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Instabilities of the Abrikosov–Suhl resonance[†]

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Abstract

We consider the possibility that instabilities of the Abrikosov–Suhl resonance lead to new fixed-point behavior of the Kondo effect in a lattice environment. In one scenario, a pairing component to the resonant scattering develops in the Kondo lattice, leading to an odd-frequency superconductor. We discuss experiments that can discriminate between this picture and d-wave pairing, and its relationship to the non-Fermi-liquid fixed point of the overscreened Kondo model.

Harry Suhl's birthday provides us with a welcome opportunity to pause and look back at early work on the Kondo effect in which he played a vital role. The Kondo or "s–d" model for magnetic ions in a metallic host dates back to work by Zener [1]. In 1956, Kasuya [2] first cast the model into its modern second quantized form

$$H = H_c + J\sum_j \boldsymbol{\sigma}_j \cdot \boldsymbol{S}_j \quad (\boldsymbol{\sigma}_j \equiv \psi^\dagger_{j\alpha}\, \boldsymbol{\sigma}_{\alpha\beta}\psi_{j\beta}). \tag{1}$$

Here $H_c = \sum \varepsilon_k \psi^\dagger_{k\alpha}\psi_{k\sigma}$ describes the conduction band and the exchange interaction is written in a tight binding form. In the early sixties Kondo [3], building on Anderson's superexchange concept [4], studied the properties of the model with antiferromagnetic rather than the ferromagnetic interactions envisaged by Zener. The famous logarithmic correction to the electron scattering rate that he derived,

$$\frac{1}{\tau} = n_i \pi J^2 \rho \left[1 + 2(J\rho)\ln\left(\frac{D}{2\pi T}\right)\right], \tag{2}$$

where ρ is the conduction electron density of states and n_i the impurity concentration, beautifully explained the resistance minimum of dilute magnetic alloys and definitively confirmed the indirect antiferromagnetic exchange between magnetic ions and conduction electrons.

Suhl was one of the first to appreciate the many body implications of this logarithmic term. In the first of two papers published in 1965 [5] he remarked "a divergence of this sort calls into question the stability of the Fermi surface". Nowadays, we view the Kondo model in the language of scaling theory, and the logarithmic terms that prompted Suhl's remark are taken as an indication that the *original* conduction sea with unquenched local moments is an unstable *fixed* point. Perturbation theory tells us that spin fluctuations are "anti-screening", causing a flow of the superexchange to strong coupling as a function of energy, according to the perturbative

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beta function

$$\frac{\partial J\rho}{\partial \ln \Lambda} = \beta(J\rho),$$

$$\beta(x) = -2x^2 + 2x^3 + \cdots \quad (x \ll 1). \tag{3}$$

Suhl's early work on the impurity model showed that the logarithmic growth of the electron scattering amplitude leads ultimately to the development of an elastic reasonant scattering center at the Fermi energy. The "Abrikosov–Suhl" resonance that he predicted [5–7] is now understood to be a renormalized Friedel–Anderson resonance.

Suhl's remark acquires a renewed significance in the light of the discovery of heavy fermion compounds. A priori, the presence of the Kondo logarithms in weak coupling tells us *nothing* about how more general Kondo models flow to strong coupling: this depends on the topology of the scaling flows. Experimentally, most heavy fermion compounds do indeed show features that demonstrate that, to some degree or another, their behavior is dominated by a flow to a Fermi-liquid fixed point. However, almost all of them show magnetic or superconducting instabilities at temperatures that are substantial fractions of the Kondo temperature: despite the itinerant aspects to these phase transitions, they are in essence *spin ordering processes*, and require descriptions where the correlation of the local moments with the conduction electron, is an integral part of the ordering process.

