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Kondo-stabilised spin liquids and heavy fermion superconductivity

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Abstract. We consider an SU(2) path integral formulation of a Kondo lattice model for heavy fermions that treats the RKKY interaction explicitly. At low temperatures we find the heavy Fermi liquid becomes unstable to the formation of a spin liquid amongst the f spins. Kondo coupling to the spin liquid stabilises it against antiferromagnetism, causing the resonating valence bonds of the spin liquid to occasionally escape into the conduction sea. This process induces off-diagonal resonant scattering in the conduction sea, thereby generating anisotropic superconductivity in the heavy fermion system.

1. Introduction

Existing theories of heavy fermion systems surmount the Nozières exhaustion problem [1–3] by generating a quasi-particle f band where the f moments passively compensate one-another via the exclusion principle. Recent two-impurity scaling results of Jones, Varma and Wilkins (JVW) [4] indicate this is an unstable state-of-affairs, showing that in the presence of an RKKY interaction, f spins actively bind into singlets, enhancing the antiferromagnetic correlations beyond that determined by a quasi-particle f band.

The JVW result suggests that an important role of the Kondo effect in heavy fermion systems is to provide a stable environment where the f moments can form short-range singlet bonds with other nearby moments, without developing long-range antiferromagnetic order. The f spin component of this state will be termed a 'spin liquid'. In isolation, such a state is expected to be unstable with respect to antiferromagnetism, acquiring only a modest proportion $\alpha = E_{SL}/E_{AFM}$ of the energy E_{AFM} in an AFM ground state. However, if we suppose that in such a spin liquid there are low-lying spin degrees of freedom on a scale of the Kondo temperature T_K, then singlet bonds will also form between conduction electrons and f spins in the spin liquid. This compensation of the spin liquid will lower its energy by an amount of order T_K per unit cell, stabilising it against magnetism (figure 1). A crude criterion for a non-magnetic ground state is then

$$T_K \gtrsim E_{SL} - E_{AFM} = -(1-\alpha)E_{AFM}. \tag{1}$$

The short-range bonds in a spin liquid help to lower its energy ($\alpha \neq 0$), making this requirement less restrictive than expected on the basis of a direct comparison of the Kondo temperature with the RKKY interaction [5]. Futhermore, in rare-earth systems T_K is enhanced by spin fluctuations into the higher-lying spin–orbit multiplets of the f

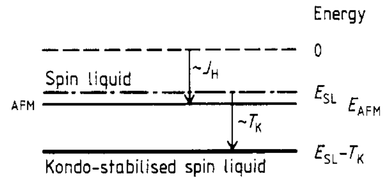

Figure 1. Energy diagram illustrating how the energy of a spin liquid can be lowered below that of an antiferromagnetic state by Kondo compensation.

states [6], and α may be large due to frustration†. A combination of these two factors will then tend to suppress development of conventional local moment magnetism.

A useful way to visualise the formation of a Kondo-stabilised spin liquid is to use Anderson's resonating valence bond picture [7] (figure 2). A pure spin liquid is visualised by linking pairs of f spins together into singlets or valence bonds. Spin exchange between sites causes the ends of the valence bonds to resonate throughout the spin system forming a sort of 'quantum spaghetti'. When we introduce Kondo coupling to the conduction electrons, the ends of the valence bonds occasionally link up with a conduction electron lying within an energy T_K of the Fermi level, resonantly scattering the electrons close to the Fermi energy. Typically, the number of conduction electrons within this energy is far smaller than the number of f spins, and in keeping with the Nozières exhaustion principle, most of the valence bonds must stay within the spin liquid.

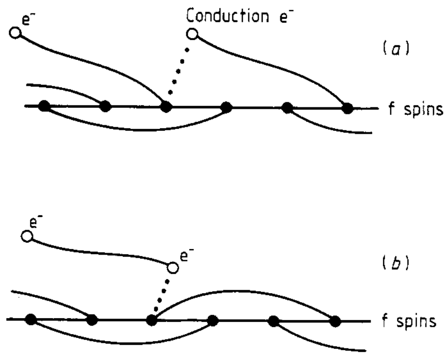

Figure 2. Illustrating how Kondo compensation of a spin liquid results in an escape of the valence bonds into the conduction sea, generating singlet pairs of conduction electrons, thereby inducing a pairing component to the resonant Kondo scattering of conduction electrons.

Occasionally however, spin exchange will occur between two valence bonds that link conduction electrons to f moments, causing the momentary escape of one valence bond entirely into the conduction sea. Such brief excursions of valence bonds into the conduction sea will produce resonant singlet pairing amongst low-energy conduction electrons, and as we shall see, this generates superconductivity in the heavy fermion system.

In this paper we examine this hypothesis within a new path integral formalism, using a lattice model for heavy fermions that contains both RKKY and Kondo interactions.

† In the 2D cuprate superconductors we believe a similar effect may also be taking place, where in this case T_K should be replaced by J_K and α is very close to unity. See [7].

We consider a simplified Kondo lattice model, valid only at temperatures that are low enough for us to integrate out the bulk of the high-lying spin fluctuations and explicitly introduce an RKKY interaction. We further simplify the problem by considering only the lowest-lying Kramers doublet of f states at each site, described by a Heisenberg spin-$\frac{1}{2}$ pseudo-spin operator, interacting with a sea of spin-$\frac{1}{2}$ conduction electrons via a Kondo exchange interaction. Our model is then

$$H = J_{\mathrm{H}} \sum_{(i,j)} \mathbf{S}_i \cdot \mathbf{S}_j + J_{\mathrm{K}} \sum_{j} c^{\dagger}{}_{j\sigma} c_{j\sigma'} (\mathbf{S}_{\sigma\sigma'} \cdot \mathbf{S}_j - \tfrac{1}{4}\delta_{\sigma\sigma'}) + \sum_{k\sigma} \epsilon_k c^{\dagger}{}_{k\sigma} c_{k\sigma}. \tag{2}$$

Here $\mathbf{S}_i = f^{\dagger}{}_{i\alpha} \mathbf{S}_{\alpha\beta} f_{i\beta}$ represents an f spin at site i, and $c^{\dagger}{}_{j\sigma} = \sum \gamma_k c^{\dagger}{}_{k\sigma} \exp(\mathrm{i}\boldsymbol{k} \cdot R_j)$ creates a conduction electron in a Wannier state at site j with the same symmetry as the f state, where γ_k is the form factor of the f state. Conduction electron energies are measured relative to the chemical potential. For simplicity, only nearest-neighbour RKKY interactions are retained. Similar models have been examined by a variety of authors, both in the context of heavy fermion superconductivity [16–18], and more recently in relation to copper oxide superconductivity [7, 8].

2. SU(2) path integral approach

Recently, we considered a two-dimensional variant of the above Kondo lattice model (KLM) in an extreme limit that we called the dual exchange model, where the conduction band width D is small compared with exchange interactions [8]. Here we extend that treatment to the opposite limit where the kinetic energy of the conduction electrons is the largest scale in the problem. The development of a path integral formalism is identical, but for clarity we shall include many more details here.

Since f charge fluctuations have been removed, the KLM is defined within the subspace constrained by the (Gutzwiller) requirement $n_f = 1$ at each site. The absence of f charge fluctuations is manifested as a local SU(2) gauge invarance of the Heisenberg spin operator $\mathbf{S}_j$ [9],

$$f^{\dagger}{}_{\sigma} \rightarrow \cos\theta\, f^{\dagger}{}_{\sigma} + \mathrm{sgn}\sigma\, \sin\theta\, f_{-\sigma}. \tag{3}$$

To illustrate this feature consider the spin raising operation S_+. This process can proceed by first annihilating a down electron, then creating an up electron, written $S_+ = f^{\dagger}{}_{\uparrow} f_{\downarrow}$. Alternatively, it can proceed by first creating an up electron, forming the $n_f = 2$ state, then annihilating a down electron, written $S_+ = -f_{\downarrow} f^{\dagger}{}_{\uparrow}$. In fact, one can accomplish the spin raising operation by an arbitrary linear combination of the above:

$$S_+ = (\cos\theta\, f^{\dagger}{}_{\uparrow} + \sin\theta\, f_{\downarrow})(\cos\theta\, f_{\downarrow} - \sin\theta\, f^{\dagger}{}_{\uparrow}). \tag{4}$$

In other words, there is no distinction between a particle or a hole when all charge fluctuations are removed. The SU(2) symmetry is a mathematical statement of this fact, and the operators $f^{\dagger}{}_{\uparrow}$ and $f_{\downarrow}$ are actually equivalent under the SU(2) group. In situations where the ground state is non-magnetic and the excitations are fermions, the SU(2) symmetry acquires great utility, and may be exploited in a path integral treatment to impose the constraint [9].

The SU(2) symmetry implies that the constraint $n_f = 1$ is actually a component of a triplet of local 'Gutzwiller constraints'

$$f^\dagger{}_{i\uparrow} f_{i\uparrow} - f_{i\downarrow} f^\dagger{}_{i\downarrow} = 0 \qquad f^\dagger{}_{i\uparrow} f^\dagger{}_{i\downarrow} = 0 \qquad f_{i\downarrow} f_{i\uparrow} = 0 \tag{5}$$

which can be written in the compact form

$$f^\dagger{}_i \tau f_i = 0 \tag{6}$$

by introducing the Nambu spinors $f^\dagger{}_i = (f^\dagger{}_{i\uparrow}, f_{i\downarrow})$. In an exact treatment of the problem, satisfaction of any one of these constraints implies satisfaction of the others. However, within a given path integral approximation scheme, all three constraints are required, for satisfaction of the first at a mean field, or Gaussian, level of approximation does *not* generally imply satisfaction of the latter two constraints at the same level of approximation. This is especially true for a superconducting state.

