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Non Fermi Liquid Dynamics of the Two-Channel Kondo Lattice

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The paramagnetic phase of the two-channel Kondo lattice model is examined with a Quantum Monte Carlo simulation in the limit of infinite dimensions. We find non-Fermi-liquid behavior at low temperatures including a finite low-temperature single-particle scattering rate, no Fermi distribution discontinuity, and zero Drude weight. Both the optical and quasiparticle mass enhancement and scattering relaxation rate show consistent evidence of non-Fermi liquid behavior. However, the low-energy density of electronic states is finite.

Keywords: non-Fermi liquid, Kondo lattice, dynamics

Introduction. The Fermi Liquid theory of Landau has provided a remarkably robust paradigm for describing the properties of interacting Fermion systems such as liquid ^3He and alkali metals (e.g., sodium). The key notion of this theory is that the low lying excitations of the interacting system possess a 1:1 map to those of the noninteracting system and hence are called “quasiparticles.” In the metallic context, one may think of the quasiparticles as propagating electron-like wave packets with renormalized magnetic moment and effective mass reflecting the “molecular field” of the surrounding medium. A sharp Fermi surface remains in the electron occupancy function $n_{\vec{k}}$ which measures the number of electrons with a given momentum, and for energies ω and temperatures T asymptotically close to the Fermi surface the excitations have a decay rate going as $\omega^2 + \pi^2(k_B T)^2$, which is much smaller than the quasiparticle energy. This generally translates into a T^2 contribution to the electrical resistivity $\rho(T)$ and an ω^2 contribution to the scattering relaxation rate $\Gamma(\omega)$ inferred from the optical conductivity, and both the optical and single-particle electronic masses are found to be enhanced but positive and finite.

The Fermi liquid paradigm appears now to be breaking down empirically in numerous materials, notably a number of fully three dimensional heavy Fermion alloys and compounds [1]. In these systems such anomalies as a conductivity with linear dependence on ω, T and logarithmically divergent linear specific heat coefficients are often observed. In addition, some heavy fermion lattice compounds, such as UPe_{13} [2] and CeCu_2Si_2 [3], the superconductivity arises in a normal state which is clearly *not* described as a Fermi liquid. Specifically, the resistivity is approximately linear in T above the transition, and the magnitude of the resistivity at the transition is high (typically $80\text{--}100\ \mu\text{--}\Omega\text{--cm}$ in UPe_{13} even in the best samples). If the quasiparticle paradigm indeed breaks down, this may require completely new concepts to explain the superconducting phases of these materials. While the Luttinger liquid theory provides an elegant way to achieve non-Fermi liquid theory in one-dimension (with, e.g., no jump discontinuity in $n_{\vec{k}}$, and separation or unbinding

of spin and charge quantum numbers), this results from the special point character of the Fermi surface. Whether the essential spin-charge separation may “bootstrap” into higher dimensions remains unclear [4]. Among the remaining theories to explain experiment are those based upon proximity to a zero temperature quantum critical point [5], those based upon disorder induced distributions of Kondo scales in local moment systems [6], and those which hope to explain the physics from impurity to lattice crossover effects in the multi-channel Kondo model [7]. Notably lacking for dimensions higher than one are rigorous solutions to microscopic models which display non-Fermi liquid behavior [8].

In this paper, we present the first rigorous solution for the dynamics of the two-channel Kondo lattice model in infinite spatial dimensions. We find that the paramagnetic phase of this model is an “incoherent metal” with finite density of states at the Fermi energy and finite residual resistivity. Both the single-particle and the optical excitations are non-Fermi liquid like; in particular, there is a finite lifetime for electrons at the Fermi energy, an ill defined quasiparticle mass, a linear low temperature electrical resistivity with a finite residual value, a negative optical mass and a linear in frequency low temperature scattering relaxation rate.

Motivation The two-channel Kondo impurity model consists of two identical species of non-interacting electrons antiferromagnetically coupled to a spin 1/2 impurity. Non-Fermi liquid behavior results because of the inability to screen out the impurity spin: it is energetically favorable for both conduction electron bands to couple to the impurity which gives a spin 1/2 complex on all length scales as the temperature goes to zero. As a result, the ground state is degenerate and the excitation spectrum non-Fermi liquid like. We believe that at least the quantitative features of the model will change once the concentration of impurities becomes finite. A single impurity always lives in a Fermi liquid host; whereas the introduction of a finite concentration of impurities into the system will mean that at some temperature, the host of each impurity will be a non Fermi liquid due to the

presence of the others. The simplest model to test this hypothesis is the fully concentrated one; ie. the two-channel Kondo lattice model.

