Competition between Singlet Formation and Magnetic Ordering in One-Dimensional Spin Systems

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We use mappings onto soluble models and Abelian bosonization to determine the phase diagram and correlation functions of a model of two coupled spin chains. We find quantum disordered singlet phases and magnetic phases and determine the phase boundaries, universality classes of transitions, and correlation functions. We believe our model captures the essential physics of the interplay between the Kondo effect and magnetic ordering, which may be important for the heavy fermion materials.

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Heavy-electron materials are a class of compounds whose chemical formula includes a rare earth or actinide element (typically Ce, Yb, or U) with a partially filled f shell. At room temperature the physics of these materials is of essentially freely fluctuating localized magnetic moments (the f electrons) weakly coupled to a wide conduction band (involving the non-f electrons) At low temperatures and energies ($T \lesssim 10$–50 K) the physical properties are approximately those of a very-large-mass (~ 100–1000 times the free electron mass) Fermi liquid; neither the local moments nor the wide band of conduction electrons seem to exist as separate excitations [1]. It is widely believed [2] that the quenching of the local moments into a heavy Fermi liquid has something to do with the Kondo effect [3]. The Kondo effect involves a single localized magnetic impurity weakly coupled to a wide conduction band; at low temperatures the local moment is quenched because it forms a singlet with a wave packet of conduction electrons. In the lattice case there are at least two possibilities: The local moments may be quenched by the conduction electrons in a lattice version of the Kondo effect, or they may couple to each other, forming a magnetically ordered state. Understanding the interplay between these two possibilities is the central unsolved problem in the theory of heavy fermion materials [4,5].

In this Letter we state and discuss our results for the behavior of a simple one-dimensional model which we hope contains the important physics of the Kondo effect and magnetic ordering. We will give the details of our calculations in a later paper [6]. Our model is a generalization of the "Kondo necklace" Hamiltonian of Refs. [5,7] and consists of two spin-$\frac{1}{2}$ chains, one representing the local moments and one representing the magnetic degrees of freedom of the conduction electrons. Within each chain there is an anisotropic Heisenberg interaction $J_x = J_y = J_\perp \neq J_z$ and between the two chains a Kondo interaction J_K. Writing $\mathbf{S}(i)$ for the spin at site i in the "local moment" chain and $\boldsymbol{\tau}(i)$ for the spin at site i in the "conduction electron" chain our Hamiltonian is

$$H = H_S + H_\tau + H_{S\tau}, \tag{1}$$

$$H_S = \sum_{i=1}^{N} J_\perp^S [S^x(i)S^x(i+1) + S^y(i)S^y(i+1)] + J_z^S S^z(i)S^z(i+1), \tag{2}$$

$$H_\tau = \sum_{i=1}^{N} J_\perp^\tau [\tau^x(i)\tau^x(i+1) + \tau^y(i)\tau^y(i+1)] + J_z^\tau \tau^z(i)\tau^z(i+1), \tag{3}$$

$$H_{S\tau} = J_K \sum_{i=1}^{N} \mathbf{S}(i)\cdot\boldsymbol{\tau}(i). \tag{4}$$

The case where only one chain has magnetic interaction, i.e., $J_\perp^S, J_z^S \to 0$ should be most closely related to actual heavy fermion materials. The symmetric case $J_\perp^\tau = J_\perp^S$, $J_z^\tau = J_z^S$ may be more easily solved. The Kondo necklace model [5] corresponds to our model for $J_\perp^S = J_z^S = J_z^\tau = 0$.

There are three separate regimes where our model is tractable: large negative J_K, large positive J_K, and small J_K. For large negative J_K we need only consider the triplet combination of S and τ on each site i; when projected into this subspace the model becomes a spin-one chain with exchange constants $J_\perp = (J_\perp^S + J_\perp^\tau)/4$ and $J_z = (J_z^S + J_z^\tau)/4$. The physics of the spin-one chain is known [8]. For large positive J_K relative to $J_\perp^{S,\tau}$ the model maps onto the Ising model in a transverse field. To perform the mapping, we label the possible states of the spin chain by the total spin $S(i)$ and total z component $M(i)$ on site i. In the limit $J_\perp^{S,\tau} = 0$ our Hamiltonian conserves all the $M(i)$ separately and there is a gap of order J_K between the ground state and any state containing a site with $M(i) \neq 0$. By identifying the $S(i) = 1$, $M_z(i=0)$ state with an Ising state with the spin down at site i and the $S(i) = 0$, $M(i) = 0$ state with an Ising state with the spin up at site i we find we may write H, Eq. (1), for $J_\perp^{S,\tau} = 0$, in the subspace $M(i) = 0$ as (here σ is a Pauli matrix)

$$H_{\text{eff}} = \sum_i J_K \sigma^z(i) + \tfrac{1}{4}(J_z^S + J_z^\tau)\sigma^x(i)\sigma^x(i+1). \tag{5}$$

