Dilute electron gas near the metal-insulator transition in two dimensions.

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In recent years systematic experimental studies of the temperature dependence of the resistivity in a variety of dilute, ultra clean two dimensional electron/hole systems have revived the fundamental question of localization or, alternatively, the existence of a metal-insulator transition in the presence of strong electron-electron interactions in two dimensions. We argue that under the extreme conditions of ultra clean systems not only is the electron-electron interaction very strong but the role of other system specific properties are also enhanced. In particular, we emphasize the role of valleys in determining the transport properties of the dilute electron gas in silicon inversion layers (Si-MOSFETs). It is shown that for a high quality sample the temperature behavior of the resistivity in the region close to the critical region of the metal-insulator transition is well described by a renormalization group analysis of the interplay of interaction and disorder if the electron band is assumed to have two distinct valleys. The decrease in the resistivity up to five times has been captured in the correct temperature interval by this analysis, without involving any adjustable parameters. The considerable variance in the data obtained from different Si-MOSFET samples is attributed to the sample dependent scattering rate across the two valleys, presenting thereby with a possible explanation for the absence of universal behavior in Si-MOSFET samples of different quality.

The resistivity in a variety of high mobility two dimensional (2D) electron/hole systems is seen experimentally to exhibit a number of interesting anomalies that do not, as yet, have an adequate theoretical understanding. (For an extensive bibliography, see Ref. 1.) The high quality of the samples allows measurements to be made at very low carrier densities corresponding to \( r_s \gtrsim 10 \), where \( r_s = E_{\text{e-e}}/E_F \) is the ratio of the Coulomb energy to Fermi energy. When the resistivity at high temperatures is comparable to or less than the quantum resistance, \( h/e^2 \), the resistivity, \( \rho(T) \), drops noticeably as the temperature is reduced [2,3]. The drop appears to be completely quenched when a magnetic field is applied parallel to the plane [4–6]. This anomalously strong positive magnetoresistance, which is obviously
related to the spin degrees of freedom, points to the importance of the electron-electron (e-e) interaction in this phenomenon.

These experimental observations have revived interest in the fundamental question of the existence of a metal-insulator transition in 2D systems in the presence of a strong e-e interaction. (We use the term “transition” to describe the qualitative change in the resistivity at the experimentally accessible temperatures, not discussing the question of the limit \( T \to 0 \).)

Although the drop in the resistivity is seen in almost all the different dilute systems studied so far, and are therefore generally considered to be universal, quantitative comparison indicates that the magnitude of the effect is very sensitive to the system used. The most pronounced anomaly has been reported in the cleanest (001) Si-MOSFET samples, where a steep drop in \( \rho(T) \) of up to five to six times has been observed.

In Fig. 1 the temperature dependence of the resistivity for different densities in a Si-MOSFET sample with a very high peak mobility of \( \mu_{\text{peak}} = 32,000 \text{ cm}^2/\text{Vs} \) (measured at \( T = 0.3\text{K} \)) has been reproduced \cite{7}. The insulating region, where the resistivity increases with decreasing temperature, is labeled as \( I \) in Fig. 1. The range of densities where the resistivity depends non-monotonically on temperature is labeled as \( C^* \) in Fig. 1. (For the specific sample used in Fig. 1, this region covers electron densities in the range \( 0.8 \times 10^{11} < n < 1 \times 10^{11}\text{cm}^{-2} \).) A narrow range of densities in between these two regions, in which the separatrix that separates the insulating phase from the metallic phase should lie (if a true metal-insulator transition exists) can be considered as the critical region \( C \). The region where no clear maximum in the resistivity is observed (unlike \( C^* \)) is labeled as \( M \) in Fig. 1. The region \( C^* \) is the subject of interest of this paper.

Since the maximum of the resistivity in the region \( C^* \) is comparable to \( \sim h/e^2 \), the transport mean free path time, \( \tau \), of the electrons here is such that \( h/\tau \lesssim E_F \). The maximum together with the steep decrease in \( \rho(T) \) occurs at low temperatures well below the Fermi energy (see Fig. 1). Therefore, the indications are that the non-monotonic behavior of the resistivity in the region \( C^* \) is a manifestation of the physics of strongly interacting electrons.
that are in the diffusive regime: $T < \hbar/\tau \lesssim E_F$.

