

## Fermi-Liquid and Non-Fermi-Liquid Phases of an Extended Hubbard Model in Infinite Dimensions

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We study an extended Hubbard model in the limit of infinite dimensions. The local correlation functions of this model are those of a generalized asymmetric Anderson model. The impurity model displays a Fermi liquid phase, a phase with neither the spin nor the charge of the impurity quenched, and an intermediate phase with the spin but not the charge of the impurity quenched. This analysis establishes the existence of metallic non-Fermi-liquid phases of the lattice model over a wide range of parameters and electron densities. The non-Fermi-liquid phases describe metals with incoherent spin and/or charge excitations and self-similar local correlation functions.

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Mott-Hubbard systems differ from simple metals in that there exist strong local interactions. The anomalous normal-state properties in high- $T_c$  copper oxides have raised the question of how these interactions might lead to metallic non-Fermi-liquid states [1, 2]. In more than one dimension, perturbative renormalization group analysis has shown that Fermi-liquid theory does describe weakly interacting fermion systems with a regular density of states [3], implying that the mechanism for the breakdown of Fermi-liquid theory is necessarily nonperturbative in the interactions.

Previous approaches to this problem analyze instabilities of the quasiparticle interaction vertex. Here, we take an alternative approach. We analyze the competition between local interactions and itinerant effects without assuming the existence of quasiparticles to begin with. We study a well defined limit (that of infinite dimensions) of a well defined model (an extended Hubbard model), by means of controlled approximations (a renormalization group in its region of validity). The limit of large dimensionality offers a remarkable simplification: the local correlation functions of a lattice model are *exactly* those of an associated impurity model, which describes the local physics of the lattice problem [4]. For the extended Hubbard model the associated impurity problem is a generalized Anderson impurity model in the mixed valence regime. Within the generalized Anderson model, we identify new states which are not described by a local Fermi liquid. The corresponding phases of the lattice problem are metallic non-Fermi-liquid states.

We study the following Hamiltonian:

$$\begin{aligned}
 H = & \sum_{i,\sigma} (\epsilon_d^0 - \mu) d_{i\sigma}^\dagger d_{i\sigma} + (U/2) \sum_{i,\sigma \neq \sigma'} d_{i\sigma}^\dagger d_{i\sigma} d_{i\sigma'}^\dagger d_{i\sigma'} \\
 & + \sum_{ij,\sigma} (t_{ij} - \mu \delta_{ij}) c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i,\sigma} t (d_{i\sigma}^\dagger c_{i\sigma} + \text{H.c.}) \\
 & + \frac{V_1}{2} \sum_{i\sigma\sigma'} c_{i\sigma}^\dagger c_{i\sigma} d_{i\sigma'}^\dagger d_{i\sigma'} + \frac{V_2}{2} \sum_{i\sigma\sigma'} c_{i\sigma}^\dagger c_{i\sigma'} d_{i\sigma'}^\dagger d_{i\sigma}.
 \end{aligned} \tag{1}$$

It describes two species of spin  $\frac{1}{2}$  electrons. The (strongly correlated)  $d$  electrons have a level  $\epsilon_d^0$ , and an on-site Coulomb interaction  $U$  which will be assumed to be infinite. The (noncorrelated) conduction electrons have a dispersion  $\epsilon_k$  determined by the hopping matrix  $t_{ij}$ , which we choose so that the corresponding density of states is a Lorentzian with width  $\Gamma$  [4, 5]. The  $d$  and  $c$  electrons are coupled locally through the hybridization  $t$ , the density-density interaction  $V_1$ , and the exchange interaction  $V_2$ .  $\mu$  is the chemical potential.

