

Fractionalized Fermi liquids

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In spatial dimensions $d \geq 2$, Kondo lattice models of conduction and local moment electrons can exhibit a fractionalized, non-magnetic state (FL^{*}) with a Fermi surface of sharp electron-like quasiparticles, enclosing a volume quantized by $(\rho_a - 1)(\text{mod } 2)$, with ρ_a the mean number of all electrons per unit cell of the ground state. Such states have fractionalized excitations linked to the deconfined phase of a gauge theory. Confinement leads to a conventional Fermi liquid state, with a Fermi volume quantized by $\rho_a(\text{mod } 2)$, and an intermediate superconducting state for the Z_2 gauge case. The FL^{*} state permits a second order metamagnetic transition in an applied magnetic field.

The physics of the heavy fermion metals, intermetallic compounds containing localized spin moments on d or f orbitals and additional bands of conduction electrons, has been of central interest in the theory of correlated electron systems for several decades [1–3]. These systems are conveniently modelled by the much studied Kondo lattice Hamiltonian, in which there are exchange interactions between the local moments and the conduction electrons, and possibly additional exchange couplings between the local moments themselves. To be specific, one popular Hamiltonian to which our results apply is:

$$H = - \sum_{j,j'} t(j,j') c_{j\sigma}^\dagger c_{j'\sigma} + \frac{1}{2} \sum_j J_K(j) \vec{S}_j \cdot c_{j\sigma} \vec{\tau}_{\sigma\sigma'} c_{j\sigma'} + \sum_{j<j'} J_H(j,j') \vec{S}_j \cdot \vec{S}_{j'} \quad (1)$$

Here the local moments are $S = 1/2$ spin \vec{S}_j , and the conduction electrons $c_{j\sigma}$ ($\sigma = \uparrow, \downarrow$) hop on the sites j, j' of some regular lattice in d spatial dimensions with amplitude $t(j, j')$, $J_K > 0$ are the Kondo exchanges ($\vec{\tau}$ are the Pauli matrices), and explicit short-range Heisenberg exchanges, J_H , between the local moments have been introduced for theoretical convenience. A chemical potential for the c_σ fermions which fixes their mean number at ρ_c per unit cell of the ground state is implied. We have not included any direct couplings between the conduction electrons as these are assumed to be well accounted by innocuous Fermi liquid renormalizations.

For simplicity, we restrict our attention here to non-magnetic states, in which there is no average static moment on any site ($\langle \vec{S}_j \rangle = 0$), and the spin rotation invariance of the Hamiltonian is preserved: the \vec{S}_j moments have been ‘screened’, either by the c_σ conduction electrons, or by their mutual interactions (there is a natural extension of our results to magnetic states). It is widely accepted [1,3–7] that such a ground state of H is a conventional Fermi liquid (FL) with a Fermi surface of ‘heavy’ quasiparticles, enclosing a volume, \mathcal{V}_{FL} determined by the Luttinger theorem:

$$\mathcal{V}_{FL} = \mathcal{K}_d [\rho_a(\text{mod } 2)]. \quad (2)$$

Here $\mathcal{K}_d = (2\pi)^d / (2v_0)$ is a phase space factor, v_0 is the volume of the unit cell of the ground state, $\rho_a = n_\ell + \rho_c$ is the mean number of all electrons per volume v_0 , and n_ℓ (an integer) is the number of local moments per volume v_0 . Note that $\rho_{c,a}$ need not be integers, and the $(\text{mod } 2)$ in (2) allows neglect of fully filled bands. In $d = 1$, (2) has been established rigorously by Yamanaka *et al.* [5]. In general d , a non-perturbative argument for (2), assuming that the ground state is a Fermi liquid, has been provided by Oshikawa [6], who also emphasized that the Luttinger theorem can be regarded as a ‘‘quantization’’ of \mathcal{V}_{FL} .

The primary purpose of this paper is to show that there exist non-magnetic, metallic states (FL^{*}) in dimensions $d \geq 2$ with a Fermi surface of ordinary $S = 1/2$, charge $-e$, sharp quasiparticles, enclosing a volume

