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Continuous-Time Monte Carlo study of the pseudogap Bose-Fermi Kondo model

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Abstract. We study the pseudogap Bose-Fermi Anderson model with a continuous-time quantum Monte Carlo (CT-QMC) method. We discuss some delicate aspects of the transformation from this model to the Bose-Fermi Kondo model. We show that the CT-QMC method can be used at sufficiently low temperatures to access the quantum critical properties of these models.

Over the past decade intermetallic compounds have served as model systems to study instabilities of metallic magnets near zero temperature [1–3]. In particular the quantum critical properties found in several heavy fermion compounds seem to be beyond the Ginzburg-Landau paradigm of criticality [4–7]. A natural explanation for the new type of criticality invokes inherently-quantum critical modes in addition to the gapless order parameter fluctuations. In the case of heavy fermion compounds, the additional critical mode has been identified with the destruction of the Kondo effect [8–10]. Since the destruction of the Kondo effect is local in space it can be systematically studied in simplified, local models. In these quantum impurity systems the critical state only appears at the (spatial) boundary of suitable hosts.

In the present article, we study the Kondo-destroying quantum critical point in the pseudogap Bose-Fermi Kondo model (PBFKM) with Ising anisotropy, defined as

\begin{equation}
H_{\text{PBFKM}} = \sum_{k,\sigma} \epsilon_k c^\dagger_{k,\sigma} c_{k,\sigma} + \sum_{q} \omega_q \phi_q^\dagger \phi_q + J S \cdot \sum_{k,k',\sigma,\sigma'} c^\dagger_{k,\sigma} \bar{\sigma} c_{k',\sigma'} + g S_z \sum_{q} (\phi_q^\dagger + \phi_q). \tag{1}
\end{equation}

Where $\epsilon_k$, $\omega_q$ are the fermionic and bosonic bath dispersions, $J$ is the Kondo coupling between the spin of the conduction electrons and the spin of the impurity, $\bar{\sigma}$ is a vector of Pauli spin matrices and $g$ is the coupling between the $z$-component of the impurity spin and the bosonic bath. We take a pseudogap density of states (DOS) for the conduction electrons, $\rho_c(\epsilon) \propto |\epsilon|^r$ for $|\epsilon| < D$ and $0 < r < 1/2$ where we have taken the Fermi energy to be zero, and a sub-ohmic density of states for the bosons, $\rho_B(\omega) = \sum_q |\delta(\omega - \omega_q) - \delta(\omega + \omega_q)| \propto \text{sgn}(\omega)|\omega|^\alpha$ up to a cutoff $\Lambda$. A perturbative renormalization group study has been used carried out for the Bose-Fermi Kondo model with non-zero conduction-electron DOS ($r = 0$) in both the Ising and continuous spin symmetry cases [11]. For the pseudogapped case ($r \neq 0$), such a study has been possible only for the continuous spin symmetry case [12]. The numerical renormalization group method, on the other hand, has been used to study the model in the Ising limit [13]. Eq. (1) has as particular

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limits the pseudogap Kondo and the Bose-Fermi Kondo models, which have recently been studied using related methods [14, 15]. Despite the seeming simplicity of Eq. (1), it is hard to study the quantum critical properties of the PBFKM directly. In particular, the quantum-relaxational regime (\(h\omega < k_B T\)) is difficult to address theoretically. The quantum-relaxational regime of the pseudogap Kondo model has been studied previously [15], by applying a CT-QMC algorithm [16–18] to the pseudogap Anderson model whose low-energy sector in the local moment regime can be mapped onto the pseudogap Kondo model via a Schrieffer-Wolff (SW) transformation. Since the Anderson model only involves fermions, standard perturbative expansion methods can be applied to it. In the CT-QMC approach, the full perturbative expansion in terms of the hybridization between conduction and localized fermions is then sampled stochastically using a Monte Carlo algorithm [16–18].

The corresponding Bose-Fermi Anderson model is

\[
H = \sum_{k,\sigma} \epsilon_k c_{k,\sigma}^\dagger c_{k,\sigma} + \epsilon_d (n^\uparrow + n^\downarrow) + U n^\uparrow n^\downarrow + \sum_{k,\sigma} (V_k d_{\sigma}^\dagger c_{k,\sigma} + V_k^* c_{k,\sigma}^\dagger d_{\sigma}) + \sum_q \omega_q \phi_q^\dagger \phi_q + g \frac{(n^\uparrow - n^\downarrow)}{2} \sum_q (\phi_q^\dagger + \phi_{-q}),
\]

where \(\epsilon_d\) is the energy level of the impurity, \(U\) is the on-site interaction, \(n_\sigma = d_{\sigma}^\dagger d_{\sigma}\), \(V_k\) is the hybridization of the impurity with the conduction electrons, and \(S_z = \frac{1}{2}(n^\uparrow - n^\downarrow)\). The CT-QMC method has been extended to treat ohmic bosonic baths coupled to the charge of the impurity by invoking a Firsov-Lang (FL) transformation [19, 20]. Here we extend this approach to treat a sub-ohmic bosonic bath that couples to the spin of the impurity and explore the possibility of using it to access the quantum critical properties. As it turns out, the generators of the FL and SW transformations do not commute, raising the important question as to which is the proper order of applying the two transformations.

