Kondo Stripes in an Anderson-Heisenberg Model of Heavy Fermion Systems

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We study the interplay between the spin-liquid and Kondo physics, as related to the non-magnetic part of the phase diagram of heavy fermion materials. Within the unrestricted mean-field treatment of the infinite-U 2D Anderson-Heisenberg model, we find that there are two topologically distinct non-degenerate uniform heavy Fermi liquid states that may form as a consequence of the Kondo coupling between spinons and conduction electrons. For certain carrier concentrations the uniform Fermi liquid becomes unstable with respect to formation of a new kind of anharmonic “Kondo stripe” state with inhomogeneous Kondo screening strength and the charge density modulation. These feature are experimentally measurable, and thus may help to establish the relevance of the spin-liquid correlations to heavy fermion materials.

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The intermetallic heavy fermion compounds based on either rare earth elements or on actinides are prototypical strongly correlated systems. In these materials, there are two types of electrons: delocalized conduction electrons (c-electrons), which derive from the outer atomic orbitals, and strongly localized f-electrons that singly occupy the inner orbitals. The interplay between the c-f hybridization and the screened on-site Coulomb repulsion, responsible for the single occupancy of f orbitals, gives rise to wide range of behaviors, including magnetic ordering, Fermi liquid and non-Fermi liquid. The magnetism arises primarily through the spin-ordering in the localized f-band. The heavy Fermi liquid (HFL) in the non-magnetic phase is believed to occur via Kondo hybridization of the f and c bands. The non-Fermi liquid behavior emerges in the vicinity of the quantum critical point separating these phases.

Recently, Senthil et al. proposed a new route to a HFL state. They considered the possibility that due to the frustrated magnetic interaction between spins in the f band, instead of forming an ordered magnetic state at low temperatures, a magnetically featureless spin liquid emerges with spin-1/2 chargeless fermionic excitations (spinons). Upon inclusion of strong enough Kondo interaction between the spinons and conduction electrons, a HFL would form, with spinons acquiring an electric charge and merging with conduction electrons to form a “large” Fermi surface. An important distinction between this scenario and the more conventional one, which does not include the possibility of a spin liquid, is that the transition occurs at a finite value of the Kondo coupling. This result in a new kind of scaling behavior near the quantum critical point separating the FL* phase of two decoupled – electron and spinon – Fermi liquids and the HFL phase of coupled spinons and electrons. Whether such a quantum phase transition remains to be seen.

Spin liquid phases have proven to be very elusive as the ground states of real materials, as well as microscopic models, particularly ones involving real electrons. However, at finite temperatures, in systems with frustrated magnetic interactions, magnetically disordered phases are well approximated by spin liquids, even if at very low temperatures a small magnetic order parameter emerges. Therefore, it is natural to ask if the spin liquid tendencies can manifest, if in the zero-temperature phase transition itself, in the structure of the “ordered” state away from the phase transition. In this Letter, we analyze in detail the structure of the heavy Fermi liquid that emerges out of the coupling of the spin liquid and the conduction Fermi liquid in the Anderson-Heisenberg lattice model. Our main findings are: First, that starting from the same spin liquid state one can obtain more than one kind of uniform heavy Fermi liquid. Second, that the spinon-electron Kondo instability can be generically inhomogeneous. The resulting structure has inhomogeneous distributions of Kondo couplings, as well as anharmonic charge density modulation, very similar to the “stripes” in the Hubbard model. A harmonic analog of this phase (without charge modulation) was recently found in a continuum model by Paul et al.

