Interference of the RKKY and Kondo interaction

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Abstract

1 Introduction

Not finalised - will come back and fix most of the narrative with regards to the Kondo effect and the aim of the project.

The Kondo problem has been one of the largest challenges in condensed matter physics. The centre of the problem lies in the understanding of local moment formation. The Anderson model (a.k.a Anderson's mean-field theory) neglects the finite quantum mechanical amplitude for the local spin to tunnel between different configurations [1]. Therefore, it fails to provide a sufficiently satisfying treatment below the so-called Kondo temperature $k_B T_K = \frac{\hbar}{\tau_{sf}}$ as perturbative methods fail below this temperature. Understanding this phenomenon requires a new understanding of the renomralization group as proposed by Ken Wilson [2–5].

In a dense Kondo lattice of local moments, the formation of quasiparticles with greatly enhanced masses, known commonly as *heavy electrons*, allows local moments in the system to interact with the sea of conduction electrons. The immersion fo a lattice of spins (normally an impurity lattice in an experiment), induces a resonances at each site of the lattice, and hence causes the conduction electrons to hybridise into a band of delocalised heavy fermions. The resultant picture is an effective dissolution of the spin in the conduction sea, causing an effective "screening" of the local moment [1].

In the meantime, local-moment metals tend to develop antiferromagnetic order at low temperatures [1]. A magnetic moment induces a cloud of Friedel oscillations in the spin density of a metal, which with coupling to a second local moment at a sufficiently close distance, shifts the energy by a small amount $J\vec{S}(\boldsymbol{x}) \cdot \left\langle \vec{M}(\boldsymbol{x}) \right\rangle$. This energy, comparable to the exchange coupling term in the Ising model, gives rise to an interaction that is a long-range magnetic interaction called the *RKKY Interaction* [1, 6].

In this project, the goal is to investigate the crossover regime between the RKKY and Kondo interaction between the f-electrons localised on impurities and the conduction electrons in the d- or p- bands of the metal. Here we aim to investigate the regime by using a mean-field technique. This analysis can be compared with the Wilson's renormalisation group analysis undergoing in UCL in conjunction with this project. The benefits of using a mean-field theory is that in addition to the mathematical simplification, it also allows the analysis of a Kondo lattice with multiple impurities, as opposed to a single impurity site in the renormalisation group treatment.

A quick analogy of the system under our analysis goes as follows: Imagine two adults with their kids in a park. The adults tend to talk to each other (RKKY) and also talk to their kids (RKKY) but the effectiveness of this

communication is "shielded" by the presence of the children annoying the adults (Kondo screening). The challenge of the project lies in the fact that the adults, instead of only having two types (spin up and down), can exist in infinite types (within the $N \to \infty$ limit). The different basis used in the Kondo effect (normally analysed in the momentum basis) and the RKKY effect (normally in the real basis) is also a centre challenge to our analysis. We will however, in this project, restrict our analysis to a small flat linear band around the Fermi energy and therefore convert the problem into the momentum basis.

2 RKKY Interaction

We start with analysing the existing RKKY interaction Hamiltonian. The aim of this section is to provide a simple treatment using the SU(N) representation of spins to analyse the RKKY interaction within the mean field approximation and hence derive an expression for the susceptibility of the system.

We start with the following Hamiltonian in the SU(N) representation:

$$H = \sum_{k\alpha} \epsilon_k c^\dagger_{k\alpha} c_{k\alpha} + J \sum_i S^z_i \cdot s^z_i \tag{1}$$

where the spin operators take the following form:

$$S^z_i = \sum_\alpha \alpha f^\dagger_\alpha f_\alpha \tag{2}$$

$$s^z_i = \sum_\alpha \alpha c^\dagger_\alpha c_\alpha \tag{3}$$

Under the mean field approximation, we can have:

$$J \sum_i S^z_i \cdot s^i_z = -\sum_i J \langle S^z_i \rangle \langle s^z_i \rangle + \sum_i J S^z_i \langle s^z_i \rangle + \sum_i s^z_i \langle S^z_i \rangle \tag{4}$$

Using Fourier transform, let us write $c_i = \frac{1}{\sqrt{N}} \sum_q c_q e^{iq\cdot x}$ and consider the perturbation part of the Hamiltonian (for conduction electrons) to be:

$$V = J \sum_i s^z_i \langle S^z_i \rangle = J \sum_{i\alpha} \langle S^z_i \rangle c^\dagger_{i\alpha} c_{i\alpha} \tag{5}$$

Therefore we have

$$\begin{aligned} s_k^z &= \frac{1}{\sqrt{N_s}} \sum_r e^{-ik\cdot r_i} s_i^z \\ &= \frac{1}{\sqrt{N_s}} \sum_{i\alpha} e^{-ik\cdot r_i} \alpha c_{i\alpha}^\dagger c_{i\alpha} \\ &= \frac{1}{\sqrt{N_s}} \sum_{r_i} e^{-ik\cdot r_i} \alpha \frac{1}{N_s} c_q^\dagger c_{q'} e^{-iqx} e^{iq'x} \\ &= \frac{1}{\sqrt{N_s}} \sum_{\alpha q q'} \alpha e^{-i(k+q-q')} c_q^\dagger c_{q'} \frac{1}{N_s} \\ &= \frac{1}{\sqrt{N_s}} \sum_{\alpha q} \alpha c_{\alpha,q}^\dagger c_{\alpha,k+q} \end{aligned} \tag{6}$$

Therefore to find the susceptibility, we find the expected value of s_k^z:

$$\langle s_k^z \rangle = \sum_{k\alpha} n(\epsilon_{k\alpha}) \langle k'\sigma | s_k^z | k'\sigma \rangle \tag{7}$$

where $|k'\sigma\rangle$ is the perturbed eigenstate. We can find this by using first-order perturbation theory:

$$|k'\sigma\rangle = |k\sigma\rangle + \sum_{q\neq k} \frac{\langle q | \hat{V} | k \rangle}{\epsilon_k - \epsilon_q} |q\sigma\rangle \tag{8}$$

so using $V = J\sum_k s_k^z \left\langle S_{-k}^z \right\rangle$ (from Fourier transform), the matrix element becomes:

$$\langle q | \hat{V} | k \rangle = \langle q | J \sum_p s_p^z \left\langle S_{-p}^z \right\rangle | k \rangle \tag{9}$$

For fixed p, we can write:

$$\begin{aligned} \langle q | \hat{V} | k \rangle &\to \langle q | J \left\langle S_{-p}^z \right\rangle \frac{1}{\sqrt{N_s}} \sum_\alpha \alpha c_t^\dagger c_{p+t} | k \rangle \\ &= \sum_\alpha J \left\langle S_{-p}^z \right\rangle \frac{1}{\sqrt{N_s}} \alpha \langle q | c_t^\dagger c_{p+t} | k \rangle \end{aligned} \tag{10}$$

We therefore need $k = p + t$ and $t = -q$, so this gives a factor $\delta_{k,p+q}$, giving

$$\langle q | \hat{V} | k \rangle = \sum_\alpha J\alpha \left\langle S_{-p}^z \right\rangle \frac{1}{\sqrt{N_s}} \delta_{k,p+q} \tag{11}$$

giving

$$|k'\sigma\rangle = |k\sigma\rangle + \sum_{q\neq k} \frac{1}{\sqrt{N_s}} \alpha J \left\langle S^z_{-p} \right\rangle \frac{\delta_{k,p+q}}{\epsilon_k - \epsilon_q} |q\sigma\rangle \tag{12}$$
$$= |k\sigma\rangle + \frac{1}{\sqrt{N_s}} \alpha J \left\langle S^z_{-p} \right\rangle \frac{1}{\epsilon_k - \epsilon_{k-p}} |k-p,\sigma\rangle$$

Therefore the expected value of s^z_t is

$$\langle s^z_t \rangle = \frac{1}{N_s} \sum_k n(\epsilon_{k\sigma}) \langle k\sigma| \sum_\gamma \gamma^2 c^\dagger_{\delta\gamma} c_{s+t,\gamma} |k-p,\sigma\rangle \frac{J \left\langle S^z_{-p} \right\rangle}{\epsilon_k - \epsilon_p} \tag{13}$$
$$+ \frac{1}{N_s} \sum_k n(\epsilon_{k\sigma}) \langle k-p,\sigma| \sum_\gamma \gamma^2 c^\dagger_{\delta\gamma} c_{s+t,\gamma} |k,\sigma\rangle \frac{J \left\langle S^z_{-p} \right\rangle}{\epsilon_k - \epsilon_p}$$

γ now being the spin projections. In the first term we set $k = s$ and $s + t = k - p$; whilst in the second term we set $k = s + t$ and $k - p = s$. This leads to $t = -p$ and $t = p$ in the two cases respectively. We therefore have

$$\langle s^z_t \rangle = \frac{J}{N_s} \sum_\gamma \gamma^2 \sum_k \frac{1}{\epsilon_k - \epsilon_{k+t}} \left[n(\epsilon_k) \langle S^z_t \rangle - n(\epsilon_{k+t}) \left\langle S^z_{-t} \right\rangle \right] \tag{14}$$

and hence from $\langle s^z_t \rangle = J\chi(t) \langle S^z_t \rangle$, if we assume that $\langle S^z_t \rangle = \left\langle S^z_{-t} \right\rangle$, then we can identify the susceptibility:

$$\chi(t) = \frac{1}{N_s} \sum_{\gamma,k} \gamma^2 \frac{n(\epsilon_k) - n(\epsilon_{k+t})}{\epsilon_k - \epsilon_{k+t}} \tag{15}$$

3 Kondo Interaction

This follows the development in Coleman [1] §17.3-6. Here we make a quick summary of the analysis given.

