disorder potential, the occupation of the states above ε_m drives the system into a regime of linear screening according to the considerations given in Ref. 19. Thus the metal-insulator transition is accompanied by a transition from nonlinear screening to linear screening; however, even in the metallic state—at least in the ''critical'' region—one expects that a significant part of the disorder potential is still screened by localized electrons.

The value of γ depends on the efficiency of nonlinear screening. The latter, in its turn, depends on the properties of the disorder potential. In particular, the spatial harmonics of a potential with a period q^{-1} larger than $n^{-1/2}$ are screened more effectively the larger q^{-1} is; indeed, the magnitude of the available screening potential is $en(q^{-1})^2/\kappa q^{-1} \propto q^{-1}$. At the same time the harmonics with $q^{-1} \ll n^{-1/2}$ are screened very poorly. Thus one can expect that the harmonics with $q^{-1} \ll n^{-1/2}$ are already strongly suppressed by the screening, and that the nonlinear screening still proceeds for harmonics with $q^{-1} \sim n^{-1/2}$. Correspondingly, the magnitude of the screening potential for these harmonics is $U_s \sim en^{1/2}/\kappa$. If one assumes that the potential of the disorder is dominated by the harmonics in question, and that the position of ε_m is scaled with the value of U_s, the parameter γ can be estimated as a derivative of U_s, with respect to the electron concentration, as

$$\gamma \sim \frac{e^2}{\kappa n^{1/2}}.$$

It is interesting to note that in the critical region when g_t can be considered equal to the 2D band, and the DOS is $2m/\pi\hbar^2$, the ratio of the terms γ and g_t^{-1} on the right-hand side of Eq. (6) is of the order of the interaction parameter $r_s = 2^{1/2}me^2/\kappa\hbar p_F$ (p_F being the Fermi momentum). Thus one could expect that the metal-insulator transition is dominated by a shift of the ''mobility edge.'' However, the detailed studies carried out for Si MOSFET's in Ref. 21 showed that the activation energy in the insulating regime (equal in our model to the difference $\varepsilon_m - \mu$) increases with a decrease of n much more slowly than would be predicted by Eq. (6) if one were to use the estimate of γ given above. Such a fact can be explained if one assumes that the disorder potential for the systems in question contains no significant contribution of spatial harmonics with $q^{-1} \sim n_c^{-1/2}$, and is dominated by harmonics with $q^{-1} \ll n_c^{-1/2}$. In this case the

sensitivity of ε_m to a variation of n is much weaker than predicted by the estimate given above, and the brackets on the left-hand side of Eq. (6) are actually dominated by g_t^{-1} which is in agreement with the experimental results of Ref. 21.

III. TEMPERATURE BEHAVIOR OF THE RESISTANCE

In our model we relate the temperature behavior of the resistance in the metallic state, in accordance with Ref. 8, to temperature-dependent disorder. That is, we assume that the ionization of strongly localized states below ε_m leads to additional scattering for the mobile electrons qualitatively in the same way as an ionization of occupied donor state creates an additional charged scatterer. Indeed, a nonlinear screening of the disorder potential by localized states is reduced when the number of localized electrons is reduced. We understand that, quantitatively, the contribution of states with large localization lengths is not expected to be similar to the contribution of donor state sufficiently separated from other localized states, but we believe that a qualitative similarity still exists. However, the efficiency of the scattering by an ionized localized state is expected to depend on the localization length of the state, and in general to increase with a decrease of a because of the larger momentum transfer corresponding to scattering centers with smaller a.

Thus the total "classical" resistance can be written as

$$\rho=\rho_0+\rho_1, \tag{7}$$

where

$$\rho_1=\hat{\rho}_1\left(\frac{T}{\tilde{T}}\right)^q \exp\left[-\left(\frac{T_s}{T}\right)\right]. \tag{8}$$

Here the exponential describes an activation and thus, according to our considerations, $T_s\sim\mu-\varepsilon_m$, while the T dependence of the preexponential (chosen as some power function) is related to a dependence of the scattering efficiency on a and thus on the energy of the state. This expression coincides with the one given in Ref. 8 for traps below the Fermi level, and is consistent with numerous experiments (for a review, see Refs. 22 and 23).

Note that the "residual" resistivity ρ_0 is also temperature dependent, due to an activation-induced increase of the concentration of mobile carriers; this dependence can be especially significant in the "critical" region where the concentrations of localized and mobile carriers can be comparable. To take this dependence into account, we apply the Drude-like relations

$$\rho_0=\frac{1}{n_m\mu_0},\quad \rho_1=\frac{1}{n_m\mu_1} \tag{9}$$

where $1/\mu_0$ and $1/\mu_1$ are the inverse mobilities controlled by the "residual disorder" and the "temperature-dependent disorder," respectively. With the simplest assumption $\partial(\mu_1^{-1})/\partial n\equiv\tilde{\mu}^{-1}=\text{const}$ (that is with a neglect of a dependence of scattering efficiency on a), one easily obtains

$$\rho(T)-\rho(0)=\left(\frac{1}{n_{m0}}-\frac{1}{n_m(T)}\right)\left(\frac{n_{m0}}{\tilde{\mu}}-\frac{1}{\mu_0}\right), \tag{10}$$

where $n_{m0}=n_m(T=0)$.

