Noninteracting Electrons and the Metal-Insulator Transition in Two Dimensions with Correlated Impurities

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While standard scaling arguments show that a system of noninteracting electrons in two dimensions and in the presence of uncorrelated disorder is insulating, in this paper we discuss the case where interimpurity correlations are included. We find that for pointlike impurities and an infinite interimpurity correlation length, a mobility edge exists in 2D even if the individual impurity potentials are random. In the uncorrelated system we recover the scaling results, while in the intermediate regime for length scales comparable to the correlation length, the system behaves like a metal but with increasing fluctuations, before strong localization eventually takes over for length scales much larger than the correlation length. In the intermediate regime, the relevant length scale is given by the interimpurity correlation length, with important consequences for high mobility systems.

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It is generally believed that a noninteracting two dimensional (2D) system in the presence of disorder is always insulating. This result is based on extensive work on scaling theory pioneered by the "gang of four" [1]. It has also received a considerable amount of numerical support [2]. The general statement can be summarized as follows. In scaling theory the localization length in 2D is given by $L_c \simeq \lambda e^{\pi k_F \lambda/2}$ [3], where λ is the elastic scattering length. Hence, as soon as λ is finite, the localization length is finite. However, because λ appears in the exponent, when $k_F\lambda \gg 1$, the localization length can be extremely large and difficult to probe experimentally. In the standard Born approximation any nonzero impurity concentration, n_I, would lead to a finite L_c, since in this approximation $\lambda^{-1} \sim n_I$. Moreover, at zero temperature a finite localization length implies that the resistance diverges exponentially for a system size exceeding the localization length. Equivalently, for an infinite system, the resistance diverges when the temperature T tends to zero because the phase coherence length l_ϕ is infinite at zero T.

When considering discrete models based on Anderson's disordered tight-binding model very similar results are obtained. All states are localized for any strength of disorder [4]. These results apply only if all sites are uncorrelated. Indeed, even in 1D there exist special long and short range correlations in the disorder, which can lead to the existence of extended states in these systems [5]. Similarly special systems can also be found in 2D [6]. The exact conditions under which these localization conditions apply has recently gained considerable interest because 2D electronic systems confined in a variety of semiconducting structures, such as Si-(MOSFET) (metal-oxide-semiconductor field-effect transistor) and p-type GaAs/AlGaAs, have shown a strong metalliclike T dependence of the resistance [7–9] down to the lowest experimental T. In metallic, we understand a positive or vanishing derivative of the resistivity as a function of the temperature, i.e., $\partial\rho/\partial T \geq 0$.

Because in these systems disorder is always present, which is expected to lead to localization, most of the recent theories have considered interactions between electrons [10] as a possible mechanism for the metallic behavior. In this work, we instead consider the case of correlations between impurities as a mechanism for delocalization. Indeed, in very high mobility 2D electronic systems such as GaAs based materials, the mobility is generally believed to be limited by background or by remote impurity scattering. Moreover, the mobility is enhanced when correlations between impurities are taken into account and this effect becomes more important at low electronic densities [11]. Hence, it is important to consider that the disorder in these low density and high mobility samples is dominated by correlated impurities. We show that these correlations can lead to a genuine metal-insulator transition for an infinite interimpurity correlation length $l \to \infty$ for the noninteracting 2D disordered system (with random potentials). Moreover, for a finite l, the crossover to localization is determined by l and not λ.

We start by considering the standard disordered tight-binding Anderson model in 2D:

$$\psi_{n+1,m} + \psi_{n-1,m} + \psi_{n,m+1} + \psi_{n,m-1} = (E - V_{n,m})\psi_{n,m}. \tag{1}$$

When $V_{n,m} = 0$ we recover the free particle case with solutions of the type $\psi_{n,m} = e^{ikn}e^{ipm}$ and eigenvalues $E = 2\cos(k) + 2\cos(p)$. When $V_{n,m}$ is random and uncorrelated, scaling theory predicts that all states are localized for any disorder strength. But when defining $V_{2n,m} = 0$ and $V_{2n+1,m}$ as random, we can write a solution to Eq. (1) as $\psi_{n,m} = \cos(n\pi/2)e^{ikm}$, corresponding to $E = 2\cos(k)$. Clearly, this is a fully extended state. The same result

