Disorder and Interactions in the Hubbard Model

Gergely T. Zimanyi
Department of Physics, University of California, Davis, California 95616

Elihu Abrahams
Serin Physics Laboratory, Rutgers University, P.O. Box 849, Piscataway, New Jersey 08855
(Received 12 March 1990)

We investigate the single-band Hubbard model with random site energies in the strong-repulsion limit, as represented by the slave-boson formulation of the t-J model. It is essential to include the correlations between the slave-boson mean field and the disorder. This leads to the widening of the non-Fermi-liquid ("generalized Mott insulating") region around half filling. In the Fermi-liquid regime we apply the renormalization-group method. The resulting phase diagram has superconducting, magnetic, and insulating phases. The disorder generally suppresses superconductivity and gives rise to the formation of localized magnetic moments.

PACS numbers: 71.30.+h, 72.15.Rn, 74.65.+n

The modern scaling theory of localization,[1,2] originally developed to describe the Anderson transition for noninteracting electrons, was later extended to include effects of electron-electron interactions.[3,4] In the absence of interactions[2] and in two dimensions, logarithmic singularities appear in the two-particle correlations as modified by the disorder. For any disorder strength, the conductivity decreases logarithmically as temperature decreases (or length scale increases). At dimensions greater than two, the logarithmic singularities sum to power-law behavior which describes the continuous disappearance of the conductivity at a mobility edge determined by a critical value of the disorder. These results were subsequently reformulated as a renormalization-group (RG) treatment of a matrix nonlinear-σ-model field theory of the long-wavelength disorder-coupled (particle-particle and particle-hole) diffusion modes of the system.[1,4,5]

Finkel'shtein[4] extended the RG treatment of the scaling theory to include interaction effects. The disorder was treated in lowest order and all interaction contributions to the leading logarithmic behavior were summed. This investigation demonstrated that the diffusive propagation of electrons due to the disorder gives rise to strongly enhanced interactions which can eventually lead to the localization of the electrons. This process is accompanied by the buildup of local magnetic moments and the vanishing of the quasiparticle diffusion constant. However, the RG equations break down in a region where the charge diffusion is still nonzero, although the spin-diffusion constant is going to zero and the spin susceptibility is diverging. Whether or not the localization of spin and charge happen simultaneously is presently a subject of active research.[6]

The failure of these earlier approaches to succeed to give a complete picture is due in part to the fact that they are essentially perturbative in that the interactions are assumed to be smaller than the bandwidth. Thus, firm conclusions cannot be drawn when the couplings scale to large values. It is therefore natural to investigate the problem starting from the strong-coupling limit at the outset. In order to approach the interplay of the Mott and the Anderson transition from a complementary angle, in the present work we investigate the strongly interacting disordered electron system using the Hubbard model. The use of the Hubbard model has the advantage that one may include the effect of commensurability, which is an essential ingredient of the Mott transition. We are then also able to draw some qualitative conclusions about the nature of the problem close to half filling where a Mott transition is expected even in the absence of disorder. Some progress describing the situation microscopically from the large-correlation limit has been made recently[7] within a Hartree-Fock treatment of the Hubbard model, with off-diagonal disorder treated exactly by numerical methods. The strong-correlation point of view is of interest not only for doped semiconductors near their metal-insulator transition[8] but also, in particular, for heavy-fermion materials and high-T_c superconductors. Since, in the weak-coupling theories,[3,4,6] the effective interactions scale to strong coupling, we expect a connection of our approach to the earlier work.

We begin with a disordered Hubbard model in the large-U limit. The disorder appears as a random distribution of local site energies (diagonal disorder). After redefining the vacuum to prevent double occupancy, one performs a t/U expansion to arrive at an effective Hamiltonian, the so-called t-J model:[9]

$$\mathcal{H} = -t\sum_{\langle i,j\rangle,\sigma} b_i^\dagger b_j c_{j,\sigma}^\dagger c_{i,\sigma} + \text{H.c.} + \sum_{i,\sigma}(\epsilon_i-\mu)c_{i,\sigma}^\dagger c_{i,\sigma} - \frac{J}{N_s}\sum_{\langle i,j\rangle\sigma,\sigma'} c_{i,\sigma}^\dagger c_{j,\sigma} c_{j,\sigma'}^\dagger c_{i,\sigma'} - \lambda\sum_i\left(\sum_\sigma c_{i,\sigma}^\dagger c_{i,\sigma} + b_i^\dagger b_i - 1\right), \quad (1)$$

where N_s is the spin degeneracy and the site energies ϵ_i

are Gaussian random variables with zero mean and rms value W. In terms of the parameters of the original Hubbard model, $J=4t^2/U$. We have utilized the slave-boson formalism[9] to perform the projection on the subspace of singly occupied sites. This constraint is enforced through the minimization of the free energy with respect to the Lagrange multiplier λ. In the following, we shall treat the slave bosons in a mean-field approximation which is justifiable only for $N_s \gg 1$.