IV. MAGNETORESISTANCE

The simplest situation corresponds to the dielectric limit ($\mu<\varepsilon_m$), with an additional assumption $g_0(\mu)>g_-(\mu)$. We recall that the index "0" corresponds to an "initial" tail of strongly localized states (spreading up to an energy ε_m) when these states are unoccupied or singly occupied. Index "-," in turn, corresponds to a band of doubly occupied states (the D^--band), where "unoccupied" states correspond to singly occupied states. Thus the condition mentioned above implies that the density of states for the second electron is at a Fermi level lower than the density of states for the first electron (the D^0 band). Correspondingly, the position of the Fermi level is controlled in this case by the D^0 band. In this situation [see Fig. 1(b) and also Appendix B] the main effect of the magnetic field is related to a shift of μ in the D^- band with a magnetic-field increase which is related to an increase of the Hubbard energy. For $T=0$ this shift is equal to $\delta\mu(H)=\mu_B gH$ (where the value of g corresponds to localized states), while for finite temperatures the position of the chemical potential in D^- band is described as (see Ref. 15)

$$\frac{\delta\mu(H)}{T}=-2\ln\left(2\cosh\frac{\mu_B gH}{2T}\right). \tag{11}$$

In the regime considered, the dominant contribution to the conductivity is related to hops within the D^- band from doubly occupied states with $\varepsilon=\mu$ to (singly occupied) states in the peak of the D^- band, since hops with spin flips from singly occupied states to singly occupied states are not allowed (as in the case of mechanism considered by Kamimura[18]).

We will begin with the case in which there is no Coulomb gap at the Fermi level, that is, when the interstate Coulomb interactions are neglected. Note that for the hopping in the band tail described by Eq. (4) with a small DOS the crucially situation depends on the relation between the width of effective hopping band $\delta\varepsilon$ and the energy scale ε_1 characterizing the DOS decay. The value of $\delta\varepsilon$ estimated for the Mott-type variable range hopping (VRH) [$g=\text{const}=g(\mu)$] is equal to

$$\delta\varepsilon\simeq\frac{T^{2/3}}{[g_c(a/2)^2]^{1/3}}\exp\frac{(\varepsilon_c-\mu)^2}{3\varepsilon_1^2}. \tag{12}$$

If $\delta\varepsilon<\varepsilon_1$, then one deals with a standard Mott-type hopping estimated for the corresponding density of states being approximately symmetric around the chemical potential.

However, when the opposite inequality holds, which can be rewritten as

$$\frac{(\varepsilon_c-\mu)^2}{\varepsilon_1^2}>2\log\left((g_c\varepsilon_1)^{1/2}\frac{a}{2}\frac{\varepsilon_1}{T}\right), \tag{13}$$

the hopping is expected to be dominated by electron hops from the Fermi level to "empty" states situated high above the Fermi level where the density of states drastically increases. (Note that "empty states" in the D^- band correspond to singly occupied states).

We believe that it is legitimate to consider this sort of hopping in a standard for the VRH way, that is, optimizing the hopping probability with respect to the typical hopping distance $\sim N_\varepsilon^{-1/2}$ (where N_ε is a density of sites with energies less than ε) and to the activation energy $\varepsilon-\mu$. Here we consider a case of a Gaussian tail, while the generalization for the exponential tail is straightforward. Taking into account that

$$N_\varepsilon=\int_\mu^\varepsilon d\varepsilon' g_c \exp-\frac{(\varepsilon_c-\varepsilon')^2}{\varepsilon_1^2}\sim g_c\varepsilon_1 \exp-\frac{(\varepsilon_c-\varepsilon)^2}{\varepsilon_1^2}$$

(where the integral is considered to be dominated by the upper limit), we obtain the following condition for the activation energy ε^*:

$$\varepsilon^*\simeq\varepsilon_c-\frac{\varepsilon_1}{\sqrt{2}}\left[\log\left(\frac{\varepsilon_1}{T}(g_c\varepsilon_1)^{1/2}\frac{4a}{2}\right)+\log\frac{\varepsilon_1}{\varepsilon_c-\varepsilon^*}\right]^{1/2}. \tag{14}$$

Since $\varepsilon_1/(\varepsilon_c-\varepsilon^*)\simeq 1$, we will neglect the last term in the brackets. Correspondingly, the temperature behavior of the conductivity is expected to obey the law

$$\sigma\propto\exp-\frac{\varepsilon_c-\mu-\frac{\varepsilon_1}{\sqrt{2}}\left[\log\left(\frac{\varepsilon_1}{T}(g_c\varepsilon_1)^{1/2}\frac{4a}{2}\right)\right]^{1/2}}{T}. \tag{15}$$

The activation energy depends logarithmically on the temperature, and slightly decreases with a temperature decrease. The difference with respect to a pure Arrhenius law originates due to a finite density of states in the tail.