Model The Hamiltonian for the two-channel Kondo lattice is

$$H = J \sum_{i,\alpha} \mathbf{S}_i \cdot \mathbf{s}_{i,\alpha} - \frac{t^*}{2\sqrt{d}} \sum_{\langle ij \rangle, \alpha, \sigma} \left(c_{i,\alpha,\sigma}^\dagger c_{j,\alpha,\sigma} + \text{h.c.} \right) - \mu \sum_{i,\alpha,\sigma} c_{i,\alpha,\sigma}^\dagger c_{i,\alpha,\sigma}, \quad (1)$$

where $c_{i,\alpha,\sigma}^\dagger$ ($c_{i,\alpha,\sigma}$) creates (destroys) an electron on site i in channel $\alpha = 1, 2$ of spin σ , \mathbf{S}_i is the Kondo spin on site i , and $\mathbf{s}_{i,\alpha}$ are the conduction electron spin operators for site i and channel α . The sites i form an infinite-dimensional hypercubic lattice. Hopping is limited to nearest neighbors with hopping integral $t \equiv t^*/2\sqrt{d}$; the scaled hopping integral t^* determines the energy unit and is set equal to one ($t^* = 1$). Thus, on each site the Kondo spin mediates spin interaction between the two different channels. This problem is non trivial, and for the region of interest in which $J > 0$ and $T \ll J$, t^* it is describable only with non-perturbative approaches. Clearly some simplifying method which allows for a solution of the lattice problem in a non-trivial limit is necessary.

Formalism and Simulation Such a method was proposed by Metzner and Vollhardt [9] who observed that the renormalizations due to local two-particle interactions become purely local as the coordination number of the lattice increases. A consequence is that the solution of most standard lattice models may be mapped onto the solution of a local correlated system coupled to an effective bath that is self-consistently determined [10]. We refer the reader to the above references and recent reviews for further details on the method [11]. In order to solve the remaining impurity problem, we use the Kondo impurity algorithm of Fye and Hirsch [12], modified to simulate the two-channel problem [13]. The results presented here are limited to the model at half filling of the conduction bands ($N = 1.0$ for $J = 0.75, 0.625, 0.5, 0.4$). A sign problem was also encountered in the QMC process which limited our access to very low temperatures. The Euclidean-time QMC results for the local greens function $G(\tau)$ were then analytically continued to real frequencies using the “annealing” Maximum Entropy method [14]. The single particle self energy may then be obtained by inverting the relation $G(\omega) = -i\sqrt{\pi}w(\omega + \mu - \Sigma(\omega))$, where $w(z)$ is the complex Fadeev function. Error bars are ill-defined for individual points in analytically continued spectra [14], and are less than 3% for the other results presented here.

Results. When the temperature is lowered below the lattice Kondo temperature T_0 [15], we find non-Fermi liquid behavior in the single-particle properties of the model. For example, the derivative of the particle distribution function $dn(\epsilon_k)/d\epsilon_k = -T \sum_n 1/(\omega_n - \epsilon_k +$

$\mu - \Sigma(i\omega_n))^2$ saturates to a finite width distribution [15], in contrast to a Fermi liquid where it would display a dominant delta function contribution as $T \rightarrow 0$, and a Luttinger liquid [4] or Marginal Fermi liquid [16] where it would have a singular divergence.

In Fig. 1 we show one electron properties of the model. Fig. 1(a) displays the single particle DOS. This has a finite value as $\omega, T \rightarrow 0$, with a peak away from the Fermi energy. Novel behavior is seen in the real part of the one electron self energy which has positive slope at $\omega \rightarrow 0$ (Fig. 1(c)). For a Fermi liquid, this slope would be negative. The physical content is important: $Z = 1/(1 - \partial \text{Re}\Sigma/\partial\omega)$ measures the overlap of the quasiparticle wave function with the original one-electron wave function having the same quantum labels. A positive slope leads to $Z > 1$ or $Z < 0$, indicating a breakdown of the quasiparticle concept. Concomitant with the finite width of $-dn/d\epsilon_k$ is a finite imaginary part to the low temperature self energy (Fig. 1(b)). This indicates that the one-electron excitations are ill defined on approach to the Fermi surface, again ruling out a Fermi liquid description. Since the low temperature thermodynamic properties such as the specific heat, uniform magnetic susceptibility, and charge susceptibility display no evidence for a gap, we believe the observed behavior indicate a new kind of metallic state.

