Hidden Caldeira-Leggett dissipation in a Bose-Fermi Kondo model

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We show that the Bose-Fermi Kondo model (BFKM), which may find applicability both to certain dissipative mesoscopic qubit devices and to heavy fermion systems described by the Kondo lattice model, can be mapped exactly onto the Caldeira-Leggett model. This mapping requires an ohmic bosonic bath and an Ising-type coupling between the latter and the impurity spin. This allows us to conclude unambiguously that there is an emergent Kosterlitz-Thouless quantum phase transition in the BFKM with an ohmic bosonic bath. By applying a bosonic numerical renormalization group approach, we thoroughly probe physical quantities close to the quantum phase transition.

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The Bose-Fermi Kondo model (BFKM) (or equivalently the spin-boson-fermion model), originally introduced by Si and coworkers\textsuperscript{1} and by Sengupta\textsuperscript{2} to describe peculiar quantum critical behaviors in heavy-fermion Kondo lattice systems, involves a single impurity spin being coupled both to a bosonic bath and to a fermionic bath. Resulting from the nontrivial competition between these distinct baths, a rich phase diagram emerges from this model (See, e.g., Refs. \textsuperscript{3} and \textsuperscript{4}). More generally, a great interest is currently devoted to the understanding of the Kondo entanglement breakdown mechanism due to the presence of extra (here, bosonic) quantum fluctuations resulting in striking quantum phase transitions. In this Letter, we revisit the case where the impurity spin $S = 1/2$ is coupled to an ohmic bosonic bath with a continuum spectrum – ohmic means that the bosonic correlation function in time $t$ decays as $1/t^2$ – through an Ising coupling. The anisotropic Hamiltonian under consideration thus takes the form:

\begin{equation}
H = \hbar S_z + H_{sf} + H_{sb},
\end{equation}

\begin{equation}
H_{sf} = \frac{J_f}{2} \left( \Psi_\uparrow(0) \Psi_\uparrow(0) S_z + \text{h.c.} \right) + v_f \sum_{\sigma = \uparrow, \downarrow} \int_{-\infty}^{\infty} dx \, \Psi_\sigma(x) i \partial_x \Psi_\sigma(x),
\end{equation}

\begin{equation}
H_{sb} = -\frac{v_b}{\sqrt{2}K_b} S_z + \frac{v_b}{4\pi} \int_{-\infty}^{\infty} dx \partial_x \Phi(x),
\end{equation}

where $\hbar$ is a magnetic field, $\Psi_\sigma(x)$ and $\Phi$ represent the fermionic and bosonic fields; $v_f$ is the velocity of the bosons and $K_b^{-1} \neq 0$ the typical coupling between the bosons and the impurity spin; Recall that $K_b^{-1} = 0$ means no coupling between the impurity spin and the bosonic environment. In Eq. (2), $v_f$ is the Fermi velocity. Without loss of generality, the one-dimensional character of the Hamiltonian $H_{sf}$ can be viewed as a result of the point-like character of the impurity and the rotational symmetry. Besides, we omit the Ising part of the Kondo coupling $J_z$ due to its minor effect (see the last page).

