Kosterlitz-Thouless Transition and Short Range Spatial Correlations in an Extended Hubbard Model

Qimiao Si and J. Lleweilun Smith
Department of Physics, Rice University, Houston, Texas 77251-1892
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We study the competition between intersite and local correlations in a spinless two-band extended Hubbard model by taking an alternative limit of infinite dimensions. We find that the intersite density fluctuations suppress the charge Kondo energy scale and lead to a Fermi liquid to non-Fermi-liquid transition for repulsive on-site density-density interactions. In the absence of intersite interactions, this transition reduces to the known Kosterlitz-Thouless transition. We show that a new line of non-Fermi-liquid fixed points replace those of the zero intersite interaction problem. [S0031-9007(96)01438-X]

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The two-band extended Hubbard model is a realistic starting point both for the high T_c cuprates and for many heavy fermion systems. The model contains a strongly correlated band and a weakly correlated one. At the phenomenological level, the low energy properties of the conventional heavy fermions (such as $CeCu_6$ and UPt_3) are well described by the Fermi liquid theory [1], while those of certain novel f-electron materials [2] and the high T_c cuprates appear not. The theoretical question, then, is: under what conditions do electron correlations lead to a non-Fermi-liquid in this model?

Recently, some progress has been made on the understanding of this model [3,4]. In the large dimensionality (D) limit, the local density-density interactions alone are found to cause Kosterlitz-Thouless [5] type quantum phase transitions from a Fermi liquid to non-Fermi-liquid metallic states. In the spinful case, the resulting non-Fermi-liquids have spin-charge separation [3,6]. The large D limit [7] has the advantage that local correlations are treated in a dynamical fashion, but the disadvantage that all intersite interactions reduce to Hartree-Fock terms; *no spatial fluctuations survive*. For physical systems in finite dimensions, intersite RKKY or superexchange type interactions are expected to compete with local correlations [8,9]. Unfortunately, for "paramagnetic" phases far away from spatial ordering transitions, there exists no controlled theoretical method to address such a competition. From the large D point of view, one way to recover spatial fluctuations is the perturbative $1/D$ expansion [10]. The practicality of this procedure is unclear at this stage. An alternative route is a loop expansion requiring that the $D = \infty$ results be recovered at the saddle-point level. This construction has so far been limited to models with certain forms of quenched disorder [11].

In this Letter, we take an alternative large D limit to study the interplay between local correlations and short range spatial fluctuations in the two-band extended Hubbard model. We introduce an explicit intersite density-density interaction and scale the interaction strength in terms of the dimensionality such that its *fluctuation part* survives the large D limit. This procedure leads to an impurity embedded in a self-consistent fermionic bath *and a self-consistent bosonic bath*. We will study primarily the spinless version of the model for which asymptotically exact results can be derived analytically. The results are of direct relevance to the charge sector of the spin-charge-separated intermediate phase of the spinful model [3,6].

The model is defined by the following Hamiltonian,

$$H = \sum_i [\epsilon_d^0 n_{d_i} + t(c_i^\dagger d_i + \text{H.c.}) + V : n_{c_i} :: n_{d_i} :] + \sum_{\langle ij \rangle} [t_{ij} c_i^\dagger c_j + (v_{ij}/2) : n_{d_i} :: n_{d_j} :]. \quad (1)$$

The spinless d electrons are dispersionless, with an energy level ϵ_d^o. The spinless c electrons have a hopping matrix t_{ij}. $\langle ij \rangle$ labels the nearest-neighbor sites. The t term describes hybridization, and the V term the on-site density-density interaction. The v_{ij} term is an intersite "charge RKKY" repulsive interaction. The standard large D limit [7] is taken with $t_{\langle ij \rangle}$ scaled to be of order $1/\sqrt{2D}$ and $v_{\langle ij \rangle}$ of order $1/D$. In this limit, only the static part of the v_{ij} term survives. Here, we scale $v_{\langle ij \rangle} = v_0/\sqrt{2D}$ and take the large D limit keeping v_0 fixed. This limit is well defined when we retain only the dynamical density modes. We achieve this through normal ordering, $: n :\equiv n - \langle n \rangle$. We focus on states without long range ordering, for which the Hartree terms can be absorbed by the chemical potential.

