Mean-Field Study of Kondo Phase Diagram

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Plan

Introduction

Kondo Model

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

Model Hamiltonian

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

Can map spin DOFs of impurity onto fermions f_σ

Path Integral → 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

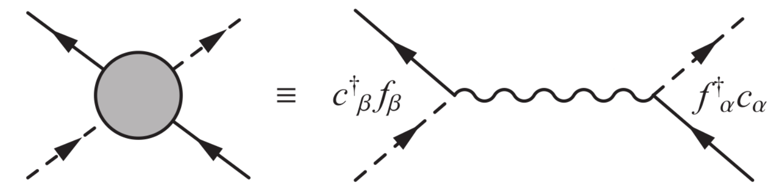
Avoid this difficult integral by making stationary phase approximation i.e. *minimise*

New Fields

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

Resolution

Introduce a new field V that mediates this interaction:



Constraints

- Making such variable changes sometimes requires **constraints**

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

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

Representation isn't faithful unless we impose the constraint:

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

- These constraints are implemented by adding Lagrange multipliers $\{\lambda_i\}$ and extremesing wrt these too - *e.g.*

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

Soft-Constraint Approach

- Now consider rewriting the same constraint:

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

- **But** this 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 stilll being possible at mean-field level

Finite Temperature Study

Solving Mean-Field Equations

Generate MF equations via minimisation:

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

Deriving Heat Capacity

Unavoidable Phase Transition?

Behaviour of Order Parameter Δ

Finite Field Study

Incorporating $B \neq 0$

Increased Difficulty of Mean-Field Equations

Conclusion

Questions?

Backup

Final Lagrangian

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