Numerical Renormalization-Group Study of the Bose-Fermi Kondo Model

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We extend the numerical renormalization-group method to Bose-Fermi Kondo models (BFKMs), describing a local moment coupled to a conduction band *and* a dissipative bosonic bath. We apply the method to the Ising-symmetry BFKM with a bosonic bath spectral function $\eta(\omega) \propto \omega^s$, of interest in connection with heavy-fermion criticality. For $0 < s < 1$, an interacting critical point, characterized by hyperscaling of exponents and ω/T scaling, describes a quantum phase transition between Kondo-screened and localized phases. A connection is made to other results for the BFKM and the spin-boson model.

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Dynamical competition between local and spatially extended degrees of freedom provides a possible mechanism for the intriguing non-Fermi-liquid behaviors observed in cuprate high-temperature superconductors [1] and in heavy-fermion systems near a quantum phase transition (QPT) [2]. The essence of this competition is embodied in a new class of quantum impurity problems: Bose-Fermi impurity models of a local moment coupled both to a fermionic band and a dissipative bosonic bath.

The key physics underlying heavy-fermion QPTs—interplay between screening of f-shell moments by conduction electrons and magnetic ordering of those moments due to the Ruderman-Kittel-Kasuya-Yosida interaction—is contained in the Kondo lattice model (KLM) [3–5]. The KLM has been studied via an extended dynamical mean-field theory (EDMFT) [5,6] that maps the lattice onto a self-consistently determined Bose-Fermi Kondo model (BFKM) in which bosons represent the fluctuating effective magnetic field generated by other f moments. Assuming the bosonic bath has a sub-Ohmic spectrum $\eta(\omega) \propto \omega^s$ $(s < 1)$, a perturbative (in $\epsilon \equiv 1 - s$) renormalization-group study [5] has found two types of antiferromagnetic ordering transition: a QPT of the usual spin-density-wave type [7] and a *locally critical* QPT, characterized by $s = 0^+$, at which divergence of the spatial correlation length coincides with critical local-moment fluctuations. There is growing evidence for the latter scenario in several materials, particularly from neutron scattering results on $CeCu_{5.9}Au_{0.1}$ [8]. Similar mappings to an effective Bose-Fermi impurity model have been applied to the *disordered* KLM [9] and to a t-J model of a highly incoherent metal close to a Mott transition, of possible relevance to the pseudogap phase of the cuprates [10]. The BFKM also describes certain dissipative mesoscopic qubit devices, e.g., a noisy quantum dot, where the bosonic bath represents gate-voltage fluctuations [11].

A satisfactory description of all these problems hinges on proper solution of the BFKM. The identification of a locally critical QPT in [5] was based on perturbative results for $\epsilon \to 1$. Most other techniques developed for conventional (pure-fermionic) impurity models [12] are inapplicable or suffer from significant limitations. For example, nonperturbative quantum Monte Carlo studies [6] of the KLM have reached conflicting conclusions concerning the existence of a locally critical QPT due to inherent limitations in accessing the lowest temperatures.

To meet the need for solutions of the BFKM that are reliable for all bath spectra and all temperatures T, we have turned to Wilson's numerical renormalization-group (NRG) technique [13], which has hitherto provided a controlled treatment of a range of fermionic impurity and lattice problems [14], and was recently applied [15,16] to the spin-boson model (SBM) of a two-level system coupled to a dissipative bosonic bath [17]. Below we report a nontrivial development of the NRG that incorporates coupling of an impurity to both a conduction band *and* a bosonic bath. We give results for the BFKM with Ising-symmetry bosonic couplings, the case most relevant to $CeCu_{5.9}Au_{0.1}$ and a noisy quantum dot. For bosonic bath exponents $0 < s < 1$, the model displays critical properties identical to those of the SBM, with exponents satisfying hyperscaling relations and ω/T scaling in the dynamics. We show directly the destruction of the Kondo resonance at the quantum-critical point (QCP). Importantly, this work opens the way for future decisive studies of the KLM, obtained by imposing EDMFT self-consistency on the BFKM solution.

