Interacting Electrons in a Two-Dimensional Disordered Environment: Effect of a Zeeman Magnetic Field

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The effect of a Zeeman magnetic field coupled to the spin of the electrons on the conducting properties of the disordered Hubbard model is studied. Using the determinant quantum Monte Carlo method, the temperature- and magnetic-field-dependent conductivity is calculated, as well as the degree of spin polarization. We find that the Zeeman magnetic field suppresses the metallic behavior present for certain values of interaction and disorder strength and is able to induce a metal-insulator transition at a critical field strength. It is argued that the qualitative features of magnetoconductance in this microscopic model containing both repulsive interactions and disorder are in agreement with experimental findings in two-dimensional electron and hole gases in semiconductor structures.

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A hundred years after the Nobel prize was awarded in 1902 for the discovery of the Zeeman effect and the subsequent explanation by Lorentz, applying a magnetic field continues to be a powerful means to elucidate puzzling phenomena in nature. One of the most recent examples is the interplay of interactions and disorder in electronic systems. This field has witnessed a revival of scientific activity after pioneering experiments in low-density silicon metal-oxide-semiconductor field-effect transistors (MOSFETs) found clear indications of a metal-insulator transition (MIT) in effectively two-dimensional (2D) systems [1]. Until then, electrons in a 2D disordered environment were thought to always form an insulating phase; this mind-set was based on the scaling theory of localization for noninteracting electrons, supplemented by perturbative treatments of weak interactions, as well as studies of the limiting case of very strong interactions. The surprising phenomena were soon confirmed in other semiconductor heterostructures, although the interpretation in terms of a quantum phase transition remains controversial, and a wide variety of experimental and theoretical approaches were unleashed at the problem [2].

Among these approaches is the application of magnetic fields. Contrary to the well-known effect of a magnetic field in weak-localization theory to disturb interference phenomena and hence *undo* localization and insulating behavior, the negative magnetoresistance effect [3], in the Si MOSFETs and similar heterostructures, the magnetic field is found to suppress the metallic behavior and therefore *promote* insulating behavior [4–6]. The effect is present for all orientations of the magnetic field relative to the 2D plane of the electrons. In particular, a Zeeman magnetic field, applied parallel to the 2D plane of electrons and therefore coupling only to the spin, and not the orbital motion of the electrons, has been used extensively. This puts into focus the important role played by the spin degree of freedom of the electron and its polarization [7–12].

In this Letter, we present a numerical study of a microscopic model for interacting electrons in a disordered environment including the effect of a Zeeman magnetic field. The present study extends our earlier work without a magnetic field [13], in which we found clear indications that interactions enhance the conductivity and lead to metallic behavior in a temperature range (about 1/10 of the Fermi energy) similar to that of experiments. Later numerical approaches have sometimes [14–17] led to different conclusions from ours, but they either treat the problem within a Hartree-Fock method, or else use diagonalization methods which deal with considerably smaller numbers of electrons than can be studied in our approach. Very recently, an improved study using the same approach as in Ref. [14] confirmed our main finding [18]. While the numerical evidence is mixed concerning the occurrence of a MIT due to interactions, there is a consensus in favor of a Zeeman magnetic field tuned transition [16,17,19,20], as we shall describe in more detail below.

The microscopic model that we study is the disordered Hubbard model defined by

$$\hat{H} = -\sum_{i,j,\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{j} n_{j\uparrow} n_{j\downarrow} - \sum_{j,\sigma} (\mu - \sigma B_{\parallel}) n_{j\sigma}, \tag{1}$$

where $c_{j\sigma}$ is the annihilation operator for an electron at site j with spin σ and $n_{j\sigma} = c^{\dagger}_{j\sigma} c_{j\sigma}$ is the occupation number operator. t_{ij} is the nearest neighbor hopping integral (i.e., $t_{ij} = 0$ if i and j are not neighboring sites), U

is the on-site repulsion between electrons of opposite spin, μ the chemical potential, and $B_\parallel$ the Zeeman magnetic field. We consider a square lattice. Disorder is introduced by taking the hopping parameters t_{ij} from a probability distribution $P(t_{ij}) = 1/\Delta_t$ for $t_{ij} \in [t - \Delta_t/2, t + \Delta_t/2]$, and zero otherwise. Δ_t measures (bond) disorder strength [21].