Our interest in the model is also motivated by the fact that this model may be realized in mesoscopic dissipative setups involving qubits, as pointed out by one of us recently\textsuperscript{5}. More precisely, the impurity spin can embody the two allowed charge states of a big metallic grain close to a given degeneracy point and $\hbar$ being proportional to the gate voltage measures deviations from this degeneracy point\textsuperscript{6}. The conduction electrons stand for the electrons both in the metallic grain ($\Psi_\uparrow$) and in a nearby reservoir electrode ($\Psi_\uparrow$), and the $J_{\perp}$ (Kondo) term denotes the tunneling process of an electron from lead to grain that flips (through the raising operator $S_z$) the charge state of the grain, and vice-versa. Note that here the spin index $\sigma = (\uparrow, \downarrow)$ is completely artificial and refers to the position of an electron in the structure (lead or grain). The original spin of the electrons are assumed to be polarized (“spinless electrons”) due to the application of a strong magnetic field. The bosons represent the electromagnetic noise in the gate voltage stemming from the finite resistance $R$ in the gate lead, and the spin-boson coupling reflects the effect of the voltage noise on the charge fluctuations of the grain. Here, $K_b \equiv R_K/2R$ with $R_K = 2\pi\hbar/e^2$ the quantum of resistance. Two of us have extended this model to one-dimensional reservoir leads being embodied by a Luttinger liquid behavior\textsuperscript{7} and also to two strongly capacitively-coupled large quantum dots (which can be reduced to a single charge qubit)\textsuperscript{8}. As a first step, the model of Eqs. (1) has been extensively studied\textsuperscript{9} by using a perturbative renormalization group (RG) approach. A quantum phase transition is discovered at the critical value of $K_b$\textsuperscript{10}:

\begin{equation}
(\bar{K}_b)_c^{-1} = J_{\perp}/\pi v_f = 2\Delta/\omega_c,
\end{equation}

where $\omega_c$ is the high energy cutoff in the theory and $\Delta = J_{\perp}\omega_c/2\pi v_f$. The RG flow equations suggest that the phase transition is of the Kosterlitz-Thouless (KT) type. On the other hand, a more rigorous approach is required in order to unambiguously prove the KT transition as well as to scrutinize the evolution of physical quantities in the vicinity of the quantum phase transition. In this Letter, we explore an exact mapping of the BFKM in Eqs. (1)\textsuperscript{11}. We properly demonstrate that this model can be mapped onto the Caldeira-Leggett (CL) model\textsuperscript{12} with the effective dissipation strength

\begin{equation}
\alpha = 1 + (4K_b)^{-1},
\end{equation}

where $\omega_c$ is the high energy cutoff in the theory and $\Delta = J_{\perp}\omega_c/2\pi v_f$. The RG flow equations suggest that the phase transition is of the Kosterlitz-Thouless (KT) type.
implies that $\phi$ to write down the $\omega$ spin gets only coupled to the parameter $\alpha$ by the local action $\exp$ The local action for the boson fields and the Hamiltonian (1) becomes that of an impurity (nation.) By performing the unitary transformation $U_k = \exp\{i\sqrt{2}\alpha\phi(0)S_z\}$ to turn the $\Delta$ term into a transverse magnetic field $\Delta S_z$, leading to

$$\tilde{H} = H_S - \sqrt{2}\alpha v_s \phi_s(0)S_z + \frac{v_s}{4\pi} \int_{-\infty}^{\infty} dx [\partial_x \phi_s(x)]^2,$$

where $H_S = hS_z + \Delta S_x$ and $\alpha$ is given in Eq. (6).

This mapping is crucial because it irrefutably reveals an originally hidden correspondence between the BFKM of Eqs. (1-3) and the CL model in which the breakdown of the Kondo physics (quantum coherence) due to dissipation is clearly established. For example, a KT type transition was predicted in Ref. 12 in the context of ohmic dissipation and this has been solidly confirmed through the NRG, either by refermionizing the bosonic degrees of freedom and then mapping the CL model onto the anisotropic Kondo model, or directly by resorting to the bosonic NRG\textsuperscript{13}. For $\Delta \rightarrow 0$ the KT transition is known to occur at $\alpha = 1$ implying in the BFKM a critical $(K_0)_c^{-1} \rightarrow 0$ from Eq. (13): since $\Delta \rightarrow 0$, the Kondo energy scale $T_K$ characterizing the emergence of a bound state between the local moment and the conduction electrons vanishes and thus the local moment remains unscreened whatever the coupling between the dissipative mode $\partial_x \phi(0)$ and the local spin.

