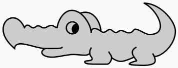

Mean-Field Study of Kondo Phase Diagram

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May 2, 2018

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Plan

1. Introduction
2. Finite Temperature Study
3. Conclusion

Introduction

Kondo Model

Single localised spin interacting with conduction electrons $c_{k,\sigma}$

Model Hamiltonian

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

- Can map impurity spin DOF to fermions f_σ
- Think of it as describing interacting fermions $c_{k,\sigma}$ and f_σ

Goal

Describe phase diagram for this model using *mean-field theory*

Path Integral $\to$ Mean-Field Theory

- Project framed in terms of path integral
- Treats Boltzmann sum as a functional integral over field configurations

Many-Body Path Integral

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

- Similar to Feynman path integral approach, but with *imaginary time* $\tau = it/\hbar$ and associated Lagrangian L

Mean-Field Theory

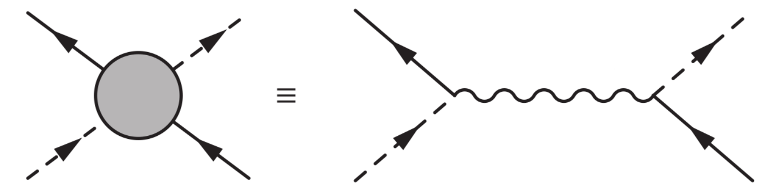
Avoid this difficult integral by making stationary phase approximation i.e. *minimise*

New Fields

- Lagrangian similar to original Hamiltonian, with extra dynamical terms: $L = H_{\text{Kondo}} + c^\dagger \partial_\tau c$
- **But**, interaction introduces difficult non-quadratic terms

Resolution

Introduce a new field V that mediates this interaction:



Constraints

- Making such variable changes may require **constraints**

e.g. Spin-1/2 $\to$ Fermion Mapping

$$s_z = \frac{1}{2}(f_\uparrow^\dagger f_\uparrow - f_\downarrow^\dagger f_\downarrow), \quad s_+ = f_\uparrow^\dagger f_\downarrow, \quad s_- = f_\downarrow^\dagger f_\uparrow$$

Unfaithful representation unless constraint imposed:

$$f_\uparrow^\dagger f_\uparrow + f_\downarrow^\dagger f_\downarrow = 1$$

- Implement constraints by adding Lagrange multipliers $\{\lambda_i\}$ and extremesing too:

$$L = \ldots + \lambda_{\mathrm{RN}}(f_\uparrow^\dagger f_\uparrow + f_\downarrow^\dagger f_\downarrow - 1)$$

Soft-Constraint Approach

- Now consider rewriting the same constraint:

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

- Equivalent **but** can't be done at mean-field level since

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

Soft-Constraint

How about introducing a new fermion h obeying $h^\dagger h = 0$, but combining these constraints by instead imposing

$$(1 - n_\uparrow - n_\downarrow)^2 - K h^\dagger h = 0 \quad ?$$

Soft-Constraint Approach

- How could $(1 - n_\uparrow - n_\downarrow)^2 - Kh^\dagger h = 0$ be any better?
- Have introduced a new free parameter K into description
- Provided $K > 0$ and $K \neq 1$, constraint operator now has positive *and* negative eigenvalues:

$$\{ \quad 1, \quad (1-K), \quad 0, \quad -K \quad \}$$

Consequence

New composite constraint picks out both constraints, while still being possible at mean-field level

Finite Temperature Study

Obtaining MF Equations

Minimise free energy $F_{\mathrm{MF}} = -k_{\mathrm{B}} T \ln Z$ wrt all variables:

$$\frac{\partial F_{\mathrm{MF}}}{\partial \Delta} = 0, \qquad \frac{\partial F_{\mathrm{MF}}}{\partial \lambda_{\mathrm{SC}}} = 0, \qquad \ldots$$

- Restricting search to reals leads to 9 equations
- Isotropy of $B = 0$ case $\implies$ 7 unique variables / equations

How does this relate to a phase diagram?

