Bose-Fermi Kondo model with Ising anisotropy: cluster-Monte Carlo approach

Stefan Kirchner a,*, Qimiao Si a,

a Department of Physics & Astronomy, Rice University, Houston, TX 77005-1892, USA

Abstract

The Bose-Fermi Kondo model (BFKM) captures the physics of the destruction of Kondo screening, which is of extensive current interest to the understanding of quantum critical heavy fermion metals. There are presently limited theoretical methods to study the finite temperature properties of the BFKM. Here we provide some of the consistency checks on the cluster-Monte Carlo method, which we have recently applied to the Ising-anisotropic BFKM. We show that the method correctly captures the scaling properties of the Kondo phase, as well as those on approach to the Kondo-destroying quantum critical point. We establish that comparable results are obtained when the Kondo couplings are placed at or away from a Toulouse point.

PACS: 05.70.Jk, 71.10.Hf, 75.20.Hr, 71.27.+a

Key words: Bose-Fermi Kondo models; quantum phase transitions; quantum-to-classical mapping; scaling properties

The sub-Ohmic Bose-Fermi Kondo models are of considerable interest in the context of quantum critical heavy fermions [1] and certain mesoscopic structures [2]. The finite temperature scaling properties of the BFKM have been studied using an $\epsilon$-expansion [3] and also at certain large-N limit [4]. At finite $\epsilon$ and $\epsilon$, standard Monte-Carlo methods [5] can be used for the Ising-anisotropic BFKM but the lowest temperature that has been reached is about $0.01 T_K^0$, where $T_K^0$ is the bare Kondo scale. Recently, we have applied a cluster-Monte Carlo method to this problem [6], which is able to reliably reach temperatures of the order of $10^{-3} - 10^{-4} T_K^0$. The purpose of this paper is two-fold. First, we demonstrate the consistency of this method for both the Kondo phase and the quantum critical regime. Second, we address the effect of the deviation from the Toulouse point on the finite-temperature scaling properties; previous studies of the Ising-anisotropic BFKM [6] have focused on the Toulouse point of the Kondo couplings.

The cluster-Monte Carlo method builds on the well-established understanding [7] that the Kondo problem in the scaling regime can be studied by a one-dimensional Ising model with long-ranged interactions. Through a Coulomb-gas picture of spin flips, the Kondo Hamiltonian, $H_K = J_{||} s_z^a s_z^b + \frac{1}{2} J_{\perp}(s_z^a s_+ + s^-_+ s_z) + H_0(c)$, is mapped onto a classical Ising chain $H_T = \sum_i K_{nn} S^i S^i_{+1} + \sum_i K_{lr} S^i S^i_{-1}$ with algebraically decaying (long-ranged) interaction $K^K_{lr}(r_i - r_j) = K/|r_i - r_j|^{2-\epsilon}$ placed at its lower critical dimension ($\epsilon = 0$) [7,5]. Here, $S$ is the impurity spin and $s$ is the electron spin density at the impurity site of the c-electrons with a featureless dispersion in its kinetic term, $H_0(c)$. $S^c_i$ is an Ising variable at the chain site $i$. The coupling constant $K_{nn}$ depends on $J_c$ while $K$ is solely a function of $J_{||}$ and can be expressed entirely through the scattering phase shift $\delta$ of the electrons, $4 \tan \delta = \pi J_{||} / \rho$, where $\rho$ is the conduction electron density of states at the Fermi energy. An extension of this equivalence has recently been used to address the quantum critical properties of Ising-anisotropic BFKMs [8,6],

$$\mathcal{H}_{\text{bkm}} = \mathcal{H}_K + \tilde{g} \sum_p S^z (\phi_p + \phi^+_{-p}) + \sum_p w_p \phi^+_p \phi_p ,$$

where the impurity spin $S$ interacts with fermions $c^\dagger_{p\sigma}$ and bosons $\phi^\dagger_p$. The spectrum of the bosonic bath is taken to be sub-Ohmic ($0 < \epsilon < 1$), $\sum_p |\delta(\omega - \omega_p) - \delta(\omega + \omega_p)| \sim |\omega|^{2-\epsilon} \text{sgn}(\omega)$ and gives rise to an interaction $K^K_{lr}(r_i - r_j) = g/|r_i - r_j|^{2-\epsilon}$ along the Ising chain on top of the $K^K_{lr}(r_i - r_j) = K/|r_i - r_j|^2$ for the Fermi-only Kondo model.

Before discussing the determination of the critical coupling $g_c$ or $g_c$, it is worthwhile discussing the $g = 0$ case in greater detail. The RG flow of the Kondo model is towards an SU(2) invariant fixed point on trajectories with $J_{||}^2(b) - J_{\perp}^2(b) = c$, where $b$ parametrizes the RG flow and $c$ is a positive constant. At the Toulouse point, the Kondo model can be mapped onto a resonant level model [10]. De-
viation from the Toulouse point is needed to restore the SU(2) symmetry at the fixed point. The Ising chain $H_I$ at $\epsilon = 0$ does not possess a continuous symmetry but undergoes a Kosterlitz-Thouless-like phase transition; the RG flow resembles that of the Kondo model away from the Toulouse point. This raises the question of whether the universal properties of the BFKM, obtained from simulating the classical Ising chain, are sensitive to whether the Kondo model is placed at or away from its Toulouse point. Previous simulations have utilized the Toulouse point, $J_{\perp} = 0$, away from Toulouse point with $g_{c} = 0$, at an intermediate coupling $g/T_{K} = 0.545$ and at the critical coupling $g_{c}/T_{K} = 0.773$ for $\epsilon = 0.4$. The divergence of $\chi(g_{c})$ is cut off due to the finite system size $L = \beta_{0}^{-1}$; the cutoff temperature decreases as $\tau_{0}$ decreases [6].

In summary, we have established that the cluster-Monte Carlo study of the classical Ising chain with long-range interaction can be used to obtain universal properties of the Ising-anisotropic Bose-Fermi Kondo model, both at and away from the Toulouse point. Because of the large temperature range it is able to reliably access, the approach is expected to be useful for studying the quantum critical behavior of not only the BFKM itself, but also the extended dynamical mean field theory of the Kondo lattice model. This work has been supported in part by NSF, the Robert A. Welch Foundation, the W. M. Keck Foundation, and the Rice Computational Research Cluster funded by NSF and a partnership between Rice University, AMD and Cray.

References
[1] Q. Si et al., Nature 413 (2001) 804.
[2] S. Kirchner et al., PNAS 102 (2005) 18824.
[3] L. Zhu and Q. Si, Phys. Rev. B 66 (2002) 024426; G. Zarand and E. Demler, ibid. (2002) 024427.
[4] L. Zhu et al., Phys. Rev. Lett. 93 (2004) 267201.
[5] D. Grempel and M. Rozenberg, Phys. Rev. B 60 (1999) 4702.
[6] S. Kirchner and Q. Si, Phys. Rev. Lett. in press and arXiv:0706.1783v1.
[7] G. Yuval and P. W. Anderson, Phys. Rev. B 1 (1970) 1522.
[8] D. Grempel and Q. Si, Phys. Rev. Lett. 91 (2003) 026401.
[9] E. Luijten and H. W. J. Blöte, Int. J. Mod. Phys. 6 (1995) 359.
[10] F. Guinea et al., Phys. Rev. B 32 (1985) 4410.