We study the Hamiltonian $H = H_F + H_B + H_{\text{int}}$, with

$$H_F = \sum_{\boldsymbol{k},\sigma} \varepsilon_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma}, \qquad H_B = \sum_{\boldsymbol{q}} w_{\boldsymbol{q}} \phi^\dagger_{\boldsymbol{q}} \phi_{\boldsymbol{q}},$$
$$H_{\text{int}} = J\boldsymbol{S} \cdot \boldsymbol{s}_c + g S_z \sum_{\boldsymbol{q}} (\phi_{\boldsymbol{q}} + \phi^\dagger_{-\boldsymbol{q}}), \tag{1}$$

which describes a spin-$\frac{1}{2}$ local moment $\boldsymbol{S}$ interacting with both the on-site spin $\boldsymbol{s}_c$ of a fermionic band and, via S_z, with a bosonic bath. The essential physics of the model, based on perturbative RG and large-N results [18–21], is the competition between the Kondo coupling J, which tends to screen the impurity moment, and the bosonic coupling g, which favors an unscreened spin. The fermionic band is assumed to be featureless with a density of states $\rho(\varepsilon) = \rho_0$ for $|\varepsilon| < D$. The impurity-boson interaction is embodied entirely in $B(\omega) = \pi g^2 \eta(\omega) = B_0 \omega^s$ for $0 \le \omega < \omega_0$, where $s > -1$. In the EDMFT problem of future interest, s will be determined self-consistently from the form of the local spin susceptibility $\chi_{\rm loc}(\omega)$ and will in general take a non-Ohmic value ($s \neq 1$) [5]. To connect with previous work [20], we write $B_0 = (K_0 g)^2$, and for convenience we set $\omega_0 = D = 1$ in the following.

NRG scheme.—The band (bath) continuum of energies $|\varepsilon| < 1$ ($0 \le \omega < 1$) is replaced by a discrete set, $\pm\Lambda^{-n}$ (Λ^{-n}) for $n = 0, 1, 2, \ldots$, where $\Lambda > 1$ parametrizes the discretization. Equation (1) may then be cast in a chain form, in close analogy to the pure-fermionic NRG, introducing a discretization error that vanishes as $\Lambda \to 1$ [13]:

$$\begin{aligned} H = {}& \sum_{n,\sigma} [\varepsilon_n f_{n\sigma}^\dagger f_{n\sigma} + \tau_n (f_{n\sigma}^\dagger f_{n-1,\sigma} + f_{n-1,\sigma}^\dagger f_{n\sigma})] \\ &+ \sum_m [E_m b_m^\dagger b_m + T_m (b_m^\dagger b_{m-1} + b_{m-1}^\dagger b_m)] \\ &+ \rho_0 J \sum_{\sigma,\sigma'} f_{0\sigma}^\dagger \boldsymbol{\sigma}_{\sigma\sigma'} f_{0\sigma'} \cdot \boldsymbol{S} + K_0 g \sqrt{\frac{F^2}{\pi}} S_z (b_0^\dagger + b_0). \end{aligned} \tag{2}$$

Here, $f_{0\sigma}$ (b_0) annihilates the unique combination of fermions (bosons) that couples to the impurity. The tight-binding coefficients ε_n, τ_n, E_m, and T_m ($m, n = 0, 1, 2, \ldots$) encoding all information about the band and the bath are determined via a Lanczos procedure. The decay of ε_n and τ_n as $\Lambda^{-n/2}$ for large n is what allows the iterative solution of the conventional Kondo problem via diagonalization of progressively longer chains [13]. Since the bath spectral function $\eta(\omega)$ vanishes for $\omega < 0$, the coefficients E_m and T_m decay faster, as Λ^{-m} for large m, as discussed previously for the SBM [15].