The conventional approach would be now to perform a translationally invariant mean-field approximation for the slave-boson field, $\langle b \rangle = (1-n_c)^{1/2}$, which yields a reduced bandwidth $t_{\rm eff} = tb^2 = t(1-n_c)$, where n_c is the number of electrons per site, and then to treat the interaction term. The insufficiency of this approach was pointed out by Rice and Ueda[10] in a slightly different context. They emphasized the importance of the correlations between the slave-boson amplitudes and the random site energies. We represent these correlations in linear response as follows: $b_i = b_0 + \chi_i \epsilon_i / 2b_0$, where $\chi_i = \partial n_{c_i}/\partial \mu \approx -\partial n_{c_i}/\partial \epsilon_i = \partial b_i^2/\partial \epsilon_i$. Here χ_i denotes the charge susceptibility. Our approximation is that the site i is imbedded in a Fermi liquid representing the average behavior ($\epsilon = 0$) of the other sites. This one-site problem is analogous to the single-Anderson-impurity problem for which the charge susceptibility is known:[11] $\chi_i \approx \chi_A = b_0^2/t$. The approximation here may be improved by including the influence of nearest-neighbor site-energy variations by means of the nonlocal charge susceptibility which may be obtained from the treatment of the two-Anderson-impurity Ruderman-Kittel-Kasuya-Yosida problem.[11] With these considerations the Hamiltonian takes the form

$$\mathcal{H} = -tb_0^2 \sum_{\langle i,j \rangle, \sigma} (1 + b_0 \epsilon_i / 2t)(1 + b_0 \epsilon_j / 2t) c_{i,\sigma}^\dagger c_{j,\sigma} + \text{H.c.} + \sum_{i,\sigma} (\epsilon_i - \mu) c_{i,\sigma}^\dagger c_{i,\sigma} - \sum_{k,k',q,\sigma,\sigma'} \frac{J(q)}{N_s} c_{k,\sigma}^\dagger c_{k',\sigma'}^\dagger c_{k-q,\sigma} c_{k'+q,\sigma'} + \mathcal{H}_{\rm constraint}, \quad (2)$$

where $J(q) = J[\cos(q_x) + \cos(q_y)]$.

Now we can make the central observation of the paper: The Hamiltonian of Eq. (2) describes an interacting disordered Fermi liquid in the weak-coupling regime [for $t(1-n_c) \gg J$)]. Therefore, the methods developed[4] for such systems can be applied, the main difference being that now the interactions are attractive, as can be seen from the sign of the interaction term in Eq. (2).

A few remarks are in order here. At present, the general belief is that close to half filling, magnetic fluctuations play an important role and possibly destroy the Fermi-liquid behavior. Thus our observation applies only farther away from half filling, as is required in any case by the above criterion for weak coupling. Second, one may wonder how the strongly repulsive model became attractive. The reason is that the repulsive core of the interaction potential is so large that on-site charge fluctuations are practically absent and therefore the core is completely excluded from the low-temperature dynamics (an effect which is insured by the slave bosons). On the other hand, the screening Friedel oscillations provide an attractive effective potential on the nearest-neighbor site, which determines the low-energy behavior. Third, most of the work on such systems concentrated on site disorder only. We have disorder in the hopping amplitudes as well; it is introduced by the constraint as seen in Eq. (2). As we demonstrate below, however, the random variables can be integrated out exactly and in a mean-field approximation the disorder on the bonds leads only to a renormalization of the parameters.

Even close to half filling some features of the model are qualitatively correct: A metal-insulator transition is expected according to the Mott scenario as we approach half filling and indeed the effective bandwidth goes to zero as $\sim(1-n_c)$; consequently, the conductivity vanishes also. Actually, we enter the strong-coupling region before reaching half filling, when $J/t_{\rm eff} \sim 1$. In this regime (which can be called the generalized Mott insulator), the still longer-range magnetic correlations render the materials insulating, as in the usual treatments of the t-J model at small dopings.[12]

The influence of disorder on this (generalized) Mott metal-insulator transition can be obtained by averaging the constraint equation:

$$1 - n_c = \langle b_i^2 \rangle = b_0^2 + \frac{1}{4b_0^2} \chi^2 \langle \epsilon_i^2 \rangle = b_0^2 \left(1 + \frac{W^2}{t^2} \right). \quad (3)$$

Thus, the effective bandwidth is reduced by the disorder according to $t_{\rm eff}^0 = t(1-n_c)/(1+W^2/t^2)$. It is seen that the weak-coupling condition breaks down further from half filling: The Mott insulating phase is *extended by the disorder*. The absence of b^2 in the last term's denominator was one of the main points of Ref. 10 in the analogous Anderson-impurity problem.

