University of Cambridge

Part III Physics

Final Project Report

Mean-Field Study of Kondo Phase Diagram

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May 8, 2018

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Abstract

1 Introduction

Metallic systems with localised magnetic impurities have, over the years, been the subject of much research in condensed matter physics, falling under the broader branch of strongly correlated systems which are characterised by interactions being significant in comparison to the kinetic energy dispersion (bandwidth).

The enormous theoretical challenge of studying strongly correlated systems, with their broad ranges of energy scales, means that one often turns to effective models to describe the low energy behaviour, introducing strict constraints that arise after *projecting out* higher energy terms. One such effective model, studied in this project, is the Kondo model. This describes conduction electrons coupled to a (single) localised spin at the origin as a model for the dilute magnetic impurities that are sometimes present in a metal.

The many rich features of the general Kondo problem have been widely studied, with some simpler formulations being amenable to an exact solution via Bethe ansatz techniques. Often times, however, it is necessary to employ approximate methods to obtain results in more general cases, one such method being mean-field theory.

Use of mean-field theory is far from ideal, however, since current formulations applied to the Kondo impurity model are known to give results in disagreement with the Bethe ansatz solution for a characteristic energy of the problem known as the Kondo temperature T_K and (by extension) the magnetic susceptibility at zero temperature. The heat capacity is also greatly underestimated by existing mean-field methods. Recently, a new mean-field approach has been proposed by Garry Goldstein, Claudio Castelnovo (supervising the project) and Claudio Chamon which has given improved estimates of these quantities, which may be a sign that this new variation is indeed an improvement over existing formulations.

One significant aspect of the Kondo model that existing mean-field formulations have thus far failed to capture properly is the crossover from a Kondo to a paramagnetic phase in the temperature-field phase diagram, instead predicting a phase transition as in Figure 1. The primary aim of this project is therefore to extend this new formulation to finite temperature, specifically to the temperature-field phase diagram and see whether a phase transition or a crossover is predicted. If the predicted behaviour is found to align with that of the exact Bethe ansatz solution, then the case for this new mean-field approach as an alternative to existing formulations would be greatly strengthened.

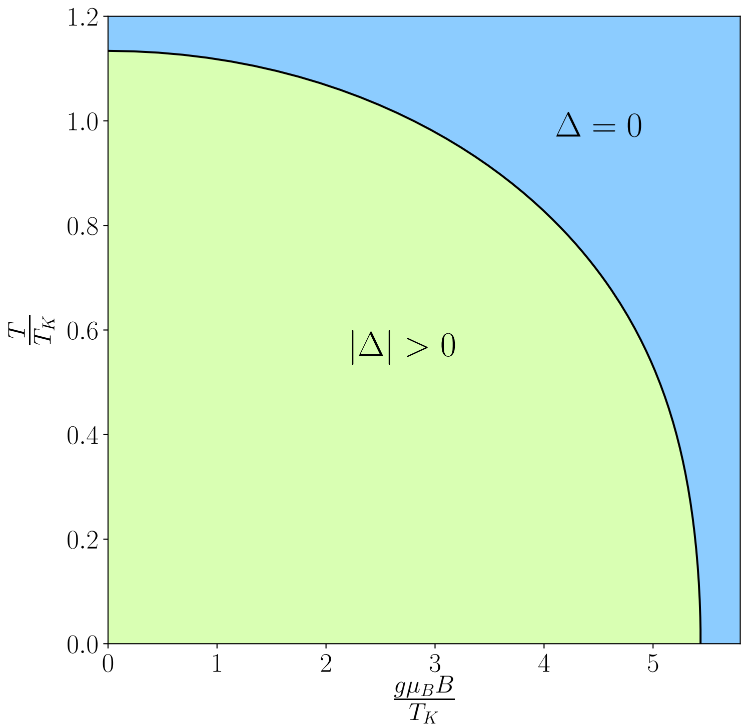

Figure 1: A representative phase diagram obtained from another mean field approach (with calculations found in [1]), which shows a distinct phase transition between two phases. The Kondo temperature T_K is used to make quantities dimensionless.

The report is structured as follows: Section 2 introduces the theoretical ideas underpinning the project; Section 3 contains the main finite-temperature investigation; Section 4 gives a brief account of the behaviour at finite-field and Section 5 concludes with a discussion of the main results of the project.

2 Theoretical Background

2.1 Kondo Model

The Kondo model made its first appearance in 1964 when theorists were attempting to explain puzzling experimental observations made 30 years earlier that certain metals containing magnetic impurities showed minima in their resistivity as a function of temperature. Jun Kondo proposed the Kondo model to describe a new scattering mechanism introduced by magnetic impurities which accounted for the functional form of the resistivity.

In its simplest single impurity flavour, the Kondo model has the following Hamiltonian:

$$H_{\text{Kondo}} = \sum_{\boldsymbol{k},\sigma} \epsilon_{\boldsymbol{k}} c^{\dagger}_{\boldsymbol{k},\sigma} c_{\boldsymbol{k},\sigma} + J\vec{S} \cdot \vec{s}(0), \tag{1}$$

in which there is a kinetic energy contribution from the conduction electrons $c_{\boldsymbol{k},\sigma}$ as well as a term describing an antiferromagnetic coupling between a spin localised at the origin and the spin density of conduction electrons at that point.[1]

2.2 Mean-Field Theory

The theoretical calculations of this project are framed in terms of the path integral, which is an approach to statistical mechanics reminiscent of Feynman's path integral formulation of quantum mechanics. The partition function can be written as the functional integral over fermionic paths:

$$Z = \operatorname{Tr} e^{-\beta H} = \int \mathcal{D}[c^{\dagger}, c] \; e^{-\int_0^{\beta} d\tau \; L} \,,$$

from which many properties of the system may then be derived.[2] Here, the equivalent *action* involves integration of the Lagrangian L over an imaginary time $\tau = it/\hbar$ with an upper limit of $\beta = \frac{1}{k_B T}$.

One then begins to employ many 'tricks' to make the problem more tractable. One such trick that proves to be useful is the introduction of new boson operators, which sometimes (as

[1] The spin density of conduction electrons is given by

$$\vec{s}(0) = \frac{1}{2} \sum_{\boldsymbol{k},\boldsymbol{k'}} \sum_{\sigma,\sigma'} c^{\dagger}_{\boldsymbol{k},\sigma} \vec{\tau}_{\sigma,\sigma'} c_{\boldsymbol{k'},\sigma'} \,,$$

where $\vec{\tau}_{\sigma,\sigma'}$ is a vector of Pauli matrices.

[2] One also replaces fermion operators with *Grassman numbers* within the integral, which have the property of anti-commutation (among others).

we shall see) necessitates that hard constraints be applied in the form of Lagrange multipliers. The way that constraints are implemented into the Lagrangian is shown in Appendix A.

The essence of mean-field theory is that we avoid performing the actual functional integration by approximating the integral by its saddle point, a step also known as the stationary phase approximation. In making this approximation, we are essentially imposing self-consistency conditions on whatever fields now appear in L, making them take on their mean values. Thankfully, these mean-field self-consistency equations are exactly what result from directly minimising the effective action with respect to the auxiliary fields, which is what this project will involve.

