Berry Phase and the Breakdown of the Quantum to Classical Mapping for the Quantum Critical Point of the Bose-Fermi Kondo model

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The phase diagram of the Bose-Fermi Kondo model contains an SU(2)-invariant Kondo-screened phase separated by a continuous quantum to classical mapping transition from a Kondo-destroyed local moment phase. We analyze the effect of the Berry phase term of the spin path integral on the quantum critical properties of this quantum impurity model. For a range of the power-law exponent characterizing the spectral density of the dissipative bosonic bath, neglecting the influence of the Berry phase term makes the fixed point Gaussian. For the same range of the spectral density exponent, incorporating the Berry phase term leads instead to an interacting fixed point, for which a quantum to classical mapping breaks down. Some general implications of our results are discussed.

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Quantum criticality has become a new paradigm in the study of the overall phase diagram of strongly correlated electron systems. Universal properties of a quantum critical point (QCP) are traditionally described in terms of a mapping to the classical critical fluctuations of an order parameter in elevated dimensions [1]. The quantum to classical mapping is based on the notion that slow fluctuations of the order parameter are the only critical degrees of freedom. This notion has been challenged in a number of contexts. In the heavy fermion metals, an anti-ferromagnetic QCP can accommodate new quantum modes, which are characterized by a critical destruction of the Kondo effect [2].

In addition to lattice Kondo systems, the critical Kondo destruction has also been studied in the Bose-Fermi Kondo model (BFKM) [6, 7]. The first indication for the violation of the quantum to classical mapping came from a study in a dynamical large-N limit of the spin-isotropic BFKM [8]. For the spectral density of the bosonic bath of the form \(|\omega|^\epsilon \text{sgn}\omega|\), that corresponds to the large-N limit yields an interacting fixed point only for \(0 < \epsilon < 1/2\) but also for \(1/2 < \epsilon < 1\). Related conclusions were drawn based on numerical renormalization group (NRG) studies of the related quantum impurity models with Ising anisotropy [9, 10]. Very recently, the results of the Ising anisotropic models have been the subject of renewed interest, in light of the contrasting behavior between the NRG results and those from Monte Carlo simulations of a classical Ising chain [11, 12, 13].

Given these recent developments, it is timely to address the issue of the quantum to classical mapping in the spin-isotropic BFKM. For this purpose, we consider the model in terms of a coherent-state spin path integral representation, which highlights the role of the Berry phase term. By separately considering the cases in the presence/absence of the Berry phase term, we establish that the breakdown of the quantum to classical mapping originates from the interference effect of the Berry phase term.

The spin-isotropic Bose-Fermi Kondo model: The model is specified by the Hamiltonian,

\[
\mathcal{H}_{\text{bfkm}} = j_K \mathbf{S} \cdot \mathbf{s} + \sum_{p\sigma} E_p c_{p\sigma}^\dagger c_{p\sigma}^\dagger + g_0 \sum_{p} \mathbf{S} \cdot (\phi_p + \phi_p^\dagger) + \sum_{p} w_p \phi_p^\dagger \phi_p. \tag{1}
\]

Here \(\mathbf{S}\) is a spin-1/2 local moment, \(j_K\) and \(g_0\) are the Kondo coupling and the coupling constant to the bosonic bath respectively, \(c_{p\sigma}^\dagger\) describes a fermionic bath with a constant density of states, \(\sum_{p} \delta(\omega - E_p) = N_0\), and \(\phi_p^\dagger\) is the bosonic bath with the spectral density:

\[
\text{Im} \chi^{-1}_0(\omega) = \sum_{p} [\delta(\omega - w_p) - \delta(\omega + w_p)] \\
\sim |\omega|^{1-\epsilon} \text{sgn}(\omega) \Theta(\omega - |\omega|). \tag{2}
\]

The partition function of this model is

\[
\mathcal{Z} = \int \mathcal{D}[\vec{c}, c_s, \vec{\phi}, \phi] \delta(\vec{n}|^2 - 1) \exp[-S(\vec{c}, c_s, \phi, \vec{n})], \tag{3}
\]

where \(c_s\) is a Grassmann variable for the fermionic coherent state, while \(\phi\) and \(\vec{n}\) are c-numbers for the bosonic and spin coherent states respectively. The action is given by

\[
S = i \text{sgn}(\omega(\vec{n})) + \int_0^\beta d\tau \sum_{p}(\Sigma \sigma \delta_{p\sigma} \partial_{\tau} c_{p\sigma} + \phi_{p} \partial_{\tau} \phi_{p}) \\
+ \int_0^\beta d\tau H_{\text{isokin}}(\vec{c}, c, \vec{\phi}, \phi, s\vec{n}). \tag{4}
\]