From our numerical results, one can show that the zero temperature self energy must be non-analytic. If the self energy is analytic everywhere in the upper half complex plane (and infinitesimal close to the real axis), then one may easily show that

$$\lim_{T \rightarrow 0} \frac{\text{Im}\Sigma(i\omega_0)}{\omega_0} = \lim_{T \rightarrow 0} \left. \frac{d\text{Re}\Sigma(\omega)}{d\omega} \right|_{\omega=0}, \quad (2)$$

where $\omega_0 = \pi T$ is the lowest Fermionic Matsubara frequency along the imaginary axis. However, we find that when $T < T_0$, $\frac{\text{Im}\Sigma(\omega_0)}{\omega_0} < 0$ and is apparently divergent; whereas, from Fig. 2 it is apparent that $\left. \frac{d\text{Re}\Sigma(\omega)}{d\omega} \right|_{\omega=0} \approx 1.5$. Thus, $\Sigma(\omega)$ cannot be analytic at the origin of the complex plane.

The non-Fermi liquid behavior also strongly effects experimentally relevant transport properties of the system. The electrical resistivity is shown in Fig. 2. We find that $\rho(T)/\rho(0)$ curves for different J values collapse onto a universal scaling curve when plotted against T/T_0 . As shown in the inset, $\rho(T) \simeq \rho(0)[1 + B(T/T_0)]$ for $T \rightarrow 0$, with $B < 0$. We interpret the finite value of $\rho(0)$ together with $-Im\Sigma(0,0)$ as “spin disorder scattering” off of the degenerate screening clouds centered about each local moment spin. Given the finite density of one particle excitations at the Fermi energy, this finite residual resistivity is indicative of an “incoherent metal phase” brought about by the disordered spin degrees of freedom, in qualitative agreement with results obtained with

a Lorentzian bare conduction DOS (which doesn't self-consistently renormalize) [17]. This surprising fact of a finite resistivity for $T \rightarrow 0$ in a translational invariant system reflects the infinitely degenerate ground state of the two channel lattice with a residual entropy.

The optical conductivity $\sigma_1(\omega)$ is measured in units of $\sigma_0 = e^2\pi/2\hbar a$, which varies between $10^{-3} \dots 10^{-2}[(\mu\Omega cm)^{-1}]$, depending on the lattice constant a . As shown in Fig. 3(a), consistent with the lack of quasiparticles, the low temperature optical conductivity displays vanishing Drude weight D . To confirm this, we also calculated D by extrapolation [18], $D \propto \chi_{jj}(q=0, i\omega_\alpha \rightarrow 0) - \chi_{jj}(q=0, i\omega_\alpha=0)$, where $\chi_{jj}(q=0, i\omega_\alpha)$ is the bulk current-current susceptibility. For each value of J and all fillings, we found that the extrapolated zero-temperature Drude weight was zero. In addition, $\sigma_1(\omega)$ has a finite-frequency ($\omega \approx 0.6J$) peak. Both these features again support our interpretation in terms of a new kind of non-Fermi liquid metallic state.

The optical conductivity of metals, even non-Fermi liquid metals [20], is usually analyzed by rewriting it in a generalized Drude form

$$\sigma(\omega) = \frac{\omega_p^2}{4\pi} \frac{1}{\Gamma(\omega) - i\omega(1 + \lambda(\omega))}, \quad (3)$$

where $\sigma(\omega) = \sigma_1(\omega) + i\sigma_2(\omega)$. The resulting mass enhancement $(1 + \lambda(\omega))$ and scattering relaxation rate $\Gamma(\omega)$ are shown in Fig. 4 when $J = 0.625$ for various temperatures. The lifetime approximation becomes exact in infinite dimensions, thus at low ω one expects $1 + \lambda(\omega) = 1 - \frac{2}{\omega}\text{Re}\Sigma(\omega/2)$ and $\Gamma(\omega) = -2\text{Im}\Sigma(\omega/2)$ [19]. At high temperatures, $\Gamma(\omega)$ and $(1 + \lambda(\omega))$ are essentially flat so a Drude peak is recovered in $\sigma_1(\omega)$; whereas at lower temperatures they become strongly frequency dependent. Here, the behavior of $\Gamma(\omega)$ is consistent with the imaginary part of the self energy, indicating that the optical and quasiparticle scattering rates are consistent for this model, even though quasiparticles do not exist. Note that when $T/T_0 = 0.20$, the low frequency optical mass is negative, $m^*(0) \approx -1.0$. This behavior is only qualitatively consistent with the mass enhancement estimated from the low temperature self energy $1 - d\text{Re}\Sigma(\omega)/d\omega|_{\omega=0} \approx -0.5$ (cf. Fig. 1). For larger values of $J > 0.75$, $m^*(0) \gtrsim 0$. Thus, the negative mass enhancement should be viewed as a sufficient but not necessary identifying feature of a non Fermi Liquid.