2.2.1 Kotliar-Ruckenstein Bosons

2.3 The Soft-Constraint Approach

One existing mean-field approach is that of Read and Newns [4], which represents the $\vec{S}_0$ term of the Hamiltonian in Eq (1) in terms of slave fermions f_σ, with occupation numbers obeying the hard constraint $\sum_\sigma f_\sigma^\dagger f_\sigma = 1$. The new mean-field approach that is being proposed reformulates this constraint as:

$$(1 - n_\uparrow - n_\downarrow)^2 = n_\uparrow n_\downarrow + (1 - n_\uparrow)(1 - n_\downarrow) = 0. \tag{2}$$

Implementing this into the Lagrangian is formally equivalent, but problematic within mean-field theory because one later imposes:

$$\langle (1 - n_\uparrow - n_\downarrow)^2 \rangle = 0\,,$$

which, for such a positive semi-definite operator, enforces the exact constraint and leads to a diverging mean-field parameter. (Appendix B gives some feeling for why this is the case.)

A resolution to this issue is to begin by introducing an auxiliary non-interacting fermion h that is constrained to be trivially empty through imposing $h^\dagger h = 0$. One then combines this constraint with that of Eq (2) by imposing instead:

$$n_\uparrow n_\downarrow + (1 - n_\uparrow)(1 - n_\downarrow) - K h^\dagger h = 0\,, \tag{3}$$

such that $K > 0, K \neq 1$ now encapsulates both constraints. Notice that this has introduced an arbitrary parameter K into the problem and thus a new degree of freedom, but has allowed us to circumvent the issues related to the previous hard constraint within mean-field theory. For this reason, this approach to mean-field theory has been internally referred to as the *soft constraint approach*.

Proceeding in a similar fashion to the Read-Newns approach and incorporating four Kotliar-Ruckenstein (KR) [3] slave bosons, one obtains the following Lagrangian:

$$
\begin{aligned}
L \quad = \quad & \sum_{\boldsymbol{k},\sigma} c^\dagger_{\boldsymbol{k},\sigma}\left(\frac{d}{d\tau} + \epsilon_{\boldsymbol{k}} - \mu\right) c_{\boldsymbol{k},\sigma} + \sum_{\sigma} f^\dagger_\sigma \frac{d}{d\tau} f_\sigma + h^\dagger \frac{d}{d\tau} h \\
& + e^\dagger \frac{d}{d\tau} e + \sum_\sigma p^\dagger_\sigma \frac{d}{d\tau} p_\sigma + d^\dagger \frac{d}{d\tau} d \\
& + \sum_\sigma \lambda_\sigma (f^\dagger_\sigma f_\sigma - p^\dagger_\sigma p_\sigma - d^\dagger d) + \lambda_{\mathrm{KR}}(e^\dagger e + \sum_\sigma p^\dagger_\sigma p_\sigma + d^\dagger d - 1) \\
& + \lambda_{\mathrm{SC}}(e^\dagger e + d^\dagger d - K h^\dagger h) \\
& + 2\frac{VV^*}{J} + \sum_{\boldsymbol{k},\sigma}\left(V^* c^\dagger_{\boldsymbol{k},\sigma} z_\sigma f_\sigma + V f^\dagger_\sigma z^\dagger_\sigma c_{\boldsymbol{k},\sigma}\right) .
\end{aligned}
\tag{4}
$$

The slave bosons e, $p_\uparrow$, $p_\downarrow$ and d represent empty, singly occupied and doubly occupied states, respectively, as long as the fermion operator is suitably transformed to 'update the books', so to speak:[3]

$$
f_\sigma \to z_\sigma f_\sigma \,, \qquad z_\sigma = e^\dagger p_\sigma + p^\dagger_{-\sigma} d\,. \tag{5}
$$

A Hubbard-Stratonovich transformation has also been applied to remove certain unpleasant terms in the Lagrangian, framing the interaction in terms of a new bosonic field V.

3 Finite-Temperature Study

As a first step towards constructing the temperature-field phase diagram, it will be useful to gain some familiarity with the mean-field equations at finite temperature by investigating the Kondo model in the absence of a magnetic field. The isotropy of this zero-field case will allow for convenient simplification of some terms in the mean-field equations.

3.1 Obtaining the Mean-Field Equations

We start by deriving the self-consistency equations that must hold for the mean-field description of the system. Since $F = -k_{\mathrm{B}} T \ln Z$ [4], searching for the minimal action is equivalent to directly minimising of F, illustrating a correspondence between the path integral and a more traditional way of approaching mean-field theory. Having introduced new bosonic fields to the Lagrangian of Eq (4), all fermionic fields may be integrated out as outlined in

[3] The conventional transformation $z_\sigma \to (1 - d^\dagger d - p^\dagger_\sigma p_\sigma)^{-1/2} z_\sigma (1 - e^\dagger e - p^\dagger_{-\sigma} p_{-\sigma})^{-1/2}$ is also applied, but is not relevant to this discussion.

[4] We shall set $k_{\mathrm{B}} = 1$ for the remainder of the project.

Appendix C to obtain an effective free energy

$$
\begin{aligned}
F \quad = \quad & \overbrace{-2T\,\Re \sum_\sigma \ln\left[\frac{\widetilde{\Gamma}(\xi_\sigma + D)}{\widetilde{\Gamma}(\xi_\sigma)}\right]}^{F_0} + \frac{2\Delta}{\pi\rho J} - \sum_\sigma \lambda_\sigma (p_\sigma^2 + d^2) \\
& + \lambda_{\mathrm{KR}}(e^2 + \sum_\sigma p_\sigma^2 + d^2 - 1) + \lambda_{\mathrm{SC}}(e^2 + d^2) \underbrace{- T \ln\left(1 + e^{\beta K \lambda_{\mathrm{SC}}}\right)}_{F_{\mathrm{h}}}
\end{aligned}
\tag{6}
$$

in terms of the *gamma function* $\widetilde{\Gamma}(z) \equiv \Gamma(\frac{1}{2} + \frac{z}{2\pi i T})$ and $\xi_\sigma = \lambda_\sigma + i|z_\sigma|^2\Delta$, a complex resonance-level energy made slightly different by the inclusion of the KR term.

Note that the temperature dependence of this free energy is solely contained in F_0 and F_{h}, which are the only terms that differ from the existing preliminary zero-temperature study of the soft-constraint approach. We now minimise this free energy to obtain a set of mean-field equations generalised to finite temperature, starting with the Hubbard-Stratonovich field

$$
\frac{\partial F}{\partial \Delta} = 0 \implies \sum_\sigma \left[\frac{\partial F_0}{\partial \xi_\sigma} - \frac{\partial F_0}{\partial \overline{\xi_\sigma}}\right] i z_\sigma^2 = -\frac{2}{\pi J \rho} \ . \tag{7}
$$

Though strictly free to only treat bosonic variables as complex numbers, we also restrict our search to real solutions, leading to one equation for each KR boson[5]:

$$
\frac{\partial F}{\partial d} = 0 \implies \sum_\sigma \left[\frac{\partial F_0}{\partial \xi_\sigma} - \frac{\partial F_0}{\partial \overline{\xi_\sigma}}\right] \frac{\partial z_\sigma^2}{\partial d}\, i\Delta = -d\, \left(\lambda_{\mathrm{KR}} + \lambda_{\mathrm{SC}} - \sum_\sigma \lambda_\sigma\right) \ , \tag{8}
$$

$$
\frac{\partial F}{\partial e} = 0 \implies \sum_\sigma \left[\frac{\partial F_0}{\partial \xi_\sigma} - \frac{\partial F_0}{\partial \overline{\xi_\sigma}}\right] \frac{\partial z_\sigma^2}{\partial e}\, i\Delta = -e\, \left(\lambda_{\mathrm{KR}} + \lambda_{\mathrm{SC}}\right) \ , \tag{9}
$$

$$
\frac{\partial F}{\partial p_\sigma} = 0 \implies \sum_s \left[\frac{\partial F_0}{\partial \xi_s} - \frac{\partial F_0}{\partial \overline{\xi_s}}\right] \frac{\partial z_s^2}{\partial p_\sigma}\, i\Delta = -p_\sigma\, \left(\lambda_{\mathrm{KR}} - \lambda_\sigma\right) \ . \tag{10}
$$

The form of the ∂z_σ^2 derivative terms are irrelevant for the time being, but are found in Appendix D. Use of the chain rule means that the difficult derivative term

$$
\frac{\partial F_0}{\partial \xi_\sigma} - \frac{\partial F_0}{\partial \overline{\xi_\sigma}} = \frac{i}{\pi} \Re(\widetilde{\psi}(\xi_\sigma + D) - \widetilde{\psi}(\xi_\sigma)) \tag{11}
$$

appears repeatedly, where $\psi(z) \equiv \frac{d}{dz}(\ln\Gamma(z))$ defines the *digamma function*.