H_{eff} has been solved by Pfeuty [9]. It has three phases: For $(J_z^S + J_z^\tau)/4J_K < -1$ the two chains are ferromagnetically ordered with $S^z(i) = -\tau^z(i)$, for $(J_\tau^S + J_z^\tau)/4J_K$

>1 each chain is antiferromagnetically ordered, and in the remaining phase there is no long-range order and there is a gap to all excitations. The phase transitions at $J_K = \pm\frac{1}{4}(J_z^S + J_z^\tau)$ are in the two-dimensional Ising universality class [9]; thus exponents and the asymptotic behavior of correlation functions may be determined. Away from the transition points there is a gap Δ, to excitations of size $|J_K - \frac{1}{4}|J_z^S + J_z^\tau||$ and all correlation functions fall off exponentially. In the ordered phases the order parameter, $\mu = \langle S^z \rangle$, grows as $\mu^{1/8}$, and at the transition the $\langle S^z(x) S^z(0) \rangle$ correlations fall off as $x^{-1/4}$. For $J_K > 0$ and $J_\perp^S = J_\perp^\tau = 0$ the model is exactly soluble and the above statements are rigorously correct. We have also shown that a small nonzero $J_\perp^S, J_\perp^\tau$ leads to corrections to $H_{\rm eff}$ of the form $C_1 \sigma^y(i)\sigma^y(i+1) + C_2 \sigma^z(i)\sigma^z(i+1)$ with $C_1, C_2 \sim J_\perp^2/J_K$. For small C_1 and C_2, these terms are irrelevant perturbations in the renormalization-group sense; this follows on general grounds from properties of the $d=2$ Ising transition [10], and we have also verified it by an explicit calculation using the methods of Ref. [9]. We note that the large J_K mapping onto the transverse-field Ising model and therefore the results concerning the order and nature of the transitions apply in any spatial dimension.

The mapping onto the Ising model in a transverse field plus irrelevant perturbations breaks down when $J_\perp^{S,\tau}/J_K$ becomes sufficiently large. To study the model for small J_K we use an expansion in J_K. A single spin-$\frac{1}{2}$ chain with $|J_z| > J_\perp$ has Ising ferromagnetic or Ising antiferromagnetic order, which is stable to small perturbations. A spin-$\frac{1}{2}$ chain with $|J_z| < J_\perp$ is in a critical state at $T=0$, with power-law decay of x-y spin correlations with exponents determined by $J_z/J_\perp$. To determine the effect of a small nonzero J_K we express $H_{S\tau}$ [Eq. (4)] in terms of the critical fields and then use standard Abelian bosonization methods [11] to determine if $H_{S\tau}$ is a relevant or irrelevant perturbation and, if relevant, to what state the system flows. We consider first a simultaneous expansion in both $J_z/J_\perp$ and $J_K/J_\perp$ in the symmetric case $J_\perp^S = J_\perp^\tau$, $J_z^S = J_z^\tau$ and then indicate the modifications arising in the more general case of arbitrary J_z and inequivalent chains. We will present the details elsewhere [6].