All the local correlation functions of this extended Hubbard model in the limit of infinite dimensions are given by the corresponding local correlators of the following generalized Anderson model:

$$\begin{aligned}
 H = & E_d^0 d_\sigma^\dagger d_\sigma + (U/2) \sum_{\sigma \neq \sigma'} d_\sigma^\dagger d_\sigma d_{\sigma'}^\dagger d_{\sigma'} \\
 & + \sum_{k\sigma} (\epsilon_k - \mu) c_{k\sigma}^\dagger c_{k\sigma} + \sum_{\sigma} t (d_\sigma^\dagger c_\sigma + \text{H.c.}) \\
 & + \frac{V_1}{2} \sum_{\sigma,\sigma'} c_\sigma^\dagger c_\sigma d_{\sigma'}^\dagger d_{\sigma'} + \frac{V_2}{2} \sum_{\sigma,\sigma'} c_\sigma^\dagger c_{\sigma'} d_{\sigma'}^\dagger d_\sigma,
 \end{aligned} \tag{2}$$

where  $\epsilon_k$  again corresponds to a Lorentzian density of states with width  $\Gamma$ , and  $E_d^0 = \epsilon_d^0 - \mu$ . The detailed derivation of this result parallels the mapping of the Hubbard model onto the Anderson impurity model [5] and will be given elsewhere [6]. As in the case of the Hubbard model [5], the assumption of a Lorentzian density of states allows us to determine the parameters of the impurity problem analytically. The parameter  $E_d^0$  is such that the density of  $d$  plus the local density of  $c$  electrons in the ground state of the impurity model Eq. (2) equals the total electron density ( $n$ ) of the original lattice problem Eq. (1):

$$\sum_{\sigma} \langle d_\sigma^\dagger d_\sigma \rangle + \sum_{\sigma} \langle c_{0,\sigma}^\dagger c_{0,\sigma} \rangle = n. \tag{3}$$

We first give a qualitative discussion of the different kinds of low energy behavior that can occur within the

impurity problem Eq. (2) [7]. The three local  $d$  states,  $|\alpha\rangle = |0\rangle$  and  $|\sigma\rangle$ , can be viewed as local spin and charge modes. The hybridization  $t$  term in the Hamiltonian (2) describes the transition from one local charge state to another (i.e., between  $|\sigma\rangle$  and  $|0\rangle$ ), while the spin flipping  $V_2^\perp$  coupling corresponds to that from one local spin state to another (i.e., among the spin doublet  $|\sigma\rangle$ ). The conduction electron bath is locally disturbed during the process of these transitions, and reacts by producing excitations in the Fermi sea. Such a reaction leads to the renormalization of the hybridization and the spin exchange couplings. Depending on the interaction strength, these couplings are renormalized differently, leading to different low energy behavior.

If these couplings grow as we go to lower energies, the transitions among the local states proceed coherently. The coherence energy scale  $E_F^*$  (to be interpreted as a renormalized Fermi energy) is the scale below which the local spin and charge modes are quenched through the formation of (heavy) quasiparticles. A scaling analysis of this Fermi-liquid regime was carried out by Haldane [8]. The renormalized theory is described by the large spin degeneracy limit of the slave boson formulation of the

model. When these couplings are irrelevant, the transitions between the local states proceed incoherently at low energies. The effective Fermi energy  $E_F^*$  vanishes, and the local charge and spin modes are not all quenched by the conduction electrons. We have a self-similar situation, a problem without scale. The local correlation functions then show algebraic behavior with nontrivial exponents. The system is an incoherent metallic state. Such states correspond to the noncondensed phase of the slave boson description. Therefore from a local point of view, the survival or the demise of Fermi-liquid theory depends on whether the transitions between the local states are relevant or not, as we go towards low energy.

To make these ideas concrete, we follow Haldane [8] and write the partition function in terms of a sum over histories of the impurity. Each history is a sequence of transitions between the three local  $d$  states  $|\alpha\rangle = |0\rangle$  and  $|\sigma\rangle$ . The transitions take place at the (imaginary) time  $0 < \tau_1 < \dots < \tau_n < \beta = \frac{1}{T}$ : along the Feynman trajectory the local state is at  $|\alpha_{i+1}\rangle$  from  $\tau_i$  to  $\tau_{i+1}$  ( $i = 1$  to  $n$ ). The partition function is now given by  $Z = \sum_{\alpha_1, \dots, \alpha_n, \alpha_{n+1}=\alpha_1} \exp(-S[\tau_1, \dots, \tau_n])$ , where the statistical weight for each history is given by