We start from the Anderson-Heisenberg lattice model with localized f-band,

\[ H = -\sum_{ij,\sigma} (t_{ij}^c + \mu \delta_{ij}) c_{i\sigma}^\dagger c_{j\sigma} + \sum_{ij,\sigma} [V_{ij} c_{i\sigma}^\dagger f_{j\sigma} + \text{h.c.}] 
+ \sum_{\sigma} (\epsilon_f - \mu) f_{i\sigma}^\dagger f_{i\sigma} + \sum_i U n_{i\uparrow} n_{i\downarrow} 
+ \frac{J_H}{2} \sum_{ij} \left( S_i \cdot S_j - \frac{n_{i\uparrow}^f n_{i\downarrow}^f}{4} \right). \]

Here \( c_{i\sigma} (c_{i\sigma}^\dagger) \) annihilates (creates) a conduction electron with spin \( \sigma \) on site \( i \); \( f_{i\sigma} (f_{i\sigma}^\dagger) \) represents the \( f \)-electron. The number operators for \( c \) and \( f \) orbitals with spin \( \sigma \) are given by \( n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma} \) and \( n_{i\sigma}^f = f_{i\sigma}^\dagger f_{i\sigma} \), respectively. The quantity \( t_{ij} \) is the hopping integral of the conduction electrons, and \( \epsilon_f \) is the local energy level of the \( f \)-electrons.
orbits. The hybridization between the conduction and $f$ bands is represented by $V_{ij}$. The $f$-electrons experience the Coulomb repulsion of strength $U$. We have included explicitly the superexchange (Heisenberg) interaction between $f$-electron spins, $\mathbf{S}_i = \frac{1}{2} \sum_{\alpha\beta} \tilde{J}^{\dagger}_{\alpha i} \sigma_{\alpha\beta} \tilde{J}^{\dagger}_{\beta i}$ with $\sigma$ the Pauli matrix. The chemical potential $\mu$ is introduced to tune the mismatch between the $c$ and $f$ patches of Fermi surface.

For simplicity, we study here the $U \to \infty$ limit, which excludes the double occupancy of the $f$-sites. This limit explicitly breaks the particle-hole symmetry in the $f$ band. We find however, that results do not qualitatively change for the Kondo-Heisenberg model \cite{1}, which contains the superexchange interaction via the Hubbard-Stratonovich transformation, the action via the Hubbard-Stratonovich transformation, the Hamiltonian \cite{1} can be written as

\[ H = - \sum_{ij,\sigma} \left( t^c_{ij} + \mu \delta_{ij} \right) c_{i\sigma}^\dagger c_{j\sigma} + \sum_{ij,\sigma} \left[ V_{ij} b_{i\sigma}^\dagger f_{j\sigma} + \text{h.c.} \right] - \sum_{ij,\sigma} [\chi_{ij} - (\epsilon_f + \lambda_i - \mu) \delta_{ij}] f_{i\sigma}^\dagger f_{j\sigma} + \sum_{i} \lambda_i (b_{i\uparrow} b_{i\downarrow} - 1) + \sum_{ij} \frac{|\chi_{ij}|^2}{J_H}. \]  

The single occupancy constraint on each site has been implemented through a Lagrange multiplier $\lambda_i$. To proceed, we make a static approximation by assuming that the slave bosons are frozen ($b_i \to \langle b_i \rangle$) and the spin liquid parameters assume their mean field values, $\chi_{ij} = (J_H/2)(f_{i\sigma}^\dagger f_{j\sigma}^\dagger)$. Moreover, for the purpose of present discussion we assume that the uniform spin liquid ($\chi_{ij} = \chi$ \cite{16}) is a good reference state for the formation of the Kondo Fermi liquid, thereby making $\chi$ an input parameter of our mean field model. Note that there is a local $U(1)$ gauge freedom present in this description: A change of phase of the slave boson on site $i$, $b_i \to b_i e^{i\phi_i}$, with the simultaneous change $f_i \to f_i e^{i\phi_i}$ and $\chi_{ij} \to e^{-i\phi_i} \chi_{ij} e^{i\phi_j}$ leaves the physical state unaltered. There are alternative mean-fields that are possible, including anomalous decoupling of the superexchange term, similar to the t-J model for cuprate superconductors \cite{17}. However, since our focus here is on possible inhomogeneous Kondo phases, we defer this possibility to a future consideration \cite{18}. In the lattice space, the Bogliubov-de Gennes (BdG) mean-field equations are:

