Theory of Metal-Insulator Transitions in Strongly Correlated Electronic Systems with Disorder

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During the next three years, a theory of metal-insulator transitions will be developed, with emphasis on systems where strong electron-electron interactions and disorder are both important. This theory will provide a simple order-parameter description of the problem, and will be used to construct the equation of state for thermodynamic and transport properties valid in a broad range of temperatures, carrier concentrations and levels of disorder. Our approach will make it possible to incorporate all the basic mechanisms of localization, including both the Mott and the Anderson route, as well as the possibility of glassy freezing of electrons. The results will be of direct relevance to many systems, ranging from doped semiconductors, disordered heavy fermion systems, layered ruthenates and manganites, two-dimensional electron gases, to high temperature superconductors.

I. INTRODUCTION

The central theme underpinning the ongoing technological revolution is the ability to design and fabricate new materials. In practice, one most often starts with some insulating compound, and then introduces charge carriers by appropriate chemical doping. As a result, materials have been obtained, ranging from insulators, to bad metals, to excellent conductors, and even high temperature superconductors. Not surprisingly, most of these interesting systems find themselves somewhere between metals and insulators. It is ironic that it is precisely in this regime, where most of the time-honored concepts and ideas of traditional solid state physics meet considerable difficulties. In fact, many of these new materials have demonstrated behavior believed impossible even a few decades ago.

Thus both from the practical and the fundamental point of view, the problem of the metal-insulator transition has emerged as one of the principal challenges in modern condensed matter science. There are several reasons why a theoretical description of this regime remains difficult. First, the electron-electron interactions become increasingly significant as the electrons become less mobile. Second, chemical doping usually introduces "dirt" or disorder, which often induces the localization of charge carriers. Typically, these two effects are of comparable magnitude, so that the interplay of electronic correlations and disorder must be addressed.

Traditional approaches to the problem of disordered interacting electrons have focused on the limit of weak disorder, and used Fermi liquid concepts to describe the effects of interactions. However, in presence of strong correlations, the Fermi liquid picture is often restricted to very low temperatures. Worse still, when disorder is added, studies on many materials have suggested that such descriptions do not apply at *any* accessible temperature. On the experimental side, many features of systems such as doped semiconductors, disordered heavy fermion metals, and even two-dimensional electron gases, have remained puzzling.

Very recently, a novel *dynamical mean-field* (DMF) approach to disordered interacting electrons has been developed and already applied with striking success to several systems. This formulation offers a unique possibility to incorporate all the basic mechanisms for electronic localization, including both the Anderson and the Mott route, as well as the description of glassy freezing of electrons. However, careful numerical and analytical work will be necessary to combine these different processes in a coherent theoretical framework, and obtain detailed predictions for realistic physical systems. In this proposal we will present a comprehensive plan for such studies, which will include: (i) transport near Mott-Anderson transitions, as a function of the doping level, the temperature and the degree of disorder; (ii) non-Fermi liquid behavior in strongly disordered metals and the origin of the two-fluid model; (iii) high temperature anomalies, the breakdown of Matthiessen's rule, and the Mooij correlations; (iv) role of glassy freezing as a driving force for the metal-insulator transition.

The proposed research will address a number of basic physics questions that for many years have remained unanswered. Some of these have recently been listed as having "high potential for important contributions by theoretical modeling" by the 1997 NSF Report of the Panel on Materials Theory. Our theoretical framework is flexible enough to incorporate all the key processes, but at the same time sets well defined goals that realistically can be achieved in a three-year period.

II. WHY IS THE METAL-INSULATOR TRANSITION IMPORTANT ?

Understanding the metal-insulator transition (MIT) poses one of the most basic questions of Condensed Matter Science. It has been been a topic of much controversy and debate starting from early ideas of Mott [1], and Anderson [2], but the problem remains far from being resolved. Having in mind the rather long history [3,4] of the subject, and in order to place the proposed research in a proper perspective, it is useful to briefly summarize the principal issues and ideas of this field.

In traditional Solid State Physics, two diametrically opposite limits are well understood: that of good metals, and that of good insulators. In both cases, a single large energy scale dominates the problem, and various material-specific details can often be treated as small "perturbations".

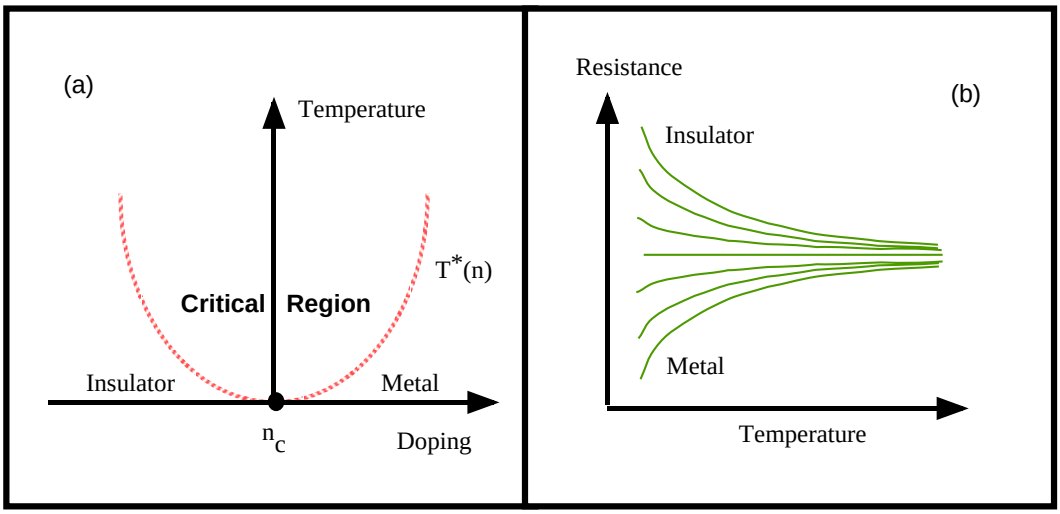

FIG. 1. Quantum critical behavior near a metal-insulator transition. Typically, one induces a metal-insulator transition by changing the carrier concentration n. Well defined metallic or insulating behavior is observed only at temperatures lower than a characteristic temperature $T^*(n)$ that vanishes at the transition. At $T > T^*$, the system is in the "quantum critical region" [5], as shown in (a). Temperature dependence of the resistance for different carrier concentrations is shown schematically in (b). As the system crosses over from metal to insulator, the temperature dependence of the resistivity changes slope from positive to negative, in violation of the Matthiessen's rule, or the Boltzmann theory predictions [6].

In the case of good metals [6], such as aluminum or copper, the large energy scale is the Fermi energy, and diluted particle-hole excitations dominate the behavior even at room temperature. For good insulators [6], charged excitations are prohibited by the existence of a large energy gap; here, the low energy excitations such as phonons or spin waves typically have a character of small "vibrations" away from a single, stable ground state.