3.1 The Read-Newns Path Integral

We begin with the Hamiltonian of the Read-Newns model for the Kondo lattice

$$H = \sum_{k\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} - \frac{J}{N} \sum_{j\alpha\beta} : \left(c^\dagger_{j\beta} f_{j\beta}\right) \left(f^\dagger_{j\beta} c_{j\alpha}\right) : \tag{16}$$

We want to carry out a Hubbard-Stratonovich transformation on the interaction

$$-\frac{J}{N} \sum_{\alpha\beta} \left(c^\dagger_{j\beta} f_{j\beta}\right) \left(f^\dagger_{j\beta} c_{j\alpha}\right) \to \sum_{\alpha} \left[\bar{V}_j \left(c^\dagger_{j\alpha} f_{j\alpha}\right) + \left(f^\dagger_{j\alpha} c_{j\alpha}\right) V_j\right] + N \frac{\bar{V}_j V_j}{J} \tag{17}$$

Let us consider the other way around, where we first construct RHS and show that it is equivalent to the expression on the LHS. We write the required the Lagrangian as

$$\begin{aligned} L\left[\psi^\dagger, \psi, \lambda\right] = &\sum_{k\sigma} c^\dagger_{k\sigma} \left(\partial_\tau + \epsilon_k\right) c_{k\sigma} + \sum_{j\sigma} f^\dagger_{j\sigma} \left(\partial_\tau + \lambda_j\right) f_{j\sigma} \\ &- \frac{J}{N} \sum_{j\alpha\beta} \left(c^\dagger_{j\beta} f_{j\beta}\right) \left(f^\dagger_{j\beta} c_{j\alpha}\right) - \sum_j \lambda_j Q \end{aligned} \tag{18}$$

For now we start on the right of the transformation and ignore the constraint $\sum_j \lambda_j Q$. Then we have

$$S'\left[c^\dagger, c, V\right] = \sum_j \left[\bar{V}_j c^\dagger_{j\alpha} f_{j\alpha} + f^\dagger_{j\alpha} c_{j\alpha} V_j + N \frac{\bar{V}_j V_j}{J}\right] \tag{19}$$

This gives

$$\mathcal{Z} = \int \mathcal{D}\left[V(\tau), \bar{V}(\tau)\right] \int \mathcal{D}\left[c(\tau), c^\dagger(\tau), f(\tau), f^\dagger(\tau)\right] e^{-S'} \tag{20}$$

where the integrals over $V(\tau)$ are over the complex plane:

$$\mathcal{D} f(\tau) := \lim_{\epsilon \to 0} \int_{-\infty}^{\infty} d\,\mathrm{Re}\, V(\tau) \int_{-\infty}^{\infty} d\,\mathrm{Im}\, V(\tau) \tag{21}$$

But the Grassman integrals are different. The definitions are similar:

$$\int \mathcal{D}f(\tau) := \lim_{\epsilon \to 0} \prod_{\tau} \int df_{\tau} \tag{22}$$

but since Grassman algebra is a type of exterior algebra - the complex conjugate is not well defined:

$$(\bar{c^{\dagger}}) = c \tag{23}$$

To illustrate this point, let us consider a general transformation in the complex plane. Our integral forms a contour along the real axis in complex plane, and we can translate the contour by any complex displacement since the integrand is analytic everywhere (Gaussian, no poles). Consider

$$z = x + iy \tag{24}$$

and effect the following transformation

$$\begin{cases} x' = x + u \\ y' = y + v \end{cases} \tag{25}$$

This gives

$$\begin{cases} z = (x' + u) + i\,(y' - v) \\ \bar{z} = x - iy = (x' - u) - i\,(y' - v) \end{cases} \tag{26}$$

Therefore, we now have:

$$\begin{cases} z = x' + iy' - u - iv = z' - (u + iv) \\ \bar{z} = x' = iy' = u + iv = \bar{z}' - (u - iv) \end{cases} \tag{27}$$

We note that $(\bar{z}') \neq (\bar{z'})$ - they are no longer complex conjugates of each other since $x', y' \in \mathbb{C}$. The two variables however cancel out such that $(\bar{z}) = \bar{z}$ overall. Therefore in this problem, V and $\bar{V}$ act as two independent variables (two $\mathbb{C}$ shifts) so can be effected by two independent shifts in the complex plane.

Let us therefore consider the map:

$$\begin{cases} \bar{V}_j \mapsto \bar{V}_j - \frac{J}{N} f^{\dagger}_{j\alpha} c_{j\alpha} \\ V_j \mapsto V_j - \frac{J}{N} c^{\dagger}_{j\beta} f_{j\beta} \end{cases} \tag{28}$$

Effecting on the action, this gives (with implicit sums following ESC[1] for Greek indices and sum over j, the site number, also implicit.)

$$\begin{aligned} S' &= \left(\bar{V}_j - \frac{J}{N} f^\dagger_{j\alpha} c_{j\alpha}\right) c^\dagger_{j\beta} f_{j\beta} + f^\dagger_{j\alpha} c_{j\alpha} \left(V_j - \frac{J}{N} c^\dagger_{j\beta} f_{j\beta}\right) \\ &+ \frac{N}{J}\left(\bar{V}_j - \frac{J}{N} f^\dagger_{j\alpha} c_{j\alpha}\right)\left(V_j - \frac{J}{N} c^\dagger_{j\beta} f_{j\beta}\right) \\ &= -\frac{J}{N} f^\dagger_{j\alpha} c_{j\alpha} c^\dagger_{j\beta} f_{j\beta} \end{aligned} \tag{29}$$

The transformation is an effective "completing the square". We can now write the partition function as

$$\mathcal{Z} = \int \mathcal{D}\left[c, c^\dagger, f, f^\dagger\right] e^{\frac{J}{N}\cdots} \int \mathcal{D}\left[V, \bar{V}\right] e^{-\frac{N}{J}\bar{V}_j V_j} \tag{30}$$

We note that the second integral in Equation 30 is a constant. the reason why the integral over $V, \bar{V}$ is constant in $f, f^\dagger, c, c^\dagger$ is because itself depends on the transformation and hence on $f, f^\dagger, c, c^\dagger$, but the contour can be shifted by Cauchy's Theorem such that it returns to be evaluated along the real axis. i.e. The contour path is independent of the choice of $f, f^\dagger, c, c^\dagger$.

If we look at this integral, we note that exponent is $\sim \frac{N}{J}\bar{V}V$, so the fluctuations in the fields δV scales like $\sim \frac{1}{\sqrt{N}}$.

Let us put in the constraint

$$\prod \delta_{n_j, Q} = \delta_{q, N_s} \tag{31}$$

where $n_j = Q$ is the decided value on the conserved charge, $q = \frac{Q}{N}$ is the f-filling factor and N_s is the total number of sites. We note here that the fermionic operators have ∂_τ terms[2]. This implies that $V, \bar{V}$ are classical fields.

We note also that the whole action scales like N.

$$\mathcal{Z} = \int \mathcal{D}\left[c, c^\dagger, f, f^\dagger\right] e^{-S} \tag{32}$$

where $S \sim \mathcal{O}(N)$. We want the variation in the action to be $\mathcal{O}(1)$.

$$|V_j| \mapsto |V_j| + \delta V_j(\tau) \tag{33}$$

[1]Einstein summation convention.