[5]This may be partly justified by the phase invariance of most terms apart from $|z_\sigma|^2$.

Finally, imposing Lagrange multiplier constraints completes the set of mean-field equations:

$$\frac{\partial F}{\partial \lambda_\sigma} = 0 \implies \left[\frac{\partial F_0}{\partial \xi_\sigma} + \frac{\partial F_0}{\partial \overline{\xi_\sigma}}\right] = (p_\sigma^2 + d^2) \ , \tag{12}$$

$$\frac{\partial F}{\partial \lambda_{\mathrm{KR}}} = 0 \implies e^2 + \sum_\sigma p_\sigma^2 + d^2 = 1 \ , \tag{13}$$

$$\frac{\partial F}{\partial \lambda_{\mathrm{SC}}} = 0 \implies e^2 + d^2 = K\langle h^\dagger h\rangle \equiv \kappa \ , \tag{14}$$

where the other combination of difficult derivatives is

$$\frac{\partial F_0}{\partial \xi_\sigma} + \frac{\partial F_0}{\partial \overline{\xi_\sigma}} = -\frac{1}{\pi}\Im(\widetilde{\psi}(\xi_\sigma + D) - \widetilde{\psi}(\xi_\sigma)) \ . \tag{15}$$

3.2 Solving the Mean-Field Equations

Our aim is to self-consistently satisfy the mean-field equations derived above. The absence of any magnetic field means that there is nothing to favour any particular configuration of the spin-$\frac{1}{2}$ magnetic impurity, so we should expect the existence of a solution with $p_\uparrow = p_\downarrow$ and $\lambda_\uparrow = \lambda_\downarrow$, allowing us to drop spin indices σ. Next, we shall make use of particle-hole symmetry to equate $e^2 = d^2$, which will dramatically simplify the mean-field equations.[6]

These simplifications mean that the occupation of each KR boson is entirely determined by κ as:

$$e^2 = d^2 = \frac{1}{2}\,\kappa \quad \text{and} \quad p^2 = \frac{1}{2}(1-\kappa) \ . \tag{16}$$

Subtracting Eq (9) and Eq (8) immediately implies $\lambda_\sigma = 0$, which means that the complex energy $\xi = iz^2\Delta$ is now purely imaginary. Combining Eq (12) and Eq (13) leads to

$$\frac{1}{2} = \frac{\partial F_0}{\partial \xi} + \frac{\partial F_0}{\partial \overline{\xi}} \approx -\frac{1}{\pi}\Im\left[\ln\frac{D}{2\pi i T} - \widetilde{\psi}(\xi)\right] \ ,$$

where we have used the large bandwidth $D \gg T, \xi$ to make the leading order approximation that $\psi(z) \approx \ln z$ for large z. Taking the principal value of the complex logarithm then leads to the result that

$$\Im\left[\psi\left(\frac{1}{2} + \frac{\xi}{2\pi i T}\right)\right] = 0 \ ,$$

which is merely consistent with the $\lambda_\sigma = 0$ conclusion that arose immediately from particle-hole symmetry and so tells us nothing new.

[6]Particle-hole symmetry comes out as a necessity in the Read-Newns mean-field approach, but here it is motivated by the belief that empty and doubly occupied pseudo-fermion states should be equally unphysical.

Turning to Eq (7) and making the same approximations, we may derive an implicit relation for Δ in terms of T and κ, similar to that found in [1]:

$$\psi\left(\frac{1}{2}+\frac{z^2\Delta}{2\pi T}\right)=\ln\frac{D}{2\pi T}-\frac{1}{J\rho z^2}\ . \tag{17}$$

Finding the finite-temperature behaviour of the order parameter is therefore a case of inverting this relation for Δ, though it will not be possible to find an expression in terms of elementary functions.

3.2.1 Importance of $\lambda_{\mathbf{SC}} \geq 0$

In identifying $\kappa = K\langle h^\dagger h\rangle$ as a free parameter, we should be certain that $\lambda_{\mathrm{SC}} > 0$, since the thermal occupation of h takes on a familiar Fermi-Dirac form

$$\langle h^\dagger h\rangle = -\frac{1}{K}\frac{\partial F_{\mathrm{h}}}{\partial\lambda_{\mathrm{SC}}}=\frac{1}{1+e^{-\beta K\lambda_{\mathrm{SC}}}}\ .$$

If one were to find that $\lambda_{\mathrm{SC}} < 0$, then the zero-temperature limit would have $\langle h^\dagger h\rangle \to 0$, thereby nullifying any freedom to choose K.

Solving the remainder of the mean-field equations for λ_{SC}, we find that

$$\lambda_{\mathrm{SC}}=\frac{2\Delta}{\pi J\rho}\frac{1-2\kappa}{\kappa(1-\kappa)}\geq 0 \quad \text{for} \quad \kappa\leq\frac{1}{2} \tag{18}$$

which means $\langle h^\dagger h\rangle \in (\frac{1}{2},\ 1)$ and so we may indeed treat κ as our free parameter (for the time being).[7]

3.3 Zero-Temperature Heat Capacity

As a quick check of validity of the above solution, one hopes that the zero-temperature limit should reproduce the leading order temperature dependence obtained from expanding the Fermi function around $T = 0$, something that has already been done using the soft-constraint approach [2].

Knowing that this particular response function is derived from the free energy as $C = \frac{\partial E}{\partial T} = -T\frac{\partial^2 F}{\partial T^2}$, we start by finding the leading order behaviour of $\frac{\partial F}{\partial T}$ from the minimised form

[7] The added restriction on the magnitude of κ is, from Eq (16), equivalent to the seemingly reasonable statement that the physical pseudo-fermion states for the impurity should be more occupied than unphysical ones.

of the free energy:

$$F^\star = \underbrace{-4T\,\Re\,\ln\left[\frac{\widetilde{\Gamma}(iz^2\Delta + D)}{\widetilde{\Gamma}(iz^2\Delta)}\right] + \frac{2\Delta}{\pi J\rho}}_{F_0^\star} + \overbrace{\kappa\lambda_{\mathrm{SC}} - T\ln\left(1+e^{\beta K\lambda_{\mathrm{SC}}}\right)}^{F_{\mathrm{h}}^\star}\ . \tag{19}$$

It can be seen that the final term $F_{\mathrm{h}}^\star \approx -\kappa\lambda_{\mathrm{SC}}e^{-\beta K\lambda_{\mathrm{SC}}}$ will vanish quickly as $T \to 0$ in comparison to the first two terms, so we may safely neglect this contribution at leading order in T.