For a single spin-$\frac{1}{2}$ chain one may write the low-energy excitations in terms of two boson fields, θ_N and θ_J. In the symmetric case of our two-chain problem we may write the Hamiltonian in terms of the symmetric (S) and antisymmetric (A) combinations of the boson fields of the two chains. The result at leading order in J_z and J_K neglecting all but the most relevant operators is [6]

$$H = \frac{1}{2}\int dx \left(1 - \frac{J_z}{\pi}\right)\left(\frac{\nabla\Theta_{N,S}^2}{2\pi}\right) + \left(1 + \frac{3J_z}{\pi} + \frac{J_K}{\pi}\right)\left(\frac{\nabla\Theta_{J,S}^2}{2\pi}\right) + \left(1 - \frac{J_z}{\pi}\right)\left(\frac{\nabla\Theta_{N,A}^2}{2\pi}\right) + \left(1 + \frac{3J_z}{\pi} - \frac{J_K}{\pi}\right)\left(\frac{\nabla\Theta_{J,A}^2}{2\pi}\right)$$
$$+ J_K (B\cos 2\Theta_{J,S} + B\cos 2\Theta_{J,A} + C\cos\Theta_{N,A}) \,. \tag{6}$$

For calculating universal quantities, the following expression for the various spin operators in terms of the phase fields is sufficient:

$$S^z(j) \to \frac{1}{2\pi}[\nabla\Theta_{S,J} + \nabla\Theta_{A,J}] + (-1)^j \mathrm{const}\cos(\Theta_{S,J} + \Theta_{A,J}) \,, \tag{7a}$$

$$S^+(j) \to (-1)^j \mathrm{const}\exp\left(i\frac{\Theta_{S,N}+\Theta_{A,N}}{2}\right) + \mathrm{const}\cos(\Theta_{S,J}+\Theta_{A,J})\exp\left(i\frac{\Theta_{S,N}+\Theta_{A,N}}{2}\right). \tag{7b}$$

The expressions for $\tau(j)$ are identical to those for $\mathbf{S}(J)$ except that $\Theta_S + \Theta_A$ is replaced by $\Theta_S - \Theta_A$. The θ fields have the commutation relations $[\nabla(\Theta_N)_A^S, (\Theta_J)_A^S] = 2\pi i \sum_n \delta(x - x' - nL)$ and $[\nabla(\Theta_N)_A^S, (\Theta_J)_S^A] = 0$; thus $(2\pi)^{-1/2} \times \nabla(\Theta_N)_A^S$ is the conjugate momentum to $(2\pi)^{-1/2}(\Theta_J)_A^S$.

We introduce rescaling factors $\lambda_{S,A}$ and velocities $v_{S,A}$ defined for small J_K, J_z as $\lambda_{S,A} = 1 + J_z/\pi \pm J_K/4\pi + \cdots$, $v_{S,A} = 1 + J_z/\pi \pm J_K/2\pi + \cdots$. After factoring out the velocities and rescaling the fields by the λ's and the canonically conjugate momenta by the λ^{-1}'s, the Hamiltonian becomes

$$H = \frac{1}{2}\int dx\, v_S \left(\frac{\nabla\tilde\Theta_{N,S}^2}{2\pi} + \frac{\nabla\tilde\Theta_{J,S}^2}{2\pi}\right) + v_A\left(\frac{\nabla\tilde\Theta_{N,A}^2}{2\pi}\right) + \left(\frac{\nabla\tilde\Theta_{J,A}^2}{2\pi}\right) + J_K\left(B\cos\frac{2}{\lambda_S}\tilde\Theta_{J,S} + B\cos\frac{2}{\lambda_A}\tilde\Theta_{J,A} + C\cos\lambda_A\tilde\Theta_{N,A}\right). \tag{8}$$

Hamiltonians of the form of Eq. (9) have been previously studied [11,12]. It is known that an operator of the form $\cos\gamma\Theta$ is relevant if $\frac{1}{2}\gamma^2 < 2$; also if an operator of the form $J\cos\Theta$ is the most relevant operator it leads to the opening of a gap $\Delta \sim J^{2/(4-\gamma^2)}$ in the excitation spectrum. For small J_z, J_K the $\cos\Theta_{N,A}$ operator is relevant and there is a gap to antisymmetric fluctuations: At low energies the two chains are locked together, either antiferromagnetically (if $J_K > 0$) or ferromagnetically (if $J_K < 0$). We must then consider the theory in the symmetric sector. For $J_K > 0$ two cases arise: If $J_z > -\frac{1}{4}J_K$ there is a gap in the symmetric sector and thus to all excitations. We interpret this as the weak coupling analog of the quantum disordered phase found in the $J_K, J_z \to \infty$ limit. For $J_z < -\frac{1}{4}J_K$ there is no gap; instead a phase with x-y correlations exists. For $J_K < 0$, similarly two phases exist. If $4J_z > |J_K|$ there is a gap to all excitations; we interpret this as the weak coupling analog of the Haldane gap phase previously discussed. For $4J_z < |J_K|$ a phase with x-y correlations exists.