As for the possible effect of the Coulomb gap, one notes that the value of $g(\mu)$ in the situation discussed is small. Correspondingly, the gap width is expected to be smaller than the characteristic energy scale ε_1, and thus the gap effects are irrelevant.

Now let us turn to the most important topic, i.e., the magnetic-field dependence. As is clearly seen, for strong magnetic fields the position of the Fermi level is significantly lowered, which leads to a dramatic decrease of the DOS at the Fermi level. In particular, the following scenario is possible. If at $H=0$ the DOS at the Fermi level is large enough [see Fig. 1(a)] that an inequality opposite to the one of Eq. (13) is satisfied, a standard VRH of Mott type or Efros-Shklovskii type is observed. Such a behavior is expected for the case when the initial position of the Fermi level corresponds to the peak region of the D^- band. However, the magnetic field shifts the position of the D^- band with respect to the Fermi level, and can finally lead to a nearly activated behavior according to Eq. (15) when $\mu_B gH>\varepsilon_1$.

One notes that hopping via the states of the D^- band actually competes with hopping over the (spin-polarized) D^0 band, that is, with hopping from an occupied state to an empty state. Correspondingly, when the magnetic-field-dependent contribution of D^- band becomes smaller than the contribution of hopping over the D^0 states, the MR saturates.

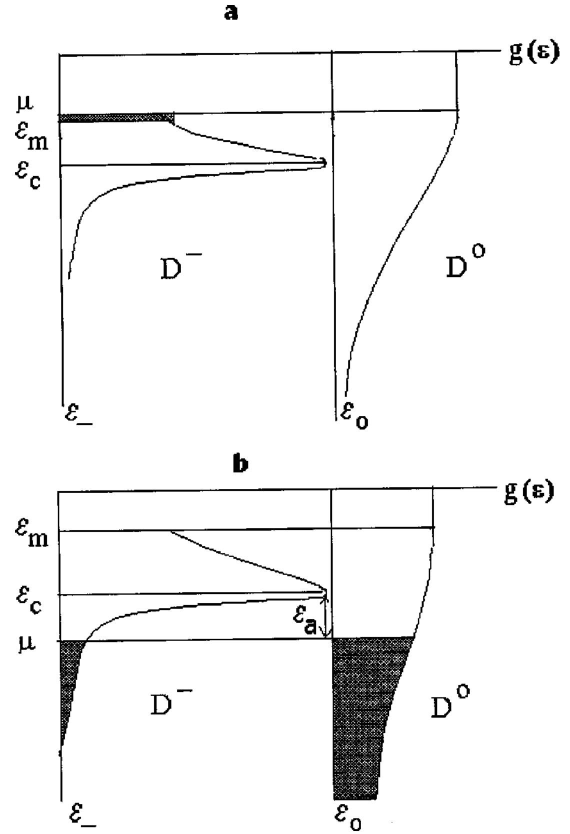

FIG. 2. (a) The structure of the subbands of doubly-occupied (left) and singly-occupied (right) localized states for an electron occupation corresponding to the metallic state in the "critical" region in the absence of a magnetic field. (b) The structure of the subbands for a high magnetic field, driving the system to strongly localized regime. Note that the position of ε_m in the D^0 band is considered to be lifted with respect to the case $H=0$ (moreover, the form of the bands is also changed), while the position of μ in the D^- band is lowered.

If we start from the metallic regime [see Fig. 2(a)], the variation of ε_m with magnetic field is of principal importance. Moreover, one expects the MR in this case to be mostly related to the variation of ε_m. Note that such a behavior is in agreement with the ideas of "magnetic-field-driven disorder" formulated in Ref. 9. An important factor is related to the fact that the metallic state corresponds in principle to linear screening, while the spin polarization of the mobile electrons is not expected to produce a strong effect on the disorder potential (see, e.g., Ref. 26). However, we believe that, at least in the critical region, a linear screening still coexists with a nonlinear one and, in particular, localized D^- states well below ε_m with relatively small localization lengths $a\leqslant n_c^{-1/2}$ cannot be efficiently screened by the mobile carriers.

Thus the depopulation of the D^- states corresponds to some suppression of the nonlinear screening which is similar to the creation of new scattering centers. Thus the polariza-

tion of localized states can lead to significant shifts of ε_m [see Fig. 2(b)]. More detailed arguments are given in Appendix B.

Estimating the variation of the electron concentration due to a depopulation of D^- states with a magnetic-field increase as

$$\delta n \simeq g_-(\mu_B g \,\delta H),$$

and applying arguments similar to those leading to Eq. (6), one obtains an estimate for the shift of the "mobility edge":

$$\delta(\varepsilon_m - \mu) \simeq \gamma g_- \mu_B g \,\delta H. \tag{16}$$

Thus one concludes that an increase of the magnetic field leads to an increase of the difference $\varepsilon_m - \mu$, and can lead to a change of a sign of this difference from negative to positive which corresponds to a suppression of the "metallic" state.