These considerations motivate us to consider possible instabilities of the Abrikosov–Suhl (AS) resonance in more general Kondo models where the appearance of new relevant variables in the Hamiltonian *diverts* the screening process into *new basins of attraction*. A simple example of this phenomenon is the impurity model with an additional screening channel coupled to the local moment,

$$H = \sum_{\alpha=1,2} H_{\text{band}}(\alpha) + J[\boldsymbol{\sigma}_1 + \lambda\boldsymbol{\sigma}_2]\cdot\boldsymbol{S}_{\text{d}}. \tag{4}$$

Here α labels the screening channel. A separatrix at $\lambda = 1$ divides the Hamiltonian flows into two distinct Fermi-liquid basins of attraction where the AS resonance resides in one channel, but is absent from the other [8, 9]. At $\lambda = 1$, the AS resonance becomes unstable, and the model scales to a non-Fermi-liquid (NFL) quantum critical point, developing a unique localized real fermion mode with a fractional entropy [10] (Fig. 1(a)). There has been much recent interest in this fixed point in connection with the possibility of a quadrupolar Kondo effect in heavy fermion systems [11].

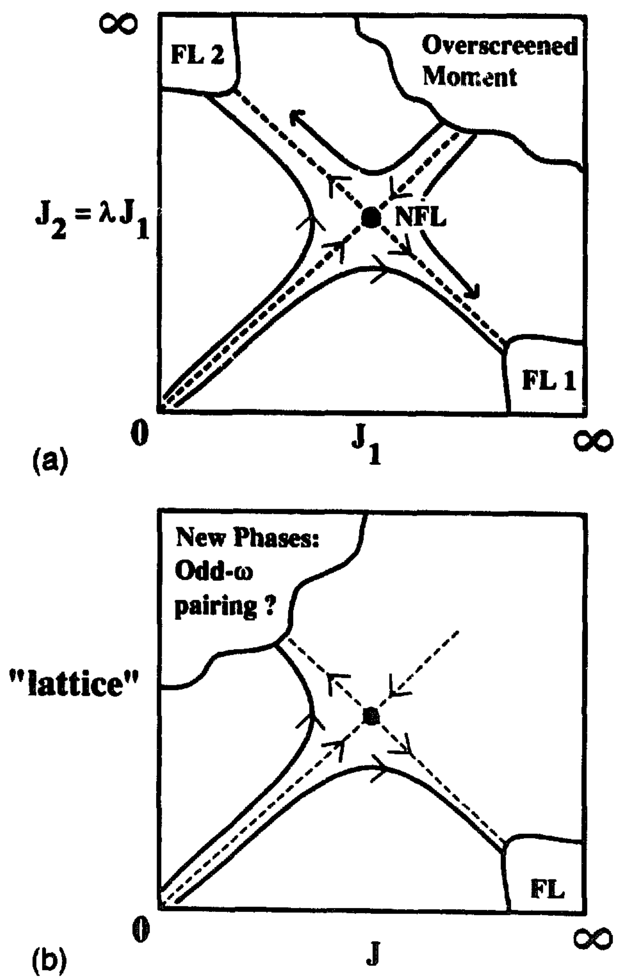


Fig. 1. (a) Scaling behavior of the two-channel Kondo model; (b) illustration of a hypothetical new fixed point in the scaling trajectories of the Kondo lattice model.

Does the lattice play a similarly relevant role in the Kondo scaling process? In the lattice, crossing a separatrix between two basins of attraction would imply a real phase transition (Fig. 1(b)) associated directly with the Kondo effect. One interesting possibility is an instability in the Abrikosov–Suhl resonance that leads it to develop an anomalous scattering component in the triplet channel, producing an odd-frequency pairing component in the electron self-energies:

$$\Delta(\kappa) = \mathrm{i}\sigma_2 d_\kappa\left(\frac{V^2}{2\omega}\right) \quad (d_\kappa = [\hat{d}_1 + \mathrm{i}\hat{d}_2]\cdot\boldsymbol{\sigma}). \tag{5}$$

This type of "odd-frequency" triplet pairing was envisaged by Berezinskii [12, 13]. Calculations that we now outline [14] indicate that such a state is stable, sharing features in common with the fixed point of the overscreened Kondo model, notably the development of neutral fermionic modes at the Fermi energy that decouple from the spin and charge degrees of freedom. The state that is formed retains certain features reminiscent of a superconductor containing a line of gap zeros, making it a conceivable alternative to the d-wave theory of heavy fermion superconductivity.