$$S[\tau_1, \dots, \tau_n] = \sum_{i < j} \sum_{\gamma} (e_{\alpha_i \alpha_{i+1}}^\gamma) (e_{\alpha_j \alpha_{j+1}}^\gamma) \ln \frac{|\tau_i - \tau_j|}{\xi_0} - \sum_i \ln(y_{\alpha_i \alpha_{i+1}}) + \sum_i h_{\alpha_{i+1}} (\tau_{i+1} - \tau_i) / \xi_0. \quad (4)$$

This statistical weight has a simple intuitive meaning. The effective "magnetic fields"  $h_\alpha$  reflect the (dimensionless) differences of the local state energies  $E_{|\alpha\rangle}$ :  $E_{|0\rangle} = 0$  and  $E_{|\sigma\rangle} = E_d$ . Specifically,  $h_0 = -\frac{2}{3} E_d \xi_0$ ,  $h_\sigma = \frac{1}{3} E_d \xi_0$ , where  $\xi_0 = 1/\Gamma$  is the ultraviolet cutoff, and  $\sum_\alpha h_\alpha = 0$ . The fugacity  $y_{\alpha_i \alpha_{i+1}}$  is the (dimensionless) amplitude associated with a transition from state  $|\alpha_i\rangle$  to state  $|\alpha_{i+1}\rangle$ . Specifically, the charge fugacity  $y_{0,\sigma} = y_{\sigma,0} = y_t = t \xi_0$ , and the spin fugacity  $y_{\sigma,\sigma' \neq \sigma} = y_j = \frac{V_2^\perp}{2} \xi_0$ .

The long range logarithmic interaction between the flipping events arises from the reaction of the conduction electron bath towards the transition between the local states. The local disturbance on the conduction electron bath during such a transition involves two factors: the absorption or emission of the local conduction electrons and the change in the local potential that the conduction electrons experience. The latter is described by the local-state-dependent potential for the spin  $\gamma$  component of the conduction electron sea:  $V_{|0\rangle}^\gamma = 0$  and  $V_{|\sigma\rangle}^\gamma = \frac{V_1}{2} + \frac{V_2^\parallel}{2} \delta_{\gamma,\sigma}$ . Both kinds of disturbances are incorporated [10] in the effective "charge,"  $e_{\alpha_j \alpha_{j+1}}^\gamma$ , associated with the transition event from  $|\alpha_i\rangle$  to  $|\alpha_{i+1}\rangle$  at time  $\tau_i$ . Specifically,  $e_{0,\sigma}^\gamma = -(1 - \frac{\delta_2}{\pi}) \delta_{\gamma,\sigma} + \frac{\delta_1}{\pi}$ , and  $e_{\sigma,\sigma'}^\gamma = (1 - \frac{\delta_2}{\pi}) (\delta_{\gamma,\sigma} - \delta_{\gamma,\sigma'})$ , where the phase shifts  $\delta_1 = \tan^{-1}(V_1/2\Gamma)$  and  $\delta_2 = \tan^{-1}(V_2^\parallel/2\Gamma)$ .

We can interpret Eq. (4) as the action associated with the partition function of a three component plasma of kinks with fugacities  $y_{\alpha\beta}$ , "charges"  $e_{\alpha\beta}^\gamma$ , and "magnetic

fields"  $h_\alpha$ . It is a special case of one dimensional classical "spin" models with  $1/r^2$  interactions considered by Cardy [11]. The "spins" can be in three states  $|\alpha\rangle$  and the Coulombic interactions between the "charges" in Eq. (4) can be transformed into a "spin-spin" interaction of the form  $\sum_{i < j} K(\alpha_i, \alpha_j) \xi_0^2 / |\tau_i - \tau_j|^2$ , where the stiffness constants  $K(\alpha, \beta) = -\frac{1}{2} \sum_\gamma (e_{\alpha,\beta}^\gamma)^2$ . Specifically,  $K(0, \sigma) = -\epsilon_0^\sigma$ ,  $K(\sigma, \sigma') = -\epsilon_j^\sigma (1 - \delta_{\sigma,\sigma'})$  where  $\epsilon_0^\sigma = \frac{1}{2} [(1 - \frac{\delta_2}{\pi} - \frac{\delta_1}{\pi})^2 + (\frac{\delta_1}{\pi})^2]$ , and  $\epsilon_j^\sigma = (1 - \frac{\delta_2}{\pi})^2$ .