To display the local symmetry explicitly, it is useful to use a generalised Nambu formalism. We begin by introducing Nambu spinors for the conduction electrons and f spins

$$f_j = \begin{pmatrix} f_{j\uparrow} \\ f^\dagger{}_{j\downarrow} \end{pmatrix} \qquad c_k = \begin{pmatrix} c_{k\uparrow} \\ c^\dagger{}_{-k\downarrow} \end{pmatrix} \tag{7}$$

where, as before, we denote the conduction Wannier states by $c_j = \sum_k c_k \exp(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{R}_j)$. It is also convenient to introduce a conjugate spinor basis

$$\tilde{f}_j = \begin{pmatrix} f_{j\downarrow} \\ -f^\dagger{}_{j\uparrow} \end{pmatrix} \qquad \tilde{c}_k = \begin{pmatrix} c_{k\downarrow} \\ -c^\dagger{}_{-k\uparrow} \end{pmatrix}. \tag{8}$$

These two types of spinors form the columns of two matrix operators

$$\begin{aligned} \mathbf{F}_j &= (f_j, \tilde{f}_j) = \begin{bmatrix} f_{j\uparrow} & f_{j\downarrow} \\ f^\dagger{}_{j\downarrow} & -f^\dagger{}_{j\uparrow} \end{bmatrix} \\ \mathbf{C}_k &= (c_k, \tilde{c}_k) = \begin{bmatrix} c_{k\uparrow} & c_{k\downarrow} \\ c^\dagger{}_{-k\downarrow} & -c^\dagger{}_{-k\uparrow} \end{bmatrix} \end{aligned} \tag{9}$$

with

$$\mathbf{C}_j = \sum_k C_k \gamma_k \exp(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{R}_j).$$

In terms of these matrices the Heisenberg spin operators in our original model can be written

$$\begin{aligned} \mathbf{S}_j &= \tfrac{1}{2}\mathrm{Tr}\left[\mathbf{S}^\mathrm{T} \mathbf{F}^\dagger{}_j \mathbf{F}_j\right] \\ \mathbf{S}_c(j) &= \tfrac{1}{2}\mathrm{Tr}\left[\mathbf{S}^\mathrm{T} \mathbf{C}^\dagger{}_j \mathbf{C}_j\right] \end{aligned} \tag{10}$$

where $\mathbf{S}^\mathrm{T}$ denotes the transpose of the spin-$\frac{1}{2}$ Pauli spin matrices. Under the local gauge transformation

$$f_j \rightarrow g_j f_j \tag{11}$$

where $g_j = \exp(\mathrm{i}\boldsymbol{W}_j \cdot \boldsymbol{\tau})$ is a unitary two-dimensional matrix, the $\mathbf{F}_j$ also transform as $\mathbf{F}_j \to g_j\mathbf{F}_j$, $\mathbf{F}^{\dagger}{}_j \to \mathbf{F}_j{}^{\dagger} g_j^{-1}$, so each component of the spin operator is SU(2) invariant.

Next, using the completeness relation

$$4\mathbf{S}^{\mathrm{T}}_{\alpha\beta} \cdot \mathbf{S}^{\mathrm{T}}_{\gamma\eta} + \delta_{\alpha\beta}\delta_{\gamma\eta} = 2\delta_{\alpha\eta}\delta_{\beta\gamma} \tag{12}$$

and the anticommutation algebra of the matrix fermion operators,

$$\{\mathbf{F}(i)_{\alpha\eta}, \mathbf{F}^{\dagger}(j)_{\eta\beta}\} = \delta_{\alpha\beta} \tag{13}$$

we rewrite the interactions as

$$\begin{aligned} J_{\mathrm{H}}(\mathbf{S}_i \cdot \mathbf{S}_j - \tfrac{1}{4}) &= -\tfrac{1}{8} J_{\mathrm{H}} \operatorname{Tr}[\mathbf{F}_i\mathbf{F}^{\dagger}{}_j\mathbf{F}_j\mathbf{F}^{\dagger}{}_i] = -\tfrac{1}{8} J_{\mathrm{H}} \operatorname{Tr}[\hat{u}_{ij}\hat{u}_{ji}] \\ J_{\mathrm{K}} c^{\dagger}{}_{i\sigma} c_{i\sigma'}(S_{\sigma\sigma'} \cdot \mathbf{S}_i - \tfrac{1}{4}\delta_{\sigma\sigma'}) &= -\tfrac{1}{8} J_{\mathrm{K}} \operatorname{Tr}[\mathbf{C}_i\mathbf{F}^{\dagger}{}_i\mathbf{F}_i\mathbf{C}^{\dagger}{}_i] = -\tfrac{1}{8} J_{\mathrm{K}} \operatorname{Tr}[\hat{v}^{\dagger}{}_i\hat{v}_i] \end{aligned} \tag{14}$$

where, following Affleck and co-workers we have introduced two pairing matrix operators [9]

$$\hat{u}_{ij} = \mathbf{F}_i\mathbf{F}^{\dagger}{}_j = \begin{bmatrix} -a^{\dagger}{}_{ij} & b_{ij} \\ b^{\dagger}{}_{ij} & a_{ij} \end{bmatrix} \tag{15}$$

$$a_{ij} = f^{\dagger}{}_{i\sigma} f_{j\sigma} \qquad b_{ij} = f_{i\uparrow} f_{j\downarrow} - f_{i\downarrow} f_{j\uparrow}$$

$$\hat{v}_i = \mathbf{F}_i\mathbf{C}^{\dagger}{}_i = \begin{bmatrix} -\alpha^{\dagger}{}_i & \beta_i \\ \beta^{\dagger}{}_i & \alpha_i \end{bmatrix} \tag{16}$$

$$\alpha_i = f^{\dagger}{}_{i\sigma} c_{i\sigma} \qquad \beta_i = f_{i\uparrow} c_{j\downarrow} - f_{i\downarrow} c_{j\uparrow}.$$

Under the local gauge transformation $f_j \to g_j f_j$, the $\hat{u}_{ij}$ and $\hat{v}_j$ matrices transform as

$$\hat{v}_j \to g_j \hat{v}_j \qquad \hat{u}_{ij} \to g_i \hat{u}_{ij} g_j^{-1} \tag{17}$$

so that the interactions are invariant under the SU(2) transformation.

The partition function for our model is given by $Z = \operatorname{Tr}[P_G \mathrm{e}^{-\beta H}]$ where $P_G = \Pi_j\, (n^f_{j\uparrow} - n^f_{j\downarrow})^2$ is the Gutzwiller projection for one f spin per site. Previous work has imposed this constraint as an integral over a U(1) group

$$(n^f_{j\uparrow} - n^f_{j\downarrow})^2 = \int \frac{\mathrm{d}\theta}{2\pi} \exp(\mathrm{i}\theta f^{\dagger}{}_j \tau_3 f_j) \tag{18}$$

where we have rewritten $n^f(\boldsymbol{R}_j) - 1 = f^{\dagger}{}_j \tau_3 f_j$ in Nambu notation. In actual fact, the SU(2) symmetry tells us that we can replace τ_3 by $\boldsymbol{n} \cdot \boldsymbol{\tau}$ where $\hat{n}$ is an arbitrary unit vector. Integrating over all possible choices $\boldsymbol{n}$ and θ enables us to rewrite the Gutzwiller projection as an integral over the SU(2) group

$$(n^f_{j\uparrow} - n^f_{j\downarrow})^2 = \int \mathrm{d}[g_j]\hat{g}_j \tag{19}$$

where $\hat{g}_j = \exp[\mathrm{i} f^{\dagger}{}_j(\boldsymbol{W}_j \cdot \boldsymbol{\tau}) f_j]$ and $\boldsymbol{W}_j = \theta\hat{n}$. The measure

$$\mathrm{d}[g] = \frac{\sin^2\theta \,\mathrm{d}\theta\, \mathrm{d}\hat{n}}{4\pi^2} \tag{20}$$

is the Haar SU(2) measure [10] (for mean-field technique see p 74 in this review) and $\theta \in [0, 2\pi]$. Rewriting $g = \mathrm{i}g^\mu\tau_\mu$ ($\mu = 0,1,2,3$, $\tau_0 = \mathrm{i}\mathbf{1}$), permits us to rewrite this measure in the alternate form

$$\mathrm{d}[g] = \pi^{-2}\prod_\mu \mathrm{d}g^\mu\delta(g^2-1) \qquad g^2 = \textstyle\sum_\mu (g^\mu)^2. \tag{21}$$

Introducing this into the partition function permits us to write it as a path integral

$$\begin{aligned} Z &= \int \mathscr{D}[f,c,W]\exp\left(-\int_0^\beta (\mathscr{L}_1 + H)\mathrm{d}\tau\right) \\ \mathscr{L}_1 &= \sum_k c^\dagger{}_k\partial_\tau c_k + \sum_j f^\dagger{}_j(\partial_\tau - \mathrm{i}W_j)f_j \end{aligned} \tag{22}$$

where $W_j = \boldsymbol{W}_j\cdot\boldsymbol{\tau}$. In the continuum time limit, the Haar measure can be replaced by the flat measure $\mathrm{d}^3W_j/4\pi^2$.

To factorise the interactions we first recognise that the pairs (a_{ij}, b_{ij}) and (α_i, β_i) are pairs of dependent operators related by an SU(2) rotation. Let us choose $D^\dagger{}_{ij} = \mathrm{Tr}[\frac{1}{2}(1-\hat{n}\cdot\boldsymbol{\tau})\hat{u}_{ij}]$ and D_{ij} as the independent operators, where $\hat{n}$ is a unit vector, then

$$J_\mathrm{H}(\mathbf{S}_i\cdot\mathbf{S}_j - \tfrac{1}{4}) = -\tfrac{1}{2}J_\mathrm{H}D^\dagger{}_{ij}D_{ij}. \tag{23}$$

We perform the Hubbard Stratonovich as follows

$$\begin{aligned} -(\tfrac{1}{2}J_\mathrm{H})D^\dagger{}_{ij}D_{ij} &\to D^\dagger{}_{ij}\phi + \bar{\phi}D_{ij} + (2/J_\mathrm{H})\bar{\phi}\phi \\ &= -\tfrac{1}{2}\mathrm{Tr}[\tilde{U}_{ij}\hat{u}_{ji} + \hat{u}_{ij}\tilde{U}_{ji}] + (1/J_\mathrm{H})\mathrm{Tr}[\tilde{U}_{ij}\tilde{U}_{ji}] \\ &= [f^\dagger{}_i\tilde{U}_{ij}f_j + \mathrm{HC}] + (1/J_\mathrm{H})\mathrm{Tr}[\tilde{U}_{ij}\tilde{U}^\dagger{}_{ij}] \end{aligned} \tag{24}$$

where $\phi = \phi_x + \mathrm{i}\phi_y$ and

$$\tilde{U}_{ij} = \phi_x(\hat{n}\cdot\boldsymbol{\tau}) + \mathrm{i}\phi_y \tag{25}$$

is a unitary matrix with $\tilde{U}_{ji} = \tilde{U}^\dagger{}_{ij}$. In the path integral we now integrate over the SU(2) group at sites i and j at each point in time. Under the SU(2) rotation, $f_j \to g_jf_j$, so that we must make the replacement $\tilde{U}_{ij} \to g_i\tilde{U}_{ij}g_j^{-1}$ inside the Lagrangian. Inserting

$$1 = \int \mathrm{d}^4U_{ij}\delta(g_i\tilde{U}_{ij}g_j^{-1} - U_{ij})$$

into the integral, where $\mathrm{d}^4U_{ij} = \Pi_\mu \mathrm{d}U^\mu_{ij}$ is a flat measure over each of the components of $U_{ij} = \mathrm{i}U^\mu_{ij}\tau_\mu$, ($\tau_0 = \mathrm{i}\mathbf{1}\boldsymbol{n}$), enables us to replace $g_i\tilde{U}_{ij}g_j^{-1}$ by U_{ij} in the Lagrangian. Next we invert the order of integration, and use the result (see Appendix)

$$\frac{1}{\pi}\int \mathrm{d}[g_i]\,\mathrm{d}[g_j]\,\mathrm{d}\phi_x\,\mathrm{d}\phi_y\,\delta(g_i\tilde{U}_{ij}g_j^{-1} - U_{ij}) = \frac{2}{\pi^2}\mathrm{Tr}[U^\dagger{}_{ij}U_{ij}]^{-1} \tag{26}$$

to determine the measure of the new variable U_{ij}

$$\mathrm{d}[U_{ij}] = \frac{2\,\mathrm{d}^4U_{ij}}{\pi^2\mathrm{Tr}[U^\dagger{}_{ij}U_{ij}]} = 2\Delta_{ij}\,\mathrm{d}\Delta_{ij}\,\mathrm{d}g_{ij} \tag{27}$$

where we put $U_{ij} = -\mathrm{i}\Delta g_{ij}$, where g_{ij} is an SU(2) matrix. As before, $\mathrm{d}g_{ij}$ is the Haar measure, which becomes flat in the time continuum limit. This is a Nambu reformulation of the matrix fermion formalism of Affleck and co-workers [9].