We first give a general formulation of this alternative large D limit. Following the standard procedure, we divide the Hamiltonian into local and intersite parts,

$$H = \sum_i h_i + \sum_{\langle ij \rangle} (h_{t,ij} + h_{v,ij}), \quad (2)$$

where h_i is on site, $h_{t,ij} = t_{ij} \psi_i^\dagger \psi_j$, and $h_{v,ij} = (v_{ij}/2) : n_{\psi_i} :: n_{\psi_j} :$. For generality, we develop the formalism with the $\psi_i^\dagger$ fields for possible multibands or spin components; for the Hamiltonian (1), $h_{t,ij} = t_{ij} c_i^\dagger c_j$, and $h_{v,ij} = (v_{ij}/2) : n_{d_i} :: n_{d_j} :$. Within

a path-integral representation, we divide the action for the lattice model into $S = S_0 + S^{(0)} + \Delta S$, where S_0, $S^{(0)}$, and ΔS are the actions associated with h_0, $\sum_{i\neq 0} h_i + \sum_{\langle ij\neq 0\rangle}(h_{t,ij} + h_{v,ij})$, and $\sum_i (h_{t,0i} + h_{v,0i} + \text{H.c.})$, respectively. Integrating out all the degrees of freedom except at site 0 leads to the following effective action, $S^{\text{eff}} = S_0 - \sum_{n=1}^{\infty}(-1)^n \times \langle(\Delta S)^n\rangle_c^{(0)}/n!$, where $\langle\,\rangle_c^{(0)}$ denotes connected correlation functions in terms of $S^{(0)}$. $\langle(\Delta S)^n\rangle_c^{(0)}$ modifies the on-site action with terms that involve n site-0 density/fermion modes. The coefficients of these operators are retarded and are given, for each n, by n-operator correlation functions with respect to $S^{(0)}$. The order in $1/D$ of each term can be determined through a cumulant expansion of the original lattice Hamiltonian [12]. We find that, to the leading order in $1/D$, no interference between $h_{t,ij}$ and $h_{v,ij}$ terms is allowed, except in local decorations. This absence of interference implies that n-point correlation functions have the usual dependence on $1/D$. As a result, for all $n > 2$, $\langle(\Delta S)^n\rangle_c^{(0)}$ vanishes as $D \to \infty$ [7]. The absence of interference also leads to separate Dyson equations for χ_{ij} and G_{ij} in terms of their respective effective cumulants. This in turn implies that $G_{ij} = G_{ii}G'_{ij}G_{jj}$, $\chi_{ij} = \chi_{ii}\chi'_{ij}\chi_{jj}$, $G_{ij}^{(0)} = G_{ij} - G_{ii}G'_{i0}G_{00}G'_{0j}G_{jj}$, and $\chi_{ij}^{(0)} = \chi_{ij} - \chi_{ii}\chi'_{i0}\chi_{00} \times \chi'_{0j}\chi_{jj}$, where $G'_{ij} \equiv \sum_{\text{paths}} t_{il_1}G_{l_1l_1}t_{l_1l_2}G_{l_2l_2}\cdots \times G_{l_nl_n}t_{l_nj}$, $\chi'_{ij} \equiv \sum_{\text{paths}} v_{il_1}\chi_{l_1l_1}v_{l_1l_2}\chi_{l_2l_2}\cdots\chi_{l_nl_n}v_{l_nj}$, and $[i, l_1, l_2, \ldots, l_n, j]$ labels a non-self-retracing path from site i to site j. It then follows that

$$\begin{aligned} G_{ij}^{(0)} &= G_{ij} - G_{i0}G_{0j}/G_{00}\,, \\ \chi_{ij}^{(0)} &= \chi_{ij} - \chi_{i0}\chi_{0j}/\chi_{00}\,. \end{aligned} \tag{3}$$