Away from the region $C^*$ and deep in the region labeled $M$ in Fig. 1 a naive estimate for $\tau$ can be extracted from the Drude expression for the resistivity, $\hbar/\tau = 4(e^2/\hbar)\rho(T = 0)E_F$, with $\rho(T = 0)$ being the extrapolated value of the resistivity at $T = 0$. This estimate gives values for $\hbar/\tau$ that are well below the Fermi energy, while the steep drop in the resistivity develops at temperatures that are comparable to or larger than $\hbar/\tau$. This implies that the anomalies in the region $M$ occur in the temperature range $\hbar/\tau \lesssim T < E_F$, and their origin may be attributed (at least partially) to a strong temperature dependence of the single particle mean free path time $\tau(T)$ [8–10]. On the contrary, the situation in the region $C^*$ is quite different since the anomalies here are in the temperature range $T < \hbar/\tau \lesssim E_F$ where disorder quenches the effects of thermal smearing on $\tau(T)$ [10].

These considerations lead us to the conclusion that the anomalous decrease in the resistivity in the two regions, $C^*$ and $M$, may have different origins and are hence best studied separately. In this paper we analyze the transport properties in the region $C^*$, close to the critical region $C$, where the transport is controlled by the propagation of diffusive collective modes. We demonstrate that the phenomenon in this region can be understood within the framework of a theory describing the effect of the $e-e$ interaction on the propagation of these modes [11]. The peculiarity of dilute conductors is that at low temperatures the antilocalizing component of this effect becomes dominant.

Although universal behavior is generally expected to hold in the critical region, no universal scaling relating the $\rho(T)$ curves from different samples has been found. In fact, considerable variance is seen even in the data obtained from different Si-MOSFET samples of similar origin, including the data from the same sample that varies due to the degradation of the high mobility sample with time. Hence, for a quantitative understanding of the temperature dependence of the resistivity in the region not far from the transition some system specific non-universal mechanism should be necessarily invoked. The conduction band of the electrons in a (001) Si-MOSFET surface has two almost degenerate valleys located at points $\pm Q_0$ ($Q_0 = 0.85 \times (2\pi/a)$, where $a$ is the lattice constant of Si) [12]. In what follows, the
sensitivity of the transport properties of the dilute electron gas to the scattering rate across the two valleys is presented as a possible explanation for the absence of this universality. At temperatures comparable to the rate of the intervalley scattering, $\hbar/\tau_\perp$, a crossover occurs between a band with two distinct valleys and a band where the two valleys are effectively unified due to the intervalley scattering. We believe that in a typical sample the value of $\hbar/\tau_\perp$ falls within the temperature interval in which measurements are made. Hence due to the crossover at $T \sim \hbar/\tau_\perp$ the resistivity $\rho(T)$ will be non-universal. Only in an ultra clean sample (like the one presented in Fig. 1), where the intervalley scattering is very weak and the two valleys are well separated, should a universal behavior hold.

To understand the temperature dependence of $\rho(T)$ in the case of two valleys, we study the interplay of the appropriate collective modes. These modes describe fluctuations of the local density of particles, spin, and in addition the fluctuations involving electron states from different valleys. The evolution of the collective modes, in the limit of long wavelengths and small frequencies, are described by a singular propagator with a diffusion pole $\propto 1/(Dq^2 - i\omega)$, where $D$ is the diffusion constant. (Note that the collective modes may exist even when a description in terms of single particle excitations is not possible.) These singular propagators when combined with the $e-e$ interaction are known in 2D to lead to the appearance of non-analytical corrections to the resistivity. On the other hand, the amplitudes of the $e-e$ interaction that affects the propagation of the collective modes are known to have divergent corrections due to the disorder. The program to self-consistently take into account these corrections, which in fact corresponds to a derivation of a system of renormalization group (RG) equations, has been realized to lowest order in the resistivity (disorder), and fortunately to all orders in the $e-e$ interaction amplitudes [13]. The latter fact is important when $r_s$ is large as then the electron liquid may be not far from some magnetic instability, implying that the Landau’s Fermi liquid amplitude $\gamma_2$ that controls the interaction of the spin-density fluctuations may be not small.