A similar decomposition is made for the Kondo term, introducing the unitary pairing matrix V_j conjugate to $\frac{1}{2}J_{\mathrm{K}}\hat{v}_j$, and writing

$$J_{\mathrm{K}}(\mathbf{S}_i \cdot \mathbf{S}_c(i) - \tfrac{1}{4}c^{\dagger}{}_{i\sigma}c_{i\sigma}) \rightarrow -\tfrac{1}{2}\mathrm{Tr}[V^{\dagger}{}_i\hat{v}_i + \hat{v}^{\dagger}{}_iV_i] + (1/J_{\mathrm{K}})\mathrm{Tr}[V^{\dagger}{}_iV_i]$$
$$= [d^{\dagger}{}_iV_ic_i + \mathrm{HC}] + (1/J_{\mathrm{K}})\mathrm{Tr}[V^{\dagger}{}_iV_i] \tag{28}$$

where integration over g_i elevates V_j to an SU(2) integration variable, with measure

$$\mathrm{d}V = V_0\,\mathrm{d}V_0 \sin^2\lambda\,\mathrm{d}\lambda\,\mathrm{d}\hat{n}/2\pi^2 \tag{29}$$

where $V = V_0 \exp(\mathrm{i}\lambda\hat{n}\cdot\boldsymbol{\tau})$.

Incorporating these expressions into the path integral permits us to write

$$Z = \int \mathscr{D}[f, c; W, V, U] \exp\left(-\int_0^{\beta} (\mathscr{L}_1 + H)\mathrm{d}\tau\right)$$
$$H = \sum_k \epsilon_k c^{\dagger}{}_k\tau_3 c_k + \sum_{(i,j)} [f^{\dagger}{}_iU_{ij}f_j + \mathrm{HC}] + \frac{1}{J_{\mathrm{H}}}\mathrm{Tr}[U^{\dagger}{}_{ij}U_{ij}]$$
$$+ \sum_i [f^{\dagger}{}_iV_ic_i + \mathrm{HC}] + \frac{1}{J_{\mathrm{K}}}\mathrm{Tr}[V^{\dagger}{}_iV_i]. \tag{30}$$

Our model now has the following time dependent SU(2) gauge invariance

$$\begin{array}{ll} f_j \rightarrow g_j f_j & V_j \rightarrow g_j V_j \\ U_{ij} \rightarrow g_i U_{ij} g_j^{-1} & W_j \rightarrow g_j \left(W_j + \mathrm{i}\partial_{\tau}\right) g_j^{-1} \end{array} \tag{31}$$

associated with the absence of f charge fluctuations. There is also the usual electromagnetic U(1) gauge symmetry associated with the charged conduction electrons, introduced via $\gamma_k \rightarrow \gamma_{k-eA}$ and $\epsilon_k \rightarrow \epsilon_{k-eA}$, where A is the electromagnetic field.

We interprete our Lagrangian as describing the motion of electrons through a pairing field generated by antiferromagnetic fluctuations. The V field describes the compensation of f spins by the conduction electrons, whilst the U field describes the mutual compensation of f spins $(J_{\mathrm{H}}(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4}) = -\mathrm{Tr}[U^{\dagger}U]/J_{\mathrm{H}})$. The SU(2) symmetry incorporates the incompressibility of the f electrons into the theory, playing the role of large on-site f interations.

3. Mean-field approach

We employ mean-field techniques similar to those developed for lattice gauge theories with continuous local symmetries [10].

Physical quantities are SU(2) gauge invariant. The most general gauge-invariant operators that are local in time are the operators

$$P_{ij\ldots l} = 2^{-L}\mathrm{Tr}[\hat{u}_{ij}\hat{u}_{jk}\ldots\hat{u}_{li}] \tag{32}$$

and

$$\underline{R}_{ij\ldots l} = \hat{v}^{\dagger}{}_i \hat{u}_{ij} \ldots \hat{u}_{kl} \hat{v}_l. \tag{33}$$

The first describes the amplitude for exchange of f spins around a loop of length L. The second is a matrix describing the interaction amongst conduction electrons via the exchange of intermediate f spins. Because of our Nambu notation this term contains off-diagonal pairing components, which are nevertherless SU(2) invariant. Translational invariance implies that the expectation values of these operators are independent of location and dependent only on the shape and size of the the loop or path.

In the mean-field approximation we replace $\hat{u}_{ij}$ and $\hat{v}_j$ by their expectation values $\langle \hat{u}_{ij} \rangle = (2/J_{\rm H}) U^{\rm o}_{ij}$, $\langle \hat{v}_j \rangle = (2/J_{\rm K}) V^{\rm o}_j$. which need only be translationally invariant up to a gauge transformation [10]. Each choice of saddle point solution for $U^{(\rm o)}_{ij}$ and $V^{(\rm o)}_j$ is a representative point on the orbit of all gauge equivalent solutions formed by the action of $g_j(\tau)$ on the U_{ij}, V_j and W_j, according to equation (31):

$$\begin{aligned} U^{\rm g}_{ij} &= g_i U^{(\rm o)}_{ij} g_j^{-1} \\ V^{\rm g}_j &= g_j V^{(\rm o)}_j \\ W^{\rm g}_j &= g_j W^{(\rm o)}_j g_j^{-1} + {\rm i} g_j \partial_\tau g_j^{-1}. \end{aligned} \tag{34}$$

Gauge invariance guarantees that all physical quantities

$$P[U^{(\rm o)}, V^{(\rm o)}, W^{(\rm o)}] \tag{35}$$

calculated in the mean-field theory, in particular the mean-field free energy $F[U, V, W]$, (but also the conduction electron propagator, the conduction electron pairing amplitude, the ring exchange operators) are invariant under this transformation,

$$P(U^{\rm g}, V^{\rm g}, W^{\rm g}) = P[U^{(\rm o)}, V^{(\rm o)}, W^{(\rm o)}]. \tag{36}$$

When we average over the the gauge orbit in the path integral, all physical quantities remain unchanged, but all gauge-dependent quantities average to zero, thus

$$\begin{aligned} \langle U_{ij} \rangle &= \int {\rm d}g\, U^{\rm g}_{ij} = 0 \\ \langle V_j \rangle &= \int {\rm d}g\, V^{\rm g}_j = 0. \end{aligned} \tag{37}$$

For this reason, although we unfold the interaction in terms of gauge-dependent fields which average to zero, the mean-field theory we use describes the physics of an entire *orbit of saddle points*. The only fluctuations that modify the physics are those perpendicular to the gauge orbit. These fluctuations cost energy, and have *finite* zero-point oscillation frequencies that we may extract, using methods well known in gauge theory.

In the calculations presented here we assume a three-dimensional simple cubic crystal structure, with a tight-binding conduction band of half width $6t$:

$$\epsilon_k = -2t(\cos k_x + \cos k_y + \cos k_z) - \mu. \tag{38}$$

Furthermore, though not essential, we take the simple case of 'point-like' f states, where $\gamma_{\boldsymbol{k}} = 1$. Finally, we restrict our attention to mean-field solutions that have the *full crystal symmetry*, choosing a gauge that is manifestly translationally invariant.

The most general translationally invariant gauge has the form

$$\begin{aligned} U(\boldsymbol{R}_i + \boldsymbol{l}, \boldsymbol{R}_i) &= U_l = -\mathrm{i}\Delta \exp(\mathrm{i}\theta_l \hat{n}_l \cdot \boldsymbol{\tau}) \qquad (l = x, y, z) \\ V_j &= -\mathrm{i} V_0 \exp(\mathrm{i}\boldsymbol{\lambda} \cdot \boldsymbol{\tau}) = V \\ W_j &= \boldsymbol{W} \cdot \boldsymbol{\tau} = W \end{aligned} \tag{39}$$

where the $\hat{n}_l$ $(l = x, y, z)$ are unit vectors. We apply a global SU(2) transformation $(g = \mathrm{i}\tau_3 \exp(-\mathrm{i}\boldsymbol{\lambda} \cdot \boldsymbol{\tau}))$ to bring V into the form $V = V_0 \tau_3$. The mean-field Hamiltonian for our ansatz is $H_{\mathrm{MF}} = \sum_{\boldsymbol{k}} \psi^{\dagger}{}_{\boldsymbol{k}} h_{\boldsymbol{k}} \psi_{\boldsymbol{k}}$, where

$$h_{\boldsymbol{k}} = \begin{bmatrix} \epsilon_{\boldsymbol{k}} \tau_3 & V^{\dagger} \\ V & W + U(\boldsymbol{k}) \end{bmatrix} \tag{40}$$

with $U(\boldsymbol{k}) = \sum_l U_l \exp(\mathrm{i}k_l) + \mathrm{HC}$, $(l = x, y, z)$ and we have defined $\psi^{\dagger}{}_{\boldsymbol{k}} = (p^{\dagger}{}_{\boldsymbol{k}}, d^{\dagger}{}_{\boldsymbol{k}})$.