Defining an Order Parameter Δ

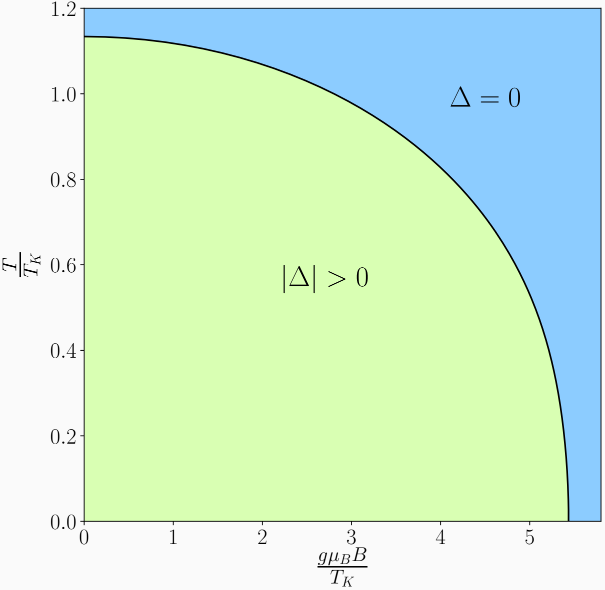
- Recall the (now constant) bosonic field V mediating the interaction

Now Define Δ

$$\Delta \propto |V|^2$$

- $\Delta \to 0$ implies $c_{k,\sigma}$ and f_σ fermions no longer interact
- Value of Δ characterises different phases

Expected Phase Diagram *(Approximate)*



Classifying Phase Transitions

- Phase transitions classified by discontinuities in successive derivatives of F wrt thermodynamic variables

Limitation of Mean-Field Theory

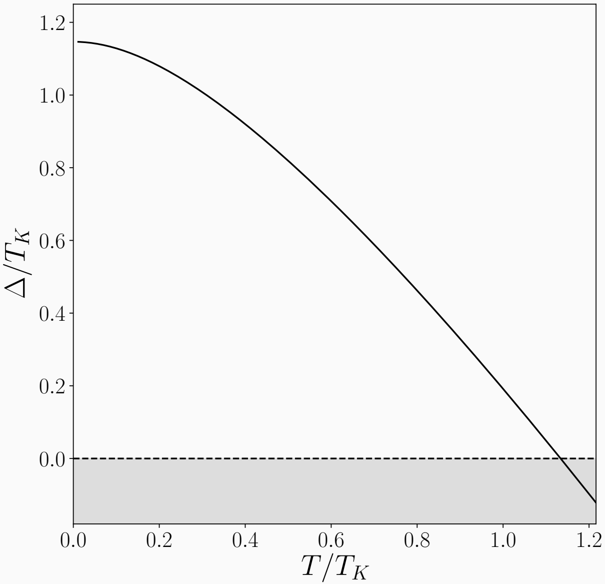
- As usual, mean-field theory predicts a phase transition
- **But**, more advanced treatments show a smooth *crossover*

- Can study nature of PT by looking at form of $F(T)$

***e.g.* Heat Capacity**

$$C = \frac{\partial E}{\partial T} = -T\frac{\partial^2 F}{\partial T^2}$$

Behaviour of Order Parameter Δ



Unavoidable Phase Transition?

Crucially, $\Delta < 0$ unphysical $\implies$ Δ assumes *piecewise* form

- **Q:** Can a piecewise function have all derivatives match?
- **A:** Not if it has a Taylor expansion.

What about non-analytic functions?

$$f(T) \approx \begin{cases} e^{-1/(T-T_c)^2} & T < T_c \\ 0 & T \geqslant T_c \end{cases}$$

Could we promote $K \to K(T)$ to remove discontinuities in $\partial^n F$?

Unavoidable Phase Transition?

- Can't seem to remove this phase transition
- K still limited by $\langle (1 - n_\uparrow - n_\downarrow)^2 \rangle \leqslant 1$
- Choosing $K(T)$ made complicated since $\widetilde{K} = K\langle h^\dagger h \rangle$
- Have thermal occupation of h fermion too:

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

Conclusion

Take Home Points

- Path integrals can describe many-body systems at finite T
- MF theory considers optimal solution only - much easier
- Soft-Constraint is an alternative approach to implementing constraints in the Lagrangian
- SC introduces a new free parameter into description, but is seemingly not enough to remove second-order PT

Backup

Final Lagrangian

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