\[ \sum_{j} \begin{pmatrix} h_{ij}^f & \Delta_{ij}^* \\ \Delta_{ji} & h_{ij}^c \end{pmatrix} \begin{pmatrix} \eta_{n\sigma}^i \\ \eta_{n\sigma}^j \end{pmatrix} = E_n \begin{pmatrix} \eta_{n\sigma}^i \\ \eta_{n\sigma}^j \end{pmatrix}, \]  

subject to the constraints

\[ \sum_{\sigma} \langle f_{i\sigma}^\dagger f_{i\sigma} \rangle + |h_i|^2 = 1, \]  

and

\[ \lambda_i b_i + \sum_{j\sigma} V_{ij} \langle c_{j\sigma}^\dagger f_{i\sigma} \rangle - \sum_{j\sigma} t_{ij}^f \langle f_{j\sigma}^\dagger f_{i\sigma} \rangle = 0. \]  

Here $h_{ij}^c = -t_{ij}^c - \mu \delta_{ij}$, $\Delta_{ij} = V_{ij} b_j^*$, and $h_{ij}^f = -\chi_{ij} + (\epsilon_f + \lambda_i - \mu) \delta_{ij}$. We solve this set of equations self-consistently via exact diagonalization on a two-dimensional square lattice. For simplicity, we consider on-site hybridization only, $V_{ij} = V \delta_{ij}$. We note, that a finite-ranged hybridization can lead to non-zero orbital momentum Kondo states with the hybridization gap anisotropic in momentum space \cite{19}. The momentum-space inhomogeneity is complementary to the real space one discussed here. Throughout this work, the quasiparticle energy is measured with respect to the Fermi energy and the energy unit $t^c = 1$ is chosen.

**FIG. 1**: (Color) A cartoon of possible Fermi surface topologies of conduction electrons and spinons. (a) The effective mass of spinons is infinite ($\chi = 0$) and no spinon Fermi surface is present; (b) $\chi \neq 0$: The Fermi surfaces of the conduction electrons and spinons, in general, are mismatched.

Within the mean-field treatment outlined above, there are two distinct uniform heavy Fermi liquid states. Suppose that we fix the gauge such that the spin-liquid parameter is positive, $\chi > 0$, and solve for Kondo hybridization, $b_i$. One possible solution is a constant, $b_i = b_0$. Another is $b_i = b_0(-1)^{x_i+y_i}$, which naively appears to break translational invariance. However, upon a gauge transformation it can be transformed to a uniform state with $b_i = b_0$ and $\chi < 0$, which is clearly uniform. The two states can be distinguished based on sign($b_i \chi_i b_j$) \cite{20}. We will denote the Kondo phase with $b_i \chi_i b_j > 0$ as “even” (eHFL) and $b_i \chi_i b_j < 0$ as “odd” (oHFL). For these two states, we can solve the above set of equations in momentum space. For eHFL, the energy dispersion has two branches given by:

\[ E_{k,\pm} = Z_k \pm \sqrt{Q_k^2 + \Delta_k^2}, \]  

where $Z_k(Q_k) = (\xi_k^c \pm \xi_k^f)/2$ with $\xi_k^c = -2t^c(\cos k_x + \cos k_y) - \mu$ and $\xi_k^f = -2(\lambda + \epsilon_f)$.
and $\Delta_k = Vb_0$. For oHLF, one only needs to replace $\chi \rightarrow -\chi$.

In Fig. 1 we provide a cartoon of possible Fermi topologies of decoupled conduction electrons and spinons. When the spinon energy is dispersionless, the Fermi surface is undefined, i.e. all spinons have the same – zero – energy in the Brillouin zone, Fig. 1(a). This is the situation of the standard Anderson lattice model. When the spinons disperse in the presence of a uniform spin liquid, the spinon Fermi surface is formed, Fig. 1(b). Again, due to the single occupancy constraint, it is pinned at half-filling, regardless of the chemical potential. The Fermi surface of the conduction electrons, $F_{S_c}$, can be tuned by the chemical potential in both cases.