To understand more deeply the connection between the CL model and the Kondo phenomenon, we can proceed from Eq. (8) along the lines of Ref. 13 and precisely recover the anisotropic Kondo model. The effective Kondo parameters here are given by $J_z = \pi v_s \Delta/\omega_c$, and $J_2 = 4\pi v_s (1-\sqrt{\alpha})$. Thus, one can clearly distinguish two phases: a Kondo (delocalized) realm when $J_z > -|J_1|$ and a ferromagnetic Kondo phase which embodies an unscreened (localized) moment when $J_z < -|J_1|$. This enables us to rigorously predict a KT phase transition in the BFKM when $J_z = -|J_1|$ which implies a critical $\alpha_c = 1 + (K_0)_c^{-1}/4 = 1 + \Delta/(2\omega_c)$ when assuming $0 < \Delta \ll \omega_c$: this reinforces the intuition gained from the perturbative RG analysis of the BFKM\textsuperscript{22}. Since Bethe-Ansatz calculation\textsuperscript{12} can only be applied to this model when $\alpha < \alpha_{c,\text{cl}}$, we seek to apply the (bosonic) NRG on Eq. (8) to probe $(S_z)$ versus $h$ and $\chi_{loc}(T)$ very close to $\alpha_c$. Those quantities have not been studied in Ref. 13.

NRG endeavors close to the transition.—The strength of the NRG lies in its nonperturbative nature and the ability to resolve arbitrarily small energies\textsuperscript{19,20,21}. This allows to provide important information in the phase transition region. For convenience, the Hamiltonian (8) can be rewritten as

$$\tilde{H} = H_S + \omega_c \int_0^1 dc \left[ -\sqrt{2}\alpha c (a + a_1^\dagger)S_z + c a_1^\dagger a c \right],$$

Conceptually, we can visualize $S_{\phi_s}$ as the action linked to an Hamiltonian $H_{\phi_s}$ with the effective velocity $v_s = \omega_c a$ ($a$ is the short-distance cutoff which will be used below) and modeling a single bosonic bath with the dissipative parameter $\alpha$ coupled to the impurity spin. The link with the CL model of a two-level system with ohmic dissipation\textsuperscript{13} becomes clear when applying the unitary transformation $U_k = \exp\{i\sqrt{2}\alpha\phi(0)S_z\}$ to turn the $\Delta$ term into a transverse magnetic field $\Delta S_z$, leading to

$$H_S - \sqrt{2}\alpha v_s \phi_s(0)S_z + \frac{v_s}{4\pi} \int_{-\infty}^{\infty} dx [\partial_x \phi_s(x)]^2, \quad (8)$$

and therefore the two models belong to the same class of universality. It immediately follows that there is a KT quantum phase transition in the BFKM, separating a Kondo phase and an unscreened spin phase. Moreover, it irrefutably demonstrates the important Eq. (4). Even though the Bethe-Ansatz method\textsuperscript{22} can be exploited in the Kondo region, it breaks down in the vicinity of the quantum phase transition \textsuperscript{22} (which must be identified as the antiferromagnetic-ferromagnetic transition in the anisotropic Kondo model). We resort to a bosonic numerical RG (NRG) technique applying to the CL model\textsuperscript{20}. Of interest to us here is the spin magnetization at temperature $T = 0$, $\langle S_z \rangle$, as well as the (local) spin susceptibility $\chi_{loc}(T)$ versus $T$. In the mesoscopic realizations, $\langle S_z \rangle = \langle Q \rangle - 1/2$, where $Q$ is the charge operator on the (large) dot, can be measured with very high precision\textsuperscript{20}.
In the fermionic case, each boson site allows for an infinite number of states, so that the result converges at large \( N \).

