Disorder Screening in Strongly Correlated Systems

D. Tanasković and V. Dobrosavljević
Department of Physics and National High Magnetic Field Laboratory, Florida State University, Tallahassee, Florida 32306, USA

E. Abrahams and G. Kotliar
Center for Materials Theory, Serin Physics Laboratory, Rutgers University, 136 Frelinghuysen Road, Piscataway, New Jersey 08854, USA

(Received 10 March 2003; published 5 August 2003)

Electron-electron interactions generally reduce the low temperature resistivity due to the screening of the impurity potential by the electron gas. In the weak-coupling limit, the magnitude of this screening effect is determined by the thermodynamic compressibility which is proportional to the inverse screening length. We show that when strong correlations are present, although the compressibility is reduced, the screening effect is nevertheless strongly enhanced. This phenomenon is traced to the same nonperturbative Kondo-like processes that lead to strong mass enhancements, but which are absent in weak-coupling approaches. We predict metallicity to be strongly stabilized in an intermediate regime where the interactions and the disorder are of comparable magnitude.

DOI: 10.1103/PhysRevLett.91.066603 PACS numbers: 72.15.Qm, 71.55.Jv

Transport in disordered metals has been studied for many years, and substantial theoretical and experimental understanding has been achieved [1] in the case of weak disorder and in the regime of weak electron-electron interaction. Much less is known about situations with strong electronic correlations; here, most research has concentrated on clean systems.

Recent experiments on two-dimensional (2D) electron gases in the zero magnetic field [2] have led to considerable renewed interest in electronic systems close to metal-insulator transitions (MITs). In these systems, well-defined metallic behavior (positive temperature coefficient of resistivity, $d\rho/dT > 0$) has been observed in the low density regime, and is characterized by a surprisingly large (up to a factor of 10) drop of resistivity at low temperatures. Here, the electron-electron interactions represent the largest energy scale in the problem [2]; this is emphasized by recent reports of substantial mass enhancement from several complementary experiments [3].

Some simple microscopic mechanisms that can produce such a resistivity drop relate to temperature-dependent screening [4–7] of the random potential. This effect obtains even in the simplest Hartree-Fock (HF) treatment of interactions, which represents the basis for the standard (Lindhard) screening theory, and applies equally well to both short-range [6] and long-range [4] forces. In this picture, the screening length is inversely proportional to the thermodynamic compressibility of the system, which therefore controls the magnitude of disorder screening. This observation immediately brings into question the relevance of such mechanisms in the regime of strong correlation, in particular, close to interaction-driven MITs. Here, one expects substantial mass enhancements, but at the same time a significant decrease of the compressibility [8]. Then, if applicable, standard screening theory (as in HF) would predict *weak* disorder screening precisely where mass is enhanced—in contrast to experiments, where the resistivity drop persists in that region (see Fig. 3, below).

In this Letter, we examine the screening of the impurity potential by focusing on a model where a reliable and controlled treatment of strong correlations is available. This is possible within dynamical mean-field theory (DMFT) [8], which is formally exact in the limit of large coordination. To investigate the regime of strong correlation, we examine a disordered Hubbard model in the vicinity of the Mott transition, a model which has recently been argued [6,9–11] to provide an appropriate description of interaction effects near the 2D-MIT. Our results demonstrate the following: (i) If DMFT equations are solved within the HF approach, we reproduce the results of standard screening theory in qualitative and even semiquantitative detail; in this picture, screening is strongly suppressed close to the Mott transition. (ii) A more accurate solution agrees with HF results far from the Mott transition, but finds diametrically opposite results in the regime of strong correlation. Here, while compressibility is reduced, both the disorder screening and the effective mass are strongly enhanced. (iii) The enhanced screening strongly stabilizes metallic behavior in the intermediate regime where the disorder and interactions are of comparable magnitude.