The diffusion propagators of the electron-hole pairs in the presence of valleys in addition to the momentum and spin quantum numbers are labeled by quantum numbers $|\tau\rangle$, where
|τ⟩ = ± are the two valley indices similar to the up and down spin states |σ⟩ =↑, ↓. Altogether there are 4 × 4 = 16 electron-hole states that break up into one singlet and fifteen multiplet states. In the case of strong intervalley scattering, however, the modes that are made of states from different valleys acquire a gap proportional to ℏ/τ⊥. This implies that for temperatures, or frequencies, less than ℏ/τ⊥ such modes do not yield diverging contributions and hence become ineffective. (This is the origin of the crossover discussed above.) As a result, off the 16 modes only one spin singlet and three spin triplet combinations retain a diffusion pole. Therefore, the situation when the two valleys are effectively unified becomes equivalent to the case with no valleys (but with the density of states doubled). In 2D the leading divergences are logarithmic and the RG equation describing the evolution of the resistivity in the absence of valleys has been previously derived [13–17]:

\[
\frac{dg}{dξ} = g^2 \left[ 1 + 1 - 3 \left( \frac{1 + \gamma_2}{\gamma_2} \ln(1 + \gamma_2) - 1 \right) \right].
\]  

(1)

Here ξ = −ln(Tτ) and the dimensionless parameter g = (e^2/πℏ)ρ; note that apart from the standard unit e^2/ℏ an additional factor 1/π has been introduced in g. In the square brackets the first term corresponds to the weak localization correction (quantum interference) [18], while the second term is the contribution of the singlet density mode which due to the long ranged nature of the Coulomb interaction is also universal [11]. The last term describes the contribution of the three triplet modes. Due to the difference in symmetry of the singlet and the triplet wave functions under exchange the last two terms have opposite signs that favor localization and antilocalization, respectively. The resulting flow of g(ξ) becomes antilocalizing when γ_2 is greater than the value γ_2^* = 2.04. This value demands, however, the presence of rather strong electron correlations. (For comparison, the effective amplitude of the e-e interaction for small momentum transfer with n valleys participating in screening equals 1/2n; the suppression occurs due to the increased screening.)

In the case of two distinct valleys, i.e., when T > ℏ/τ⊥, Eq. 1 can be easily generalized as:

\[
\frac{dg}{dξ} = g^2 \left[ 2 + 1 - 15 \left( \frac{1 + \gamma_2}{\gamma_2} \ln(1 + \gamma_2) - 1 \right) \right].
\]  

(2)
The difference between the numerical factors in Eq. 1 and Eq. 2 are easily accounted for in terms of the number of degrees of freedom in each case. Naturally, the weak localization term becomes twice as large because of the presence of two valleys. Although the $e$-$e$ amplitude controlling the interaction in the singlet channel is reduced by a factor of two as electrons from both valleys participate in screening, after adding together the contributions from each valley the second term in Eq. 2 remains the same as that in Eq. 1 [11]. Finally, the difference in the number of the multiplet modes increases the coefficient of the $\gamma_2$ term from 3 to 15. (Now, $\gamma_2$ is the Fermi liquid amplitude that controls the $e$-$e$ interaction in all the multiplet channels. Like in Eq. 1 this dimensionless parameter is normalized by the density of states for a single spin and valley species.) As a result of these modifications the value of $\gamma_2$ required for the flow of $g(\xi)$ to become antilocalizing is considerably reduced to $\gamma_2^* = 0.45$. (This value is not too far from the $e$-$e$ interaction amplitude for small angle scattering, that we use to compare, which equals 0.25 for $n = 2$.) The reduction of $\gamma_2^*$ from 2.04 to 0.45 makes it easier in the case of two valleys to reach the stage where the resistivity starts to decrease.