To set up the renormalization group (RG) we use Cardy's procedure extended to account for an effective "magnetic field" in the Coulomb gas representation of Eq. (4). The inclusion of such an effective "field" in the RG is essential, since it would be generated in the course of renormalization due to the particle-hole asymmetry even if we start with zero field. In the following we will assume that the "field" is small (which is justified near the pinned density regime to be discussed shortly). The RG equations describe the flow of the dimensionless couplings as the bandwidth  $1/\xi$  is reduced. They are given by

$$\begin{aligned} dy_t/d \ln \xi &= (1 - \epsilon_t) y_t + y_t y_j, \\ dy_j/d \ln \xi &= (1 - \epsilon_j) y_j + y_t^2, \\ d\epsilon_t/d \ln \xi &= -6\epsilon_t y_t^2 + \epsilon_j (y_t^2 - y_j^2), \\ d\epsilon_j/d \ln \xi &= -2\epsilon_j (y_t^2 + 2y_j^2), \\ dE_d \xi/d \ln \xi &= (y_t^2 - y_j^2) + E_d \xi (1 - 3y_t^2), \end{aligned} \quad (5)$$

where the “field” is written in terms of  $E_d \xi = h_\sigma - h_0$ . The cross terms in the scaling of the fugacities  $y_t$  and  $y_j$  reflect the coupling between spin and charge channels, while the first term in the renormalization of  $E_d \xi$  arises due to the particle-hole asymmetry. Our RG equations represent a systematic generalization of those of Haldane to incorporate all couplings which can be generated in the renormalization process [8, 12].

We stress that, *in the region where the charge fugacity is renormalized to zero*, there is a *range of electron density  $n$*  over which the *renormalized  $d$  electron level* equals the chemical potential, i.e.,  $E_d^* = 0$ , in order to obey Eq. (3). In the absence of the hybridization, this result was established analytically in Ref. [13], by showing that the total density at zero temperature develops a discontinuity when the renormalized  $d$  level crosses  $E_d^* = 0$  corresponding to a critical chemical potential. Our RG equations imply that, when the charge fugacity is renormalized to zero, it is possible to adjust the initial conditions of the flow so that  $E_d^* = 0$ . In this case, the charge of the  $d$  level is well defined asymptotically, and the total density at zero temperature is again discontinuous at the critical chemical potential  $\mu_c$ . The physical content of this condition is the absence of energy barriers for charge fluctuations in an incoherent metallic state. From a formal point of view,  $E_d$  plays the role of a mass in a field theory. And by choosing to work in the pinned density region, we are studying the renormalization of model Eq. (2) at a massless point.

Our RG equations lead to three kinds of fixed points:

(a) For  $\epsilon_t < 1$ , both the charge and spin fugacities are relevant. The resulting *strong coupling fixed point* is beyond the reach of perturbative RG. However, it is similar to that of the usual asymmetric Anderson model. At low energies, the hybridization quenches both the local spin and charge, leading to a singlet ground state.

(b) When the renormalized  $\epsilon_t^* > 1$  and  $\epsilon_j^* > 1$ , both the charge and spin fugacities are irrelevant, leading to *weak coupling fixed points*. Here, neither the local spin nor the local charge degrees of freedom is quenched. In terms of the original interaction parameters, this occurs in a range of attractive density-density and ferromagnetic exchange couplings.