We consider a disordered Hubbard model described by the Hamiltonian

$$H = -\sum_{ij\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \sum_{i\sigma} \varepsilon_i n_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}. \qquad (1)$$

Here t_{ij} are the hopping matrix elements, c and $c^{\dagger}$ are fermionic creation and annihilation operators, $n = c^{\dagger} c$ is the number operator, and σ labels the spin projection. U represents the Hubbard on-site repulsion, and the disorder

is introduced by random site energies ε_i, as specified by a distribution function $P(\varepsilon_i)$.

Disorder renormalization (screening).—Within DMFT [8], a quasiparticle is characterized by a self-energy function $\Sigma(\omega)$, which is assumed to be purely local (momentum independent). In a random system [12], this quantity, though still local, is now site dependent $\Sigma_i(\omega) = \Sigma(\omega, \varepsilon_i)$ which explicitly depends only on the corresponding local site energy ε_i [13]. The renormalized disorder potential (as seen by the quasiparticle at the Fermi energy) can thus be defined by

$$v_i(\varepsilon_i) = \varepsilon_i + \Sigma_i(\omega = 0) - \mu - \delta\mu, \tag{2}$$

where μ is the chemical potential. These renormalized energies are defined with respect to a reference energy $\delta\mu$ chosen such that $\overline{v}_i = \int d\varepsilon_i\, P(\varepsilon_i) v_i(\varepsilon_i) = 0$, i.e., that their site average vanishes. In a case of particle-hole symmetry $\delta\mu = 0$. Since there are no vertex corrections within DMFT, the $T = 0$ dc resistivity [8,12] depends only on the variance of this renormalized disorder, viz. $\rho \sim \overline{v}_i^2$. The self-energies $\Sigma_i(\omega)$ must be calculated by solving an ensemble of Anderson impurity problems supplemented by a self-consistency condition [8,12].

Weak coupling (Hartree-Fock) solution.—In the HF approximation for the Hubbard model, $\Sigma_i(\omega) = U\langle n_i\rangle$; here $\langle\cdots\rangle$ represents the quantum average (for a given disorder configuration). Within DMFT, the local occupation $\langle n_i\rangle$ depends only on the local (renormalized) site energy, and for moderate disorder [6] we find

$$\frac{\overline{v}_i^2}{\overline{\varepsilon}_i^2} = [1 + U\chi_{ii}]^{-2}, \tag{3}$$

where $\chi_{ii} = -\partial\langle n_i\rangle/\partial\varepsilon_i$ is the local compressibility [14]. This result, although based on a local approximation, proves to provide qualitative and even semiquantitative agreement with more standard screening theory. Just as in Refs. [4–6], for reasonable values of the interaction strength ($U \lesssim$ bandwidth), the screening of the random potential cannot be very large (resistivity drop by a factor of 2 at most [4]).

Strongly correlated regime.—We approach a $T = 0$ Mott transition at half filling. In general, the DMFT equations cannot be solved in closed form, but extensive work [8] has shown that most qualitative and even quantitative features of the $T = 0$ solution can be reproduced using simple analytical approximations. Here, we use the four-boson mean-field method of Kotliar and Ruckenstein (KR) [15], which is equivalent to the well-known Gutzwiller variational approximation, but can be readily generalized to disordered systems. This approach provides a parametrization of the low-energy (quasiparticle) part of the local Green function which, in our case, takes the form ($\hbar = c = 1$)

$$G_i(\omega_n) = \frac{Z_i}{i\omega_n - \tilde{\varepsilon}_i - Z_i\Delta(\omega_n)}. \tag{4}$$