First, as a point of reference, we consider the case of dispersionless spinons, $\chi = 0$. In Fig. 2(a) we show the slave boson field (effective $c$-$f$ band hybridization) and the mean-field $f$-site energy, as a function of the coupling parameter $V$. In Fig. 2(b), we show the projected density of states (DOS). There is a pronounced hybridization gap that appears above the Fermi energy in both projected conduction and $f$-electron DOS.

Now we turn to the case of dispersive spinons. For zero chemical potential $\mu = 0$, the uncoupled Fermi surfaces of the conduction electrons, $F_{S_c}$, and spinons, $F_{S_f}$, coincide, i.e., the red line in Fig. 1(b) overlaps the blue one. In this case, there is a perfect nesting across the two Fermi surfaces. This has important consequences for the Kondo hybridization, breaking the degeneracy between the odd and even Kondo phases, which existed in the $\chi = 0$ case. Qualitatively, the energetic preference of the odd Kondo phase can be seen from the approximate correspondence between the present model and the repulsive Hubbard model. Spin up (down) electrons in the Hubbard model correspond to $c$ ($f$) electrons here. In the Hubbard model, the dominant instability at half filling occurs at momentum $(\pi, \pi)$ and corresponds to antiferromagnetism. In the present model, antiferromagnetism clearly corresponds to the odd Kondo phase.

In Fig. 3, we present the self-consistent numerical results for the odd and even uniform Kondo phases. One can see from Fig. 3, the quantum critical points separating the FL* phase from the odd and even Kondo (heavy Fermi liquid) states occur at different values of interband coupling parameter $V$. Comparison of free energies (see the inset of Fig. 3), as expected, reveals that the odd Kondo phase has lower energy than the even phase. That the odd Kondo phase takes better advantage of the Fermi surface geometry is prominently manifested in the DOS. For the even Kondo state, although there is a depression exhibited in the projected conduction electron DOS, the projected $f$-electron DOS shows a broad band behavior (see Fig. 3(a)). However, for the odd Kondo state, an $s$-wave-like gap opens in both the projected conduction electron and $f$-electron DOS (see Fig. 3(b)).

A finite chemical potential breaks the particle-hole symmetry in the conduction band and introduces a mismatch between the Fermi surfaces of the conduction electrons, $F_{S_c}$, and spinons, $F_{S_f}$. In this case, an instability to a state modulated at an incommensurate wavevector, related to the mismatch between $F_{S_c}$ and $F_{S_f}$, is possible. Indeed, in the continuum, an incommensurate harmonic Kondo wave has been recently found for circular Fermi surfaces [12]. Here, we explore the real-space modulation pattern, by solving the BdG equations on a
finite size $(24 \times 24)$ lattice self-consistently via exact diagonalization. To facilitate numerical convergence, we considered only unidirectional patterns. This was achieved by “seeding” them as an initial guess, and iterating until convergence. We found that this procedure leads to convergence to a local minimum, without changing the initially imposed spatial period. The optimal modulation pattern is anharmonic, in close analogy to the stripes found in the mean-field treatment of the Hubbard model \[1\]. For a fixed coupling parameter $V$, we find that there is a critical value of $\mu$, below which a modulated Kondo state occurs.

In Fig. 5 we show the spatial dependence of the slave-boson $b$ field, the Kondo hybridization $b_i (c_d^\dagger f_i)$, the local $f$-electron density, and the local $c$-electron density (the latter three quantities are gauge-invariant). We see clearly the emergence of an anharmonic Kondo stripe state when the system is deeply in the heavy fermion liquid phase. In this strong coupling limit, the hole density in the $f$-band is rather high, which leads to a short periodicity. We also notice that in the strong coupling limit, the “domain wall” between the regions of constant sign of $b_i$ is bond centered. We anticipate that by reducing the coupling strength $V$ toward the Kondo breakdown critical point, the anharmonicity will be suppressed along with a reduction of the modulation amplitude, leading to a nearly-harmonic Kondo wave \[12\]. However, system size limitations and problems with numerical convergence in this parameter regime, prevented us from verifying this directly. The Kondo stripes are closely analogous to the antiferromagnetic (AF) stripes in the mean-field treatment of the repulsive Hubbard model \[11\]. The field $b(r)$ plays the role of the AF order parameter $M(r)$, and the electron density $\rho(r)$ corresponds to the hole density $\rho(r)$. The lowest-order symmetry-allowed coupling in the Kondo stripe free energy (which also follows from the constraint) is $[b(r)]^2 \rho(r)$, which corresponds to $S^2(r)\rho(r)$ term for AF stripes \[21\].