Quite generally, when a system is neither a good metal nor a good insulator, both the localized and the itinerant aspects of the problem are important. In this intermediate regime, several competing processes can be simultaneously present. As a result, the system cannot "decide" whether to be a metal or an insulator until a very low temperature T^* is reached, below which a more conventional description applies. This situation is typical of systems close to a quantum critical point [5], which describes a zero temperature second order phase transition between two distinct states of matter. Here, a characteristic, energy scale T^* vanishes as the transition is approached from either side, as shown in Figure 1. Experimentally, such behavior has been observed in a number of systems, ranging from doped semiconductors [7–9], and doped Kondo insulators [10], to two-dimensional electron gases [11–13].

Investigating the approach to such a quantum critical point is clearly a subject of a fundamental significance. Perhaps more importantly, understanding the nature of low energy excitations in the intermediate regime between a metal and an insulator is of crucial importance for the progress in material science. In fact, it cannot be overemphasized that almost each and every example of the novel exotic materials finds itself in this regime, where traditional physical pictures and ideas offer little help.

III. WHY IS THE MIT PROBLEM DIFFICULT ?

Experimental results on many systems have demonstrated that the metal-insulator transition shows many features expected at a quantum critical (QC) point. In particular, a characteristic *scaling* behavior of the conductivity has been observed [8,9,11–13], as a function of carrier concentration, temperature and the magnetic field. However, in contrast to standard critical phenomena [16], in the case of the MIT it is by no

means obvious what *order parameter* should be considered, or what symmetry is broken. It is precisely this genuine ambiguity that has represented the main stumbling block in formulating theoretical approaches to the MIT problem.

Even worse, no general principle dictates that the MIT must be a critical point, since the metal and the insulator are not related by an obvious symmetry. In fact, for clean systems, several theories [1] have predicted that interactions should induce a first order (discontinuous) metal-insulator transition. Here, the presence of disorder can be expected to be crucial. In particular, general arguments [14] have suggested that sufficiently strong disorder can induce a second order phase transition, even if a first order transition is found in the clean limit.

On the other hand, simple physical arguments have been presented a long time ago, outlining the main physical processes that could localize the electrons. The first ideas on the subject date back to Mott [1], who realized that in narrow-band systems, electron-electron interactions can lead to a formation of a magnetic insulator even for partially filled bands. Some years later, Anderson [2] emphasized that even for noninteracting electrons, sufficiently strong disorder can "trap" the electrons and lead to insulating behavior at $T = 0$. Both the Mott and the Anderson problem have a simple and robust physical basis and offer a reasonably clear picture of the relevant processes. Nevertheless, a theoretical description comparable to that of classical critical phenomena has not been easy to find, despite years of effort [3,4].

The primary reason for the difficulties is related to the fact that both the Mott and the Anderson transition find themselves in regimes where traditional, perturbative approaches [3] cannot be straightforwardly applied. To make the problem even more difficult, simple estimates [1] are sufficient to appreciate that in many situations the effects of interactions and disorder are of comparable magnitude. Furthermore, it has been suggested a long time ago [15] that the two mechanisms will in fact *reinforce* each other in the transition region, and thus both should be simultaneously considered. So far, very few approaches have attempted to explicitly incorporate these two basic routes to localization.

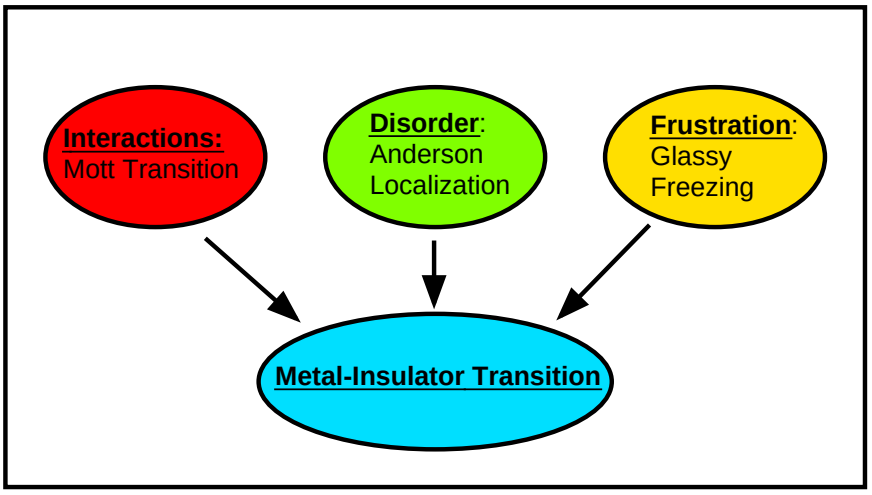

FIG. 2. Three basic routes to localization

Another aspect of disordered interacting electrons poses a fundamental problem. Very generally, the Coulomb repulsion favors a uniform electronic density, while the disorder favors local density fluctuations. When these two effects are comparable in magnitude, one can expect many different low energy electronic configurations. i. e. the emergence of many *metastable states*. Similarly as in other "frustrated" systems with disorder, such as spin glasses [17], these processes can be expected to lead to *glassy* behavior of the electrons, and the associated anomalously slow relaxational dynamics. Indeed, both theoretical [18] and experimental [19–21] work has found evidence of such behavior deep on the insulating side of the transition. However, at present very little is known as to the precise role of such processes in the critical region. Nevertheless, it is

plausible that the glassy freezing of the electrons must be important, since the associated slow relaxation clearly will reduce the mobility of the electrons. From this point of view, the glassy freezing of electrons may be considered, in addition to the Anderson and the Mott mechanism, as a third fundamental route to electron localization.

IV. TRADITIONAL APPROACHES TO DISORDERED INTERACTING ELECTRONS

The existence of a sharp metal-insulator transition at $T = 0$ has been appreciated for many years [1]. Experiments on many systems indeed have demonstrated that a well defined critical carrier concentration can easily be identified. On the theoretical side, ambiguities on how to describe or even think of the metal-insulator transition have made it difficult to directly address the nature of the critical region. Instead, most studies carried out over the last twenty years have focused on the limit of weak disorder [3], where considerable progress has been achieved.

Here, for noninteracting electrons the conductance was found to acquire singular (diverging) corrections in one and two dimensions, an effect known as "weak localization" [22,3]. According to these predictions, for $d \leq 2$ the conductivity would monotonically decrease as the temperature is lowered, and would ultimately lead to an insulating state at $T = 0$. Interestingly, similar behavior was known in Heisenberg magnets [23,16], where it resulted from $d = 2$ being the *lower critical dimension* for the problem.

This analogy with conventional critical phenomena was first emphasized by the "gang of four" [22] , as well as Wegner [23], who proposed an approach to the metal-insulator transition based on expanding around two dimensions. For this purpose, an effective low energy description was constructed [23,58], which selects those processes that give the leading corrections at weak disorder in and near two dimensions. This "non-linear sigma model" formulation [23,58] was subsequently generalized to interacting electrons by Finkelshtein [25], and studied using renormalization group methods in $2 + \varepsilon$ dimensions [25,26]. In recent years, the non-linear sigma model of disordered interacting electrons has been extensively studied by several authors [4].