One concludes that in this regime the saturation of the MR corresponds to a stabilization of ε_m, which corresponds to a total polarization of the electron system including the localized states. The saturation field H_{sat} corresponds to lifting the bottom of the D^- band to the position of the chemical potential. Note that this scenario is similar to the one considered by Pudalov *et al.* Ref. 11.

As for the final state of the system, for $H > H_{sat}$ it obviously depends on the initial electron concentration. If this is large enough, in the final state the chemical potential is still larger than ε_m and the system persists in a metallic state. Moreover, we believe that deep in the metallic state linear screening dominates, and the MR can be related to mechanisms of the sort considered in Ref. 26. Thus we do not intend to analyze this regime in detail.

V. DISCUSSION

Let us compare the predictions of our model with the existing experimental data. We shall start with the temperature behavior of resistance. According to Eq. (10), the sign of the temperature coefficient of the resistance depends on the sign of the second set of brackets in Eq. (10). Moreover, Eq. (10) describes a "metal-insulator transition" under a purely classical regime. Indeed, for

$$n_{m0} = \tilde{\mu}/\mu_0 \equiv n_{mc}$$

$\rho(T) = \text{const}$. Note that this result is in agreement with the almost temperature-independent behavior of resistance for the "critical" concentration reported in Ref. 27.

The critical value of the resistivity is given as

$$\rho_c = \frac{1}{n_{m0}\mu_0} = \frac{1}{\tilde{\mu}}.$$

Thus, in our model, this quantity is controlled by the scattering efficiency of a depopulated localized state rather than by the total number of scattering centers. This fact is in agreement with the surprising experimental results of Ref. 24, demonstrating smaller values of the critical conductance for samples with larger peak mobilities. Indeed, samples with larger mobilities also exhibited smaller values of the critical concentration, which can result in less effective screening and, correspondingly, in a larger scattering efficiency for a single scatterer.

For smaller values of $n_{m,0}$ the temperature behavior of the resistance is dominated by the activation of electrons from localized states to delocalized ones (in accordance with observations reported in Ref. 11):

$$\rho \propto \exp\left(\frac{\varepsilon_m - \mu}{T}\right). \tag{17}$$

One notes that within the framework of a purely classical description our model exhibits, with an exponential accuracy, a scaling behavior of $\rho(T, n_s)$ which is symmetric with respect to the "critical" curve with $\varepsilon_m - \mu = 0$ if one assumes a constant DOS at the "critical region," since in the latter case

$$n_s - n_c = g_t(\mu - \varepsilon_m).$$

This behavior is in agreement with experiment (see, e.g., Ref. 6). For a strongly localized system when $\varepsilon_m - \mu$ is large enough, the system exhibits variable range hopping which is in agreement with experimental data (see, e.g., Ref. 6).

Actually quantum effects cause the system to become an insulator for $T \to 0$, since the states above the cutoff energy $\tilde{\varepsilon}_m$ discussed in Sec. II are described by the STL. This scenario was considered in detail in Ref. 8. Correspondingly, the metal-insulator transition discussed above is not a true quantum phase transition according to our model.

Now let us discuss the MR. As mentioned above, we are mostly interested in the insulating limit because, in our opinion, it can give more information about the system's properties than the metallic limit. Thus we would first like to compare our predictions concerning the MR in the strongly insulating limit with existing experimental data.

As reported (see, e.g., Refs. 6 and 12), the high-field insulator regime typically exhibits a nearly activated temperature dependence of the magnetoconductivity. We shall start from the experiment reported in Ref. 13, where a δ-doped GaAs/Al_xGa_{1-x}As heterostructure was studied. Although this system does not exhibit a 2D MIT, it demonstrates a strong positive MR starting from hopping regime. A specific feature was a gradual transition from variable range Efros-Shklovskii hopping to nearly activated hopping. In our previous paper[16] we tried to fit the experimental curves according to a pure Arrhenius law, ascribing the deviations from experimental behavior to a neglect of the nonzero DOS in the band tail.

Now we are going to compare the experimental data of Ref. 13 with our present theory which directly takes into account a Gaussian tail of the D^- band. In Fig. 3 we plot the theoretical curves corresponding to Eq. (15), calculated for $\varepsilon_c - \mu(H=0) = 0.234$ meV ($H = 8$T), 0.219 meV ($H = 6$ T), $\varepsilon_1 = 0.14$ meV, $g_0 a^2 = 0.93$ meV^{-1}, and $g = 0.12$. As seen, there is a good agreement between the experimental data and our theoretical prediction which supports our interpretation.

