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Phase diagram of the metal-insulator transition in two-dimensional electronic systems

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We investigated the interdependence of the effects of disorder and carrier correlations on the metal-insulator transition in two-dimensional electronic systems. We present a quantitative metal-insulator phase diagram. Depending on the carrier density we find two different types of metal-insulator transition—a continuous localization for $r_s \lesssim 8$ and a discontinuous transition at higher r_s. The critical level of disorder at the transition decreases with decreasing carrier density. At very low carrier densities we find that the system is always insulating. The value of the conductivity at the transition is consistent with recent experimental measurements. The self-consistent method that we have developed includes the effects of both disorder and correlations on the transition using a density relaxation theory, with the Coulomb correlations determined from numerical simulation data. [S0163-1829(99)51208-3]

A metal-insulator transition has now been observed in a number of different two-dimensional electronic systems over a wide range of carrier densities and levels of disorder. At the transition the carrier density parameter r_s, which measures the strength of the carrier correlations, covers values $7 \lesssim r_s \lesssim 23$.[1–3] The strength of disorder at the transition also covers a wide range, and depends on the value of the critical r_s. In Si/SiGe,[3] the transition occurs at low carrier densities and high mobilities. For the transition in Si metal-oxide-semiconductor field-effect transistors (MOSFET's) that occurs at higher densities, the mobilities are much smaller. A recent experimental phase diagram[4] provides a relation between the strength of the correlations and the disorder. It shows that the critical level of the disorder at the transition diminishes as the correlations grow stronger.

In spite of a great deal of experimental and theoretical work the nature of the conducting state remains unclear and controversial. Unlike conventional metals, its Coulomb interaction energy is typically much larger than its Fermi energy. Numerous proposals have been made about the causes of the stabilization of this conducting phase. These include strong Coulomb repulsions between the carriers,[5,6] or an anomalous enhancement of the spin-orbit interaction due to the broken inversion symmetry of the confining potential well in Si MOSFET's.[7] References[8] proposed that the conducting phase is superconducting, with the pairing of the carriers being mediated by the dynamic correlation hole surrounding each carrier. Thakur and Neilson[9] demonstrated the existence of superconducting pairing due to strong Coulomb correlations in the presence of disorder. They found up to levels of disorder typical of high quality Si MOSFET's that the superconductivity persists.

The conducting phase is destroyed at low carrier densities.[1] Recently, it has been reported[4,10] that the conducting phase also becomes unstable if the carrier density is increased above a critical value. The system enters another insulating phase that has the characteristics of a single-particle localized state. In contrast there is evidence that the insulating phase at low densities is a coherent insulator with properties similar to a Wigner crystal or glass.[11] The critical density for the second transition is still not high enough for electron interactions to be neglected. In this paper we treat Coulomb interactions and disorder on an equal footing in order to investigate the transitions at both small and large r_s.

In the strong correlation limit and in the absence of disorder, electrons localize to form a Wigner solid with long-range crystalline order. Here we consider interacting charge carriers in the presence of weak disorder that would destroy any long-range order. We have previously proposed that strong Coulomb correlations in the presence of disorder can localize electrons into a coherent glassy insulator with liquidlike short-range order, leading to a metal-insulator transition.[5] The possibility of localization into such a glassy state has been discussed more recently by Chakravarty *et al.*[12]

We define the order parameter for the glass state as $f(q) = \lim_{t\to\infty} \Phi(q,t)$, where $\Phi(q,t) \equiv (N(q,t)|N(q,0))$ is the Kubo-relaxation function for the normalized dynamical density variable $N(q,t) = \rho(q,t)/\sqrt{\chi(q)}$, where $\rho(q,t)$ is the usual density fluctuation operator and $\chi(q)$ is the static susceptibility. When the order parameter is nonzero, spontaneous density fluctuations do not decay at infinite time and the system is an insulator. Conversely, if $f(q)$ is zero then our system is in a conducting phase.