Finally, we mention the possible applicability of our results to concentrated heavy Fermion systems. Three systems display resistivity of the form $\rho(T) \approx \rho(0)[1 + B(T/T_0)^\alpha]$ for $T < T_0$, with $\rho(0)$ of order the unitarity limit and $\alpha \approx 1$. They are: $\text{UCu}_{5-x}\text{Pd}_x$ (with $B < 0$) [1], UBe_{13} ($B > 0$) [2,21,22], and CeCu_2Si_2 ($B > 0$) [3]. UBe_{13} and CeCu_2Si_2 are ordered compounds which have been proposed as possible two-channel lattice systems (see Refs. [7](b,c)), while $\text{UCu}_{5-x}\text{Pd}_x$ is a possible

example of the distribution of Kondo scales scenario [6]. In both UBe_{13} [23] and $\text{UCu}_{5-x}\text{Pd}_x$ [20] the measured $\sigma_1(\omega)$ and $\Gamma(\omega)$ are strikingly similar to those displayed in Figs. 3 and 4.

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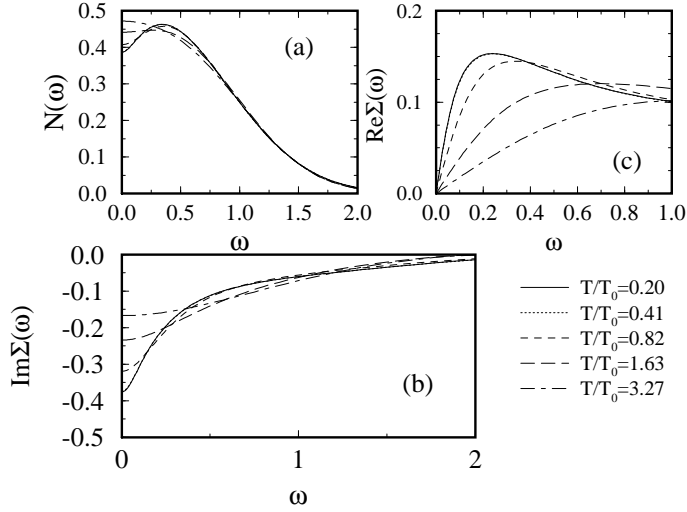


FIG. 1. Single particle properties of the two-channel Kondo lattice in infinite dimensions when $J = 0.625$ and $N = 1.0$. (a) Single-particle density of states (DOS). At high temperatures $T \gg T_0$ (not shown), the DOS is a Gaussian, crossing over to the peaked distribution with relative suppression at $\omega \rightarrow 0$ for lower temperatures when $T \ll T_0$. (b) Imaginary part of the self energy. As the temperature is lowered the self energy does not approach a Fermi liquid form $\text{Im}\Sigma(\omega) \propto -T^2 - \omega^2$, but rather appears to approach the non-analytic form (see text) $\text{Im}\Sigma(\omega) \propto -c + |\omega|$. (c) The real part of the self energy $\text{Re}\Sigma(\omega)$, is also anomalous since its initial slope is positive indicating a quasiparticle renormalization factor which is greater than one.

