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Part III Physics

Final Project Report

Mean-Field Study of Kondo Phase Diagram

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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 which (in its simplest single impurity flavour) has the following Hamiltonian:

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

in which conduction electrons $c_{k,\sigma}$ have a Hamiltonian composed of the usual kinetic energy term as well as a term coupling the spin density of conduction electrons at the location of a (single) localised spin $\vec{S}$.

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. Since then, much attention has been devoted to other rich features of the general Kondo problem, 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.

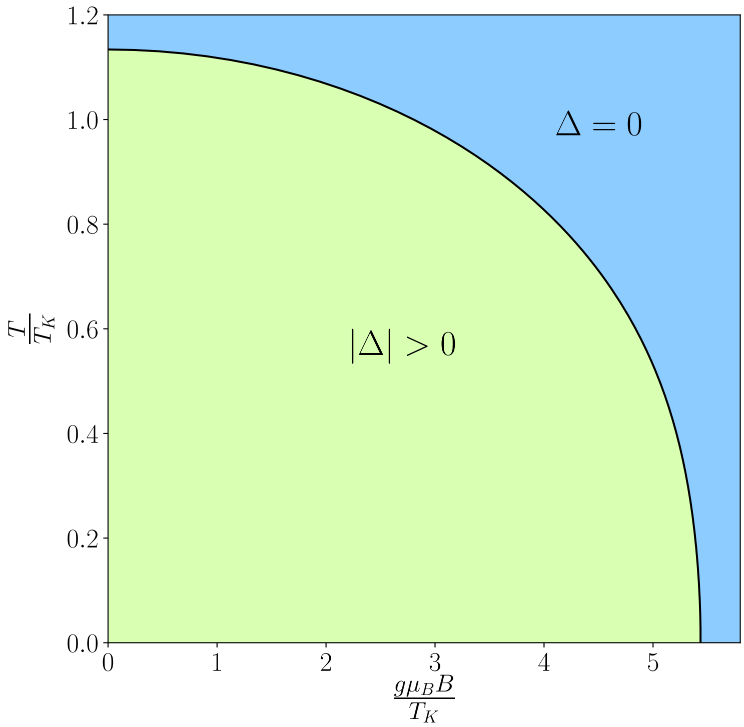

Figure 1: A representative phase diagram obtained from another mean field approach (with calculations found in [1]), which shows a distinct phase transition between two phases. The Kondo temperature T_K is used to make quantities dimensionless.

2 Theoretical Background

2.1 Kondo Model

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:

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

from which many properties of the system may then be derived. [1] 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 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.

2.3 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*.

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

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

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

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: [2]

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

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 Mean-Field Equations

We start by deriving the self-consistency equations that must hold for the mean-field description of the system. Since $F=-k_{\mathrm{B}}T\ln Z$ [3], 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 Appendix C to obtain an effective free energy

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

[2]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.

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

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 [4]:

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

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

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

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

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 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

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

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. [5]

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) immediatley 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

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

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.

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 $\lambda_{\mathrm{SC}} \geq 0$

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

$$\lambda_{\mathrm{SC}} = \frac{2\Delta}{\pi J\rho}\left(4 + \frac{1}{\kappa} + \frac{1}{1-\kappa}\right) \geq 0\ , \tag{18}$$

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).

[5] 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.

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 of the free energy:

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

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 $\ln\Gamma(u)$ [6], is calculated as $\left[\frac{d\psi}{du}\right]^{-1} = u - \frac{1}{2} + \frac{1}{12u} + \dots$. 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

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

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

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

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.

3.4 Investigating the Nature of the Transition

4 Finite Magnetic Field

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 $Pe^{-\int d\tau \bar{\lambda} P} = 0$ 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,

$$\begin{aligned} L &= \sum_\sigma \begin{pmatrix} \cdots & c^\dagger_{k,\sigma} & \cdots & f^\dagger_\sigma \end{pmatrix} \begin{pmatrix} (\epsilon_k + \partial_\tau)\delta_{k,k'} & V^* z_\sigma \\ V z^\dagger_\sigma & (\lambda_\sigma + \partial_\tau) \end{pmatrix} \begin{pmatrix} \vdots \\ c^\dagger_{k',\sigma} \\ \vdots \\ f^\dagger_\sigma \end{pmatrix} \quad + \quad \cdots \\ &\to \quad \sum_{\sigma,n} \ln\det \begin{pmatrix} (\epsilon_k - i\omega_n)\delta_{k,k'} & V^* z_\sigma \\ V z^\dagger_\sigma & (\lambda_\sigma - i\omega_n) \end{pmatrix} \quad + \quad \cdots \quad , \end{aligned}$$

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

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

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:

$$\frac{\partial z_\sigma^2}{\partial d} = \left(\frac{d}{1 - d^2 - p_\sigma^2} + \frac{p_{-\sigma}}{e p_\sigma + p_{-\sigma} d} \right) z_\sigma^2 \, , \quad \frac{\partial z_\sigma^2}{\partial e} = \left(\frac{e}{1 - e^2 - p_{-\sigma}^2} + \frac{p_\sigma}{e p_\sigma + p_{-\sigma} d} \right) z_\sigma^2 \, , \tag{22}$$

$$\frac{\partial z_\sigma^2}{\partial p_\sigma} = \left(\frac{p_\sigma}{1 - d^2 - p_\sigma^2} + \frac{e}{e p_\sigma + p_{-\sigma} d} \right) z_\sigma^2 \, , \quad \frac{\partial z_\sigma^2}{\partial p_{-\sigma}} = \left(\frac{p_\sigma}{1 - e^2 - p_\sigma^2} + \frac{d}{e p_\sigma + p_{-\sigma} d} \right) z_\sigma^2 \, . \tag{23}$$

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