Mean Field Theory of the Mott-Anderson Transition

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We present a theory for disordered interacting electrons that can describe both the Mott and Anderson transitions in the respective limits of zero disorder and zero interaction. We use it to investigate the $T = 0$ Mott-Anderson transition at a fixed electron density, as the disorder strength is increased. Surprisingly, we find *two* critical values of disorder W_{nfl} and W_c. For $W > W_{\mathrm{nfl}}$, the system enters a "Griffiths" phase, displaying metallic non-Fermi liquid behavior. At even stronger disorder, $W = W_c > W_{\mathrm{nfl}}$ the system undergoes a metal-insulator transition, characterized by the linear vanishing of both the *typical* density of states and the *typical* quasiparticle weight.   [S0031-9007(97)03117-7]

The nature of the metal-insulator transition is a fundamental problem in condensed matter science. There are two basic mechanisms that cause electron localization. Mott demonstrated that electron-electron interactions can produce a metal-insulator transition (MIT) even in a clean system [1]. Anderson discovered that disorder, i.e., strong spatial fluctuations in the potential due to impurities [2], can drive a metal-insulator transition in a system of noninteracting electrons.

Following these early ideas, important advances were made following the application of scaling approaches [3–10] to the problem. In the interacting case, these formulations turned out to be closely connected to Fermi liquid ideas [7].

These efforts notwithstanding, many basic questions remain. In particular, it proved very difficult to incorporate the effects of strong electronic correlations, such as the formation of local magnetic moments, in a comprehensive theory of the MIT. This is a serious shortcoming, since it is well established experimentally that the metallic state close to the MIT is characterized by a divergent magnetic susceptibility and linear specific heat coefficient. These observations form the basis of the two fluid phenomenology [11].

Very recently, a new approach [12] to the strong correlation problem has been developed and successfully applied to systems in the vicinity of the Mott transition. This dynamical mean field theory is in its spirit quite similar to the well known Bragg-Williams theory of magnetism, and as such becomes exact in the limit of large coordination. The approach has furthermore been extended to disordered systems [13], and used to investigate phenomena such as disorder-induced local moment formation [14]. However, if formulated in its strict large-coordination limit, the theory misses strong spatial fluctuations, and thus cannot incorporate Anderson localization effects.

The goal of the present study is to present a theory that can describe both the Mott and Anderson routes to local-

ization, and therefore address the interplay of these effects. We follow an approach very similar to the well known Thouless-Anderson-Palmer formulation of the mean field theory of spin glasses [15]. Specifically, we treat the correlation aspects of the problem in a dynamical mean field theory fashion, but allow *spatial variations* of the order parameter in order to allow for Anderson localization effects. The theory is then exact in the noninteracting limit, and reduces to the standard dynamical mean field theory in absence of disorder.

For simplicity, we consider a simple single-band Hubbard model with random site energies, as given by the Hamiltonian

$$H = \sum_{ij} \sum_{\sigma} (-t_{ij} + \varepsilon_i \delta_{ij}) c_{i,\sigma}^{\dagger} c_{j,\sigma} + U \sum_i c_{i,\uparrow}^{\dagger} c_{i,\uparrow} c_{i,\downarrow}^{\dagger} c_{i,\downarrow}.$$

Within the dynamical mean field theory, all local correlation functions can be evaluated using a single-site effective action of the form

$$\begin{aligned}
S_{\mathrm{eff}}(i) = \sum_{\sigma} \int_o^{\beta} d\tau \int_o^{\beta} d\tau' \, c_{i,\sigma}^{\dagger}(\tau) \\
\times [\delta(\tau - \tau')(\partial_{\tau} + \varepsilon_i - \mu) + \Delta_{i,\sigma}(\tau, \tau')] \\
\times c_{i,\sigma}(\tau') + U \int_o^{\beta} d\tau \, n_{i,\uparrow}(\tau) n_{i,\downarrow}(\tau).
\end{aligned} \tag{1}$$