### NRG Results

In Fig. 1 (left) we show the flow of the ground state expectation value \( \langle S_z \rangle \) as a function of the iteration variable \( N \). At small \( \Delta/\omega_c \), for \( \alpha = 1.4 \) and for any \( h < 0 \), after a few iterations we find that \( \langle S_z \rangle \) flows rapidly to 1/2, which is in agreement with the localized (dissipative) phase of the CL model as well as with the perturbative RG analysis of the BFKM. This corresponds to an unscreened local spin or a particle which is localized in one of the two allowed levels. A strong dissipative Ising coupling with the bosonic bath definitely hinders the Kondo effect to develop. In contrast, for \( \alpha = 0.6 \), we show that \( \langle S_z \rangle \) flows to saturating values which deviate from 1/2 and fall drastically with the decreasing \( h \). Moreover, \( \langle S_z \rangle \) yields a linear dependence versus \( h \) around \( h = 0 \) which indicates a fully screened Kondo effect.

We have fitted the NRG curve for \( \alpha = 0.6 \) (which is sufficiently far from \( \alpha_c \)) with Bethe-Ansatz results applying to the Kondo regime. The dependence of \( \langle S_z \rangle \) on \( h \) at various \( \alpha \) for \( \Delta = 0.01 \) and \( \omega_c = 1 \) is displayed in Fig. 1.

We have carefully followed the progressive destruction of the delocalized Kondo regime when approaching the quantum phase transition at different applied magnetic fields. More specifically, we can infer the Kondo temperature \( T_K \) from \( \langle S_z \rangle \) versus \( h \) based on the following scaling argument. The (Kondo) Fermi liquid type state emerging for \( \alpha < \alpha_c \) is embodied by a constant (local) spin susceptibility \( \chi_{\text{loc}} \approx \eta \) which must be identified as the.

In Fig. 2 (left) we show the local susceptibility \( \chi_{\text{loc}}(T) \) as a function of \( T \). The open circles are the numerical data for \( T = T_N = 1.1\Delta^{-N} \) and lines are guides to the eyes. The open circles are the numerical data and the dashed line represents the fitting curve \( \ln T_K = -4.67/(1.15 - \alpha) \). The NRG parameters, \( \Delta \) and \( \omega_c \), are the same as in Fig. 1.

[Diagram of flow of the ground state expectation value of \( S_z \) as a function of iteration variable \( N \).]

**FIG. 1:** (color online) Left: Flow of \( \langle S_z \rangle \) with the iteration \( N \). The dashed line is for \( h = -0.0001 \) (unscreened realm). All the solid lines correspond to \( \alpha = 0.6 \) (Kondo regime), and from top to bottom, to \( h = -10^{-4}, -5 \times 10^{-5}, -5 \times 10^{-4}, -10^{-6}, -10^{-6} \). Right: \( \langle S_z \rangle \) as a function of \( h \). The open circles sitting on top of the \( \alpha = 0.6 \) curve are the Bethe-Ansatz results. Parameters are \( \Delta = 0.01 \) and \( \omega_c = 1 \). The NRG parameters are \( \Lambda = 2, N_l = 100, N_h = 8 \), and \( N_d = 500 \).

In Eq. (10) the spin gets only coupled to the first (0th) site of the bosonic chain, and the remaining part of the chain is characterized by on-site energies \( \epsilon_n \) and hopping parameters \( t_n \). They satisfy a set of recursion relations and their derivations as well as for the precise definition of the \( b_n \) boson operators. It is important to note that both \( \epsilon_n \) and \( t_n \) decay exponentially as \( \Lambda^{-n} \) as a result of the logarithmic discretization. This allows us to solve the model in Eq. (10) in an iterative way: first we diagonalize \( H_N \) exactly, keep the \( N_s \) lowest energy levels and then use the recursion relation between \( H_{N+1} \) and \( H_N \) derived from Eq. (11) to diagonalize \( H_{N+1} \). Typically, the result converges at large \( N \approx 25 \). In contrast to the fermionic case, each boson site allows for an infinite number of bosons and hence a truncation of the \( (N_h + 1) \) boson states is necessary. Throughout this paper, we use \( N_s = 100 \) and \( N_h = 8 \) (except the 0th site for which \( N_d = 500 \)); those values are approximately those used in Ref. 13. We have also used another set of parameters \( (N_s = 150 \) and \( N_h = 12 \) and found a good agreement. The quantities \( \langle S_z \rangle(h) \) and \( \chi_{\text{loc}}(T) = d\langle S_z \rangle(T)/dh \mid_{h=0} \) are also calculated iteratively.