Within the Mori-Zwanzig formalism[13] $\Phi(q,t)$ is calculated in terms of the memory function $M(q,t)$, which we evaluate using mode-coupling theory.[14] In the limit $t \to \infty$ the relaxation function reduces to

$$f(q) = \frac{1}{1+\Omega(q)/M(q)}, \tag{1}$$

where $\Omega(q) = q^2/[m^\star \chi(q)]$ and $M(q) = \lim_{t\to\infty} M(q,t)$. $m^\star$ is the carrier effective mass. We express $M(q) = M_{cc}(q) + M_{ic}(q)$, where

$$M_{cc}(q) = \frac{1}{2m^* q^2} \sum_{q'} \{V(q')(\boldsymbol{q}\cdot\boldsymbol{q}') + V(|\boldsymbol{q}-\boldsymbol{q}'|) \times [\boldsymbol{q}\cdot(\boldsymbol{q}-\boldsymbol{q}')]\}^2 \chi(q')\chi(|\boldsymbol{q}-\boldsymbol{q}'|) f(q') f(|\boldsymbol{q}-\boldsymbol{q}'|),$$

$$M_{ic}(q)=\frac{1}{m^*q^2}\sum_{q'}\left[n_i\langle|U_{\rm imp}(q)|^2\rangle+\langle|W_{\rm surf}(q)|^2\rangle\right]\times(\boldsymbol{q}\cdot\boldsymbol{q}')^2\chi(|\boldsymbol{q}-\boldsymbol{q}'|)f(|\boldsymbol{q}-\boldsymbol{q}'|). \quad (2)$$

The $M_{cc}(q)$ part of the memory function originates from the interactions between the carriers, and the $M_{ic}(q)$ from the carrier-disorder interactions. $V(q)=2\pi e^2/\epsilon q$ is the Coulomb potential with dielectric constant ϵ. $U_{\rm imp}(q)$ is the impurity potential for randomly distributed monovalent Coulombic impurities of density n_i that are embedded in the carrier layer. $W_{\rm surf}(q)$ is the surface roughness scattering term. Details of the disorder potentials used are given in Ref. 5.

To evaluate the static susceptibility $\chi(q)$ with correlations, we use the generalized random-phase approximation expression,

$$\chi(q)=\chi_0(q)/\{1+V(q)(1-G(q))\chi_0(q)\}, \quad (3)$$

where $\chi_0(q)$ is the Lindhard function for noninteracting electrons. The local-field factor $G(q)$ accounts for the correlations between the carriers. We evaluate $G(q)$ from ground-state properties of the electron liquid[15] using the fluctuation-dissipation theorem.[16]

The memory functions $M_{cc}(q)$ and $M_{ic}(q)$ mutually influence each other through $f(q)$. The nature of the localized state at the transition is largely determined by which of these memory functions is dominant.

At low densities and small levels of disorder the interactions between the carriers dominate and $M_{cc}(q)$ is much larger than $M_{ic}(q)$. In this case the localization is primarily caused by many-body effects and the localized state is a coherent frozen insulator. At the transition the order parameter $f(q)$ jumps from zero to nonzero and the system undergoes a discontinuous transition from delocalized to localized state. This solid is not a Wigner crystal but a frozen macroscopically coherent state with liquidlike short-range order. It is quite different from the frozen state obtained from localized electrons interacting with a disordered medium discussed in Ref. 17. Our localization is driven by the increasing relative size of the exchange-correlation hole as the density decreases.[15] For $r_s\gtrsim 10$ the exchange-correlation hole excludes all other electrons as if each electron had a hard core.[5] With decreasing electron density the fraction of the total area occupied by these excluded regions approaches the close packing limit[18] and it becomes difficult for electrons to pass by each other. A small amount of disorder introduces impurity pinning centers. The electron-electron correlations are crucial for this phase. If we neglect them by using a Hubbard-like expression for $\chi(\boldsymbol{q})$ in Eq. (2) we do not get the transition.

At high densities and high levels of disorder we find $M_{ic}(q)$ is much larger than $M_{cc}(q)$. Carrier-disorder scattering dominates over electron interactions and the localization transition is to a noncoherent state. For noncoherent localization many-body effects are not central. The carriers localize independently, similar to single-particle localization. The localization is continuous, with the order parameter $f(q)$ steadily increasing with disorder. We conclude in our model that there are two distinct transitions, from conductor to a coherent insulator for larger r_s, and from conductor to a noncoherent insulator for smaller r_s.