The value of the effective g factor is about four times lower than the handbook values for GaAs. However, one has

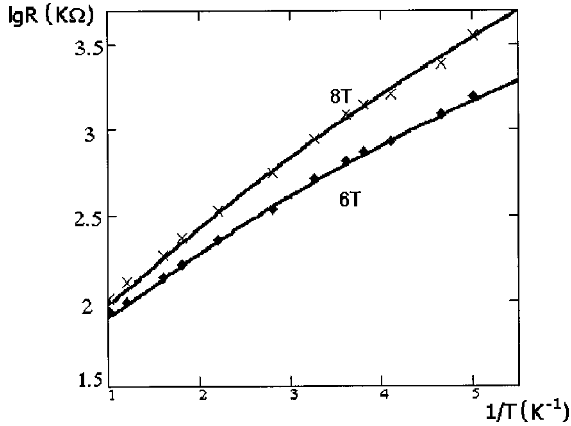

FIG. 3. Resistivity vs temperature for a Si δ-doped GaAs-Al_xGa_{1-x}As heterostructure of Ref. 13 for $B=6$ (full squares) and 8 Tesla (crosses) at $n=9.52\times10^{10}$ cm^{-2}. Solid lines are theoretical curves corresponding to Eq. (15) calculated for $\varepsilon_c-\mu=0.234$ meV ($H=8$ T), 0.219 meV ($H=6$ T), $\varepsilon_1=0.14$ meV, $g_0a^2=0.93$ meV^{-1}, and $g=0.12$.

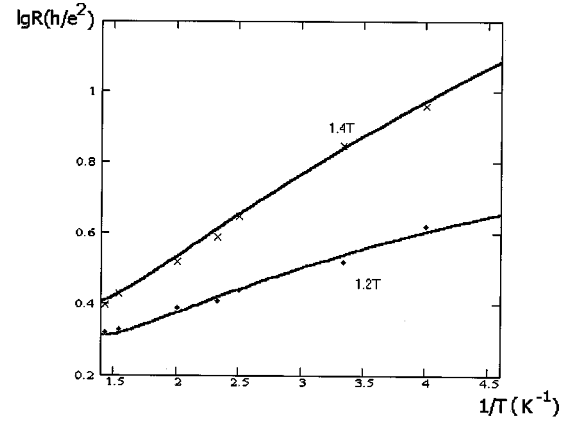

FIG. 4. Resistivity vs temperature for rhe Si MOSFET of Ref. 2 for $B=1.2$ (full squares) and 1.4 (crosses) at $n=8.83\times10^{10}$ cm^{-2}. Solid lines show the theoretical curves calculated on the basis of Eq. (15) with the values of the parameters $\varepsilon_c-\mu=0.147$ meV ($H=1.4$ T), 0.126 meV ($H=1.2$ T), $\varepsilon_1=0.1$ meV, $g_0a^2=1.2$ meV^{-1}, and $g=1.7$.

to keep in mind that we deal with an Al_xGa_{1-x}As-GaAs heterostructure rather than with bulk GaAs. The g-factor values for Al_xGa_{1-x}As quantum wells were calculated theoretically.[28] It was shown that due to the fact that in such structures one has a mixture of GaAs states (for which the g factor ~ -0.45 is negative) and Al_xGa_{1-x}As states (where the g factor is positive) the effective g factor depends on the well width. In the case of the gated heterostructure under discussion, the effective width of the potential well is controlled by the gate voltage V_g, and thus the effective g factor is expected to depend on V_g. The corresponding behavior was considered in some detail in our previous paper,[16] and was shown to be in agreement with the experimental data of Ref. 13.

In addition, we have compared our results with MR data of Simonian *et al.*[2] The data obtained for Si MOSFET's demonstrated a suppression of the metallic state in strong parallel magnetic fields, and a transition to a localized state. Since our model gives most definite quantitative predictions for insulating limit, we analyzed the data on temperature behavior of the MR reported in Ref. 2 for the strongest magnetic fields (1.4 and 1.2 T). In Fig. 4 we present both experimental data and theoretical curves calculated on the base of Eq. (15) for the values of the parameters $\varepsilon_c-\mu=0.147$ meV($H=1.4$ T), 0.126 meV($H=1.2$ T) $\varepsilon_1=0.1$ meV, $g_0a^2=1.2$ meV^{-1}, and $g=1.7$. It is seen that there is a good agreement between theoretical and experimental results. The value of the g factor estimated in this way is close to the handbook values for Si. Note that in the insulating limit the Fermi-liquid renormalization of g factor is irrelevant.

Following the same ideas, we have also analyzed the MR in the insulating limit for p-type GaAs-Al_xGa_{1-x}As heterostructures exhibiting a metal-insulator transition.[5] The extracted value of the g factor appeared to be equal to 0.025–0.04. This is in agreement with the fact that the expected value of the g factor for heavy holes is zero; this effect is related to an admixture of light-hole states.

Reference 2 reported a suppression of the metallic phase at a strong magnetic field, followed by a saturation of the resistance. The behavior exhibits an H/T scaling, while the most representative data correspond to the dielectric side of the MIT. This behavior is in agreement with Eq. (11) which predicts the H/T scaling for the MR activation exponent.

An important feature of the MR in systems exhibiting a 2D MIT is its saturation at high fields. According to our model, the nature of this effect can be different for different regimes.

For systems initially in a strong insulating limit (when the disorder potential is not significantly affected by the magnetic field), the saturation field H_{sat} is related to a competition between contributions of D^- and D^0 subbands, and thus depends mostly on the forms of the subbands.

