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Strong correlations and disorder in $d = \infty$ and beyond

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The behavior of strongly correlated electrons in disordered systems is investigated using a functional integral formulation of the problem. In the mean-field approximation, which becomes exact in the limit of large spatial dimensionality, the problem reduces to the solution of an *ensemble* of self-consistently determined Anderson impurity models. The methods are applied to different classes of disorder, and the possible phases of the system are analyzed. We present results for the behavior of the thermodynamic and transport properties near the metal-insulator transitions for each case considered. When strong hopping disorder is present, disorder-induced local-moment formation is found, leading to qualitative modifications of metallic phases even away from the transition. Finally, we indicate how our approach can be systematically extended beyond the mean-field limit, where the presence of *spatial* fluctuations makes it possible to address the problem of Anderson localization in strongly correlated electronic systems.

I. INTRODUCTION

After more than 30 years[1] of intense research, a comprehensive description of disordered interacting electrons still remains elusive. Much of the current knowledge about the problem relies on numerous investigations, both experimental and theoretical, of the weakly disordered limit[2] where satisfactory understanding is achieved. In such systems, both the disorder and the interactions can typically be treated in a perturbative fashion, and the behavior can be described using a generalized Fermi-liquid phenomenology.[3]

For stronger disorder, the situation becomes more complicated. As the disorder increases, the Anderson localization effects[2] gradually lead to the breakdown of the metallic phase, and eventually the metal-to-insulator transition (MIT) takes place. In order to understand these disorder-induced transitions, scaling theories of localization were developed.[4–6] Here the MIT is viewed as a critical point where the physics is dominated by long-wavelength (hydrodynamic) fluctuations. The approach was extended to interacting electrons by Finkelshtein,[7] who constructed a long-wavelength effective Lagrangian for the relevant degrees of freedom and used renormalization-group (RG) methods in $2+\varepsilon$ dimensions to analyze the critical point. This theory, based on Fermi-liquid ideas,[3] offered a consistent scenario for the MIT in systems where spin is not conserved (e.g., in the presence of external magnetic fields or magnetic impurities). In the situation when the spin *is* conserved, the RG flows take the system to the regime of strong correlations but weak disorder, and the *perturbative* solution near two dimensions breaks down. It has been suggested that this signals some magnetic instability,[7] or that it indicates a continuous Fermi-liquid-to-insulator transition with a divergent specific heat coefficient, but with a discontinuous jump in the conductivity.[8] Other interpretations have also been proposed.[9]

More recently, increasing experimental[10] and theoretical[11,12] evidence has been pointing to the limitations of the Fermi-liquid picture of disordered metals near the MIT. Numerous experiments with doped semiconductors,[10] carried out down to mK temperatures, showed seemingly diverging magnetic susceptibilities and specific-heat coefficients even on the metallic side of the transition. To account for these findings, disorder-induced local-moment formation[13] has been advocated, and a two-fluid description[14] of the low-energy excitation proposed. These local moments are viewed to exist on short-distance scales, and as such were ignored in the derivation of the effective long-wavelength theories of Finkelshtein.

Another route to the metal-insulator transition follows from the presence of strong electronic correlations even in the absence of disorder. This phenomenon, known as the Mott transition,[15] takes place when the kinetic energy gained by delocalization becomes insufficient to compensate for the potential energy cost of charge-density fluctuations. The transition can also be described as the point at which low-lying excitations transform themselves from quasiparticles to spins—all the electrons become local moments. Historically, this mechanism for localization was put forward as one of the first explanations for the MIT in uncompensated doped semiconductors.[15] The experimental values of the critical concentration where the transition occurs are indeed consistent with simple estimates by Mott which ignored the disorder. Still, as the MIT is approached by reducing the dopant concentration, *both* the correlation's strength *and* the amount of disorder are increased—making it difficult to assess which effect is the dominant one.

All the above facts suggest that a proper treatment of strong electronic correlations in disordered systems could very well be a central piece in the puzzle of dirty metals. In this paper we present an approach to the problem, which builds nonperturbative strong correlation effects as

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a starting point. We identify a class of models that can be solved exactly in the limit of large spatial dimensions,[16] where a mapping onto impurity models greatly facilitates the theoretical analysis.[17] In the large-d limit, the disordered problem reduces to self-consistently solving an *ensemble* of Anderson impurity models. The method provides an intuitively appealing *local* picture of the interplay of strong correlations and disorder, and thus represents a natural language for the study of phenomena such as disorder-induced local-moment formation or the disorder-modified Mott transition.

In the rest of the paper, we begin by presenting a detailed description of our formalism, and the derivation of the self-consistency conditions in the $d\rightarrow\infty$ limit. We discuss various directions in which the method can be used to obtain systematic corrections to this mean-field limit. We stress the technical advantage of dealing with the spatially disordered situation, and the possibility of carrying a controlled *loop expansion*.[18] Many aspects of disorder-interacting electrons could be studied in this framework, but in this paper we restrict our attention to the following two basic physical questions: (1) What is the behavior of thermodynamic and transport properties in the vicinity of the MIT? (2) Can the interplay of strong correlations and disorder lead to *qualitative* modifications of metallic phases?

In the exactly solvable $d=\infty$ limit, we have been able to answer these questions. The results are presented for several models of disorder and types of transitions. We discuss the general successes and limitation of the mean-field picture, and compare our findings with experimental results for doped semiconductors. Finally, we indicate various possible extensions of our theory, and comment on the most promising directions for future work. A short report on this work has been presented earlier.[19] We mention that a related study of disordered interacting electrons, based on the $d=\infty$ limit, has been carried out independently in Ref. 20. However, the authors addressed questions other than those studied in the present work. Also, that approach was restricted to $d=\infty$, and did not indicate how systematic corrections to mean-field theory could be obtained.

II. PURE HUBBARD MODELS

The main object of this paper is to study the effects of disorder on strongly correlated metals. To put the problem in perspective and to set up the methodology, we briefly review the results obtained with the mean-field method in the pure limit, following Refs. 21–23.

The mean-field approach based on taking the limit of large spatial dimensionality represents a general method for the study of many-body systems.[17,24] The basic idea, which goes back to the early work of Bragg and Williams,[25] is to focus on a given lattice site and construct an effective theory for *local* properties. In this language, the local site is viewed as embedded in an effective field, the *cavity field*.[26] When the given site has *many neighbors,* i.e., large coordination (large spatial dimensionality), the *spatial* fluctuations of the cavity field are suppressed, and its value is determined self-consistently. The general formulation closely parallels the standard mean-field theory of (for example) classical Ising models of magnetism. In contrast, when the approach is applied to quantum fermionic problems, an additional feature emerges—the cavity field acquires nontrivial *time dependence,* allowing a nonperturbative treatment of *local dynamics,* which proves to be of crucial importance for strongly correlated electrons. In particular, the approach incorporates *incoherent* (inelastic) processes even on this mean-field level, as opposed to most other treatments. As a result, the formulation can be used even in the study of *non-Fermi-liquid* metallic phases, for example in extended Hubbard models.[27] In the following, we limit our attention to simple Hubbard models of correlated electrons; the generalization to more complicated models is straightforward.[24]

The phase diagram of the pure Hubbard model on a Bethe lattice at half-filling has a Néel phase at low temperatures, and a paramagnetic phase at high temperatures. However, the value of the Néel temperature can be made arbitrarily low by increasing the frustration, a situation which is even more relevant to disordered systems like Si:P, which do not order magnetically down to mK temperatures[10] due to a wide distribution of random antiferromagnetic exchanges. In this case, a Mott transition was found.[21–23] The phase diagram of the fully frustrated Hubbard model,[22] which remains paramagnetic at all temperatures, is schematically shown in Fig. 1.

The two possible paramagnetic phases of the Hubbard model are separated by a first-order boundary which terminates in two second-order points. One is at finite temperatures, which has a character of a liquid-gas transition, while the other is a zero-temperature critical point

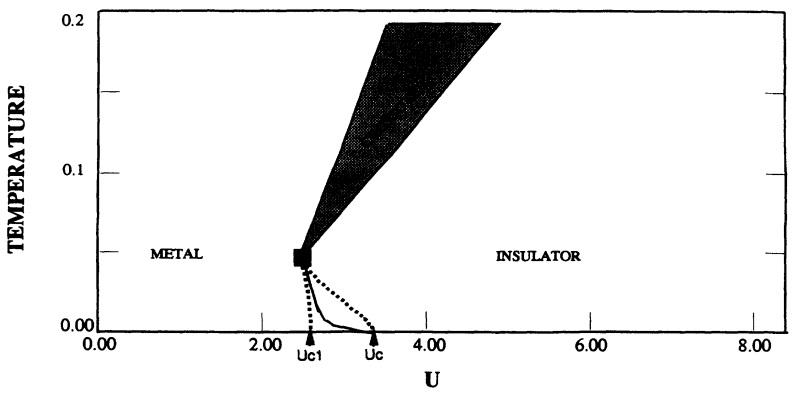

FIG. 1. Phase diagram of the pure Hubbard model in $d=\infty$ (following Ref. 22), as a function of correlation strength U and temperature T. The finite temperature first-order metal-to-insulator transition is shown by a full line, and the boundaries of the coexistence region by dashed lines. At $T=0$ the metallic solution is lower in energy throughout the coexistence region, and so $U=U_c$ represents the zero-temperature transition point.

at $U=U_c$ reminiscent of the Brinkman-Rice scenario, as extensively discussed in Ref. 22. For the purpose of our discussion, we will concentrate on the behavior near U_c, which will be the metal-insulator transition in a disordered system. On general grounds,[28] in the presence of disorder we expect the first-order line found at finite temperatures to be suppressed, but the zero-temperature critical point at U_c to remain.

From the technical point of view, the central tool that we shall use is the mapping of a lattice problem onto an Anderson impurity model, which allows us to study the *local* physics with a mean-field-like approach.[17] For example, all the local correlation functions of the Hubbard model on a Bethe lattice can be calculated from an impurity action of the general form

$$S_{\rm imp}[G_0]=\int c_\sigma^\dagger G_0^{-1} c_\sigma + U\int n_\uparrow n_\downarrow \ , \tag{1}$$

provided that G_0 obeys the self-consistency condition

$$G_0^{-1}=i\omega_n+\mu-t^2\langle c^\dagger c\rangle_{\{G_0\}} \ . \tag{2}$$

The Hamiltonian version of the action of Eq. (2) is an Anderson impurity model;[29] in the following, we will show that in a random medium this statement can be generalized to map the local physics of a random Hubbard model onto a *collection* of Anderson impurity problems.

III. DISORDER IN $d=\infty$

As we have seen, the main idea of the $d=\infty$ approach is to obtain a local description of the problem. This is accomplished by formally integrating out all the degrees of freedom outside the site considered. The procedure can in principle be performed in general dimensions, but then the resulting contribution to the local effective action—the cavity field—takes an arbitrarily complicated form. In the presence of disorder the situation is even more complex: the cavity field varies from site to site, reflecting the random environments in which a given site is embedded.

The problem again simplifies when the number of neighbors is large, in which case the cavity fields become *self-averaging,* i.e., independent of the disorder, and only *local* disorder fluctuations survive. The theory thus assumes a mean-field character, in the sense that the *spatial* fluctuations (but not the temporal ones) are ignored, and as a consequence, phenomena such as Anderson localization will be absent in the strict $d=\infty$ limit. Nevertheless, even at the $d=\infty$ level, the approach is sufficiently flexible to allow for a detailed study of numerous questions relevant to the interplay of strong correlations and (local) disorder.

The derivation of mean-field equations for disordered interacting electrons in $d=\infty$ can be carried out systematically for any special type of disorder or lattice form.[30] However, there are two general classes of models, for which the formulation can be implemented in a particularly elegant fashion, which also allow for controlled extensions *away* from the $d=\infty$ limit. In this paper, we will limit our attention to classes of models in question, since in other cases the modifications lead to technical complications, but the physical behavior remains *qualitatively* unchanged.