(c) When  $\epsilon_t^* > 1$  and  $\epsilon_j < 1$ ,  $y_j$  increases while  $y_t$  decreases initially. Eventually, the large  $y_j$  will start to drive  $y_t$  to increase. However, this late stage is already beyond the reach of perturbative RG. From bosonization as well as a strong coupling analysis,  $y_t$  can be shown to remain irrelevant at *these intermediate coupling fixed points* [6, 14]. The basin of attraction is given by the condition that the charge stiffness  $\epsilon_t^{**}$ , further renormalized from  $\epsilon_t^*$  due to the relevant spin fugacity, is larger than 1. In terms of the original coupling, this corresponds to a range of attractive density-density and antiferromagnetic exchange couplings.

We now discuss the qualitative physics of each regime:

(a) In the strong coupling regime, we can infer from

our knowledge of the usual Anderson model that the low energy physics is characterized by a nonzero renormalized hybridization. The RG equations establish that [8], as the chemical potential (and hence  $E_d^*$ ) is varied, the mixed valence singlet state occurs as a crossover from the empty orbital to local-moment singlet states. This crossover occurs for  $E_d^*$  extending over a range determined by the renormalized resonance width  $\Delta^* = \pi \rho_0 (t^*)^2$ . This strong coupling phase can also be established explicitly in the large  $N$  limit [15].

(b) In the weak coupling regime, the renormalized hybridization is zero. Therefore, the analog of the mixed valence crossover regime of the strong coupling case occurs at one particular  $E_d^* = 0$  corresponding to the critical chemical potential  $\mu_c$ : it turns into a critical point at which the mixed valence behavior persists to zero energy. For chemical potentials away from  $\mu_c$ , the mixed valence state occurs above a finite crossover energy scale.

Within the weak coupling mixed valence regime, the correlation functions at low frequencies have a *regular perturbation expansion* in the running fugacities,  $t^* = t(\omega/\Gamma)^{\epsilon_t^*}$ , and  $(V_2^\perp)^* = V_2^\perp (\omega/\Gamma)^{\epsilon_j^*}$ . This allows us to calculate the one particle local Green's functions.  $G_{cc}$  is not renormalized from its fixed point  $1/\tau$  form by the fugacities since the  $c$  electron does not create a kink. On the other hand,  $G_{dc}(\omega) \sim \omega^{-1+\alpha}$  and  $G_{dd}(\omega) \sim \omega^{-1+\beta}$  at low frequencies. Here the exponents are given, to leading order, by  $\alpha = -(\delta_1^* + \delta_2^*)/\pi + [(\delta_1^* + \delta_2^*)/\pi]^2 + (\delta_1^*/\pi)^2$  and  $\beta = [(\delta_1^* + \delta_2^*)/\pi]^2 + (\delta_1^*/\pi)^2$ . For the conduction electron self-energy  $\Sigma_{cc} = (G_0^{-1})_{cc} - (G^{-1})_{cc}$ ,

$$\text{Im} \Sigma_{cc}(\omega + i0^+) \sim (\omega)^{2\epsilon_t^* - 2}. \quad (6)$$

The multiparticle correlation functions also show power law behavior. For example,

$$\begin{aligned} \langle d_\sigma^\dagger d_{\sigma'}(\tau) d_\sigma^\dagger d_\sigma(0) \rangle &\sim (\tau)^{-\alpha_1}, \\ \langle d_\sigma^\dagger c_{\sigma'}(\tau) c_{\sigma'}^\dagger d_\sigma(0) \rangle &\sim (\tau)^{-\alpha_2}, \\ \langle d_\sigma^\dagger c_{\sigma'}^\dagger(\tau) c_{\sigma'} d_\sigma(0) \rangle &\sim (\tau)^{-\alpha_3}, \end{aligned} \quad (7)$$