While the sigma model approach presented considerable formal complexity, its physical content in fact proved to be remarkably simple. As emphasized by Castellani, Kotliar and Lee [27], one can think of the sigma model of disordered interacting electrons as low energy *Fermi liquid* description of the system. Here, the low energy excitations are viewed as weakly interacting quasi-particles that, at least for weak disorder, can be described by a small number of Fermi liquid parameters such as the diffusion constant, the effective mass, and the interaction amplitudes. In this approach, one investigates the evolution of these Fermi liquid parameters as weak disorder is introduced. The metal-insulator transition is then identified by the *instability* of this Fermi liquid description, which in $d = 2 + \varepsilon$ dimensions happens at weak disorder, where controlled *perturbative* calculations can be carried out.

Remarkably, by focusing on such a stability analysis of the metallic state, one can obtain a description of the transition which does not require an *order parameter* description, as in usual critical phenomena [16]. This is a crucial advantage of this approach, precisely because of the ambiguities associated with deciding what an appropriate order parameter description should be. On the other hand, it is important to stress that by construction, the sigma model focuses on those physical processes that dominate the perturbative, weak disorder regime. In real systems, the metal-insulator transition is found at strong disorder, where a completely different set of processes could be at play.

V. LIMITATIONS OF THE CONVENTIONAL SCENARIO

In recent years, an increasing number of experimental findings seem to bring into question the "weak coupling" picture of disordered interacting electrons. Some of the most striking results can be summarized as follows:

(1) In doped semiconductors [7], the low temperature conductivity displays a simple power-law behavior $\sigma \sim (n - n_c)^{\mu}$ [28] in a very broad range of concentrations, all the way to several n_c. However, the

value of the critical exponent μ shows strong dependence on the degree of compensation [7] and the magnetic field [29].

(2) Thermodynamic response on the metallic side of the transition shows singular behavior, such that the susceptibility χ and the specific heat coefficient γ seem to *diverge* at low temperatures. Such behavior is observed in doped semiconductors [30], and also in several disordered heavy fermion systems [31], but is inconsistent with Fermi liquid predictions [27,4].

(3) The temperature dependence of the resistivity in the transition region shows a characteristic behavior as shown in Fig. 1(a). Here, the slope of the temperature dependence changes sign as the disorder is increased, and the system crosses from metal to insulator. Such anomalies have first been observed in A15 (rare earth) compounds [32], but recent work finds very similar behavior [10] in doped semiconductors [33], doped Kondo insulators [10], transition metal oxides [34], high temperature superconductors [35], and even two-dimensional electron gases [11–13]. Remarkably, this behavior is *not* restricted to low temperatures, but in some cases has been found to persist all the way to the (effective) Fermi temperature [10–13]. In temperature this range, Fermi liquid descriptions certainly cannot apply.

(4) Very recently, striking evidence of a metal-insulator transition in two-dimensional electronic systems in zero magnetic fields has been discovered [11–13]. These findings have challenged long-held beliefs that all the electronic states are localized at $T = 0$ in two dimensions, and that $d = 2$ should play a role of the lower critical dimensionality in this problem.

From the theoretical point of view, several studies have suggested what may be missing in the conventional scenario. To explain the thermodynamic anomalies, a phenomenological "two-fluid" model [36] of doped semiconductors has been proposed, resulting from disordered-induced local moment formation [37,40]. This view portrays a strongly inhomogeneous picture of the system, where rare events [38,39,41] may dominate the low temperature behavior, as in "Griffiths phases" [42]. Furthermore, strong correlation effects may be enhanced by disorder [15,3], leading to enhanced electron-electron scattering at finite temperature, and result in non-Fermi liquid behavior [38,39,41]. However, the sigma model cannot be used to investigate the approach to the Mott transition and the resulting formation of the highly correlated electron gas. Finally, we note that an attempt to an order parameter description of the non-linear sigma model has been attempted, based on a $6 - \varepsilon$ expansion approach [43]. Interestingly, the formal structure of this problem has displayed striking similarities with the random-field Ising model [44] and other glassy [17] systems. Based on these findings, it has been suggested [43,45] that nonperturbative effects may play a crucial role near the metal-insulator transition, but that a solution will require a different theoretical formulation.

VI. DMF APPROACH TO DISORDERED INTERACTING ELECTRONS

As we have seen, a number of experimental and theoretical investigations have suggested that the conventional picture of disordered interacting electrons may be incomplete. Most remarkably, the characteristic "critical" behavior seen in many experiments covers a surprisingly broad range of temperatures and densities. This is more likely to reflect an underlying "mean-field" behavior of disordered interacting electrons than the asymptotic critical behavior described by an effective long-wavelength theory.

What seems to be needed is a simple mean-field description that would provide the equivalent of a Van der Waals equation of state, for disordered interacting electrons. Such a theory has long been elusive, primarily due to a lack of a simple order-parameter formulation for this problem. Very recently, an alternative approach to the problem of disordered interacting electrons has been formulated, based on dynamical mean-field (DMF) methods [46]. This formulation is largely complementary to the scaling approach, and has already resulting in several striking predictions. In the following, we briefly describe this method, and summarize the main result that have been obtained so far.

A. The DMF formulation

The main idea of the DMF approach is in principle very close to the original Bragg-Williams (BW) mean-field theories of magnetism [16]. It focuses on a single lattice site, but replaces [46] its environment by a self-consistently determined "effective medium", as shown in Fig. 3.

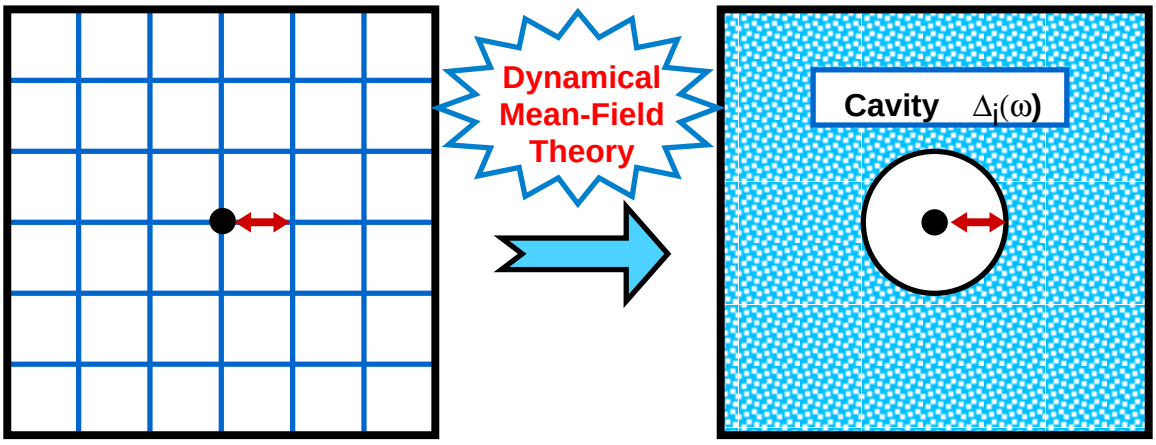

FIG. 3. In dynamical mean-field theory, the environment of a given site is represented by an effective medium, represented by its "cavity spectral function" $\Delta_i(\omega)$. In a *disordered* system, $\Delta_i(\omega)$ for different sites can be very different, reflecting Anderson localization effects.