A key step in our work is to bypass the difficulties of gauge theory approaches to the Kondo lattice model, replacing the commonly used Abrikosov pseudo-fermion representation of spins with a more ancient, Majorana representation that avoids the constraints. This method, in a different guise, was used by Spencer and Doniach [15] in their early work on the Kondo model under the name of "Drone fermions", but has since been neglected. The essence of the method is to generlize the fermionic properties of Pauli matrices to a lattice. Recall that Pauli matrices anticommute $\{\sigma_a, \sigma_b\} = 2\delta_{ab}$ which implies they are real or "Majorana" ($\boldsymbol{\sigma}^\dagger = \boldsymbol{\sigma}$) fermions. Their Fermi statistics guarantee that the "spin" operator $\boldsymbol{S} = -(\mathrm{i}/4)\,\boldsymbol{\sigma}\times\boldsymbol{\sigma}$ is a faithful representation of a spin $-1/2$. We generalize this property to the lattice by introducing a three-component Majorana fermion $\boldsymbol{\eta}_i$ at each site i, which satisfies the algebra $\{\eta_i^a, \eta_j^b\} = \delta_{ij}\delta^{ab}$ $(a, b = 1, 2, 3)$. The corresponding spin operators are then

$$\boldsymbol{S}_j = -\frac{\mathrm{i}}{2}\boldsymbol{\eta}_j \times \boldsymbol{\eta}_j. \tag{6}$$

In terms of Majorana fermions, the Kondo exchange interaction can be written as

$$H_{\mathrm{int}}[j] = -\frac{2}{J}\hat{V}_j^\dagger \hat{V}_j, \tag{7}$$

where

$$\hat{V}_j = \begin{pmatrix} \hat{V}_{j\uparrow} \\ \hat{V}_{j\downarrow} \end{pmatrix} = -\frac{J}{2}[\boldsymbol{\sigma}\cdot\boldsymbol{\eta}_j]\psi_j \tag{8}$$

is a charge e spinor formed between the conduction electron and local moment. This form suggests the possibility that electrons and local moments will condense to develop a vacuum expectation value

$$\begin{pmatrix} V_{j\uparrow} \\ V_{j\downarrow} \end{pmatrix} = \begin{pmatrix} \langle\phi|\hat{V}_{j\uparrow}|\phi\rangle \\ \langle\phi|\hat{V}_{j\downarrow}|\phi\rangle \end{pmatrix}. \tag{9}$$

Defects of a charge e spinor correspond to π changes in the order parameter phase and carry the same flux quantum as a charge $2e$ scalar. Spinor order of this type generates a nontrivial correlation between the spin of the local moments and the conduction electron pair degrees of freedom:

$$\langle \tau_\alpha(x) S^\beta(x)\rangle = g\mathcal{M}_\alpha^\beta(x) \quad (\alpha, \beta = 1, 2, 3). \tag{10}$$

Here $\boldsymbol{\tau}(x)$ is the conduction electron "isospin": z components describe the number density, $\tau_3 = \frac{1}{2}(\rho(x) - 1)$, and transverse components describe the pairing $\tau_+(x) = \psi_\uparrow^\dagger(x)\psi_\downarrow^\dagger(x)$. The quantity $g \sim V_j^2/J^2$ defines the magnitude of the order parameter and $\mathcal{M}$ is an orthogonal matrix whose orientation is set by the components of V.