We solve the discretized BFKM via an iterative scheme that adds a site to the fermionic chain at each step, but extends the bosonic chain only at every second step. Since $T_{2n} \sim \tau_n$, this ensures that fermions and bosons of the same energy scale are treated at the same step. The number of particles per bosonic site is in principle unlimited, but is restricted in practice to a finite maximum N_b. For the conventional Kondo model, the basis must be truncated after only a few iterations, saving only the lowest N_s eigenstates of one step to form the basis (of $4N_s$ states) for the next step. Truncation is required even sooner in the BFKM, where the basis grows by a factor of $4(N_b + 1)$ at each step at which bosons are added.

It is not obvious *a priori* that the approach outlined above should capture the physics of the BFKM QCP [22], but it is validated by the results presented below. These results are converged with respect to the truncation parameters, $8 \le N_b \le 12$ and $500 \le N_s \le 2000$ typically sufficing. Calculated critical exponents prove insensitive to the choice of Λ (see Table I), so to reduce computer time $\Lambda = 9$ was used, except where noted otherwise.

TABLE I. Critical exponents for $\Lambda = 9$, $s = 0.2$ and 0.8. Parentheses surround the estimated nonsystematic error in the last digit. The insensitivity to Λ is illustrated by the $s = 0.2$ values $\nu = 4.90(5)$, $x = 0.200(1)$ for $\Lambda = 5$, and $\nu = 4.9(1)$, $x = 0.199(4)$ for $\Lambda = 3$.

s	ν	x	$1/\delta$	β	γ
0.2	4.99(5)	0.200(1)	0.665(5)	1.99(2)	1.00(1)
0.8	2.11(2)	0.803(3)	0.106(2)	0.209(1)	1.67(2)

Critical coupling.—For $s \le 1$ the NRG flow of effective couplings has two stable limits: a Kondo fixed point at $J = \infty$, $g = 0$, describing a phase in which conduction electrons screen the local moment and the single-particle spectrum exhibits a Kondo resonance; and a "localized" fixed point at $J = 0$, $g = \infty$, where the impurity dynamics are controlled by the coupling to the bath. A third, unstable fixed point—the QCP at $J^* \neq 0$, $g^* \neq 0$—is reached for bare couplings lying precisely on the boundary $g = g_c(J)$ between the Kondo and localized phases. For $s > 1$, by contrast, the Kondo fixed point is reached for all $J > 0$. At $s = 1$ the critical point is Kosterlitz-Thouless-like [11], while for $-1 < s < 0$ it is noninteracting. We restrict attention henceforth to the range $0 < s < 1$, over which the QCP exhibits properties (shown below) characteristic of an interacting critical point. (For the case $s = 0$ of interest in connection with local criticality, logarithms replace power laws at the QCP.)

Correlation length exponent.—The crossover from the quantum-critical regime to a stable low-temperature regime defines a scale that vanishes at the critical coupling: $T^* \sim |g - g_c|^\nu$ [Fig. 1(a)]. The correlation length exponent $\nu(s)$, which can be determined from the NRG many-body spectrum or from properties such as the local susceptibility or the single-particle spectrum, diverges for $s \to 0^+$ and $s \to 1^-$, indicative of qualitative changes at these limiting values of the bath exponent. For small s, $\nu \simeq 1/s$ [fit in Fig. 1(b)], which becomes asymptotically exact

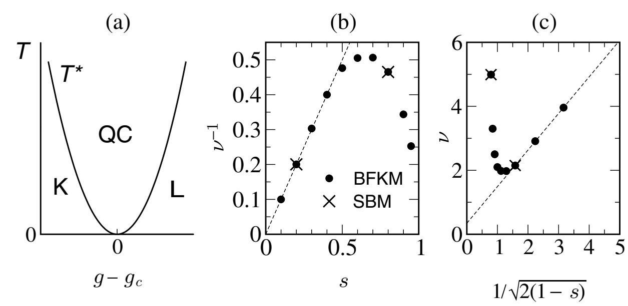

FIG. 1. (a) Schematic phase diagram for the BFKM, showing Kondo (K), localized (L), and quantum-critical (QC) regimes separated by a crossover scale $T^* \propto |g - g_c|^\nu$ that vanishes at the QCP. (b),(c) Correlation length exponent ν as a function of bath exponent s. Crosses (at $s = 0.2$ and 0.8) show representative results for the SBM. Dashed lines are the linear fits discussed in the text.