Here, the local quasiparticle weight $Z_i = 2[1 - (e_i^2 - d_i^2)^2]^{-1}(e_i + d_i)^2[1 - (e_i^2 + d_i^2)]$, as well as parameters e_i, d_i, and $\tilde{\varepsilon}_i$, are site-dependent [14] quantities, determined by the KR equations [15]

$$-\frac{\partial Z_i}{\partial e_i}\frac{1}{\beta}\sum_{\omega_n}\Delta(\omega_n)G_i(\omega_n) = Z_i(\mu + \tilde{\varepsilon}_i - \varepsilon_i)e_i, \tag{5}$$

$$-\frac{\partial Z_i}{\partial d_i}\frac{1}{\beta}\sum_{\omega_n}\Delta(\omega_n)G_i(\omega_n) = Z_i(U - \mu - \tilde{\varepsilon}_i + \varepsilon_i)d_i, \tag{6}$$

$$\frac{1}{\beta}\sum_{\omega_n}G_i(\omega_n) = \frac{1}{2}Z_i(1 - e_i^2 + d_i^2). \tag{7}$$

Half filling can be enforced by the requirement $\overline{e}_i^2 = \overline{d}_i^2$. Finally, a self-consistency condition [12] determines the "hybridization function" $\Delta(\omega) = \Delta_o[\omega - \Sigma_{av}(\omega)]$ describing the environment of a given site. Here $\Delta_o(\omega) = \omega + \mu - [G_o(\omega)]^{-1}$, $G_o(\omega)$ being the lattice Green's function corresponding to no disorder and $U = 0$. The "average" self-energy $\Sigma_{av}(\omega)$ is defined via the disorder-averaged Green's function $\overline{G}(\omega) = \int d\varepsilon_i\, P(\varepsilon_i)G_i(\omega)$: $\overline{G}(\omega) \equiv G_o[\omega - \Sigma_{av}(\omega)]$. Thus, $\Sigma_{av}(\omega) = \omega + \mu - \Delta(\omega) - [\overline{G}(\omega)]^{-1}$. It follows that $\delta\mu = \int d\varepsilon_i\, P(\varepsilon_i)\tilde{\varepsilon}_i/Z_i$, and $v_i = \tilde{\varepsilon}_i/Z_i - \delta\mu$.

Phase diagram.—These equations can be easily solved for an arbitrary band structure and distribution of disorder, but such details do not affect the qualitative form of the solution, which proves to depend only on the presence or absence of particle-hole symmetry. We first examine the particle-hole symmetric situation, and as an illustration we concentrate on a model with a semicircular band of width $4t$ at half filling, and site energies uniformly distributed in the interval $(-W/2, W/2)$. The resulting $T = 0$ phase diagram, as obtained from a full numerical solution, is shown in Fig. 1. The Mott insulating phase is completely suppressed for $W > U$, since the disorder tends to fill in the Hubbard-Mott gap. The phase boundary separating the correlated metal and the Mott insulator (full line) is identified by the simultaneous vanishing of the quasiparticle weights Z_i on all lattice sites. All quantities display simple critical behavior close to this phase boundary, the form of which can be analytically obtained for weak disorder, but which proves to remain qualitatively correct along the entire critical line. To second order in ε_i, we find $Z_i = Z_0(1 + C\varepsilon_i^2)$, where $Z_0 \equiv Z_i(\varepsilon_i = 0) = 2(1 - U/U_c)$ linearly goes to zero at the critical interaction $U_c(W) = U_c^0(1 + \frac{2}{5}C\overline{\varepsilon}_i^2)$. This corresponds to the well-known effective mass enhancement ($m^* \sim 1/Z$) in the strongly correlated regime. Here the constant $C = 10/(U_c^0)^2$, and $U_c^0 = 64t/3\pi$ for the considered band structure.

Scattering rate.—To determine the effects of correlations on transport, we calculate the scattering rate $1/\tau = 1/\tau = -2\,\mathrm{Im}\,\Sigma_{av}(\omega = 0) = -2\,\mathrm{Im}\,G_o(0)\overline{v}_i^2$. We find that scattering is strongly reduced near the Mott transition, corresponding to correlation-enhanced screening.