In contrast to the BW theory, the environment cannot be represented by a static external field, but instead must contain the information about the dynamics of an electron moving in or out of the given site. Such a description can be made precise by formally integrating out [46] all the degrees of freedom on other lattice sites. In presence of electron-electron interactions, the resulting local effective action has an arbitrarily complicated form. Within DMF, the situation simplifies, and all the information about the environment is contained in the local single particle spectral function $\Delta_i(\omega)$. The calculation then reduces to solving an appropriate quantum impurity problem supplemented by an additional self-consistency condition that determines this "cavity function" $\Delta_i(\omega)$.

The precise form of the DMF equations depends on the particular model of interacting electrons and/or the form of disorder, but most applications [46] to this date have focused on Hubbard and Anderson lattice models. The approach has been very successful in examining the vicinity of the Mott transition in clean systems [47–49], in which it has met spectacular successes in elucidating various properties of several transition metal oxides [50]. Applications to heavy fermion systems and Kondo insulators [51] have been equally impressive, in particular in regards to the description of finite temperature properties, and the crossover from coherent to incoherent behavior. In fact, perhaps the most significant feature of the DMF formulation resides in its ability to treat *incoherent* processes, resulting from inelastic electron-electron scattering, in a nonperturbative fashion. As a result, the DMF method is not restricted to Fermi liquid regimes, in contrast to most other theoretical approaches. This feature is likely to be most significant for *disordered* systems, where the coherence temperature can be considerably depressed, resulting in non-Fermi liquid metallic behavior [41].

B. DMF as an order-parameter theory for the MIT

The central quantity in the DMF approach is the local "cavity" spectral function $\Delta_i(\omega)$. From the physical point of view, this object essentially represents the *available electronic states* to which an electron can "jump" on its way out of a given lattice site. As such, it provides a natural order parameter description for the MIT. Of course, its form can be

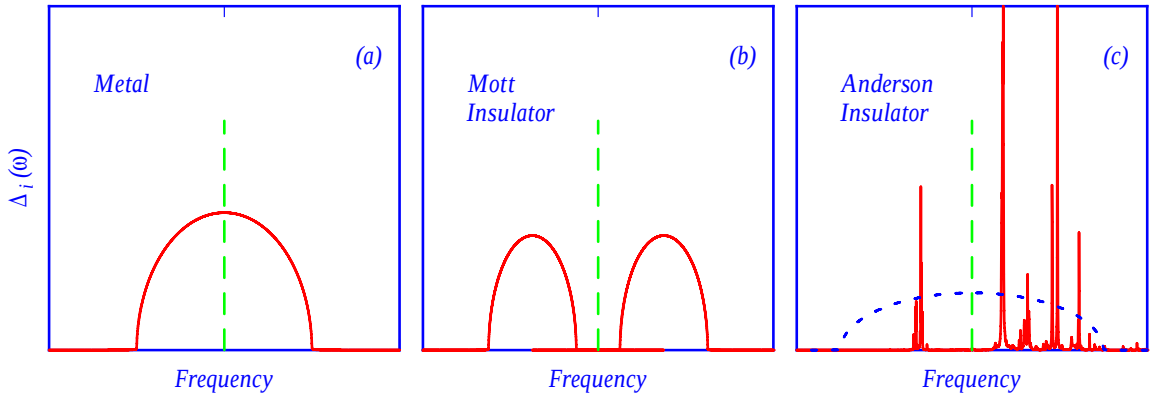

FIG. 4. The local cavity spectral function $\Delta_i(\omega)$ as the order parameter for the MIT. In a metal (a) there are available electronic states near the Fermi level (dashed line) to which an electron from a given site can delocalize. Both for a Mott insulator (b) and the Anderson insulator (c) the Fermi level is in the gap, and the electron cannot leave the site. Note that the *averaged* spectral function (dotted line in (c)) has no gap for the Anderson insulator, and thus cannot serve as an order parameter.

substantially modified by either the electron-electron interactions or disorder, reflecting the corresponding modifications of the electron dynamics. According to the Fermi's golden rule, the transition rate to a neighboring site is proportional to the density of final states - leading to insulating behavior whenever $\Delta_i(\omega)$ has a gap at the Fermi energy. In the case of a Mott transition in absence of disorder, such a gap is a direct consequence of the strong on-site Coulomb repulsion, and is the same for every lattice site.

The situation is more subtle in the case of disorder-induced localization, as first noted in the pioneering work of Anderson [2]. Here, the *average* value of $\Delta_i(\omega)$ has no gap and thus cannot serve as an order parameter. However, as Anderson noted a long time ago, "...no real atom is an average atom..." [15]. Indeed, in an Anderson insulator, the environment "seen" by an electron on a given site can be very different from its average value. In this case, the *typical* "cavity" spectral function $\Delta_i(\omega)$ consists of several delta-function (sharp) peaks, reflecting the existence of localized (bound) electronic states, as shown in Fig. 4(c). Thus a *typical* site is embedded in an environment that has a *gap* at the Fermi energy - resulting in insulating behavior. We emphasize that the location and width of these gaps strongly vary from site to site. These strong fluctuations of the local spectral functions persist on the metallic side of the transition, where the typical spectral density $\Delta_{typ} = \exp < \ln < \Delta_i >$ can be much smaller than its average value. Clearly, a full *distribution function* is needed to characterize the system. The situation is similar as in other disordered systems, such as spin glasses [17]. Instead of simple averages, here the entire distribution function plays a role of an order parameter, and undergoes a qualitative change at the phase transition.

When both strong electron-electron interactions and disorder are present [40,52,50], the situation is even more complicated. In general, the presence of interaction reduces the spectral weight near the Fermi energy, which can be characterized by a local quasiparticle (QP) weight Z_i. For clean systems, this leads to an effective mass enhancement $m^*/m \sim Z^{-1}$ [46], which results in significant modifications of thermodynamic behavior. In presence of disorder, the local QP weight Z_i can have strong spatial fluctuations [40,41], and again, the full distribution function must be evaluated, and plays a role of an additional order parameter. In particular, in presence of sufficiently strong disorder, the distribution function $P(Z_i)$ can become singular (diverge at $Z_i \to 0$), which results in non-Fermi liquid metallic behavior [38–41,52,50], as observed in a

number of systems.

The DMF formulation thus naturally introduces self-consistently defined order parameters that can be utilized to characterize the qualitative differences between various phases. In contrast to clean systems, these order parameters have a character of distribution functions, which change their qualitative form as we go from the normal metal to the non-Fermi liquid metal, to the insulator.

VII. PROPOSED RESEARCH

Our existing work [40,52,50,41,55] has already demonstrated that the DMF methods offer a new non-perturbative approach to the MIT in disordered systems. They provide insight into previously inaccessible regimes, and can be easily adapted to study a number of physical systems and situations. However, only the first steps have been taken, indicating directions for research, rather than providing definitive answers. In the next three years, we will focus on several aspects that seem particularly promising, and in the process will address some basic questions about the MIT in general.