as $s \to 0$, while for $s \to 1$ the exponent approaches $\nu = 1/\sqrt{2(1-s)} + C$ [fit in Fig. 1(c)]. Our ν values are essentially in exact agreement with NRG for the SBM [15] and, for $s \to 0$, with perturbative RG for the BFKM expanding about $s = 0$ [23].

Local magnetic response.—Central to the EDMFT of future interest is the local susceptibility $\chi_{\rm loc}$: the response to a magnetic field h acting solely on the impurity. Figure 2 shows the static local susceptibility $\chi_{\rm loc}(T; \omega = 0)$ vs T for $s = 0.2$. The two phases are readily distinguished. For $g < g_c$, screening of the impurity moment is signaled for $T \lesssim T^*$ by a constant value $\chi_{\rm loc}(T; \omega = 0) \propto (g_c - g)^{-\gamma}$ that diverges as $g \to g_c^-$. For $g > g_c$, by contrast, there is free-moment behavior with a Curie constant $T\chi_{\rm loc}(T; \omega = 0) \propto (g - g_c)^{\lambda}$ (see inset of Fig. 2). At criticality, it is found that

$$\chi_{\rm loc}(T; \omega = 0, g = g_c) \propto T^{-x}, \tag{3}$$

with $x = s$ for all $0 < s < 1$, as predicted by the ϵ expansion [20]. We have also calculated exponents defined by $M_{\rm loc}(g > g_c, T = 0, h = 0) \propto (g - g_c)^{\beta}$ and $M_{\rm loc}(g = g_c, T = 0) \propto |h|^{1/\delta}$, where $M_{\rm loc} \equiv \langle S_z \rangle$ serves as an order parameter for the localized phase. Table I shows exponents obtained for two representative cases.

Starting from a scaling ansatz for the critical part of the free energy, $F_{\rm crit} = Tf(|g - g_c|/T^{1/\nu}, |h|/T^b)$, it is readily shown that $\delta = (1 + x)/(1 - x)$, $\lambda = 2\beta = \nu(1 - x)$, and $\gamma = \nu x$. The exponents obtained numerically for $0 < s < 1$ obey these hyperscaling relations, indicating that the critical point is interacting [7].

We now turn to the imaginary part of the dynamical local susceptibility, $\chi''_{\rm loc}(\omega)$. Figure. 3 shows $\chi''_{\rm loc}(\omega; T = 0, g = g_c)$ vs ω for $s = 0.2$. The exponent y, defined via

$$\chi''_{\rm loc}(\omega; T = 0, g = g_c) \propto |\omega|^{-y}\,{\rm sgn}(\omega), \tag{4}$$

is found to satisfy $y = s$ for all $0 < s < 1$. The static local susceptibility $\chi_{\rm loc}(T)$ is also shown, from which it is evident that $x = y$, which likewise holds over the entire s range. Because of truncation, the NRG method is known to be unreliable for $|\omega| \lesssim T$ [24]. However, the result $y = x$ for $0 < s < 1$ (obtained in [6] for the particular case $s = 0^+$) is consistent with ω/T scaling at the QCP and reflects the interacting nature of the fixed point [7]. Specifically, we find for $\omega \ll T_K$ that

$$T_K \chi''_{\rm loc}(\omega, T; g = g_c) \sim \left(\frac{T}{T_K}\right)^{-s} \phi_s\left(\frac{\omega}{T}\right), \tag{5}$$

with ϕ_s a universal function of its argument as demonstrated in the lower part of Fig. 3. A similar result has recently been obtained for the multichannel BFKM in the large-N limit [25].