[2]This is because they have non-zero commutators whereas for the fields $V, \bar{V}$, we have $\left[V, \bar{V}\right] = 0$.

where $\delta V_j(\tau) \sim \mathcal{O}(\frac{1}{\sqrt{N}})$. The condition we have is to restrict the overall charge of the system. In the large N limit, we can write the condition by doing the following approximation

$$\prod_j \delta_{n_j,Q} \approx \delta_{\sum n_j,Q} \approx \delta_{N_s,Q} \tag{34}$$

We note that we can write $V_j \to V$ and $\bar{V}_j \to \bar{V}$ since we have Lorentz invariance and the mean field approximation. The action is therefore

$$S = |\bar{V}| c_j^\dagger f_j + f_j^\dagger c_j |V| \tag{35}$$

We know that constraint can be introduced through a Lagrange multiplier field:

$$S = S_0 - \lambda_j Q = S_0' + \sum_j \lambda_j \left(n_{jj} - Q\right) \tag{36}$$

Hence we know that $\delta\lambda \sim \mathcal{O}\left(\frac{1}{\sqrt{N}}\right)$, so we can go back and put λ and V to be constant at around the stationary point. $\lambda(\tau, j)$ is a dynamical field. We can make a set of gauge transformations known as the Read-Newns gauge transformation.

$$\begin{cases} f_{j\sigma} \mapsto e^{i\phi_j} f_{j\sigma} \\ V_j \to e^{i\phi_j} |V_j| \\ \lambda_j \mapsto \lambda_j - i\dot{\phi}_j \end{cases} \tag{37}$$

Note that for the scalar fields V and $\bar{V}$ we are simply redefining the field (i.e. rewriting the field). Then we have

$$S_K = \int_0^\beta d\tau \left[f_{j\alpha}^\dagger \left(\partial_\tau + \lambda_j\right) f_{j\alpha} + \left(|V_j| e^{-i\phi_j} c_{j\alpha}^\dagger f_{j\alpha} + |\bar{V}_j| e^{i\phi_j} f_{j\alpha}^\dagger c_{j\alpha} \right) + N \frac{|V_j|^2}{J_K} - \lambda_j Q \right] \tag{38}$$

$$\mapsto \int_0^\beta d\tau \left[f_{j\alpha}^\dagger \left(\partial_\tau + \lambda_j + i\dot{\phi}_j\right) f_{j\alpha} + |V_j| \left(c_{j\alpha}^\dagger f_{j\alpha} + f_{j\alpha}^\dagger c_{j\alpha} \right) + N \frac{|V_j|^2}{J_K} - \lambda_j Q \right] \tag{39}$$

where we have effected the f_j transformation. Now write $\lambda_j(\tau) = \lambda_j + i\dot{\phi}_j$, giving

$$S_K(j) = \int_0^\beta d\tau \left[f_{j\alpha}^\dagger \left(\partial_\tau + \lambda_j(\tau)\right) f_{j\alpha} + |V_j| \left(c_{j\alpha}^\dagger f_{j\alpha} + f_{j\alpha}^\dagger c_{j\alpha} \right) + N \frac{|V_j|^2}{J_K} - \lambda_j Q \right] \tag{40}$$

$$+ iQ \int_0^\beta d\tau \dot{\phi}_j$$

Notice we can write the last term in the following way:

$$iQ\int_0^\beta d\tau\dot{\phi}_j = iQ\Delta\phi_j = i2\pi Qn \tag{41}$$

However $e^{i2\pi Q} = 1$ in the overall phase since $Q \in \mathbb{N}$. Therefore, we can ignore this term.

3.2 Effective Hamiltonian

We can now write the effective Hamiltonian in a quadratic form. Proceed to write the mean field Hamiltonian in the following form:

$$H_{MFT} = \sum_{k\alpha} \begin{pmatrix} c^\dagger_{k\alpha} & f^\dagger_{k\alpha} \end{pmatrix} \begin{pmatrix} \epsilon_k & V \\ V & \lambda \end{pmatrix} \begin{pmatrix} c_{k\alpha} \\ f_{k\alpha} \end{pmatrix} + N\mathcal{N}_s \left(\frac{|V|^2}{J} - \lambda q \right) \tag{42}$$

or simply,

$$\sum_{k\alpha} \psi^\dagger_{k\alpha} \underline{\underline{h}}(k) \psi_{k\alpha} + N\mathcal{N}_s \left(\frac{|V|^2}{J} - \lambda q \right) \tag{43}$$

where

$$\psi_{k\alpha} = \begin{pmatrix} c_{k\alpha} \\ f_{k\alpha} \end{pmatrix} \tag{44}$$

$$\underline{\underline{h}}(k) = \begin{pmatrix} \epsilon_k & V \\ V & \lambda \end{pmatrix} \tag{45}$$

Here we have also assumed for simplicity the case $V = \bar{V}$. We diagonalise the system by writing it in the following form:

$$H_{MFT} = \begin{pmatrix} a^\dagger_{k\alpha} & b^\dagger_{k\alpha} \end{pmatrix} \begin{pmatrix} E_{k^+} & 0 \\ 0 & E_{k^-} \end{pmatrix} \begin{pmatrix} a_{k\alpha} \\ b_{k\alpha} \end{pmatrix} + N\mathcal{N}_s \left(\frac{|V|^2}{J} - \lambda q \right) \tag{46}$$

The eigenvalues are

$$E_k = \frac{\epsilon_k + \lambda_k}{2} \pm \sqrt{\left(\frac{\epsilon_k - \lambda_k}{2} \right)^2 + |V|^2} \tag{47}$$

Eigenvectors are obtained as follows:

$$\begin{cases} (\epsilon_k - E_k)\, u_k + V v_k = 0 \\ V u_k + (\lambda - E_k)\, v_k = 0 \end{cases} \tag{48}$$

$$\implies u_k^2 \,(E_k - \epsilon_k) = v_k^2 \,(E_k - \lambda_k) \tag{49}$$

Normalisation requires $u_k^2 + v_k^2 = 1$. Therefore substituting and a bit algebra later, we obtain

$$u_k^2 = \frac{1}{2} \pm \frac{(\epsilon_k + \lambda_k)/2}{2\sqrt{\left(\frac{\epsilon_k - \lambda_k}{2}\right)^2 + |V|^2}} \tag{50}$$

Hence the eigenvectors are

$$\begin{pmatrix} u_k \\ v_k \end{pmatrix} = \left[\frac{1}{2} \pm \frac{(\epsilon_k + \lambda_k)/2}{2\sqrt{\left(\frac{\epsilon_k - \lambda_k}{2}\right)^2 + |V|^2}} \right]^{\frac{1}{2}} \tag{51}$$

which is indeed in BCS form.

Now we can use the free energy expansion to obtain a relationship between V and T. We first develop an effective action for the large N-expansion. We start with the Read-Newns path integral (with no gauge fixing)

$$e^{-N\mathcal{S}\left[\bar{V},V,\lambda\right]} \equiv \mathcal{Z}_E\left[\bar{V},V,\lambda\right] = \int \mathcal{D}\left[\psi^\dagger,\psi\right] e^{-\mathcal{S}\left[\bar{V},V,\lambda,\psi^\dagger,\psi\right]} \tag{52}$$

So we have defined $\mathcal{Z}_E = e^{-N\mathcal{S}_E}$. Now,

$$\mathcal{S} = \int_0^\beta d\tau \left[\sum_k c_{k\alpha}^\dagger \left(\partial_\tau + \epsilon_k\right) + \sum_j \left(f_{j\alpha}^\dagger \left(\partial_\tau + \lambda_j\right) f_{j\alpha} + \bar{V}_j c_{j\alpha}^\dagger f_{j\alpha} + V_j f_{j\alpha}^\dagger c_{j\alpha} + N\frac{|V_j|^2}{J} - \lambda_j Q \right) \right] \tag{53}$$

At large N the integration is dominated by its stationary points (i.e. the saddle point approximation):

$$\mathcal{Z} = \int \mathcal{D}\left[\bar{V},V,\lambda\right] e^{-N\mathcal{S}_E\left[\bar{V},V,\lambda\right]} \approx \exp\left\{\left(-N\mathcal{S}_E\left[\bar{V},V,\lambda\right]\right)\right\} \tag{54}$$

Identify $N\mathcal{S}_E = \log \mathcal{Z}_E \implies N\delta\mathcal{S}_E = \frac{\delta\mathcal{Z}_E}{\mathcal{Z}_E}$. The saddle-point conditions impose the following self-consistent relations:

$$\begin{cases} \frac{\delta N\mathcal{S}_E}{\delta \bar{V}_j(\tau)} = \frac{1}{\mathcal{Z}_E}\int \mathcal{D}\left[\psi^\dagger,\psi\right]\left(c_{j\alpha}^\dagger f_{j\alpha}\frac{NV_j}{J}\right)e^{-\mathcal{S}} = \left\langle c_{j\alpha}^\dagger f_{j\alpha}\right\rangle(\tau) + \frac{N}{J}V_j(\tau) = 0 \\ \frac{\delta N\mathcal{S}_E}{\delta \lambda_j(\tau)}\frac{1}{\mathcal{Z}}\int \mathcal{D}\left[\psi^\dagger,\psi\right](n_f(j,\tau) - Q)e^{-\mathcal{S}} = \langle n_f(j,\tau) - Q\rangle = 0 \end{cases} \tag{55}$$

The first relation is the mean field self-consistency associated with the Hubbard-Stratonovich transformation. We use the radial gauge to absorb the phase of the hybridisation such that $\bar{V}_j(\tau) = V_j(\tau) = |V_j|, \lambda_j(\tau) = \lambda_j$. Then the saddle-point partition function $\mathcal{Z}_E\left[V,\lambda\right]$ is simply the partition function of

the static MF Hamiltonian $H_{MF} = H[V, \lambda]$, $\mathcal{S}_E = \mathrm{Tr}\, e^{-\beta H_{MF}}$. Write the action in the following form:

$$\mathcal{S} = \int_0^\beta d\tau \left[\sum_\alpha \psi_\alpha^\dagger \left(\partial_\tau + \underline{\underline{h}} \right) \psi_\alpha + \sum_j \left(N \frac{V_j^2}{J} - \lambda_j Q \right) \right] \tag{56}$$

Now do the Fermi integral.