Anticipating that explicitly calculating the inverse of Eq (17) will be somewhat difficult, we may find an expression for $\frac{d\Delta}{dT}$ by inverting the chain rule

$$\frac{d\psi}{dT} = \frac{d\psi}{du}\frac{\partial u}{\partial\Delta}\frac{d\Delta}{dT} + \frac{d\psi}{du}\frac{\partial u}{\partial T} \implies \frac{d\Delta}{dT} = \left(\frac{d\psi}{dT}\left[\frac{d\psi}{du}\right]^{-1} - \frac{\partial u}{\partial T}\right)\left[\frac{\partial u}{\partial\Delta}\right]^{-1},$$

where $u \equiv \frac{1}{2} + \frac{z^2\Delta}{2\pi T}$ denotes the argument of $\psi(u)$. Thus, the only non-trivial derivative term left to calculate is $\left[\frac{d\psi}{du}\right]^{-1}$ which, using the asymptotic expansion of $\ln\Gamma(u)$ [8], is $\left[\frac{d\psi}{du}\right]^{-1} = u - \frac{1}{2} + \frac{1}{12u} + \dots$. This gives the leading-order temperature dependence of the order parameter as

$$\frac{d\Delta}{dT} \approx -\frac{\pi^2}{3}\frac{T}{z^4\Delta}\ , \tag{20}$$

reproducing a previous result in [2].

The remaining derivative may be performed by using the same asymptotic expansion of the first line of

$$\begin{aligned}
-\frac{1}{4}\frac{dF_0^\star}{dT} &= \Re\ln\widetilde{\Gamma}(iz^2\Delta + D) - \Re\ln\widetilde{\Gamma}(iz^2\Delta) - \Re\left[\frac{D}{2\pi iT}\ \widetilde{\psi}(iz^2\Delta + D)\right] \\
&\quad + \frac{z^2}{2\pi}\left(\frac{d\Delta}{dT} - \frac{\Delta}{T}\right)\Re\left[\widetilde{\psi}(iz^2\Delta + D) - \widetilde{\psi}(iz^2\Delta)\right] \\
&= -\frac{\pi}{6}\frac{T}{z^2\Delta} + \frac{1}{2\pi J\rho}\frac{d\Delta}{dT} + \dots\ .
\end{aligned}$$

Upon combining all derivative terms, the zero-temperature heat capacity is found to be

$$C = \frac{2\pi}{3}\frac{T}{z^2\Delta} + \dots\ , \tag{21}$$

once again reassuringly consistent with the result obtained from the first-order correction to the Fermi function [2]. The finite-temperature mean-field equations therefore provide an alternative derivation of this limit of the heat capacity.

[8] The asymptotic expansion of $\ln\Gamma(u)$, known as *Stirling's series*, is given by [5]

$$\ln\Gamma(u) = \frac{1}{2}\ln 2\pi + u(\ln u - 1) - \frac{1}{2}\ln u + \frac{1}{12u} - \frac{1}{360u^3} + \dots\ .$$

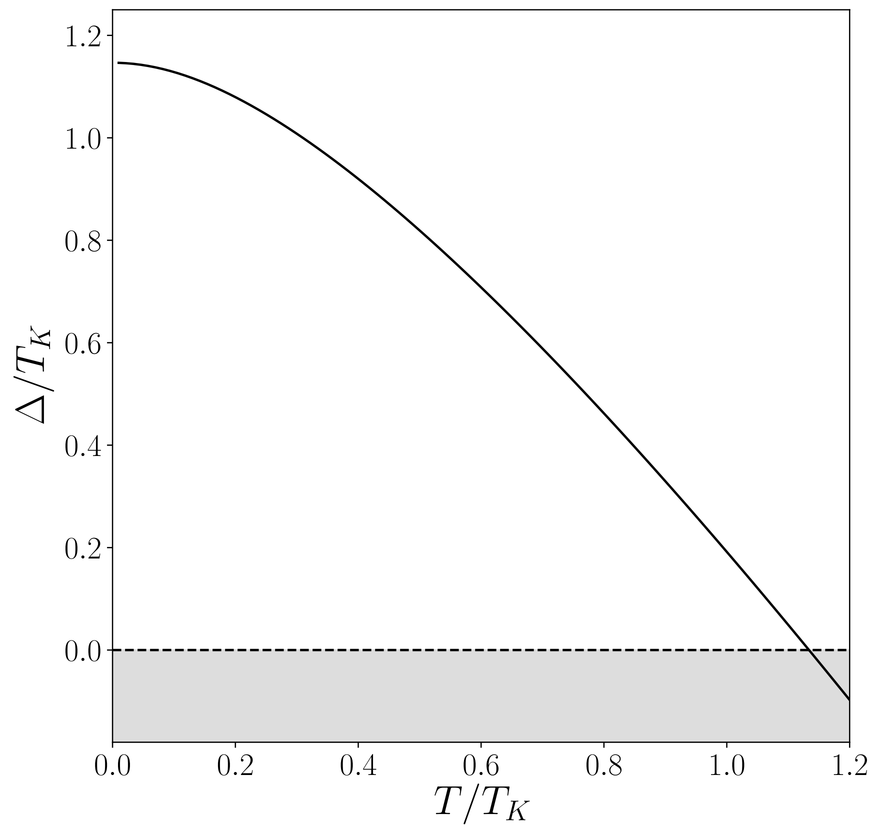

Figure 2: A plot of the order parameter Δ against the temperature T, with both axes normalised by the Kondo temperature T_K. The shaded region below the $\Delta = 0$ line indicates a non-physical region of the order parameter. The phase transition occurs at $T_c \approx 1.13\ T_K$.

3.4 Plotting the Mean-Field Solution

Satisfied that the zero-temperature limit of Eq (17) reproduces familiar results, we may use this implicit equation to plot the temperature dependence of the Δ in the case of κ being constant[9], as shown in Figure 2.

From this plot it may be seen that the first derivative, $\frac{d\Delta}{dT}$, is discontinuous at $T = T_c$ if intervening by not allowing Δ to become negative. This has the consequence that $\frac{d^2F}{dT^2}$ is also discontinuous, characteristic of a second-order phase transition as opposed to a crossover. In Section 3.6 we shall investigate whether judiciously choosing the temperature dependence of the original soft-constraint parameter $K \to K(T)$ can remove this phase transition.

[9]Here, κ is once again chosen such that $z^{-2} = 1 - \frac{1}{2}\rho J \ln(\rho J)$, which reproduces the two-loop Kondo temperature $T_K = D\sqrt{\rho J} e^{1/(\rho J)}$ [2].

3.5 Limitations of a Constant Soft-Constraint Parameter

Before starting to artificially influence the temperature dependence of the model, one might question whether or not this is a natural thing to do. In solving the mean-field equations as we did in Section 3.2, we absorbed the analytically difficult $\langle h^\dagger h \rangle$ term into a free parameter κ that allowed us to reduce the mean-field equations to a single equation, namely Eq (17). However, this strategy came at the cost of expressing Δ in terms of κ and *not* the elementary parameter K which originally appeared in the introduction to the soft-constraint approach. We shall now observe the behaviour that would arise if K were instead held constant.

Keeping the mean-field equations in terms of K and T, we are left to solve two simultaneous equations involving λ_{SC} and Δ:

$$\psi\left(\frac{1}{2} + \frac{z^2\Delta}{2\pi T}\right) = \ln\frac{T}{T_K} - \ln\left(2\pi\sqrt{\rho J}\right) + \frac{1}{\rho J}\left[1 - \frac{1}{z^2}\right] , \tag{22}$$

$$\lambda_{\mathrm{SC}} = \frac{8}{\pi\rho J}\frac{\Delta}{z^2}\left(1 - \frac{2K}{1 + e^{-\beta K \lambda_{\mathrm{SC}}}}\right) , \tag{23}$$

where $z^2 = 4K\left(1 - K/(1 + e^{-\beta K\lambda_{\mathrm{SC}}})\right) / \left(1 + e^{-\beta K\lambda_{\mathrm{SC}}}\right)$. It may be appreciated that obtaining a closed-form solution for Δ is now made impossible.

