Hubbard Models with Random Hopping in $d = \infty$

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A class of Hubbard models with random hopping is examined as models of strongly correlated electrons in disordered systems. In the limit of large spatial dimensionality the problem is reduced to solving an ensemble of self-consistently determined Anderson impurity models. Even at intermediate correlation, disorder-induced local moment formation occurs, leading to a diverging specific heat coefficient *inside* the metallic phase. For stronger correlation, the system undergoes a metal-insulator transition where the dc conductivity abruptly drops to zero, displaying minimum metallic conductivity.

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The thermodynamic and transport properties of disordered interacting electrons near the metal-insulator transition (MIT) represent a subject of considerable current interest [1]. Many such systems have been studied experimentally; some of them seem to exhibit a continuous transition [2] at zero temperature, while a minimum metallic conductivity interpretation has been advocated for others [3]. The description of the metallic state near the transition in terms of Fermi-liquid ideas [4] has been questioned [5,6], and the role of low energy local magnetic fluctuations (local moments) has been stressed [7,8].

Theoretically, very little is understood. For interacting electrons, a long wavelength effective Lagrangian was derived by Finkelshtein [9] who devised a renormalization group (RG) procedure for this model. The theory is closely related to Fermi-liquid concepts [10] and does not contain explicitly the local moments which might be present at short distance scales. The RG analysis of this long wavelength theory near two dimensions has so far been inconclusive, because the RG flow leads to a strong coupling running away of the triplet interaction amplitude, which cannot be treated systematically. It has been suggested that this signals some magnetic instability [9], 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 [10]. Other interpretations have also been proposed [11].

Given the approximations involved in the derivation of the long wavelength theory [9] and the known shortcomings of the perturbative $2+\varepsilon$ expansion [12], it is clearly of interest to study other limits of this problem where one can obtain reliable results by means of controlled approximations. In this Letter we examine a class of models of interacting disordered electrons in the limit of infinite dimensions.

The physical questions that we would like to address include the following: (1) Does spin localization precede charge localization, or do they occur simultaneously at the metal-insulator transition? (2) How does the conductivity behave in the vicinity of the MIT? In the framework of our model we have been able to answer these questions. At finite temperature, the thermodynamics is dominated by local moments and spin localization precedes the metal-insulator transition. The energy of the system is additive, and can be thought of as a sum of two components: local moment and conduction electrons, providing a microscopic justification for the success of the "two fluid" picture of Ref. [7]. For sufficiently long-tailed distributions of hopping elements, this leads to a divergent specific heat coefficient at $T \to 0$, even *inside* the metallic phase. At $T=0$, a metal-insulator transition is found where the conductivity discontinuously jumps to zero, displaying minimum metallic conductivity.

The class of models that we consider are Hubbard models with off-diagonal disorder, corresponding to a Hamiltonian of the form

$$H=\sum_{ij}\sum_{\sigma}[-t_{ij}+\varepsilon_i\delta_{ij}]c_{i,\sigma}^{\dagger}c_{j,\sigma}+U\sum_i c_{i,\uparrow}^{\dagger}c_{i,\uparrow}c_{i,\downarrow}^{\dagger}c_{i,\downarrow}\,. \tag{1}$$

The random hopping elements are assumed to take the form $t_{ij}=y_{ij}f(x_i,x_j)$, and in addition, there can be an arbitrary distribution of site energies ε_i. Here, the y_{ij}'s are independent bond variables with a symmetric distribution, i.e., $\overline{y_{ij}^{2n+1}}=0$, and $f(x_i,x_j)$ is an arbitrary function of local site variables x_i.

In general, finding exact solutions of such models is not possible, but considerable simplifications occur in the limit of large spatial dimensionality [13,14]. In this limit, all local correlation functions can be evaluated with respect to a local effective action of the form

$$\begin{aligned}S_{\rm eff}(i)=&\sum_{\sigma}\int_0^{\beta}d\tau\int_0^{\beta}d\tau' c_{i,\sigma}^{\dagger}(\tau)[\delta(\tau-\tau')(\partial_\tau+\varepsilon_i-\mu)\\&+W_{i,\sigma}(\tau,\tau')]c_{i,\sigma}(\tau')\\&+U\int_0^{\beta}d\tau\, c_{i,\uparrow}^{\dagger}(\tau)c_{i,\uparrow}(\tau)c_{i,\downarrow}^{\dagger}(\tau)c_{i,\downarrow}(\tau)\,.\end{aligned} \tag{2}$$