From Eq. (3), $\langle :n_i: \rangle^{(0)} \equiv \langle n_i\rangle^{(0)} - \langle n_i\rangle$ is of order $1/D$. Hence, in the large D limit, $\langle\Delta S\rangle^{(0)}$ also vanishes; only $\langle(\Delta S)^2\rangle_c^{(0)}$ survives, leading to

$$S^{\text{eff}} = -\int_0^\beta d\tau \int_0^\beta d\tau' [\psi_0^\dagger(\tau)g_0^{-1}(\tau-\tau')\psi_0(\tau') + :n_{\psi_0}(\tau): \chi_0^{-1}(\tau-\tau'):n_{\psi_0}(\tau'):] + S_0\,. \tag{4}$$

Here, $g_0^{-1}(\tau-\tau')$ and $\chi_0^{-1}(\tau-\tau')$ are the Fourier transforms of

$$\begin{aligned} g_0^{-1}(i\omega_n) &= -\sum_{ij} t_{i0}t_{0j}G_{ij}^{(0)}(i\omega_n)\,, \\ \chi_0^{-1}(i\nu_n) &= \sum_{ij} v_{i0}v_{0j}\chi_{ij}^{(0)}(i\nu_n)\,, \end{aligned} \tag{5}$$

where $i\omega_n$ and $i\nu_n$ are the fermionic and bosonic Matsubara frequencies, respectively. The Dyson equations of the lattice Hamiltonian implies that G_{ij} is determined by the on-site self-energy alone; χ_{ij} is determined by the on-site effective cumulant, or, equivalently, the on-site part of the vertex function irreducible in terms of both the particle hole bubble and the single v_{ij} line. All these local quantities can be calculated directly in terms of S^{eff}. Therefore, given an S^{eff}, we can calculate all G_{ij} and χ_{ij} and hence, via Eq. (5), $g_0^{-1}(i\omega_n)$ and $\chi_0^{-1}(i\nu_n)$. The self-consistent equations (3)–(5) indeed close. They define the dynamical mean field equations. We note that related mean field equations arise in the metallic spin-glass problem [13]. The retarded g_0^{-1} can be represented by a self-consistent noninteracting fermionic bath [7]. Similarly, an additional noninteracting *bosonic* bath can be used to represent the retarded χ_0^{-1} term. We have therefore a self-consistent Anderson-like impurity model coupled to screening bosons [14].

We now apply this formalism to the extended Hubbard model (1). The self-consistent impurity model is a resonant-level model with an additional bosonic bath,

$$\begin{aligned} H_{\text{imp}}^{\text{eff}} &= E_d^0 d_0^\dagger d_0 + H_0 + t(c_0^\dagger d_0 + \text{H.c.}) \\ &\quad + V :n_{c_0}::n_{d_0}: + \sum_q W_q\rho_q^\dagger\rho_q \\ &\quad + \sum_q F_q :n_{d_0}:(\rho_q + \rho_{-q}^\dagger)\,, \end{aligned} \tag{6}$$

where $E_d^0 = \epsilon_d^0 - \mu$, and H_0 describes the local c_0 electron coupled to a noninteracting fermionic bath whose dispersion, together with the parameters associated with the bosonic bath, W_q and F_q, are determined from the self-consistency Eqs. (5). In the remainder of this Letter, we focus on the $D = \infty$ Bethe lattice. This has the advantage that the bare density of states is bounded. For $v_0 = 0$, it was shown both analytically [3] and numerically [15] that the density of states of the self-consistent fermionic bath is nonsingular in the metallic regime. We find this continues to be the case for finite v_0. This then allows an asymptotically exact analytic analysis of our self-consistent problem. Note that the spectral function of the bosonic bath is arbitrary (and is in fact non-Ohmic in the non-Fermi-liquid case; see below).