The Green function corresponding to H_{MF} is $\mathcal{G}_{\boldsymbol{k}}(\mathrm{i}\omega_n) = (\mathrm{i}\omega_n - h_{\boldsymbol{k}})^{-1}$. The mean-field free energy per unit cell is

$$F[U, V, W] = T \sum_{\boldsymbol{k}, \mathrm{i}\omega_n} \mathrm{Tr}\, \ln[\mathcal{G}_{\boldsymbol{k}}(\mathrm{i}\omega_n)] + 2V_0^2/J_{\mathrm{K}} + 6\Delta^2/J_{\mathrm{H}} \tag{41}$$

where T is the temperature. This must be stationary with respect to variations in U, V and W, which generates three mean-field equations.

$$\begin{aligned} 0 &= \langle f^{\dagger}{}_i \boldsymbol{\tau} f_i \rangle = T \sum_{\boldsymbol{k}, \mathrm{i}\omega_n} \mathrm{Tr}[\boldsymbol{\tau} \mathcal{G}^{ff}_{\boldsymbol{k}}(\mathrm{i}\omega_n)] \\ U_l &= J_{\mathrm{H}} \langle f_{i+l} f^{\dagger}{}_i \rangle = -T\, J_{\mathrm{H}} \sum_{\boldsymbol{k}, \mathrm{i}\omega_n} \mathcal{G}^{ff}_{\boldsymbol{k}}(\mathrm{i}\omega_n) \exp(\mathrm{i}\boldsymbol{k}_l) \\ V &= J_{\mathrm{K}} \langle f_i c^{\dagger}{}_i \rangle = -T\, J_{\mathrm{K}} \sum_{\boldsymbol{k}, \mathrm{i}\omega_n} \gamma_{\boldsymbol{k}} \mathcal{G}^{fc}_{\boldsymbol{k}}(\mathrm{i}\omega_n) \end{aligned} \tag{42}$$

where the superscripts on $\mathcal{G}$ label the block-diagonal components. The first imposes the three Gutzwiller constraints, on the average, and the other two self-consistently determine U and V.

By solving these mean-field equations we are carrying out a path integral version of the Gutzwiller approximation

$$H P_G = P_G H_{\mathrm{MF}}. \tag{43}$$

If $|\tilde{\psi}\rangle$ is a ground-state wavefunction for H_{MF}, then the corresponding approximation to the ground-state wavefunction of H is $|\psi\rangle = P_G |\tilde{\psi}\rangle$. If g is an arbitrary SU(2) transformation, then all unprojected states $|\psi(g)\rangle = g|\psi\rangle$ are equivalent under the Gutzwiller projection $|\psi\rangle = P_G |\tilde{\psi}(g)\rangle$.

We now demand that the eigenvectors of $h_{\boldsymbol{k}}$ are invariant under 90° rotations $\boldsymbol{k} \to R\boldsymbol{k}$, from which it follows that $h_{R\boldsymbol{k}} = \pm D_R h_{\boldsymbol{k}} D^{\dagger}{}_R$, where D_R is a unitary matrix. (The $\pm$ in this equation occurs because the eigenvalues of $h_{\boldsymbol{k}}$ come in pairs $(E_\alpha, -E_\alpha)$

due to the spin rotational invariance of the problem.) Since D_R must be $\boldsymbol{k}$ independent, it can be divided into four identical 2×2 block elements d_R. This implies that

$$\tau_3 = \pm d_R \tau_3 d^{\dagger}{}_R \qquad U(R\boldsymbol{k}) = \pm d_R U(\boldsymbol{k}) d^{\dagger}{}_R \tag{44}$$

so rotations in real space correspond to orthogonal transformations in particle–hole space that interchange (up to an inversion) the axes $\hat{n}_l$ whilst leaving the z axis unchanged, up to an inversion. The explicit form of $U(\boldsymbol{k})$ is

$$U(\boldsymbol{k}) = 2\Delta \sum_l (\cos\theta\, \sin k_l + \sin\theta\, \cos k_l \hat{n}_l \cdot \boldsymbol{\tau}). \tag{45}$$

Since a unit matrix is unchanged by a unitary transformation, the term proportional to a unit matrix cannot give rotationally invariant physics, so $\theta = \pi/2$. For the trivial case $d_R = 1$, $U(\boldsymbol{k})$ is explicitly rotationally invariant and the vectors $\hat{n}_l$ must be parallel: $U(\boldsymbol{k}) = 2\Delta \sum_l \cos k_l \hat{n}\cdot\boldsymbol{\tau}$. In the non-trivial representation $d_R \neq 1$, d_R will only leave the z axis unchanged (up to an inversion) for all rotations of the point group, if the vectors $\hat{n}_l$ form the prongs of a 'tripod' whose axis lies in the $\hat{z}$ direction, also parallel to $\boldsymbol{W}$ (figure 3):

$$\hat{n}_i \cdot \hat{n}_j = \cos n \qquad (i \neq j) \qquad \boldsymbol{W}_0 = W\hat{z} \qquad \sum_l \hat{n}_l \propto \hat{z}. \tag{46}$$

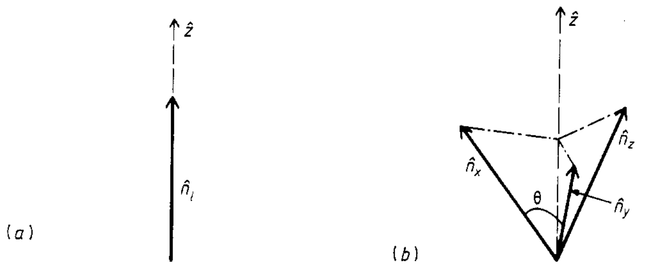

Figure 3. Showing the configuration of the SU(2) vectors $\hat{n}_l$ in (a) the Fermi liquid and (b) the superconducting phase.

In both cases, the mean-field Hamiltonian can be written in a more conventional form:

$$H_{\mathrm{MF}} = \sum_{svk\sigma} \left[\epsilon_k c^{\dagger}{}_{k\sigma} c_{k\sigma} + V_0 (c^{\dagger}{}_{k\sigma} f_k + \mathrm{HC}) + u_k f^{\dagger}{}_{k\sigma} f_{k\sigma}\right] + \sum_k (\Delta_k f^{\dagger}{}_{k\uparrow} f^{\dagger}{}_{-k\downarrow} + \mathrm{HC}). \tag{47}$$

Here

$$\begin{aligned} u_k &= W_z + 2\Delta_z \sum_l \cos k_l \\ \Delta_k &= W_x + \mathrm{i} W_y + \sqrt{6}\Delta_\perp \phi_k \end{aligned} \tag{48}$$

where $\Delta\hat{n}_l = \Delta_z \hat{z} + \Delta_\perp \hat{n}_{l\perp}$ and the $\hat{n}_{l\perp}$ lie in the x–y plane.

In the trivial case $d_R = 1$, ϕ_k has s symmetry under 90° rotations:

$$\phi_k = \sqrt{\tfrac{2}{3}} \sum_l \cos k_l \qquad \text{extended s wave.} \tag{49}$$

In the non-trivial case $d_R \neq 1$, $W_\perp = 0$, $W_z = W$ and ϕ_k has d symmetry

$$\begin{aligned} \phi_k &= e^{i\alpha}(\zeta_k \pm i\eta_k) \\ \eta_k &= (c_x - c_y)/\sqrt{2} \\ \zeta_k &= (c_x + c_y - 2c_z)/\sqrt{6} \qquad \text{d wave} \end{aligned} \tag{50}$$

and the $\hat{n}_{l\perp}$ lie at 120° to each other. We have taken the convention $\hat{n}_{z\perp} = \cos\alpha\hat{y} + \sin\alpha\hat{x}$ and the sign in ϕ_k is the sign of $(\hat{n}_x \times n_y)\cdot\hat{z}$.

We shall shortly show that exchange energy is gained when the directions of the $\hat{n}_l$ are well separated, energetically favouring the higher symmetry state with d symmetry. This state will be the main focus of our attention.

Now we diagonalise H_{MF} in terms of two quasi-particle bands $(n = +, -)$,

$$H_{\mathrm{MF}} = \sum_{kn} E_{kn}(a^\dagger{}_{kn\uparrow} a_{kn\uparrow} - a_{kn\downarrow} a^\dagger{}_{kn\downarrow}) \tag{51}$$

where $(n = \pm)$ and

$$\begin{aligned} E_{k\pm} &= \left\{ \left[(\boldsymbol{u}_k^2 + \boldsymbol{e}_k^2)/2 + V_0^2 \right] \pm \left[(\boldsymbol{u}_k^2 - \boldsymbol{e}_k^2)^2/4 + V_0^2(\boldsymbol{u}_k + \boldsymbol{e}_k)^2 \right]^{1/2} \right\}^{1/2} \\ \boldsymbol{e}_k &= \epsilon_k \hat{z} \\ \boldsymbol{u}_k &= 2\Delta \sum_l \cos k_l \hat{n}_l. \end{aligned} \tag{52}$$

The free energy may be expressed in terms of these eigenvalues as

$$F[U, V, W] = -T \sum_{k, n=\pm 1} 2\ln[\cosh(\beta E_{kn}/2)] + 2V_0^2/J_{\mathrm{K}} + 6\Delta^2/J_{\mathrm{H}} \tag{53}$$

The requirement that F is stationary with respect to Δ_z, $\Delta_\perp$, V and W generates four scalar mean-field equations for case (ii)

$$\sum_{kn} \tanh\left(\frac{\beta E_{kn}}{2}\right) \nabla_U E_{kn} \cdot \begin{bmatrix} \hat{z} \\ \Sigma_l \hat{z}\cos k_l \\ \Sigma_l \hat{n}_{l\perp} \cos k_l \end{bmatrix} = \begin{bmatrix} 0 \\ 6/J_{\mathrm{H}} \\ 6/J_{\mathrm{H}} \end{bmatrix} \tag{54}$$

$$\sum_{kn} \tanh\left(\frac{\beta E_{kn}}{2}\right) \frac{\partial E_{kn}}{\partial V} = 4V/J_{\mathrm{K}} \tag{55}$$

where

$$\nabla_{\boldsymbol{u}} E_{kn} = \frac{1}{2E_{kn}} \left(\boldsymbol{u} + n \frac{\frac{1}{2}(\boldsymbol{u}^2 - \boldsymbol{e}^2)\boldsymbol{u} + V_0^2(\boldsymbol{u} + \boldsymbol{e})}{[\frac{1}{2}(\boldsymbol{u}^2 - \boldsymbol{e}^2)^2 + V_0^2(\boldsymbol{u} + \boldsymbol{e})^2]^{1/2}} \right). \tag{56}$$

We shall not list the mean-field equations for the unstable s-wave state.

There are two phases that arise in solution of the mean-field equations: (i) a Fermi liquid phase and (ii) an anisotropic superconducting phase. We now discuss these phases in turn.

3.1. Fermi liquid ($\Delta_\perp = 0$)

At finite temperatures, entropy effects favour the formation of a Fermi liquid state in which the vectors $\hat{n}_l$ lie along the $\hat{z}$ axis. This state is formed by the action of the Kondo effect which binds the low-lying conduction electrons to the f spins in singlet states. This process removes a spin from the f fluid, and adds a charge, thereby forming a charged mobile 'f hole'. Before discussing this process in detail let us first summarise the mean-field equations.