An important observation is that all critical exponents of the Ising-symmetry BFKM are in numerical agreement with those of the corresponding sub-Ohmic SBM [15,16]. This clearly indicates that the two QCPs belong to the same universality class (as implied in Ref. [6(a)]).

Spectral function.—Finally, we calculate $A(\omega) = -\frac{1}{\pi}\,{\rm Im}\langle\langle d; d^{\dagger}\rangle\rangle_{\omega}$ for the Ising-symmetry Bose-Fermi Anderson model described by

$$H_{\rm int} = \sum_{\sigma}\left(\varepsilon_d + \frac{1}{2}Un_{d,-\sigma}\right)n_{d\sigma} + V\sum_{\boldsymbol{k},\sigma}(d_{\sigma}^{\dagger}c_{\boldsymbol{k}\sigma} + {\rm H.c.}) + \frac{1}{2}g(n_{d\uparrow} - n_{d\downarrow})\sum_{\boldsymbol{q}}(\phi_{\boldsymbol{q}} + \phi_{-\boldsymbol{q}}^{\dagger}). \tag{6}$$

Here, $n_d = d_{\sigma}^{\dagger}d_{\sigma}$ is the spin-σ occupancy of an impurity level of energy ε_d, U is the on-site interaction, and V is the hybridization between the impurity and the conduction band. The coupling to the bosons is again through the z component of the effective impurity spin. In the regime $U, |\varepsilon_d| \gg \Gamma_0 \equiv \pi\rho_0 V^2$ where charge fluctuations are sup-

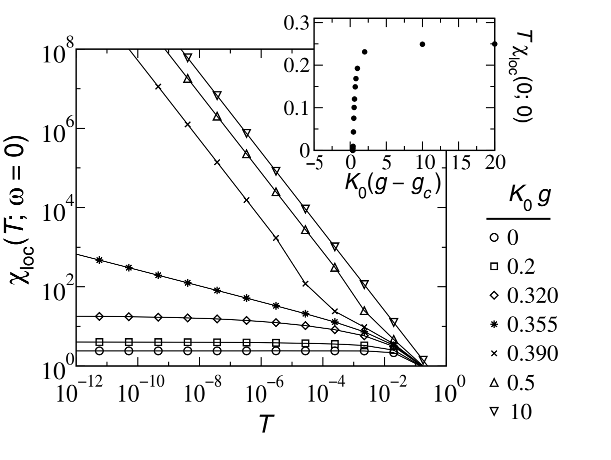

FIG. 2. Static local susceptibility $\chi_{\rm loc}(T; \omega = 0)$ vs T for $s = 0.2$ and $\rho_0 J = 0.5$, where $K_0 g_c \simeq 0.355$. The inset shows the vanishing of $T\chi_{\rm loc}(0; 0)$ for $g \to g_c^+$.