$$I_F = \int \mathcal{D}\left[\psi^\dagger, \psi\right] \exp\left\{ \left[- \int_0^\beta d\tau \sum_\alpha \psi_\alpha^\dagger \left(\partial_\tau + \underline{\underline{h}} \right) \psi_\alpha \right] \right\} \tag{57}$$

$$\begin{aligned} I_F &= \left(\det\left\{ \left[\partial_\tau + \underline{\underline{h}} \right] \right\} \right)^N \\ &= \exp\left\{ \left[N \log \det\left\{ \left[\partial_\tau + \underline{\underline{h}} \right] \right\} \right] \right\} \\ &= \exp\left\{ \left[\mathrm{tr} \log \left[\partial_\tau + \underline{\underline{h}} \right] \right] \right\} \end{aligned} \tag{58}$$

Then we have

$$N\mathcal{S}_E[V, \lambda] = N \left[- \mathrm{tr} \log \left(\partial_\tau + \underline{\underline{h}} \right) + \sum_j \int_0^\beta d\tau \left(\frac{|V_j|^2}{J} - \lambda_j q \right) \right] \tag{59}$$

Now since $\mathcal{Z}_E = e^{-\beta F_{MF}} = e^{-N\mathcal{S}_E}$ where F_{MF} is the mean field free energy, it follows that

$$F_{MF}[V, \lambda] = \frac{1}{\beta} \mathcal{S}[V, \lambda] = - \frac{N}{\beta} \mathrm{tr} \log \left(\partial_\tau + \underline{\underline{h}}[V, \lambda] \right) + \sum_j \left(\frac{N|V_j|^2}{J} - \lambda_j Q \right) \tag{60}$$

So replacing $\partial_\tau \to -i\omega_n$, the Mastsubara frequencies:

$$F_{MF} = -NT \sum_{i\omega_n} \mathrm{tr} \log \left[\mathcal{G}^{-1}(i\omega_n) \right] + \sum_j \left(\frac{N|V_j|^2}{J} - \lambda_j Q \right) \tag{61}$$

and

$$\mathcal{G}^{-1} = \left(i\omega_n - \underline{\underline{h}}[V, \lambda] \right) \tag{62}$$

Diagonalise the Hamiltonian such that $\underline{\underline{h}} \to E_\zeta \delta_{\zeta,\zeta'}$, then $\mathrm{tr} \log \left[-i\omega_n + \underline{\underline{h}} \right] = \sum_\zeta \log\left(E_\zeta - i\omega_n \right)$. We should also do the Matsubara sum, where:

$$-T \sum_{i\omega_n} \log\left(-i\omega_n + E_\zeta \right) \to -T \log\left(1 + e^{-\beta E_\zeta} \right) \tag{63}$$

We can therefore write the free energy as:

$$F_E[V, \lambda] = -NT \sum_\zeta \log\left(1 + e^{-\beta E_\zeta} \right) + \sum_j \left(\frac{N|V_j|^2}{J} - \lambda_j Q \right) \tag{64}$$

4 A combined model

In this section we try and develop a simplified model that takes into account both the effects of Kondo screening and the RKKY interaction. We take the following assumptions:

1. The spin can be treated in the $SU(N)$ representation.
2. The system can be treated within the mean field approximation, with a small perturbation from the mean field homogeneous solution.
3. There exists a possible Hubbard-Stratonovich transformation that decouples the fields in the Kondo channel.
4. We only first consider one impurity in the system.

We begin the analysis with the Kondo Hamiltonian,

$$H_K = -\frac{J}{N}\sum_{\alpha\gamma}(c^\dagger_\alpha f_\alpha f^\dagger_\gamma c_\gamma) \tag{65}$$

Here J is the coupling constant for the Kondo interaction, N is the number of spin projections, i.e. $N = 2s + 1$ where s is the maximal spin projection of the electron. $c^{(\dagger)}$ and $f^{(\dagger)}$ represent the lowering (raising) operators of the conduction and f-impurity electrons in the system.

We look for an SU(N) representation for the Ising (Heisenberg) Hamiltonian. We postulate that it takes the form:

$$H_I = -\frac{j_z}{N}\sum_\alpha \alpha c^\dagger_\alpha c_\alpha \sum_\gamma \gamma f^\dagger_\gamma f_\gamma \tag{66}$$

To check this, we note that

$$\hat{s}_j = c^\dagger_{j\alpha}\vec{\sigma}_{\alpha\gamma}c_{j\gamma} \tag{67}$$

where Einstein summation convention is assumed on the greek indices and $\vec{\sigma}$ are the Pauli matrices in SU(2). The natural generalisation for the SU(N) algebra is therefore:

$$s_j = \sum_\alpha \alpha c^\dagger_{j\alpha}c_{j\alpha} \tag{68}$$

for each site j.

The Hamiltonian is our analysis is the Kondo Hamiltonian. We write it in the following form:

$$H_K = H_I + (H_K - H_I) \tag{69}$$

where we decouple the first term H_I in the RKKY channel but the second term $H_K - H_I$ in the Kondo channel. It is the second term that is central to the whole analysis of the problem.

4.1 Hubbard-Stratonovich Transformation

We consider the second term in Equation 69 in the Kondo channel - i.e. we carry out a Hubbard-Stratonovich transformation on the Hamiltonians by introducing new scalar fields $V_{\alpha\gamma}$ now dependent on the spin. As before, our goal is to obtain something in the following form (with indices on the V fields suppressed):

$$\mapsto \bar{V} c_\alpha^\dagger f_\alpha + (f_\beta^\dagger c_\beta) V + N \frac{V\bar{V}}{J} \tag{70}$$

In general, we can consider the transformation of the form:

$$-A c_\alpha^\dagger f_\beta g^{-1}_{(\alpha\beta)(\gamma\delta)} f_\gamma^\dagger c_\delta \mapsto g_{(\alpha\beta)(\gamma\delta)} \bar{V}_{(\alpha\beta)} V_{(\gamma\delta)} + \bar{V}_{(\alpha\beta)} c_\alpha^\dagger f_\beta + V_{(\alpha\beta)} f_\beta^\dagger c_\alpha \tag{71}$$

where A is an appropriate normalising factor. Let us change the notation to make this a bit easier. The term we want to end up with is in the following form:

$$\bar{V}_i g_{ij} V_j + \bar{V}_i \omega_i + x_j V_j \tag{72}$$

where ω_i is the vector with $c_\alpha^\dagger f_\beta$ as its components and x_i is the vector with $f_\beta^\dagger c_\alpha$ as its components. Let us consider the Hubbard-Stratonovich transformation of the following form:

$$V_i \mapsto -g_{ij}^{-1} \omega_j + V_i \tag{73}$$

$$\bar{V}_j \mapsto -x_i g_{ij}^{-1} + \bar{V}_j \tag{74}$$

Therefore, we can map

$$\begin{aligned} \bar{V}_i g_{ij} V_j + \bar{V}_i \omega_i + x_j V_j \mapsto{}& \bar{V}_i g_{ij} V_j + \left(-x_k g_{ki}^{-1}\right) g_{ij} V_j + \bar{V}_i g_{ij} \left(-g_{jk}^{-1} \omega_k\right) \\ &+ x_k g_{ki}^{-1} g_{ij} g_{jl}^{-1} \omega_l - x_l g_{li}^{-1} \omega_i + \bar{V}_i \omega_i - x_i g_{ij}^{-1} \omega_i + x_i V_i \\ ={}& \bar{V}_i g_{ij} V_j + x_k \delta_{kj} g_{jl}^{-1} \omega_l - 2 x_i g_{ij}^{-1} \omega_j \\ ={}& \bar{V}_i g_{ij} V_j - x_k g_{ij}^{-1} \omega_j \end{aligned} \tag{75}$$

The last line being the term we start with in the Hamiltonian to be decoupled in the Kondo channel plus a term involving the interacting Hubbard-Stratonovich fields.

The form of g_{ij} is difficult to obtain in general. We analyse the form of this metric in the simplest non-trivial case, that being the $N = 3$, or spin 1 case. Here, if we take the latin indices to have the following correspondence with the Greek indices:

i	(α, β)
1	(1,1)
2	(1,0)
3	(1,-1)
4	(0,1)
5	(0,0)
6	(0,-1)
7	(-1,1)
8	(-1,0)
9	(-1,-1)

Figure 1: A table showing the correspondence between latin and greek indices in g_{ij} or $g_{(\alpha\beta)(\gamma\delta)}$ for the spin 1 case.