The eigenenergies E_{kn} revert to the simpler form

$$E_{kp} = (\epsilon_k + u_k)/2 + p[(\epsilon_k - u_k)^2/4 + V_0^2]^{1/2} \qquad (p = n\,\mathrm{sgn}(\epsilon_k + u_k) = \pm)$$
$$u_k = W + 2\Delta \sum_l \cos k_l. \tag{57}$$

The corresponding quasi-particle operators are

$$a^\dagger{}_{kp\sigma} = \cos\delta_{kp} c^\dagger{}_{k\sigma} + \sin\delta_{kp} f^\dagger{}_{k\sigma} \qquad \tan\delta_{kp} = V_0/(E_{kp} - u_k) \tag{58}$$

and the corresponding normal ground state would then be

$$|\Psi_{\mathrm{FL}}\rangle = P_G|\tilde{\Psi}_{\mathrm{FL}}\rangle \qquad |\tilde{\Psi}_{FL}\rangle = \prod_{E_{k_p}<0} a^\dagger{}_{kp\sigma}|0\rangle. \tag{59}$$

The mean-field equations assume the following form

$$\sum_{kp} p \tanh\left(\frac{\beta E_{kp}}{2}\right) \frac{1}{[(\epsilon_k - u_k)^2 + 4V_0^2]^{1/2}} = 2/J_{\mathrm{K}}$$
$$\sum_{kp} \tanh\left(\frac{\beta E_{kp}}{2}\right) \frac{V_0^2}{V_0^2 + (E_{kp} - u_k)^2} \begin{bmatrix} 1 \\ \Sigma_l \cos k_l \end{bmatrix} = \begin{bmatrix} 0 \\ 6\Delta_z/J_{\mathrm{H}} \end{bmatrix}. \tag{60}$$

Setting $V_0 = 0$ determines the temperature scale of the crossover into this Fermi liquid phase, which is given by $T_{\mathrm{FL}} = \lambda T_{\mathrm{K}}$, where

$$T_{\mathrm{K}} = 6t \exp(-1/J_{\mathrm{K}}\rho_0) \tag{61}$$

defines the Kondo temperature and

$$\ln\lambda = \psi(\tfrac{1}{2}) + \lim_{D\to 0} \frac{1}{2\rho_0} \int \mathrm{d}\epsilon\, \rho(\epsilon) \left|\frac{\epsilon}{\epsilon^2 + D^2}\right| + \ln\frac{D}{6t}. \tag{62}$$

Note how the exponent is correctly given for our original definition of the coupling constant, although the prefactor will depend on the treatment of fluctuations. As in earlier treatments, the mean-field theory does not contain the critical fluctuations required to reduce this false phase transition to a crossover.

To elucidate the effect of Kondo binding of conduction electrons to f spins, it is helpful to 'integrate out' the conduction electron degrees of freedom, defining an effective Hamiltonian for the f electrons. The conduction electrons introduce a self-energy into the f electron propagator given by

$$\Sigma_f(\boldsymbol{k},\omega) = V_0^2/(\omega - \epsilon_{\boldsymbol{k}}\tau_3) \simeq t_{\boldsymbol{k}}\tau_3 \qquad (\omega \ll V_0 \sim (T_{\rm K}/\rho_0)^{1/2})$$
$$t_{\boldsymbol{k}} = -V_0^2/\epsilon_{\boldsymbol{k}} \sim T_{\rm K} \tag{63}$$

leading to an f propagator of the form

$$\mathscr{G}_f(\boldsymbol{k},\omega) = [\omega - (u(\boldsymbol{k}) + W + t_{\boldsymbol{k}})\tau_3]^{-1}. \tag{64}$$

The effective Hamiltonian describing these 'f electrons' takes the form

$$H = \sum_{i,j} \tfrac{1}{2}\tilde{t}_{ij}[f^{\dagger}{}_{i\sigma}f_{j\sigma} + \mathrm{HC}]$$
$$\tilde{t}_{ij} = \sum_{\boldsymbol{k}}[u(\boldsymbol{k}) + W + t_{\boldsymbol{k}}]\exp[\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{R}_i - \boldsymbol{R}_j)]. \tag{65}$$

We can interprete these fermions as the charged particles formed when low-energy conduction electrons bind to f spins. To see that these excitations are indeed charged, we appeal to arguments of gauge invariance. In a slowly varying vector potential field $\boldsymbol{A}$, $\epsilon_{\boldsymbol{k}} \to \epsilon_{\boldsymbol{k}-e\boldsymbol{A}}$, shifting the momenta of conduction electrons by an amount $e\boldsymbol{A}$. Since $V_j = J_J\langle c_j f^{\dagger}{}_j\rangle$, in a field V_j acquires a phase factor $V_j \to \exp(\mathrm{i}e\int^j \boldsymbol{A}\cdot \mathrm{d}\boldsymbol{r}\,\tau_3)V_j$, so the mean-field Hamiltonian takes the form

$$H_{\rm MF} = \sum_{\boldsymbol{k}\sigma}[\epsilon_{\boldsymbol{k}-e\boldsymbol{A}}c^{\dagger}{}_{\boldsymbol{k}\sigma}c_{\boldsymbol{k}\sigma} + V_0(c^{\dagger}{}_{\boldsymbol{k}\sigma}f_{\boldsymbol{k}-e\boldsymbol{A}} + \mathrm{HC}) + u(\boldsymbol{k})f^{\dagger}{}_{\boldsymbol{k}\sigma}f_{\boldsymbol{k}\sigma}]. \tag{66}$$

By redefining $f'_{\boldsymbol{k}\sigma} = f_{\boldsymbol{k}+e\boldsymbol{A}\ \sigma}$, we see that the effects of a slowly varying vector potential on the phases associated with resonant Kondo scattering can be absorbed by a shift $u(\boldsymbol{k}) \to u(\boldsymbol{k}-e\boldsymbol{A})$. In other words, the quasi-particle energies transform as $E_{\boldsymbol{k}p} \to E_{\boldsymbol{k}-e\boldsymbol{A},p}$ in a vector potential, showing that the quasi-particles do indeed carry a charge $-e$. We may regard these excitations as holes in the background of f spins, formed by the formation of singlet pairs between the conduction and f spins, in fact this interpretation is internally consistent, because the curvature of $t_{\boldsymbol{k}}$ is opposite to the curvature of the original conduction band. These f holes are actually composite objects in terms of the original model, and the SU(2) symmetry is now hidden as an internal symmetry.

The non-local interactions in this phase contain a strong $\boldsymbol{q}$ dependence because of the extended nature of the RKKY interaction. These interactions induce direct binding between the f spins, which in our approach is modelled by the development of $U \neq 0$. In the high-temperature Fermi liquid regime, the mutual compensation of f spins, expressed by $U = \Delta\tau_3$, is mainly passive in nature, and would be present even if the RKKY interactions could be turned off. The principal effect of this term is to renormalise the dispersion of the f electrons over and above the contribution from the Kondo effect.

At low temperatures, where the entropy associated with the low-lying excitations of a Fermi liquid is less important, the tripod of vectors $\hat{n}_l$ now unfolds and U acquires an off-diagonal component. The condition

$$\Delta_{\perp} \neq 0 \tag{67}$$

cannot occur without an RKKY interaction, so $\Delta_\perp$ can be regarded as an order parameter signalling the development of 'active' mutual f spin compensation. In general, the conduction electron self-energy has the form

$$\Sigma_c(\boldsymbol{k},\omega) = \frac{V_0^2}{\omega - \left(\boldsymbol{W} + 2\Delta\sum_l \cos k_l \hat{n}_l\right)\cdot\boldsymbol{\tau}} \tag{68}$$

describing resonant scattering of conduction electrons by the Kondo effect. Once $\Delta_\perp \neq 0$, σ acquires *off-diagonal* components in Nambu space, inducing 'resonant superconductivity' in the conduction fluid.

To investigate this instability, we set $\Delta_\perp = 0^+$ in the mean-field equations, yielding

$$\begin{aligned} 1/J_{\mathrm{H}} &= \Pi^{\mathrm{s,d}}(T) \\ \Pi^{s,d}(T) &= \sum_{kp} \frac{1}{2E_{kn}} \tanh(\beta E_{kn}/2) g_{kp} |\phi_k^{\mathrm{s,d}}|^2 \\ g_{kp} &= \frac{1}{2} + p\,\mathrm{sgn}(\epsilon_k - u_k)\left(\frac{V_0^2 + (u_k^2-\epsilon_k^2)/2}{\left[(u_k^2-\epsilon_k^2)^2 + 4V_0^2(U_k+\epsilon_k)^2\right]^{1/2}}\right) \end{aligned} \tag{69}$$

where $\phi_k^{\mathrm{s,d}}$ is determined by the symmetry of the pairing field, as given previously. This determines the superconducting transition temperature of the heavy Fermi liquid. In a one-band Cooper instability, the factor g_{kp} would be weakly energy dependent and of order one, reflecting the constant attractive interaction between the quasi-particles in the vicinity of the Fermi energy. In this case

$$g(\boldsymbol{k}p) = \begin{cases} 1 & E_{kp} \ll V \sim \sqrt{T_{\mathrm{K}}/\rho_0} \\ (V/\epsilon_k)^4 & E_{kn} \gg V \sim \sqrt{T_{\mathrm{K}}/\rho_0} \end{cases} \tag{70}$$

and the strength of the attractive interaction is roughly determined by the degree of f admixture in the quasi-particles, being strongest where the f admixture is higher.

Since $|\phi_k^{\mathrm{d}}|^2 - |\phi_k^{\mathrm{s}}|^2 = -2(c_xc_y + c_yc_z + c_zc_x)$, if the f Fermi surface is concentrated in regions where $\sum_l \cos k_l \sim 0$, then the average value of $(c_xc_y + c_yc_z + c_zc_x)$ is negative and d-wave pairing is favoured. If the f Fermi surface is situated in regions where the magnitude of $\sum_l \cos k_l$ is large, then $(c_xc_y + c_yc_z + c_zc_x)$ is positive and extended s-wave pairing is favoured. In practice the former case seems to prevail becuse the f Fermi surface is determined by the term $2\Delta\sum_l \cos k_l$ in u_k. Figure 4 displays the predictions of a more detailed calculation comparing the d- and s-wave transition temperatures. In the next section we will advance energetic reasons for the d-wave preference in this Cooper instability.