Nevertheless, it is still possible to make some progress by parameterising the above equations in terms of $s \equiv \beta\lambda_{\mathrm{SC}}$, and plotting the quantities Δ/T_K and T/T_K along both axes according to:

$$\left(\frac{T}{T_K}\right) = \frac{1}{2\pi\sqrt{\rho J}}\, e^{(1-z^{-2})/(\rho J)}\ \exp\left[-\psi\left(\frac{1}{2} + \frac{\rho J\ z^4\ s}{16(1 - 2K/(1 + e^{-Ks}))}\right)\right] , \tag{24}$$

$$\left(\frac{\Delta}{T_K}\right) = \frac{\pi\rho J\ z^2}{8(1 - 2K/(1 + e^{-Ks}))}\left(\frac{T}{T_K}\right) s\ . \tag{25}$$

The resulting parametric plot, Figure 3, has a catastrophically problematic shape in which there are no mean-field solutions beyond a certain temperature, but two extremal values of Δ below this temperature.[10] This suggests a breakdown of the mean-field equations and from this clearly unphysical behaviour we conclude that K must indeed have some temperature dependence if it is to accurately describe any finite-temperature features of the model at all.

[10]This strange behaviour may look suspiciously like an artefact of the algebraic manipulations used to achieve the parametric form of Eq (24) and Eq (25), but this functional form is also reproduced when numerically solving the mean-field equations.

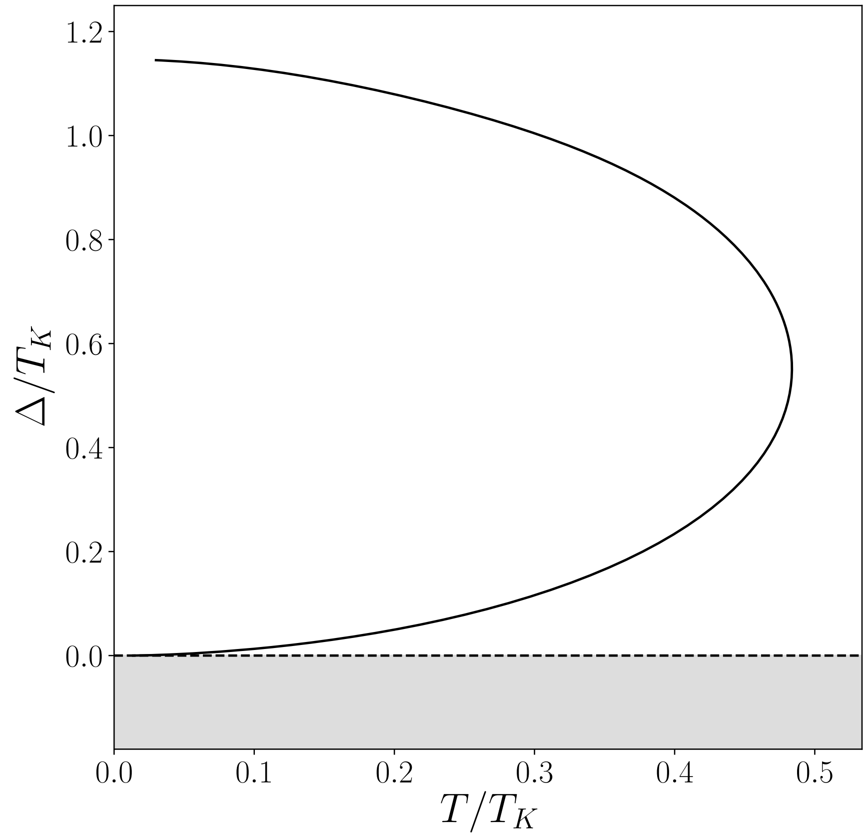

Figure 3: A plot of the order parameter Δ against the temperature T, produced parametrically for the case of constant K. The one-to-many mapping is not a physical function and so indicates a breakdown of the mean-field equations.

3.6 Manipulating the Nature of the Phase Transition

We have seen that neither constant K nor κ can reproduce a crossover from a strongly-coupled to weakly-coupled phase at finite temperature, so we now investigate whether a suitable choice of $\kappa \to \kappa(T)$ can remove this second-order phase-transition.

The first question to ask is whether it is possible for mean-field Δ to only *asymptotically* approach the weakly-coupled phase as temperature is increased, thereby not assuming a piecewise form. Consider choosing a different value for the soft-constraint parameter $\widetilde{\kappa}$ such that $z^2 \to \widetilde{z^2} = \alpha z^2$. To see whether the form of $\Delta(T)$ will change significantly upon making this choice, one can look at the new mean-field equation for Δ:

$$\psi\left(\frac{1}{2} + \frac{\alpha z^2 \Delta}{2\pi T}\right) = \ln \frac{D}{2\pi T} - \frac{1}{J\rho\ \alpha z^2}\ . \tag{26}$$

When rescaling axes according to

$$\widetilde{T} = T \cdot e^{-\left(\frac{1}{\alpha}-1\right)/(J\rho z^2)}\ , \quad \widetilde{\Delta} = \Delta \cdot \alpha e^{-\left(\frac{1}{\alpha}-1\right)/(J\rho z^2)}\ , \tag{27}$$

this equation reduces to nothing more than the original mean-field equation of Eq (17), but in terms of $\widetilde{\Delta}$ and $\widetilde{T}$. Therefore, choosing a different constant value of κ cannot change the shape of Δ. Consequently, even if we promote $\kappa \to \kappa(T)$, the above mean-field condition will have an unavoidable $\Delta = 0$ solution at some finite-temperature.[11]

Another option is to attempt to match successive derivatives of Δ at the transition such that F will be continuous in all its derivatives. Trying to match all derivatives of a piecewise function that is analytic on both sides is conceptually problematic, however. To see this, one could imagine that if all successive derivatives *were* chosen to match, then both sides would share a Taylor series expansion about that point and hence be described by the same function, without need for a piecewise definition. Unless resorting to non-analytic functions, increasing the order of the phase transition is the closest one could get to a crossover.

With this in mind, we shall now see what can nevertheless be achieved by choosing the form of $\kappa(T)$. For example, let κ_0 be the value of the soft-constraint parameter that correctly picks out the Kondo temperature T_K.[12] Constructing $\kappa(T)$ as:

$$\kappa(T) = \kappa_0 + \delta \cdot \left[\operatorname{sech}\left(\frac{T}{t_1}\right) + \tanh\left(\frac{T - T_c}{t_2}\right)\right] \ , \tag{28}$$

can allow the order parameter to more gradually approach $\Delta = 0$, as shown in Figure 4, provided that t_1, t_2 and δ are suitably chosen. The choice of the hyperbolic tangent above is somewhat arbitrary, but illustrates the principle that switching between $(\kappa_0 - \delta)$ and $(\kappa_0 + \delta)$ near the transition temperature can reduce the gradient to zero at the transition. (The hyperbolic secant term, on the other hand, serves to recover some of the zero-temperature behaviour.) There likely exist other, better choices for $\kappa(T)$, depending on the desired functional form of $\Delta(T)$; the only requirement is that $\frac{d\Delta}{dT} \to 0$ as $\Delta \to 0$, which can be achieved by tuning the parameters of the function such that

$$\left.\frac{d\kappa}{dT}\right|_{T=T_c} = \frac{4J\rho}{T_c}\frac{\kappa_0^2(1-\kappa_0)^2}{(1-2\kappa_0)} \quad \text{and} \quad \kappa(T_c) = \kappa_0 \ . \tag{29}$$

One glaring deficiency of this analysis is that it is still unclear how $K(T)$ should be chosen in the first place, since it would in general[13] require solving

$$\kappa(T) = \frac{K(T)}{1 + e^{-\beta\lambda_{\mathrm{SC}}K(T)}} \ , \tag{30}$$

[11] After all, any temperature-dependent $\kappa(T)$ is just switching between different 'constants'.