In the most general case, the Hamiltonian of a disordered Hubbard model takes the form

$$H=\sum_{ij}\sum_{\sigma}[-t_{ij}+\varepsilon_i\delta_{ij}]c_{i,\sigma}^\dagger c_{j,\sigma}+U\sum_i c_{i,\uparrow}^\dagger c_{i,\uparrow}c_{i,\downarrow}^\dagger c_{i,\downarrow} \ . \tag{3}$$

Using a functional integral representation for quantum averages, and the replica method for disorder averaging, the (replicated) partition function of the model can be written[7] as

$$\bar{Z}^n=\int D\varepsilon_i P_S[\varepsilon_i]Dt_{ij}P_H[t_{ij}]\int D\bar{c}_i Dc_i \exp\{-S\} \ , \tag{4}$$

with the action $S=S_{\rm loc}+S_{\rm hop}$ consisting of a local part (that includes the Hubbard interaction)

$$\begin{aligned} S_{\rm loc}&=\sum_i S_{\rm loc}(i) \\ &=\sum_i\left[\sum_{\alpha,s}\int_0^\beta d\tau\,\bar{c}_{s,i}^\alpha[\partial_\tau+\varepsilon_i-\mu]c_{s,i}^\alpha \right. \\ &\qquad \left. +U\sum_\alpha\int_0^\beta d\tau\,\bar{c}_{\uparrow,i}^\alpha c_{\uparrow,i}^\alpha \bar{c}_{\downarrow,i}^\alpha c_{\downarrow,i}^\alpha\right] \ , \end{aligned} \tag{5}$$

and a hopping part

$$\begin{aligned} S_{\rm hop}&=\sum_{\langle ij\rangle} S_{\rm hop}(i,j) \\ &=\sum_{\langle ij\rangle}\left[-t_{ij}\sum_{\alpha,s}\int_0^\beta d\tau[\bar{c}_{s,i}^\alpha c_{s,j}^\alpha+{\rm H.c.}]\right] \ . \end{aligned} \tag{6}$$

Here, $\bar{c}_{s,i}^\alpha$ and $c_{s,i}^\alpha$ are the electronic (Grassmann) fields with spin $s=\uparrow,\downarrow$, replica index $\alpha=1,\ldots,n$ at lattice site i, and β is the inverse temperature. The random site energies ε_i are described by their probability distribution $P_S[\varepsilon_i]$, and the random hopping elements t_{ij} by the corresponding distribution $P_H[t_{ij}]$.

A. Disordered Bethe lattices and the $1/d$ expansion

The first class of models that we consider consists of Hubbard models with *arbitrary* disorder, but restricted to Bethe lattices. In this case, the problem can be reduced to a certain integral equation, even for a finite coordination number, which is convenient for performing extensions away from infinite dimensionality. Furthermore, the Bethe lattice has a bounded density of states even in the $d\to\infty$ limit, a feature that is convenient in the study of the Mott transition.

1. *Integral equation*

To derive the integral equation, we concentrate on a particular site, and perform a partial trace (in the replicated partition function) over all the sites in the $m=z-1$ (z is the coordination number, m the "branching ratio") branches (all but one) that come out of the given site. Because all sites of a Bethe lattice are only singly connected, the result of this partial trace will be a

functional *only* of the fields living on this site (call it the ith site). If we denote this functional by $\Xi[i]$, it is not difficult to see that the functional satisfies the following integral equation:

$$\Xi[i]=\left[\int D\bar{c}_j Dc_j D\varepsilon_j P_S(\varepsilon_j) Dt_{ij} P_H(t_{ij}) \times \exp\{-S_{\rm hop}(i,j)-S_{\rm loc}(j)\}\Xi[j]\right]^m . \quad (7)$$

In the noninteracting limit, static disorder conserves energy, so that different frequencies decouple and Eq. (7) reduces to an ordinary integral equation; a similar equation was a basis of studies of localization on Bethe lattices[31] giving an Anderson transition. When interactions are present, there is frequency mixing, and we have to solve a *functional* integral equation. This is difficult, but the problem simplifies in the large-m limit.

2. $d\to\infty$ limit

To obtain meaningful results in this limit, an appropriate scaling of the hopping elements[16] has to be performed, and we replace $t_{ij}\to t_{ij}/\sqrt{m}$. In order to let $d\to\infty$ (i.e., $m\to\infty$), we take the logarithm of Eq. (7) and expand in powers of $S_{\rm hop}\sim 1/\sqrt{m}$. To leading order in $\sqrt{m}$, the *local effective action* $S_{\rm eff}(i)=S_{\rm loc}(i)-\ln\Xi(i)$ takes the form

$$S_{\rm eff}(i)=\sum_s \int_0^\beta d\tau \int_0^\beta d\tau'\, \bar{c}_{i,s}(\tau)[\delta(\tau-\tau')(\partial_\tau+\varepsilon_i-\mu)+W_{i,s}(\tau,\tau')]c_{i,s}(\tau')+U\int_0^\beta d\tau\, \bar{c}_{i,\uparrow}(\tau)c_{i,\uparrow}(\tau)\bar{c}_{i,\downarrow}(\tau)c_{i,\downarrow}(\tau) . \quad (8)$$

The self-consistency condition determining the "Weiss" (cavity) field is obtained by expanding the integral equation (7), giving

$$W_{i,s}(\omega_n)=\int d\varepsilon_j P_S(\varepsilon_j)\int dt_{ij} P_H(t_{ij}) t_{ij}^2 G_{j,s}(\omega_n) = \overline{t_{ij}^2 G_{j,s}(\omega_n)} , \quad (9)$$

where

$$G_{j,s}(\omega_n)=\langle \bar{c}_{j,s}(\omega_n)c_{j,s}(\omega_n)\rangle_{S_{\rm eff}(j)} \quad (10)$$

are the local Green's functions evaluated with respect to the *single-site* effective action of Eq. (8). In deriving Eq. (8), we have restricted our attention to nonsuperconducting phases ($\langle \bar{c}_s \bar{c}_{-s}\rangle=0$), so that $W_{i,s}$ does not have anomalous components. We have also used the fact that, due to spin conservation, $\langle \bar{c}_s c_{s'}\rangle\sim\delta_{s,s'}$ as well as that for $\alpha\neq\alpha'$, $\langle \bar{c}^\alpha c^{\alpha'}\rangle=\langle\bar{c}\rangle\langle c\rangle=0$ (particle conservation). The replicas decouple at $m=\infty$, reflecting the absence of Anderson localization, and we can let $n\to 0$, eliminating the replicas in the rest of the calculation.

We note that the local effective action of Eq. (7) is identical to the action of an Anderson impurity model[29] with a given hybridization function $\Delta(\omega_n)\sim W(\omega_n)$. We see that, even for disordered systems, the solution of a Hubbard model in infinite dimensions can be reduced to solving an *ensemble* of Anderson impurity models with an additional self-consistency condition that includes disorder averaging. Once the local effective action is self-consistently determined, it is possible to compute all correlation functions of the Hubbard model from the corresponding (local) correlation functions of the Anderson model. Because the solution defines an ensemble of local impurity problems, it determines the *probability distributions* for local quantities (e.g., the local Kondo temperatures) that fluctuate from site to site in a disordered system.

3. 1/d expansion

The self-consistent equations presented are exact on the Bethe lattice with an infinite branching ratio. However, the integral equation (7), which is exact for *any* m can be used to generate an expansion in $1/m$, which brings in spatial fluctuations to the cavity field $W(i)=-\ln\Xi[i]$. The expansion generates higher-order terms to the effective action, which take the general form

$$S_{\rm eff}^{(n)}\sim\int \Gamma^{(n)}(1,\ldots,n)\bar{c}(1)\ldots c(n) , \quad (11)$$

where the vertex functions $\Gamma^{(n)}(1,\ldots,n)$ obey self-consistency conditions of the form

$$\Gamma^{(n)}(1,\ldots,n)\sim\langle\bar{c}(1)\ldots c(n)\rangle_{S_{\rm eff}} . \quad (12)$$

The above infinite set of coupled equations is exact for any m, and in fact is just a way to rewrite a functional integral equation (7). However, it is not hard to see that $\Gamma^{(n)}(1,\ldots,n)\sim 1/m^{(n-2)/2}$, so that at *large but finite* m one can obtain a self-consistent $1/m$ expansion by truncating the expansion of the effective action at a desired level. The first nontrivial term in this expansion generates $S_{\rm eff}^{(4)}\sim\Gamma^{(4)}$, which is a connected vertex function of four arguments that has a very transparent physical interpretation. That is, at $m=\infty$ the Hubbard model is mapped to an Anderson impurity problem in a self-consistently determined electronic band, but the on-site interaction U remains *unrenormalized*. At next to leading order, the presence of $S_{\rm eff}^{(4)}$ in the effective action indicates that the first effect of spatial fluctuations in finite dimensions brings in a (self-consistent) renormalization, and *retardation* of the Hubbard U.

We thus conclude that our approach offers a natural way to extend the large dimensionality methods, and to study the effects of spatial fluctuations in a systematic fashion. We note that the $1/m$ expansion, as presented above, effectively generates an expansion in the power of hopping elements. It thus represents a *locator* expansion,[1] that describes the *short-ranged* spatial correlations,

i.e., is similar in spirit to cluster generalizations of standard mean-field theories. It is worth pointing out that such an expansion, if truncated to any finite order, can never account for the presence of *long-wavelength* spatial fluctuations (such as spin waves) that are expected to play a crucial role in determining the critical behavior of the system. In situations where the long-wavelength modes are important, one expects that an alternative expansion around the mean-field theory, namely a *loop expansion,* should be more useful. In Sec. III B we will present a class of models that allow for a natural formulation of such a loop expansion, while reducing to the same mean-field equations as presented above, when restricted to $d=\infty$.

B. Gauge-invariant models and the loop expansion

In this section, we consider a different class of models, that can be formulated on an *arbitrary* lattice, but correspond to a special form of disorder. In this class, the random hopping elements are assumed to take the form

$$t_{ij}=y_{ij}g(x_i,x_j)\ , \tag{13}$$

and in addition there can be an arbitrary distribution of site energies ε_i. Here y_{ij}'s are independent *bond* variables with a symmetric distribution, i.e., $\overline{y_{ij}^{2n+1}}=0$, and $g(x_i,x_j)$ is an arbitrary function of local *site* variables x_i.

The special class of models which have a symmetric distribution of hopping elements has a very simple physical interpretation. As first observed by Wegner,[5] in these "gauge-invariant" models, the phases of the electrons undergo random shifts at every lattice hop, and so the mean free path l reduces to one lattice spacing. On general grounds, on length scales longer than l the details of the lattice structure are washed out by disorder, so that for gauge-invariant models in the large dimensionality limit, the details of the lattice structure become irrelevant. We contrast this with the models with arbitrary disorder, discussed in Sec. III A, which have a well-defined pure limit, and accordingly can also have an arbitrarily large mean free path. The presence of this intermediate length scale (l can be much larger than the lattice spacing a, but much smaller than the localization length ξ) is often irrelevant to both long-wavelength phenomena such as localization, and local phenomena such as the Mott transition. The gauge-invariant models avoid these unnecessary complications, without disrupting any of the qualitative properties on either very short or very long length-scales.

The general properties are the same for all the models in this class, but for the simplicity of our presentation we will restrict our attention to the separable case,[32] where $g(x_i,x_j)=x_ix_j$, with an arbitrary distribution $P_X(x_i)$ for the site variables x_i. For a trivial choice of $P_X(x_i)=\delta(x_i-1)$, the models reduce to the gauge-invariant models of Wegner.[5] Nontrivial distributions $P_X(x_i)$ which extend to small values of the variable x_i are useful for the study of disorder-induced local-moment formation.[13] Those sites with x_i small represent the sites with weak hybridization. At intermediate correlation, we expect the sites with small x_i to behave as local moments and make large contributions to thermodynamic quantities such as the specific-heat coefficient $\gamma=C/T$, while other sites remain in the itinerant regime.

Also, we take the y_{ij}'s to be Gaussian random variables with zero mean, and with the variance

$$\overline{y_{ij}^2}=\frac{1}{z}f_{ij}t^2\ . \tag{14}$$

Here the (uniform) matrix f_{ij} specifies the lattice structure

$$f_{ij}=\begin{cases}1 & \text{for connected sites}\\ 0 & \text{for disconnected sites}\ ,\end{cases} \tag{15}$$

and we have scaled the (square of the) hopping elements by the coordination number $z=\sum_j f_{ij}$, in order to obtain a finite result in the $z\to\infty$ limit.

1. Functional integral formulation

At this point, it is convenient to perform explicitly the averaging over the Gaussian random (bond) variables y_{ij}, after which the hopping part of the action takes the form

$$S_{\rm hop}=\tfrac{1}{2}t^2\sum_{ij}\frac{1}{z}f_{ij}x_i^2x_j^2\left[\sum_{\alpha,s}\int_0^\beta d\tau[\bar{c}_{s,i}^{\alpha}(\tau)c_{s,j}^{\alpha}(\tau)+\text{H.c.}]\right]^2\ . \tag{16}$$

As we can see from this expression, the averaging over disorder has generated a *quartic* term in the action,[5] that is nonlocal in (imaginary) time, spin, and replica indices. We are now in a position to introduce collective Q fields[5,7] of the form (in terms of Matsubara frequencies $\omega=2n\pi T$; the indices "n" are omitted for brevity)

$$Q_{\omega_1\omega_2}^{\alpha_1\alpha_2,s_1s_2}(i)=\frac{1}{z}\sum_j f_{ij}x_j^2\bar{c}_{j,s_1}^{\alpha_1}(\omega_1)c_{j,s_2}^{\alpha_2}(\omega_2)\ , \tag{17}$$

by decoupling the (quartic) hopping term using a Hubbard-Stratonovich transformation. For simplicity, as before, we will ignore the superconducting phases as well as fluctuations in the particle-particle (Cooper) channel, so that the Q field does not have anomalous components. (The procedure can be straightforwardly generalized[6] to include the omitted terms.)