The asymptotically exact analysis is carried out by writing the partition function of $H_{\text{imp}}^{\text{eff}}$ in a kink-gas representation. The procedure parallels what was detailed in Ref. [3]. We only note that the effect of the additional bosonic bath on the action of a particular history can be treated by a time-dependent canonical transformation, for the *arbitrary form of the boson spectral function*. The resulting kink-gas action is

$$S(\tau_{2n},\ldots,\tau_1) = -2n\ln(y) + \sum_i (-1)^i h(\tau_{i+1}-\tau_i)/\xi_0 + \sum_{i<j}(-1)^{i+j}\left[2\epsilon\ln\frac{\tau_j-\tau_i}{\xi_0} + K(\tau_j-\tau_i)\right]. \tag{7}$$

Here, $[\tau_{2n},\ldots,\tau_1]$, for $n = 1, 2, \ldots$, labels a sequence of kink events along the imaginary time axis. The fugacity is given by $y = t\rho_c$, where ρ_c is the density of states of the self-consistent fermionic bath at the Fermi energy. $\epsilon = (1/2)\{1 - (1/\pi)\{\tan^{-1}[\pi\rho_c(1 - n_d)V] + \tan^{-1}(\pi\rho_c n_d V)\}\}^2$ is the stiffness constant. The logarithmic interaction among the kinks is mediated by the fermionic bath. $h = E_d^0\xi_0$ is the symmetry breaking field. Finally, $K(\tau)$ describes an additional long

range interaction of the kinks induced by the bosonic bath. Because of the self-consistency, $K(\tau)$ is determined entirely by the full local susceptibility

$$\partial^2 K(\tau)/\partial\tau^2 = v_0^2 \chi(\tau). \tag{8}$$

Anticipating the possible $1/\tau^\alpha$ form for the local susceptibility, we first solve the kink-gas action (7) with

$$K(\tau) = \lambda[(\tau/\xi_0)^{2-\alpha} - 1]/(2-\alpha) \tag{9}$$

for a fixed α value. We will consider the case with vanishing renormalized symmetry breaking field, h^*. We have derived the renormalization group (RG) equations for α close to 2,

$$\begin{aligned} dy/d\ln\xi &= y[1 - (\epsilon + \lambda/2)], \\ d\epsilon/d\ln\xi &= -4\epsilon y^2, \\ d\lambda/d\ln\xi &= \lambda[(2-\alpha) - 4y^2], \\ dh/d\ln\xi &= h(1 - 2y^2), \end{aligned} \tag{10}$$

valid for small h. The RG flow is given in Fig. 1. The flow in the y-ϵ plane (the dotted lines) describes a Kosterlitz-Thouless transition. It goes to a strong coupling fixed point when $\epsilon < \epsilon^{\rm crit} = 1$, and to a line of weak coupling fixed points when $\epsilon > \epsilon^{\rm crit}$. The flow in the y-λ plane (the dashed lines) are those of the Ising model with a long range $1/\tau^\alpha$ interaction [16,17]. There exists an unstable fixed point at $(y^*, \lambda^*) = (\sqrt{2-\alpha}/2, 2)$, which describes a second order phase transition. Close to the origin, the separatrix has the form $\lambda^{\rm sep} \approx 2[y/(2-\alpha)]^{2-\alpha}$. The flow goes to a strong coupling fixed point for $\lambda < \lambda^{\rm sep}$, and to a weak coupling fixed point when $\lambda > \lambda^{\rm sep}$. In the language of the long range Ising model, $\alpha = 2$ is the lower critical range, and $\alpha = 3/2$ the upper critical range [16]. The RG flows in between these two planes (solid lines) interpolate between these two limits. There exist a line of weak coupling fixed points with $y^* = 0$, $\lambda^* = \infty$, and a finite ϵ^*.

These results can be used to solve our self-consistent problem. We focus on the mixed valence regime only.