For systems initially in the "critical" region (no matter on what side of the transition) the initial evolution of the MR is related to a shift of ε_m, although at high fields a competition between hopping processes in D^- and D^0 bands is still possible. In both regimes mentioned above, the value of H_{sat} is expected to be sample dependent. Note that such a behavior was reported in Ref. 11.

Although from the very beginning we have not intended to discuss properties of systems where the initial electron density was significantly larger than the critical one, we would like to make some comments about this regime as well. In particular, even for systems initially deep in the metallic regime but still containing a significant density of localized states, the value H_{sat} is not expected to be universal, since the form of the D^- band is obviously sample dependent. Moreover, the possible exchange of electrons between the conducting band and states spatially separated from the conducting paths (discussed in Appendix B) does not allow one to relate the total electron concentration to the position of the chemical potential in the conducting band. In addition, one also notes that the value of the g factor for mobile electrons is renormalized due to exchange interactions, and is concentration dependent; in any case its value is different

from the corresponding value for localized states. Thus we believe that the saturation field for the metallic regime does not give proper information concerning, in particular, the value of the g factor. This conclusion is especially important for samples with concentrations close to the critical one.

Note that if H_{sat} corresponds to a crossover from a ''metallic'' state to an ''insulating'' state then—at least for magnetic fields close to H_{sat}—the chemical potential crosses the peak of the D^- band. This factor can explain the enhanced DOS at the Fermi level for the ''critical'' state (with respect to the standard one for the ideal 2D conduction band) observed in Ref. 25.

We would also like to note that the ''final'' insulating state achieved in strong magnetic fields is different from the insulating state existing for $H=0$ at small enough electron concentrations. In particular, the latter situation is characterized by the presence of a peak of the D^- band close to ε_m which is absent for the former situation. Correspondingly, electrons in the metallic state close to the ''critical'' state for $H=0$ are expected to suffer an additional mechanism of inelastic scattering related to the activation of D^- states which is absent for the spin-polarized situation. This latter factor can enhance the role of weak localization for $H>H_{sat}$. In any case, according to convincing calculations of Ref. 22, the behavior of the ''critical'' states is strongly sensitive to the system parameters. This fact, taking account of the factor mentioned above, explains a difference in behavior of the ''critical states'' for the cases of $H=0$ and $H>H_{sat}$ reported in Ref. 25.

We believe that the surprising evolution of the temperature coefficient of the resistance in the course of a magnetic-field increase (being ''metalliclike'' in $H=0$ and $H>H_{sat}$, and ''insulatinglike'' for some intermediate fields close to H_{sat}) reported in Ref. 12 can be related to the evolution of a position of the D^- band with respect to the Fermi level. Indeed, one can expect that the presence of quasilocalized states at the Fermi level, at the moment when the peak of the D^- band coincides with μ, can significantly affect both classical and quantum contributions to the resistance.

VI. SUMMARY

We have demonstrated that the main features of a 2D MIT apparently observed recently in different systems can be explained within the framework of a simple two-band model. The latter is based on the assumption that a transitionlike behavior takes place in the disorder-induced ''tail'' of the 2D conductance band where the lower, strongly localized states are not described by scaling theory of localization starting from the large conductance limit. An important role among these states is played by doubly occupied states coexisting in general with the singly occupied ones. The role of the D^- states is emphasized by the fact that as a result of the energy dependence of the Hubbard energy their DOS is peaked near the bottom of the 2D conductance band. We also emphasize the role of the nonlinear screening of a disordered potential by localized electrons. The ''metalliclike'' temperature behavior of the conductivity is related to the activation of localized carriers to the conductance band leading to an ''undressing'' of the disorder potential due to a partial suppression of the nonlinear screening. The strong positive MR on the dielectric side is related to a suppression of activated hopping to the peak of the D^- band as a result of lowering the chemical potential with respect to the D^- band. The suppression of the metallic state in a strong magnetic field is explained as a result of the depopulation of the doubly occupied localized states participating in the nonlinear screening of the disorder potential. A comparison of theoretical predictions with existing experimental data exhibits at least a qualitative agreement, while the values of g factors extracted from the MR data for the strongly insulating limit according to our model are in quantitative agreement with the values known for localized states in corresponding materials.

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APPENDIX A: FORM OF THE D BAND

We start from the density of states corresponding to singly occupied states (characterized by energies ε_0) $g(\varepsilon_0)$. The energies of doubly occupied states are shifted (with respect to the energies ε_0) by the Hubbard energy. We take into account that, according to our assumption, the localization length for the strongly localized states can be written as

$$a(\varepsilon_0)=a_B\left(\frac{\varepsilon_B}{\varepsilon_m-\varepsilon_0}\right)^{\nu},$$

where ε_B is the energy width of the band of localized states, while a_B is the minimal localization length available for these states. Thus, for the energy of the doubly occupied state ε_-, we have

$$\varepsilon_-=\varepsilon_0+U_0\left(\frac{\varepsilon_m-\varepsilon_0}{\varepsilon_B}\right)^{u} \tag{A1}$$

(where $U_0=e^2/\kappa a_B$). The DOS for the doubly occupied states should be written in terms of the total energies ε_-; then one should also take into account the Jacobian related to a change of variables from ε_0 to ε_-. Correspondingly, the DOS in the D^- band is given as[18]

$$g_-(\varepsilon_-)=g[\varepsilon_0(\varepsilon_-)]\left(\frac{\partial\varepsilon_-}{\partial\varepsilon_0}\right)^{-1}, \tag{A2}$$

where the functional dependence of $\varepsilon_0(\varepsilon_-)$ is given by the solution of Eq. (A1).