**Berry phase of the coherent-state spin path integral:** Eq. (4) is written in terms of the spin (or SU(2)) coherent states [14, 15]. Just like bosonic coherent states, spin coherent states are generated by a unitary operator

\[
|\xi> = T(\xi)|0> \quad T(\xi) = e^{i \mathbf{J}^r - \xi \mathbf{J}^z} \tag{5}
\]
acting on a suitably defined vacuum $|0>$. $J^+ / J^-$

is the raising/lowering operator of the spin algebra, and

$\xi$ is a $c$-number. Alternatively, the coherent state can

be represented as a point on the three-dimensional unit

sphere, $\hat{n}$, which is parameterized by the two angles $\Theta$

and $\phi$; $\xi = (1/2) \Theta e^{i \phi}$.

In Eq. 4, the path integral runs over all periodic paths, i.e. $\hat{n}(0) = \hat{n}(\beta)$. $\omega(\hat{n})$ is a geometrical phase

and equals the area on the unit sphere enclosed by $\hat{n}(\tau)$. $s$

is the spin of the local moment. In the following, we

will be considering the appropriate SU(N) or O(N) generalizations of the SU(2) model.

Model in the absence of the Berry phase: We consider first the quantum critical properties of the BFKM without the Berry phase term. Simply removing the Berry phase term from the functional integral, Eq. 4, results in an ill-defined measure. Restraining however the spin path integral to a subset of paths with identical Berry phase, e.g. the subset of all great circles, the Berry phase term can be absorbed into the normalization of the partition function. After integrating out the bosonic bath, this leads to

$$\mathcal{L} = i\mu(\tau) \sum_i n_i^2 - 1 + J_K \tilde{n}(\tau) \cdot \tilde{c}(\tau) \tilde{\sigma} c(\tau)$$

$$+ \sum_{\sigma} \int_0^\beta dt' \tilde{c}_\sigma(\tau) G_{\tilde{c}}^{-1}(\tau - \tau') c_{\sigma}(\tau')$$

$$+ g^2 \int_0^\beta d\tau' \tilde{n}(\tau) G_\phi(\tau - \tau') \tilde{n}(\tau'),$$

with $i\mu(\tau)$ being a Lagrangian multiplier enforcing the constraint $\sum_i n_i^2 = 1$, $J_K = sj_K/2$, and $g = sg_0$. $G_c = \langle T_\tau \tilde{c}_\sigma(\tau) c_{\sigma}(0) \rangle_0$, and $G_\phi = \langle T_\tau \phi(\tau) \phi(0) \rangle_0$. The terms involving the electron fields are quadratic in them, so the electron fields can be exactly integrated out as well:

$$\mathcal{Z} = \int \mathcal{D}[\hat{n}] \text{Det} \left[ G_{\tilde{c}}^{-1}(\tau - \tau') \delta_{\sigma,\sigma'} + J_K \tilde{n}(\tau) \cdot \tilde{\sigma} \delta(\tau - \tau') \right]$$

$$\times \exp\left[-\int_0^\beta d\tau i\mu(\tau) \sum_i n_i^2(\tau) - 1 \right]$$

$$+ g^2 \int_0^\beta d\tau \int_0^\beta d\tau' \tilde{n}(\tau) G_\phi(\tau - \tau') \tilde{n}(\tau') \right].$$

With the help of $\exp[\ln\text{Det}M] = \exp[\text{Tr}\ln M]$ the effective action can be expressed as

$$S = \int_0^\beta d\tau i\mu(\tau) \sum_i n_i^2 - 1$$

$$+ g^2 \int_0^\beta d\tau \int_0^\beta d\tau' \tilde{n}(\tau) G_\phi(\tau - \tau') \tilde{n}(\tau')$$

$$+ \text{Tr} \ln(-G_{\tilde{c}}^{-1} \delta_{\sigma,\sigma'})$$

$$+ \text{Tr} \ln(1 - J_K G_c \tilde{n}(\tau) \cdot \tilde{\sigma} \delta_{\sigma,\sigma'} \delta(\tau - \tau')).$$

The logarithm can be expanded in powers of $J_K G_c \tilde{n}(\tau) \cdot \tilde{\sigma} s_{\sigma,\sigma'} \delta(\tau - \tau')$. The odd powers in this expansion vanish, since the Pauli matrices are traceless.