It is now possible to formally integrate out the electron (Grassmann) fields, and the resulting action for the Q fields can be written as

$$S[Q]=S_{\rm hop}[Q]+S_{\rm loc}[Q]\ . \tag{18}$$

The nonlocal part of the action $S_{\rm hop}[Q]$ takes a simple quadratic form in terms of the Q fields

$$S_{\rm hop}[Q]=-\tfrac{1}{2}t^2\sum_{ij}\sum_{\alpha_1\alpha_2}\sum_{s_1s_2}\sum_{\omega_1\omega_2}K_{ij}Q^{\alpha_1\alpha_2,s_1s_2}_{\omega_1\omega_2}(i)Q^{\alpha_2\alpha_1,s_2s_1}_{\omega_2\omega_1}(j)\ , \tag{19}$$

where, $K_{ij}=(1/z)f_{ij}^{-1}$ is the inverse lattice matrix, scaled by coordination number z. In contrast, all the nonlinearities are contained in the *local* part of the action:

$$S_{\rm loc}[Q]=-\sum_i \ln\int dx_i P_X(x_i)\int d\varepsilon_i P_S(\varepsilon_i)\int D\bar{c}_i Dc_i \exp\{-S_{\rm eff}[\bar{c}_i,c_i,Q_i,x_i,\varepsilon_i]\}\ , \tag{20}$$

where the effective action for on-site electrons takes the form

$$S_{\rm eff}[\bar{c}_i,c_i,Q_i,x_i,\varepsilon_i]=-\sum_{\alpha_1\alpha_2}\sum_{s_1s_2}\sum_{\omega_1\omega_2}\bar{c}^{\alpha_1}_{i,s_1}(\omega_1)[(i\omega_1+\mu-\varepsilon_i)\delta_{\alpha_1\alpha_2}\delta_{s_1s_2}\delta_{\omega_1\omega_2}-x_i^2t^2Q^{\alpha_1\alpha_2,s_1s_2}_{\omega_1\omega_2}(i)]c^{\alpha_2}_{i,s_2}(\omega_2)$$
$$+U\sum_{\alpha}\sum_{\omega_1+\omega_3=\omega_2+\omega_4}\bar{c}^{\alpha}_{i,\uparrow}(\omega_1)c^{\alpha}_{i,\uparrow}(\omega_2)\bar{c}^{\alpha}_{i,\downarrow}(\omega_3)c^{\alpha}_{i,\downarrow}(\omega_4)\ . \tag{21}$$

The local effective action $S_{\rm eff}[\bar{c}_i,c_i,Q_i,x_i,\varepsilon_i]$ is identical to the action of a (generalized) Anderson impurity model embedded in an electronic bath characterized by a hybridization function $x_i^2t^2Q^{\alpha_1\alpha_2,s_1s_2}_{\omega_1\omega_2}(i)$. We can thus interpret our system as a *collection* of Anderson impurity models[29] that are "connected" through the existence of collective Q fields. Here we note that, in contrast to an ordinary Anderson model, the hybridization function is now *nondiagonal* in frequency, spin, and replica indices. Physically, this reflects the fact that in general dimensions a given site can be regarded as an Anderson impurity model in a *fluctuating* bath, which breaks local translational invariance in time, space, and spin.

2. Saddle-point solution

The action has a general form which is very similar to standard lattice models investigated in statistical mechanics.[33] As usual, the problem simplifies considerably in the limit of large coordination number, when the spatial fluctuations of the Hubbard-Stratonovich field (Q in our case) are suppressed, and the mean-field theory becomes exact. It is worth pointing out that there are two classes of lattices which can have large coordination.

(a) Lattices with short-range bonds but living in a space of *large dimensionality*. For example, on a hypercubic lattice with nearest-neighbor hopping in d dimensions, $z=2d$.

(b) Lattices embedded in a finite dimensional space, but having a *long hopping range*. In this case, the lattice matrix f_{ij} takes the form

$$f_{ij}=\begin{cases}1 & |i-j|<L\\ 0 & \text{otherwise}\ ,\end{cases} \tag{22}$$

and the coordination number $z\sim L^d$.

In either case, when $z\to\infty$, the functional integral over Q fields, representing the partition function, can be evaluated (exactly) by a saddle-point method, and we obtain mean-field theory. In order to derive the mean-field equations in our case, we look for extrema of the action $S[Q]$ with respect to the variations of the Q fields, i.e.,

$$\frac{\delta S[Q]}{\delta Q^{\alpha_1\alpha_2,s_1s_2}_{\omega_1\omega_2}(i)}=0\ . \tag{23}$$

Since the saddle-point solution is translationally invariant in time and space, and conserves spin, it is *diagonal* in all indices:

$$[Q^{\alpha_1\alpha_2,s_1s_2}_{\omega_1\omega_2}(i)]|_{\rm SP}=\delta_{\alpha_1\alpha_2}\delta_{s_1s_2}\delta_{\omega_1\omega_2}Q_s^{\rm SP}(\omega)\ , \tag{24}$$

and the saddle-point equations assume the form

$$Q_s^{\rm SP}(\omega)=\int d\varepsilon_i P_S(\varepsilon_i)\int dx_i P_X(x_i)x_i^2G_{i,s}(\omega)\ , \tag{25}$$

where

$$G_{i,s}(\omega)=\langle\bar{c}_s(\omega)c_s(\omega)\rangle_{S_{\rm eff}[\bar{c},c,Q^{\rm SP},x_i,\varepsilon_i]}\ . \tag{26}$$

If we identify

$$W_{s,i}(\omega)\equiv x_i^2t^2Q_s^{\rm SP}(\omega)\ , \tag{27}$$

we see that our saddle-point equations become *identical* as the $d\to\infty$ equations on a Bethe lattice [Eqs. (8)–(10)] when applied to the appropriate model of hopping disorder. We emphasize that the present equations are exact at $z\to\infty$ for an *arbitrary* lattice, due to the presence of the "gauge-invariant" form of the hopping disorder. Since the saddle-point equations determine the local effective action, this means that all *local* correlation functions will be insensitive to the lattice structure in this mean-field limit. However, other properties, such as the tendency to the formation of the spin and charge-density wave, *are* very sensitive to the details of the lattice structure.

As an example, we can compare the case of a simple hopping disorder $t_{ij}=y_{ij}$ on the case of a bipartite lattice, such as the Bethe lattice, and the case of a lattice with infinite range hopping [the limit $L\to\infty$ of model (b) above]. The self-consistency (mean-field) equations are *identical* in the two cases, and in fact reduce to those of a *pure* Hubbard model on a Bethe lattice with hopping t. On the other hand, it is well established[22] that in the first case the system is unstable toward the formation of an antiferromagnetic ground state, even for arbitrarily small U/t, while in the second the system remains paramagnet-

ic for any U/t, due to large frustration. In many physical systems, such as doped semiconductors,[10] disorder introduces large amounts of frustration, and magnetic ordering does not occur, even though the system is strongly correlated. In order to study such situations, it is useful to have at hand microscopic models that have a nonmagnetic ground state, and allow one to study the approach to the metal-insulator transition which occurs at $T=0$.

3. Loop expansion

The present approach is particularly convenient for studying the effects of strong correlations on *disorder-driven* transitions, and the interplay of Anderson localization and strong correlations in general. This is especially true since Anderson localization is not present in $d=\infty$ (or infinite range) models, and so one has to extend the approach to include the presence of spatial fluctuations missing from the mean-field description. In order to systematically study the fluctuation effects, we proceed to carry out an expansion in terms of the deviations of the collective Q fields from their saddle-point value, i.e., in powers of $\delta Q(i)=Q(i)-Q^{\mathrm{SP}}$. This procedure, also known as a *loop expansion,*[33] has been used in other disordered problems, such as spin glasses,[34] to generate systematic corrections to the mean-field theory. The method is particularly convenient when applied to long-range models[34] [class (b) above], since in that case the loop corrections are ordered by a small parameter $1/z$. The loop expansion can be applied also to large dimensionality models [class (a) above], but in that case a given order in a loop expansion can be considered to be an infinite resummation of the simple $1/d$ expansion,[35] since each term contains all powers of $1/d$.

When the expansion of the effective action in terms of δQ's is carried to lowest, quadratic order, we obtain a theory describing Gaussian fluctuations around the saddle point that represent weakly interacting collective modes.[5,7] Higher-order terms in the expansion then generate effective interactions of these modes, which under appropriate conditions can lead to fluctuation-driven phase transitions. In practice, if all components of the collective Q fields are retained in this analysis, the theory becomes prohibitively complicated and cumbersome. However, in order to analyze the *critical behavior,* it is not necessary to keep track of all the degrees of freedom, but is enough to limit the analysis to *soft modes,* i.e., those that represent low-energy excitations. In disordered metallic phases, charge and spin conservation laws lead to the existence of *diffusion modes* which are the hydrodynamic modes describing charge- and spin-density relaxation. In the Fermi-liquid regime,[3] all other collective excitations require higher energies, and can be neglected in a hydrodynamic description of the system. One is then led to construct a theory of interacting diffusion modes, as a theory of critical phenomena for disordered interacting systems.

This line of reasoning was used in field-theoretical approaches to the localization problem of noninteracting electrons, as first developed by Wegner.[5] In this theory, collective Q fields, similar to the ones presented in this paper, are introduced. At the saddle-point level, no phase transition occurs, and all the states are extended. An analysis of the fluctuations of the Q fields is then performed, and a *subset* of those fluctuations identified that represents the hydrodynamic (diffusion) modes. Only the fluctuations of these modes are retained, and an effective hydrodynamic theory constructed—the *nonlinear sigma model*.[5] The interactions of these modes lead to the metal-insulator (localization) transition, which was analyzed using renormalization-group techniques and $2+\varepsilon$ expansions. In subsequent work, Finkelshtein[7] was able to apply a similar procedure to *interacting* disordered electrons. However, this theory is based on a number of implicit assumptions that restrict its validity to *Fermi-liquid* regimes. In the language of Q fields, one again expands around a noninteracting saddle point, and the interaction effects appear only at the level of the fluctuation corrections.

When strongly correlated electronic systems are considered, much of the physics relates precisely to the *destruction of coherent quasiparticles* by inelastic processes, so that one needs a description that is not limited to Fermi-liquid regimes. In the language of hydrodynamics, additional soft modes appear that indicate the tendency for interaction-driven instabilities. In particular, strong correlations can lead to local-moment formation and the Mott transition. In both cases, the charge fluctuations are suppressed, and low-energy spin fluctuations dominate the physics.

In the present approach, in contrast to the work of Wegner and Finkelshtein, the strong correlations are already treated in a nonperturbative fashion at the saddle-point (mean-field) level, so that *all* soft modes can be systematically included. In particular, even at a one-loop level, we can address the question of how the disorder-induced local-moment formation and the approach to the Mott transition affect the weak localization (diffusion) corrections. Ultimately, our approach indicates how a more general low-energy theory can be constructed that extends the σ-model description to include strong correlation effects.

In the present paper, we will limit our attention to the form of the Gaussian fluctuations of the Q fields, that allow one to compute the leading corrections to mean-field theory. The Gaussian part of the action takes the form

$$S^{(2)}[Q]=-\tfrac{1}{2}t^2\sum_{l_1\ldots l_4}\int\frac{dk}{(2\pi)^d}\delta Q_{l_1l_2}(k)[(L^2k^2+1)\delta_{l_1l_4}\delta_{l_2l_3}-t^2W(l_1)W(l_3)\delta_{l_1l_2}\delta_{l_3l_4}+t^2\Gamma(l_1\ldots l_4)]\delta Q_{l_3l_4}(-k)\,. \quad (28)$$

This expression is appropriate for the long-ranged model (b) above, in which case the inverse lattice matrix in momentum space takes the form $K(k)\approx 1+L^2k^2$, and we cut off the momentum integrals at $\Lambda=2\pi/L$. Note that the coefficient of k^2, which can be interpreted as *stiffness* of the δQ modes, is $\sim L^2$, so we see that indeed the fluctuations

are suppressed at $L \to \infty$. In the above formula, the index l_m is used to represent the frequency, spin, and replica indices. The local vertex function $\Gamma(l_1 \ldots l_4)$ is given by

$$\Gamma(l_1 \ldots l_4) = \int d\varepsilon_i P_S(\varepsilon_i) \int dx_i P_X(x_i) x_i^4 \langle \bar{c}_i(l_1) c_i(l_2) \bar{c}_i(l_3) c_i(l_4) \rangle_{S_{\text{eff}}[Q^{\text{SP}}]} . \tag{29}$$

At this level, the dynamics of the collective fluctuations δQ is governed by the form of $S^{(2)}[\delta Q]$, which is expressed in terms of the *local correlation functions* of the saddle-point theory, i.e., of the $d=\infty$ disordered Hubbard model. Accordingly, a detailed study of the $d=\infty$ limit does not only provide a mean-field description of the problem, but also determines the form of the leading corrections resulting from fluctuations. In the rest of this paper, we will limit our attention to the mean-field limit, and study the effects of the various types of disorder present. Extensions of the theory to include fluctuation corrections remain to be addressed in greater detail in future work.