holds in 1D but for a single energy [12]. The main difference in the 2D case compared to 1D is the existence of a band of extended states for $-2 \leq E \leq 2$. For every energy in this band there is exactly one wave function, which can be written in this form, hence there is no degeneracy. Therefore, when evaluating the two-terminal conductance of the system one obtains $G = 2e^2/h$ for $-2 \leq E_F \leq 2$ and $G = 0$ otherwise, since all other states are localized. This gives rise to a band of extended states around the band center and leads to a metal-insulator transition when the Fermi energy crosses $E = -2$ and $E = 2$, which is very similar to the 3D Anderson model. Similarly, when only the $V_{an,m}$'s are random, but all other potentials are zero, the system has conductance steps at $E = \pm 2 + 2\cos(l\pi/a)$, with $l = 1, 2, 3, \ldots, a - 1$ and a an integer $a \geq 2$. We have evaluated the conductance numerically as a function of the Fermi energy and the results are presented in Fig. 1. In order to calculate the temperature dependence of the conductance we simply used $G(T) = \int dE f_T'(E - E_F)G(E)$, where f_T is the Fermi-Dirac distribution function. For noninteracting electrons this is the dominant temperature dependence since inelastic scattering is strongly suppressed at low temperatures. Moreover, because E_F is equivalent to the density, this system exhibits a genuine metal-insulator transition as a function of density.

The continuous case can be treated in an analogous way by considering δ impurities with random amplitudes on a lattice, which is similar to the 1D case discussed in Ref. [13]. In this case the random potential is $V(x, y) = \sum_{n,m} V_{n,m}(y)\delta(na - x)\delta(ma - y)$, where $V_{n,m}$ are random. The special energies for the conductance steps are now given by $E = n^2\hbar^2\pi^2/2ma^2$, where a is the corresponding lattice constant of the random impurities, m the effective mass, and $n = 1, 2, \ldots$. The corresponding conducting wave functions (extended states) are simply given by $\psi(x, y) = \sin(n\pi x/a)e^{iky}$ for $E = [n^2 + (ka/\pi)^2]\hbar^2\pi^2/2ma^2$. In the inset of Fig. 2 the zero temperature conductance, G, is shown as a function of the Fermi energy.

The temperature dependence is shown for different values of E_F in Fig. 2. Hence, in this simple model in which δ impurities are on a lattice with random amplitudes, we have a E_F induced metal-insulator transition at $E_C = \hbar^2\pi^2/2ma^2$, independent of the disorder strength. This is generic for pointlike impurities on a lattice, and Azbel used a similar model but with impurity D-function potentials on a lattice, which also exhibits a mobility edge at E_C [14]. We obtained the temperature dependence by using the Fermi-Dirac distribution $R^{-1} = \int dE f_T'(E - E_F)G(E)$. It is quite striking to note that the overall shapes of the curves are very similar to the experimental ones in high mobility 2D systems [8]. The temperature scale in these experiments is typically close to the Fermi temperature T_F, which is of the order of 1 K and very similar to the relevant scale in our simple model.

In the above discussion we considered the two-terminal conductance of the system. Experimentally, this is the quantity which is normally measured. However, in order to neglect the contact resistance, four-terminal measurements are typically performed, but at zero magnetic field this is equivalent to a two-terminal measurement assuming zero contact resistance. In addition, in 2D the value of the conductance is converted to conductivity by taking into account the geometry of the sample. Hence the conductivity in our case would be $\sigma = G/\text{square}$. It is interesting to note that the conductance of our model does not depend on the geometry of the sample. At first, this does not seem physical, but since an isotropic experimental system has a finite l_ϕ at nonzero T equal in every direction, the relevant geometry for comparison with experiments is a square; hence $\sigma = G$. Indeed, we could model the experimental system as a network of quantum coherent squares coupled classically and we would

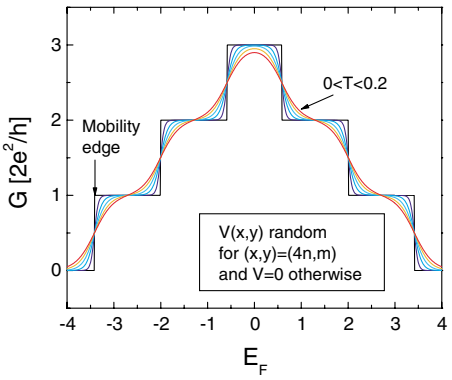

FIG. 1 (color online). Fermi energy dependence of the two-terminal conductance with $V_{4n,m}$ random and all others zero. The results are obtained from the tight-binding Hamiltonian and for different temperatures.