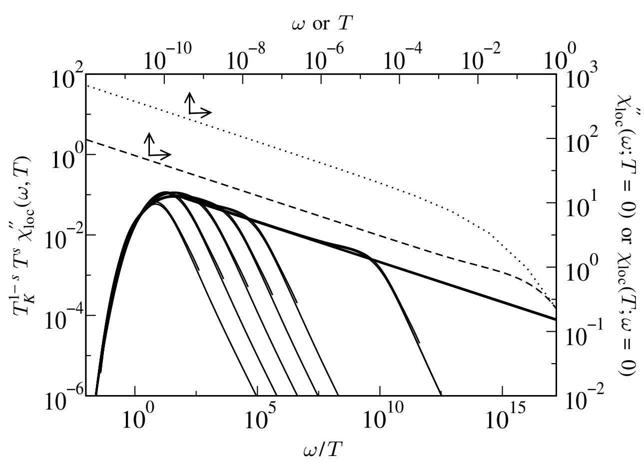

FIG. 3. Upper-right axes: $\chi''_{\rm loc}(\omega; T = 0)$ (dashed line) and $\chi_{\rm loc}(T; \omega = 0)$ (dotted line) at the QCP for $s = 0.2$ and $\rho_0 J = 0.5$, showing that $x = y = s$; see Eqs. (3) and (4). Lower-left axes: Finite-T scaling of $\chi''_{\rm loc}(\omega, T)$ at the QCP as described by Eq. (5). Data are shown for $s = 0.2$, $\rho_0 J = 0.1$ (thin line) and 0.25 (thick line) with $g = g_c$ in each case, and for temperatures $T/T_K = 10^{-1}$, 10^{-2}, 10^{-3}, 10^{-4}, 10^{-5}, 10^{-10}, and 10^{-20}. The curves have a common form for $\omega/T \ll T_K/T$.

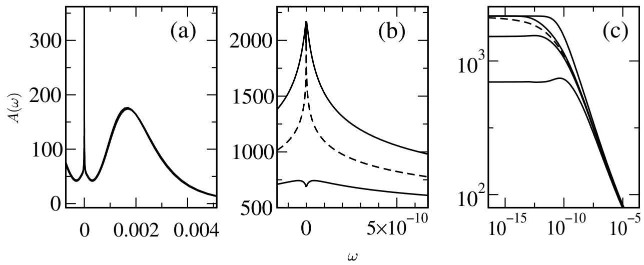

FIG. 4. Single-particle spectrum vs ω for bath exponent $s = 0.7$, impurity parameters $U = -2\varepsilon_d = 0.002$ [such that $A(\omega) = A(-\omega)$], hybridization strength $\Gamma_0 = 1.5 \times 10^{-4}$, and discretization $\Lambda = 3$. Shown for $B_0 - B_{0,c} = 0$ (dashed line), $\pm 10^{-4}$ on (a) the scale of U and (b) the scale set by the central feature. (c) Shown on a logarithmic scale for $B_0 - B_{0,c} = 0$ (dashed line), $\pm 10^{-5}$, $\pm 10^{-4}$.

pressed, this Anderson model maps onto the BFKM under a Schrieffer-Wolff transformation [12].

The QCP is manifest in the single-particle spectrum as a collapse of the central Kondo resonance. Figure 4 shows $A(\omega)$ vs ω close to and at the QCP. On the scale of the Hubbard satellite bands [Fig. 4(a)], the spectra are barely distinguishable. Figure 4(b) shows the same spectra on the scale of the central feature. For $B_0 < B_{0,c}$ the integrity of the Kondo resonance is preserved; it remains pinned at the Fermi level, $A(\omega = 0) = (\pi\Gamma_0)^{-1}$, as required by Fermi-liquid theory for the conventional Anderson model [12]. Close to the transition, the lowest-frequency (Fermi-liquid) behavior $1 - \pi\Gamma_0 A(\omega) \propto \omega^2$ crosses over above a scale $|\omega| \approx \omega^*$ to a power-law characteristic of the QCP itself. For $B_0 = B_{0,c}$ [dashed line in Fig. 4(b)], $\omega^* = 0$; i.e., the spectrum remains pinned but the lowest-frequency behavior is non-Fermi-liquid in nature. For $B_0 > B_{0,c}$ the Kondo resonance collapses and $A(\omega = 0)$ decreases with increasing B_0. Near the critical coupling there is a crossover, seen as a weak maximum in $A(\omega)$ at $|\omega| = \omega^*$ [Fig. 4(c)], to the quantum-critical behavior described above. The correlation length exponent may also be calculated from the vanishing of ω^* at the transition, and agrees with the results of Fig. 1 to within numerical error.

Summary.—We have developed the NRG method to treat coupling of a quantum impurity to both a conduction band and a bosonic bath, as described by Bose-Fermi Kondo and Anderson models. Our approach provides a good account of the critical properties of the Ising-symmetry BFKM with a power-law bath spectrum. Over the range of bath exponents $0 < s < 1$, the competition between fermionic and bosonic couplings gives rise to an interacting fixed-point, exhibiting hyperscaling of critical exponents and ω/T scaling in the impurity dynamics, which belongs to the same universality class as the critical point of the SBM. The method can readily be extended to models having multiple bosonic baths, such as the *XY* and isotropic BFKMs. This work also opens the way for EDMFT treatments of the Kondo lattice down to $T = 0$ that will shed much-needed light on the possibility of local criticality in heavy-fermion systems.