[12] It is known from previous work that $\kappa_0 = \frac{1}{2}\left(1 - \sqrt{-\frac{1}{2}\rho J \ln \rho J}\right)$ [2].

[13] Note that a simple relation $K(T) \approx 2\kappa(T)$ holds near $T \approx T_c$, since $\lambda_{\mathrm{SC}} \approx 0$.

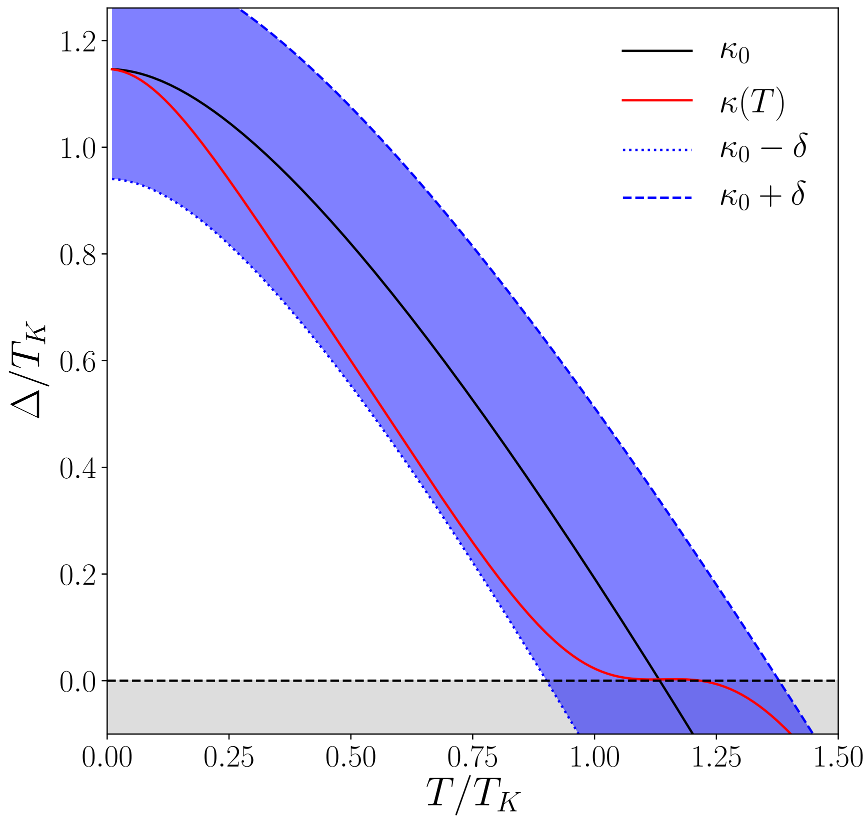

Figure 4: A plot where the form of $\kappa(T)$ is chosen to increase the order of the transition. Here, $\kappa(T)$ is given by Eq (30) (with $\delta \approx 0.018$, $t_1 \approx \frac{1}{5}T_K$ and $t_2 \approx \frac{4}{17}T_K$) and switches from one constant κ curve to another. This allows the order parameter to take on any shape bounded by the blue shaded region, whose width is determined by the magnitude of δ.

4 Finite Magnetic Field

Having explored the finite-temperature predictions for the soft-constraint in the absence of a magnetic field, we now introduce a finite magnetic field B, breaking the previous isotropy of the problem. One can include the effects of the magnetic field by introducing a Zeeman term for the magnetic impurity:

$$F_B = -g\mu_B B\left(f_\uparrow^\dagger f_\uparrow - f_\downarrow^\dagger f_\downarrow\right) = -g\mu_{\mathrm{B}} B \sum_\sigma \sigma p_\sigma^2 \ ,$$

where g is the *Landé g-factor* and the effect on the conduction electrons has been ignored.

4.1 Effect on the Mean-Field Equations

The inclusion of a magnetic field leaves the previous mean-field equations of Section 3.1 largely unchanged apart from the equation for the singly-occupied KR boson, which now becomes

$$\frac{\partial F}{\partial p_\sigma} = 0 \implies \sum_s \left[\frac{\partial F_0}{\partial \xi_s} - \frac{\partial F_0}{\partial \overline{\xi_s}}\right] \frac{\partial z_s^2}{\partial p_\sigma}\, i\Delta = -p_\sigma\left(\lambda_{\mathrm{KR}} - \lambda_\sigma - \sigma g\mu_B B\right) \ . \tag{31}$$

Without isotropy, however, solving the mean-field equations becomes appreciably more difficult, but searching for the location of the phase boundary $\Delta = 0$ in the $B - T$ plane is a slightly simpler task because it allows particle-hole symmetry to be justifiably used again.

4.2 Plotting the Phase Boundary

Setting $\Delta = 0$, the mean-field Lagrange multipliers are found to be:

$$\lambda_{\mathrm{KR}} = 0 \ , \quad \lambda_{\mathrm{SC}} = 0 \ , \quad \lambda_\sigma = -\sigma g\mu_B B \ . \tag{32}$$

Proceeding with this fixed B-field, we obtain the condition that the occupancy of the impurity is given by

$$p_\sigma^2 = \frac{1}{2}(1-\kappa) + \sigma\frac{1}{\pi}\Im\left[\psi\left(\frac{1}{2} + \frac{g\mu_B B}{2\pi i T}\right)\right] \ , \tag{33}$$

which is problematic because $\Im\left[\psi\left(\frac{1}{2} + \frac{g\mu_B B}{2\pi i T}\right)\right] \to -\frac{\pi}{2}$ in the large B limit, such that $p_\downarrow^2$ would become negative. Physically, this corresponds to one spin-state of the impurity being heavily favoured compared to the other, but this mean-field solution requires intervention with a piecewise definition to ensure that both p_σ^2 saturate sensibly.

Making a parametric plot of the phase boundary in terms of $b = \frac{g\mu_B B}{T}$ according to

$$\left(\frac{T}{T_K}\right) = \frac{1}{2\pi\sqrt{\rho J}} e^{\left(1-z^{-2}\right)/(\rho J)} \exp\left[-\Re\, \psi\left(\frac{1}{2} + \frac{b}{2\pi i}\right)\right] \quad \text{and} \quad \frac{g\mu_B B}{T_K} = \left(\frac{T}{T_K}\right) b \tag{34}$$

reveals a further problem with this approach, namely that the behaviour is dominated by the $\frac{1}{\rho J z^2}$ that appears in the exponential. If κ is left constant, then this leads to a phase boundary that curves upwards at large magnetic fields, as shown in Figure , because z^2 includes other field-dependent terms. This is despite the fact that the rest of the expression behaves similarly to the large-N limit found by Piers Coleman [1], which was used to create the original phase diagram of Figure 1.