In summary, we have considered a lattice model of coupled conduction electrons and spinons, as a model of a heavy Fermi liquid (Kondo) state. We found that for nearest-neighbor hopping models, two distinct heavy Fermi liquid states are possible. We also point out that in the generic case of mismatched electron and spinon Fermi surfaces, electronically inhomogeneous heavy Fermi liquid phases (Kondo stripes) are expected to appear. These phases exhibit inhomogeneous Kondo hybridization and charge density, which should manifest in both local and bulk probes. Identifying these phases experimentally may help to determine the relevance of the spin-liquid physics to heavy fermion materials.

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[1] G. R. Stewart, Rev. Mod. Phys. 56, 755 (1984).
[2] H. Tsunetsugu, M. Sigrist, and K. Ueda, Rev. Mod. Phys. 69, 809 (1997).
[3] G. R. Stewart, Rev. Mod. Phys. 73, 797 (2001); 78, 743 (2006).
[4] P. Gegenwart, Q. Si, and F. Steglich, Nature Phys. 4, 186 (2008).
[5] T. Senthil, S. Sachdev, and M. Vojta, Phys. Rev. Lett. 90, 216403 (2003).
[6] T. Senthil, M. Vojta, and S. Sachdev, Phys. Rev. B 69, 035111 (2004).
[7] P. Coleman, J. B. Marston, and A. J. Schofield, Phys. Rev. B 72, 245111 (2005).
[8] A. J. Millis and P. A. Lee, Phys. Rev. B 35, 3394 (1987); P. Coleman, Phys. Rev. B 35, 5072 (1987); D. M. Newns and N. Read, Adv. Phys. 36, 799 (1987); M. Grilli, G. Kotliar, and A. J. Millis, Phys. Rev. B 42, 329 (1990); A. M. Sengupta and A. Georges, Phys. Rev. B 52, 10295 (1995).
[9] C. Pepin, Phys. Rev. Lett. 98, 206401 (2007); C. Pepin, preprint \url{arXiv:0802.1498} (2008).
[10] J. A. Hertz, Phys. Rev. B 14, 1165 (1976); A. J. Millis, Phys. Rev. B 48, 7183 (1993); T. Moriya and T. Takimoto, J. Phys. Soc. Jpn. 64, 960 (1995); S. Kambe et al.,
ibid. 65, 3294 (1996).
[11] J. Zaanen and O. Gunnarsson, Phys. Rev. B 40, 7391 (1989).
[12] I. Paul, C. Pepin, and M. R. Norman, Phys. Rev. Lett. 98, 026402 (2007).
[13] A. C. Hewson, *The Kondo Problem to Heavy Fermions* (Cambridge University Press, Cambridge, 1993).
[14] S. E. Barnes, J. Phys. F 6, 1375 (1976).
[15] P. Coleman, Phys. Rev. B 29, 3035 (1984).
[16] G. Baskaran, Z. Zou, and P. W. Anderson, Solid State Commun. 63, 973 (1987).
[17] P. A. Lee, N. Nagaosa, and X.-G. Wen, Rev. Mod. Phys. 78, 17 (2006).
[18] Jian-Xin Zhu, unpublished.
[19] P. Ghaemi and T. Senthil, Phys. Rev. B 75, 144412 (2007).
[20] S. Sachdev, private communication.
[21] L. Pryadko *et al.*, Phys. Rev. B 60, 7541 (1999).