IV. THERMODYNAMIC AND TRANSPORT PROPERTIES

As we saw in Sec. III, the solution of $d=\infty$ Hubbard models with disorder reduces to solving a set of self-consistency conditions determining the local effective action. The solution of the self-consistent equations immediately gives the single-particle local spectral functions, but we would also like to use these results to calculate other thermodynamic and transport properties of the system. In this section, we indicate how these quantities can be obtained in the $d=\infty$ framework.[36]

A. Thermodynamics

Once the local Green's functions are determined self-consistently, we can immediately obtain all the thermodynamic properties from the calculation of the energy $E(T)$. Using standard methods,[37] it is possible to express the energy in terms of single-particle Green's functions. To do this, we use the Heisenberg equations of motion for the field operators $c_{i,s}(\tau)$, for a given *fixed* realization of disorder, which (for $s=\uparrow$) takes the form

$$[\partial_\tau + \varepsilon_i - \mu] c_{i,\uparrow}(\tau) = + \sum_j t_{ij} c_{j,\uparrow}(\tau) - U c_{i,\uparrow}(\tau) c_{i,\downarrow}^\dagger(\tau) c_{i,\downarrow}(\tau) , \tag{30}$$

and similarly for $s=\downarrow$. Multiplying this equation by $c_{i,\uparrow}^\dagger(\tau)$, and performing the summation over $s=\uparrow,\downarrow$ and the site index i, we can relate the interaction energy

$$V = U \sum_i c_{i,\uparrow}^\dagger c_{i,\uparrow} c_{i,\downarrow}^\dagger c_{i,\downarrow} \tag{31}$$

to the kinetic energy

$$K = \sum_{ij} \sum_s [-t_{ij} + \varepsilon_i \delta_{ij}] c_{i,s}^\dagger c_{j,s} , \tag{32}$$

and find

$$V = -\frac{1}{2} \left[K + \sum_{i,s} c_{i,s}^\dagger(\tau) [\partial_\tau - \mu] c_{i,s}(\tau) \right] . \tag{33}$$

Using the definition of the single-particle Green's function,

$$G_s(i\tau, j\tau') = \langle c_{i,s}^\dagger(\tau) c_{j,s}(\tau') \rangle , \tag{34}$$

we obtain an expression for the energy $E = \langle K \rangle + \langle V \rangle$ of the form

$$E(T) = \tfrac{1}{2} \sum_{ij,s} [-t_{ij} + \varepsilon_i \delta_{ij}] G_s(i\tau, j\tau) + \lim_{\tau' \to \tau} \tfrac{1}{2} \sum_{i,s} [-\partial_\tau + \mu] G_s(i\tau', i\tau) . \tag{35}$$

This expression for the energy is valid for a Hubbard model with an arbitrary realization of disorder, and in arbitrary dimension. In the limit of large coordination, the hopping elements are rescaled as $t_{ij} \to t_{ij}/\sqrt{z}$,[16] and the leading contributions can be obtained by an expansion in powers of $t_{ij}/\sqrt{z}$. To leading order, and for the classes of models that we consider, the off-diagonal element of the Green's-function *factors*

$$G_s(i,j;\omega_n) = \frac{1}{\sqrt{z}} t_{ij} G_s(i,i;\omega_n) G_s(j,j;\omega_n) + O\left[\frac{1}{z}\right] . \tag{36}$$

The expression for the energy for the models of Sec. III then assumes a simpler form

$$E(T) = \int d\varepsilon_i P_S(\varepsilon_i) \int dx_i P_H(x_i) \times \frac{1}{\beta} \sum_n [i\omega_n + \mu + \varepsilon_i + W_i(\omega_n)] \times G_i(\omega_n) . \tag{37}$$

The expression is valid in the paramagnetic phase, where we have performed the spin sum. It is important to note that the energy takes an *additive form* with respect to sites having energies ε_i and hopping parameters x_i. Once the energy is known as a function of temperature, we can calculate quantities such as the specific heat, entropy, etc. We immediately conclude that the specific heat is also additive, reminiscent of the phenomenological "two-fluid model" of doped semiconductors; we will discuss the relevance of our results to such systems in more detail in Sec. VI. Finally, the procedure can easily be generalized to include external uniform or staggered magnetic fields, allowing the calculation of the appropriate susceptibilities.

B. Conductivity

Transport coefficients can be expressed quite generally using the Kubo formulation,[37] and the calculation reduces to computing appropriate electronic correlation

functions. In particular, the real part of the conductivity can be expressed as

$$\sigma_R(\omega)=\frac{1}{\omega}\frac{1}{\Omega}\mathrm{Im}\sum_{i,i'}\chi_{jj}(i,i';\omega)\ , \tag{38}$$

where $\chi_{jj}(i,i';\omega)$ is the retarded current-current correlation function corresponding to lattice sites i and i', and Ω is the volume of the system. For the lattice models we consider, the current operator takes the form

$$\mathbf{j}(\mathbf{i})=-iat\sum_s[c^\dagger_{s,\mathbf{i}}c_{s,\mathbf{i}+\mathbf{a}}-c^\dagger_{s,\mathbf{i}}c_{s,\mathbf{i}-\mathbf{a}}]\ . \tag{39}$$

Here we have used the units in which $\hbar=e=1$, and $\mathbf{a}$ is the unit lattice vector in the direction of the current.

As for other quantities, considerable simplifications occur in the $d=\infty$ limit, essentially due to the cancellation of the vertex corrections, as first pointed out by Khurana.[38] For general models of disorder, it is then possible to express the conductivity in terms of the (averaged) local spectral functions—a feature reminiscent of the coherent-potential approximation (CPA).[26] In fact, in the noninteracting limit, our self-consistency conditions reduce to the CPA, which is consistent with the absence of Anderson localization in $d=\infty$.

The specific expressions for the conductivity take different forms depending on the precise form of disorder, but as in Sec. III we limited our attention to two classes of models where the results take a particularly simple form.

1. Gauge-invariant models

This class of models is characterized by hopping elements with random signs, which correspond to a mean free path of one lattice spacing. Upon averaging, all off-diagonal (nonlocal) elements of the single-particle Green's function vanish, and the result is expressed entirely in terms of the local spectral functions:

$$\sigma_R(\omega)=4\pi a^2\frac{t^2}{z}\int d\omega'\rho_W(\omega')\rho_W(\omega'+\omega)\times\frac{f(\omega')-f(\omega'+\omega)}{\omega}\ , \tag{40}$$

where $f(\omega)$ is the Fermi function, and $\rho_W(\omega)$ is the *local* spectral function corresponding to the averaged cavity field

$$\rho_W(\omega)=-\frac{1}{\pi}\mathrm{Im}\int d\varepsilon_i P_S(\varepsilon_i)\int dx_i P_H(x_i)x_i^2 G_i(\omega+i\eta)\ . \tag{41}$$

We note at this point that, since the conductivity is an off-diagonal correlation function, the *leading* contribution is $\sigma\sim 1/z$ (after rescaling the hopping elements), and in the $z\to\infty$ limit one should consider a *rescaled* quantity $\sigma\to z\sigma$. In the following, we consider this rescaled conductivity, which remains finite in the $z\to\infty$ limit.

At $\omega=0$ and low temperatures, after performing the spin sum, the expression reduces to

$$\sigma_{\mathrm{dc}}(T)=4\pi a^2 t^2\rho_W^2(\omega=0,T)\ . \tag{42}$$

The result coincides with the expression obtained by Wegner,[5] for noninteracting electrons in the presence of gauge-invariant hopping disorder with N orbitals per site, in the $N\to\infty$ limit.

As we can see from this expression, the conductivity is finite in the metallic region $[\rho^2(\omega=0,T)\neq 0]$, in contrast to the case of pure lattices where the resistance (inelastic scattering) vanishes at $T\to 0$. For gauge-invariant models, the pure limit cannot be obtained by tuning a parameter (disordered strength) since the mean free path l cannot exceed one lattice spacing ($l\to\infty$ in the pure limit). However, as we will see, these models with hopping randomness (in addition to possible site randomness) display *generic* behavior at the metal-insulator transition, which presumably is relevant for realistic systems.

2. Models with site randomness

The other class of models that we consider corresponds to pure site randomness, in contrast to gauge-invariant models that possess hopping randomness. In this class, which can be formulated on an arbitrary lattice, the disorder strength can be arbitrarily weak, allowing the study of the correlation screening of the disorder that will be discussed in Sec. V. For models with site randomness in $d=\infty$, the conductivity expression[38] is almost identical to that in the pure Hubbard model:[21]

$$\sigma_R(\omega)=\frac{2}{dV}\sum_{\mathbf{k}}v_{\mathbf{k}}^2\int d\omega'\bar{\rho}(\mathbf{k},\omega')\bar{\rho}(\mathbf{k},\omega'+\omega)\times\frac{f(\omega')-f(\omega'+\omega)}{\omega}\ , \tag{43}$$

where

$$\bar{\rho}(\mathbf{k},\omega)=-\frac{1}{\pi}\mathrm{Im}\frac{1}{\omega+i\eta+\mu-\varepsilon_{\mathbf{k}}-\Sigma_{\mathrm{dis}}(\omega+i\eta)} \tag{44}$$

is the spectral function (at momentum $\mathbf{k}$) corresponding to the single-particle Green's function *averaged* over disorder. Here $\varepsilon_{\mathbf{k}}$ describes the electronic dispersion in the pure noninteracting limit, and $\mathbf{v}_{\mathbf{k}}=\partial\varepsilon_{\mathbf{k}}/\partial\mathbf{k}$ is the corresponding lattice velocity; their specific form depends on the details of the lattice structure. This expression is identical to the familiar CPA expression[26] for noninteracting electrons. In our case, $\bar{\rho}(\mathbf{k},\omega)$ is the *fully renormalized* quantity with respect to interactions, and thus acquires a strong frequency and temperature dependence in the strongly correlated region. Note the difference in the way the momentum summation enters the conductivity expression, as compared to the gauge-invariant models, where the expression involves *local* spectral functions only.

In $d=\infty$ the self-energy $\Sigma_{\mathrm{dis}}(\omega_n)$ is *momentum independent,* and so can be calculated from the *local* (averaged) Green's function

$$\bar{G}(\omega_n)=\int d\varepsilon_i P_E(\varepsilon_i)G_i(\omega_n)\ , \tag{45}$$

where $G_i(\omega_n)$ is the solution of the $d=\infty$ mean-field equations, Eqs. (8)–(10). Once $\bar{G}(\omega_n)$ is known, the quantity $\Sigma_{\mathrm{dis}}(\omega_n)$ can be obtained from Eq. (44), which upon momentum summation can also be written as

$$\overline{G}(\omega_n)=g_0[\omega_n-\Sigma_{\rm dis}(\omega_n)]\ , \tag{46}$$

where $g_0(\omega_n)$ is the bare local Green's function (in the absence of interactions and disorder). In particular, for a Hubbard model with pure site randomness with a bare semicircular density of states (DOS), we can write

$$\Sigma_{\rm dis}(\omega_n)=i\omega_n+\mu-t^2\overline{G}(\omega_n)-[\overline{G}(\omega_n)]^{-1}\ . \tag{47}$$

We emphasize the distinction between $\Sigma_{\rm dis}(\omega_n)$ and the self-energy $\Sigma_i^A(\omega_n)$ of the local Anderson model corresponding to a given site i. Physically, $\Sigma_A(\varepsilon_i,\omega_n)$ measures only the local *inelastic scattering* from electron-electron interactions, while $\Sigma_{\rm dis}(\omega_n)$ measures the total scattering that includes both the inelastic and elastic (impurity) contributions. In the presence of disorder, the scattering rate $1/2\tau=-{\rm Im}\Sigma_{\rm dis}(\omega=0)$ remains finite even at $T=0$, reflecting the presence of elastic impurity scattering. At sufficiently weak disorder, $1/2\tau$ can be arbitrarily small, and we get a Drude-like expression $\sigma_{\rm dc}\sim\tau$, resulting in arbitrarily large dc conductivity.

V. METAL-INSULATOR TRANSITIONS

After describing the formal aspects of the $d=\infty$ approach to correlated disordered electrons, we now present our findings obtained by applying the methods to various physical situations. In practical terms, solving the mean-field equations reduces, even in the presence of disorder, to the solution of Anderson impurity models supplemented by additional self-consistency conditions. From the technical point of view, the problem is of the same level of difficulty as in the pure limit. Over the last few years, a number of exact numerical and approximate analytical techniques[21–23,39] useful for solving such equations have been developed and tested. Since the same technical approaches can be employed even in the disorder case, we will not spend much time elaborating on the various methods that can be used to solve the mean-field equations. Instead, in the following we shall concentrate on making a clear summary of our conclusions for the various models of disorder considered, and their implication for realistic experimental systems.