Here, the Fermi fields $c_{i,\sigma}(\tau)$ represent electrons of spin σ on site i, μ is the chemical potential, and β is the inverse temperature. The "Weiss field" $W_{i,\sigma}(\tau,\tau')$ is obtained by formally integrating out all the degrees of freedom on other sites in the lattice, in the large d limit. The self-consistency condition determining $W_{i,\sigma}$ is

$$W_{i,\sigma}(\omega_n)=\sum_j t_{ij}^2 G_{j,\sigma}(\omega_n)\overset{d\to\infty}{\longrightarrow}\overline{t_{ij}^2 G_{j,\sigma}(\omega_n)}\,, \tag{3}$$

where $G_{j,\sigma}(\omega_n)=\langle c_{j,\sigma}^{\dagger}(\omega_n)c_{j,\sigma}(\omega_n)\rangle$ are the local Green's

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functions evaluated with respect to the effective action of Eq. (2). For the considered class of models with random hopping, these expressions are valid on an *arbitrary* lattice. The same expressions are also valid for a Bethe lattice with an *arbitrary* form of disorder. Similar expressions can be derived for other lattices and forms of disorder [15], but will not be discussed here, since these modifications do not lead to qualitative changes. The results are obtained by an appropriate scaling [16] of the hopping elements, so that the kinetic energy remains finite as $d \rightarrow \infty$, and keeping only the leading terms in the $1/d$ expansion. Note that in the large d limit, due to self-averaging, the sum in Eq. (3) is replaced by an average over disorder, and $W_{i,\sigma}$ becomes a function of local disorder parameters only.

The special class of models which have a symmetric distribution of hopping elements has a very simple physical interpretation. As first observed by Wegner [17], 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 in this large dimensionality limit, the local effective action, Eq. (2), for every lattice becomes identical as on the Bethe lattice.

In order to clarify the generality of our methods, we have developed an alternative derivation of the self-consistent equations, Eqs. (2) and (3), by using a saddle-point approach. In this formulation, which we will only sketch here, one first formally integrates out the random bond variables y_{ij} by using the replica trick. The new term coming from disorder is then decoupled by introducing collective Q fields by a Hubbard-Stratonovich transformation, similarly as in the approaches of Wegner [17] and Finkelshtein [9]. The resulting partition function can be calculated by carrying out a saddle-point analysis in the Q fields, which becomes exact as $d \rightarrow \infty$. The saddle-point value of the collective field Q is the "Weiss field" $W(\omega_n)$, and we recover the self-consistency equations, Eqs. (2) and (3). The details of the calculation will be discussed elsewhere. Here we just observe that our approach represents a particularly elegant method for purposes of extending the theory to finite dimensions, by simply performing a loop expansion around the $d \rightarrow \infty$ saddle point. Note that this theory, in contrast to the formulation of Finkelshtein, builds nonperturbative strong correlation effects even at the saddle-point level, which in principle allows a detailed study of the interplay of the localization physics with strong correlation aspects.

We have argued that for the considered class of models, the *local* properties such as the local density of states do not depend on the nature of the lattice, but only on the (average) number of neighbors. In contrast, various instabilities such as the spin and charge density wave formation depend very strongly on the nesting properties of the lattice. A number of strongly correlated disordered systems such as doped semiconductors [2,3] do have random hopping, but do not have magnetic instabilities, presumably due to the large frustration introduced by random arrangements of dopant atoms. To study such systems, we can limit our attention to such lattices where geometric frustration disfavors magnetic ordering, but does not modify local properties. In the clean case, a number of such lattices have been discussed in the literature [13,18,19]. In the following, we will limit our attention to paramagnetic solutions appropriate to the physical systems in question.

The local effective action of Eq. (2) is identical to the action of an Anderson impurity model [20] with a given hybridization function $\Delta(\omega_n) \sim W(\omega_n)$, so that the problem is reduced to solving an *ensemble* of Anderson impurity models with an additional self-consistency condition that includes disorder averaging. Using the known theorems for Anderson models, it is now possible to make several exact statements about the model.

