Co-operative Two-Channel Kondo Effect

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We discuss how the properties of a single-channel Kondo lattice model are modified by additional screening channels. Contrary to current wisdom, additional screening channels appear to constitute a relevant perturbation which destabilizes the Fermi liquid. When a heavy Fermi surface develops, it generates zero modes for Kondo singlets to fluctuate between screening channels of different symmetry, producing a divergent composite pair susceptibility. Additional screening channels couple to these divergent fluctuations, promoting an instability into a state with long-range composite order.

A puzzling question that arises in trying to understand heavy fermion superconductors is how the localized moments seen in high temperature properties participate in the pair condensate. In these systems a significant fraction of the entropy associated with the local moments appears to be involved with the superconducting condensation process: for $UB\text{e}_{13}$, the spin-condensation entropy is about $0.2k_B\ln 2$ per spin. The concept of “composite pairing”, where a Cooper pair and local moment form a bound-state combination that collectively condenses may provide a way to understand this large spin-condensation entropy. Recent studies of the one-dimensional Kondo lattice at strong-coupling and the infinite dimensional two-channel Kondo lattice have both given indication of a composite pairing instability.

In this paper we discuss how the properties of a single-channel Kondo lattice model for heavy fermion systems are modified by coupling to additional screening channels. Current wisdom, based on the naive extrapolation from single impurity models, regards these additional couplings to be irrelevant. We shall show that an entirely different state of affairs arises in a two-channel Kondo lattice where the scattering channels of different local symmetry are obliged to share a single Fermi sea. This allows for the possibility of a constructive interference between the two channels which drives the development of composite order.

Consider a sea of conduction electrons coupled to an N-site lattice of spin-1/2 local moments via two channels:

$$H = H_o + \sum_j \{ J_1 \psi_{1j}^\dagger \sigma \psi_{1j} + J_2 \psi_{2j}^\dagger \sigma \psi_{2j} \} \cdot S_j, \quad (1)$$

where $H_o = \sum_{k \Gamma} \epsilon_{k \sigma} c_{k \sigma}^\dagger c_{k \sigma}$ describes a single electron band and

$$\psi_{1j}^\dagger = N^{-\frac{1}{2}} \sum_k \Phi_{k \Gamma} c_{k \sigma}^\dagger e^{-ik \cdot R_j}, \quad (\Gamma = 1, 2) \quad (2)$$

creates an electron at site $j$ in one of two orthogonal Wannier states, with form-factor $\Phi_{k \Gamma}$. We are motivated to include a weak second-channel coupling into a Kondo lattice model by the observation that interactions in the conduction generally cause the spin-exchange to spill over from the primary (f-) channel into a weaker, secondary screening channels. We shall also introduce a “control” model (II), where

$$H_{o}^{(II)} = \sum_{k \Gamma \sigma} c_{k \sigma}^\dagger \Gamma \sigma \psi_{1k \sigma}$$

simply describes a band of electrons carrying a conserved channel quantum number $\Gamma = 1, 2$. In the control, electrons in different channels do not mix, and the absence of a composite pairing instability in this model provides confirmation that that composite pairing effects are a consequence of channel interference.

To examine the effect of second-channel couplings, we introduce the composite operator

$$\Lambda = \sum_j -i \psi_{1j}^\dagger \sigma_{12} \psi_{2j}^\dagger \cdot S_j, \quad (4)$$

which transfers singlets between channels by simultaneously adding a triplet and flipping the local moment. We now show that channel interference causes the susceptibility of this composite operator to diverge in Fermi liquid ground-state of channel one.

Suppose $J_2 << J_1$ so that a Kondo effect develops in channel one. At low energies, the operator $(S_j \cdot \sigma_{\alpha \beta}) \psi_{1\beta}$ then behaves as a single bound-state fermion, represented by the contraction

$$(S_j \cdot \sigma_{\alpha \beta}) \psi_{1\beta}(j) = z f_{j\alpha}. \quad (5)$$

where $z$ is the amplitude for bound-state formation. Hybridization between these composite bound-states and
conduction electrons forms the heavy-fermion quasiparticles, with energy $E_k$ and an enlarged Fermi surface whose enclosed volume counts both conduction and composite f-electrons.