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[1] M. R. Norman and C. Pépin, Rep. Prog. Phys. **66**, 1547 (2003).
[2] G. R. Stewart, Rev. Mod. Phys. **73**, 797 (2001).
[3] P. Coleman, Physica (Amsterdam) **259B–261B**, 353 (1999).
[4] P. Coleman, C. Pépin, Q. Si, and R. Ramazashvili, J. Phys. Condens. Matter **13**, R723 (2001).
[5] Q. Si, S. Rabello, K. Ingersent, and J. L. Smith, Nature (London) **413**, 804 (2001); Phys. Rev. B **68**, 115103 (2003).
[6] (a) D. R. Grempel and Q. Si, Phys. Rev. Lett. **91**, 026401 (2003); (b) J.-X. Zhu, D. R. Grempel, and Q. Si, Phys. Rev. Lett. **91**, 156404 (2003); (c) P. Sun and G. Kotliar, Phys. Rev. Lett. **91**, 037209 (2003).
[7] S. Sachdev, *Quantum Phase Transitions* (Cambridge University Press, Cambridge, England, 1999).
[8] H. v. Löhneysen *et al.*, Phys. Rev. Lett. **72**, 3262 (1994); A. Schröder *et al.*, *ibid.* **80**, 5623 (1998); O. Stockert *et al.*, *ibid.* **80**, 5627 (1998); A. Schröder *et al.*, Nature (London) **407**, 351 (2000).
[9] D. Tanasković, V. Dobrosavljević, and E. Miranda, cond-mat/0412100.
[10] K. Haule, A. Rosch, J. Kroha, and P. Wölfle, Phys. Rev. Lett. **89**, 236402 (2002).
[11] K. Le Hur, Phys. Rev. Lett. **92**, 196804 (2004).
[12] A. C. Hewson, *The Kondo Problem to Heavy Fermions* (Cambridge University Press, Cambridge, England, 1993).
[13] K. G. Wilson, Rev. Mod. Phys. **47**, 773 (1975).
[14] A. C. Hewson, S. C. Bradley, R. Bulla, and Y. Ono, Int. J. Mod. Phys. B **15**, 2549 (2001).
[15] R. Bulla, N. Tong, and M. Vojta, Phys. Rev. Lett. **91**, 170601 (2003).
[16] R. Bulla, H. Lee, N. Tong, and M. Vojta, Phys. Rev. B **71**, 045122 (2005).
[17] A. J. Leggett *et al.*, Rev. Mod. Phys. **59**, 1 (1987).
[18] J. L. Smith and Q. Si, Europhys. Lett. **45**, 228 (1999).
[19] A. M. Sengupta, Phys. Rev. B **61**, 4041 (2000).
[20] L. Zhu and Q. Si, Phys. Rev. B **66**, 024426 (2002).
[21] G. Zaránd and E. Demler, Phys. Rev. B **66**, 024427 (2002).
[22] The chain mapping of the bosons may fail deep inside the BFKM localized regime due to a divergence of the mean site occupancy. In this case, an alternative mapping proposed for the SBM [16] may prove more successful.
[23] M. Vojta, N. Tong, and R. Bulla, Phys. Rev. Lett. **94**, 070604 (2005).
[24] T. A. Costi, A. C. Hewson, and V. Zlatić, J. Phys. Condens. Matter **6**, 2519 (1994); K. Ingersent and Q. Si, Phys. Rev. Lett. **89**, 076403 (2002).
[25] L. Zhu, S. Kirchner, Q. Si, and A. Georges, Phys. Rev. Lett. **93**, 267201 (2004).