A. Previous work: weak disorder in strongly correlated systems

The most straightforward formulation of disordered interacting electron is obtained in the large coordination limit ($z \rightarrow \infty$) [40], where the DMF theory becomes exact. The situation is the simplest on Bethe lattices, where the local cavity spectral function can be written as [52,50]

$$\Delta_i(\omega) = \frac{t^2}{z} \sum_{i=1}^{z} \rho_i(\omega).$$

Here, $\rho_i(\omega)$ is the local density of states (LDOS) on a neighboring site. Generally, in a strongly disordered system, the LDOS will have strong fluctuations, as in Fig. 4(c). However, in the large coordination ($z \rightarrow \infty$) limit [40], $\Delta_i(\omega)$ has contributions from a large number of sites, and is replaced by its *average* value. As a result, the the LDOS fluctuations are suppressed, leading to the absence of Anderson localization. Still, this limitation is not too serious at weak disorder, where this formulation can be considered reliable. In the noninteracting limit, the disorder is treated on the level of the "coherent potential approximation" (CPA) [40], but in presence of strong correlations, qualitatively new behavior can emerge.

In particular, even if the cavity spectral function $\Delta_i(\omega)$ is replaced by its average value, various *local* quantities such as the local QP weight Z_i can still show strong spatial fluctuations. This possibility has been explored in the context of Hubbard models with random hopping elements [40], which has been proposed as a model of doped semiconductors. In the DMF picture, each lattice site is viewed as an Anderson impurity model, and the corresponding Kondo temperature T_K is proportional to the local QP weight Z_i. In presence of sufficiently strong disorder, a finite concentration of sites have very low Kondo temperature, and thus behave as local magnetic moments. This model was therefore successful in demonstrating the disorder-induced local moment formation [40], as proposed by both experiments [36] and earlier theoretical efforts [37]. Furthermore, the resulting distribution of Kondo temperatures was found to be sufficiently singular to account for diverging spin susceptibility χ and specific heat coefficient $\gamma = C/T$, even in the metallic phase - thus allowing for non-Fermi liquid (NFL) behavior [40] observed in experiment.

A similar NFL behavior has been observed in several classes of disordered heavy fermion compounds [31]. In recent work [41], we have applied the $z = \infty$ DMF formulation to disordered Anderson lattice models, and examined both the thermodynamic and transport properties. For an appropriate model of disorder, the results were found to be in remarkable agreement with experiments on several materials, and were successful in describing most anomalies. This formulation was able to account not only for the temperature dependence of thermodynamic quantities [41], the DC resistivity [41], but also of the optical conductivity [53], the dynamic susceptibility [41], and the magnetoresistance [54].

An important feature of this theory needs to be emphasized. As we have described, for an appropriate form of disorder, the resulting distribution of QP weights, i. e . Kondo temperatures can assume the required

singular form. However, the precise form of the resulting distribution is very sensitive to the detailed model of disorder chosen. In a sense, one has to "fine-tune" the model of disorder to get the desired results, even though a single model can account for numerous experimental probes. On the other hand, the experimentally observed NFL behavior [31], at least in Kondo alloys is remarkably universal. Such universality cannot be explained by the $z = \infty$ DMF model, and remains an important open problem in this field. Very recently [55], we have extended the DMF formulation in order to incorporated the Anderson localization effects. Preliminary results seem to indicate that the resulting distributions may assume a universal form, but much more detailed work will be necessary to achieve a satisfactory understanding of this fascinating phenomenon.

B. The Mott-Anderson transition

Once the system approaches the metal-insulator transition, the Anderson-localization effects cannot be ignored. Very generally, one expects that near a quantum critical point the system is characterized by a small energy scale (the coherence temperature T^* near the MIT). As a result, in this regime even moderate amounts of disorder can be expected to lead to substantial modifications, and thus must be carefully considered.

In order to incorporate the Anderson localization effects, in very recent work [52,50], we have extended the DMF formulation to finite coordination lattices. This formulation closely resembles the TAP [56,17] approach to spin glasses, where the interactions are treated in a mean-field approach for a fixed realization of disorder, but the order parameter is allowed to spatially fluctuate. In the DMF case, the role of the order parameter is played by the local cavity spectral function Δ_i. In analogy with the TAP equations, the DMF equations [52,50] relate the order parameter Δ_i on a given site to similar objects on the neighboring sites. Since the procedure is carried out at fixed disorder, it is exact in absence of interactions, and reduces to the standard DMF formulation in absence of disorder.

While in principle this formulation can be applied to any lattice in finite dimensions, the resulting equations assume the simplest form on a Bethe lattice. Here, the DMF equations take a form of recursion relations, relating the order parameters on neighboring sites. The noninteracting limit of this model has been examined many years ago by Abou-Chacra et al. [57], and shows an Anderson transition. In this limit, much progress can be made, since the recursion relations can be recast [57] as a nonlinear integral equation for a distribution function of the local density of states (LDOS). This equation can be solved analytically [58,59] in the vicinity of the transition, and the critical behavior of various quantities has been obtained.

In the interacting case, similar recursion relations have been derived [52,50], but assume a much more complicated form. Here, due to inelastic electron-electron scattering, the energy is not conserved, and one needs to consider a probability distribution for the full *function* $\Delta(\omega)$. Such an equation is not easy to solve analytically, but a solution can be obtained using a simulation approach, by numerically sampling the corresponding distribution function. We have applied this approach to a doped Mott insulator in Ref. [52], where a disorder driven MIT has been examined.

We have obtained several striking results, including:

- For strong disorder, a non-Fermi liquid (NFL) metallic phase has been identified preceding the actual MIT. This phase appears for disorder strength $W > W_{c1}$, at which point the distribution function $P(Z_i)$ becomes singular. As a result, singular thermodynamic response is found at low temperatures, for example $\gamma = C/T \to \infty$ as $T \to \infty$.

- At stronger disorder , a metal-insulator transition is found where both $\Delta_{typical}$ and $Z_{typical}$ vanish. This has been interpreted as the process where a *finite fraction* of sites become singly occupied, and thus turn into localized magnetic moments. Thus the transition has both a character of an Anderson and Mott transition, and also provides a clear microscopic justification for the two-fluid model [36].

- Evidence has been obtained suggesting that the transport properties have a strong doping dependence, and that at least two different universality classes for the MIT should exist.

- The critical behavior that we find is qualitatively different than in the noninteracting case, providing evidence for the key role of the correlation effects.

The described results have been obtained for a very specific model, motivated by the physics of doped Mott insulators. The approach can be easily generalized to other models and physical situations. However, even for the considered model, the obtained results can only be considered as firsts steps in the analysis of the metal-insulator transition. Still, even at the existing level, the result have already elucidated several puzzling features of doped semiconductors.