It is instructive to relate this instability to the original Heisenberg interaction. The Heisenberg interaction may be written in the form

$$J_{\mathrm{H}} \sum_{(i,j)} \mathbf{S}_i \cdot \mathbf{S}_j = -J_{\mathrm{H}} \sum_{k,\,k',\,q} (\phi_k^{\mathrm{s}}\phi_{k'}^{\mathrm{s}} + \eta_k\eta_{k'} + \zeta_k\zeta_{k'})\hat{\Delta}^\dagger{}_k(\boldsymbol{q})\hat{\Delta}_{k'}(\boldsymbol{q}) \tag{71}$$

where $\hat{\Delta}^\dagger{}_k(\boldsymbol{q}) = f^\dagger{}_{k+q/2\uparrow} f^\dagger{}_{-k+q/2\downarrow}$. When we integrate out the fluctuations in U, this introduces a temperature-dependent interaction whose $\boldsymbol{q} = 0$ component is given by

$$-\sum_{k,\,k'} [J_s(T)\phi_k^{\mathrm{s}}\phi_{k'}^{\mathrm{s}} + J_d(T)(\eta_k\eta_{k'} + \zeta_k\zeta_{k'})]\hat{\Delta}^\dagger{}_k(0)\hat{\Delta}_{k'}(0) \tag{72}$$

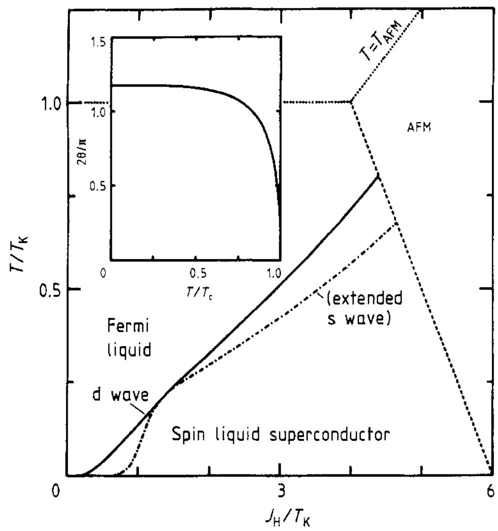

Figure 4. Mean-field phase diagram, calculated for the case $\mu/t = -1.5$, $T_K/t = 0.01$. Dotted curves indicate crossover to a heavy Fermi liquid, full curve the calculated d-wave instability, chain curve the lower extended s-wave T_c instability. For completeness, the broken curve indicates the anticipated position of the transition between an antiferromagnet (in 3D) and superconductor, which cannot be calculated in the current theory. Inset: variation of the angle θ between the SU(2) vectors $\hat{n}_l$ as a function of temperature ($U_l = \Delta\hat{n}_l \cdot \boldsymbol{\tau}$, $\hat{n}_i \cdot \hat{n}_j = \cos\theta$). The parameters chosen were $J_H/T_K = 0.5$, for which $T_c/T_K = 0.04$. Note how the tripod opens up as the temperature is lowered, and that even though $J_H/T_K < 1.0$, the zero-temperature value of θ is very close to the 90° favoured in the idealised spin liquid.

where

$$J_{s,d}(T) = \frac{J_H}{1 - J_H \Pi^{s,d}(T)}. \tag{73}$$

Thus anisotropic superconductivity is associated with a divergence in the forward-scattering d-wave component of the RKKY interaction. This divergence is of magnetic origin, in fact, when $J_H \gtrsim T_K$, $\Pi^{s,d}(T) \sim 1/4T$, and we find that

$$J_{s,d}(T) = \frac{J_H}{1 - (J_H/4T)}. \tag{74}$$

This is precisely the divergence that generates mean-field antiferromagnetism. However, in this case the Kondo effect pre-empts magnetism. Since formation of a magnetic ground state would entail losing $-V_0^2/J_K$ of compensation energy, the system compromises by forming a Kondo-stabilised spin liquid.

There are two regimes along the superconducting phase boundary. When $J_H \ll T_K$, T_c is small, the superconductivity is weak coupling and the integral in the gap eqaution is dominated by the logarithmic singularity in the Cooper channel at the Fermi surface. Define the quasi-particle density of states

$$\rho^*(\epsilon) = \sum_{kp} \delta(\epsilon - E_{kp}) \tag{75}$$

which is approximately given by $\rho_0 V_0^2/W^2 = \alpha/T_K$, where α is of order one . We also define the Fermi surface average of $|\phi_k^d|^2$:

$$\phi^2(\epsilon)\rho^*(\epsilon) = \sum_{kp} |\phi_k^d|^2 \delta(\epsilon - E_{kp}). \tag{76}$$

Using these definitions, and putting $g_k \simeq 1$ near the Fermi surface, we find that the weak coupling T_c is

$$T_c = \eta T_K \exp\left(-\frac{1}{J_H \phi^2(0)\rho^*(0)}\right) = \eta T_K \exp\left(-\frac{T_K}{\alpha J_H \phi^2(0)}\right) \qquad (J_H \ll T_K) \tag{77}$$

where η is given by

$$\ln \eta = \psi(\tfrac{1}{2}) + \lim_{D\to 0} \frac{1}{2\rho^*|\phi^d(0)|^2} \int d\epsilon\, \phi^2\rho^*(\epsilon) \left|\frac{\epsilon}{\epsilon^2 + D^2}\right| + \ln \frac{D}{T_K}. \tag{78}$$

We see that the coupling constant is of order J_H/T_K, as might expected from Fermi liquid arguments.

A more extensive portion of the phase diagram is *not* dominated by the weak-coupling instability. When J_H/T_K approaches unity, the detailed dispersion of the lower f band ceases to be of importance in the gap equation. To get an approximate estimate for T_c we consider the limit in which $\beta E_{kp} \to 0$. Setting $g_{kp} \simeq 1$, $\tanh(\beta E_{kp}/2) \simeq \beta E_{kp}/2$, gives

$$T_c \simeq J_H/4 \qquad (J_H \sim T_K). \tag{79}$$

(In actual fact, the finite dispersion derived from $\Delta_z \neq 0$ depresses the phase diagram slightly below this value, as can be seen in figure 4.) In this regime, the superconductor can be regarded as a Kondo-stabilised spin liquid, as we now discuss.

3.2. Anisotropic superconductor ($U_l \propto \hat{n}_l \cdot \boldsymbol{\tau}$, V, $W \neq 0$)

Below T_c, the size of $\Delta_\perp$ grows to minimise the RKKY superexchange energy. To gain insight into this process it is helpful to first ignore the Kondo effect of the conduction electrons on the f spins. This provides us with a 'spin liquid' starting point with which we can compare the f spin correlations of the superconducting phase. Such a starting point only makes sense if the Kondo effect helps to stabilise the spin liquid.

In the absence of the Kondo exchange term, there is perfect particle–hole symmetry in the f fluid, so $W = 0$. Taking $\hat{n}_i \cdot \hat{n}_j = \alpha$, then the quasi-particle energies are

$$E_k = 2\Delta \left[(1-\alpha)\sum_l \cos^2 k_l + \alpha\left(\sum_l \cos k_l\right)^2\right]^{1/2} \tag{80}$$

and $\alpha = 0$ maximises the sum $\sum_k E_k$. The mean-field ground-state energy is $E_0 = 6\Delta^2/J_H - 2\sum_k E_k$. At the saddle point, $\partial E_0/\partial\Delta = 0$, or $6\Delta^2/J_H = \sum_k E_k$, so $\alpha = 0$ maximises Δ, thereby minimising the total exchange energy $-6\Delta^2/J_H$. Thus in an idealised spin liquid we expect the $\hat{n}_l$ to be *orthogonal* to one another [11].

The Kondo exchange effectively shifts the z component of $\boldsymbol{u}_k$ according to

$$\Delta_z(c_x + c_y + c_z) \to \Delta_z(c_x + c_y + c_z) + W - V_0^2/\epsilon_k. \tag{81}$$

However, on the average the shift in W compensates the effect of the 'hybridisation' term $-V_0^2/\epsilon_k$, since the constraint equation $\langle f^\dagger \tau_3 f\rangle = 0$ implies

$$\begin{aligned} 0 &= \sum_k \frac{1}{2|E_k|}\left(\Delta_z(c_x + c_y + c_z) + W - \frac{V_0^2}{\epsilon_k}\right) \\ &\simeq \sum_k \frac{1}{2|E_k|}\left(W - \frac{V_0^2}{\epsilon_k}\right) \end{aligned} \tag{82}$$

where we have restricted our attention to the lower quasi-particle band $E_k = E_{k-}$. Consequently, the distortion induced in the spin liquid state is minimised. Numerical work shows that even when the Kondo coupling is considerable, at $T = 0$, $\hat{n}_i \cdot \hat{n}_j \simeq 0$ in the superconducting ground state .

Since the U_l of the superconducting phase are quite close to those of the spin liquid, this implies that short-range equal-time spin correlations in the superconductor closely resemble those of a spin liquid. For instance, the nearest-neighbour spin correlations are determined by

$$\langle \mathbf{S}_i \cdot \mathbf{S}_j\rangle = \tfrac{1}{4} - \mathrm{Tr}\, U^\dagger U/(J_\mathrm{H})^2 = \tfrac{1}{4} - 2(\Delta/J_\mathrm{H})^2. \tag{83}$$

Similarly, the amplitude for ring exchange around a single square plaquet

$$\langle P_\mathrm{R}\rangle = (1/J_\mathrm{H}^4)\mathrm{Tr}\, U_{ij}U_{jk}U_{kl}U_{li} = -2(\Delta/J_\mathrm{H})^4 \tag{84}$$

is negative, as in the pure spin liquid.

It is instructive to examine the ground-state wavefunction of our Kondo-stabilised spin liquid in Anderson's RVB language. If we take the pure spin liquid, then this may be written in the form

$$\begin{aligned} |\psi\rangle &= P_G \prod_k (1 - \alpha_k \exp(-\mathrm{i}\theta_k) f^\dagger{}_{k\uparrow} f^\dagger{}_{-k\downarrow})|0\rangle \\ \alpha_k &= \left(\frac{(\sum_l c_l^2)^{1/2} + c_z}{(\sum_l c_l^2)^{1/2} - c_z}\right)^{1/2} \\ \tan\theta_k &= c_y/c_z. \end{aligned} \tag{85}$$

A weak Kondo effect adds a perturbation $H = \sum_k (c^\dagger{}_k \tau_3 f_k + \mathrm{HC})$ to the mean-field Hamiltonian. To leading order in V_0, this replaces

$$f^\dagger{}_{k\sigma} \to f^\dagger{}_{k\sigma} + \frac{V_0}{u_k - \epsilon_k} c^\dagger{}_{k\sigma} \tag{86}$$

in the quasi-particle operators, and the modified wavefunction takes the form

$$\begin{aligned} |\psi_{KSSL}\rangle &= P_G \prod_k [1 - \alpha_k \exp(-\mathrm{i}\theta_k)\tilde{b}^\dagger{}_k]\,|0\rangle \\ \tilde{b}^\dagger{}_k &= \left(f^\dagger{}_{k\uparrow} f^\dagger{}_{-k\downarrow} + \frac{V_0}{u_k - \epsilon_k}(c^\dagger{}_{k\uparrow} f^\dagger{}_{-k\downarrow} + f^\dagger{}_{k\uparrow} c^\dagger{}_{-k\downarrow}) + \frac{V_0^2}{(u_k - \epsilon_k)^2} c^\dagger{}_{k\uparrow} c^\dagger{}_{-k\downarrow}\right). \end{aligned} \tag{87}$$

We may interprete the terms involving conduction electrons as describing the 'escape' of resonating valence bonds into the conduction sea. Thus

$$\alpha_{cf}(\boldsymbol{r}) = \sum_k \frac{\alpha_k V_0}{u_k - \epsilon_k} \exp(-\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{r}) \tag{88}$$

is the amplitude for forming a singlet bond of length r between the conduction fluid and f spins, whilst

$$\alpha_{cc}(\boldsymbol{r}) = \langle c^\dagger{}_\uparrow(\boldsymbol{r}) c^\dagger{}_\downarrow(0)\rangle = \sum_k \frac{\alpha_k V_0^2}{(u_k - \epsilon_k)^2} \exp(-\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{r}) \tag{89}$$

is the pairing amplitude for total escape of a valence bond into the conduction sea. Whilst α_{cf} is not SU(2) invariant, reflecting the overcomplete nature of the RVB basis set, this last pairing term *is* SU(2) invariant, and therefore survives the Gutzwiller projection. Consequently, the escape of valence bonds into the conduction sea generates a physical off-diagonal long-range order in the conduction sea.