If one is truly interested in the case of the Kondo model in a fixed magnetic field, then it appears that κ would have to acquire a (likely complicated) B-field dependence to tame this behaviour, even before starting to manipulate the *nature* of the transition. One way to circumvent this issue could be to say that one is actually interested in the case where B is not fixed, but rather a uniformly distributed stochastic field $\widetilde{B} \in [-B/2,\ B/2]$. In this case the imaginary part of $\widetilde{\psi}(g\mu_B\widetilde{B})$ averages to zero and the same large-N limit of the phase boundary is recovered for constant κ.

5 Discussion

A Constraints in the Lagrangian

The way that constraints can be implemented into the Lagrangian is illustrated in the following example. Suppose that we wanted to implement the constraint $\sum_\sigma f_\sigma^\dagger f_\sigma = 1$, say, which would be equivalent to having a partition function

$$Z = \mathrm{Tr}\left[e^{-\beta H} \, \delta\left(\sum_\sigma f_\sigma^\dagger f_\sigma - 1 \right) \right].$$

We could then express the constraint as

$$\delta\left(\sum_\sigma f_\sigma^\dagger f_\sigma - 1 \right) = \int_0^{2\pi} \frac{d\alpha}{2\pi} \, e^{-i\alpha(\sum_\sigma f_\sigma^\dagger f_\sigma - 1)} = \int_0^{2\pi i k_B T} \frac{d\lambda}{2\pi i k_B T} e^{-\beta\lambda(\sum_\sigma f_\sigma^\dagger f_\sigma - 1)},$$

where we have written $\lambda = i\alpha k_B T$. Absorbing various factors into the measure of integration, we may now write:

$$Z = \int \mathcal{D}[\lambda] \; \mathrm{Tr}\left[e^{-\beta H} e^{-\beta\lambda(\sum_\sigma f_\sigma^\dagger f_\sigma - 1)} \right].$$

Imposing this constraint can therefore be seen to be equivalent to modifying the original path integral and including an extra term in the Lagrangian:

$$L \to L + \lambda \left(\sum_\sigma f_\sigma^\dagger f_\sigma - 1 \right).$$

In fact, this is actually the Read-Newns constraint that is imposed on the occupation of the fermions f_σ (with $\sigma \in \{\uparrow, \downarrow\}$) representing the localised spin of the magnetic impurity.

B Divergent Mean-Field Parameter

To see why imposing $\langle (1 - n_\uparrow - n_\downarrow)^2 \rangle = 0$ leads to a divergent mean-field parameter, one may appreciate that by virtue of positive semi-definiteness, the mean-field condition

$$\left. \frac{\delta Z}{\delta \lambda(\tau)} \right|_{\bar{\lambda}} = 0$$

essentially becomes a condition on the integrand itself (namely something like $P e^{-\int d\tau \bar{\lambda} P} = 0$ for the constraint P), which forces $\bar{\lambda} \to \infty$.

C Deriving the Helmholtz Free Energy

The Lagrangian of Eq (4) now has all fermionic fields in quadratic form, since this was the purpose of the auxiliary bosons in the first place. One may therefore perform standard Gaussian integration over the Grassman variables to get an expression involving the determinant of the action,

$$L = \sum_\sigma \left(\cdots \quad c_{k,\sigma}^\dagger \quad \cdots \quad f_\sigma^\dagger \right) \begin{pmatrix} (\epsilon_k + \partial_\tau)\delta_{k,k'} & V^* z_\sigma \\ V z_\sigma^\dagger & (\lambda_\sigma + \partial_\tau) \end{pmatrix} \begin{pmatrix} \vdots \\ c_{k',\sigma}^\dagger \\ \vdots \\ f_\sigma^\dagger \end{pmatrix} + \cdots$$

$$\to \sum_{\sigma,n} \ln\det \begin{pmatrix} (\epsilon_k - i\omega_n)\delta_{k,k'} & V^* z_\sigma \\ V z_\sigma^\dagger & (\lambda_\sigma - i\omega_n) \end{pmatrix} + \cdots ,$$

which involves a summation over Matsubara frequencies ω_n. The mean-field impurity electron contribution to the Helmholtz free energy is therefore

$$F = -T \sum_{\sigma,n} \ln \left(-i\omega_n + \lambda_\sigma + \sum_k \frac{z_\sigma^2 |V|^2}{i\omega_n - \epsilon_k} \right) + \cdots ,$$

where $\cdots$ now includes the conduction electron contribution and all the other constraint terms previously present in the Lagrangian.

D Further Details of the Mean-Field Equations

The derivatives of z_σ^2 may be calculated quite easily as:

$$\frac{\partial z_\sigma^2}{\partial d} = \left(\frac{d}{1 - d^2 - p_\sigma^2} + \frac{p_{-\sigma}}{ep_\sigma + p_{-\sigma}d} \right) z_\sigma^2 , \quad \frac{\partial z_\sigma^2}{\partial e} = \left(\frac{e}{1 - e^2 - p_{-\sigma}^2} + \frac{p_\sigma}{ep_\sigma + p_{-\sigma}d} \right) z_\sigma^2 , \quad (35)$$

$$\frac{\partial z_\sigma^2}{\partial p_\sigma} = \left(\frac{p_\sigma}{1 - d^2 - p_\sigma^2} + \frac{e}{ep_\sigma + p_{-\sigma}d} \right) z_\sigma^2 , \quad \frac{\partial z_\sigma^2}{\partial p_{-\sigma}} = \left(\frac{p_\sigma}{1 - e^2 - p_\sigma^2} + \frac{d}{ep_\sigma + p_{-\sigma}d} \right) z_\sigma^2 . \quad (36)$$

E Impossibility of Asymptotically Approaching $\Delta = 0$

The mean-field condition

$$\Re\left[\psi\left(\frac{1}{2} + \frac{iz^2\Delta + D}{2\pi iT}\right) - \psi\left(\frac{1}{2} + \frac{iz^2\Delta}{2\pi iT}\right)\right] = \frac{1}{J\rho\, z^2}\ , \tag{37}$$

is incompatible with a limit in which $\Delta \to 0$ as $T \to \infty$ [14], unless one could also have $z^2 = 4\kappa(1-\kappa)$ also diverging which, by the restriction on the magnitude of κ for validity of the soft-constraint approach, is forbidden.

F Relating $\frac{d^2F}{dT^2}$ to $\frac{d\Delta}{dT}$

G Code Excerpts

This section contains code used to plot figures in this report. Code for the entire project, along with version history, may be found in the following *GitHub* repository:

`https://github.com/ElisR/Kondo-Soft-Constraint`

G.1 Solving the Equations in Parametric Form

```python
# Trying to recreate previous plots without resorting to iterative solutions

import numpy as np
import scipy.special as special
import scipy.optimize as optimize


global rho, J
rho = 0.4
J = 0.4


# TODO: Fix the vectorised form of this equation
def MF_lambda_SC(Temp):

    K_T = 0.5 - 0.5 * np.sqrt(1 - 1 / (1 - 0.5 * rho * J * np.log(rho * J)))

    def MF_equation_lambda(lambda_SC, T):

        k_T = K_T / (1 + np.exp(- K_T * lambda_SC / T))
        z2 = 4 * k_T * (1 - k_T)

        eq = special.digamma(0.5 + J * rho * z2 * z2 * lambda_SC /
                             (16 * T * (1 - 2 * k_T))) +\
            np.log(T) + np.log(2 * np.pi) +\
            0.5 * np.log(rho * J) - (1 - 1 / z2) / (rho * J)
```