By applying this contraction procedure we see that the action of the composite operator $\Lambda$ on the heavy fermion ground-state creates a pair:

$$\Lambda|\Phi\rangle = -i \sum_j \mathbf{S}_j \cdot (\psi_{1j}^\dagger \sigma \sigma_2 \psi_{2j}^\dagger)|\Phi\rangle = z \sum_{k,\sigma} \sigma \psi_{2k\sigma}^\dagger f_{-k-\sigma}^\dagger|\Phi\rangle \quad (6)$$

In the control model, $\psi_{2k}^\dagger$ and $f_{-k}^\dagger$ are light and heavy electrons on different Fermi surfaces. The mismatch between the decoupled Fermi surfaces for channel one and two assures that the excitation energy $\epsilon_k + E_k$ is always finite. By contrast, in the physical model, $\Lambda$ creates: (I) a pair of heavy fermions (channel interference ) and (II) a heavy and light electron (channel conservation).

It follows that composite pair susceptibility $\chi_\Lambda$ must contain a singular term, directly proportional to the anisotropic pair susceptibility of the heavy quasiparticles, $\chi_\Lambda \propto \sum_k \tanh (\beta E_k) \left( \Phi_{1k} \Phi_{2k}^\dagger \right)^2 \propto \ln (T_{K1}/T) \quad (8)$

where $T_{K1}$ is the Kondo temperature for channel one. Any finite $J_2$ will polarize the transfer of singlets into channel two, thereby coupling $J_2$ to this divergent susceptibility. This will cause $J_2$ to scale to strong-coupling. A similar conclusion will hold when $J_2$ is large, and $J_1$ is small. Since both Fermi-liquid fixed points are unstable (Fig. 3), continuity of the renormalization flows at strong and weak coupling leads us to conclude that the physical two-channel Kondo lattice possesses a new attractive fixed point which is common to both channels.

One of the distinct features of this new lattice fixed point is the development of off-diagonal composite order,

$$\langle \hat{\Lambda}(x) \rangle \neq 0. \quad (9)$$

This type of order involves the explicit participation of two screening channels and the local moments in the pair condensate. To explore the nature of this new phase, we present a simple extension of the existing mean-field theory of the Kondo lattice. If we employ the pseudo-fermion representation of the local moments

$$S_j = \frac{1}{2} f_j^\dagger \sigma f_j$$

then the associated constraint $\langle f_j f_j^\dagger \rangle = 1$ at each site leads to a local $SU(2)$ symmetry

$$f_{j\sigma} \rightarrow \begin{cases} e^{i\theta} f_{j\sigma}, \\ \cos \phi f_{j\sigma} + \sin \phi f_{j-\sigma}^\dagger. \end{cases} \quad (10)$$

The Lagrangian for the f-electrons is

$$L_f = \sum_j \tilde{f}_j^\dagger \left( \partial_\tau + \mathbf{W} \cdot \mathbf{\tau} \right) \tilde{f}_j, \quad (11)$$

where the tilde field $\tilde{f}_j^\dagger = (f_j^\dagger f_j^\dagger, f_{j\uparrow}^\dagger)$ denotes a Nambu spinor representation of the f-electron and $\mathbf{W}$ is a fluctuating gauge field which imposes the constraint. The $SU(2)$ symmetry makes it possible to simultaneously factorize $H_f$ in both particle-hole and Cooper channels.
$$H_I = \sum_{i,j} \left\{ [\hat{f}_j^\dagger V^I_i \hat{\psi}_{ij} + H.c.] + \frac{1}{2J_F} \text{Tr}[V^I_j V^I_j] \right\}, \quad (12)$$

where \( \hat{\psi}_{ij} = (\hat{\psi}_{ij}^\dagger, \psi_{ij}) \). The field

$$V^I_j = i \left[ -\Delta^* \frac{\Lambda_j}{V^*} \right]_j,$$  

is directly proportional to an SU(2) matrix.