There is, of course, an important energetic difference between our state and a pure spin liquid, for the mean-field ground-state energy per unit cell contains both Heisenberg and Kondo components, given by

$$E_0 = -\frac{6\Delta^2}{J_{\mathrm{H}}} - \frac{2V_0^2}{J_{\mathrm{K}}} \simeq -\frac{6\Delta^2}{J_{\mathrm{H}}} - \frac{T_{\mathrm{K}}}{J_{\mathrm{K}}\rho_0} \tag{90}$$

where we have put $V_0^2\rho \sim T_{\mathrm{K}}$. The second term arises from the Kondo effect. Thus although the spin correlations bear close resemblance to those of a spin liquid, the ground-state energy is significantly *stabilised* by the Kondo effect. This result also explains why d-wave pairing is favoured, for the d-wave instability forces the 'arms of the tripod' defined by $\hat{n}_l$ to separate, lowering the exchange energy.

To complete this section we remark briefly on what is to be expected when T_{c} becomes comparable with the Kondo temperature. In our mean-field approach, there is another phase boundary separating the superconducting state from the pure spin liquid state. Setting $V = 0^+$ in the mean-field equations, and taking the $\hat{n}_l$ to be orthogonal, we find that an instability in V occurs at a temperature T^* given by

$$\frac{1}{J_{\mathrm{H}}} = \sum_{kp=\pm} \frac{1 - f(E_k) - f(p\epsilon_k)}{2(E_k + p\epsilon_k)} \left(1 + p\frac{c_x + c_y + c_z}{[3(c_x^2 + c_y^2 + c_z^2)]^{1/2}}\right). \tag{91}$$

A similar result was obtained for two dimensions, where we *do* expect a spin liquid to be stable at finite temperatures. However, in three dimensions, we expect an antiferromagnetic phase transition, probably first order in nature to pre-empt the phase transition into a pure spin liquid state. The situation is more subtle in quasi-two-dimensional situations, where the interesting possibility of a second-order phase transition between the Kondo-stabilised spin liquid superconductor and a finite-temperature quantum antiferromagnet with no long-range order is not precluded.

4. Discussion: dilute systems and quasi-particle interactions

The notion of Kondo-stabilised spin liquids has interesting consequences for dilute Kondo impurity systems that shed light on the underlying mechanism of the superconductivity in the dense system. The first appearance of the RKKY interaction occurs in the two-impurity Kondo problem. However, the essential feature of a spin liquid, namely a quantum resonance of spin-singlet bonds, that is needed to gain a large proportion of the antiferromagnetic exchange energy, cannot develop until there are at least three impurity spins. Our mean-field theory gives results that are consistent with this reasoning.

Consider the Heisenberg component of the mean-field theory for two and three equally spaced impurities

$$H_2 = \Delta({f^\dagger}_2 \hat{n} \cdot \boldsymbol{\tau} f_1 + \mathrm{HC}) + 2\Delta^2/J_{\mathrm{H}}$$
$$H_3 = \Delta({f^\dagger}_1 \hat{n}_3 \cdot \boldsymbol{\tau} f_3 + {f^\dagger}_3 \hat{n}_2 \cdot \boldsymbol{\tau} f_2 + {f^\dagger}_2 \hat{n}_1 \cdot \boldsymbol{\tau} f_1 + \mathrm{HC}) + 6\Delta^2/J_{\mathrm{H}}. \qquad (92)$$

For two impurities, the eigenvalues of H_2 are $\pm 2\Delta$ for all values of $\hat{n}$. In this case the mean-field energy in the presence of spin compensation ($V = V_0\tau_3$ in the uniform gauge) depends only on the cosine of the angle between $\hat{n}$ and $\hat{z}$: $E = E(\cos \hat{n} \cdot \hat{z})$. This energy is extremal only for $U \propto \tau_3$, and consequently, the conduction electron self-energy is diagonal. At the mean-field level, this implies that the results of an SU(2) analysis of the two-impurity model will correspond to those of a large-N treatment [12]. In the special case considered by JVW, the conduction band is completely symmetric, and at the mean-field level, there is no dependence of the total energy on the angle between $\hat{n}$ and the $\hat{z}$ axis†.

For the three-impurity case, however, we can choose the $\hat{n}_j$ to be the prongs of a tripod with axis along the $\hat{z}$ direction. In this case the MF energy eigenvalues are

$$E_n = 2\Delta|\cos(\rho + 2\pi n/3)| \qquad (n = 1, 2, 3) \qquad (93)$$

where $\sin\rho = (\sqrt{3}/2)\cos(\hat{n}_1 \cdot \hat{z})$. Filling the lowest three eigenstates, the mean-field free energy of the pure spin liquid is then $-\sum_n E_n = -\sqrt{3}\Delta\cos(\rho - \pi/6)$. The mean-field energy is minimised by the choice $\rho = \pi/6$ for which the $\hat{n}_i$ all lie at right angles to one another. In this configuration, the conduction electron self-energy is off-diagonal for any orientation of the tripod described by $\hat{n}_1$, $\hat{n}_2$ and $\hat{n}_3$ relative to the $\hat{z}$ axis. Of course, until the concentration of impurities becomes dense, fluctuations in the phase of the pairing order parameter will suppress a true superconducting phase transition, leading to strong local superconducting fluctuations at low temperatures. Unusual magnetic resonance properties recently measured in dilute Kondo systems may be intimately related to this feature [13].

We now go on to discuss the quasi-particle interactions in the normal Fermi liquid. Computation of these interactions from the Gaussian fluctuations about the mean-field theory follows lines similar to those used in large-N approaches, but the calculation is slightly complicated by the delicate issue of removing the large class of zero-gauge modes from the fluctuations. This task is accomplished using the Fadeev–Popov method. First we decide in advance the coordinate system that defines the fluctuations about the gauge orbit, defining a plane $f(U, V, W) = 0$: thereby 'fixing the gauge'. We then integrate over the gauge orbits passing through this plane, introducing a Fadeev–Popov determinant $Y(U, V, W)$ into the path integral that measures the 'length' of the

† We have not examined this special case in detail, however, it is tempting to suggest that, for a perfectly symmetric band, fluctuations about the mean-field theory might select $\hat{n}$ perpendicular to $\hat{z}$, which would then give rise to identical scattering phase shifts in the even- and odd-parity scattering channels, as discovered in the Wilson scaling. This behaviour would disappear in the presence of an asymmetric conduction band.

gauge orbit:

$$\int d[U,V,W] = \int d[U,V,W]\, Y(U,V,W)\, \delta(f[U,V,W])$$
$$Y(U,V,W)^{-1} = \int dg\, \delta(f[U^g,V^g,W^g]). \tag{94}$$

The most convenient choice of gauge is an 'axial gauge'. Consider an arbitrary fluctuation (U',V',W'), in which we write $V' = -\mathrm{i}(V_0+\delta V)\exp(\mathrm{i}\boldsymbol{\lambda}\cdot\boldsymbol{\tau})\tau_3$ This fluctuation lies on the same gauge orbit as the point (U'^g, V'^g, W'^g). Choosing $g = \exp(-\mathrm{i}\boldsymbol{\lambda}\cdot\boldsymbol{\tau})$, brings us to the unique point on the orbit where $V = (V_0+\delta V)\tau_3$, so the choice $V \propto \tau_3$ fixes the gauge. This gauge choice is the SU(2) analogue of the Newns and Read 'radial gauge' employed in the large-N approach to the Kondo problem [14]. The determinant for the axial gauge is a constant†, so the measure for V fluctuations in this gauge is simply

$$d[V]_a = \prod_j V_0(j)\, dV_0(j) \tag{95}$$

(where the subscript denotes 'axial'). For small fluctuations, the measures for V and U may be linearised

$$d[V]_a \simeq \prod_j dV_0(j)$$
$$d[U] \simeq \prod_{(i,j)} d\Delta_{ij}\, d^3 W_{ij} \tag{96}$$

where $U_{ij} = -\mathrm{i}\Delta_{ij}\exp(\mathrm{i}\boldsymbol{W}_{ij}\cdot\boldsymbol{\tau})$. This permits us to examine the Gaussian fluctuations that couple the charged quasi-particle excitations in the normal phase.

† To calculate the determinant $Y[V]$ for the axial gauge, we consider one site and write

$$d[V]_{\mathrm{axial}} = d[V]\, Y[V] \prod_{i=0,2} \delta[h_i]$$

where we have put $V = V_0 h$ where h is an SU(2) matrix $h = h_\mu \tau^\mu = \boldsymbol{h}\cdot\boldsymbol{\tau} - \mathrm{i}h_0\mathbf{1}$. Using the Fadeev–Popov method

$$Y[V]^{-1} = \int d[g] \prod_{\mu=0,2} \delta[h^g_\mu]$$
$$h^g = gh = h^g_\mu \tau^\mu.$$

This is a constant, independent of V_0, that factors out of the path integral. For completeness, note that $d[g] = d[h^g]$, thus

$$Y[V]^{-1} = \int d[h^g] \prod_{\mu=0,2} \delta[h^g_\mu] = \frac{1}{\pi^2}\int d^4 h\,\delta\left(1-\sum_\mu h^2_\mu\right) \prod_{\mu=0,2} \delta[h_\mu] = \frac{2}{\pi}.$$