We now sketch the extension of our results to larger J_z. For $J_K \to 0$ the most relevant operators induced by J_K have the form given in Eq. (8) with $\lambda_S^2 = \lambda_A^2 = 1 + J_z/\pi$. In a single spin chain as J_z is decreased past the ferromagnetic Ising point $(J_z = -J_\perp)$ a first-order transition occurs, and the bosonization description breaks down. For all negative J_K the transition remains first order with the transition line at $J_z = -J_\perp$ because the fully polarized ferromagnetic state is an eigenstate which maximizes $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$, $\langle \boldsymbol{\tau} \cdot \boldsymbol{\tau}_j \rangle$, and $\langle \mathbf{S}_j \cdot \boldsymbol{\tau}_j \rangle$; and for $-J_z > J_\perp$ it is the nondegenerate ground state. For small $J_K > 0$ the transition remains first order but the boundary will curve. At the antiferromagnetic Heisenberg $J_z = J_\perp$ point of a single spin chain, another operator, not explicitly written in Eqs. (6) or (9), becomes marginal and, for $J_z > J_\perp$, relevant. The flow equations for this variable are Kosterlitz-Thouless type and predict that the Ising order parameter grows as $\exp[-1/(J_z - J_\perp)^{1/2}]$. In addition, as J_z goes to $J_\perp$ from below, the dimension of all of the operators multiplying J_K in Eq. (8) approaches 1, so near the antiferromagnetic Heisenberg point all gaps scale as $(J_K)^\eta$ with $\eta \approx 1$, but the gap to antisymmetric fluctuations need not be larger than the gap to symmetric fluctuations. The proper description of the small $J_K, (J_z - J_\perp)$ region requires solution of coupled multivariable scaling equations and will be discussed in detail elsewhere [6]. We find that the phase boundary has the essential singularity form shown in Fig. 1. At the transition between the gapped and Ising phases the antisymmetric fluctuations between the chains become gapless, as in the $J_K, J_z \to \infty$ limit.

We have also considered the case of two coupled inequivalent spin chains, so $\mathbf{J}^S \neq \mathbf{J}^\tau$. This is more complicated because the problem does not separate into symmetric and antisymmetric sectors, and the various operators produced by J_K pick out different linear combinations of fluctuations between the two chains. Nevertheless we believe the important features of the phase diagram turn out to be equivalent to that of the two equivalent chains. We sketch the argument here and give the details elsewhere [6]. We consider first two inequivalent chains with (for $J_K = 0$) velocities $v_1 \sim J_\perp^1$ and $v_2 \sim J_\perp^2$ and rescaling factors λ_1 and λ_2, with $\lambda_1, \lambda_2 < \sqrt{2}$ so neither chain is Ising ordered. To leading order in J_K the leading relevant operator in Eq. (6) is $J_K \cos(\theta_{N1} - \theta_{N2})$. This leads to a gap in a sector rotated from the antisymmetric sector by an angle determined by the anisotropy. Projecting the remaining terms onto the orthogonal, ungapped sector $\bar{S}$ leads to an operator of the form $J_K \cos 2\theta_{J\bar{S}}/\bar{\lambda}$, with effective exponent $\bar{\lambda}$ given by a complicated combination of $v_1, \lambda_1, v_2, \lambda_2$. The J_K operator is relevant or irrelevant according [13] to whether $\bar{\lambda}$ is greater or less than 1, and

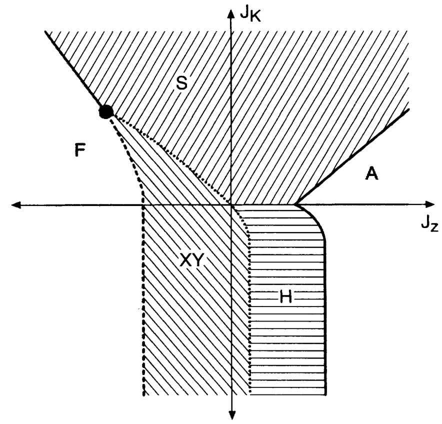

FIG. 1. Phase diagram for two coupled spin chains, described by Eqs. (1)-(4) of the text. J_K is the coupling between chains; $J_K > 0$ means antiferromagnetic coupling. J_z is the Ising coupling in one chain; the units are chosen such that the x-y coupling $J_\perp = 1$. Phase S is a singlet phase with a gap to all excitations, phase H is the Haldane gap phase of the $S=1$ antiferromagnet, phases F and A are Ising ferromagnet and antiferromagnet, respectively, and in phase XY there are power-law x-y correlations. The heavy solid line indicates a second-order transition, the dashed line a first-order transition, and the dotted line a Kosterlitz-Thouless transition.