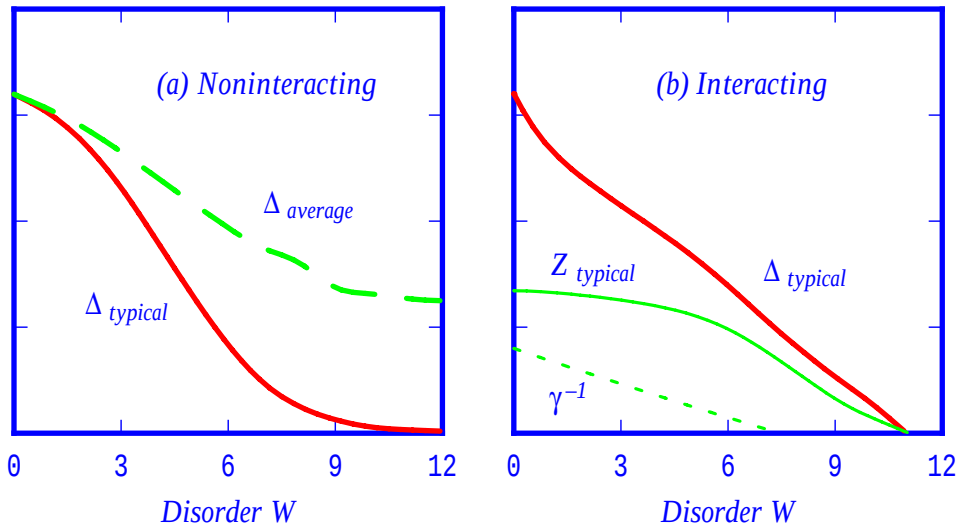

FIG. 5. Critical behavior at the Mott-Anderson transition at $T = 0$. Results taken from Ref. [ ] are shown for the typical and the average spectral function Δ, the typical quasiparticle weight Z, and the specific heat coefficient $\gamma = C/T$. In the noninteracting case (a), only $\Delta_{typical}$ is critical, and vanishes *exponentially* at the transition. In presence of interactions (b) all quantities show simple *linear* critical behavior.

1. Conductivity in the critical regime

A clear difference between a metal and an insulator exists only at zero temperature. In fact, the transition point is most easily identified by measuring the DC conductivity at low temperatures, which typically shows an abrupt change of behavior in a narrow parameter range. On the other hand, the solution of the DMF equations does not directly provide predictions for the behavior of the conductivity. Instead, it defines local order parameters that can be self-consistently determined and may be used to differentiate the metal from the insulator.

In particular, the *typical* local spectral density Δ_{typ} was shown to vanish as the transition is approached from the metallic side. This quantity does provide [50] information about the transport properties, since it is proportional to a typical transition rate of an electron to a neighboring site. Furthermore, at least for the noninteracting electrons near an Anderson transition on a Bethe lattice, it was shown [58,59] to have the same critical behavior as the conductivity. Still, in order to allow direct comparisons with experiments, an explicit calculation of the DC conductivity needs to be performed.

In order to investigate the critical behavior of the conductivity near a Mott-Anderson transition, we will focus on disordered Hubbard models, and solve the DMF equations using a simulation approach, following Ref. [52]. The conductivity will be computed using two different methods:

- A direct evaluation will be carried out by calculating the density-density correlation function, and extracting from it the diffusion constant, following the approach of Ref. [58,59]. The conductivity will then be obtained from the Einstein relation $\sigma = (dn/d\mu)D$.
- A simpler expression for the conductivity will be obtained near the MIT, where it can be related to local spectral function, as in Ref. [61].

Of particular interest is the dependence of this critical behavior on the doping (compensation) level. On general grounds [3], one expects the effects of the electronic correlations to be the strongest near half-filling (one electron per site). In that case, the on-site repulsion can lead to strong suppression of density fluctuations, resulting in large effective mass enhancements near the Mott transition. If the average occupation is lower, the electrons can more easily "avoid each other", and the correlation enhancements are reduced. This reasoning immediately suggests that the critical behavior of transport quantities should be very sensitive to the doping level. So far only the behavior of $\Delta_{typical}$ has been investigated as a function of doping. Preliminary theoretical results [50] do demonstrate that at least two universality classes can be expected, but explicit calculations of the conductivity need to be performed before this question is settled.

Experimentally, the question of the doping dependence of transport has been examined by investigating the effects of compensation in doped semiconductors [7]. In the uncompensated case (one electron per site), the conductivity exponent μ was found to be close to $\mu = 1/2$, but was shown to reduce to $\mu = 1$ upon compensation (less than one electron per site). An interesting open question is whether *a finite* or an infinitesimal amount of compensation is needed to modify the critical behavior. Within the DMF theory, a finite fraction of sites acquire local magnetic moments at the MIT. This fact would suggest that the change of critical behavior occurs at a finite critical compensation, perhaps at the point where these "Mott droplets" stop percolating. Interestingly, this idea seems to find preliminary support in very recent experimental work [62].

2. Exact DMF critical behavior

In contrast to the noninteracting limit, the DMF equations are not easy to solve analytically even on Bethe lattices. For this reason, the existing results [52,50] have been obtained by sampling the desired distribution functions using a simulation approach. This approach has been able to reproduce the known analytical results [58,59] for the Anderson transition of noninteracting electrons on a Bethe lattice. Here, the $\Delta_{typical}$ (as well as the conductivity) is known to depend *exponentially* on the distance to the transition. Near the transition, the conductivity therefore assumes exponentially small, yet finite values, in an appreciable range of disorder. This unusual behavior is believed to reflect anomalously large spatial fluctuations of the order parameter in the critical region, presumably reflecting the possibility that the upper critical dimensions for Anderson localization may be infinite [63]. As a result, the analytical solution of this problem assumes an extremely complex [58,59] form that took years to unravel. From the numerical point of view, the fact that the order parameter is exponentially small in the critical region makes it very difficult to obtain reliable results or even deduce the precise critical value of disorder. This behavior is illustrated in Figure 5 (a) where numerical results for $\Delta_{typical}$ as a function of disorder are plotted for noninteracting electrons on a Bethe lattice.

Results in the interacting case have also been obtained, by examining the example of a doped Mott insulator in presence of disorder. Figure 5 (b) shows the behavior of the order parameters as a function of disorder strength W. Somewhat surprisingly, in the interacting case the behavior is *simpler*, and all the order parameters behave in a mean-field-like *linear* fashion as the transition is approached. This fact is not only striking from a general point of view, but also tremendously simplifies the numerical solution, leading for example to a clearly defined critical value of disorder. It is worth recalling that for most models in statistical mechanics, the solution on the Bethe lattice assumes a simple, mean-field form. This reflects an effective infinite dimensionality of the Bethe lattice, which thus exceeds the upper critical dimensions for the problems in question. Accordingly, the following possibilities becomes apparent:

- The simple linear behavior of the order parameters may reflect the possibility that the upper critical dimensionality is *finite* in the interacting case. Similar suggestions have emerged from recent field-theoretical studies [43] based on the non-linear sigma model approaches.

- If this is true, then a simple *analytical* solution of the DMF equations must exist for the critical region. Similar ideas have been the basis for the "projective self-consistent" methods [46] used to analyze the critical behavior near the Mott transition in the DMF formulation. In the case of the Mott-Anderson transition the entire distribution functions play the role of the order parameters. However, these

distribution functions may be possible to *parameterize* in a simple fashion, resulting in simple *algebraic* equations for the appropriate parameters.