Here, we have used functional integration over Grassmann fields $c_{i,\sigma}(\tau)$ that represent electrons of spin σ on site i, and $n_{i,\sigma}(\tau) = c_{i,\sigma}^{\dagger}(\tau) c_{i,\sigma}(\tau)$. The "hybridization function" $\Delta_i(\tau, \tau')$ is obtained by formally integrating out all the degrees of freedom on other sites in the lattice, and is given by

$$\Delta_i(\omega_n) = \sum_{j=1}^{z} t_{ij}^2 G_j^{(i)}(\omega_n). \tag{2}$$

The sum over j runs over the z neighbors of site i, and $G_j^{(i)}(\omega_n) = \langle c_j^{\dagger}(\omega_n) c_j(\omega_n) \rangle$ are the local Green functions evaluated on site j, but with site i removed. For z

finite, and arbitrary lattices, $G_j^{(i)}(\omega_n)$ cannot be expressed through *local* Green's functions only, but the situation is simpler on a Bethe lattice [16], where a simple recursion relation can be written for this object, expressing it through similar objects on neighboring sites. In particular, $G_j^{(i)}(\omega_n)$ can be computed from a local action of the form identical as in Eq. (2), except that in the expression for $\Delta_j(\tau, \tau')$, the sum now runs over $z - 1$ neighbors, excluding site i.

We note that this local action is identical as the action of an Anderson impurity model embedded in a sea of conduction electrons described by a hybridization function $\Delta_j(\tau, \tau')$. We conclude that the objects $G_j^{(i)}(\omega_n)$ are related by a stochastic recursion relation, which involves solving Anderson impurity models with random on-site energies ε_i.

To make further progress, it is crucial to identify appropriate order parameters that can characterize different phases of the system and describe quantitatively the approach to the transition. In early work, it has already been stressed by Anderson [2] that a proper description of disordered systems should focus on distribution functions, and that *typical* rather than the average values should be associated with physical observables. Our formalism maps the original model onto an ensemble of Anderson impurity models, and its low energy behavior is naturally described in terms of the distribution function of the corresponding local density of states (DOS), defined as $\rho_j = -\operatorname{Im} G_j(0)$ [17]. From this distribution we can extract the typical DOS $\rho_{\text{typ}} = \exp\{\langle \ln \rho \rangle\}$, which is a natural order for the metal-insulator transition.

On the metallic side of the transition, the distribution function of a second quantity, the local *quasiparticle* (QP) weight, which is obtained from the Green functions as $q_j = \frac{\partial}{\partial\omega} \operatorname{Re}[G_j^{-1} - \Delta_j]|_{\omega=0}$, is necessary to characterize the low energy behavior near the transition. Important information is obtained from the typical value of the random variable q_j, defined as $q_{\text{typ}} = \exp\{\langle \ln q_j \rangle\}$, which emerges as a natural order parameter from previous studies of the Mott transition.

It is also useful to consider the average QP density of states $\rho_{\text{QP}} = \langle \rho_j/q_j \rangle$. This object is very important for thermodynamics, since it is directly related to quantities such as the specific heat coefficient $\gamma = C/T$, or the local spin susceptibility χ_{loc}.

It is instructive to discuss the behavior of these order parameters in the previously studied limiting cases. In the limit of large lattice coordination spatial fluctuations of the bath function $\Delta_i(\omega_n)$ are unimportant, and there is no qualitative difference between typical and average quantities. In the Mott insulating phase there is a gap in the density of states, while there is a finite density of states on the metallic side of the transition. As the MIT is approached from the metallic side, ρ_{typ} remains finite, but q_{typ} is found [13] to linearly go to zero.

Another well studied limit is that of noninteracting electrons on the Bethe lattice, which is known [2,5,16,18] to

display an Anderson transition. In the Anderson insulator phase the local density of states has strong spatial fluctuations; few sites with discrete bound states near the Fermi level have large density of states while the density of states in most of the sites is zero. The average DOS is *finite* in both the insulating and metallic phases, and is noncritical at the transition. Similarly, by definition $q_{\text{typ}} = 1$ in this noninteracting limit, so it also remains noncritical. On the other hand, the typical density of states ρ_{typ} is finite in the metal and zero in the Anderson insulator. This quantity is critical, and is found to vanish exponentially [19] with the distance to the transition.

Equation (2) is a system stochastic equation, i.e., it depends on the realization of the random variables describing the disorder. To calculate the probability distributions of ρ_j and q_j we use a simulation approach, where the probability distribution for the stochastic quantity $G_j^{(i)}(\omega_n)$ is sampled from an ensemble of N sites, as originally suggested by Abou-Chacra *et al.* [16]. To solve Anderson impurity models for given bath functions $\Delta_j(\tau, \tau')$ we use the slave boson mean field theory [20,21], which is known to be qualitatively and even quantitatively correct at low temperature and low energies.