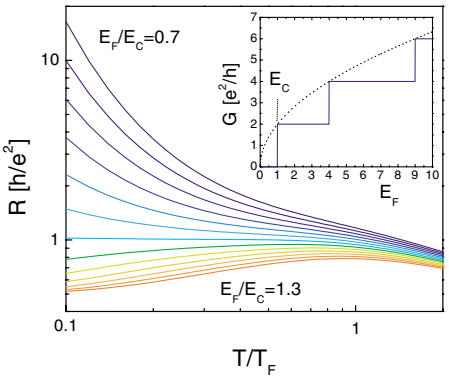

FIG. 2 (color online). Temperature dependence of the two-terminal resistance for various values of E_F. The inset shows the zero temperature dependence of the conductance as a function of E_F and the dotted line illustrates the overall square root dependence of the conductance steps.

recover $\sigma = G$, where the value of the critical conductivity does not depend on the geometry.

Experimentally, a large applied parallel magnetic field tends to exponentially increase the resistivity in low density GaAs based systems [15]. In a noninteracting picture a parallel field would simply shift the two spin subbands and therefore not significantly alter the overall behavior, although it could decrease the critical transition density. However, when comparing to experimental systems in a parallel field other effects become very important too. For instance, the 2D plane is not entirely flat because there are micron sized in-plane deviations, which are of the order of 4 to 30 nm high vertically [16], which can allow random fluxes to penetrate the 2D system and induce additional localization. These effects are beyond the scope of this work and will not be considered further.

Coming back to our model, where the disorder is confined to a regular lattice, we could show that there is a well-defined metal-insulator transition, very similar to the experimental situation. We now turn to the more general case of finite l. We start by considering the case, where the impurities are uncorrelated $l = 0$ and where the density of impurities is low before we turn to the more general case of arbitrary l.

For the numerical calculation we considered the tight-binding equation (1) with finite extent L in the n direction and infinite in m. Without disorder we have plane wave solutions of the type $\psi_{n,m}^{(p)} = \sin(np\pi/L)e^{ikm}$, with $E = 2\cos(p\pi/L) + 2\cos(k)$. This system can be viewed as a quasi-1D quantum wire, where the degeneracy of states depends on L and E and the conductance is simply $2e^2/h$ multiplied by the degeneracy. In the middle of this system we now add N_I punctual impurities in a rectangle of size (width $= L$) $\times$ (length $= L$). For the contact region we use a much larger width than the disordered region, which does not affect the overall dependence of the conductance. This model is illustrated in Fig. 3, where the source and drain region has no disorder and is much wider (width $= 384$) than the disordered region. We evaluated numerically the conductance of the system using standard transfer matrix techniques and show the conductance as a function of the number of impurities for different sizes of the disordered region in Fig. 3. In our model we used a square geometry $L \times L$, which has the particularity that at the band center the conductance G is independent of L for $V = 0$ and $\sigma = G$. The curves were obtained by averaging over ten different disorder configurations.

Figure 3 clearly shows that σ depends only on the number of impurities and not on the size of the system. Hence the dependence is simply $\sigma(N_I) = \sigma(L^2 n_I)$. This dependence holds for the entire range until σ saturates to the value where $n_I \simeq 1$. At a large enough number of impurities and in the strong localization regime we have an excellent fit to the expression $\sigma(N_I) \sim e^{-\alpha\sqrt{N_I}} \sim e^{-\alpha\sqrt{n_I}L}$, where α depends only on the impurity strength and $L_c^{-1} = \alpha\sqrt{n_I}$. The quality of the fit and the simplicity of the fitting expression is quite remarkable. This result also implies that for any nonzero uncorrelated impurity density the system is always insulating, which is consistent with the scaling analysis.

However, when the impurities are distributed on a lattice, i.e., $l = \infty$, as in Fig. 1, we also obtain a universal dependence only on N_I independent of L, i.e., $\sigma(N_I)$. The result is shown in Fig. 4. The only difference here is that $\sigma(N_I \to \infty) = 2e^2/h$ instead of zero. For this data set we considered that only every second site is random, which in this case leads to a metallic conductance of $2e^2/h$ at the band center. This data set was obtained without averaging over different disorder configurations and each data point represents an independent impurity configuration.