We proceed analogously to Finkel'shtein's treatment[4] by introducing a functional integral over (Matsubara) frequency-dependent Grassmann variables to represent the fermions. The quenched average over the random configurations is achieved by the usual replica trick.[4,13] The disorder is integrated out exactly over a Gaussian distribution of width W. Since the terms linear in the ϵ_i have coefficients bilinear in the c's, this procedure yields a translationally invariant action with a mixed replica four-fermion interaction, as in Ref. 4. However, the terms of Eq. (2) which contain the charge susceptibility introduce, in addition to the usual on-site terms, a coupling between nearest-neighbor sites as well. The mean-field factorization of the on-site terms defines a lifetime τ. A new feature comes from the similar treatment of the nearest-neighbor term. A further reduction of the effective bandwidth is found: $t_{\text{eff}} = t^0_{\text{eff}}(1 - W^2/4t^2)$.

The next task is to carry out a two-step renormalization procedure. First, all states outside an energy strip around the Fermi level of width $1/\tau$ are integrated out through, e.g., a mean-field or a random-phase approximation. It has been shown[12] in the nondisordered case that the mean-field approach yields the enhancement of some of the effective dimensionless couplings Γ (where $\Gamma_0 = J/t_{\text{eff}}$), primarily in the d-wave superconducting channel, with a lesser rise in the s-wave superconducting and magnetic channels. On the other hand, the coupling in the particle-hole charge channel is suppressed. Since in this energy region the length scales are shorter than the elastic mean free path l, this behavior of the effective couplings is not changed qualitatively by the disorder.

In the second stage of the scaling, one integrates out the states within the $1/\tau$-wide strip around the Fermi energy. Here, the disorder averages out the anisotropies of the physical quantities, preserving only their s-wave components. In this long-wavelength regime, the momenta are confined to small values and $J(q)$ can be approximated by its $q=0$ value. This effect appears formally as a strong suppression of the energy-dependent effective non-s-wave components of the couplings. This has been shown, for example, for the d-wave superconducting amplitude:[14]

$$\Delta(k) \approx \Delta_s \left[1 + \frac{\gamma^d(k)}{1 + i/2\omega\tau} \right], \tag{4}$$

where $\gamma^d(k)$ is the d-wave structure factor. Therefore, we neglect the anisotropic amplitudes and utilize the known scaling relations for the isotropic short-range couplings:[4]

$$\frac{dg}{dx} = \frac{g(2-d)}{2} + g^2 \left[4 - 3\frac{1+\gamma_s}{\gamma_s}\ln(1+\gamma_s) - \gamma_C \right], \tag{5a}$$

$$\frac{d\gamma_s}{dx} = \frac{g}{2}[(1+\gamma_s)^2 + 2\gamma_C(1+3\gamma_s+2\gamma_s^2)], \tag{5b}$$

$$\frac{d\gamma_C}{dx} = \frac{g}{2}[1+3\gamma_s+\gamma_C-\gamma_C(3\gamma_s+2\gamma_C)] - \gamma_C^2, \tag{5c}$$

where g is the dimensionless measure of the disorder. It is proportional to W and its bare value is $g_0 = 1/\epsilon_F\tau$, where ϵ_F is the Fermi energy. In the noninteracting case it is equal to the resistance of the sample and in the interacting case it is still simply related to it.[4] d is the dimension and $\gamma_{s,C} = \Gamma_{s,C}/z$, where z is the wave-function (or frequency) renormalization factor and the s and C subscripts refer to the spin and Cooper channels. Finally, the scaling variable $x = -\ln(l^2_{\text{in}})$, where l_{in} is an inelastic-scattering length proportional to some negative power of the temperature; thus x is proportional to the logarithm of the temperature. Only two Fermi-liquid channels are shown because a constraint uniquely determines the behavior of the third (charge) channel.[3,4]

To obtain the phase diagram of the model, we integrate the scaling equations. The phases should be identified by the divergence of the corresponding effective Fermi-liquid coupling γ_i. Since the scaling equations were derived perturbatively, we can fix the phase boundaries at the places where the corresponding γ_i's reach unity. In Fig. 1, we show the phase diagram in two and three dimensions. The displayed surface separates the "high-temperature" superconducting phase from the other phases. By this we mean the superconducting phase of the mean-field treatment of the ordered model, which has a high value of T_c.[12] For $g=0$, this