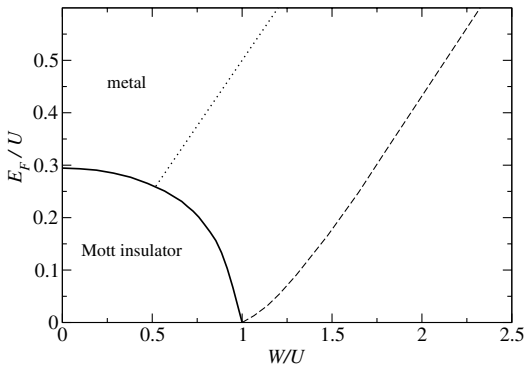

FIG. 1. DMFT phase diagram of the Hubbard model with random site energies. The Mott insulator can be suppressed by sufficiently strong (bare) disorder $W > U$. Also shown is an estimate of the regime where Anderson localization effects are important, as obtained by comparing the Fermi energy E_F to bare disorder W (dotted line) or screened disorder $\tilde{W}$ (dashed line). Localization is strongly suppressed by correlation effects in the intermediate regime where the disorder is comparable to the on-site repulsion U.

To show this analytically, we note that in the critical regime the spectral weight corresponding to $\Delta(\omega)$ is of the order of Z_o. We expand Eq. (7) with respect to $\tilde{\varepsilon}_i/Z_i$: To leading order, $\tilde{\varepsilon}_i/Z_i \sim -e_i^2 + d_i^2 \sim \mathcal{O}(Z_i)$. Therefore $\tilde{\varepsilon}_i/Z_i \equiv v_i \sim Z_i \to 0$ as $U \to U_c(W)$, and we conclude that random site energies are *perfectly screened* at the metallic side of the Mott transition [16]. The same conclusion remains valid even for an asymmetric distribution of disorder, in which case particle-hole symmetry is restored as the transition is approached. For weak disorder, we obtained a simple formula for the scattering rate close to the Mott transition:

$$\frac{1}{\tau} = \frac{2}{t}\left[\frac{3\pi t}{4U_c}\left(1 - \frac{U}{U_c}\right)\right]^2 \overline{\varepsilon}_i^2. \tag{8}$$

Typical numerical results obtained for disorder ranging from weak to strong are shown in Fig. 2(a). We find that disorder is strongly screened even relatively far from the transition, for $U/U_c(W) \gtrsim 0.5$.

Particle-hole asymmetry.—For a particle-hole asymmetric model (generally appropriate for realistic materials), we find that for $U \to U_c(W)$ the energies v_i remain finite, although still much smaller than W. The disorder screening nevertheless remains very strong, which persists even in the case of fairly strong particle-hole asymmetry and strong disorder. Typical numerical results are shown in Fig. 2(b), where the full line corresponds to the symmetric semicircular density of states, and the dashed line is obtained for the particle-hole asymmetric lattice described by the Green function $G_{oa}(\omega) = [\omega - t^2 G_o(\omega + a)]^{-1}$. In this plot, the asymmetry parameter a is chosen to be $0.15D$ (strongly asymmetric lattice), where D is the bandwidth. For weak disorder and moderate particle-hole asymmetry, we were able to obtain a quantitative estimate of the screening effect, and we find that close to the transition the scattering rate approaches a very small asymptotic value $1/\tau \sim (\delta\mu)^2 \overline{\varepsilon}_i^4 \sim W^4$, instead of $1/\tau \sim W^2$ as for weak interactions. In addition, for any realistic lattice at half filling, $\delta\mu$ is a small number (≤ 0.1), explaining the smallness of the scattering rate.