We focus on the particle-hole symmetric case, \(U = -2\epsilon_d\). First, we perform the FL transformation to eliminate the term linear in \(\phi\) exactly. We choose a generator \(S_{FL} = g S_z \sum q \frac{1}{\omega_q} (\phi_q^\dagger - \phi_{-q})\) and the transformed Hamiltonian \(\tilde{H} = e^{S_{FL}} H e^{-S_{FL}}\) is

\[
\tilde{H} = \sum_{k,\sigma} \epsilon_k c_{k,\sigma}^\dagger c_{k,\sigma} + \epsilon_d (n^\uparrow + n^\downarrow) + \tilde{U} n^\uparrow n^\downarrow + \sum_{k,\sigma} (V_k \tilde{d}_{\sigma}^\dagger c_{k,\sigma} + V_k^* c_{k,\sigma}^\dagger \tilde{d}_{\sigma}) + \sum_q \omega_q \phi_q^\dagger \phi_q,
\]

where \(\tilde{d}_{\sigma} = d_{\sigma} \exp(\frac{\sigma g}{2} \sum q \frac{1}{\omega_q} (\Phi_q^\dagger - \Phi_{-q}))\), \(\sigma = \pm 1\) for \(\uparrow/\downarrow\), \(\tilde{U} = U + \frac{1}{2} g^2 \sum q \frac{1}{\omega_q}\), and \(\tilde{c}_d = -\tilde{U}\). Note that \(\tilde{n}_\sigma = n_\sigma\) and the transformation does not destroy particle-hole symmetry.

A modified transformation [21] is used to eliminate the hybridization term in Eq. (3). We only consider the Kondo limit, and for simplicity neglect the \(k\) dependence of \(V_k = V\). The generator \(S_{SW}\) is standard but with \(U, \epsilon_d, d, d^\dagger\) replaced by \(\tilde{U}, \tilde{c}_d, \tilde{d}, \tilde{d}^\dagger\), namely \(S_{SW} = \sum_{k,\sigma} V \left(\frac{1-n_\sigma}{\epsilon_d - \epsilon_k} + \frac{n_\sigma}{\epsilon_d + U - \epsilon_k}\right) (\tilde{d}_{\sigma}^\dagger c_{k,\sigma} - c_{k,\sigma}^\dagger \tilde{d}_{\sigma})\). Writing the Hamiltonian in Eq. (3) as \(\tilde{H} = H_0 + H_1 + \tilde{H}_h\) where \(H_0 = \epsilon_d (n^\uparrow + n^\downarrow) + \tilde{U} n^\uparrow n^\downarrow + \sum_{k,\sigma} \epsilon_k c_{k,\sigma}^\dagger c_{k,\sigma} + \sum_q \omega_q \phi_q^\dagger \phi_q\) and \(\tilde{H}_h = \sum_{k,\sigma} V (\tilde{d}_{\sigma}^\dagger c_{k,\sigma} + c_{k,\sigma}^\dagger \tilde{d}_{\sigma})\), we have \(H' = e^{S_{SW}} \tilde{H} e^{-S_{SW}} \approx H_0 + H_1 + \left[S_{SW}, H_0\right] + \frac{1}{2} [S_{SW}, \tilde{H}_h]\).

Projecting out unoccupied and doubly occupied states we arrive at

\[
H' = \sum_{k,\sigma} \epsilon_k c_{k,\sigma}^\dagger c_{k,\sigma} + \sum_q \omega_q \phi_q^\dagger \phi_q + \sum_{k,k',\sigma} \left(\frac{1}{2} \tilde{W}_{k,k'} + \frac{1}{4} \tilde{J}_{k,k'}\right) c_{k,\sigma}^\dagger c_{k',\sigma}^\dagger c_{k',\sigma} c_{k,\sigma} - \sum_{k,k'} \tilde{J}_{k,k'} \left(\frac{1}{2} (s_{k,k'}^+ \tilde{S}^+ + s_{k,k'}^- \tilde{S}^-) + s_{k,k'}^+ \tilde{S}^+\right),
\]

where \(\tilde{W}_{k,k'} = V^2 (\frac{1}{\epsilon_k - \epsilon_{k'}} + \frac{1}{\epsilon_d - \epsilon_{k'}}), \tilde{J}_{k,k'} = V^2 (\frac{1}{\epsilon_k - \epsilon_{k'}} - \frac{1}{\epsilon_d - \epsilon_{k'}} - \frac{1}{\epsilon_d - \epsilon_{k'}})\) is the Kondo coupling, \(\tilde{S}^+ = S^+ \exp(g \sum_q \frac{1}{\omega_q} (\Phi_q - \Phi_{-q}))\), \(\tilde{S}^- = S^- \exp(-g \sum_q \frac{1}{\omega_q} (\Phi_q - \Phi_{-q}))\).
The single particle Green function, \( \langle \hat{S}_k \rangle \), reduces the Hamiltonian in Eq. (2) to the resonant level model with a pseudogap. The impurity to unity. For small \( g = 0 \) the bosonic bath decouples from the problem and can be ignored, and taking for large \( g \), we obtain quantitative agreement, within numerical accuracy, in the long time behavior for both \( G \) and \( \chi \).