The essential observation is that the onsite product of the two fields \( \mathcal{M}(x_j) = V^I_j V^I_j \) is invariant under local SU(2) gauge transformations \( V^I_j \rightarrow g_j V^I_j \). \( \mathcal{M}(x) \) therefore represents a physical quantity. Careful re-expression of this matrix in an operator form reveals that its components are directly related to the composite order that develops between the two channels

$$\left\{ \begin{array}{l} \langle F(x) \rangle \\ -\Lambda_j(x) \end{array} \right\} = \frac{\langle V^I_j(x) V^I_j(x) \rangle}{J_I J_2}, \quad (14)$$

where \( F(x_j) = \psi_{ij}^\dagger \sigma \psi_{ij} \cdot \mathbf{S} \) represents composite charge order and \( \Lambda(x) \) is the composite pair density. The product form of this result establishes that composite order is a consequence of interference between the Kondo effect in the two channels.

By removing the site indices on the hybridization and constraint field we obtain the mean-field Hamiltonian

$$H_{MF} = \sum_k (\epsilon^+_k, f^+_k) \left[ \epsilon_k \tau_j \frac{V^I_k}{W \cdot \tau} \right] (\epsilon_k, f_k), \quad (15)$$

where the one-band character of the model forces the order parameter for each channel to enter into the hybridization \( V^I_k = V^I_1 \Phi_{1k} + V^I_2 \Phi_{2k} \). This provides the origin of the interference between the two channels. Choosing the gauge where \( V^I_1 = iv_2 \mathbf{1} \), then a stable composite-paired solution emerges with \( V^I_2 = v_2 \mathbf{1}, \mathbf{W} = (0,0,\lambda) \). After some work, we find that the eigenvalue spectrum of [13] has two branches, where

$$E_{k,\pm} = \sqrt{\alpha_k \pm (\alpha_k^2 - \gamma_k^2)^{1/2}}, \quad (16)$$

where \( \alpha_k = v^2_1 + \frac{1}{2}(\lambda^2 + c_k^2), \gamma_k = [\lambda \epsilon_k - V^2_1] \pm 2v_1 v_2 \mathbf{1}^2 \) and we have defined \( \nu_{\Gamma,\tau} = v_1 \Phi_{\Gamma,\tau}, V_{k,\pm} = v_{1k} \pm v_2 \mathbf{1} \). The requirement that the Free energy per site

$$F = -2T \sum_{k,\alpha = \pm} \ln \left[ 2 \cosh(\beta E_{k,\alpha}/2) \right] + \sum_{r=1,2} \frac{(\nu_r)^2}{J_F}, \quad (17)$$

is stationary with respect to variations in \( v_2, v_1 \) and \( \lambda \) gives rise to three mean-field equations. Two classes of solution exist:

- **Normal state**: \( v_1 \) or \( v_2 = 0 \). Two normal state phases exist corresponding to a single-channel Kondo effect in channel one or two. The Fermi surface geometries of the two phases are topologically distinct, and at half filling these phases evolve into two different Kondo insulating phases.

- **Composite paired state**: \( v_1 v_2 > 0 \). When channel conservation is absent, a Kondo effect in both channels leads to a paired state with an anisotropic heavy electron gap function \( \Delta_k \sim \sqrt{T_K I K_2} \Phi_{1k} \Phi_{2k} \).

Setting \( v_2 = 0^+ \) in the mean-field equations, the transition from the one-channel Fermi liquid into the composite paired state is given by \( J_2 \chi_\Lambda(T) = 1 \) where

$$\chi_\Lambda(T) = \sum_{\mathbf{k} \alpha} \text{th}(\frac{E_{k,\alpha}}{2T}) \left\{ \left[ \frac{\Phi_{1k}}{E_{k,\alpha} - E_{k,\alpha - \epsilon_k}^2} \right] + \left[ \frac{\Phi_{2k}^2}{E_{k,\alpha} - E_{k,\alpha + \epsilon_k}^2} \right] \right\}, \quad (18)$$

is the composite pair susceptibility. There are two important contributions to this integral: a high energy, single-ion part where \( E_{k,\pm} \approx |\epsilon_k| > T_{K1} \) and a low energy “Fermi surface” contribution where the term in square brackets is proportional to \( (\Phi_{1k})^2 \), so that