In general, when either sufficiently strong correlations or disorder is present, metal-to-insulator transitions (MIT's) can take place. In the $d=\infty$ framework, Anderson localization effects are absent, but the MIT can still take place because of strong correlation effects. In the following, we discuss the possible classes of MIT's present in $d=\infty$ models, and make predictions about the behavior of thermodynamic and transport properties as the transition is approached.

A. Hopping disorder

In a number of materials that display a metal-insulator transition such as uncompensated doped semiconductors, the main source of disorder stems from the random position of dopant atoms, thus leading to strong hopping randomness. In order to study such situations, we begin our analysis by examining models with pure hopping randomness.

As a first example, we consider the case of simple uncorrelated hopping disorder, of the form $t_{ij}=y_{ij}$, with y_{ij} Gaussian-distributed random numbers with variance t^2. In that case, the self-consistency condition determining the effective action are identical to the pure Hubbard model on the $d=\infty$ Bethe lattice. The solution of this model is well known,[21–23] as discussed in Sec. II. At moderate correlation strength, the system is metallic, and displays the usual Fermi-liquid behavior. At $T=0$, a Mott-Hubbard transition takes place at a critical interaction strength U_c, where the quasiparticle band vanishes and a gap for charged excitations appears, leading to an insulating state. As the transition is approached, the effective mass, and thus also the specific heat, is found to diverge as $\gamma\sim(U_c-U)^{-1}$.

While these properties are identical, as in the pure model, the behavior of the conductivity proves to be more sensitive to the presence of disorder. By using the expressions for the conductivity of Sec. IV, and the well-known results for the local spectral functions,[21–23] we can readily compute the transport properties at arbitrary temperature T and interaction strength U. At $T=0$ the behavior of the dc ($\omega=0$) conductivity is particularly simple, and can be computed analytically. In this limit, Fermi-liquid theorems for the Anderson model assert that, in the metallic phase, the imaginary part of the Anderson model self-energy vanishes (physically this reflects the absence of *inelastic* scattering at $T=0$). When this result is applied to the $d=\infty$ model, we conclude that at half-filling (at particle-hole symmetry), the local spectral function $\rho(\omega=0,T=0)$ is *pinned* to its *noninteracting* value $\rho_0=(\pi t)^{-1}$. As a result the $T=0$ value of the dc conductivity is *also pinned,* i.e.,

$$\sigma_{\rm dc}(T=0)=\sigma_0=4a^2/\pi \tag{48}$$

throughout the metallic phase. Although the precise value of σ_0 given here is appropriate only for this particular model of hopping randomness, the proof for the conductivity pinning can easily be generalized to more complicated situations. In fact, pinning is obeyed at $T=0$ for any model obeying (local) particle-hole symmetry, i.e., models at half-filling with arbitrary form of hopping randomness. Random *site* energies *break* local particle-hole symmetry, and thus violate the pinning condition; in that case $\sigma_{\rm dc}(T=0)$ can depend on U.

Thus we have shown that for models with hopping randomness, the conductivity at $T=0$ remains constant inside the metallic phase, and then abruptly *jumps* to zero as the system becomes a Mott insulator. The behavior can be described as a manifestation of *minimum metallic conductivity,* in agreement with early ideas of Mott.

At finite temperature, the pinning condition is violated due to *inelastic* scattering, and we have to solve the self-consistency equations at $T\neq0$ explicitly in order to obtain results for the conductivity. As we have seen above, in the present model the calculations for the conductivity reduce to calculating the local DOS, which is the same as in the pure model with hopping t. Explicit results for the conductivity as a function of U at finite temperature have

been presented in Ref. 19. The jump in the conductivity was found to persist at small but finite temperatures $T<T^*$, which is of the order of 1% of the bandwidth. At higher temperatures, the conductivity is a smooth function of U, and *continuously* drops to exponentially small values as U is increased, reflecting the destruction of the coherent quasiparticles by thermal inelastic scattering.

B. Correlated hopping randomness

Before leaving models with pure hopping disorder, we would like to comment on possible modifications of the transition in the presence of more complicated models of random hopping. The generalizations we have in mind correspond to correlated hopping disorder where, in addition to random bond variables y_{ij}, the hopping elements can take a more general form $t_{ij}=y_{ij}x_ix_j$, where we can have arbitrary distributions of random site variables x_i. These models, useful for the study of disorder-induced local-moment formation, are designed to implement the strong fluctuations of the *local hybridization* of a given site to its environment, an effect which is important in realistic systems, but drops out in the $d=\infty$ limit if models with bond randomness only are considered. In another interpretation, fluctuations in the local site variable x_i, which do survive in the $d=\infty$ limit, represent the fluctuations of the *local bandwidth* of the Hubbard model.

For these models with correlated hopping disorder, the behavior of the system proves to be very sensitive to the detailed form of the *probability distribution* $P_X(x_i)$ for random variables x_i. If the *low-x* tail of the distribution extends to very small values, local-moment formation occurs, and even the qualitative nature of the metallic phase can be modified; this effect will be discussed in more detail in Sec. VI. On the other hand, it is the form of the *high-x* tail that is the most relevant to the metal-insulator transitions.

On general grounds, we expect that sufficiently long high-x tails can completely suppress the existence of the Mott gap at any value of U, even at $T=0$. In principle, it would be desirable to be able to obtain precise criteria about the forms of $P_X(x)$ that result in the suppression of the Mott phase. Unfortunately, with few exceptions, closed-form (analytical) solutions of the $d=\infty$ mean-field equations are not available, so obtaining exact criteria is difficult. Still, much can be learned from approximate schemes used in solving the equations. In particular, an approximate solution to the mean-field equations can be obtained by solving the appropriate Anderson impurity problem using the approach of Yosida and Yamada[40,17] (YY) using second-order perturbation theory in U. This method, often called the iterated perturbation theory (IPT) (Refs. 22 and 23) has been found to be quite useful in obtaining information about the problem.

In the present case, the IPT is particularly useful, as it allows a simple derivation of an approximate criterion for the destruction of the Mott phase by strong hopping disorder. To obtain this criterion, we examine the stability of the insulating solution under an iterative procedure. In this iterative method, one makes an initial guess for a form of the cavity field $W_x(\omega_n)$. This defines a specific form for the local effective action, Eq. (8). Within the IPT, the corresponding Anderson model is solved in perturbation theory, and an expression for $G_x(\omega_n)$ is obtained. The procedure is repeated for every value of x by sampling the distribution $P_X(x)$. A new value of the cavity field $W_x(\omega_n)$ is obtained from the self-consistency condition Eq. (9) [in the present case $P_S(\varepsilon_i)=\delta(\varepsilon_i)$—no site randomness]. Finally, the procedure is iterated until convergence is found.

The procedure is typically implemented numerically, but a stability criterion which is *exact* within the IPT can be derived analytically, as follows. In the present model of hopping randomness, it is useful to consider the quantity [compare Eq. (25)]

$$Q(\omega_n)=\int dx\, P_X(x)x^2G_x(\omega_n)\ , \tag{49}$$

which represents the part of the cavity field which is *independent* of the local disorder parameter x, so that

$$W_x(\omega_n)=x^2t^2Q(\omega_n)\ . \tag{50}$$

If we assume that at some stage N of the iteration, the solution is insulating, i.e., there is a *gap* in the single-particle excitation spectrum, then the local Green's functions assume a linear form at $\omega_n\to 0$:

$$G_x^{(N)}(\omega_n)\sim -i\omega_n+\cdots\ , \tag{51}$$

and the same is true for the cavity field. Here we have specialized to half-filling ($\mu=U/2$), where particle-hole symmetry holds even in the presence of hopping randomness. To proceed, it is convenient to parametrize the corresponding [Eq. (49)] low-frequency form of $Q(\omega_n)$ as

$$Q^{(N)}(\omega_n)=-\alpha_N t^{-2}(i\omega_n)+\cdots\ . \tag{52}$$

Physically, the parameter α_N measures the gap size ($\alpha\to\infty$ if the gap closes). According to Yosida and Yamada,[40] the Anderson model is solved in second-order perturbation theory with respect to the nonmagnetic Hartree-Fock solution, and so the expressions involve "bare" propagators of the form

$$G_0^{(N)}(x;\omega_n)=[i\omega_n-W_x(\omega_n)]^{-1}\ , \tag{53}$$

which, using the above form of the cavity field, take a singular form

$$G_0^{(N)}(x;\omega_n)=(1+x^2\alpha_N)^{-1}(i\omega_n)^{-1}+(\text{regular terms})\ . \tag{54}$$

As the YY expression for the self-energy of the Anderson model $\Sigma_A(x;e\omega_n)$ involves a third-order convolution of $G_0(x;\omega_n)$'s, it is not hard to see that the result is also singular:

$$\Sigma_A^{(N)}(x;e\omega_n)=\tfrac{1}{4}U^2(1+x^2\alpha_N)^{-3}(i\omega_n)^{-1}+(\text{regular terms})\ . \tag{55}$$

Using Dyson's equation

$$G_x(\omega_n)=[G_0^{-1}(x;\omega_n)-\Sigma_A(x;\omega_n)]^{-1}\ , \tag{56}$$

and the self-consistency condition Eq. (46), we find a new value of the cavity field:

$$Q^{(N+1)}(\omega_n)=-\left[\int dx\, x^2(1+x^2\alpha_N)^3\right](i\omega_n)+\cdots . \tag{57}$$

Comparing this with Eq. (49), we obtain a *recursion relation* for the parameter α_N, of the form

$$\alpha_{N+1}=\frac{4}{U^2}[M_2+3M_4\alpha_N+3M_6\alpha_N^2+M_8\alpha_N^3] , \tag{58}$$

where we have introduced the *moments* of the probability distribution $P_X(x)$, defined as

$$M_l=\int dx\, x^l P_X(x) . \tag{59}$$

In order for the insulating solution to exist, there has to be a nontrivial solution of the equation $\alpha_{N+1}=\alpha_N$. A graphic solution of this algebraic equation is schematically presented in Fig. 2. Since all the moments M_l are positive, the function $\alpha_{N+1}(\alpha_N)$ is monotonically increasing, as are all its derivatives. Clearly, for finite moments M_l, and small values of U, the solution does not exist, and $\alpha_N\to\infty$ under iteration, indicating that the Mott gap closes. On the other hand, for U larger than some critical value U_{c1}, the insulating solution does exist. The precise value of U_{c1} depends on the value of the moments M_l; a closed form expression for U_{c1} can be derived, but will not be presented here. Experience with pure models[22] showed that the value U_{c1}, where the insulating solution disappears, is generally *smaller* than the value U_c where the metal is destroyed and the MIT takes place (the metallic solution is typically lower in energy). Nevertheless, the value of U_{c1} can be used as a *lower bound* on the critical interaction strength where the MIT occurs.

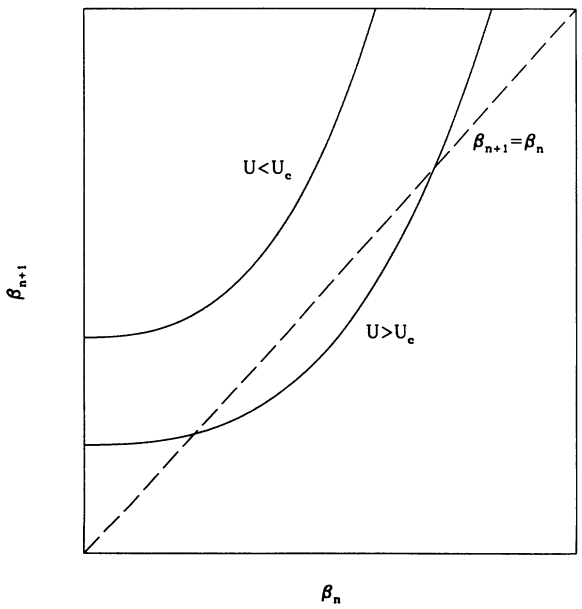

FIG. 2. Graphic solution of the equation determining the stability of the insulating solution, Eq. (58). A nontrivial solution exists only for $U>U_{c1}$, the value of which depends on the distribution $P_X(x_i)$ for the local hopping parameters.