We now discuss our results for the nontrivial situation where both the disorder and interactions are present. We consider a $z = 3$ Bethe lattice, in the limit of infinite on-site repulsion U at $T = 0$ and fixed filling $n = 0.3$, in the presence of a uniform distribution of random site energies ε_i of width W (following the notation of Ref. [16], W is measured units of the hopping element t). We begin by concentrating on the evolution of the probability distribution of the local quasiparticle weights q_i, as the disorder is increased. The sites with $q_i \ll 1$ represent [13,14] disorder-induced local magnetic moments, and as such will dominate the thermodynamic response (see the definition of ρ_{QP}). For weak disorder we expect relatively few local moments and the quasiparticle weight distribution is peaked at a finite value. As the disorder is increased, the distribution of q_j's broadens. At a critical value of the disorder W_{nfl}, a transition to a *non-Fermi liquid* (NFL) metallic state takes place. To illustrate this behavior we display the integrated distribution of the variable q, $n(q)$ for different values of disorder in Fig. 1(a). If $n(q) \sim q^\alpha$, as $q \to 0$, and $\alpha \leq 1$, then $P(q) \to +\infty$ in this limit. Since the local Kondo temperatures $T_K^{(i)} \sim q_i$ [13], this behavior reflects a singular distribution of Kondo temperatures. As a result, we immediately obtain NFL behavior [22–25] with diverging γ and χ_{loc} at $T = 0$. As we can see, there is a well defined value of disorder $W_{\text{nfl}} \sim 7$, beyond which the slope of $n(q)$ at $q = 0$ diverges, and we enter the NFL phase. It is worth mentioning that a similar transition to a NFL metal, well before the MIT, has been found from the field-theoretical approaches in $2 + \varepsilon$ dimensions [6–8,10]. In the NFL phase the thermodynamics is dominated by disorder-induced local moments.

The probability distribution of the second order parameter ρ, $P(\ln \rho)$, for different values of the disorder
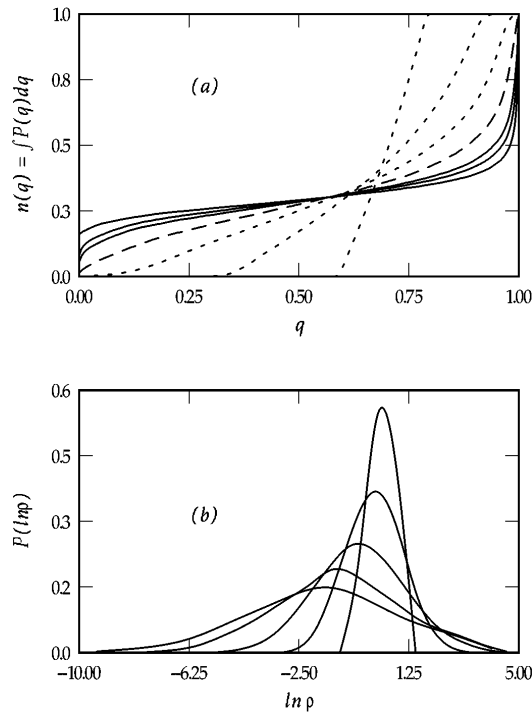
FIG. 1. Evolution of probability distributions for *interacting* electrons as a function of disorder at $T = 0$: (a) integrated distribution for local quasiparticle weights (local Kondo temperatures). Results are presented for $W = 1, 3, 5$ (dotted lines), $W = 7$ (dashed line), and $W = 9, 10, 11$ (full lines). The transition to the NFL regime is signaled by the divergence of the *slope* of $n(q)$ at $q = 0$. (b) The evolution of the local DOS distribution is presented by plotting $P(\ln \rho)$ for $W = 3, 5, 7, 9, 10$. We find that the *maximum,* i.e., $\langle \ln \rho \rangle$ shifts, as the transition is approached. Note also the extremely large *width* of the distribution, so that ρ now spans many orders of magnitude.