In order to systematically study this action, we will first generalize it in such a way that the fluctuations around a saddle point vanish. To do so, we extend the O(3) invariance of the action to an $O(N^2 - 1)$ symmetry, with $\hat{n}$ containing $M = N^2 - 1$ components. This corresponds to a generalization of Eq. 4 to the case with an $O(N^2 - 1) \times SU(N)$ symmetry. We rescale the coupling constants $J_K$ and $g$ in terms of $N$, so that a non-trivial large-N limit ensues. The required rescaling of $J_K$ is determined by the N-dependence of the quadratic term in the expansion of the logarithm of Eq. 4. $Tr(J_K \tilde{n} \cdot \tilde{A} G_c) = Tr(J_K \sum_{i=1}^N n_i A_i G_c)^2$, where the trace is over the (extended) spin space. The $A_i$ are Hermitian $N \times N$ matrices of unit determinant. We make use of the invariance of the trace and expand the generators in terms of $N \times N$ matrices $B^l_l (l = 1, \ldots, N^2)$: $A_i = \sum_i n_i B_i^l$. The set $B^l_l$ is chosen such that the $l$th matrix $B^l_l$ has $B^l_l s_{t,s} = e^{i\phi}$ and $B^l_l t_{t,s} = e^{-i\phi}$ if and only if $l = N(s - 1) + t$ with $s = 1, \ldots, N$ and $t = 1, \ldots, N$. All other elements of $B^l_l$ vanish identically. The particular value of $\phi$ is left unspecified since it will only affect the expansion coefficients $a_{l,s}$. $G_c$ is diagonal in the spin space. Therefore, the quadratic term should scale as $N \cdot M$. Rescaling $J_K \rightarrow J_K^2 / M = J_K^2$ renders the second term proportional to $N$. Rescaling $g \rightarrow g/N = \tilde{g}$ has the same effect on the similar term in the effective action involving the bosonic bath. Finally, the constraint needs to be generalized to $\sum_i n_i^2 = q_0 N$.

Taking all these together, the large-N limit of the $O(N^2 - 1) \times SU(N)$ model leads to a saddle-point equation

$$\chi^{-1}_{\text{loc}}(\tau) = \mu_0 + J_K^2 G_{c,\tau}(\tau) G_{c,\tau}(\tau) + \tilde{g}^2 G_\phi(\tau).$$

(9)

At the saddle point, $i\mu(\tau) = \mu_0$ satisfies

$$\sum_n \chi_{\text{loc}}(\omega_n) = \mu_0.$$

(10)

The second term of the RHS of Eq. 4 is just the particle hole bubble of the conduction electrons, with $G_{c,\tau}(\tau) G_{c,\tau}(\tau) \sim 1/\tau^2$. The long-time behavior of $G_\phi(\tau)$ is specified by Eq. 4, $G_\phi(\tau) \sim 1/\tau^{2-\gamma}$. Solving the saddle point equation for a diverging $\chi_{\text{loc}}(\tau)$ results in a critical $\chi_{\text{loc}}$ with $\chi_{\text{loc}}(\tau) \sim 1/\tau^{\gamma}$, implying

$$\chi_{\text{loc}}(\omega, T = 0) \sim 1/(i\omega)^{1-\gamma}.$$
to a quartic coupling of the field \( u(\tau) \):

\[
\frac{u}{N} \prod_i \int d\omega_i n(\omega_i).
\]

The scaling dimension of the field \( n(\omega) = (2 - \epsilon)/2 \) follows from Eq. (2). As a result, the scaling dimension of the quartic coupling is \( u = 2(\frac{4}{3} - \epsilon) \). For \( \epsilon < 1/2 \), \( u \) is a relevant perturbation and the low-energy properties of the system will be governed by an interacting fixed point with \( u^* \neq 0 \) and consequently hyperscaling and \( \omega/T \)-scaling. This interacting fixed point is the Ginzburg-Wilson-Fisher fixed point of the local \( \phi^4 \)-theory. For \( 1/2 \leq \epsilon < 1 \), \( u \) is irrelevant and will flow to zero; the Gaussian fixed point will be stable. A vanishing quartic coupling makes the approach to the fixed point singular; in other words, \( u \) is dangerously irrelevant and therefore spoils hyperscaling and \( \omega/T \)-scaling. In the context of the long-ranged Ising model this process has been discussed recently in [11]. The dangerously irrelevant coupling leads to

\[
\chi_{loc}(\omega = 0, T) \sim 1/\omega^2.
\]

Comparing Eqs. (11) and (13) shows that \( \chi_{loc}(\omega, T) \) disobey an \( \omega/T \)-scaling.