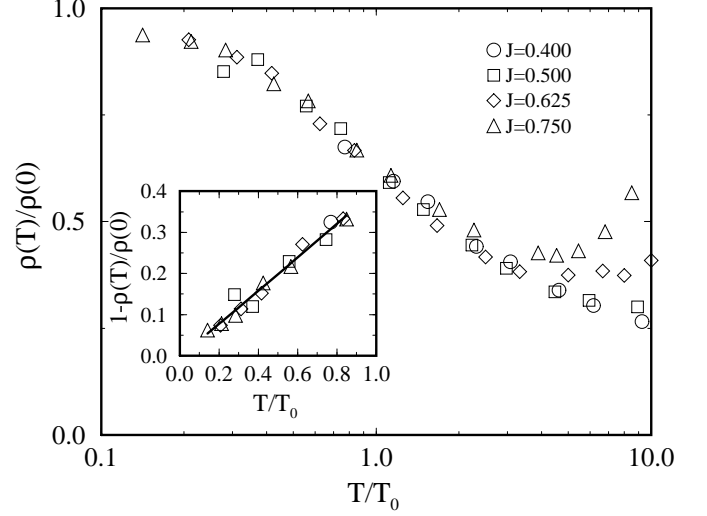


FIG. 2. Resistivity of the two-channel Kondo lattice. $\rho(T)/\rho(0)$ is plotted versus T/T_0 for various values of J . In the inset, the lowest temperature data (for $T/T_0 < 1$, shown as open circles) was fit to $\rho(T)/\rho(0) = 1 + B(T/T_0)^\alpha$, with $B = -0.4$ and $\alpha = 1.03$.

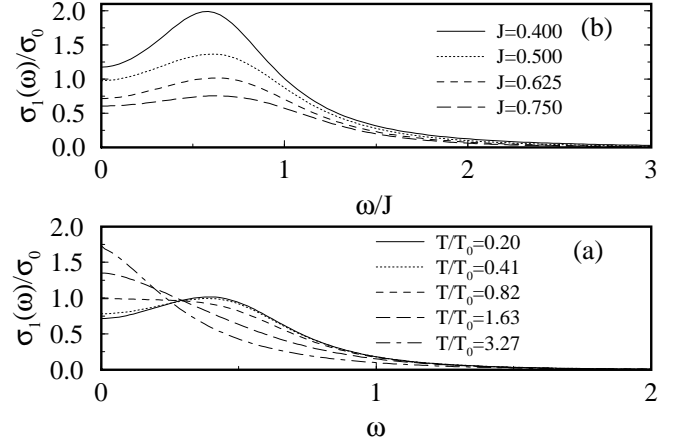


FIG. 3. Optical conductivity of the two-channel Kondo lattice. (a) Optical conductivity when $J = 0.625$. As the temperature is lowered $T < T_0$, the optical conductivity develops a pseudogap at low frequencies. No evidence of a finite Drude weight, D , can be seen, consistent with estimates of D obtained from extrapolation of Matsubara-frequency results [18]. (b) The optical conductivity vs. ω/J when $T = 0.0156$ for various values of J . $\sigma_1(\omega)$ displays a finite-frequency peak at roughly $\omega \approx 0.6J$.

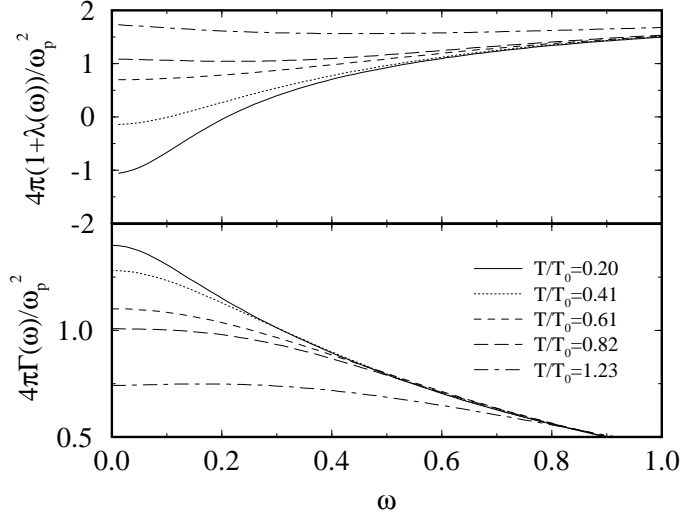


FIG. 4. Optical scattering rate $\Gamma(\omega)$ (a) and mass enhancement $(1 + \lambda(\omega))$ (b) obtained from the optical conductivity shown in Fig. 2(a) using Eq. 3. For $T/T_0 \ll 1$ both $\Gamma(\omega)$ and $(1 + \lambda(\omega))$ display non fermi liquid behavior: $\Gamma(\omega)$ is roughly linear in ω and $m^*(0) < 0$. Typical Fermi liquid behavior is recovered when $T/T_0 \gtrsim 1$, since both $\Gamma(\omega)$ and $(1 + \lambda(\omega))$ become weakly frequency dependent consistent with the recovery of the Drude peak in Fig. 3(a).