At this point we observe that if *any* of the moments M_l ($l=2$, 4, 6, and 8) are *infinite,* there cannot be a solution to the above equation, and thus the insulating phase is suppressed. This can occur if the probability distribution has algebraically long tails, characterized by sufficiently small exponents. We conclude that within the IPT, the following criterion applies: *If the probability distribution has the asymptotic form* $P_X(x)\sim x^{-\gamma}$, *at* $x\to\infty$, *with* $\gamma\leq 9$, *the Mott insulating phase cannot exist at any value of U.*

It is interesting to note that the IPT criterion for the stability of the insulating solution involves only low-order moments (M_l, $l=2$, 4, 6, and 8) of the probability distribution. This feature is clearly an artifact of the IPT, since the expression for the self-energy Σ_A stops at $O(U^2)$, and so the recursion relation for α_N stops at the cubic order. Clearly, if higher-order [e.g., $O(U^4)$] corrections were included in the calculation of the self-energy, there would be higher-order terms in Eq. (58), which in turn would involve higher *moments* of the probability distribution $P_X(x)$. This suggests that even in the situation where only the moments of relatively high order diverge, the insulator would still be unstable. The above argument also points to the limitations of the IPT, which for these pathological distributions would be more significant than in the absence of disorder.

Based on the above arguments, we suspect that in the exact solution of the $d=\infty$ mean-field equations *any* algebraically long tails would lead to the destruction of the Mott phase. This result—that the metallic phase can survive at arbitrarily strong disorder—is almost certainly an artifact of the $d=\infty$ limit. In finite dimensions we expect that localization and/or percolation effects restore the insulator at sufficiently strong disorder. From a physical point of view, the presence of long tails in the distribution of hopping elements simply reflects the occurrence of rare bonds with anomalously large values of the hopping elements. In realistic systems such as doped semiconductors, such events correspond to closely spaced pairs or clusters of dopant atoms. Loosely speaking, if these clusters are far from each other, electrons can be trapped inside each cluster, but still not strictly localized on one atomic site. It is plausible that a Mott-like transition still takes place, but this time on a slightly longer length scale—where the cluster (long tail) effects are irrelevant. These interesting modifications of the Mott scenario by finite dimensional fluctuations remain to be addressed by extending our approach to large but finite dimensions.[41]

We conclude this section by illustrating how modifications of the probability distribution for hopping elements $P_X(x)$ affect the transport properties of the system. At $T=0$ the general theorem discussed above guarantees that σ_{dc} remains *pinned,* i.e., independent of U all the way to the transition. On the other hand, at finite temperature, the pinning is violated and the effects of disorder are more apparent. As an example, we have calculated σ_{dc} for a Gaussian distribution

$$P_X(x)=(2\pi\Delta)^{-1/2}\exp\{-(x-x_0)^2/2\Delta^2\} . \quad (60)$$

The calculations were performed numerically using the IPT scheme described above, and the results for $T=0.05D$ presented in Fig. 3. We have chosen $x_0=1$, so that for $\Delta=0$ the model reduces to the model with uncorrelated hopping elements of Wegner (see Sec. III), for which the mean-field equations for the local DOS are identical as in the pure case.[21-23] In this limit, the local Kondo temperatures (local quasiparticle bandwidths) are identical on all the sites, and we find an abrupt decrease in the conductivity at $T_k \sim T$, which in the present case (full line in Fig. 3) occurs at $U \sim 2.5$ (in units of D). When additional randomness in the local hopping parameters x_i is present ($\Delta=0.1$ and 0.2), there is a *distribution* of local Kondo temperatures, and the destruction of local coherence leading to the decrease in the conductivity takes place more gradually (dashed and dotted lines in Fig. 3).

It is interesting to note that by introducing fluctuations (thermal in this case) the *effective exponent* characterizing the behavior of the conductivity, is *increased* from $\mu=0$ at $T=0$ (minimum metallic conductivity) to a small but finite value $\mu \sim 0.5$ at $T \neq 0$. The addition of local hopping disorder (random x_i's) also helps increase this effective exponent. On general grounds, we can speculate that even at $T=0$, but in finite dimensions, the *quantum and disorder fluctuations* absent in $d=\infty$ might play a similar role—to *increase* the value of the conductivity exponent to small but finite values observed in uncompensated doped semiconductors.[10]

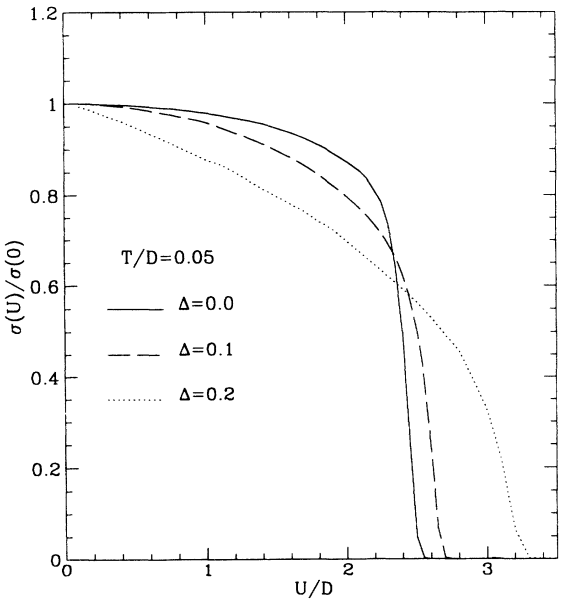

FIG. 3. Conductivity dependence on the correlation strength at finite temperature $T=0.05D$, at three different values of the disorder strength Δ. The combination of thermal fluctuations and disorder leads to a finite value of the effective conductivity exponent $\mu_{\rm eff} \sim 0.5$. Quite generally, we expect that any small perturbation leads to the rounding of the $T=0$ jump found in the $d=\infty$ mean-field theory. Such small conductivity exponents are difficult to obtain in other approaches (Ref. 7), but are readily observed experimentally in doped semiconductors (Ref. 10).

C. Combined hopping and site randomness

In addition to hopping disorder, in realistic systems one also expects some degree of site randomness, which can originate, for example, from the presence of long-ranged electrostatic fields due to charged impurities (acceptors). As discussed above, random site energies locally break the particle-hole symmetry, even if the system on average is at half-filling. One could speculate that the presence of site randomness might lead to a qualitatively different scenario, and bring into question the relevance of results obtained with pure hopping randomness.

Motivated by these considerations, we have examined Hubbard models with random site energies ε_i. We recall (Sec. III) that the *same* $d=\infty$ equations correspond to either (a) Bethe lattices with pure site randomness or (b) arbitrary lattices with site randomness *in addition to uncorrelated* random hopping elements $t_{ij}=y_{ij}$. The resulting local spectral functions are identical in the two cases, but the transport properties are very different (Sec. IV).

We studied these self-consistency conditions using a combination of several different techniques, including numerically exact quantum Monte Carlo methods,[21,22] Lanczos diagonalization approaches,[39] and approximate slave-boson methods.[42] Detailed results, and predictions for the case of *pure* site randomness, will be presented elsewhere.[43] Here we just comment on the consequences of these results for the case of combined hopping and site randomness. As we have seen, in this case (the gauge-invariant models of Sec. III) the conductivity can be expressed entirely in terms of *local* spectral functions $\rho_W(\omega_n)$. Our result demonstrated that $\rho_W(0)$ remains *finite* all the way to the MIT, so according to Eq. (42) the *jump* of $\sigma_{\rm dc}$ ("minimum metallic conductivity") persists even in the presence of combined hopping and site randomness. Our *qualitative* conclusions for the MIT scenario remain unchanged.

D. Other types of transitions in $d=\infty$

In this paper, we have concentrated much of our attention on metallic phases, assuming the absence of spin- or charge-density-wave formation, since these phenomena typically do not occur in disordered systems of interest. Nevertheless, one can consider systems on lattices with perfect nesting, which then leads to various instabilities that can open a gap on the Fermi surface, and thus induce metal-insulator transitions. Typically, such effects are not associated with strong correlations, since perfect nesting leads to instabilities even in weakly correlated systems. For example, pure Hubbard models on hypercubic or Bethe lattices have antiferromagnetic (insulating) ground states for arbitrary small U. One could also investigate situations where disorder is added to such systems, and examine the resulting thermodynamic and transport properties near the transitions using the $d=\infty$ methods.

Studies of this type have recently been carried out by Janis, Ulmke, and Vollhardt[20] for antiferromagnetic in-

stability. The presence of sufficiently strong disorder was found to suppress the antiferromagnetism, as can be expected, since randomness washes out the perfect nesting and leads to a broadening of the electronic bands. In another study, Uhrig and Vlaming[20] examined charge-density-wave formation in the case of disordered *spinless* electrons. In the absence of spin, there is no Kondo effect, and an associated heavy quasiparticle band at the Fermi surface found in Hubbard models. As a result, the conductivity was found to continuously decrease to zero, as expected in ordinary band-crossing transitions.

In general, spin- and charge-density-wave instabilities are found even on a single-particle (Hartree-Fock) level of description. (Note that for spinless electrons the Hartree-Fock approximation becomes exact[20] in $d=\infty$.) We expect the role of further (many-body) correlations to be limited to quantitative modifications of the effective band structure near such transitions. The behavior of thermodynamic and transport properties in this case is thus most likely to remain qualitatively the same as in ordinary (noninteracting) band-crossing transitions.

VI. DISORDERED METALLIC PHASES: THE FORMATION OF LOCAL MOMENTS

Most metallic systems, both in the pure limit and in the presence of small amounts of disorder, can be understood by using Fermi-liquid concepts.[3] In such situations, elementary excitations can be described as a set of weakly interacting quasiparticles, leading to universal properties at low temperatures. Of course, this simplified description is valid only at temperatures $T<T_{\rm coh}$, where the "coherence" temperature $T_{\rm coh}$ represents the energy scale associated with coherent quasiparticles, which depends on the relative strength of the correlations in the system.

In a disordered system, the parameter that measures the relative interaction strength $u=U/t$, where U is the on-site (Hubbard) interaction, and t the hopping element ($t\sim$bandwidth) is also a *random function of position.* Those sites which are weakly hybridized with the rest of the system (small t) will be in the strong correlation regime (large u) where *local* charge fluctuations can be ignored, and local-moment formation[29,13] occurs even if the system is not very close to the Mott transition. For a broad distribution of hoppings, only a few of the sites are expected to correspond to $u\gg 1$, and thus represent well-formed local moments. Instead, most of the sites will be in the intermediate regime $u\sim O(1)$, where the charge fluctuations cannot be ignored, and the coupling of the local moments to conduction electrons is appreciable. We expect a broad distribution of these "Kondo" couplings, leading to an even broader distribution of the corresponding "Kondo temperatures" which represent characteristic energy scales at which *local* Fermi-liquid behavior sets in.

If the resulting distribution of the local Kondo temperatures T_k is sufficiently broad and extends all the way to $T_k=0$, one can expect the behavior of the system to be *qualitatively* changed,[11,12] and the Fermi-liquid regime is not restored at any $T\neq 0$. This kind of *non-Fermi-liquid* behavior, characterized, for example, by a diverging specific-heat coefficient $\gamma=C/T$ at $T\to 0$, is indeed observed in a number of materials containing strong hopping disorder, such as doped semiconductors.[10] The presence of this "disorder-induced local-moment formation" is also expected to play a crucial role in determining the transport properties near the metal-insulator transition.

Disorder-induced local-moment formation in a Hubbard model with random hopping was recently investigated in a Hartree-Fock framework.[13] This approach clearly indicated the presence of *instabilities* to local-moment formation, but did not address the nature of local moments, or their interaction with the conduction electrons needed to determine the properties of the ground state. In contrast, the present approach based on the $d=\infty$ formulation offers a natural language for problems involving the interplay of local disorder fluctuations and strong correlation effects. Furthermore, our approach is *not* limited to a particular temperature interval and thus can be used to obtain results in the entire temperature range.

In order to study the physics of the disordered metallic phase, and the associated disorder-induced local-moment formation, it is useful to consider models of correlated hopping randomness of the form $t_{ij}=y_{ij}x_ix_j$ introduced in Sec. III. In realistic systems such as doped semiconductors, there are large fluctuations in the local hybridization of a given site with its environment originating from randomness in the position of dopant atoms. To represent such systems in our $d=\infty$ framework, it is useful to consider models with broad distributions of local hopping parameters x_i.

A. Binary hopping disorder: two-fluid model

As the simplest example, we consider binary disorder, where the hopping parameter x_i assumes two values x_A and x_B with probabilities c and $1-c$, respectively. This model could represent an alloy[32] with two types of atoms, here denoted by A and B. To study disorder-induced local-moment formation, we consider a situation where one type of site (A sites) has appreciably smaller hybridization (hopping) than the other type (B sites). As the correlation U is increased, the A sites will enter the local-moment regime, whereas the B sites still remain itinerant. This would be the simplest possible scenario, in which the system can be described by a phenomenological "two-fluid" model[14] often used to interpret experiments in materials such as doped semiconductors. Our approach provides a controlled microscopic derivation of the two-fluid model, and permits detailed investigations in the limits of its validity. In particular, the method clearly includes not only the mechanism for local-moment formation, but also the feedback effects associated with the interaction between the two fluids (local moments on sites A, and itinerant electrons on sites B). When the correlation is increased even further, both types of sites enter the local-moment regime, but with different Kondo temperatures T_K^A and T_K^B which define characteristic energy scales of low-energy (delocalized) quasiparticles. Both Kondo temperatures decrease as the correlation is increased, and eventually vanish at the

Mott transition when a gap for charged excitations opens.