We use the determinant quantum Monte Carlo (QMC) method, which has been applied extensively to the Hubbard model, both with and without disorder [13,21–23]. While disorder and interaction can be varied in a controlled way and strong interaction is treatable, QMC is limited in the size of the lattice, and the *sign problem* restricts the temperatures which can be studied. To alleviate the sign problem, we use off-diagonal rather than diagonal disorder, and tune the value of μ such that density $\langle n \rangle = 0.5$ (where the sign problem is less severe). Interestingly, the sign problem is also reduced by the presence of disorder [13].

The quantity of immediate interest when studying possible metal-insulator transitions is the *conductivity* and, in particular, its T and $B_\parallel$ dependences. By the fluctuation-dissipation theorem σ_{dc} is related to the zero-frequency limit of the current-current correlation function. A complication of the QMC simulations is that the correlation functions are obtained as a function of *imaginary* time. To avoid a numerical analytic continuation procedure to obtain frequency-dependent quantities, which would require Monte Carlo data of higher accuracy than can be produced in the presence of even a tolerable sign problem and the need for disorder averaging, we employ an approximation to obtain σ_{dc} from the wave vector- and imaginary-time-dependent current-current correlation function (see, e.g., [13], where also tests of the approximation are discussed). Another interesting quantity to study in conjunction with the magnetoconductivity is the degree of spin polarization P of the electronic system: $P = (n_\downarrow - n_\uparrow)/(n_\downarrow + n_\uparrow)$, where $n_\downarrow, n_\uparrow$ are the average spin densities of the corresponding number operators in (1).

In order to study the effect of the Zeeman magnetic field $B_\parallel$ on the metallic behavior, we start from the case with density $\langle n \rangle = 0.5$ and disorder strength $\Delta_t = 2.0$ for which the model exhibits clear metallic behavior: σ_{dc} rising when lowering temperature T [13]. Figure 1 shows that turning on $B_\parallel$ reduces the conductivity and suppresses the metallic behavior; at field strength $B_\parallel = 0.4$, σ_{dc} appears T independent (within the error bars), and at larger field strengths shows a tendency to decrease upon lowering T. We do not expect σ_{dc} to go to zero, as for a real insulator, unless very low T and very large lattices (out of reach of our computational approach) are employed. Nevertheless, Fig. 1 shows the qualitative features of a magnetic-field-driven metal-insulator transition, similar to what is seen in experiment [4–6]. Previous numerical approaches using different techniques have also produced this effect [16,17,19].

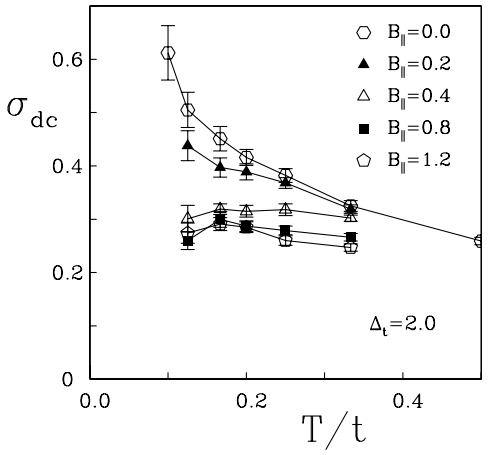

FIG. 1. Conductivity σ_{dc} (in units of $e^2/\hbar$) as a function of temperature T for various strengths of Zeeman magnetic field $B_\parallel$. As $B_\parallel$ increases, a transition from metallic to insulating behavior is seen in σ_{dc}. Calculations are performed on 8×8 lattices for $U/t = 4$ at density $\langle n \rangle = 0.5$ with disorder strength $\Delta_t = 2.0$ (see text); error bars result from averaging over typically 16 quenched disorder realizations. $B_\parallel$ and Δ_t are given in units of t.