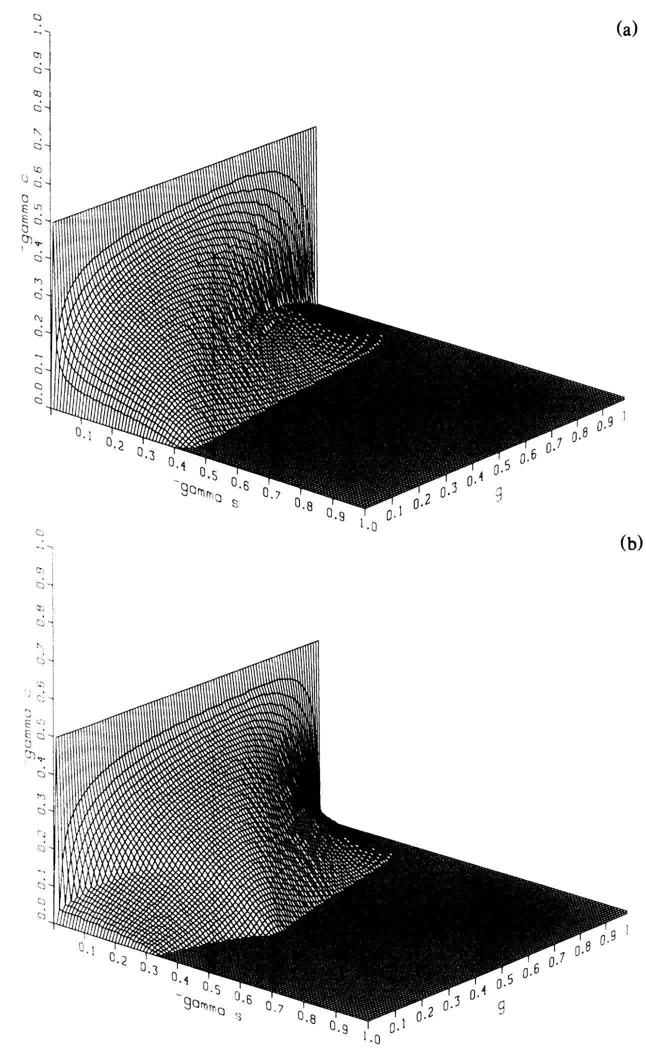

FIG. 1. (a),(b) The phase diagram of the disordered Hubbard model in two and three dimensions, respectively. g is the measure of the disorder, and γ_s and γ_C are the dimensionless vertices in the magnetic and superconducting channels, respectively.

superconducting phase is dominant. However, for nonzero disorder and for small values of the γ_i, superconductivity is generally suppressed. This effect is stronger in two dimensions as is witnessed by the bulging of the surface. Those trajectories which start below the surface exit the unit cube at one of the side walls. In so doing, the iteration decelerates, so that the divergence of the effective couplings occurs at lower temperatures. Therefore we can distinguish two further regions in the parameter space: The first is a low-temperature superconducting regime, which is connected to the high-T_c phase through a crossover; here T_c is lower, but γ_C is still the dominant singularity (this happens for $|\gamma_C| \gg |\gamma_s|$, both of them below the displayed surface). The second is a disordered magnet phase, where superconductivity is suppressed and γ_s is diverging. In the latter case, γ_s is changing sign as well, so we are back at the scenario of the weakly interacting disordered electron gas; i.e., one expects the formation of localized magnetic moments and possibly spin-glass behavior.[7,15] The dominance of magnetism is ensured by the appearance of ferromagnetic correlations, since they suppress superconductivity, as can be seen from Eq. (5c). It is noteworthy that for intermediate couplings [when the term in square brackets in Eq. (5c) is negative], increasing disorder may in fact increase T_c. The effect is strongest for larger values of γ_s, i.e., closer to a phase boundary with magnetism.