We solve Eqs. (1) and (2) self-consistently for the order parameter $f(q)$. We vary the strength of the disorder potential by varying the impurity density n_i while keeping the surface roughness at each r_s fixed.

In Fig. 1 we show the order parameter $f(q)$ for three values of $r_s=8$, 12, and 18. The multiple curves for each fixed r_s correspond to increasing levels of disorder. The peak in $f(q)$ at $q=2k_F$ is a result of the well-known cusp in the two-dimensional $\chi_0(q)$ and is of no importance here.

At the highest carrier density corresponding to $r_s=8$, Fig. 1(a), the localization is dominated by the $M_{ic}(q)$ part of the memory function. There is no conducting phase, $f(q)$ being nonzero for any disorder and increasing continuously with impurity density. These features, and the dominance of the impurity-carrier part of the memory function, are characteristic of carriers localizing independently. In Anderson localization the carriers also localize independently and are localized for arbitrarily small disorder. Nevertheless the mechanism here is different. Anderson localization is associated with phase interference of the single-particle propagators, while our localization is driven by the interactions between density fluctuations and the impurities. Our noncoherent insulator, unlike an Anderson insulator, should persist in weak magnetic fields since the localization is not caused by interference.

In Fig. 1(b) for $r_s=12$ the order parameter remains zero for small nonzero levels of disorder. This indicates the existence of a conducting phase. If we increase the level of disorder, a critical value is passed at which $f(q)$ jumps discontinuously to nonzero values and at that point there is a metal-insulator transition.[5] The short-range coherent order of the insulator state is reflected by a peak in $f(q)$ at the reciprocal nearest-neighbor distance, $q\approx 2.4k_F$. In the range $8\lesssim r_s\lesssim 18$, the critical level of disorder at the transition decreases with increasing r_s. Beyond the transition if we increase the disorder further for fixed r_s, the $f(q)$ increases continuously. For very high levels of disorder the overall shape of the $f(q)$ evolves towards a Gaussian indicating the development of a noncoherent insulator.

By $r_s=18$ the system localizes without disorder and there is no conducting phase. This large r_s localization is driven purely by the correlations between the carriers. In Fig. 1(c), $f(q)$ is nonzero for $n_i=0$ and no surface roughness scattering (dashed line). Without disorder the $f(q)$ goes to zero as q goes to zero. The solid lines show $f(q)$ with surface roughness scattering included.

The property that the critical level of disorder for the metal-insulator transition is dependent on the carrier density is associated with the changing strength of the correlations. The zero temperature phase diagram in Fig. 2 shows the relationship between the carrier density and the critical level of disorder at the transition. Disorder includes both n_i and surface roughness.

Around $r_s=8$ to 9 our transition is not very well defined since here the order parameter $f(q)$ grows slowly and continuously with decreasing r_s for fixed n_i, and the localization is continuous with the disorder. This localization should