We recall that the Hamiltonian we want to decouple is of the following form:

$$H = H_K - H_I = -\frac{J}{N}\sum_{\alpha\beta} : \left(c^\dagger_\alpha f_\alpha f^\dagger_\beta c_\beta\right) : + \frac{j_z}{N}\sum_{\alpha\beta}\left(\alpha\beta c^\dagger_\alpha c_\alpha f^\dagger_\beta f_\beta\right) \tag{76}$$

Therefore we can use this to find that the corresponding g^{-1}_{ij} is of the following form (subject to the constraint that the spin projections are conserved during hopping between the conduction band and the impurity site) :

$$[g^{-1}]_{ij} = -\frac{1}{N}\begin{pmatrix} -J+j_z & 0 & 0 & 0 & -J & 0 & 0 & 0 & -J \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -j_z & 0 & 0 & 0 & 0 & 0 & \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -J & 0 & 0 & 0 & -J & 0 & 0 & 0 & -J \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -j_z & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -J & 0 & 0 & 0 & -J & 0 & 0 & 0 & -J+j_z \end{pmatrix} \tag{77}$$

This matrix can be indeed written in block diagonal form, with only one 3×3 matrix with a nontrivial inversion:

$$\begin{pmatrix} -J+j_z & -J & -J \\ -J & -J & -J \\ -J & -J & -J+j_z \end{pmatrix}^{-1} = \begin{pmatrix} \frac{1}{j_z} & -\frac{1}{j_z} & 0 \\ -\frac{1}{j_z} & -\frac{2J+j_z}{Jj_z} & -\frac{1}{j_z} \\ 0 & -\frac{1}{j_z} & \frac{1}{j_z} \end{pmatrix} \tag{78}$$

Hence the metric takes the form:

$$[g]_{ij} = -N \begin{pmatrix} \frac{1}{j_z} & 0 & 0 & 0 & -\frac{1}{j_z} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{j_z} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{1}{j_z} & 0 & 0 & 0 & -\frac{2J+j_z}{Jj_z} & 0 & 0 & 0 & -\frac{1}{j_z} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{1}{j_z} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{1}{j_z} & 0 & 0 & 0 & \frac{1}{j_z} \end{pmatrix} \tag{79}$$

4.2 RKKY Mean Field Decoupling

Now we consider the decoupling in the RKKY channel. We start with the Ising Hamiltonian:

$$H_I = -\frac{j_z}{N} \sum_{\alpha} \alpha c_{\alpha}^{\dagger} c_{\alpha} \sum_{\gamma} \gamma f_{\gamma}^{\dagger} f_{\gamma} \tag{66}$$

which can be written as:

$$H_I = -\frac{j_z}{N} \left(\hat{S}_z \cdot \hat{s}_z \right) \tag{80}$$

where $\hat{S}_z$ and $\hat{s}_z$ are the spin projection operators for the f- and c- electrons respectively. We use the Mean-Field approach:

$$S_z \mapsto \langle S_z \rangle + (S_z - \langle S_z \rangle) \tag{81}$$

$$s_z \mapsto \langle s_z \rangle + (s_z - \langle s_z \rangle) \tag{82}$$

Therefore the Hamiltonian becomes:

$$H_I = -\frac{j_z}{N} \left(S_z - \langle S_z \rangle \right) \left(s_z - \langle s_z \rangle \right) \tag{83}$$

$$= -\frac{j_z}{N} \left(S_z \langle s_z \rangle + \langle S_z \rangle s_z - \langle S_z \rangle \langle s_z \rangle + \mathcal{O}\big(\delta S_z^2\big) \right) \tag{84}$$

We note here that the constant term gives a non-convergent Gaussian integral in the analysis when the two fields are antiferromagnetic (i.e. of opposite signs) but for a sufficiently local search of saddle points we for now assume that this should not affect our approach.

4.3 The full Hamiltonian and method of analysis

The full Hamiltonian now becomes the following after the decoupling in the two separate channels.

$$\begin{aligned} H_K = &-\frac{j_z}{N}\left[\langle s_z\rangle \sum_\gamma (\gamma f_\gamma^\dagger f_\gamma) + \langle S_z\rangle \sum_\alpha (\alpha f_\alpha^\dagger f_\alpha)\right] \\ &+ \sum_{\alpha\gamma} \bar{V}_{\alpha\gamma} c_\alpha^\dagger f_\gamma + \sum_{\alpha\gamma} V_{\alpha\gamma} c_\alpha f_\beta^\dagger \\ &+ \frac{j_z}{N}\langle S_z\rangle \langle s_z\rangle + \sum_{\alpha\gamma\delta\epsilon} \bar{V}_{\alpha\gamma} g_{(\alpha\gamma)(\delta\epsilon)} V_{\delta\epsilon} \end{aligned} \tag{85}$$

where the last line are constant terms. Similarly to §3 above, we can then add in the energy band structure of the conduction band electrons and a constraint for the f-impurity electrons as follows:

$$\Delta H = \sum_{\alpha k} \epsilon_k c_{\alpha k}^\dagger c_{\alpha k} - \lambda\left(\sum_\gamma f_\gamma^\dagger f_\gamma - 1\right) \tag{86}$$

where λ is a Lagrange multiplier field. The full Hamiltonian can therefore be written in the following form[3]:

$$\begin{aligned} H_f = &\sum_{\alpha\gamma} \begin{pmatrix} c_\alpha^\dagger & f_\beta^\dagger \end{pmatrix} \begin{pmatrix} \frac{1}{N}\left(-\frac{j_z}{N}\langle S_z\rangle \alpha + \epsilon_k\right) & \bar{V}_{\alpha\beta} \\ V_{\alpha\beta} & \frac{1}{N}\left(-\frac{j_z}{N}\langle s_z\rangle \beta - \lambda\right) \end{pmatrix} \begin{pmatrix} c_\alpha \\ f_\beta \end{pmatrix} \\ &+ \lambda + \frac{j_z}{N}\langle S_z\rangle \langle s_z\rangle + \sum_{\alpha\gamma\delta\epsilon} \bar{V}_{\alpha\gamma} g_{(\alpha\gamma)(\delta\epsilon)} V_{\delta\epsilon} \end{aligned} \tag{87}$$

[3]We have taken a small flat band around the Fermi surface and therefore have assumed that the operators c_k in the Fourier space are similar to that of the real space c. (Dubious assumption?)

5 The free energy problem

Now to continue the analysis we consider the free energy of the problem:

$$\Phi = -k_B T \log \Xi = -\frac{1}{\beta} \log \Xi \tag{88}$$

where Ξ is the grand partition function of the problem:

$$\Xi = \sum_{\{n_i\}} \exp^{-\beta H(\{n_i\})} \tag{89}$$

with $\{n_i\}$ being the possible combinations of number occupations.

5.1 RKKY model

In order to perform a comprehensive analysis of the problem, let us begin our analysis with the original RKKY model. The Hamiltonian is of the following form:

$$H_{\text{Ising}} = \frac{j_z}{N_0} \sum_j \left(\sum_\alpha \alpha f^\dagger_{\alpha j} f_{\alpha j} \right) \left(\sum_\beta \beta c^\dagger_{\beta j} c_{\beta j} \right) - \lambda \sum_{\alpha j} f^\dagger_{\alpha j} f_{\alpha j} + \sum_{\beta k} \epsilon_k c^\dagger_{\beta k} c_{\beta k} \tag{90}$$

Under the mean field approximation, our Hamiltonian becomes:

$$\begin{aligned} H_I^{MF} = &- \sum_j \frac{j_z}{N_0} \langle S^z \rangle \langle s^z \rangle + \frac{j_z}{N_0} \sum_j \langle s^z \rangle \left(\sum_\alpha f^\dagger_{\alpha j} f_{\alpha j} \right) \\ &+ \frac{j_z}{N_0} \sum_j \langle S^z \rangle \left(\sum_\gamma f^\dagger_{\gamma j} f_{\gamma j} \right) - \lambda \sum_{\alpha j} f^\dagger_{\alpha j} f_{\alpha j} + \sum_{\gamma k} c^\dagger_{\gamma k} c_{\gamma k} \end{aligned} \tag{91}$$

Let us impose the following assumptions:

1. Only 1 site for the impurity so the sum over j is trivial.
2. Consider for now a flat band, i.e. choose arbitrarily that ϵ_k is integrated over a small band $\int \rho d\epsilon_k$ where ρ is the density of states.
3. We for now assume that $c_k \simeq c_j$ in this small band limit from the Fermi surface.
4. For now say the number of spin degeneracy is N_0.

We can then construct the free energy of the system. The problem however now lies: which of the following free energy expressions are true? (One of them takes into the account that there is a maximum of 1 electron in each of the impurity and the conduction site, and the other allows both spin up and down states to be simultaneously occupied for the f- and c- electrons.) Listing them out for the spin-1/2 case:

$$\begin{aligned}\Phi_1 = &-\frac{j_z}{N_0}\langle s^z\rangle\langle S^z\rangle \\ &-\frac{1}{\beta}\log\left[1+\exp\left\{-\beta(\epsilon_k+\frac{j_z}{2N_0}\langle S^z\rangle)\right\}+\exp\left\{-\beta(\epsilon_k-\frac{j_z}{2N_0}\langle S^z\rangle)\right\}\right] \\ &-\frac{1}{\beta}\log\left[1+\exp\left\{\beta(\lambda+\frac{j_z}{2N_0}\langle s^z\rangle)\right\}+\exp\left\{\beta(\lambda-\frac{j_z}{2N_0}\langle s^z\rangle)\right\}\right]\end{aligned} \tag{92}$$

$$\begin{aligned}\Phi_2 = &-\frac{j_z}{N_0}\langle s^z\rangle\langle S^z\rangle-\frac{1}{\beta}\log\left[1+\exp\left\{-\beta(\epsilon_k+\frac{j_z}{2N_0}\langle S^z\rangle)\right\}\right] \\ &-\frac{1}{\beta}\log\left[1+\exp\left\{-\beta(\epsilon_k-\frac{j_z}{2N_0}\langle S^z\rangle)\right\}\right]-\frac{1}{\beta}\log\left[1+\exp\left\{\beta(\lambda+\frac{j_z}{2N_0}\langle s^z\rangle)\right\}\right] \\ &-\frac{1}{\beta}\log\left[1+\exp\left\{\beta(\lambda-\frac{j_z}{2N_0}\langle s^z\rangle)\right\}\right]\end{aligned} \tag{93}$$

The first free energy has 9 terms in total. The second one has 16 terms in total. In order to investigate this, I have used a simple Mathematica script to analyse this problem (in this specific case the programme is written for spin 1). The idea of the programme is as follows:

1. First differentiate the free energy expressions with respect to $\langle S^z\rangle$, $\langle s^z\rangle$ and λ. Set this to zero and obtain three simultaneous equations.