$$\mathcal{V}_{FL^*} = \mathcal{K}_d [(\rho_a - 1)(\text{mod } 2)] \quad (3)$$

over a finite range of parameters. For $n_\ell = 1$ \mathcal{V}_{FL^*} is determined by the density of conduction electrons alone. A number of earlier works [8–10] have considered a Fermi surface of conduction electrons alone, decoupled in mean-field from the local moments. Here we establish the conditions under which (3) characterizes a stable phase of matter for generic couplings, beyond simple decoupled models. One of our findings is that any FL^{*} state must be *fractionalized* [11] *i.e.* it possesses $S = 1/2$ neutral spinon excitations (which are entirely distinct from the Fermi surface quasiparticles) which carry a charge under a gauge group which characterises the topological order in the FL^{*} state. We will consider here only the simplest case of a Z_2 gauge group [11,12], in which case the Z_2 FL^{*} state possesses a gap to topologically non-trivial ‘vison’ states [11,13,14] which carry Z_2 flux. The connection with a Z_2 (or other) gauge theory explains why the FL^{*} is not possible in $d = 1$: a translationally invariant deconfined phase of the gauge theory is only present for $d \geq 2$. We will also discuss the quantum transition between the Z_2 FL^{*} state and the conventional FL state

as the exchange couplings are varied: this transition is preempted by a superconducting state.

We note that the FL* state does not contradict the non-perturbative computation by Oshikawa [6] of \mathcal{V}_{FL} ; on the contrary, this argument helps establish the intimate connection between (3) and topological order. Oshikawa placed the system on a torus, and considered the adiabatic evolution of the ground state upon threading a magnetic flux of hc/e felt by the electrons with spin up (in some basis) through one of the holes of the torus. For insulating antiferromagnets with a fractionalized spin liquid ground state (a resonating valence bond (RVB) state), this procedure connects two of the topologically distinct states which become degenerate in the thermodynamic limit in a toroidal geometry [14–16] *i.e.* it connects states with and without a vison threading the hole of the torus. The FL* state of the Kondo lattice models we are discussing here has a similar topological order, and the toroidal system has global vison excitations which are degenerate with the ground state in the thermodynamic limit. Oshikawa did not consider such excitations, and only included the electron-like Fermi surface quasiparticles. Consequently, his argument does not directly apply to the FL* state, and a modification accounting for vison excitations shows that the volume \mathcal{V}_{FL^*} is allowed. In other words, the Fermi volume is still quantized, but differently from that in a Fermi liquid.

The volume \mathcal{V}_{FL} is observed in many compounds, and in particular in those with weak direct exchange J_H between different local moments. Doniach [17] pointed out that increasing J_H would lead to magnetically ordered states. However, the effective exchange interactions between the local moments are strongly frustrated in many common lattices, so that the magnetic order may be very fragile or entirely absent: it is these frustrated systems which are favorable candidates for displaying a non-magnetic FL* state. The generic appearance of superconductivity in the crossover between the Z_2 FL* and FL states is experimentally significant: this may be regarded as a proposed ‘mechanism’ for superconductivity in heavy fermion systems, which bears some similarity to the RVB theory [18]. The critical temperature (T) for the onset of superconductivity, T_c , can be small.

The $T > 0$ behavior of the Z_2 FL* state depends on d , as discussed for other fractionalized states in Ref. [11]. In $d = 3$ there is a finite temperature phase transition associated with the onset of topological order. This is absent in $d = 2$ where the topological order is present only at $T = 0$. In layered quasi-two dimensional materials, both types of behavior (corresponding to two distinct $T = 0$ phases) are possible.

To understand the origin of our results in the context of (1), consider first the limiting case $J_K = 0$, when the c_σ fermions and the \vec{S}_j spins are decoupled. While the c_σ fermions will occupy states inside a Fermi surface enclos-

ing volume $\mathcal{K}_d[\rho_c(\text{mod } 2)]$, there are two distinct classes of possibilities for a non-magnetic ground state for the \vec{S}_j spins interacting via J_H .

The first is a ground state with confinement of spinons and a unit cell with n_ℓ even; this may require breaking of translational symmetry by the appearance of bond order [19]. In this case $\rho_a = \rho_c(\text{mod } 2)$, and turning on a finite J_K leads to a FL state, possibly with co-existing bond order, with the Fermi volume \mathcal{V}_{FL} equal to that at $J_K = 0$.