FIG. 2. Order parameters as functions of the disorder strength W. In the noninteracting limit (a), the typical DOS vanishes exponentially with disorder, while the average DOS is noncritical. When interactions are present (b), the typical DOS decreases *linearly* with disorder, while at the same time the average one *diverges*. The divergence is clearly seen by plotting $1/\langle \rho \rangle_{ab}$ (dotted line), which vanishes *linearly* as the critical disorder is approached. Both quantities are found to be critical at $W = W_c \approx 11$. Also shown is $1/\langle \rho \rangle_{QP}$ (thin full line), which vanishes at $W = W_{nfl} \approx 7$. Finally, we show in (c) the critical behavior of the typical QP weight, which also vanishes linearly at $W = W_c$, similarly as in a Mott transition.

strength is shown in Fig. 1(b). Notice that not only the width, but also the maximum of the distribution shifts with disorder, a behavior reminiscent of an ordinary Anderson transition. The typical DOS is strongly depressed at strong disorder. This behavior is even more clearly seen if we plot the DOS averages at the Fermi energy as a function of disorder, as presented in Fig. 2(b). The typical DOS decreases in a clearly *linear fashion,* as the transition at $W = W_c \approx 11$ is approached. This should be contrasted [26] to the $U = 0$ Anderson transition, where we find [see Fig. 2(a)] the decrease to be exponential in agreement with analytical results [18]. We mention that at least in the noninteracting limit [18], the typical DOS behaves in a fashion which is qualitatively identical to that of the diffusion coefficient. Having this in mind, one is tempted to interpret our results as indicating linear behavior of the conductivity near the transition, as found experimentally in many "compensated" systems.

Even more dramatic is the behavior of the average DOS which is noncritical both near a conventional $U = 0$ Anderson transition, and near a clean Mott transition. This quantit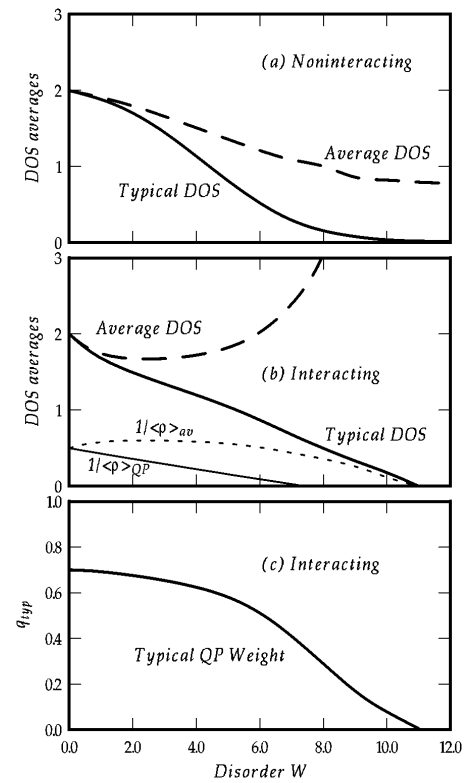y is found to *diverge* at the same value of disorder where the typical DOS vanishes. The fact that we indeed have the divergence is further confirmed by plotting $1/\langle \rho \rangle_{av}$ as a function of disorder, as shown by a dotted line in Fig. 2(b). This quantity vanishes linearly at the same critical disorder $W = W_c \approx 11$. Also in Fig. 2(b) we exhibit the divergence of the QP DOS, at the transition to the NFL phase. Finally, we consider the behavior of q_{typ}, which is also found to vanish linearly at $W = W_c$, similarly as in the case of the Mott transition, but in contrast to the noninteracting scenario. Physically, this indicates that a *finite fraction* of electrons turn into strictly localized magnetic moments at the metal-insulator transition.

To summarize, in this Letter we have presented a new self-consistent theory of disordered interacting electrons that can describe both the Anderson and Mott routes to localization. In this approach, the typical local DOS and the typical local resonance width play the role of order parameters, but the entire *probability distributions* are needed to fully characterize the behavior of the system.

Our equations take a form of stochastic recursion relations for these quantities that involves solving an ensemble of Anderson impurity models. As a specific application of this approach, we have considered a large U limit of the Hubbard model at a fixed electron density, and investigated effects induced by gradually turning on the disorder. We find that the correlations effects produce dramatic modifications of the conventional Anderson scenario. At intermediate disorder, there is a transition to a non-Fermi liquid phase, characterized by singular thermodynamics, but conventional transport. At larger disorder a metal-insulator transition takes place. This is a *new type* of transition, having some of the features of both the Anderson and Mott scenarios. Remarkably, the main features our treatment, a non-Fermi liquid phase before the metal insulator transition and a linearly vanishing conductivity are found in compensated doped semiconductors.

Our framework suggests several research directions. One would like to relate response functions that determine the transport coefficients to the local order parameters, as was done in the noninteracting case by Efetov and Viehweger [18]. Our calculations should be extended to the vicinity of half filling where correlation effects should be even more pronounced. This study could cast some light on the different types of metal-insulator transitions that occur in compensated and uncompensated doped semiconductors.

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