As in the large-N approach, the Gaussian fluctuaions define a 'quasi-particle interaction Hamiltonian' H_I whose expectation value in a two-quasi-particle state defines the Landau interaction constants

$$f_{\sigma,\sigma'}(\boldsymbol{k},\boldsymbol{k}') = \langle \boldsymbol{k}\sigma,\boldsymbol{k}'\sigma|H_I|\boldsymbol{k}\sigma,\boldsymbol{k}'\sigma'\rangle \qquad |\boldsymbol{k}\sigma,\boldsymbol{k}'\sigma'\rangle = a^{\dagger}{}_{kp_F\sigma}a^{\dagger}{}_{k'p'_F\sigma'}|\widetilde{FL}\rangle \tag{97}$$

where $|\widetilde{FL}\rangle$ is the mean-field Fermi liquid ground state and $a^{\dagger}{}_{kp_F\sigma}$ the corresponding quasi-particle operators (band index p_F chosen for band at Fermi surface). It is interesting to contrast the interactions obtained in the SU(2) approach with those obtained in the large-N approach to the Kondo lattice model. Like the large-N expansion, the zero-frequency fluctuations in the constrained Lagrange multiplier field W give rise to a repulsive interaction between the f components of the quasi-particles. In the axial gauge, the fluctuations in W may be separated into components perpendicular and parallel to the SU(2) $\hat{z}$ axis.

$$\langle \delta W_\alpha(1)\delta W_\beta(2)\rangle = \delta_{\alpha\beta}D_\alpha(1-2) \qquad (D_1 = D_2 = D_\perp). \tag{98}$$

Fluctuations in W_3 generate a repulsive interaction in the particle–hole channel:

$$H_3 = \frac{1}{2}\sum_{kk'q\sigma\sigma'} U_{\boldsymbol{q}} f^{\dagger}{}_{k+q\sigma} f^{\dagger}{}_{k'\sigma'} f_{k'+q\sigma'} f_{k\sigma}$$
$$U_{\boldsymbol{q}} = D_3(\boldsymbol{q},\omega)|_{\omega=0}. \tag{99}$$

When a quasi-particle propagates, the surrounding medium responds via this interaction by reducing the f charge density, preserving a constant f charge density ($f^{\dagger}\tau_3 f = 0$). Unlike the large-N approach, analogous terms are generated in the Cooper channel by the fluctuations in $\boldsymbol{W}_\perp$ normal to the charge direction

$$H_\perp = \sum_{kk'q\sigma\sigma'} \Gamma_{\boldsymbol{q}} f^{\dagger}{}_{k'+q\uparrow} f^{\dagger}{}_{-k'\downarrow} f_{-k\downarrow} f_{k+q\uparrow}$$
$$\Gamma_{\boldsymbol{q}} = 2D_\perp(\boldsymbol{q},\omega)|_{\omega=0}. \tag{100}$$

The perpendicular fluctuations arise because of the need to impose on the x and y components of the vector SU(2) the constraint $f^{\dagger}{}_j\boldsymbol{\tau} f_j = 0$ when additional quasi-particles are added to the system. This interaction is not explicitly present in the large-N approach. However, like the diagonal terms, these terms are also repulsive of order T_K and mainly local in character.

At the Fermi surface, the quasi-particle excitations are almost entirely of f character ($\cos\delta_{k_F} \sim 1$), so the local constraints generate the following contributions to the Fermi liquid interaction

$$f_{\uparrow\uparrow}(\boldsymbol{k},\boldsymbol{k}') = f_{\downarrow\downarrow}(\boldsymbol{k},\boldsymbol{k}') = U_0 - U_{\boldsymbol{k}-\boldsymbol{k}'}$$
$$f_{\uparrow\downarrow}(\boldsymbol{k},\boldsymbol{k}') = f_{\downarrow\uparrow}(\boldsymbol{k},\boldsymbol{k}') = U_0 + \Gamma_{\boldsymbol{k}+\boldsymbol{k}'}. \tag{101}$$

Note how the transverse fluctuations enhance the spin dependence of the interactions. In the one-impurity problem there is no q dependence of interactions, so the parallel spin interaction vanishes. This feature, combined with the zero f charge susceptibility is necessary for a Wilson ratio 2.

There are also fluctuations in the U field, corresponding to the renormalised RKKY interaction. These interactions are non-local in character, containing terms of the form

$$H_{RKKY} = \sum_{(i,j),\ (l,l')} \hat{u}(\boldsymbol{R}_i + \tfrac{1}{2}\hat{l}, \boldsymbol{R}_i - \tfrac{1}{2}\hat{l}) K(\boldsymbol{R}_i - \boldsymbol{R}_j) \hat{u}(\boldsymbol{R}_j - \tfrac{1}{2}\hat{l}', \boldsymbol{R}_j + \tfrac{1}{2}\hat{l}') \qquad (l, l' = x, y, z) \tag{102}$$

where the $\hat{u}$ are the bond operators introduced in (15), $\hat{u}K\hat{u}$ denotes $\hat{u}_{\alpha\beta}K_{\alpha\beta\delta\gamma}\hat{u}_{\delta\gamma}$ and

$$K_{\alpha\beta,\gamma\nu}[\boldsymbol{R}_i - \boldsymbol{R}_j] = \langle [\delta U_l(\boldsymbol{R}_i)]_{\alpha\beta} [\delta U_{l'}(\boldsymbol{R}_j)]_{\gamma\nu} \rangle_{\omega=0}. \tag{103}$$

The forward-scattering component of these interactions in the Cooper channel generates pairing of the quasi-particles, whilst the q-independent part generates the renormalised nearest-neighbour RKKY interaction. Near the superconducting transition temperature, the forward scattering component of this interaction in the d-channel diverges.

To conclude, we mention some general implications of our Kondo-stabilised picture of heavy fermion superconductivity. Firstly, we note that it is intrinsically a strong-coupling mechanism, relying on two basic pieces of physics:

(i) that the Kondo effect preferentially stabilises a spin liquid against magnetism;

(ii) that the coherent coupling of a spin liquid to a conduction sea necessarily results in superconductivity.

Transition temperatures that are a large fraction of the Kondo temperature are encompassed in this picture, once J_H becomes comparable with or greater than T_K. In this regime, superconductivity can occur before a fully developed Fermi liquid has formed. The superconductor UBe_{13} is a good candidate for this scenario.

Secondly, we note that our mechanism has a new temperature scale associated with the mean-field T_c. It is quite likely that fluctuation effects will suppress the actual T_c well below this value, and the mean-field T_c will be marked by a substantial growth in the short-length f spin correlations. Experimentalists have long explained the sudden changes in transport and thermodynamic properties of heavy fermion systems at low temperatures in terms of a phenomenological 'coherence temperature'. This second scale, where the spin liquid starts to form and f spin correlations start to grow, would provide a convenient explanation of the 'coherence temperature'.

Finally, we mention the possibility of a unifying link between heavy fermion and cuprate superconductivity. Earlier we noted an interesting phase boundary between the superconducting and spin liquid phases which is probably not realised in three dimensions due to the formation of an antiferromagnet in preference to a pure spin liquid. However, in two dimensions, long-wavelength fluctuations affect an antiferrmomagnetic state quite differently to a superconducting spin liquid. The long-wavelength spin fluctuations suppress T_{AFM} to zero, or to the three-dimensional ordering temperature. By contrast, the mean-field transition temperature between the spin liquid and superconductor should give a good estimate of a Kosterlitz–Thouless transition into a superconducting state, and furthermore, a tiny three-dimensional Josephson coupling will drive a KT superconductor into a conventional 3D superconductor [15]. Hence, in a quasi-two-dimensional situation, a spin-liquid to superconducting transition may become feasible. We speculate that heavy fermion superconductivity and cuprate superconductivity are both forms of a Kondo-stabilised spin liquid, arrived at through different sequences of spin compensation. We are actively engaged in exploring this possiblity.

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Appendix

We now evaluate

$$f(U) = \frac{1}{\pi}\int \mathrm{d}[g_i]\,\mathrm{d}[g_j]\,\mathrm{d}\phi_x\,\mathrm{d}\phi_y\,\delta(g_i\tilde{U}_{ij}g_j^{-1} - U) \tag{A1}$$

where

$$\tilde{U}_{ij} = \phi_x(\hat{n}\cdot\boldsymbol{\tau}) + \mathrm{i}\phi_y \tag{A2}$$

and $U = [\boldsymbol{u}\cdot\boldsymbol{\tau} + \mathrm{i}u_0]$. First note that $f(U)$ does not depend on the choice of $\hat{n}$, because of the integration over the gauge orbits of g_i and g_j, so we shall arbitrarily choose $\hat{n} = \hat{x}$. Second, note that we can rewrite the four-dimensional delta function as $\delta(\tilde{U}_{ij} - g_i^{-1}Ug_j)$, so $f(g_a^{-1}Ug_b) = f(U)$ is invariant under arbitrary gauge transformations of U. Next, note that ϕ_x, ϕ_y and u_α ($\alpha = [0, 1, 2, 3]$) each have the dimensions of energy, so the dimension of $f(U)$ is $[U^{-2}]$. The only gauge-invariant function with this dimension is proportional to $1/\mathrm{Tr}[U^\dagger U]$, hence

$$f(U) = \frac{\alpha}{\mathrm{Tr}[U^\dagger U]}$$

where the constant α is to be determined. To evaluate α, set $U = \mathrm{i}\mathbf{1}$, then

$$\alpha = \frac{2}{\pi}\int \mathrm{d}[g_i]\,\mathrm{d}[g_j]\,\mathrm{d}\phi_x\,\mathrm{d}\phi_y\,\delta(\tilde{U}_{ij} - \mathrm{i}g_i^{-1}g_j). \tag{A3}$$

Changing variables from (g_i, g_j) to $(g_i, \tilde{g} = g_i^{-1}g_j)$, and using the gauge invariance of the measures $\mathrm{d}[g_i]\,\mathrm{d}[g_j] = \mathrm{d}[g_i]\,\mathrm{d}[g_i^{-1}g_j]$, the integral over g_i then factors out to give

$$\alpha = \frac{2}{\pi}\int \mathrm{d}[\tilde{g}]\,\mathrm{d}\phi_x\,\mathrm{d}\phi_y\,\delta(\tilde{U}_{ij} - \mathrm{i}\tilde{g}). \tag{A4}$$

Finally, putting $\hat{n} = \hat{x}$, $g = h_0 + \mathrm{i}\boldsymbol{h}\cdot\boldsymbol{\tau}$, $\boldsymbol{h} = (h_1, h_2, h_3)$, $\mathrm{d}[\tilde{g}] = \pi^{-2}\mathrm{d}^4h_\mu\,\delta[h^2 - 1]$, ($h^2 = \sum_\mu h_\mu^2$, $\mu = 0, 1, 2, 3$) then gives

$$\begin{aligned}\alpha &= \frac{2}{\pi^3}\int \mathrm{d}^4h\,\mathrm{d}\phi_x\,\mathrm{d}\phi_y\,\delta[h^2 - 1]\,\delta[h_1 - \phi_x]\,\delta[h_0 - \phi_y]\,\delta[h_2]\delta[h_3] \\ &= \frac{2}{\pi^3}\int \mathrm{d}h_0\,\mathrm{d}h_1\,\delta[h_0^2 + h_1^2 - 1] = \frac{2}{\pi^2}.\end{aligned} \tag{A5}$$

yielding our final result $f(U) = 2/[\pi^2\mathrm{Tr}(U^\dagger U)]$.

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