If $u>1 g_-$ diverges at some $\varepsilon_{0,c}$ corresponding to a vanishing of the derivative in Eq. (A2),

$$\varepsilon_B=uU_0\left(\frac{\varepsilon_m-\varepsilon_{0,c}}{\varepsilon_B}\right)^{u-1}. \tag{A3}$$

This is related to the fact that the function $\varepsilon_0(\varepsilon_-)$ is a double-valued one, and a vanishing of the derivative in question corresponds to the coincidence of these solutions. One branch of the solutions corresponds to the singly occupied states above $\varepsilon_{0,c}$, while another one corresponds to the states below $\varepsilon_{0,c}$.

Now, one concludes that if

$$\varepsilon_m-\varepsilon_{0,c}\simeq\varepsilon_B\left(\frac{u\varepsilon_B}{U_0}\right)^{1/(u-1)}$$

is small enough with respect to ε_B, the lowest localized states will allow only single-electron occupation. Indeed, the Hubbard energy for these states appears to be too high, and the corresponding doubly occupied states float to the region of mobile carriers.

We take into account that there is an upper cutoff for the localization lengths $\tilde{a}$ imposed by the STL (discussed at the beginning of Sec. II). This results in a lower cutoff for the difference $\varepsilon_m-\varepsilon_0$. Our considerations hold if the energy $\varepsilon_{0,c}$ is not affected by this cutoff; the corresponding criterion is

$$\frac{\tilde{a}}{a_B}>\left(\frac{\varepsilon_B}{\varepsilon_m-\varepsilon_{0,c}}\right)^{\nu}.$$

In what follows we will assume this criterion to hold.

The critical value of the energy of a doubly occupied state $\varepsilon_{-,c}$ is related to $\varepsilon_{0,c}$ by Eq. (A1). To estimate the energy dependence of g_- near a critical value of ε_-, we take into account that, for ε_0 close to $\varepsilon_{0,c}$,

$$\frac{\partial\varepsilon_-}{\partial\varepsilon_0}\simeq\frac{\partial^2\varepsilon_-}{\partial\varepsilon_0^2}(\varepsilon_0-\varepsilon_{0,c}). \qquad \text{(A4)}$$

Aiming to rewrite this equation in terms of ε_-, we take into account that

$$\varepsilon_--\varepsilon_{-,c}\simeq\left.\frac{\partial\varepsilon_-}{\partial\varepsilon_0}\right|_{\varepsilon_0=\varepsilon_c}+\frac{1}{2}\frac{\partial^2\varepsilon_-}{\partial\varepsilon_0^2}(\varepsilon_0-\varepsilon_{0,c})^2. \qquad \text{(A5)}$$

Keeping in mind that the first derivative vanishes, we are left with

$$(\varepsilon_0-\varepsilon_{0,c})\simeq\left(\frac{1}{2}\frac{\partial^2\varepsilon_-}{\partial\varepsilon_0^2}\right)^{-1/2}(\varepsilon_--\varepsilon_{-,c})^{1/2}, \qquad \text{(A6)}$$

where

$$\frac{\partial^2\varepsilon_-}{\partial\varepsilon_0^2}\simeq\frac{u-1}{\varepsilon_m}\left(\frac{uU_0}{\varepsilon_m}\right)^{1/(u-1)}.$$

Correspondingly, for ε_- close to $\varepsilon_{-,c}$ (but still above $\varepsilon_{-,c}$) we have

$$g_-=\frac{2^{1/2}g[\varepsilon_0(\varepsilon_-)]}{(\varepsilon_--\varepsilon_{-,c})^{1/2}}\left(\frac{\varepsilon_m}{u-1}\right)^{1/2}\left(\frac{\varepsilon_m}{uU_0}\right)^{1/2(u-1)}. \qquad \text{(A7)}$$

According to these considerations (also see Ref. 18) g_- vanishes for $\varepsilon_-<\varepsilon_{-,c}$. Note that in a realistic situation such a sharp edge of the DOS singularity is expected to be smeared in some way. In particular, one can expect local fluctuations of the parameter U_0 due to local fluctuations of the dielectric function. It is natural to assume that fluctuations of U_0 correspond to a Gaussian distribution with some variance δU_0. As can be easily followed, these fluctuations give rise to Gaussian fluctuations of the energy $\varepsilon_{-,c}$ with a variance

$$\varepsilon_1\sim\delta U_0\frac{1}{u-1}\left(\frac{u\varepsilon_m}{U_0}\right)^{1/u-1}.$$