To illustrate this scenario, we have used the IPT discussed in Sec. IV to solve explicitly the self-consistency conditions for the considered model of binary hopping randomness. The results are presented in Fig. 4, where we plot the partial and the average densities of state (DOS's) for $t_B=4t_A$ ($t_{A/B}\equiv x^2_{A/B}t$) and $c=\frac{1}{2}$, at $T=0$ and for half-filling, in three correlation regimes. In Fig. 4(a), we show a weak correlation situation $U/D=0.1$ ($D\equiv 2\bar{t}$), where both types of sites are itinerant and the corresponding DOS's are broad, featureless distributions. At intermediate correlation, $U/D=1.6$, the B sites are still delocalized, but the A sites develop local moments; this is most clearly seen by considering the partial DOS's of the two species, as shown in Fig. 4(b). Note the upper and lower Hubbard bands forming on the A sites, as well as the corresponding sharp Kondo resonance at the Fermi surface. Finally, Fig. 4(c) shows the regime of strong correlation $U/D=3.2$, where local moments form on both types of sites, but the system is still metallic due to the Kondo effect.

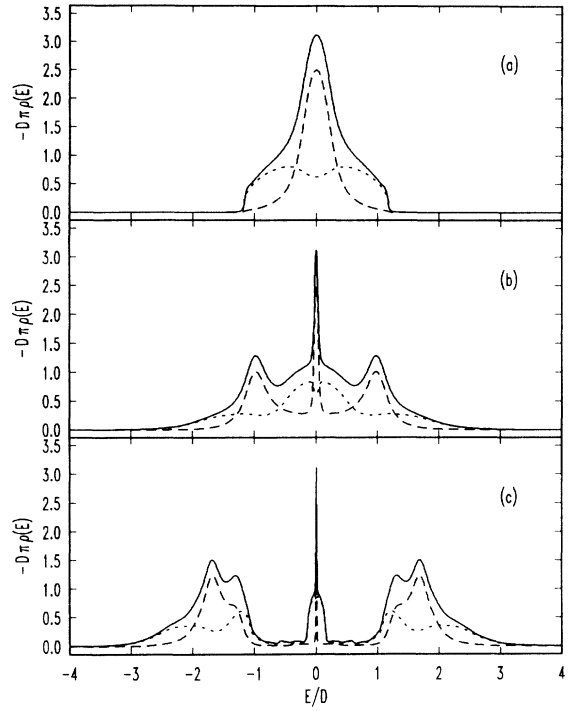

FIG. 4. (a) Single-particle density of states (DOS) as a function of energy (after analytical continuation $i\omega_n\rightarrow E+i\eta$), in the weak correlation regime $U/D=0.1$. The average DOS is shown by a full line, whereas the partial DOS's corresponding to the A and B sites (see text) are plotted by dashed and dotted lines, respectively. (b) Intermediate correlation $U/D=1.6$. Note that the partial DOS of the A site (dashed line) has a form characteristic of a local moment, with the upper and lower Hubbard bands appearing, and a sharp Kondo resonance at the Fermi surface. The B sites (dotted line) are still itinerant. (c) DOS close to the Mott transition, $U/D=3.2$ (strong correlations). In this regime, all sites are in the local moment regime, but with different Kondo temperatures $T_K^A\ll T_K^B$. The system is still metallic due to the Kondo delocalization.

The approach to the Mott transition is easiest to monitor by evaluating the effective masses of each "fluid," which we define from the corresponding self-energies of the Anderson models. These "partial" self-energies are given by

$$\Sigma_A(x;\omega_n)=i\omega_n+\mu-W_x(\omega_n)-[G_x(\omega_n)]^{-1}\ ; \quad (61)$$

the effective masses are then defined by the standard expression

$$m^*_{A/B}/m=\lim_{\omega_n\rightarrow 0}\left[1-\frac{\partial}{\partial i\omega_n}\Sigma_A(x_{A/B};\omega)\right]\ . \quad (62)$$

The variation of these effective masses with the correlation is presented in Fig. 5. As expected, both inverse masses vanish at the same point which signals the disappearance of the quasiparticle bands and the opening of the gap at the Fermi surface–the Mott transition.

The formation of the local moments is even more apparent if we calculate the thermodynamic response of the system. Using the expressions of Sec. III, and the above solution of the self-consistency conditions, it is not difficult to calculate the energy, and thus the specific heat of the system.

The calculation is particularly simple at $T=0$, where the linear coefficient of the specific heat $\gamma=C/T$ can easily be obtained. In the noninteracting limit γ is simply proportional to the DOS, but in the presence of interaction effective-mass corrections have to be introduced. In our case, we find

$$\frac{\gamma}{\gamma_0}=c\frac{m^*_A}{m}\rho_A(0)+(1-c)\frac{m^*_B}{m}\rho_B(0)\ . \quad (63)$$

The partial DOS's $\rho_{A/B}(0)$ are pinned at the noninteracting values, but a strong correlation dependence comes from effective masses. As we can see from Fig. 5, even in the intermediate correlation regime the effective mass on the A sites is strongly enhanced, and thus we conclude that the specific heat will be dominated by the contribu-

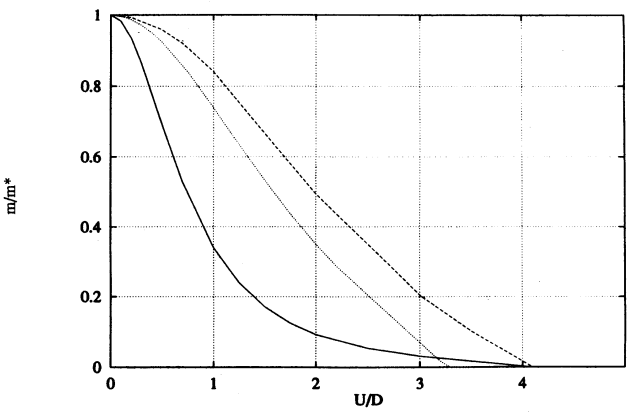

FIG. 5. Inverse effective masses corresponding to the weakly hybridized A sites (full line), and the strongly hybridized B sites (dashed line). Both masses diverge at $U/D=4.1$, signaling the Mott transition. For comparison, we also show the effective mass in the absence of disorder (dotted line); in this limit the Mott transition occurs at a slightly lower correlation.

tion from the "heavy electrons" resulting from local-moment formation.

The calculation can also be extended to $T\neq 0$, and in Fig. 6 we present the resulting specific heat as a function of temperature in the intermediate correlation regime [Fig. 4(b)], corresponding to the coexistence of the local moment and the conduction electrons. As expected, we find linear specific heat at the lowest temperatures $T \ll T_k^A$, where the Fermi-liquid behavior is restored. We also note the presence of a peak in $C(T)$ at $T \sim T_k^A$, typical of the presence of local moments. As in a usual Schottky anomaly, such a peak in the specific heat reflects the presence of a local excitation of energy $E_k^A \sim T_k^A$, in this case corresponding to the energy needed to destroy the local Kondo singlet. It is interesting to observe that at higher temperatures ($T \gg T_k^A$) the specific heat takes an approximately linear form, but with a *finite* $T=0$ *intercept*, so that we can write

$$\gamma(T)=\frac{C(T)}{T}\approx\gamma_0+\frac{T_0}{T} \ . \tag{64}$$

This expression is very similar to the phenomenological two-fluid model[14] of local-moment and conduction electrons, recently advocated as an accurate representation of experimental findings in doped semiconductors[10] near the metal-insulator transition.

Finally, we examine how this disorder-induced local-moment formation modifies the transport properties, in particular the temperature dependence of the conductivity. Typical results are presented in Fig. 7, where we plot the conductivity as a function of temperature for the binary model corresponding to the same parameters as in Fig. 6. As expected in the presence of local moments, the conductivity shows a sharp increase at $T \sim T_k^A$, since at that point the spin-flip scattering from the local moments (on the A sites) is dramatically reduced due to Kondo screening by conduction electrons (on the B sites).

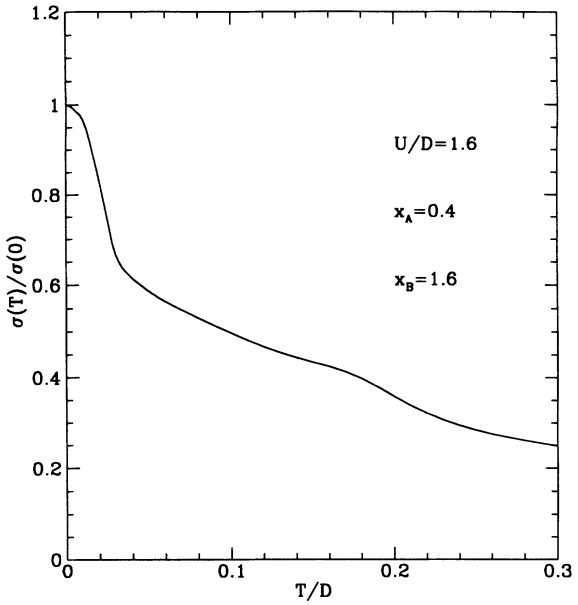

FIG. 7. Temperature dependence of the dc conductivity for the model of Fig. 6. Note the sharp increase in the conductivity at low temperatures, reflecting the onset of coherence due to Kondo screening of the local moments. Low-temperature *enhancements* of the conductivity have been observed in uncompensated doped semiconductors (Ref. 10), but until now this effect was attributed to hydrodynamic interaction effects (Ref. 2) which are absent in our theory.

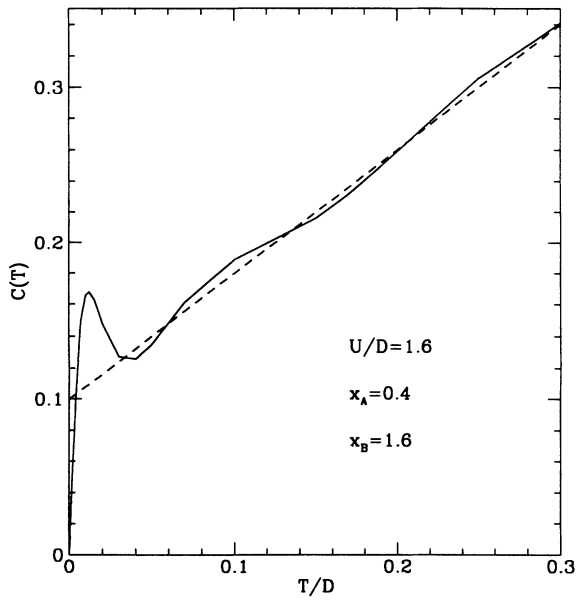

FIG. 6. The specific heat for the binary model of hopping randomness, at an intermediate correlation corresponding to coexistence of local moments and conduction electrons [as in Fig. 4(b)]. Fermi-liquid behavior (linear specific heat) occurs at low temperatures $T < T_k^A \sim 0.01D$. At higher temperatures, the temperature dependence is reminiscent of the phenomenological two-fluid model (Ref. 14) of doped semiconductors [see Eq. (64)].

B. Continuous distributions of hopping: non-Fermi liquids

As we have seen in the above example, in the case of *bounded* distributions of hopping elements x_i, although the local moment formation does occur, the Fermi-liquid behavior is restored below a certain low temperature $T_k^{(\min)}$. On the other hand, if the distribution $P_X(x_i)$ extends all the way to $x_i=0$, the behavior of the thermodynamic and transport properties will display *non-Fermi-liquid* aspects[11,12] even at arbitrarily low temperatures. Some explicit results for the specific heat in the case of a continuous distribution displaying non-Fermi-liquid behavior were presented in Ref. 19. In this paper, we will not present further numerical results for a realistic distribution of disorder and general temperature ranges; these studies will be presented elsewhere. Here we will limit our presentation to a discussion of the asymptotic *low-temperature* behavior that can be determined *analytically* for an arbitrary form of $P_X(x_i)$.

1. Specific heat

We begin with an analysis of the low-temperature form of the specific heat in the present case. To obtain the *leading* temperature dependence as $T \to 0$, we use arguments similar to those used by Bhatt and Fisher[11] and Dobrosavljević, Kirkpatrick, and Kotliar[12] in previous work. As we have seen in Sec. IV, the energy of the system takes an *additive* form with respect to contributions coming from different sites. Those sites that have their respective Kondo temperatures $T_k(i)$ lower than the temperature of the system T, will provide the dominant contributions to the specific heat. To leading order, we can ignore the temperature as well as frequency dependence of the Weiss field $W_i(\omega_n)$. In that case, the contribution from a given site is just that of an Anderson model with hybridization $\Delta(i)=x_i^2\Delta_0$, where Δ_0 is the energy scale corresponding to the *typical* hybridization in the system. Since the sites in question, having very weak hybridization, act as local moments in the Kondo regime, the corresponding Kondo temperature is given by

$$T_k(x_i) \approx D_0 \exp\{-U/x_i^2\Delta_0\} , \tag{65}$$

where D_0 is an energy of the order of the typical bandwidth in the system.