where to leading order,  $\alpha_1 = 2\epsilon_j^*(1 - \delta_{\sigma,\sigma'})$ ,  $\alpha_2 = 2\epsilon_t^* \delta_{\sigma,\sigma'} + 2\epsilon_{tj}^*(1 - \delta_{\sigma,\sigma'})$ , and  $\alpha_3 = 2\epsilon_t^* (-\frac{\delta_1^*}{\pi}, -\frac{\delta_2^*}{\pi}) \delta_{\sigma,\sigma'} + 2\epsilon_{tj}^* (-\frac{\delta_1^*}{\pi}, -\frac{\delta_2^*}{\pi})(1 - \delta_{\sigma,\sigma'})$ . Here,  $\epsilon_{tj}^*(\frac{\delta_1^*}{\pi}, \frac{\delta_2^*}{\pi}) = \frac{1}{2} [(1 - \frac{\delta_1^*}{\pi})^2 + (\frac{\delta_1^*}{\pi} + \frac{\delta_2^*}{\pi})^2]$ . Therefore, the  $d^\dagger c^\dagger$  superconducting correlation function is divergent, while the excitonic and  $d$ -electron correlation functions vanish.

(c) In the intermediate coupling regime, the mixed valence regime again persists to zero energy at a critical chemical potential  $\mu_c$ , and above a finite energy scale for  $\mu$  away from  $\mu_c$ . Since the spin channel is relevant, the spin excitations are coherent and are described by a resonance. The local spin susceptibility is regular. On the other hand, no resonance forms in the charge channel, and the local charge susceptibility retains the algebraic behavior. Meanwhile, the single particle spectral function is a convolution of the spin and charge sectors, which therefore again has the algebraic form. The super-

conducting  $d^\dagger c^\dagger$  susceptibility still diverges at low frequencies algebraically.

These results establish the existence of three phases in the extended Hubbard model (1). The Fermi-liquid phase corresponds to the strong coupling phase. The non-Fermi-liquid phases associated with both the weak coupling and the intermediate coupling states occur *over a range of electron density and interaction strength*. The weak coupling phase has incoherent charge and spin excitations, while the intermediate coupling phase has incoherent charge but coherent spin excitations. They both have vanishing quasiparticle residue.

The results we have established so far are exact for the extended Hubbard model in infinite dimensions with a Lorentzian density of states. For a bounded density of states, our RG analysis applies when high energy (nonuniversal) states are integrated out. This initial stage of renormalization determines the initial conditions of the RG flow. In addition, when the system is metallic, it is indeed consistent to have a nonzero density of states of the conduction electron at the chemical potential leading to the *finite* imaginary part of the Weiss-field  $G_0^{-1}$ , which can be effectively described by the width of the Lorentzian for low energy behavior [6]. Therefore, our results are relevant to the metallic phases of the (extended) Hubbard model with short range hopping parameters.

Recently non-Fermi-liquid states have been studied in impurity models with additional channels of screening electrons [16]. This corresponds to adding to the impurity Hamiltonian a term  $V' \sum_i \sum_{\sigma'=1}^M (n_d)_i S_{i\sigma'}^\dagger S_{i\sigma'}$ , where  $S^\dagger$  creates electrons in the screening channels. In our framework of analyzing impurity models this addition modifies the bare values of the stiffness:  $\epsilon_t^0 \rightarrow \epsilon_t^0 + \frac{1}{2}M(\frac{\delta'}{\pi})^2$ , where the phase shift  $\delta' = \tan^{-1}(V'\xi_0)$ . This moves the initial conditions of the RG flow towards the basin of attraction of the zero charge fugacity fixed points.

In summary, we found two novel kinds of mixed valence states of the generalized asymmetric Anderson model, which characterize metallic non-Fermi-liquid phases of the extended Hubbard model in infinite dimensions. For a finite range of electron density, there exist transitions between Fermi-liquid and metallic non-Fermi-liquid phases when the strength of the local interactions is varied. We note that the non-Fermi-liquid phases have a large ground state degeneracy. This degeneracy may be lifted below some finite temperature due to the onset of an ordering transition. Our description of the non-Fermi-liquid normal phase applies above this temperature, in the same spirit that the paramagnetic Mott insulating phase describes the half-filled Hubbard model [17] above

the Néel temperature. In the non-Fermi-liquid phases the diverging pair susceptibility suggests an ordering transition into a superconducting state. On the other hand, the slowed charge dynamics suggest that a small random potential may cause an Anderson localization transition.

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