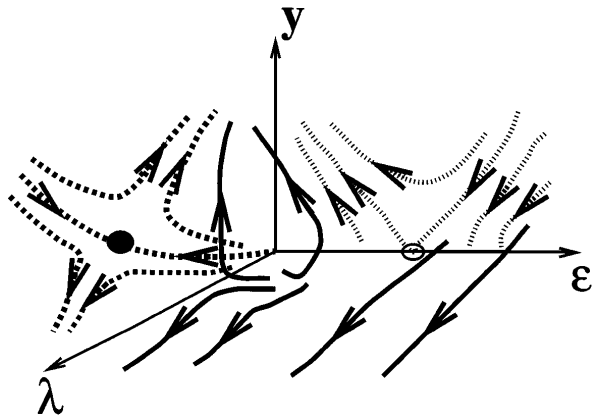

FIG. 1. The RG flow of the kink-gas action Eqs. (7) and (9) for $\alpha <\sim 2$ and vanishing renormalized symmetry breaking field.

We specify the phase diagram in terms of the three-dimensional parameter space spanned by $g_t = t\rho_0$, $g_V = [1 - (2/\pi)\tan^{-1}(\pi\rho_0 V/2)]$, and $g_v = \rho_0 v_0$, where ρ_0 is the bare density of states of the conduction electrons at the Fermi energy. The Kosterlitz-Thouless transition at $g_v = 0$ describes the charge Kondo effect [18]. The critical value $g_V^{\rm crit}$ corresponds to an attractive $V^{\rm crit}$ such that $\rho_c V^{\rm crit} = -(2/\pi)\tan[(\sqrt{2}-1)\pi/2]$. When $g_V < g_V^{\rm crit}$, i.e., $-V < V_0^{\rm crit}$, the solution is a Fermi liquid with the usual form for the local density susceptibility,

$$\chi(\tau) \sim (1/\Delta^*\tau)^2 \quad \text{for } \tau \gg 1/\Delta^*, \tag{11}$$

where Δ^* denotes the charge Kondo energy scale, which acts as the renormalized Fermi energy. As V approaches V_c from the Fermi liquid side, Δ^* vanishes in the Kosterlitz-Thouless fashion, $\Delta^* \approx (\rho_c)^{-1} \times \exp[-1/\sqrt{\epsilon^{\rm crit} - \epsilon}]$. For $g_V > g_V^{\rm crit}$, i.e., $-V > V_0^{\rm crit}$, the solution is a line of non-Fermi-liquids with the connected local density susceptibility

$$\chi(\tau) \approx |\rho_c/\tau|^\alpha. \tag{12}$$

The exponent α is interaction dependent, increasing from 0 to 2 as one moves away from the critical point [19,20].

The intersite interaction v_0 modifies the phase diagram in several ways. Consider first $g_V > g_V^{\rm crit}$. The line of fixed points of the $v_0 = 0$ problem becomes unstable. In terms of the parameters appropriate for the kink-gas action Eq. (7), the RG flow is towards an infinite value of the λ coupling. Usually, one cannot specify the resulting fixed points when a coupling constant flows towards infinity. Remarkably, in our case we can determine the correlation functions in the new fixed points due to the special feature of the solution to the kink-gas action Eqs. (7) and (9): the local susceptibility has an algebraic time dependence with an exponent identical to that of the range of $K(\tau)$ [21,20]. The RG flow is towards another line of fixed points with an infinite λ^*, a finite ϵ^*, and a vanishing hybridization y^*. The connected local susceptibility remains to have the algebraic $1/\tau^{\alpha^*}$ form, with the exponent α^* entirely determined by ϵ^*.

For $g_V < g_V^{\rm crit}$, we are able to establish the existence of a phase transition as v_0 is increased. First, the solution must be a non-Fermi-liquid for sufficiently strong v_o. Suppose that it is a Fermi liquid, with a renormalized Fermi energy E^*. Then the local susceptibility has a long time $(1/E^*\tau)^2$ dependence for τ longer than $1/E^*$. At times up to $1/E^*$, if the local susceptibility decays slower than $1/\tau^2$, then the corresponding $K(\tau)$ in this intermediate time range has the form Eq. (9) with $\alpha < 2$ and $\lambda = v_0^2 A$, where A is the prefactor in the decay of the local susceptibility. The scaling equations (10) imply that, for $\epsilon + \lambda/2 > 1$, the fugacity decreases in this time range. If the local susceptibility decays faster than $1/\tau^2$, one can still choose a v_0 sufficiently large such that the fugacity does not increase up to the time scale $1/E^*$. In both cases, at times beyond $1/E^*$, the kink-gas action corresponds to a Coulomb gas with a stiffness constant