**Model in the presence of the Berry phase**: In order to generalize SU(2) to SU(N) within a path integral formulation it is necessary to use proper coherent states over SU(N). Such coherent states can be constructed in analogy to the SU(2) case and a corresponding Berry phase term for the SU(N) spin path integral with similar topological properties emerges [15, 16, 21]. This model in the presence of the Berry phase term can be studied in a dynamical large-N limit of the SU(N) \( \times \) SU(\( \kappa \)) NBFKM:

\[
\mathcal{H}_{\text{MBFK}} = (J_K/N) \sum_\alpha S \cdot s_\alpha + \sum_{p, \alpha, \sigma} E_p c^\dagger_{p, \alpha, \sigma} c_{p, \alpha, \sigma} + (g/\sqrt{N}) S \cdot \Phi + \sum_p w_p \Phi^\dagger_{p, \alpha} \Phi_{p, \alpha},
\]

where \( \sigma = 1, \ldots, N \) and \( \alpha = 1, \ldots, M \) are the spin and channel indices respectively, and \( \Phi \equiv \sum_p (\Phi^\dagger_{p, \alpha} \Phi_{p, \alpha}) \) contains \( N^2 - 1 \) components. The local moment is expressed in terms of pseudo-fermions \( S_{\sigma, \sigma'} = f^\dagger_{\sigma} f_{\sigma'} - \delta_{\sigma, \sigma'} Q/N \), where \( Q \) is related to the chosen irreducible representation of SU(N) [16, 21]. The quartic term between conduction electrons and pseudo-fermions is expressed in terms of a bosonic decoupling field \( B_\alpha \). The large-N saddle-point equations are

\[
\begin{align*}
\Sigma_B(\tau) &= -G_c(\tau) G_f(-\tau); \\
\Sigma_f(\tau) &= \kappa G_c(\tau) G_B(\tau) + g^2 G_f(\tau) \Phi(\tau); \\
G_B^{-1}(i\omega_n) &= 1/J_K - \Sigma_B(i\omega_n); \\
G_f^{-1}(i\omega_n) &= i\omega_n - \lambda - \Sigma_f(i\omega_n);
\end{align*}
\]

(15)

together with a constraint \( G_f(\tau \to 0^-) = Q/N \). Here, \( \kappa = M/N \) and \( \lambda \) is a Lagrangian multiplier. The analytically continued equations (15) can be self-consistently solved for any frequency (\( \omega \)) and temperature (\( T \)) [8]. Eqs. (15) completely capture the (full) quantum dynamics of the problem and contain the effect of the Berry phase in the path integral approach. At the QCP, the order parameter susceptibility [8] behaves as

\[
\chi_{loc}(\omega = 0, T) \sim 1/\omega^{1-\epsilon}; \quad \chi_{loc}(\omega = 0, T) \sim 1/T^{1-\epsilon}
\]

(16)

for all \( 0 < \epsilon < 1 \). Fig. (a) shows the \( \omega - T \)-scaling of \( \chi_{loc}(\omega, T) \) for \( \epsilon = 2/3 > 1/2 \). The numerical parameters are \( \kappa = 1/2, Q/N = 1/2, \) and \( N_0(\omega) = (1/\pi) \exp(-\omega^2/\pi) \) for the conduction electron density of states. The nominal bare Kondo scale is \( T_K^0 = \min(1, 0.05) \), with the exponent very close to 1. Fig. 1(b) shows the \( \omega - T \)-scaling, see Fig. 1(b). By contrast, at the Gaussian fixed point \( \chi_{loc}(\omega, T) \) is solved for any frequency (\( \omega \)) and temperature (\( T \)) [8].
The exponent in this temperature dependence is shown in Fig. 2(b) for \( \omega / T \).

Since the exponent in this temperature dependence is the same as that of its frequency dependence at \( T = 0 \), it cannot be modified by any subleading temperature-dependent terms that could possibly be generated by a dangerously irrelevant coupling at a finite \( N \). [By contrast, in the absence of the Berry phase term, the temperature dependence \( \Delta M(\omega, T) = M(\omega, T) - M(\omega = 0, T = 0) \), is shown in Fig. 2(b) for \( \omega = 0 \). It has the important property

\[
\Delta M(\omega = 0, T) \sim T^{1-\epsilon}.
\]

(18)

Without the Berry phase term, an interacting fixed point with the \( \omega / T \)-scaling occurs for \( 0 \leq \epsilon < 1/2 \) but a Gaussian fixed point spoiling the \( \omega / T \)-scaling arises for \( 1/2 \leq \epsilon < 1 \). With the Berry phase term, the Bose-Fermi Kondo model shows an interacting fixed point with \( \omega / T \)-scaling over the entire range \( 0 < \epsilon < 1 \).

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[22] [0 > for SU(2) coherent states can be any of the 2s+1 states \( |s, m > \) with \( m = -s, \ldots, s \). Customary choices are \( |0 > = |s, s > \) or \( |0 > = |s, -s > \), so that the coherent states can be generated by either \( J^- \) or \( J^+ \) alone. The determination of the normalizing factor which gives rise to the Berry phase in the path integral requires the proper use of the Baker-Cambell-Hausdorff formula in...
analogy to bosonic coherent states, \( T(z) = e^{[za^\dagger - za]} = e^{-|z|^2/2}e^{za^\dagger}e^{za}. \)