In order to examine these possibilities, we will first use the existing simulation approaches to obtain detailed information about the behavior of the entire probability distributions near the transition. Such results are not available at present, since only the simplest features of the transition have been studied so far. Simple parametrization schemes will then be attempted, and compared with the numerical data. For example, preliminary work suggested that the distribution function $P(\Delta_i)$ can be well represented by a log-normal distribution, which can be parameterized by its average and the typical value, both showing simple linear critical behavior. The desired analytical solution for the DMF critical behavior would offer a tremendous conceptual and practical advantage in examining the details of the MIT. This would represent the equivalent of a Van der Waals equation of state for this problem. Note that although similar attempts have been presented in earlier work [43], these theories could not explicitly incorporate the Anderson localization effects, nor the possibility for a clean Mott transition, both of which are included in the present formulation.

C. Disorder-induced non-Fermi liquid behavior

One of the main characteristics of strongly correlated systems is a dramatic reduction of the "coherence temperature" T^* below which the Fermi liquid description applies. This behavior is well documented in many clean systems such as heavy fermion materials and transition metal oxides. In other materials containing disorder, recent work [31] has suggested that T^* may be vanishingly small, resulting in anomalous temperature dependences of most physical properties.

A consistent description of such situations has emerged from the DMF formulation [41,55], and has met considerable success explaining a number of experiments. In particular, we have identified such non-Fermi liquid (NFL) metallic behavior near the Mott-Anderson transition [52,50], as shown in Fig. 5 (b). Here, the $T = 0$ specific heat coefficient $\gamma = C/T$, was found to diverge at a critical value for disorder $W = W_{c1}$, much before the MIT (at $W = W_{c2} > W_{c1}$) is reached. We have obtained similar results for disordered Anderson lattice models [55], where the corresponding critical disorder strength was again identified. It is interesting that for $W \to W_{c1}$, γ diverges in a simple linear fashion (γ^{-1} vanishes linearly), whereas the transport behavior (at least Δ_{typ}) seems noncritical [52,50]. However, just as for the critical behavior near the MIT, the existing evidence for this transition to the NFL metallic phase is limited to results of numerical simulations [52,50]. Several basic questions that will be examined in this context will inculude the following:

- The transition to the metallic NFL behavior occurs when the distribution function for local quasiparticle weights $P(Z_i)$ becomes singular, viz. $P(Z_i) \to \infty$ at $Z_i \to 0$. Precisely how this happens near $W = W_{c1}$ will be explicitly examined, and the precise critical behavior will be determined. In particular, a central issue is whether only the form of the *tail* of this distribution becomes sufficiently long, as in usual quantum Griffiths phases [64], or an actual phase transition happens, where the entire distribution is affected. The latter possibility would be analogous to an Anderson transition [2], where the entire $P(\Delta_i)$ collapses. This issue is of crucial importance, since it is not clear whether two different metallic *phases* can exist. As for the MIT behavior, the observed linear behavior of γ near $W = W_{c1}$ offers hope that a simple analytical description of this transition may be possible. As for the critical behavior near the MIT, we will search for such a solution, by examining various parametrization schemes for the relevant distribution functions.

- The temperature dependence of the transport properties such as the conductivity will be investigated in the metallic NFL regime. This question has attracted considerable recent interest, since according to the phenomenological "two-fluid" model [36] of doped semiconductors, thermodynamics may be singular, and dominated by disorder-induced local moments. At the same time, transport may be unaffected, or very weakly affected, since the conduction electrons may find routes that avoid these local moments. This conjecture finds some support in recent experiments [8], but remains to be elucidated theoretically. In contrast, experiments in Kondo alloys [31] seem to suggest that *both* thermodynamic and transport properties [41] can be modified in the NFL regime. These discrepancies

may reflect the differences between the respective physical systems. In particular, the local moments in question are believed to be dynamically generated near a Mott-Anderson transition ("disorder-induced local moment formation" [37,40]), but are pre-formed in Kondo alloys. As a result the degree of local moment - conduction electron coupling may be very different in the two systems. To elucidate this point, comparative studies of disordered Hubbard and Anderson lattice models will be carried out.

D. High temperature anomalies

In recent work, experimental evidence has been obtained on the transport properties of a number of strongly correlated systems near a metal-insulator transition [7–10,34,35,11–13]. While the detailed behavior at the lowest temperatures may depend on the particularities of a given system, new features emerge if one considers a broader temperature interval, comparable to the *Fermi* energy. Here striking similarities are discovered between systems as different as doped semiconductors [7], doped Kondo insulators [10], underdoped cuprates [35], transition metal oxides [34] and even two-dimensional electron gases in zero magnetic field [11–13]. Very roughly, the situation is illustrated in Figure 1 (b), where a change in slope of the temperature dependence of the resistivity is seen. Similar behavior has been observed many years ago in the so-called A15 compounds [32], and is often referred to as the "Mooij correlation" [65,3].

From the theoretical point of view, this behavior has proved to be a long-standing challenge. In fact, it has long been appreciated that such breakdown of the Mathiessen's rule [3] cannot be obtained using standard Boltzmann equation approaches [6]. Instead, this behavior is believed [3,61] to reflect the interplay of Anderson localization and interaction effects. While there have been some early attempts [61] to address this question, not much progress has been made, principally due to difficulties in describing inelastic scattering processes in a broader temperature range.

We have already emphasized that one of the main advantages of the DMF approach [46,50] is the fact that it is not restricted to low-temperature, coherent regimes. Since it can also incorporate the Anderson localization effects [52,55], this approach is practically the only reliable avenue for addressing these high temperature anomalies. On the other hand, much of the work [52,50,41,55] using the DMF approach for disordered interacting electrons has been restricted to $T = 0$, where slave-boson methods [52,41,55] have been used to solve the local impurity problem.

In order to investigate this high temperature regime, a new set of tools will be developed in order to solve the DMF equations. In applications to disordered electronic systems, numerically exact methods [46], such as the quantum Monte Carlo, or exact diagonalization approaches are not efficient enough, since an entire *ensemble* [40,52] of Anderson impurity models needs to be considered. Instead, calculations will be performed at finite temperature using iterated perturbation theory (IPT) [46] and non-crossing approximation (NCA) [66] approaches. Numerical codes for the implementation of these approaches are readily available at present, and will readily be adapted to the disordered situation.

Alternatively, recent work on clean systems [67] has revealed that excellent *analytical* approximations for the DMF equations can be formulated for the high temperature behavior. This approach will be used to examine the leading high temperature dependence of the resistivity in the transition region, which may be sufficient to explain many experimental features.

E. Glassy behavior and the metal-insulator transition

Glassy behavior is often associated with the competition between strong interactions and disorder, and is well known in systems such as spin glasses [17]. In the context of disordered electronic systems [3], the role of glassy freezing is most obvious in the insulating limit. Here, the electrons tend to populate the lowest potential wells, but at the same time must keep apart from each other - as dictated by the Coulomb repulsion. Many such low energy configurations are possible, resulting in an extensive number of metastable states characteristic of glassy systems. The fact that this interaction-induced rearrangement of electrons can directly influence transport has first been pointed out by Efros and Shklovskii [68]. According to this theory, the Coulomb interactions lead to a depletion of energy states from the vicinity of the Fermi level, and the

formation of a soft "Coulomb gap". As a result the hopping law is modified at the lowest temperatures, as confirmed by a large number experimental studies [3].