the transition when λ_{eff} passes through 1 is Kosterlitz-Thouless as before. However, for $v_1 \gg v_2$, $\lambda \sim (v_2/v_1)^{1/4} \ll 1$. For $v_1/v_2 \gtrsim 14$, the gapless regime extends to the Heisenberg point for infinitesimal J_K. Clarifying the nonzero J_K behavior there requires a more sophisticated analysis which we have not yet completed.

In the Kondo necklace model [5], $v_2 \to 0$ at fixed J_K and there is an x-y anisotropy. For $J_K \to \infty$ our analysis shows a singlet phase where a gap to excitations occurs. Our small-J_K results are based on an expansion in $J_K/(v_1 v_2)^{1/2}$, which obviously breaks down as $v_2 \to 0$. A different approach would be required to determine whether the Kondo necklace model has an XY phase as $J_K \to 0$.

By connecting up the weak coupling and strong coupling results we obtain the phase diagram shown in Fig. 1. We have inferred the existence of the multicritical point where phases F, XY, and S meet from the absence of the XY phase in the large-J_K calculation and its presence in the small-J_K calculation. The H-A and S-A boundaries are Ising transitions because a Z_2 symmetry is broken. The Heisenberg antiferromagnetic point $J_z = |J_\perp|$ must be analyzed by more sophisticated methods. For the $J_z < 0$ region, we have already argued that for $J_K \leq 0$ the transition between phases XY and F is first order. However, the transition from phase F to phase S is Ising for $J_K \to +\infty$. We believe that the order of the phase transition changes at the multicritical point whose existence we inferred above. The XY-S line is known [11,12] to be Kosterlitz-Thouless at weak coupling, where a single operator, $\cos 2\Theta_{J,S}$, becomes relevant. The XY-H

line is a continuation of the XY-S line and is Kosterlitz-Thouless for the same reason as the XY-S line, in agreement with previous results [8] for $J_K \to -\infty$.

The Kondo and Anderson lattice models, more realistic models which include the charge degrees of freedom of the conduction electrons and (for the Anderson model) the possibility of valence fluctuations on the local moment site, have also been studied numerically in one dimension [13,14]. At band fillings corresponding to one conduction electron and one local moment electron per site, the ground state was found to be insulating with no long-range magnetic order and a gap to both charge and spin excitations. The spin degrees of freedom of a one-dimensional Fermi gas cannot be simply modeled as a spin chain. However, we believe that the magnetic excitations of this model are described by our Hamiltonian with $J_K > 0$, and antiferromagnetic Heisenberg interactions in both chains. For these parameters we find the ground state to be nonmagnetic in at least qualitative agreement with the numerical results.

In conclusion, we comment on implications of our results for theories of heavy fermion metals. Some mean-field theories predict that one has either a Kondo phase with no magnetic correlations or a magnetic phase with no Kondo correlations, with a strongly first-order transition separating the two phases [15]. By contrast, the transitions we find between Kondo and magnetic states are conventional second-order (or Kosterlitz-Thouless) $T=0$ phase transitions produced by tuning a parameter, in qualitative agreement with a previous suggestion of Doniach [16], although we do not find any evidence of the unusual critical behavior suggested in Ref. [16]. The short length scale physics varies smoothly near the transitions. We suspect that these will be generic features of models of heavy fermion materials with magnetic interactions. One aspect of our results which we believe is not generic is the persistence of the quantum disordered phases S and H for not too asymmetric chains and arbitrarily small values of J_K over a range of J_z. We believe that this is an effect peculiar to one-dimensional half-filled bands and that in higher-dimensional generalization of our model magnetic order would occur for sufficiently small J_K.