2. For the first two equations (the ones for $\langle S^z\rangle$ and $\langle s^z\rangle$), there is a linear term in each equation (given by the first term in the free energy expressions above). This is used to solve the equations iteratively as in the form:

$$\langle S^z\rangle \to f(\langle s^z\rangle, \langle S^z\rangle) \tag{94}$$

$$\langle s^z\rangle \to g(\langle s^z\rangle, \langle S^z\rangle) \tag{95}$$

where f and g are continuous functions ($\to$ means the two expressions are not equivalent, see below). The λ constraint equation is solved by finding a root in the equation in each iterative cycle.

3. In each cycle, the procedure is to calculate $\langle s^z \rangle$, $\langle S^z \rangle$ and λ in that order but within each step the set values will be updated by the most recently calculated one. The integration performed over the set of values ϵ_k is as follows. The free energy expression obtained from differentiating is rearranged and integrated:

$$\langle S^z \rangle = \int f(\langle s^z \rangle, \langle S^z \rangle) \rho d\epsilon_k \tag{96}$$

$$\langle s^z \rangle = \int g(\langle s^z \rangle, \langle S^z \rangle) \rho d\epsilon_k \tag{97}$$

where the integration range is set from $-\Lambda$ to Λ and $\rho = \frac{1}{2\Lambda}$ is the constant density of states.

4. The program is tested for different temperatures $\beta = \frac{1}{k_B T}$ and different sizes of bands. For $\Lambda \ll 1$, this is the thin band limit and it should recover the flat band limit, i.e. setting $\epsilon_k \to 0$. For $\Lambda \gg 1$, this should be the zero-temperature limit and a finite field should be found.

However the current conclusion is, upon setting $N = 2, 3, 4$ and 5, the program only gives a non-zero $\langle s^z \rangle$ and $\langle S^z \rangle$ for the first free energy expression for the thick band limit or the zero-temperature limit. The questions remained to be asked are:

- Why is this the case?
- Currently can't think of a sensible way to generalise this to the full model (if the sum over the spin indices is not outside the logarithm). How should one do that?—
- Physically does this free energy expression (the first one) makes sense? This restricts the amount of fermions in each site to be 1 in all possible occupations.

6 A new model

Let us consider decoupling the Hamiltonian in a different way compared to that suggested in §4. We begin again with the full Hamiltonian of the form.

$$H = H_0 + H_K + H_a \tag{98}$$

where the Kondo Hamiltonian as of the form:

$$H_K = J \sum_{\alpha\beta} f_\alpha^\dagger f_\beta c_\beta^\dagger c_\alpha \tag{99}$$

and the intrinsic Hamiltonian for the c-electrons and the anisotropy Hamiltonian are respectively:

$$H_0 = \sum_{k\alpha} c_{k\alpha}^\dagger c_{k\alpha} \tag{100}$$

$$H_a = \sum_{\alpha} \epsilon_a f_\alpha^\dagger f_\alpha \tag{101}$$

We note that the crystal fields in the anisotropy Hamiltonian makes some of the projections α more energetic. In this Hamiltonian, we have the following ordering parameters:

1. Kondo ordering parameter:

$$\left\langle f_\alpha^\dagger c_\alpha \right\rangle = V \tag{102}$$

$$\left\langle c_\alpha^\dagger f_\alpha \right\rangle = \bar{V} \tag{103}$$

2. Magnetic ordering parameter along the z-axis:

$$\left\langle f_\alpha^\dagger f_\alpha \right\rangle = t_\alpha \tag{104}$$

$$\left\langle c_\alpha^\dagger c_\alpha \right\rangle = u_\alpha \tag{105}$$

3. No magnetic order along the $x - y$ axis:

$$\left\langle f_\alpha^\dagger f_\beta \right\rangle = \left\langle c_\alpha^\dagger c_\beta \right\rangle = 0 \tag{106}$$

   if $\alpha \neq \beta$.

Now note that in general if we have two operators $\hat{A}$ and $\hat{B}$, then

$$\begin{aligned}\hat{A}\hat{B} &= \left[\langle A\rangle + \left(\hat{A} - \langle A\rangle\right)\right]\left[\langle B\rangle + \left(\hat{B} - \langle B\rangle\right)\right] \\ &\simeq -\langle A\rangle\langle B\rangle + \hat{A}\langle B\rangle + \hat{B}\langle A\rangle\end{aligned} \tag{107}$$

So let us split up the Kondo Hamiltonian in the following way:

$$H_K = J\left[\delta\sum_{\alpha\beta}\left(f_\alpha^\dagger f_\beta \cdot c_\beta^\dagger c_\alpha\right) - (1-\delta)\left(f_\alpha^\dagger c_\alpha \cdot c_\beta^\dagger f_\beta\right)\right] \tag{108}$$

where

$$\begin{array}{cc}\delta = 0 & \text{Kondo MF} \\ \delta = \frac{1}{2} & \text{Unbiased decoupling} \\ \delta = 1 & \text{RKKY MF}\end{array}$$

We can write the order parameter in the following more compact form:

$$\begin{cases}\left\langle f_\alpha^\dagger f_\beta\right\rangle = \delta_{\alpha\beta}t_\alpha \\ \left\langle c_\beta^\dagger c_\alpha\right\rangle = \delta_{\alpha\beta}u_\alpha\end{cases} \tag{109}$$

Therefore, using the mean field approximation, we can write

$$\begin{aligned}H_K \simeq J\delta\sum_{\alpha\beta}&\left(-\left\langle f_\alpha^\dagger f_\beta\right\rangle\left\langle c_\beta^\dagger c_\alpha\right\rangle + f_\alpha^\dagger f_\beta\left\langle c_\beta^\dagger c_\alpha\right\rangle + \left\langle f_\alpha^\dagger f_\beta\right\rangle c_\beta^\dagger c_\alpha\right) \\ - J(1-\delta)\sum_{\alpha\beta}&\left(-\left\langle f_\alpha^\dagger c_\alpha\right\rangle\left\langle c_\beta^\dagger f_\beta\right\rangle + f_\alpha^\dagger c_\alpha\left\langle c_\beta^\dagger f_\beta\right\rangle + \left\langle f_\alpha^\dagger c_\alpha\right\rangle c_\beta^\dagger f_\beta\right)\end{aligned} \tag{110}$$

Therefore using the order parameter relations, we can obtain:

$$\begin{aligned}H_K = J\delta\sum_\alpha&\left(-t_\alpha u_\alpha + t_\alpha c_\alpha^\dagger c_\alpha + u_\alpha f_\alpha^\dagger f_\alpha\right) \\ &+ J(1-\delta)\sum_{\alpha\beta}V_\alpha\bar{V}_\beta - V_\alpha c_\beta^\dagger f_\beta - \bar{V}_\beta f_\alpha^\dagger c_\alpha\end{aligned} \tag{111}$$

We can introduce the average of the V fields:

$$v = \frac{1}{N}\sum_\alpha V_\alpha \tag{112}$$

then we have

$$\begin{aligned}H_K = J\delta\sum_\alpha&\left(-t_\alpha u_\alpha + t_\alpha c_\alpha^\dagger c_\alpha + u_\alpha f_\alpha^\dagger f_\alpha\right) \\ &J(1-\delta)N^2v^2 - J(1-\delta)Nv\sum_\alpha c_\alpha^\dagger f_\alpha - J(1-\delta)N\bar{v}\sum_\alpha f_\alpha^\dagger c_\alpha\end{aligned} \tag{113}$$

and therefore in matrix form:

$$H_K = -J\delta \sum_\alpha t_\alpha u_\alpha + J(1-\delta)N^2 v^2 \tag{114}$$
$$+ \sum_\alpha \begin{pmatrix} c_\alpha^\dagger & f_\alpha^\dagger \end{pmatrix} \begin{pmatrix} J\delta t_\alpha & -J(1-\delta)Nv \\ -J(1-\delta)N\bar{v} & J\delta u_\alpha \end{pmatrix} \begin{pmatrix} c_\alpha \\ f_\alpha \end{pmatrix}$$

We can use Parsaval's Theorem which gives:

$$\sum_i c_i^\dagger c_i = \sum_k c_k^\dagger c_k \tag{115}$$

so the full Hamiltonian now gives:

$$H_0 + H_a + H_K = -J\delta \sum_\alpha t_\alpha u_\alpha + J(1-\delta)N^2 v^2 \tag{116}$$
$$+ \alpha \begin{pmatrix} c_{k\alpha}^\dagger & f_{k\alpha}^\dagger \end{pmatrix} \begin{pmatrix} J\delta t_\alpha + \epsilon_k & -J(1-\delta)Nv \\ -J(1-\delta)N\bar{v} & J\delta u_\alpha + \epsilon_\alpha - \lambda \end{pmatrix} \begin{pmatrix} c_{k\alpha} \\ f_{k\alpha} \end{pmatrix}$$

where we fix the Lagrangian multiplier field λ by

$$\frac{1}{N_s} \sum_{k\alpha} f_{k\alpha}^\dagger f_{k\alpha} = 1 \tag{117}$$

We have neglected the term

$$\left\langle \sum_{\alpha\beta} \delta A_\alpha \delta B_\beta \right\rangle \sim N \ll N^2 \tag{118}$$

which scales with N so when $N \to \infty$ this term is negligible when compared to the energy/ mean field terms of the Hamiltonian i.e. the fluctuation term is negligible. This can be physically attributed to the fact that if α and β are sufficiently far apart then they should not be strongly correlated. Our saddle point solution should therefore be exact in this limit.