$\epsilon' = \epsilon(\xi = 1/E^*) + (v_0/\sqrt{2}\,E^*)^2$ and a small fugacity y'. When v_0 becomes sufficiently large, (ϵ', y') will lie in the weak coupling side of the RG flow, making $E^* = 0$. Therefore, the Fermi liquid solution cannot occur. The only self-consistent solution in this large v_0 regime is one similar to what we found for the $g_V > g_V^{\rm crit}$ case, characterized by a $y^* = 0$, a finite ϵ^*, and an infinite λ^*. The local susceptibility has the form of Eq. (12), with $\alpha < 2$. Physically, the intersite density-density interactions provide charge screening, which contribute to the orthogonality effect [4,14]. In the mixed valence regime, this orthogonality helps realize the weak coupling fixed point with incoherent charge excitations.

For sufficiently small v_0, on the other hand, the Fermi liquid solution is stable. This can be seen by a v_0 expansion around the $v_0 = 0$ solution. We replace $K(\tau)$ in Eq. (7) by what we would get from Eq. (8) with the local susceptibility $\chi(\tau)$ of the $v_0 = 0$ problem, Eq. (11). At the time scale $\xi' = 1/\Delta^*$, $\epsilon(\xi') < \epsilon(\xi_0) < 1$, and $K(\tau) = (v_0/\Delta^*)^2 \ln(\tau/\xi')$. From Eq. (8), the kink-gas action at $\xi > \xi'$ is a Coulomb gas with a stiffness constant $\epsilon' = \epsilon(\xi') + (v_0/\sqrt{2}\,\Delta^*)^2$. For sufficiently small v_0, $\epsilon' < \epsilon^{\rm crit} = 1$. In this range, the Fermi liquid solution is self-consistent. Self-consistency, however, will modify the renormalized Fermi energy, making it unlikely that the phase transition is of the Kosterlitz-Thouless type. The precise nature of the transition is beyond the reach of our RG formalism. The schematic phase diagram is given in Fig. 2.

As a result, non-Fermi-liquids with self-similar correlation functions occur even for repulsive values of the on-site density-density interaction.

In the non-Fermi-liquid case, that the renormalized λ^* is infinite is one indication that the ground state cannot be the paramagnetic metallic state. The fact that the Ising model corresponding to the kink-gas action Eqs. (7) and (9) has a divergent free energy at zero temperature for $\alpha < 1$ implies the same physics. The precise nature of the ordering depends on the details of the band structure and the intersite interactions.

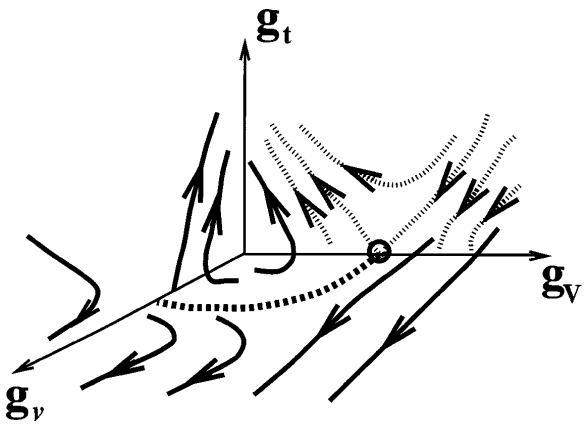

FIG. 2. The phase diagram of the Hamiltonian Eq. (1) in the mixed valence regime. The dashed line is schematic.

Our results apply at temperatures above the ordering temperature.

The extension to the spinful extended Hubbard model is straightforward. The form of the scaling equations implies that our results carry over to the charge sector of the spin-charge-separated intermediate phase.

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Note added.—After the completion of this work, we learned of the independent work of Kajueter and Kotliar [22] who constructed related mean field equations in the context of a spinless one-band fermion model with semicircular density of states and found no numerical evidence for non-Fermi-liquids in that model.

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