In particular, for particle-hole symmetric situations [hopping disorder and half filling $(\mu - U/2)$] at $T=0$, the self-energy of the Anderson model $\Sigma(\omega=0) - U/2$ as long as $\Delta(0) \neq 0$ (in the metallic phase), so that both $W_{i,\sigma}(\omega=0)$ and $G_{i,\sigma}(\omega=0)$ remain *pinned* to their respective noninteracting values. As we will show, the result is that the dc conductivity at $T=0$ remains unrenormalized in the metallic phase. We calculate the conductivity in a model with uncorrelated random hopping elements with a symmetric distribution, i.e., $t_{ij} = y_{ij}$ (see above), and $\overline{y_{ij}^2} = t^2$. More complicated forms of hopping disorder lead to no qualitative changes in behavior of the conductivity. Using a Kubo formula [21] to relate $\sigma(\omega)$ to the current-current correlation function, it is possible to show that in this case a particularly simple expression for the real part of $\sigma(\omega)$ can be obtained:

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

where $\rho(\omega)$ is the single-particle spectral function (at temperature T) of the *pure* Hubbard model with hopping t with a semicircular density of states, and $f(\omega)$ is the Fermi function. Using the methods of Refs. [13,14] for the calculation of $\rho(\omega)$, we have plotted σ_{dc} at half filling in Fig. 1, as a function of the interaction U and the temperature T. At $T=0$, pinning is observed and σ_{dc} remained unrenormalized by the interactions until U_c is reached, where it discontinuously jumps to zero, displaying minimum metallic conductivity. The first order jump persists at finite but very low 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. Interestingly, a very similar scenario was advocated as a phenom-

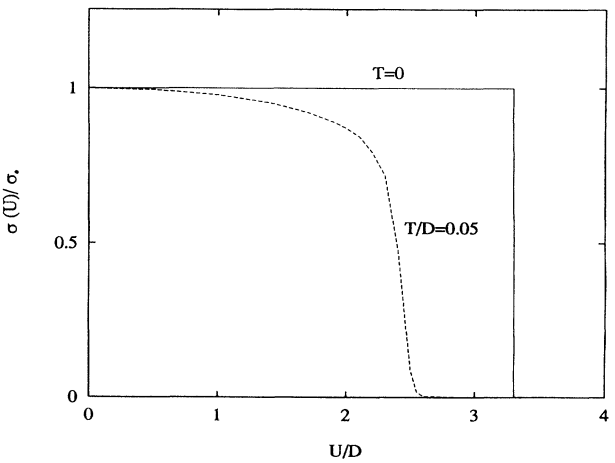

FIG. 1. dc conductivity of the infinite dimensional Hubbard model with random hopping, at half filling. σ_{dc} is plotted in units of σ_0, the $U=0$ value. The full line shows the $T=0$ behavior, displaying minimum metallic conductivity. At finite temperature $T=0.05>T^*$ (in units of the half bandwidth $D=2t$), σ_{dc} decreases *continuously* as the correlations grow, as shown by the dashed line.

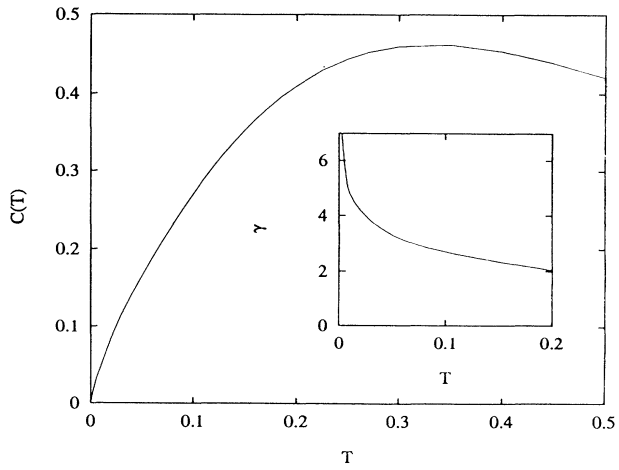

FIG. 2. The specific heat of the infinite dimensional Hubbard model with random hopping, at intermediate correlation. All the energies are measured in units of $U=x_0$ (see text). In contrast to the pure case $C(T)$ is *not linear* even at the lowest temperatures, displaying *non-Fermi-liquid* behavior. This is presented even more clearly by plotting the specific heat coefficient $\gamma=C/T$ as a function of temperature (inset), which is found to *diverge* as $T\to 0$.

enological description of experimental findings in some materials near the MIT [3]. In these materials, the disorder largely originates from the random positions of dopant atoms, so the above scenario that considers the particle-hole symmetric situation can be expected to be an appropriate one. In realistic systems, *in addition* to random hopping there is also randomness in the site energies. Although in that case the pinning condition is not observed, and thus the dc conductivity is not strictly independent of the correlation U, preliminary work [22] shows that even in that case our *qualitative* conclusions remain valid.