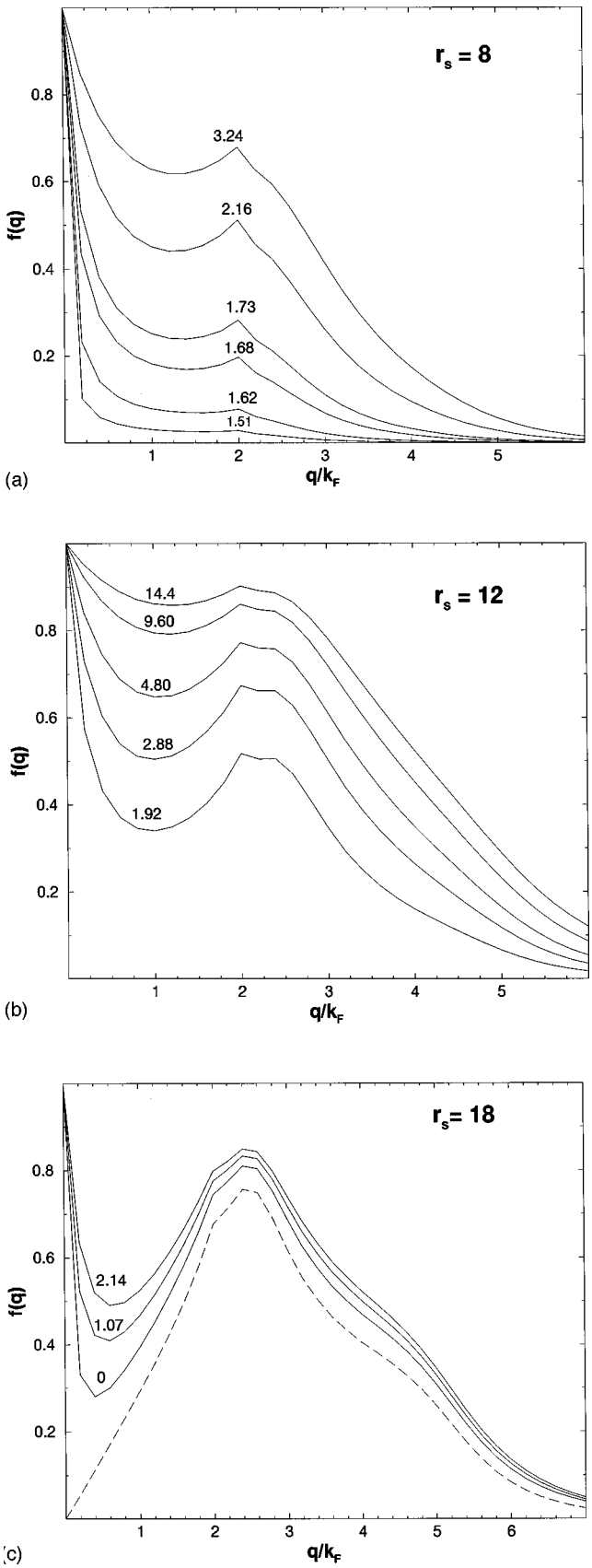

FIG. 1. Order parameter $f(q)$. Curve labels are impurity densities n_i. Surface roughness is included in all cases. (a) $r_s=8$. n_i is in units of $10^{10}\,\mathrm{cm}^{-2}$. (b) $r_s=12$. n_i is in units of $10^9\,\mathrm{cm}^{-2}$. $f(q)$ is zero for $n_i<1.92\times10^9\,\mathrm{cm}^{-2}$. (c) $r_s=18$. n_i is in units of $10^8\,\mathrm{cm}^{-2}$. The dashed line is $n_i=0$ with no surface roughness.

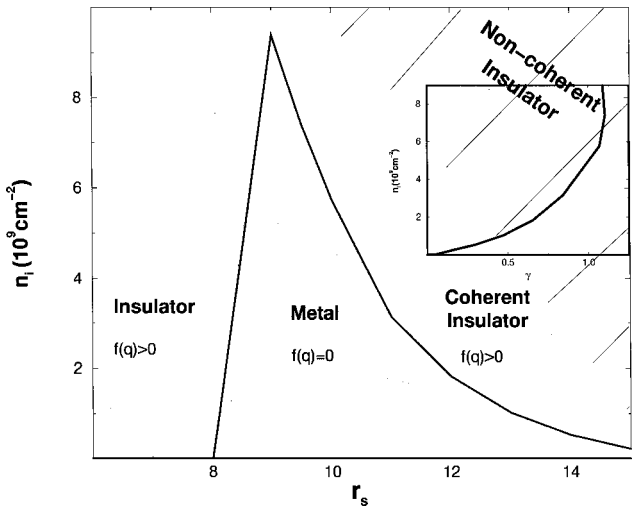

FIG. 2. Zero temperature phase diagram. Axes are impurity density n_i and carrier density parameter r_s. In the insulating phases the order parameter $f(q)>0$. In the conducting phase $f(q)=0$. The transition at higher densities is continuous. When $r_s>9$ the $f(q)$ discontinuously jumps from zero to nonzero values at the transition. The inset shows the corresponding scattering rate $\hbar\gamma$ at the transition as a function of n_i.