On a bipartite lattice, the lowest energy stable mean field solution is produced by a staggered pairing field of the form

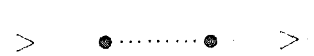
$$V_j = \mathrm{e}^{\mathrm{i}(\boldsymbol{Q}\cdot\boldsymbol{R}_j/2)}\frac{V}{\sqrt{2}}\mathcal{Z}, \tag{11}$$

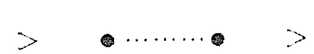
where $\boldsymbol{Q} = (\pi, \pi, \pi)$ and $\mathcal{Z}$ is a unit spinor. The mean field Hamiltonian describes a mixing between local moments and conduction electrons, where the hybridization is a spinor:

$$H_{\mathrm{mft}} = \sum_k \left\{\tilde{\varepsilon}_k \psi_k^\dagger \psi_k + \frac{V}{\sqrt{2}}\left[\psi_k^\dagger(\boldsymbol{\sigma}\cdot\boldsymbol{\eta}_k)\mathcal{Z} + \mathrm{h.c.}\right]\right\} + N|V|^2/J \tag{12}$$

(here the staggered phase has been gauge transformed to the conduction electrons by the replacement $\varepsilon_k \to \tilde{\varepsilon}_k = \varepsilon_{k-Q/2}$). When a conduction electron hybridizes with the zero energy Majorana modes, it develops a self-energy component proportional to $1/\omega$. Since the Majorana fermion is neutral, the scattered fermion can emerge as either electron or hole (see below), thereby developing an odd-frequency pairing term in the conduction electron self-energy.

Diagrammatically, this process is represented as

 $= \frac{V^2}{2\omega}\underline{1}$,

 $= \frac{V^2}{2\omega}\underline{\tau}_1$, (13)

where a dotted line indicates the intermediate resonance and we have used a Nambu notation to denote anomalous pairing components. For example, if $\mathcal{Z} = \binom{0}{1}$ then the down electrons experience this resonant pairing, with self-energy

$$\Sigma_{\downarrow}(\omega) = \frac{V^2}{\omega}\underline{\mathscr{P}}, \tag{14}$$

where $\underline{\mathscr{P}} = \frac{1}{2}[\underline{1} + \tau_1]$ is a projection operator that projects out a Majorana component of the down conduction sea: the remaining half does *not* couple to the odd-frequency triplet pairing field and forms a novel band of decoupled gapless excitations. If we decompose the conduction electron spinor into constituent "Majorana" components,

$$\psi_k = \frac{1}{\sqrt{2}}[\psi_k^0 + \mathrm{i}\boldsymbol{\psi}_k\cdot\boldsymbol{\sigma}]\mathscr{Z}, \tag{15}$$

the zeroth component, $\psi_k^0 = -(\mathrm{i}/\sqrt{2})[\psi_{k\downarrow} - \psi^{\dagger}_{-k\downarrow}]$, is decoupled from the local moments. The other three components of the conduction bands develop a gap $\Delta_g \sim V^2/D$ (where D is the bandwidth) that decouples them from the gapless mode, rendering it both neutral and spinless. The gapless excitations consequently have vanishing spin/charge coherence factors at the Fermi energy which vanish linearly with energy:

$$\langle k|\begin{Bmatrix}\tau^3\\ \sigma^z\end{Bmatrix}|k\rangle = \omega_k\left(\frac{2\mu}{V^2+\mu^2}\right) \quad (\omega_k \ll \Delta_g), \tag{16}$$

where μ is the chemical potential and ω_k the quasiparticle energy. Linear coherence factors lead to power laws in the nuclear magnetic relaxation

$$\frac{1}{T_1} \propto T^3$$

that coexist with a linear specific heat capacity. Unlike a d-wave superconductor with lines of zeroes, this T^3 NMR relaxation rate will persist even when the linear specific heat is large. In a dirty d-wave superconductor, we expect a Korringa relaxation in the superconducting state once it develops a linear specific heat. Figure 2 contrasts the linear specific heat and NMR relaxation rate for the simple mean field theory outlined here, demonstrating these features.