We now will discuss the opposite order of transformations, namely, \( H'' = e^{SFL}e^{SW}H e^{-SW}e^{-SFL} \). Applying the SW transformation, projecting out charge fluctuations and then applying the FL transformation arrives at equation (4), however with \( W_{k,k'} \), \( J_{k,k'} \) replaced by \( W_{k,k'}, J_{k,k'} \). We see that applying first the SW transformation, which is not exact, completely ignores the bosonic baths’ influence on the charge degrees of freedom of the impurity. Whereas applying the FL transformation first, which is exact, correctly captures the bosonic baths’ influence on the Anderson model which lowers the Kondo coupling. The non-commutativity of the two transformations quantitatively affects the effective Kondo scale at the quantum critical point, but it does not change the universal scaling behavior of the quantum critical properties because the critical value of the Kondo coupling is not universal.

As a check on the CT-QMC approach we first compare the single particle Green function and the spin susceptibility for the numerical result with \( U = g = 0 \). Comparing the exact calculation and the CT-QMC result we see agreement for both \( G \) and \( \chi \).

\[
\chi(\tau, T) = \frac{1}{2} \sum_{\alpha, \beta} \sum_{k,k'} \frac{\tilde{\sigma}_{\alpha, \beta} \tilde{\sigma}_{\alpha, \beta}}{\omega - \epsilon_d - \sum_{k,k'} \frac{|V_k|^2}{|\omega - \epsilon_k|^2}}
\]

The imaginary time Green function can then be obtained by Fourier transform, \( G(\tau, \beta) = \int_{-\infty}^{\infty} d\omega \frac{e^{-i\omega\tau}}{e^{\beta\omega} - 1} \text{Im}(G(\omega + i0^+)) \) and the local spin susceptibility can be constructed \( \chi(\tau, \beta) = -\frac{1}{2} G(\tau, \beta) G(-\tau, \beta) \). As seen in figure 1 we obtain quantitative agreement, within numerical accuracy, in the long time behavior for both \( G(\tau, \beta) \) and \( \chi(\tau, \beta) \).

We now turn to the quantum-critical properties of the PBFKM defined in Eq. (2) by measuring the static spin susceptibility, described below. In what follows we fix \( r = 0.4 \) and \( g = 0 \). After the (FL) transformation, the Hamiltonian in Eq. (3) can be expanded in the hybridization term. We use the CT-QMC algorithm to calculate the partition function, the single particle Green function and the local spin susceptibility. Fixing \( U = 0.025D \) and varying \( g \) we can tune the model to a quantum critical point (QCP). Within the CT-QMC approach we measure the local spin susceptibility \( \chi(\tau, \beta) = (T, S_z(\tau)S_z(0)) \) and then calculate the static susceptibility \( \chi_{\text{stat}}(\beta) = \int_0^\beta d\tau \chi(\tau, \beta) \), where we have set the Lande g-factor and Bohr magneton to unity. For small \( g \), the finite \( U \) gives rise to a Kondo screened local moment; the static susceptibility approaches a constant for temperatures well below the Kondo temperature, \( T_K \).

For large \( g \), the impurity spin decouples from the conduction band and follows the fluctuations of the bosonic bath; the static susceptibility takes the Curie-Weiss form, \( \chi_{\text{stat}}(T) \sim T^{-1} \). At the QCP, the bosonic bath acts to decohere and destroy the Kondo effect [14]. Consequently, at the
Figure 2. Static susceptibility in the vicinity of the quantum critical point, \( g_c \approx 0.18D \). For \( r = 0 \) the Kondo temperature is, \( T_K \approx 0.029D \). Well below \( T_K \) we see divergence of the static susceptibility as \( \chi_{\text{stat}} \sim T^{-0.609} \).

QCP the scaling of \( \chi_{\text{stat}}(T) \) acquires an anomalous exponent \( \chi_{\text{stat}}(T) \sim T^{-\alpha} \) for temperatures well below \( T_K \). As seen in figure 2, using the CT-QMC approach we obtain \( g_c \approx 0.18D \) and in the vicinity of the quantum critical point, \( \chi_{\text{stat}}(T) \sim T^{-x} \) with \( x = 0.609 \). Our calculated exponent agrees with the numerical renormalization group result within numerical accuracy [13]; the same exponent is also expected in related pseudogap Bose-Fermi Kondo model with continuous spin symmetry [12] or the Bose-Fermi Kondo model with Ising symmetry but with \( r = 0 \) [11].

In conclusion, we have shown that the low energy properties of the pseudogap Bose-Fermi Kondo model can be addressed within a continuous-time quantum Monte Carlo approach. We have demonstrated that this approach correctly reproduces the exactly solvable limit of the pseudogap resonant level model, and been able to determine the critical behavior of the static local spin susceptibility in an interacting case.

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