persist in a small magnetic field. These properties are consistent with those of the new insulating state reported recently for $r_s\leqslant 8$.[4]

For $8<r_s<18$ the order parameter is zero for n_i less than a critical value and we have the conducting phase. Since our order parameter would be zero for any conducting phase it gives no indication about the precise nature of the conducting phase. At the right phase boundary the transition to the insulating phase is discontinuous and $f(q)$ jumps discontinuously to nonzero values as we cross it. The critical level of disorder for the transition decreases with decreasing density. Near the phase boundary when the disorder level is slightly larger than the critical value the system is in the coherent insulating state. The characteristic properties of our coherent insulator are consistent with those of the collective insulating state discussed by Pudalov *et al.*[11] For very large disorder

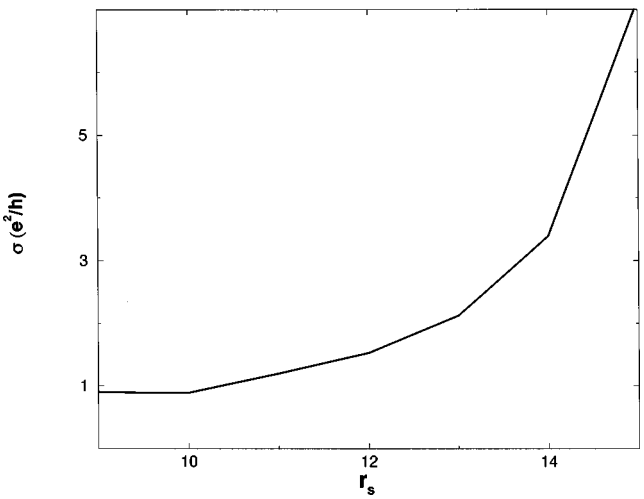

FIG. 3. Conductivity σ at the critical disorder for the transition as a function of r_s.

the $f(q)$ has evolved into a Gaussian-like shape [see Fig. 1(b)] and the system becomes a noncoherent insulator. For $r_s \gtrsim 18$ the order parameter is nonzero without disorder and the conducting phase has disappeared. Our phase diagram has common features with the conceptual phase diagram discussed by Chakravarty *et al.*[12]

The inset in Fig. 2 shows the relation between n_i and the scattering rate γ off the disorder. Within the memory function formalism the nonlinear equation for γ is given by[19]

$$i\gamma = -\frac{1}{2m^{\star}n_c}\sum_q q^2[n_i\langle|U_{\rm imp}(q)|^2\rangle + \langle|W_{\rm surf}(q)|^2\rangle] \times\left(\frac{\chi(q)}{\chi^{(0)}(q)}\right)^2 \frac{\phi_0(q,i\gamma)}{1+i\gamma\phi_0(q,i\gamma)/\chi^{(0)}(q)}, \quad (4)$$

where $\phi_0(q,i\gamma)=(1/i\gamma)[\chi^{(0)}(q,i\gamma)-\chi^{(0)}(q)]$ is the relaxation spectrum for noninteracting carriers that scatter off the disorder. Thakur and Neilson[9] showed for the density range $5 \leqslant r_s \leqslant 10$ that the superconducting phase persists at least up to values of $\hbar\gamma = 1$ (expressing $\hbar\gamma$ in units of twice the Fermi energy). They also showed that the effective potential becomes more strongly attractive as r_s increases. This suggests that our conducting phase in Fig. 2, which is only found for $\hbar\gamma \lesssim 1$, is a superconductor.

Using the Drude model, γ can be related to the zero temperature conductivity, $\sigma/(e^2/h) = 1/(\hbar\gamma)$. In Fig. 3 we show σ at the transition as a function of r_s. In the range $9 < r_s < 14$, σ lies between $1 \lesssim \sigma/(e^2/h) \lesssim 3$. This is consistent with experimental values. At lower densities the σ calculated within the Drude model increases rapidly. This is associated with the decrease in the critical level of disorder at the transition. Since the Drude approximation is inapplicable for large r_s this increase in σ at low density should not necessarily be seen experimentally.

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