In conventional conductors the initial values of the amplitude $\gamma_2$ are small, and the net effect is in favor of localization. In dilute systems, however, this amplitude is enlarged due to $e$-$e$ correlations. In addition, in 2D the amplitude $\gamma_2$ also experiences logarithmic corrections due to the disorder [13–17]. The equation describing the RG evolution of $\gamma_2$ is the same for both one and two valleys:

$$\frac{d\gamma_2}{d\xi} = g \frac{(1 + \gamma_2)^2}{2}.$$  \hspace{1cm} (3)

It follows from this equation that as the temperature is lowered $\gamma_2$ increases monotonically. When it increases beyond the value $\gamma_2^*$ the resistivity will pass through a maximum. Although the initial values of $g$ and $\gamma_2$ are not universal and depend on the system, the flow of $g$ according to the RG equations can be described by a universal function $R(\eta)$ [13]:

$$g = g_{\text{max}} R(\eta) \quad \text{and} \quad \eta = g_{\text{max}} \ln(T_{\text{max}}/T),$$  \hspace{1cm} (4)
where $T_{\text{max}}$ is the temperature at which $g$ reaches its maximum value $g_{\text{max}}$, i.e., $\gamma_2(T_{\text{max}}) = \gamma^*_2$. For the case of two valleys, the function $R(\eta)$ is found here by numerically integrating Eq. 2 and Eq. 3 with the boundary conditions: $g(\xi = 0) = g_{\text{max}} = 1$ and $\gamma_2(\xi = 0) = \gamma^*_2 = 0.45$.

Thus, if the experimental data of the resistivity are scaled with respect to the maximum value as $g/g_{\text{max}}$ and plotted against $\eta$, which involves scaling the log of the temperature by $g_{\text{max}}$, then the data should collapse on the function $R(\eta)$. This analysis has certain limitations, however. The RG equations have been derived in the lowest order in $g$ and therefore cannot be applied in the critical region $C$ where $g \gtrsim 1$. On the other hand, for $g \ll 1$ exponentially small temperatures are needed for changes in the resistivity to become noticeable. In addition, some other (not yet completely identified) mechanism operating in the region $M$ may mask the discussed logarithmic corrections that are very weak when $g \ll 1$.

For these reasons, only curves in the region $C^*$ with maximum $g$ ranging from $g_{\text{max}} \approx 0.3$ to $g_{\text{max}} \approx 0.6$ have been used to test the RG analysis. The result is presented in Fig. 2, where the data has been scaled as in Eq. 4. The decrease in the resistivity up to five times together with its saturation has been captured in the correct temperature interval by this analysis. Note that no adjustable parameters were used in the procedure.

We emphasize again that this universal behavior will be observed only in ultra clean samples, and will not be found in samples that are only moderately clean, because of the crossover at $T \sim \hbar/\tau_\perp$. Next, in samples with a low mobility, where a description in terms of an effective single valley is relevant, the large value for $\gamma^*_2 = 2.04$ makes it difficult for the non-monotonicity to be observed as the initial values of $\gamma_2$ are, most probably, far away from 2.04. Then, to scale the amplitude $\gamma_2$ till the value $\gamma^*_2$ will, for $g \ll 1$, demand exponentially small temperatures as the corrections depend on the temperature only logarithmically. On the other hand, for $g$ near the critical region, where changes in the resistivity develops rapidly, the resistivity flows to such large values that the system instead of passing through the maximum becomes insulating. To summarize, we have argued that it is not the large
value of \( r_s \) that makes the physics of the region not far from the transition in high mobility MOSFET samples so different from that in lower mobility samples, but the difference in their number of effective valleys. Note that in some samples the discussed anomalies have not been observed even for \( r_s \approx 10 \).

The strong magnetoresistance in a parallel magnetic field can be also understood by the reduction of the number of diffusion modes that contribute to the antilocalizing corrections [19,20]. Here, the Zeeman splitting induces a gap in the propagators of the diffusion modes that are made of states with different spin projections. As a result these modes will no longer contribute to the antilocalization corrections. In a very strong magnetic field when the electrons are completely polarized, the system becomes identical to one with no valleys with the original valleys acting as fictitious spin projections. The difference in the resistivity of two- and one-valley systems, which is large at low enough temperatures, will be recovered as the magnetic field is applied resulting in a very strong positive magnetoresistance.