$$\chi_\Lambda \approx 2N(0) \left\{ \langle \Phi_{2k}^2 \rangle \ln \left( \frac{D}{T_{K1}} \right) + \langle \Phi_{1k}^2 \Phi_{2k}^2 \rangle \ln \left( \frac{T_{K1}}{T} \right) \right\}, \quad (19)$$

where \( \langle \ldots \rangle \) denotes an angular average, \( D \) and \( N(0) \) are the conduction electron band-width and density of states respectively. Notice how the second interference term largely compensates for the single-ion cut-off \( (T_{K1}) \) in the first term. A composite pair instability occurs at

$$T_c \sim D(D/T_{K1})^{-1} \exp \left\{ \frac{1}{2(\Phi_{1k}^2 \Phi_{2k}^2) N(0) J_2} \right\}. \quad (20)$$

where \( \zeta = \langle \Phi_{2k}^2 \rangle / (\langle \Phi_{1k} \Phi_{2k} \rangle^2) \).

To illustrate this conclusion we have used a two-dimensional model where the local moments couple to a tight-binding lattice of conduction electrons via an “s-” and “d-” channel:

![FIG. 3. Phase diagram for a two channel Kondo lattice with “s” and “d-wave” screening channels. Composite pairing develops in shaded region.](image-url)
Fig. 4. Phase diagram for two-channel Kondo insulator. “K.I 1” and “K.I 2” denote Kondo insulating phases in channel one and two respectively. In the intermediate gapless phase both channels participate coherently in the composite pairing process.

\[ \Phi_{1k} = 1, \quad \Phi_{2k} = [\cos(k_x) - \cos(k_y)]. \]

Fig. 3 shows the phase diagram computed using the mean-field equations. When \( J_2 \sim J_1 \) the mean-field transition temperature for composite order is comparable with the single-site Kondo temperature.

An interesting prediction of the theory is the existence of a second-order superconducting-insulating transition. At half-filling the normal state is a Kondo insulating ground-state in channel one or two. Beyond a critical value \( J_2 > J_2^* \), a Kondo insulator in channel 1 becomes unstable with respect to a composite-paired state. Even though this phase forms in the complete absence of a Fermi surface, the superfluid stiffness

\[ \rho_s = \left( \frac{2}{d} \right) \sum_k \left( \frac{V_{\Omega_k}}{V_{k^+}} \right)^2 \frac{\left( \Phi_{1k} \nabla \Phi_{2k} - \Phi_{2k} \nabla \Phi_{1k} \right)^2}{\left( \varepsilon_k / 2 \right)^2 + V_{k^+}^2} \]

is positive (where \( d \) is the dimensionality). At a higher value \( J_2 > J_2^* \), the Kondo effect in channel one is finally suppressed, forming a second Kondo insulating state. Fig. 4 shows how the Kondo-insulating ground-states become unstable to a composite paired state at strong coupling.

In closing, it is perhaps instructive to contrast composite and magnetically mediated pairing. The latter is maximized in the vicinity of an anti-ferromagnetic quantum-critical point. By contrast, the composite pairing described here is driven by a constructive interference between two rival normal phases, and requires no fine tuning. The gap function is determined by an interference product of two Wannier functions, \( \Delta_k \propto \Phi_{1k} \Phi_{2k} \), predicting an intimate relationship between the gap symmetry and local quantum chemistry. When the primary spin exchange occurs in the f-channel, a small exchange coupling to a p-channel will develop a composite paired state with a gap symmetry \( \Phi_1 \times \Phi_p \). For transition metal systems, admixture between a primary d-channel and a secondary s-channel will provide a gap with d-symmetry.

We should like to thank N. d’Abrumenil, R. Ramazashvili and A. Finkelstein for helpful comments relating to this work. Research was supported in part by the National Science Foundation under Grants NSF DMR 96-14999, the EPSRC, UK during a sabbatical stay at Oxford and NATO grant CRG. 940040. HYK is grateful for support from a Korea Research Foundation grant.

* On sabbatical leave from Rutgers University.

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