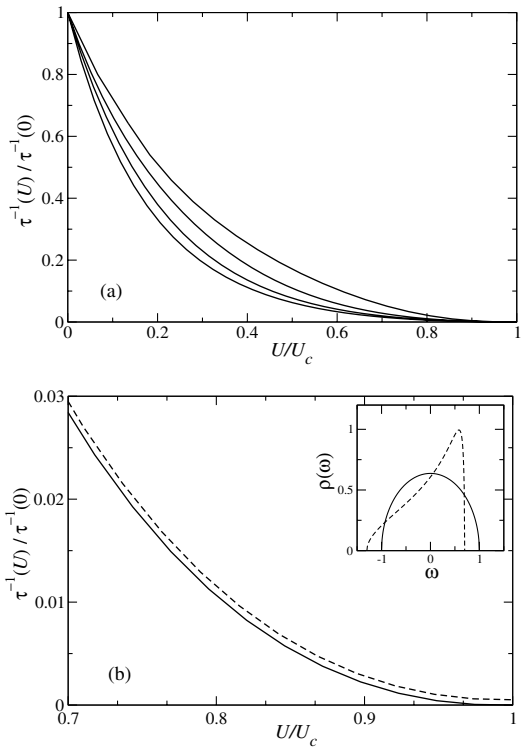

FIG. 2. Scattering rate normalized with the noninteracting value. (a) From the lower to the upper curves: $W = 0.1, 1, 2, 4$. (b) Results close to U_c for the particle-hole symmetric lattice (full line), and the asymmetric lattice (dashed line), with $W = 1$. The inset shows the density of states in these two cases.

Breakdown of conventional theory.—In the strongly correlated regime our DMFT results are in sharp discrepancy with results obtained within Hartree-Fock, as shown in Fig. 3. For small U, both methods give similar results, but closer to the transition HF theory (dashed line) predicts a reduced disorder screening, while full DMFT (full line) shows that the screening remains strongly enhanced. The reduction of screening found in HF reflects the decrease of the compressibility near the Mott transition. This is a result of a Stoner instability in the magnetic HF solution, which sets in for $U = 1/\rho_0(0) = \pi D/2$ as a precursor to a gap opening at the transition [17]. We emphasize that the direct relation between compressibility and screening as in Eq. (3) is a general feature of weak-coupling approaches, and its applicability is seriously limited in the strongly correlated regime.

Enhanced screening as "Kondo pinning."—In the DMFT approach [8] that we use, the solution of the full Hubbard model is mapped to solving an ensemble [12] of auxiliary Kondo-Anderson impurity problems. Accordingly, the approach to the Mott transition can be described as the decrease of the local Kondo temperature,

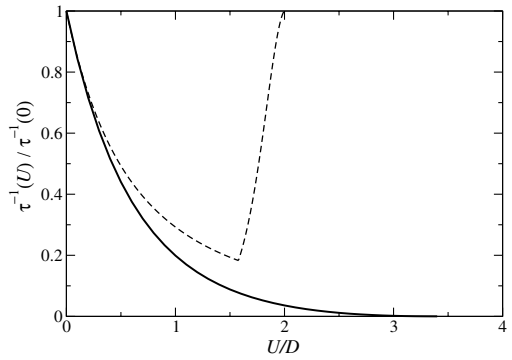

FIG. 3. Normalized scattering rate for weak disorder as a function of U, from the full DMFT solution (full line), and the corresponding Hartree-Fock (HF) approximation (dashed line). For moderate interaction both methods predict the same screening, but diametrically opposite results are obtained in the strongly correlated regime, where DMFT predicts enhanced screening, while a strong suppression is obtained within HF theory.

corresponding to the reduction of the local quasiparticle weight. In this language, the renormalized energy level v_i can be identified as the position of the Kondo resonance, which is well known to "pin" to the Fermi energy in the Kondo limit $Z_i \to 0$. We can thus interpret the surprising enhancement of disorder screening in the strongly correlated regime as reflecting the nonperturbative Kondo physics captured by our DMFT method, but not by standard weak-coupling theories. This mechanism is very closely related to the Kondo enhancement of resonant tunneling through quantum dots, as observed in recent experiments [18]. Our discussion makes it clear why site randomness is strongly suppressed, but also indicates that, if additional hopping randomness [12] is introduced, the same mechanism would *not* apply, as we have verified by explicit calculations. In realistic systems, we expect the disorder to be strongly but not perfectly screened even in the vicinity of the Mott transition.