The second possibility, of central interest in this paper, is that \vec{S}_j moments form a fractionalized spin liquid ground state with n_ℓ odd [11,12,20]: this happens on frustrated lattices, as has been supported by studies [21] on the triangular lattice. A fundamental property of such a state is its topological stability [11], and the associated gap towards creation of vison excitations which carry unit flux of a Z_2 gauge field. The $S = 1/2$ spinon excitations above this state carry a unit Z_2 gauge charge. Now turn on a small $J_K \neq 0$. The key argument of this paper is that the resulting ground state is smoothly connected to the $J_K = 0$ limit: the quantum numbers of the latter state and its excitations are topologically protected, the vison gap will survive for a finite range of J_K values, and perturbation theory in powers of J_K is non-singular. So we obtain our advertised FL* state, with a Fermi surface of spin-1/2, charge $-e$, quasiparticles enclosing the volume \mathcal{V}_{FL^*} equal to that at $J_K = 0$, along with a separate set of spin-1/2 neutral spinon excitations [22]. Physically, each local moment has formed a singlet with another local moment in an RVB spin liquid state - the Kondo coupling with the conduction electrons is ineffective in breaking these singlets. The Fermi surface quasiparticles have a weak residual interaction, arising from exchanges of pairs of spinons, which could lead to their pairing in a high angular momentum channel at some very low T : this produces an exotic superconductor which co-exists with a fractionalized spin liquid [23] which we will not discuss further—the superconductivity discussed elsewhere in this paper is more robust and a qualitatively different state.

As we continue to increase J_K , the physics of the Kondo effect will eventually be manifest: it will become favorable for a local moment to form a Kondo singlet with the conduction electrons rather than with other local moments. This may be formalized as follows, for the case in which the spinons are fermions: Representing the \vec{S}_j moments by $S = 1/2$ fermions $f_{j\sigma}$ ($\vec{S}_j = f_{j\sigma}^\dagger \vec{\tau}_{\sigma\sigma'} f_{j\sigma'}/2$ with the single-occupancy constraint $f_{j\sigma}^\dagger f_{j\sigma} = 1$), the formation of Kondo singlets is signaled by a non-zero hybridization between the f_σ and the c_σ fermions. This can be expressed more precisely in terms of the composite boson fields $B_1 = f_\sigma^\dagger c_\sigma$ and $B_2 = \varepsilon^{\sigma\sigma'} f_\sigma c_{\sigma'}$, where ε is the antisymmetry tensor with $\varepsilon^{\uparrow\downarrow} = 1$. Both of these fields have a unit Z_2 gauge charge, an electromagnetic

charge e and are spin singlet: Condensation of these bosons implies a non-zero amplitude that a local moment has formed a Kondo singlet with the conduction electrons. This condensation indicates that the Z_2 gauge theory enters a Higgs phase which can also be identified with a phase in which Z_2 charges are confined [24]. Moreover, as the spinon pairing amplitude $\langle \varepsilon^{\sigma\sigma'} f_\sigma f_{\sigma'} \rangle$ is generically non-zero in the small J_K fractionalized phase [11], the condensation of B_1 implies condensation of B_2 (and vice-versa), and there is only a single Z_2 confinement transition. More importantly, the pairing of the spinons and the condensation of $B_{1,2}$ implies that the resulting phase also has pairing of the conduction electrons, and is a superconductor at $T = 0$.

Consider now the behavior when $J_K, t \gg J_H$. In the limit $J_H = 0$, the usual FL state is expected (at least at generic incommensurate conduction electron density). Turning on a weak non-zero J_H potentially introduces a weak instability toward superconductivity, as will be the case in our mean-field theory below. However, the FL state may still be stabilized by a weak nearest neighbor repulsive interaction between the conduction electrons.

The general considerations above can be illustrated by a simple mean-field computation of the phase diagram of H . We applied the large N method associated with a generalization of H to $\text{Sp}(N)$ symmetry [25] on the triangular lattice. It is important to note that both the symmetry group and the lattice have been carefully chosen to allow for a mean field state with Z_2 topological order, stable under gauge fluctuations [12]; in particular, there are topologically distinct mean-field ground states in a toroidal geometry, differing in the Z_2 flux through the holes of the torus. Other choices [8] for the lattice or the symmetry group lead to mean-field solutions which are generically disrupted by $\text{U}(1)$ or $\text{SU}(2)$ gauge fluctuations in $d = 2$. We used self-conjugate, fully anti-symmetric (fermionic) representations for the spin states, and the computations were then similar to earlier work on the t - J model [25]. For $J_K = 0$ and nearest neighbor J_H , these representations yields globally stable solutions in which the \vec{S}_j spins are paired in fully dimerized states which break lattice symmetries. As we are not interested in such states here, we restricted our analysis to saddle points which preserve all lattice symmetries. Such RVB saddle points can be stabilized by additional couplings between the local moments; they are also stable for nearest-neighbor J_H for bosonic spin representations [26,25], but these, unfortunately, do not allow a simple description of the FL state at large J_K . It is possible that the spinons undergo a change from bosonic to fermionic statistics with increasing J_K within the Z_2 FL* state, but this will not be captured by our present mean field theory which has only fermionic spinons.