**FIG. 2:** (color online) The local susceptibility \( \chi_{\text{loc}}(T) \) as a function of \( T \). The open circles are the numerical data for \( T = T_N = 1.1\Delta^{-N} \) and lines are guides to the eyes. Inset: Logarithm of the Kondo energy scale \( T_K \) versus \( \alpha \) for \( \alpha \) close to \( \alpha_c \). The solid circles are the numerical data and the dashed line represents the fitting curve \( \ln T_K = -4.67/(1.15 - \alpha) \). The NRG parameters, \( \Delta \) and \( \omega_c \), are the same as in Fig. 1.
we reach $\alpha_c(\Lambda \rightarrow 1) = 0.98 (\approx 1)$. The effect of the dissipative coupling becomes weaker when increasing $\Delta$. For each $\Delta$, we have repeated the above-mentioned extrapolation procedure and precisely extracted $\alpha_c$ which basically corresponds to the critical bosonic coupling at which the Kondo scale strictly vanishes. The resulting $\alpha_c$ as a function of $\Delta$ obeys $\alpha_c(\Delta) = 0.974 + 0.537\Delta/\omega_s$ which clearly agrees with our expectation from the CL mapping. The formation of a Fermi liquid ground state in the Kondo realm is also clearly observed in Fig. 2 through the $\chi_{\text{loc}}(T)$ versus $T$ plot: For $\alpha < \alpha_c = 1.15$, $\chi_{\text{loc}}(T)$ saturates to a constant for $T < T_K$ whereas for $T$ above $T_K$ the Curie’s law $\chi_{\text{loc}} \propto 1/T$ is well satisfied. At the transition point, we clearly observe that the $\chi_{\text{loc}}(T) \propto 1/T$ behavior persists down to the lowest temperatures.

Finally, we would like to briefly comment on the effect of the Ising coupling term $J_z$ between the spin and the fermions, originally present in the heavy-fermion systems but absent in the mesoscopic realizations under consideration, close to the phase transition point. For $\alpha \rightarrow 1$, $\varphi \approx \varphi_s$ and thus the second term in the right hand side of Eq. $\varphi$ becomes $\sqrt{\mathfrak{A}}(\mathfrak{J}_z - \mathfrak{A}\mathfrak{J}_s)\partial_x\varphi_s(0)\mathfrak{S}_z$. This immediately leads to a critical $\alpha_c \approx 1 + O(\Delta) + O(J_z)$, which is qualitatively consistent with Ref. $\mathfrak{2}$.

**Conclusion.**—We have demonstrated that the BFKM, with an ohmic bosonic bath and an Ising-type coupling between the latter and the impurity spin, and the CL model belong to the same class of universality. This unambiguously proves the existence of a KT phase transition at zero temperature in the former model when tuning the Ising dissipative coupling. We have chosen to resort to the bosonic NRG to investigate in detail physical quantities like the spin magnetization $\langle S_z \rangle$ versus the magnetic field $h$ close to the quantum phase transition where Bethe-Ansatz calculations break down. The latter clearly reflects two phases: the “localized” phase typical of an unscreened moment and the “delocalized” Kondo realm characterized by a Kondo energy scale which goes to zero exponentially fast close to the KT transition. Comparing with the recent fermionic NRG of the BFKM, the bosonic NRG approach can be extended to the case of a sub-ohmic bath, which might be relevant for the quest of quantum criticality in heavy-fermion systems.$\mathfrak{2}$

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