6.1 The code

We first test this model for the $N = 3$ case (i.e. the spin one case). The code used is similar to the one used before for the old model, where the Hamiltonian in Equation 116 is used to construct a free energy expression, which is then minimised and solved iteratively to find a suitable saddle point solution.

Here we detail the part where the integration comes in. When solving for the sum over k, we treat the system to have a small perturbation around the Fermi energy surface. Therefore, we do the following substitution:

$$\sum_k \mapsto \int_{-\Lambda}^{\Lambda} \rho d\epsilon_k \tag{119}$$

where we call Λ to be the (half)-bandwidth of the system and we assume the density of states is constant at $\rho = \frac{1}{2\Lambda}$. By setting Λ to different values, we obtain two different limits as detailed below:

6.1.1 Zero band limit

This is the simplest limit where we set $\epsilon_k = 0$. Physically, this means that the energy value in real-space is constant, so the system is localised to the Fermi energy surface.

6.1.2 Thin band limit

This is the limit where we take $\Lambda \to 0$. As we take this limit in the integral, the density of states simply turns into a delta function centred at $\epsilon_k = 0$ (i,e. $\delta\epsilon_k$). Therefore this has the same effect as the zero band limit.

6.1.3 Broad band/ low temperature limit

This is the limit where we take $\beta \to 0$. Let us investigate this limit analytically. Without loss of generality, we set $\langle S_z \rangle > 0$. In the RKKY limit, the iteration equation for $\langle s_z \rangle$ reduces to:

$$\begin{aligned} \langle s_z \rangle &= \int_{-\Lambda}^{\Lambda} \left[\frac{1}{1 + e^{\beta\left(\frac{j_z \langle s_z \rangle}{N_0} + \epsilon_k\right)}} - \frac{1}{1 + e^{\beta\left(-\frac{j_z \langle s_z \rangle}{N_0} + \epsilon_k\right)}} \right] \\ &\simeq \rho \left(-\frac{j_z \langle S_z \rangle}{N_0} + \Lambda \right) - \rho \left(\frac{j_z \langle S_z \rangle}{N_0} + \Lambda \right) \\ &\simeq -\frac{2 j_z \langle S_z \rangle}{N_0} \rho \end{aligned} \tag{120}$$

Here we note that we have assumed the fact that the Fermi energy is much smaller than the bandwidth:

$$\epsilon_F = -\frac{j_z \langle S_z \rangle}{N_0} \ll \Lambda \tag{121}$$

and we integrate up to the Fermi energy if β is sufficiently large enough (as in any Fermi system).

The equation for $\langle S_z \rangle$ is

$$\langle S_z \rangle = \frac{1}{1 + e^{\beta\left(\frac{j_z \langle s_z \rangle}{N_0} - \lambda\right)}} - \frac{1}{1 + e^{-\beta\left(\frac{j_z \langle s_z \rangle}{N_0} + \lambda\right)}} \tag{122}$$

In the large β limit, only the lowest energy limit is occupied - which has the energy $-\frac{j_z \langle s_z \rangle}{N_0} - \lambda$, which in our notation corresponds to the $m = 1$ state. In this limit we simply have:

$$\langle S_z \rangle \to +1 \tag{123}$$

as we only have 1 electron occupying the $+1$ projection state. The Lagrange multiplier field must satisfy:

$$0 < -\lambda \tag{124}$$

so

$$\frac{j_z \langle s_z \rangle}{N_0} < \lambda < 0 \tag{125}$$

where we note that $s_z < 0$. This analysis applies to the corresponding fields: $S_z \mapsto t_\alpha$ and $s_z \mapsto u_\alpha$, where α are the spin projections. So to conclude in this limit we have:

$$\begin{cases} \beta \to 0 \\ \langle s_z \rangle \to -\frac{2\rho j_z}{N_0} = -\frac{j_z}{N_0 \Lambda} \\ \langle S_z \rangle \to 1 \end{cases} \tag{126}$$

6.2 Some First Results

Let us first investigate the thin band limit and see how introducing the Kondo interaction changes the picture. Here we first investigate the relationship between β, the inverse temperature and t_{-1}, the mean field for impurities of $\alpha = -1$.

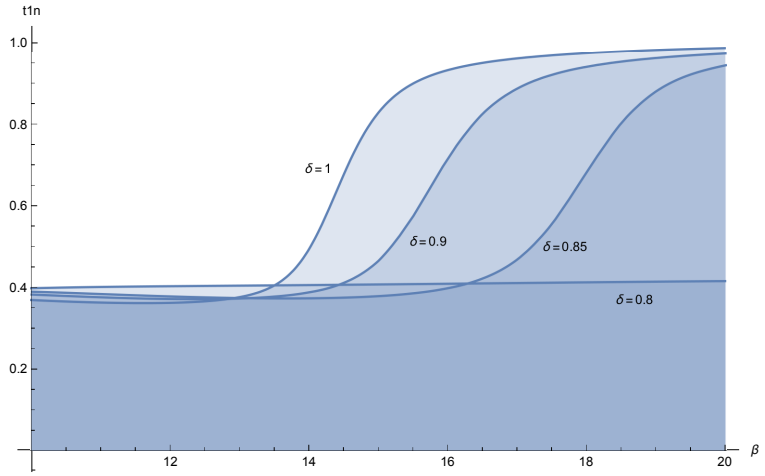

Figure 2: A plot of the evolution of system for the mean field t_{-1} (denoted t_{1n}) against β the inverse temperature for different values of δ. We can see that when the Kondo interaction is gradually turned on, the transition temperature reduces, which is as expected due to the shielding effect. A funny thing occurs at around $\delta = 0.83$, where the transition graph flattens out quickly - this is worth investigating later.

I have also investigated the relationship between β and the Hubbard-Stratonovich field v.

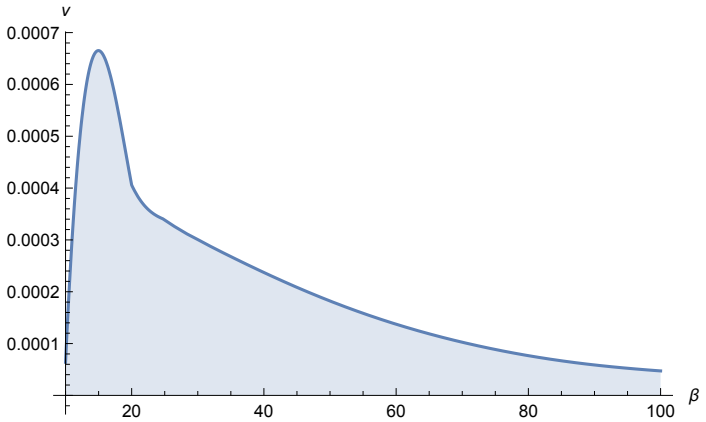

Figure 3: A plot of the evolution of system for the mean HS field v against β the inverse temperature for $\delta = 0.9$. This shows the typical shape of the growth of the field - it peaks at around the transition and slowly drops down.

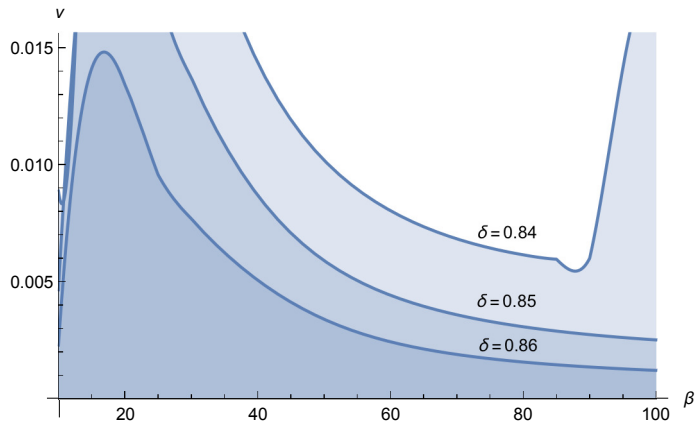

Figure 4: A plot of the evolution of system for the mean HS field v against β the inverse temperature for different values of δ. A few things can be observed: Firstly, the HS field v grows when δ is increased, as expected since the Kondo interaction is increased. Secondly, the peak of the transition is shifted to lower temperatures, which agrees with the above results. There is also a growth of v for high β at $\delta = 0.84$, something worth investigating later.