Screening and localization.—The DMFT approach is too simple to describe Anderson localization effects, which cannot be neglected for strong enough randomness. Nevertheless, it is interesting to estimate the disorder strength necessary for localization. In the absence of interactions, localization is expected [1] to set in when the disorder scale W is comparable to the kinetic (i.e., Fermi) energy, as indicated by a dotted line in Fig. 1. However, we have shown that correlations lead to strong screening, with a renormalized disorder scale $\tilde{W} \sim (\overline{v_i^2})^{1/2} \ll W$, which we can numerically compute for any U and W, and analytically in several limits. In particular, in the atomic limit ($E_F \to 0$), we find $\tilde{W} \sim (1 - U/W)^{3/2}$. In the presence of interactions, the onset of localization should be estimated by comparing $\tilde{W}$ to E_F, and the resulting boundary is shown by a dashed line in Fig. 1. Interestingly, the metallic phase is found to be strongly stabilized by screening in the intermediate regime $W \sim U$. Of course, such interplay of correlation and localization should be studied in more detail by extensions of DMFT which can explicitly incorporate the localization effects [19], but this fascinating issue remains a challenge for future work.

We thank C. Busser, A. Georges, S. Das Sarma, D. Popović, and Z. Radović for useful discussions. This work was supported by the NHMFL and NSF Grants No. DMR-9974311 and No. DMR-0234215 (D. T., V. D.), No. DMR-9976665 (E. A.), and No. DMR-0096462 (G. K.). V. D. and E. A. also thank the Aspen Center for Physics where part of this work was carried out.

[1] P. A. Lee and T.V. Ramakrishnan, Rev. Mod. Phys. **57**, 287 (1985).
[2] E. Abrahams *et al.*, Rev. Mod. Phys. **73**, 251 (2001).
[3] V. M. Pudalov *et al.*, Phys. Rev. Lett. **88**, 196404 (2002); A. A. Shashkin *et al.*, Phys. Rev. B **66**, 073303 (2002).
[4] S. Das Sarma and E. H. Hwang, Phys. Rev. Lett. **83**, 164 (1999).
[5] V. T. Dolgopolov and A. Gold, JETP Lett. **71**, 27 (2000).
[6] I. F. Herbut, Phys. Rev. B **63**, 113102 (2001).
[7] G. Zala *et al.*, Phys. Rev. B **64**, 214204 (2001).
[8] A. Georges *et al.*, Rev. Mod. Phys. **68**, 13 (1996).
[9] L. Candido *et al.*, Phys. Rev. Lett. **86**, 492 (2001).
[10] V. T. Dolgopolov, JETP Lett. **76**, 377 (2002).
[11] V. Dobrosavljević *et al.*, Phys. Rev. Lett. **90**, 016402 (2003).
[12] V. Dobrosavljević and G. Kotliar, Phys. Rev. Lett. **71**, 3218 (1993); Phys. Rev. B **50**, 1430 (1994).
[13] Within DMFT for disordered systems [12], the environment of a given site is replaced by its disorder-averaged value.
[14] The role of the local compressibility in determining the renormalization of parameters in the presence of strong correlation and disorder and the fact that the quasiparticle parameters are site-dependent was emphasized in early work by G. T. Zimanyi and E. Abrahams, Phys. Rev. Lett. **64**, 2719 (1990).
[15] G. Kotliar and A. E. Ruckenstein, Phys. Rev. Lett. **57**, 1362 (1986).
[16] We emphasize that the approach to the Mott transition considered in this work does not correspond to the physical trajectory describing the reduction of density in 2D electronic systems [2]. There $(E_F/U) \sim n^{1/2}$, while $(W/U) \sim n^{-1/2}$, where n is the electron density. Applications of our theory to experimental situations will be addressed elsewhere.
[17] This ferromagnetic instability is well known to be an artifact of the HF theory for a half-filled Hubbard model, and follows from the neglect of the correlation energy in this approach.
[18] D. Goldhaber-Gordon *et al.*, Phys. Rev. Lett. **81**, 5225 (1998).
[19] V. Dobrosavljević and G. Kotliar, Phys. Rev. Lett. **78**, 3943 (1997).