The contribution of a given site to γ is then approximately given by

$$\gamma(x_i) \sim \begin{cases} \dfrac{1}{T}, & T_k(x_i) < T \\ \dfrac{1}{T_k}, & T_k(x_i) > T \ . \end{cases} \tag{66}$$

Collecting the contributions from all the sites with $T_k(x_i) < T$, we find that to leading order

$$\gamma(T) \sim \frac{1}{T} n_{\rm fr}(T) \ . \tag{67}$$

Here the number (fraction) of "free spins"

$$n_{\rm fr}(T) = \int_0^{x^{\max}(T)} dx_i P_H(x_i) \ , \tag{68}$$

and

$$x^{\max}(T) = \left[\frac{\Delta_0}{U} \ln \frac{D_0}{T} \right]^{-2} \ . \tag{69}$$

Using these expressions, it is not difficult to see that for any distribution $P_H(x_i)$ which extends all the way to $x_i = 0$, and having a low-x_i tail longer than exponential (e.g., power law or log normal), the resulting $\gamma(T)$ *diverges* as $T \to 0$. The precise form of this singularity depends on the details of $P_H(x_i)$. However, for any power-law or even log normal form of the low-x_i tail, the quantity $n_{\rm fr}(T)$ decreases to zero as $T \to 0$ *more slowly than any power*, giving an anomalously slow decrease of the number of "free" spins with temperature, and a large anomaly in $\gamma(T)$.

The above arguments rigorously show that for a large class of models with continuous distributions of hopping our $d = \infty$ equations admit *non-Fermi-liquid* metallic solutions. We expect this non-Fermi-liquid behavior of disordered metallic phases to be a generic feature and thus persist even beyond mean-field theory. However, the dependence on the details of the probability distribution for disorder is likely to be an artifact of the $d = \infty$ mean-field theory. Arguments presented in Ref. 12, as well as those in Ref. 44, suggest that fluctuations present in finite dimensions will lead to a *renormalized* distribution of randomness which takes a *universal* form, insensitive to the microscopic details of the system. The fluctuations could also modify the behavior of the conductivity near the metal-insulator transition, possibly leading to modifications in the values of the appropriate critical exponents. We emphasize that the present approach allows for a systematic study of these fluctuation effects, by performing a loop expansion around the mean-field solution.

2. Conductivity

As we saw in Sec. IV, the "pinning condition," which is valid for any model of hopping randomness, guarantees that at particle-hole symmetry (half-filling) the $T=0$ value of the conductivity in the metallic phase remains unaffected by the interactions, and thus by the associated disorder-induced local-moment formation. However, the presence of local moments does induce *anomalous low-temperature corrections* to $\sigma_{\rm dc}$ which could be crucial to understanding the transport properties in systems such as doped semiconductors.

To determine the leading temperature corrections to $\sigma_{\rm dc}$, we proceed in a fashion similar to the discussion of the specific heat. In Sec. III, we saw that, for the models under consideration, the conductivity is expressed through an averaged spectral function $\rho_W(\omega_n)$ that can be written as

$$\rho_W(\omega_n) = \int dx_i P_X(x_i) x_i^2 \rho_i(\omega_n) \ . \tag{70}$$

In this expression, $\rho_i(\omega_n)$ is the local spectral function (of the Anderson model) corresponding to a given site i, and we assume hopping disorder only. In the strongly correlated regime, $\rho_i(\omega_n)$ has a sharp (Kondo) peak near the Fermi surface, describing the coherent quasiparticles. As the temperature is increased from zero, inelastic scattering will destroy the existence of this coherent peak at a characteristic temperature T_k. However, in a *random* system, this process takes place *locally*, and a given *site* becomes "incoherent" at $T \sim T_k(x_i)$, when this Kondo resonance is washed out. Thus, in contrast to the thermodynamic response, appreciable contributions to the conductivity come from those sites with $T_k(x_i) > T$, which remain coherent. More precisely,

$$\rho_i(\omega_n \to 0) \sim \begin{cases} 0, & T_k(x_i) < T \\ \dfrac{1}{x_i^2 \Delta_0}, & T_k(x_i) > T \ . \end{cases} \tag{71}$$

Again, to leading order we can ignore the frequency dependence of $\rho_i(\omega_n)$, and we find (at $\omega_n \to 0$)

$$\rho_W(T)\sim\int_{x_{\max}(T)}^{+\infty}dx_i P_\chi(x_i)\ . \tag{72}$$

By using this result and Eq. (42), we conclude that the leading low-temperature correction to the dc conductivity assumes the form

$$\delta\sigma_{\rm dc}(T)=\sigma_{\rm dc}(T)-\sigma_{\rm dc}(0)\sim -n_{\rm fr}(T)\ , \tag{73}$$

i.e., we find an anomalous increase as $T\to 0$.

It is interesting to note that, although $n_{\rm fr}(T)$ vanishes more slowly than any power as $T\to 0$, for realistic distributions[11,12] one can write

$$n_{\rm fr}(T)=T^{\alpha(T)}\ , \tag{74}$$

where $\alpha(T)$ only very weakly, typically *logarithmically*[11,12] depends on temperature. Experimentally, one expects to measure some *effective* exponent α. As $\alpha\to 0$ at $T\to 0$, one expects these effective exponents to be small. This behavior should be contrasted with the fact that similar, nonanalytic finite temperature corrections to the conductivity of dirty metals follow from *weak localization and interaction* effects.[2] Our results suggest that such temperature dependence could have an entirely different origin—due to disorder-induced local-moment formation. Of course, a full theory should include both the local moments and the aforementioned hydrodynamic (diffusion) corrections.[2,7] In the framework of our approach these additional terms would appear at the level of *one-loop* corrections to the $d=\infty$ (mean-field) expressions.

VII. COMPARISON WITH EXPERIMENTS

After three decades of intensive investigations, there are various constraints on theoretical models of uncompensated doped semiconductors. In the following, we list these constraints and comment on how our perspective fares *vis a vis* the experiments.

(1) At the accessible temperatures, the thermodynamic quantities χ and γ vary smoothly[10] as a function of concentration across the transition, and are increasing functions of the inverse temperature even throughout the metallic phase.

(2) The NMR experiments[46] portray a strongly inhomogeneous picture. There is a wide distribution of Knight shifts on the phosphorus sites. As the transition is approached, a large number of sites acquire Knight shifts that are larger than the measurable range, indicating the formation of local moments. The Knight shift on Si is a smoother function of concentration,[46] suggesting that the metal-insulator transition takes place in the phosphorus impurity band. Furthermore, $1/T_1T$ obeys the Korringa law, suggesting that the susceptibility is momentum independent.

(3) Finkelshtein has emphasized[47] that the electron-spin resonance (ESR) linewidth[48] $\Delta H_{1/2}$ is proportional to χ. Since $\Delta H_{1/2}$ is proportional to $\sum_q \chi(q)$, this indicates that the *divergent* part of the susceptibility is roughly q independent.

(4) The thermodynamic behavior should be contrasted with measurements of charge transport, which vary much more rapidly near the transition. The $T=0$ extrapolated value[10] of the conductivity vanishes with an exponent μ which is thought to be close to $\frac{1}{2}$. However, no dynamical scaling range in temperature and concentration has been observed, making the determination of the exponents ambiguous. In particular, values of the conductivity exponent ranging from $\mu=0$ (Ref. 49) to 1 (Ref. 50) have been obtained on the basis of the *same* data.

(5) Small amounts of compensation or the external magnetic field are very relevant perturbations[10] that alter dramatically the critical behavior of the conductivity. Significant differences between compensated and uncompensated samples are also seen in the high-temperature extrapolation of the linear term in the specific heat[51] $\gamma_{\rm HT}$. The compensated sample has a $\gamma_{\rm HT}$ which varies smoothly at the transition, while in the uncompensated case $\gamma_{\rm HT}$ drops sharply at n_c indicating the presence of a Mott-Hubbard gap.

(6) Spin-orbit scattering, however, is an *irrelevant* perturbation[52] since Si:B (where spin-orbit scattering is dominant) shows a behavior similar to Si:P.

The approach presented in this paper, on the most qualitative level, is consistent with all these observations *on the metallic side.* The collection of Anderson impurity models as a mean-field theory of the disordered Hubbard model provides a microscopic realization of the two-fluid model which phenomenologically explains (1)–(3). The local inhomogeneity of the system described in (2) is naturally captured in our formulation. The weakly coupled sites can be thought of as the P donors, where the wave functions of the delocalized electrons are concentrated. The q independence of the thermodynamic response discussed in (2) and (3) is directly built in our formulation at the mean-field level. The loop expansion corrections will bring possible departures from this behavior.

Underlying this picture is a broad distribution of energy scales which makes the Mott transition in dirty systems very different from those in the pure case. The conductivity goes discontinuously to zero at $T=0$, but at any finite temperature is a rapidly varying continuous function. This observation may account for the lack of scaling, but here the loop corrections to mean-field theory might modify the effective exponents. In our model, the relevant perturbations are those that cause departures from *particle-hole symmetry.* Our approach thus justifies the fact that the *uncompensated* semiconductors represent a unique universality class.

VIII. CONCLUSIONS

In summary, we have presented a nonperturbative approach to strongly correlated disordered electrons. Even on a mean-field level, our results agree with many of the surprising features found in doped semiconductors. Furthermore, our formulation also allows for systematic corrections to the mean-field description, which makes possible a detailed investigation of the interplay of the Anderson localization and strong correlation effects. A large number of problems could be addressed using our approaches, but several specific directions appear particularly promising.

One of the most interesting results that we found is that the combination of hopping randomness and strong correlation can lead to disordered-induced local-moment formation, resulting in *non-Fermi-liquid* metallic behavior even away from the transition. By performing a loop expansion around such solutions, we can study the effect of local moments on weak localization and interaction effects[2] which were the focus of the scaling theories of localization. One could also study how these hydrodynamic effects would be affected by the approach to the *Mott transition,* where low-energy spin fluctuations emerge. In this way, our approach shows explicitly how the existing theories for the metal-insulator transition[5–9] should be modified to account for strong correlation effects.

Our theory can also be extended to models that display *non-Fermi-liquid* behavior, even in the absence of disorder. For example, extended Hubbard[27] models and multichannel Kondo lattice models[24] can be formulated and solved in the $d = \infty$ framework. Effects of weak disorder in such incoherent metals could then be examined by performing a loop expansion around the mean-field solution. In this way, one could make predictions about the weak localization corrections in materials such as high-T_c compounds.

Another interesting direction involves developing a mean-field theory for the metal-insulator transition that would encompass both Anderson and Mott mechanisms for localization on the same footing. In the framework of the large dimensional approach, such a theory can be formulated by examining disordered Hubbard models on Bethe lattices with large but finite coordination. For these models, the problem can be reduced[41] to the solution of a coupled set of stochastic equations describing an ensemble of Anderson impurity models. Such equations can be studied by a variety of methods, ranging from numerically exact simulation techniques to approximate analytical schemes. Once these equations are solved, an interesting picture will emerge, bringing us closer to the long-awaited solution of the Anderson-Mott problem.

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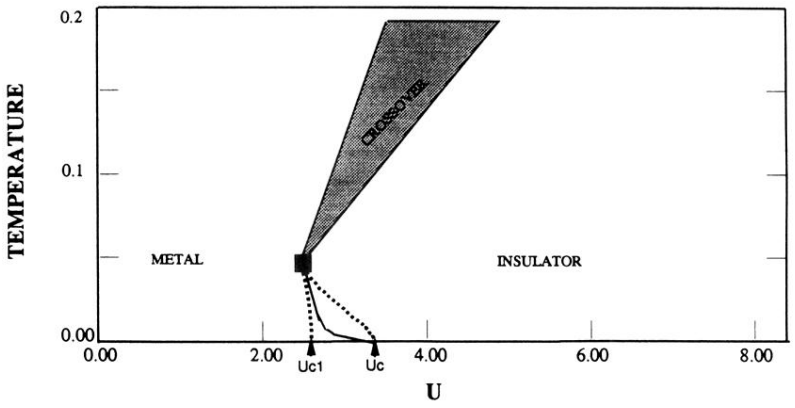

FIG. 1. Phase diagram of the pure Hubbard model in $d = \infty$ (following Ref. 22), as a function of correlation strength U and temperature T. The finite temperature first-order metal-to-insulator transition is shown by a full line, and the boundaries of the coexistence region by dashed lines. At $T = 0$ the metallic solution is lower in energy throughout the coexistence region, and so $U = U_c$ represents the zero-temperature transition point.