Our results may also be relevant for the newly discovered "heavy fermion insulator" compounds [17]. In these materials, because of the band filling, the Kondo effect apparently leads at low temperatures not to a heavy Fermi liquid but to a small-gap insulator. The low-temperature magnetic susceptibility $\chi(q,\omega=0)$ of these materials has been measured via neutron scattering [18] and found to be q independent for some range of q. It has been suggested [18] that this q independence is a generic property of the heavy fermion insulator state. Our model (except for the restriction to one spatial dimension) should be directly relevant to these materials. In it the susceptibility is in general not q independent; indeed the $q=0$ component of χ_{xx} or χ_{zz} diverges at the transitions between the nonmagnetic phase S and the ferromagnetic phases XY or F and the $q=\pi$ component of χ_{zz} diverges at the S-A transition. Therefore we believe that within the Kondo lattice model the observed q independence of $\chi(q,\omega=0)$ in the heavy fermion insulator compounds simply implies that a parameter (equivalent to our J_z) happens to have some particular value.

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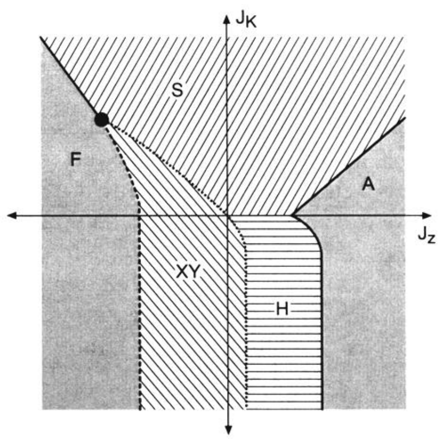
[1] G. R. Stewart, Rev. Mod. Phys. **56**, 755 (1984).
[2] P. A. Lee *et al.*, Condens. Matter Phys. B **12**, 99 (1986).
[3] See, e.g., P. Nozières, in *Proceedings of the Fourteenth International Conference on Low Temperature Physics*, edited by M. Krusius and M. Vuorio (North-Holland, Amsterdam, 1975).
[4] C. M. Varma, Rev. Mod. Phys. **48**, 219 (1978); S. Doniach, Physica (Amsterdam) **91B**, 231 (1977).
[5] R. Jullien, N. Fields, and S. Doniach, Phys. Rev. B **16**, 4889 (1977).
[6] S. P. Strong and A. J. Millis (unpublished).
[7] R. Jullien and P. Pfeuty, J. Phys. F **11**, 353 (1981).
[8] F. D. M. Haldane, Phys. Lett. **93A**, 464 (1983); H. J. Schulz, Phys. Rev. B **34**, 6372 (1986); H. J. Schulz and T. Ziman, Phys. Rev. B **33**, 6546 (1986).
[9] P. Pfeuty, Ann. Phys. (N.Y.) **57**, 79 (1970).
[10] See, e.g., S. K. Ma, *Modern Theory of Critical Phenomena* (Benjamin/Cummings, Reading, MA, 1976), especially Chaps. VII and VIII, Sec. 5.
[11] A. Luther and I. Peschel, Phys Rev. B **9**, 2911 (1974); F. D. M. Haldane, J. Phys C **14**, 2585 (1981).
[12] I. Affleck, in *Fields, Strings and Critical Phenomena*, Proceedings of the Les Houches Summer School Session XLIX, edited by E. Brezin and J. Zinn-Justin (Elsevier, Amsterdam, 1989).
[13] K. Ueda, H. Tsunetsunga, and M. Sigrist, Phys. Rev. Lett. **68**, 1030 (1992).
[14] R. M. Fye and D. J. Scalapino, Phys. Rev. B **44**, 7486 (1991).
[15] See, e.g., H. Shiba and P. Fazekas, Prog. Theor. Phys. Suppl. **101**, 403 (1990).
[16] S. Doniach, in *Theoretical and Experimental Aspects of Valence Fluctuations and Heavy Fermions*, edited by L. C. Gupta and S. K. Malik (Plenum, New York, 1987), p. 179.
[17] M. F. Hundley, P. C. Canfield, J. D. Thompson, Z. Fisk, and J. M. Lawrence, Phys. Rev. B **42**, 6842 (1990).
[18] T. E. Mason *et al.*, Phys. Rev. Lett. **69**, 430 (1992).



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