The phase diagram is shown in Fig 1 as a function of J_K and T for fixed J_H , t , and ρ_c .

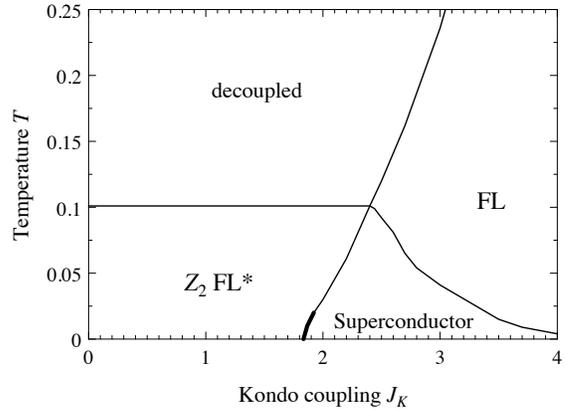


FIG. 1. Mean field phase diagram of H on the triangular lattice. We used fermionic representations of $\text{Sp}(N)$ for the spins, and restricted attention, by hand, to saddle points which preserve all lattice symmetries. We had nearest-neighbor $t = 1$, $J_H = 0.4$, and $\rho_c = 0.7$. The superconducting T_c is exponentially small, but finite, for large J_K , while it is strictly zero for small J_K . Thin (thick) lines are second (first) order transitions. The transitions surrounding the superconductor will survive beyond mean field theory, while the others become crossovers.

In addition to the Z_2 FL* and FL states, and an intermediate superconducting state, whose character we have already discussed, there is also a high temperature “decoupled” state. Here, in the mean field saddle point, the spins are mutually decoupled from each other, and from the conduction electrons. This decoupling is, of course, an artifact of the saddle point, and it points to a regime where all excitations are incoherent but strongly interacting with each other. For the case where the superconducting phase is present only at very low temperatures (as may well be the case beyond mean field theory), this incoherent regime represents the quantum-critical region of the Z_2 FL*-FL transition. A separate description of this incoherent quantum critical dynamics was provided by the large-dimensional saddle point studied by Burdin *et al.* [10], where it was related to the gapless spin liquid state of Ref. [27].

An interesting $T = 0$ quantum phase transition appearing in Fig 1 is that between the FL* and superconducting states. As we discussed earlier, this transition is associated with the condensation of the charge e bosons $B_{1,2}$. A critical theory of the transition can be written down in terms of $B_{1,2}$ and the conduction electrons: the methods and resulting field theory are identical to those discussed in Ref. [28]. The renormalization group analysis shows that the $T = 0$ transition can be either first or second order, depending upon the values of microscopic parameters. The gapped vison excitations in the FL* state may be detected through the flux trapping experiments discussed in Ref. [29]. Furthermore, provided the transition is not too strongly first order, the presence of a critical charge e bosonic mode implies that the su-

perconducting state in the vicinity of this transition is a candidate for displaying stable hc/e vortices [30,11].

Interesting physics obtains in the presence of an external uniform Zeeman magnetic field in the FL* state. As the local moment and conduction electron systems are essentially decoupled in this phase, they both respond independently to the magnetic field. If the spinons are gapped in the fractionalized phase, then there would be a critical field B_c associated with the onset of magnetization in the local moment system. Experimentally, this would be seen as a “metamagnetic” transition in the response of the system to an applied field. Interestingly, this onset transition could clearly be generically (*i.e.* without any fine tuning) second order. Metamagnetic quantum criticality in strongly correlated systems has been the subject of some recent experimental [31] and theoretical studies [32], although accidental fine tuning has been invoked to obtain a second order transition.

This paper has established that metals with local moments in dimensions $d \geq 2$ can have non-magnetic ground states (FL*) which are distinct from the familiar heavy Fermi liquid state (FL). The latter state has a Fermi surface enclosing a volume \mathcal{V}_{FL} determined by the density, ρ_a , of both the conduction electrons and local moments; our topologically ordered FL* state has sharp electron-like excitations on a Fermi surface enclosing a volume \mathcal{V}_{FL^*} determined by $(\rho_a - 1)$ (for $n_\ell = 1$ this is the density of conduction electrons alone), along with additional ‘fractionalized’ excitations. In between these FL and FL* states, a plethora of additional states associated with magnetic, superconducting, and charge order appear possible, along with non-trivial quantum critical points between them. We believe this rich phenomenology should find experimental realizations in the heavy fermion compounds.

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