In order to ascertain that we are indeed dealing with a critical phenomenon and in order to locate the critical field strength, we focus on fields close to $B_\parallel = 0.4$. It is important to note that the effect of $B_\parallel$ is to polarize the electronic system (with our choice in (1), $n_\downarrow$ is promoted at the expense of $n_\uparrow$) and therefore a large enough $B_\parallel$ will result in electrons with spin down only and, because of the nature of the Hubbard interaction, in a noninteracting system [24]. Consequently, in the limit of large 2D lattices and low temperature, the hopping disorder will force the conductivity to vanish. Subtracting out the nonzero value of σ_{dc} that we obtain at very large $B_\parallel$ is then a systematic way to correct for finite size and nonzero T. In Fig. 2, we show the resulting $\delta\sigma_{dc}$ vs $B_\parallel$ for our lowest temperatures. A rather abrupt onset appears of $\delta\sigma_{dc}$ below $B_\parallel \approx 0.5$, which agrees with the field value where the curves of σ_{dc} vs T change from insulating to metallic (Fig. 1). Our data for a 2D system in Fig. 2 are consistent with a linear vanishing of $\delta\sigma_{dc}$ as the (quantum) critical point is approached. At present, our results, while presenting compelling evidence for the transition itself, are clearly not precise enough to obtain critical exponents. Interestingly, a transition from insulator to metal upon increasing magnetic field, i.e., the known negative magnetoresistance effect, occurs in an amorphous three-dimensional Gd-Si alloy (showing a MIT at zero field), also with a linear vanishing of the conductivity [25].

In Fig. 3, we show the *resistivity* ρ ($\equiv 1/\sigma_{dc}$) as a function of $B_\parallel$ for low T. The crossing point ($B_\parallel = 0.35 \pm 0.10$) demarks a critical field strength B_c which separates

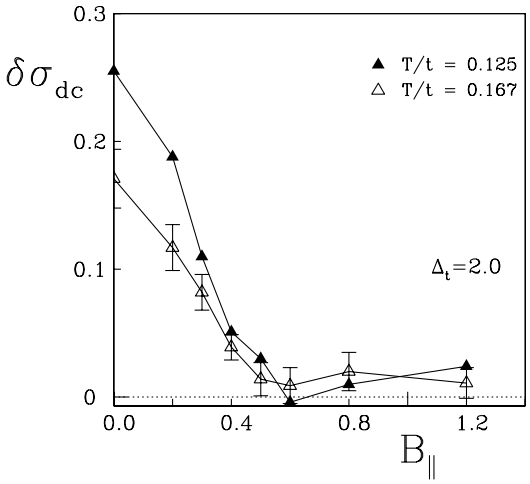

FIG. 2. Conductivity with value at very high B field subtracted, $\delta\sigma_{dc} \equiv \sigma_{dc}(B_{\|}, T) - \sigma_{dc}(B_{\|} = 4, T)$, as a function of $B_{\|}$ for low temperature T. A sharp onset of conductivity is seen at a Zeeman field at which the slope of $\sigma_{dc}(T)$ changes sign in Fig. 1. Computational details and units are as in Fig. 1; for clarity, only error bars on $T = t/6$ data are shown; those on $T = t/8$ data are typically slightly larger (cf. Fig. 1).

fields for which the resistivity decreases when lowering temperature (low-field metallic behavior) from fields for which ρ increases upon lowering T (high-field insulating behavior). It is especially noteworthy that the critical field strength (which can be roughly estimated to lie between 0.3 and 0.5 from Figs. 2 and 3) is clearly lower than the field for which full spin polarization sets in. Indeed, in Fig. 4, we show how the spin polarization P, defined above, behaves as a function of $B_{\|}$ at the lowest temperature used: there is no reflection of the critical field strength in the behavior of the polarization and full spin polarization only happens for $B_{\|} > 1.2$. This feature of our data is in agreement with recent experiments performed on 2D electron and hole gases in GaAs and AlAs [11,12]. Since complete spin polarization is equivalent to a noninteracting system, the separation of the two field strengths and the incomplete polarization at the MIT present evidence that the Zeeman field tuned MIT must be seen as a property of a fully interacting many-body system, at least in the 2D disordered Hubbard model.

Another interesting feature of Fig. 3 is what appears to be the saturation of resistivity at a field not much higher than B_c. Experiments also show this behavior [8,11]. For AlAs the saturation is shown to coincide with full spin polarization [11], but for Si inversion layers [9], as in our results, saturation happens before full spin polarization. We argue that the on-site nature of the interactions in the Hubbard model makes the saturation happen at much reduced field strength compared to that of complete polarization: at our rather low total density the minority spin species will effectively be decoupled from the majority spin species and both spin species form noninteracting subsystems at a field where the minority spin has not disappeared completely. Increasing magnetic field further at constant total density will then not change the conducting properties anymore.