[14] Not that the Kondo model would be valid at such a temperature, in any case.

```

        return eq

    return optimize.fsolve(MF_equation_lambda, 0, args=(Temp))


def F(s):
    """
    Returns the mean field free energy
    Function of the non-affine parameter
    """

    z2 = 4 * k(s) * (1 - k(s))
    D = np.exp(1 / (rho * J)) / np.sqrt(rho * J)

    F_orig = (s * z2 / (2 * (1 - 2 * k(s))) -
              4 * np.real(
        special.loggamma(0.5 +
                         s * J * rho * z2 * z2 / (16 * (1 - 2 * k(s))) +
                         D / (2 * np.pi * 1j * t(s))) -
        special.loggamma(0.5 +
                         s * J * rho * z2 * z2 / (16 * (1 - 2 * k(s)))))
              ) * t(s)

    F_extra = t(s) * (K(s) * s / (1 + np.exp(- K(s) * s)) -
                      np.log(1 + np.exp(- K(s) * s)))

    return (F_orig + F_extra)

def K(s):
    """
    Returns the value of the soft-constraint parameter
    """

    K_0 = 0.5 - 0.5 * np.sqrt(1 - 1 / (1 - 0.5 * rho * J * np.log(rho * J)))

    #return K_0 * (1 + np.exp(- K_0 * s * (1 + np.exp(- K_0 * s * (1 + np.exp(- K_0 *
    ↪  s))))))
    #return K_0 * (1 + 0.5 * np.exp(- 1 * s))
    return K_0


def k(s):
    """
    Returns the value of the modified soft-constraint parameter
    Modification comes from thermal occupation of "empty" pseudo-fermions
    """

    return K(s) / (1 + np.exp(- K(s) * s))


def t(s):
    """
    Returns normalised temperature for given value of non-affine parameter
    """

    T = (1 / (2 * np.pi)) * (1 / np.sqrt(rho * J)) *\
        np.exp((1 - 1 / (4 * k(s) * (1 - k(s)))) / (rho * J)) *\
        np.exp(- special.digamma(
               0.5 + J * rho * s * np.square(k(s) * (1 - k(s))) /
               (1 - 2 * k(s))))

    return T


def delta(s):
    """
    Returns the mean-field hybridisation field at a given non-affine parameter
    """

    k_T = k(s)
    z2 = 4 * k_T * (1 - k_T)

    d = np.pi * J * rho * z2 * s * t(s) / (8 * (1 - 2 * k_T))

    return d
```

G.2 Plotting Δ Parametrically

```python
import New_Term_Parametric as parametric_SC

import numpy as np
import matplotlib.pyplot as plt


def plot_delta_vs_T():
    """
    Plotting delta vs T using a robust parametric plot, with extra term
    """

    ss = np.linspace(0, 250, 1500)

    ts = parametric_SC.t(ss)
    deltas = parametric_SC.delta(ss)

    fig = plt.figure(figsize=(8.4, 8.4))

    plt.rc('text', usetex=True)
    plt.rc('font', family='serif')

    plt.fill_between(np.linspace(-0.2, np.max(ts) + 0.2, 10),
                     0, -0.5, color='#dddddd')

    # Plot the figure
    plt.plot(ts, deltas, "k-")

    plt.xlabel(r'$ T / T_K $', fontsize=26)
    plt.ylabel(r'$ \Delta / T_K $', fontsize=26)

    ax = plt.gca()
    ax.set_xlim([0, np.max(ts) + 0.05])
    ax.set_ylim([-0.18, 1.25])
    ax.tick_params(axis='both', labelsize=20)

    plt.axhline(y=0, linestyle='--', color='k')


    plt.savefig("new_delta_vs_T_parametric.pdf",
                dpi=300, format='pdf', bbox_inches='tight')
    plt.clf()


def plot_F_vs_T():
    """
    Plotting the free energy against temperature
    """

    ss = np.linspace(0, 45, 1000)

    ts = parametric_SC.t(ss)
    Fs = parametric_SC.F(ss)

    fig = plt.figure(figsize=(8.4, 8.4))

    plt.rc('text', usetex=True)
    plt.rc('font', family='serif')

    plt.plot(ts, Fs, "k-")

    plt.xlabel(r'$ T / T_K $', fontsize=26)
    plt.ylabel(r'$ F / T_K $', fontsize=26)

    ax = plt.gca()
    ax.tick_params(axis='both', labelsize=20)

    plt.savefig("new_F_vs_T_parametric.pdf",
                dpt=300, format='pdf', bbox_inches='tight')
    plt.clf()


def plot_lambda_vs_T():
```

```python
    """
    Trying to nail down the form of lambda_SC against temperature
    """

    Ts = np.linspace(0.2, 1.2, 250)

    lambdas = np.zeros(np.size(Ts))

    ss_parametric = np.linspace(0, 45, 1000)
    ts = parametric_SC.t(ss_parametric)
    lambdas_parametric = np.multiply(ss_parametric, ts)

    for i in range(np.size(Ts)):
        T = Ts[i]

        lambdas[i] = parametric_SC.MF_lambda_SC(T)
        lambdas[i] = (lambdas[i] >= 0) * lambdas[i]

    fig = plt.figure(figsize=(8.4, 8.4))

    plt.rc('text', usetex=True)
    plt.rc('font', family='serif')

    plt.plot(Ts, lambdas, "r-", label="fsolve")
    plt.plot(ts, lambdas_parametric, "k--", label="parametric")

    plt.xlabel(r'$ T / T_K $', fontsize=26)
    plt.ylabel(r'$ \lambda $', fontsize=26)

    ax = plt.gca()
    ax.tick_params(axis='both', labelsize=20)
    ax.legend()

    plt.savefig("s_vs_T.pdf",
                dpi=300, format='pdf', bbox_inches='tight')


def plot_eq_vs_lambda():
    """
    Investigating the nature of the MF equation
    """

    T = 0.6

    lambdas = np.linspace(-20, 20, 250)

    eqs = np.zeros(np.size(lambdas))

    for i in range(np.size(eqs)):
        eqs[i] = MF_equation_lambda(lambdas[i], T)

    fig = plt.figure(figsize=(8.4, 8.4))

    plt.rc('text', usetex=True)
    plt.rc('font', family='serif')

    plt.plot(lambdas, eqs, "r-", label=("T = " + str(T)))

    plt.xlabel(r'$ \lambda $', fontsize=26)
    plt.ylabel(r'$ MF_{eq}(\lambda) $', fontsize=26)

    ax = plt.gca()
    ax.tick_params(axis='both', labelsize=20)
    ax.legend()

    plt.savefig("eq_vs_lambda.pdf",
                dpi=300, format='pdf', bbox_inches='tight')


def main():
    # Setting various parameters of the problem

    global rho, J
    rho = 0.4
    J = 0.4

```

```
    plot_delta_vs_T()
    plot_F_vs_T()


if __name__ == '__main__':
    main()
```

References

[1] P. Coleman *Introduction to Many Body Physics* Cambridge University Press (2015)

[2] G. Goldstein, C. Castelnovo and C. Chamon *Mean-Field Method for Handling Null Constraints on Positive-Semidefinite Operators* Draft (2017)

[3] G. Kotliar and A. E. Ruckenstein *New Functional Integral Approach to Strongly Correlated Fermi Systems: The Gutzwiller Approximation as a Saddle Point* Phys. Rev. Lett. **57**, 1362 (1986)

[4] N. Read, and D. M. Newns *A New Functional Integral Formalism for the Degenerate Anderson Model.* Journal of Physics C: Solid State Physics 16.29 (1983)

[5] M. Abramowitz *Handbook of Mathematical Functions, With Formulas, Graphs, and Mathematical Tables* Dover Publications, Inc. (1974)