We now consider the most interesting case, where we change the interimpurity correlation length l. The results in Fig. 5 illustrate three cases ($l = 0$, $l \neq 0$, $l = \infty$) for a fixed system size L since σ does not depend explicitly on L but only on N_I. In order to vary l we chose to introduce two types of impurities N_I^{corr} and N_I^{uncorr} and $N_I = N_I^{\text{corr}} + N_I^{\text{uncorr}}$. The N_I^{corr} impurities will fall randomly on the

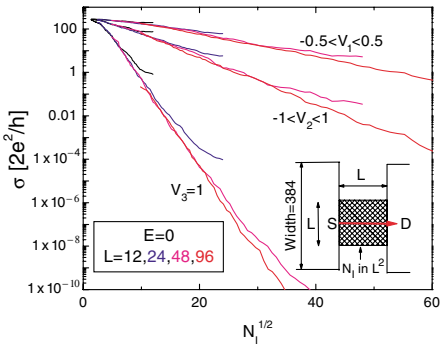

FIG. 3 (color online). The conductivity as a function of the number of impurities for different sizes and values of the impurity potential, with $-0.5 < V_1 < 0.5$, $-1 < V_2 < 1$, and $V_3 = 1$.

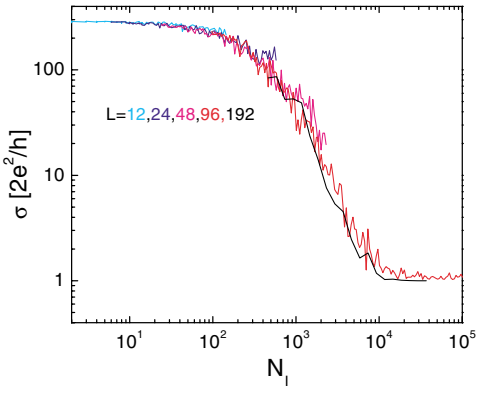

FIG. 4 (color online). The conductivity as a function of the number of impurities for different sizes and for $-1 < V_2 < 1$. Here only every second site is disordered.

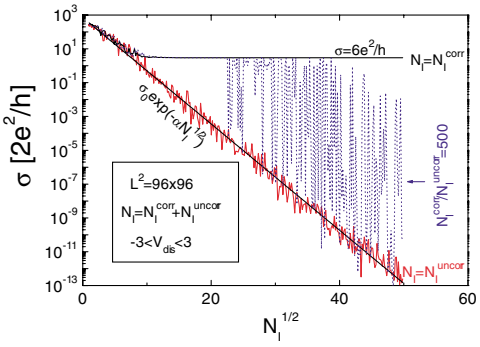

FIG. 5 (color online). The conductivity as a function of the number of impurities for different ratios of correlated to uncorrelated impurities. The straight line is the fit $\sigma \sim \exp(-\alpha N_I^{1/2})$ and the dotted line corresponds to the intermediate case.

lattice (of spacing 4 for Fig. 5), whereas the N_I^{uncorr} impurities are not correlated to any site. The correlation length is therefore determined by the density of uncorrelated impurities $l^2 = L^2/N_I^{\text{uncorr}}$.

Overall, the conductivity remains metallic for length scales comparable to the correlation length and the conductance fluctuations are close to zero in this metallic regime. For length scales exceeding the correlation length we first have increasing conductance fluctuations before the system eventually localizes at large enough length scales $L \gg l$ with a localization length equal to the uncorrelated case. The fluctuations in the intermediate regime are much larger than for the uncorrelated system and constitute an important signature of the correlation in the "metalliclike" state. Interestingly, a very similar enhancement of the conductance fluctuations is seen close to the transition from the metallic to insulating behavior in Si-MOSFET and GaAs systems [17]. In our model of correlated impurities it is therefore the interimpurity correlation length l, which controls the range of metallic behavior and not the semiclassical elastic scattering length λ, which can be much smaller than l. Hence, a large l can significantly enhance the range of metallic behavior in 2D, which constitutes one of the main results of this Letter. This is in stark contrast to the case where the impurity range is increased, which is appropriate to describe experimental systems because charged impurities are screened by electrons. In this case it was shown that a larger impurity range enhances localization if impurities remain uncorrelated [18]. However, the situation with correlated impurities was not considered. Hence, this shows that interimpurity correlations suppress localization whereas large impurity ranges enhance localization. In an applied perpendicular magnetic field, it was recently shown that a long-range disorder potential might induce a metal-insulator transition [19] too. Clearly, correlations between impurities have a significant impact on the localization properties and have to be considered when comparing to experimental systems along with electron-electron interactions.

In conclusion, we have analyzed the impact of interimpurity correlations on the localization properties of a noninteracting 2D electronic system. For impurities on a lattice and with random potentials, corresponding to an infinite interimpurity correlation length, the system exhibits a true metal-insulator transition. A finite correlation length enhances the scale over which the system is conducting before the system is eventually localized. A large correlation length can explain the large conductance fluctuations and metallic behavior of experimental systems. We also showed that the conductivity is only a function of the number of impurities, N_I, and that the localization length is given by $L_c \sim N_I^{-1/2}$ for $L \gg l$.

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