As in all mean field theories, issues of stability and fluctuations are of paramount importance. Uniform odd-frequency states appear in general to be unstable [14]. Here the staggered phase stabilizes the state, producing a finite Meissner stiffness. Since there are no awkward gauge modes, fluctuations about the odd-ω state are similar to zero-point fluctuations in a Heisenberg magnet. The corresponding "Ising limit" where these

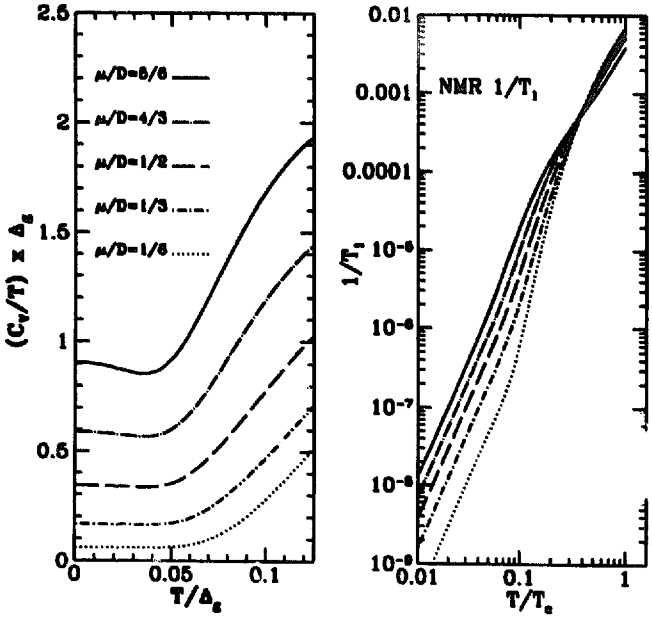


Fig. 2. C_v/T and NMR $1/T_1$ calculated for a variety of chemical potential values illustrating the failure to develop a Korringa relaxation in the presence of severe gaplessness.

fluctuations vanish is produced by adding an additional term to the Kondo interaction that couples the conduction electron *isospin* to the local moment as follows:

$$H = H_c + J\sum_j(\boldsymbol{\sigma}_j + \lambda\boldsymbol{\tau}_j)\cdot\boldsymbol{S}_j. \tag{17}$$

The new term polarizes the composite order parameter, stabilizing a phase with $\mathscr{M} = \underline{1}$. Decomposing the conduction electron into four Majorana components as in Eq. (15), then

$$\boldsymbol{\sigma}_j + \boldsymbol{\tau}_j = -\mathrm{i}\boldsymbol{\psi}_j\times\boldsymbol{\psi}_j, \qquad \boldsymbol{\sigma}_j - \boldsymbol{\tau}_j = 2\mathrm{i}\psi_j^0\boldsymbol{\psi}_j. \tag{18}$$

Thus, in the special case $\lambda = 1$, the zeroth Majorana component *explicitly decouples* from the local moments, as in the mean field theory.

One fascinating feature of the isospin Kondo model, is its precise equivalence to the two-channel Kondo model in the one impurity limit. In the one-impurity version of this model the conduction sea is one-dimensional and near the Fermi surface, spin–charge decoupling means that the isospin and spin of the conduction electron behave as two independent spin degrees of freedom, precisely emulating the two screening channels of the two-channel Kondo model[16]. This isomorphism is lost for multi-site or lattice models. In fact, NFL properties are far more stable in the isospin model, which manifestly preserves the decoupling of the neutral Majorana mode in the lattice at $\lambda = 1$. Furthermore, the gap in the other three Majorana bands will preserve the decoupling of the neutral mode in a finite region about $\lambda = 1$. Careful quantitative calculations of the zero-point fluctuations are required to establish if the domain of attraction of the odd-ω state extends all the way to the $\lambda = 0$ Kondo lattice (dimensionality plays an important role here). Clearly though, these simple considerations establish an important link between the existence of a lattice analog of the two-channel Kondo fixed point and the development of odd-frequency pairing.

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