From the renormalized value of g one can also obtain the temperature dependence of the resistivity ($\rho = l^{d-2} \times gz$); we show its behavior for a few initial conditions in Fig. 2. Two features are important: In contrast to the weak-coupling approach,[3,4] the resistivity $\rho(T)$ is always

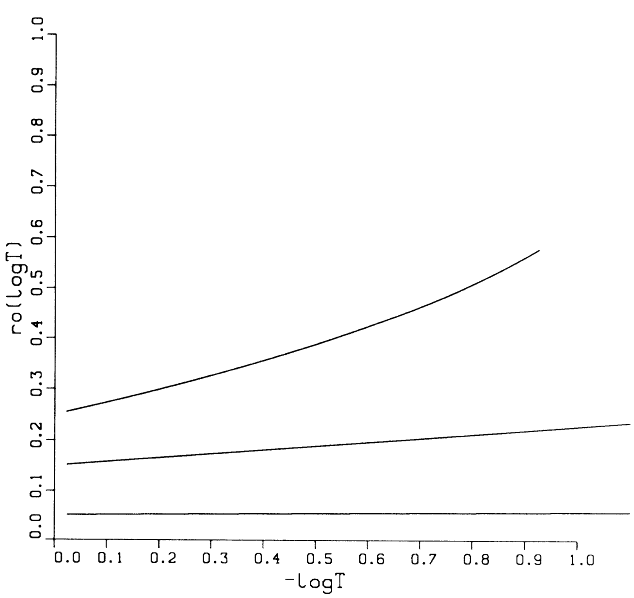

FIG. 2. The temperature dependence of the resistivity for typical bare values of the vertices $-\gamma_s = 0.25$, $-\gamma_C = 0.25$ in three dimensions.

rising, a clear indication of the localizing effect of disorder. For the low-temperature superconductor region and for the magnetic phase, this temperature dependence is much weaker than for the high-T_c phase.

In this paper we investigated the effect of disorder on the strongly interacting electron gas, in other words the interplay of the Mott and Anderson scenarios for the metal-insulator transition. The strong correlations were treated through a slave-boson formalism. In the framework of a correlated mean-field approach we mapped the problem onto a weakly interacting attractive Fermi liquid. First, the generalized Mott insulating region around half filling was qualitatively shown to expand due to the disorder. Second, a renormalization-group approach was used to determine the phase diagram. The high-T_c superconductor phase gives way to a disordered magnet and a low-T_c superconductor with increasing disorder. However, disorder can in fact enhance T_c when the system is close to the superconductor–disordered-magnet phase boundary. Finally, the monotonic temperature dependence of the resistivity shows the effects of localization. This approach will be improved by including slave-boson fluctuations around the mean-field solution.

We have benefited from conversations with P. Coleman, G. Forgacs, G. Kotliar, D. H. Lee, and P. A. Lee. This work was supported in part by National Science Foundation Grants No. DMR 85-20190 and No. DMR 89-06958. G.T.Z. was also supported by an INCOR grant from the Los Alamos National Laboratory.

[1]F. J. Wegner, Z. Phys. B **35**, 207 (1979).

[2]E. Abrahams, P. W. Anderson, G. Licciardello, and T. V. Ramakrishnan, Phys. Rev. Lett. **42**, 673 (1979).

[3]B. L. Altshuler, A. G. Aronov, and P. A. Lee, Phys. Rev. Lett. **44**, 1288 (1980).

[4]A. M. Finkel'shtein, Zh. Eksp. Teor. Fiz. **84**, 168 (1983) [Sov. Phys. JETP **57**, 97 (1983)]; C. Castellani, C. DiCastro, P. A. Lee, and M. Ma, Phys. Rev. B **30**, 527 (1984); C. Castellani, G. Kotliar, and P. A. Lee, Phys. Rev. Lett. **59**, 323 (1987).

[5]S. Hikami, Phys. Rev. B **24**, 2671 (1981).

[6]D. Belitz and T. Kirkpatrick, Phys. Rev. Lett. **63**, 1296 (1989).

[7]M. Milovanovic, S. Sachdev, and R. N. Bhatt, Phys. Rev. Lett. **63**, 82 (1989).

[8]P. W. Anderson, Science **235**, 1196 (1987).

[9]D. J. Klein and W. A. Seitz, Phys. Rev. B **10**, 3217 (1974).

[10]T. M. Rice and K. Ueda, Phys. Rev. B **34**, 6420 (1986).

[11]P. Coleman, Phys. Rev. B **35**, 5072 (1987); N. Read and D. Newns, Adv. Phys. **36**, 799 (1987).

[12]G. Kotliar, P. A. Lee, and N. Read, Physica (Amsterdam) **153B&C**, 538 (1988); M. Inui, S. Doniach, P. Hirschfeld, and A. E. Ruckenstein, Phys. Rev. B **37**, 2320 (1988).

[13]S. F. Edwards and P. W. Anderson, J. Phys. F **5**, 965 (1975).

[14]D. Markowitz and L. P. Kadanoff, Phys. Rev. **131**, 563 (1963).

[15]R. N. Bhatt and P. A. Lee, Phys. Rev. Lett. **48**, 344 (1982).