**In conclusion**, we have demonstrated that in an ultra clean (100) Si-MOSFET the temperature behavior of the resistivity in the region \( C^* \) is well described by the RG analysis of the interplay of the \( e-e \) interaction and disorder when the electron band has two distinct valleys. For \( g \) not too large, the system of RG equations in the case of two valleys is an internally consistent theory (for all practical purposes), unlike that for a single valley where \( \gamma_2 \) diverges at \( \eta \approx 1 \) after the maximum of \( g \) is passed. This divergence points to some instability of a magnetic nature in the electron gas, beyond which the RG analysis in its present form does not hold anymore. This instability also occurs in the case of two valleys but at such low temperatures that it has no practical significance.

Finally, a few remarks concerning the electron gas in Si-MOSFETs.

The intervalley scattering involves a transfer of a large momentum \( 2Q_0 \) in the direction perpendicular to the conduction plane. The width of the extension \( z_0 \) of the electrons inside the inversion layer is larger than the atomic scale \( a \), with \( z_0 \) becoming even larger when the electron density decreases. Therefore, the calculation of the intervalley scattering amplitudes involves an integration of smooth electron wave functions together with a fast
oscillating factor with $2Q_0$ Fourier component. As a result one gets amplitudes proportional to a high power of the parameter $1/(Q_0 z_0)$, which is small. Hence, the amplitudes of this process involving Coulomb interactions are very weak. The imperfections on the interface, on the other hand, can be of the atomic scale and their matrix element will contain Fourier components of high momenta. We assume, therefore, that the rate of the intervalley scattering is controlled by the quality of the interface, which is sample dependent.

Some information about the rate of the intervalley scattering can be obtained from the magnetoresistance measurements in a weak magnetic field perpendicular to the conduction plane. The results of these measurements [21], which yield a negative magnetoresistance, have been fitted with a standard expression containing the Digamma function, $\Psi$. Depending on the rate of the intervalley scattering, the theory predicts different values for the prefactor $\alpha$ in this expression: $\alpha = 1$ in the absence of the intervalley scattering and $\alpha = 0.5$ in the case of strong intervalley scattering [22]. The experimental situation for the sample used in Fig. 1 (but after some age degradation, however) remains uncertain. The optimal fit gives values for $\alpha$ between 0.6 and 0.8, with a tendency to be larger when the density decreases [23]. We consider the fact that $\alpha$ is noticeably larger than 0.5 as an indication that the intervalley scattering is not too strong in the system at low density.

In our analysis throughout we have ignored the valley splitting. In the absence of intervalley scattering the valley splitting does not influence the magnetoresistance. However, the combined effect of the intervalley scattering and the valley splitting will suppress the coefficient $\alpha$ below 0.5. Since the actual coefficient is larger than 0.5, we have ignored the valley splitting. It is also known from theoretical calculations that the valley splitting is small at low densities that are of interest to us here [12].

The chiral splitting of the electron band due to the spin orbit interaction in the presence of the asymmetric interface potential has been often discussed in connection with the dilute electron gas. This mechanism is, however, incompatible [24–26] with the observed negative magnetoresistance in MOSFETs [23]. Since actually there are no reasons to expect a considerable chiral splitting in n-type semiconductors, we have ignored the spin orbit effects in
our analysis of the dilute electron gas in Si-MOSFETs.
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We have benefited greatly from numerous discussions with V. M. Pudalov and we appreciate his contribution to our understanding of the experimental data. This work was supported by the Israel Science Foundation - Centers of Excellence Program, and by the German Ministry of Science (DIP). A. P. acknowledges the support of the Feinberg Graduate School of the Weizmann Institute of Science.
FIGURES

FIG. 1. Resistivity of a high mobility Si-MOSFET sample for various densities as a function of temperature. The electron densities, $n$, are defined in units of $10^{11}\text{cm}^{-2}$. Data are reproduced from Fig. 1(a) of Ref. 7. I labels the insulating region, and C labels the critical region. $C^*$ is the region near the critical region where a clear maximum is observed in the temperature dependence of the resistivity and is the region that is studied in the text. M labels the region further away from the critical region where such a maximum is not observed.

FIG. 2. The data corresponding to $n = 0.83, 0.88$, and $0.94 \times 10^{11}\text{cm}^{-2}$ in Fig. 1 are scaled according to Eq. 4. The solid line corresponds to the solution of the renormalization group Eqs. 2 and 3; no adjustable parameters have been used in this fit.
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Figure 2., A. Punnoose, A. M. Finkel'stein