The notion of a predictable and straightforward effect of $B_{\|}$ is also concordant with the phenomenon that $\rho(B_{\|})$ behaves qualitatively the same in the metallic and insulating phases (see, e.g., Ref. [2]), and therefore the same physical mechanism seems at play in both cases. Our results suggest the reduction of the effective interaction by spin polarization as a likely candidate for this mechanism.

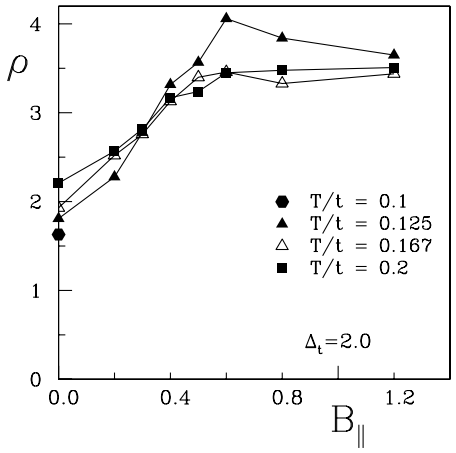

FIG. 3. Resistivity ρ as a function of $B_{\|}$ for various low T. The crossing point provides another estimate for the critical field strength. Computational details and units are as in Figs. 1 and 2; for clarity the error bars have been omitted, but can be estimated from Figs. 1 and 2.

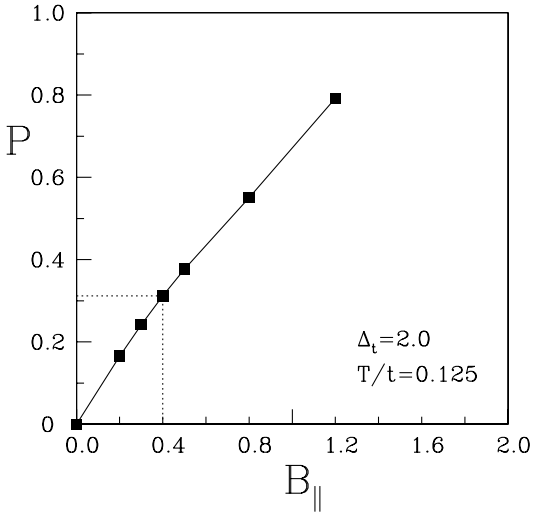

FIG. 4. Degree of spin polarization $P = (n_{\downarrow} - n_{\uparrow})/(n_{\downarrow} + n_{\uparrow})$ (see text) as a function of $B_{\|}$ for fixed low $T = t/8$. The polarization shows little change through the metal-insulator transition and is only 0.31 at the estimated critical field strength.

In summary, applying a Zeeman magnetic field in the 2D disordered Hubbard model reduces the effect of the Hubbard interaction and is able to bring about a transition from a metallic phase to an insulator at a critical field strength. We find this critical field is considerably less than the field required for full spin polarization, emphasizing that, for the disordered Hubbard model, the metal-insulator transition occurs in a region where a considerable degree of electronic correlation remains. This is in good qualitative agreement with experimental observations when a magnetic field is applied parallel to a 2D electron or hole gas in GaAs- and AlAs-based heterostructures [11,12]. For Si MOSFETs, the general phenomenon of suppression of the metallic behavior is in agreement, but the issue of the critical field being smaller than a saturating field is less clear [8,10]. In earlier work, we studied the T dependence of σ_{dc} for various Δ_t without a B field and showed that the Hubbard interaction enhances σ_{dc} and leads at low T to metallic behavior that can be turned into insulating behavior by sufficiently strong disorder. Our present results concerning the effect of a magnetic field are consistent with that conclusion: the rather strong interactions that caused the conducting phase at disorder strength $\Delta_t = 2.0$ (below the critical disorder strength of approximately 2.4 above which the system is insulating) without B field are reduced by a B field which is able to drive the system back to its insulating phase. The latter is also its natural state in the absence of interactions. We believe that this consistency indicates that the disordered Hubbard model provides a coherent, qualitative picture of the phenomena in 2D electronic, disordered systems both in the presence and the absence of a Zeeman magnetic field.

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