7 Investigations of the new model

In this section we present some investigations of the new model, starting with the analysis of the $N_0 = 3$ ($s = 1$) numerical model coded in *Mathematica*.

7.1 Investigation of Bandwidth and the Transition Temperature

Consider the case $\delta = 1$. This represents the RKKY limit of the current model. In the previous section, we highlighted that there is a continuous phase transition as temperature is lowered (i.e. β is increased) where the system spontaneously magnetises. From Coleman, the transition temperature for the RKKY model is put at:

$$T_{RKKY} = J\rho^2 \tag{127}$$

where ρ is the density of states of the system. It can be shown that we should expect:

$$\beta_{RKKY} \sim \Lambda \tag{128}$$

where Λ is the half-bandwidth. The results for the $N_0 = 3$ limit is as follows:

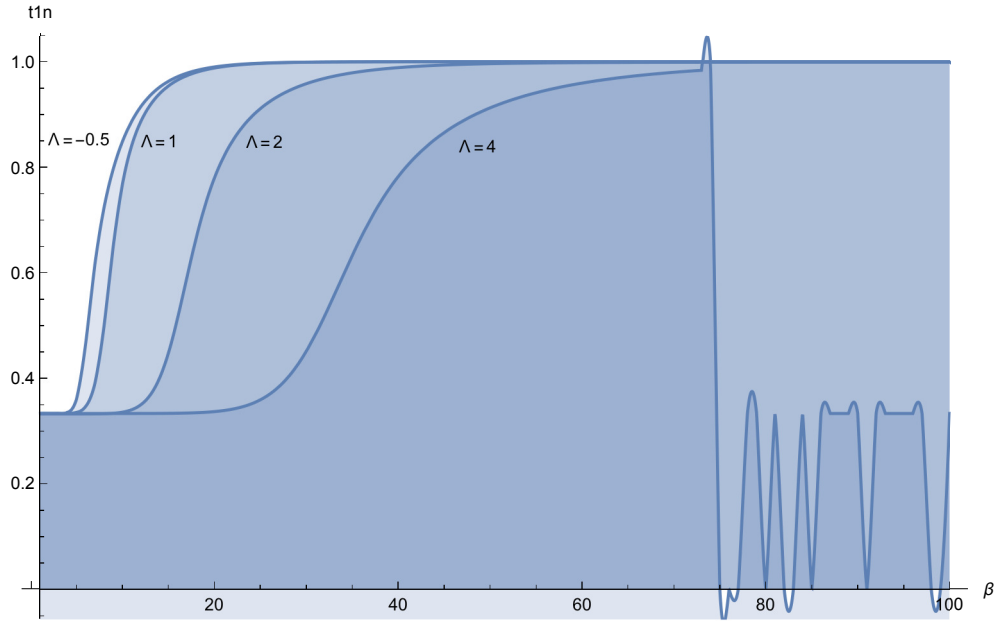

Figure 5: The transition plot of the t_{-1} field against inverse temperature β for different values of Λ in the RKKY limit of the model $\delta = 1$. We note that the plots and transition temperatures, the latter taken to be the midpoint of the transition curves, broadly agrees with the relationship $\Lambda \sim \beta$. The $\Lambda = 4$ curve exhibits abnormalities at high values of β (low temperatures) due to the numerical problems with Fermi functions in the model.

The conclusion is our current programme works well for the bandwidth from about $\Lambda = 0.5 - 3.0$. We will for now limit our analysis to this bandwidth for some preliminary results.

7.2 Determining the lowest energy state

The next obvious step is to determine the actual physical state of the system. Since δ is not a physical observable (it is a mere theoretical variable to determine the mixing/ coupling strength between the two Hamiltonians), our theoretical must predict something physical - here we introduce a variable that only has two values $z_0 \mapsto \pm 1$ - this measures whether the system is magnetising (in this case $z \mapsto 1$) or non-magnetising ($z \mapsto -1$). This can be easily seen in the transition shown in Figure 6.2 - the state labelled $\delta = 0.9$ is magnetising, whilst the state labelled $\delta = 0.8$ is non-magnetising.

Determination of z The procedure of determining z is described as follows. For each set of parameters (number of sites N_s, number of spin pro-

jections $N_0 = 2s + 1$, Half-bandwidth Λ and coupling strength J), we first compute the ground state energy of the system for different δ. This is done with the *Freeenergyof*δ function. The *Searchfor*δ*tomin*Φ finds the minimum of this energy and determines the δ that minimises this energy. We then use this δ to investigate whether this is magnetised state and assign the value of z to the system based on whether the t_{-1} field exhibits a transition.

For example, one data set is obtained as follows:

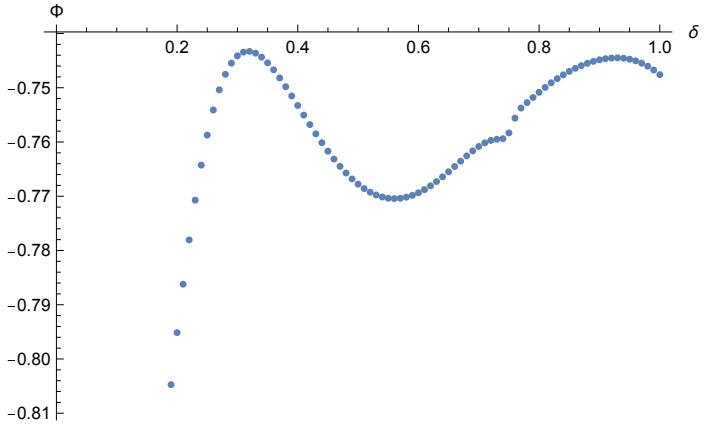

Figure 6: Plot of the free energy against δ. The parameters of the system is $\beta = 20$, $N_s = 1$, $N_0 = 3$, $J = 1$, $\Lambda = 1$. The scattered plot involves points $\delta = 0.1 - 1.0$ at intervals of $\Delta\delta = 0.01$.

An interpolation of the plots is performed.

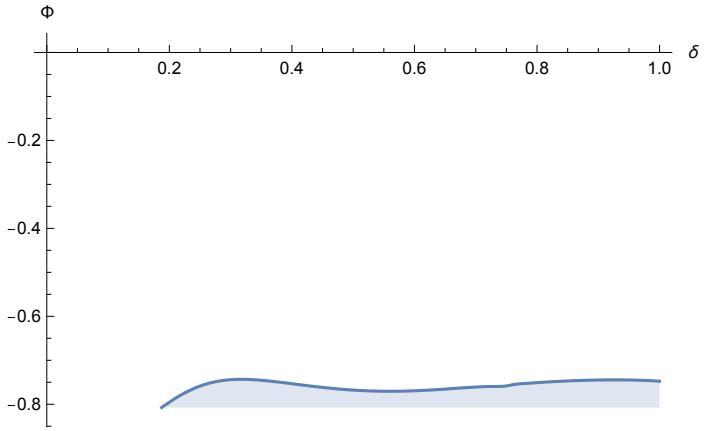

Figure 7: Plot of interpolation function of the previous scattered plot of the free energy against δ. The parameters of the system is $\beta = 20$, $N_s = 1$, $N_0 = 3$, $J = 1$, $\Lambda = 1$. The minimum of the function is at $\delta = 0.560372$, giving $\Phi_{min} = -0.770438$. This is taken as the δ that minimises the free energy.

This δ is then used to compute the evolution plot of t_{-1} with temperature (inverse temperature β). The result is as follows:

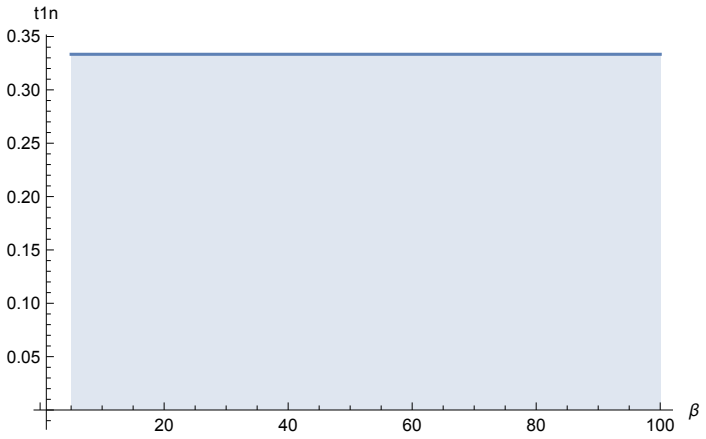

Figure 8: Plot of the impurity field t_{-1} against inverse temperature β. The expected value of the field t_{-1} stays at about $\frac{1}{3}$ so the system exhibits no magnetic transition. This allows us to assign these set of parameters with a value of $z = 1$.

The question remains: Do I need to compute a variation method with the range of β?

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