In many systems near the MIT, the thermodynamics was found to be consistent with the presence of local magnetic moments [2,3], even in situations without extrinsic magnetic impurities. It has been suggested that such behavior originates from disorder-induced local moment formation [8], in particular on those sites which are only weakly hybridized with the rest of the system. In order to study this behavior, we turn our attention to a model of hopping randomness of the form $t_{ij}=y_{ij}x_ix_j$, where x_i are local random variables. Those sites with x_i small represent the sites with weak hybridization. In this model of correlated hopping randomness, local disorder fluctuations survive even in the $d\to\infty$ limit, permitting the study of disorder-induced local moment formation. Similar results can be obtained for other models of hopping randomness. At intermediate correlation, we expect the sites with x_i small to behave as local moments and give large contributions to the thermodynamic quantities such as the specific heat coefficient $\gamma=C/T$, while other sites remain in the itinerant regime.

These ideas can be made more specific by calculating the energy [21] of the system, which in the $d\to\infty$ limit assumes the form

$$E(T)=\int dx\,P(x)\frac{1}{\beta}\sum_n [i\omega_n+\mu+W_x(\omega_n)]G_x(\omega_n)\,, \quad (5)$$

where $P(x)$ is the probability distribution for the local random variable x, and W_x and G_x correspond to sites with a given value of x. As an illustration, we have examined a continuous distribution $P(x)\sim x^2, x\in(0,x_0)$ and calculated the specific heat $C(T)=\partial E(T)/\partial T$ as a function of temperature. The value of U was taken to be $U=x_0$, so as to correspond to intermediate correlation (U of the order of half the average bandwidth). By using the methods of Refs. [13,14], we have obtained an essentially exact numerical solution of the self-consistency equations for the considered model of randomness. The results presented in Fig. 2 show that, in contrast to the pure case, $C(T)$ *does not* behave linearly with temperature in *any* temperature range, so that $\gamma=C/T$ (shown in the inset) diverges as $T\to 0$. Such *non-Fermi-liquid* [5,6] behavior has been observed in a number of dirty metals near the MIT. It simply reflects the existence of a wide distribution of local Kondo temperatures [5,6] in a random system. Using arguments similar to those in Refs. [5] and [6], we have constructed an analytic proof that γ indeed diverges as $T\to 0$ in our model. The asymptotic form of $\gamma(T)$ can be obtained, and proves to depend on the details of the probability distribution for disorder [23]. For bounded distributions of hopping elements, $\gamma(T)$ saturates to a large but finite value at $T=0$, and the

Fermi-liquid behavior is restored. Again, additions of random site disorder will only quantitatively modify our results. The present approach is to our knowledge the first calculation to display such an exotic behavior as a solution of a microscopic model containing both strong correlations and disorder. We emphasize that our methods allow us to obtain results in the *entire* temperature range, where the behavior can be dominated by *incoherent* processes, which are ignored in most other treatments.

In conclusion, we have examined a class of microscopic models that permit detailed investigations of disordered interacting electrons. As we have shown, a *qualitatively* new metallic behavior results from the interplay of disorder and strong correlations. Earlier work [9,10] suggested that in the general case the interplay of disorder and interactions can drive the system (in the RG sense) to a regime of strong correlations but weak disorder. This is the regime studied in the present paper. The metal-insulator transition that we find is driven by the interaction effects in a diffusive regime, since the localization effects are absent in infinite dimensions. However, by performing a loop expansion around our mean-field solution, this work can be extended to large but finite dimensions where the details of the interplay of Anderson localization and strong correlations can be studied in a controlled fashion.

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[23] We expect the 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. [6], as well as those in Ref. [24], 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 fluctuations effects, by performing a loop expansion around the mean-field solution.

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