Averaging the form-factor function of Eq. (A7),

$$\frac{1}{(\varepsilon_--\varepsilon_{-,c})^{1/2}}\theta(\varepsilon_--\varepsilon_{-,c})$$

$[\theta(x>0)=1,\theta(x<0)=0]$ with respect to the fluctuations in question, one easily obtains that the averaged form factor has a form

$$[(\varepsilon_--\varepsilon_{-,c})+\varepsilon_1]^{-1/2}, \quad \varepsilon_->\varepsilon_{-,c}$$

$$\left[\varepsilon_1\exp-\left(\frac{\varepsilon_--\varepsilon_{-,c}}{\varepsilon_1}\right)^2\right], \quad \varepsilon_-<\varepsilon_{-,c}. \qquad \text{(A8)}$$

As a result one expects the D^- band to have its own tail corresponding to a nonzero but quickly decreasing DOS at $\varepsilon_-<\varepsilon_{-,c}$,

$$g_-\simeq g_c\exp-\left(\frac{\varepsilon_c-\varepsilon}{\varepsilon_1}\right)^2, \qquad \text{(A9)}$$

where we have omitted $-$ indices for the energy terms, implying that the function $g_-(\varepsilon)$ has an energy argument corresponding to D^- band.

APPENDIX B: EFFECT OF MAGNETIC FIELD ON THE D^- BAND

The problem of extreme importance for us is related to a variation of μ with a variation of the magnetic field. The presence of the field leads to the Zeeman addition $\mu_B gH$ in Eq. (A1). Since this term is not energy dependent, it does not change the value of $\varepsilon_{0,c}$ discussed above, but shifts the bottom of the D^- band $\varepsilon_{-,c}$ toward a "mobility edge" corresponding to the majority spins. Finally the value $\varepsilon_{-,c}$ coincides with ε_m, which obviously corresponds to

$$\varepsilon_m-\varepsilon_{-,c}(H=0)=\mu_B gH. \qquad \text{(B1)}$$

After this only singly occupied states exist below ε_m.

As for the position of the Fermi level, for a fixed number of electrons it should be calculated taking account of the balance between the number of electrons in singly and doubly occupied states. For a system deep in the insulating state, such an analysis was made in Ref. 15 with an assumption that the DOS of the doubly occupied states at the Fermi level

is much less than the DOS for singly occupied states. In this case the position of μ in the D^0 band is fixed, while its position in the D^- band is lowered according to considerations given above.

The picture is not as simple if we start from the metallic state. If we deal only with band tail states, the depopulation of doubly occupied states (including the localized D^- states) would inevitably lead to a rise of the chemical potential for the majority electrons. Note that for conducting (delocalized) electrons the value of the g factor can be renormalized due to Fermi-liquid effects (see, e.g., Ref. 29).

Thus these simple considerations concerning the evolution of the chemical potential with the increase of the magnetic field cannot explain the strong positive MR in the metallic state, since the rising of the chemical potential for spin-polarized electrons is not expected to decrease the conductivity significantly. In our opinion, the MR can be related to the evolution of the position of the "mobility edge" ε_m with an increase of the field. This argument is supported by the estimate given in Sec. II, which shows that, at least at the critical region, the evolution of ε_m can dominate the evolution of μ.

Two possible scenarios can be discussed. First, one can expect that the depopulation of the doubly occupied D^- states (that is, the redistribution of electrons between doubly and singly occupied localized states) leads to an enhancement of the disorder and to an increase of ε_m. Indeed, one must keep in mind that the occupation of localized states by electrons corresponds to a screening of this potential, and that the screening is expected to be more effective if there exists an additional choice between double and single occupations. Indeed, the additional degree of freedom can allow one to lower the total electrostatic energy of the system. According to the arguments given above, the evolution of ε_m can dominate over the inevitable increase of μ related to the depopulation of D^- states.

Another possibility corresponds to the presence of a subband of strongly localized states assumed to coexist with the 2D band states (including the band tail states), but spatially separated from the band states. (Note that such a scenario is similar to the one considered in Refs. 11 and 9) These localized states are expected to have a "mobility edge" much higher than ε_m, and much larger Hubbard energies, preventing the double occupation of these states. Such an assumption is a realistic one, since, for small electron concentrations, the percolation character of the electron transport is expected to be due to the presence of a large-scale potential.[19] In this case electrons from D^- states are, in particular, redistributed to these states, decreasing the density of electrons in the band tail. Thus the nonlinear screening of localized states becomes less effective, while a rise of the chemical potential is suppressed. As a result, the difference $\mu(H)-\varepsilon_m(H)$ can at some $H=H_c$ change its sign, which corresponds to a crossover to the insulating limit.

Although a possible shift in ε_m with an increase of carrier concentration was disputed in Ref. 25 we would like to note those authors based their considerations on the absence of significant shifts of ε_m for small variations of electron concentration around its critical value. In our opinion, this argument does not hold for our picture, since the redistribution of electrons due to spin polarization is expected to be pronounced in contrast to the case of a small variation of n.

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