Most theoretical studies of this "electron glass" have been restricted to classical models [18], which are most relevant deep in the insulating regime. More recently, complementary field-theoretical [43] studies have suggested that glassy freezing [45] may be crucial even in the critical regime of the metal-insulator transition, but so far no consistent microscopic scheme has been presented that could address this question.

Within the DMF approach [46,50], most efforts so far have focussed on Hubbard models with on-site repulsion only. In order to incorporate glassy phenomena, it is necessary to extend the DMF formulation and incorporate the nonlocal electron-electron interaction V_{ij} between pairs of sites. Since the physics of the electron glass reflects the existence of many competing rearrangements of the electronic *charge* density, the simplest nontrivial model that can display such phenomena considers *spinless* interacting electrons in presence of random site energies ε_i, as given by the Hamiltonian

$$H = \sum_{<ij>} (-t_{ij} + \varepsilon_i \delta_{ij}) c_i^\dagger c_j + \sum_{<ij>} V_{ij} c_i^\dagger c_i c_j^\dagger c_j \,. \tag{1}$$

In the classical ($t_{ij} = 0$) limit, and for $V_{ij} = e^2/r_{ij}$, this is nothing but the model considered by Efros and Shklovskii [68]. Here, many aspects have been elucidated, but the attempts to incorporate quantum effects have largely been limited to first principal numerical approaches [18].

In preliminary (unpublished) work [69] we have been able to formulate an extended DMF approach to this model, which is very similar to the well-known mean-field theories for spin glasses [17], as well as our previous approaches to disordered Hubbard models [40,52,50]. As in other DMF theories, one can derive a local effective action for this problem that in the standard Grassmannian-replica formulation [40] takes the form [69]

$$S_{eff}(i) = \sum_a \int_o^\beta \int_o^\beta d\tau d\tau' \, [c_i^{\dagger a}(\tau)(\delta(\tau-\tau')\partial_\tau + \varepsilon_i + t^2 G(\tau,\tau'))c_i^a(\tau')$$
$$+ \frac{1}{2} V^2 \delta n_i^a(\tau) \chi(\tau,\tau') \delta n_i^a(\tau')] + \frac{1}{2} V^2 \sum_{a \neq b} \int_o^\beta \int_o^\beta d\tau d\tau' \, \delta n_i^a(\tau) \, q_{ab} \, \delta n_i^b(\tau'). \tag{2}$$

This result is formally exact in an appropriate large coordination limit [40], where nearest-neighbor interactions V_{ij} have been rescaled as $V_{ij} \to V_{ij}/\sqrt{z}$. Here, the local single-particle Green's function $G(\tau,\tau')$, the Edwards-Anderson order parameter q_{ab} and the local density-density correlation function $\chi(\tau,\tau')$ are determined by appropriate self-consistency conditions.

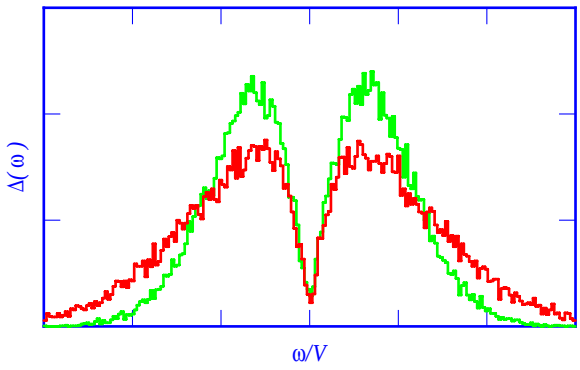

FIG. 6. Average single particle spectral function $\Delta(\omega) = -ImG(\omega)$ in the classical ($t = 0$) limit at $T = 0$, as a function of disorder strength W. Results are shown for $W/V = 0.5$ and $W/V = 1.0$. The gap size remains almost independent of the disorder strength. Similar results have been obtained [71] by numerical simulations for long-range Coulomb interactions in $d = 3$.

In this formulation, a number of nontrivial results can be obtained by analytical and modest numerical calculations. In particular, interesting behavior is found even in the classical ($t_{ij} = 0$) limit, where the model maps to the familiar random-field Ising model [44,73]. Here, a finite glass transition temperature can be identified by carrying out a replica-symmetry-breaking [17,70] stability analysis. As a result of such glassy freezing, a soft gap in the single-particle spectral function emerges, reminiscent of the "Coulomb gap" of Efros and Shklovskii [68] ; preliminary results showing this behavior are presented in Figure 6. It is remarkable that several features of this model show striking similarities to those obtained for more realistic Coulomb interactions in three dimensions [71]. In particular, the low energy form of the gap shows a universal from that seems independent of disordered strength. Furthermore, the presence of a static, but non-uniform electronic density in the glass phase results in an enhancement of the *effective disorder* seen by the electrons. In this way, glassy freezing can strongly enhance the electron localization processes.

The preliminary results that we have obtained using the DMF formulation of the electron glass demonstrate that this approach can be effectively used to investigate many nontrivial consequences of the non-local Coulomb interactions. In a sense, one may think of the considered large coordination limit as a way to mimic the long range form of the more realistic Coulomb interactions. In this context, a number of key questions will be examined, as follows

- Effects of quantum fluctuations induced by finite electron tunneling t_{ij} will be investigated. Preliminary results [69] have already shown that sufficiently large tunneling can result in melting of this electron glass, even at $T = 0$, but the details of the corresponding quantum critical behavior need to be determined. For this regime, techniques similar to those used in other quantum spin glass problems [72] may be useful, and will be adapted to the electronic case.

- The simplest DMF formulation of the electron glass problem focuses on the large coordination limit. Here, the Anderson localization effects are absent [40], so the $T = 0$ glass transition does not represent a realistic description of the MIT. This difficulty can be overcome by following the approaches previously used in examining the Mott-Anderson transition [52,50,55]. To do this, the DMF formulation will be extended to models on finite coordination lattices, where the interplay of Anderson localization and the glass transition will be examined.

- Our studies will be extended to models with spin. This will be done by examining disordered Hubbard models with both the on-site interactions U and the inter-site interaction V_{ij}. The former can lead to formation of localized magnetic moments in the insulating regime and the large effective mass renormalizations in the metal, while the latter can induce the glassy freezing of electrons. The nontrivial interplay of all these effects will be examined, giving a new nonperturbative picture of the MIT.

VIII. CONCLUSIONS

Recent years have witnessed enormous renewed interest in the metal-insulator transition. Scores of new and fascinating materials are being fabricated, with properties that could not be anticipated. A common theme in many of these systems is the presence of both strong electron-electron interactions and disorder, a situation which proved difficult to analyze using conventional theoretical methods. In this proposal, we have described a novel approach to this difficult problem, and shown that it can capture most relevant processes. This formulation can easily be adapted to many realistic situations and will open new avenues for the development of materials science research.

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