Kondo effect in a quantum critical ferromagnet

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We study the Heisenberg ferromagnetic spin chain coupled with a boundary impurity. Via Bethe ansatz solution, it is found that (i) for $J>0$, the impurity spin behaves as a diamagnetic center and is completely screened by $2S$ bulk spins in the ground state, no matter how large the impurity spin is; (ii) the specific heat of the local composite (impurity plus $2S$ bulk spins which form bound state with it) shows a simple power law $C_{loc}\sim T^{3/2}$; (iii) for $J<0$, the impurity is locked into the critical behavior of the bulk. Possible phenomena in higher dimensions are discussed. [S0163-1829(99)02521-7]

Kondo problem or the magnetic impurity problem in an electron host plays a very important role in modern condensed-matter physics. It represents a generic nonperturbationable example of the strongly correlated many-body systems. Recently, with the development of research on some low-dimensional systems[1] and the observation of unusual non-Fermi-liquid behavior in some heavy fermion compounds,[2] the interest in this problem has been largely renewed. The multichannel Kondo problem[3] provided an example of impurity systems which show non-Fermi-liquid behavior at low temperatures.[4] In a Luttinger liquid, the impurity behaves rather differently[5,6] from that in a Fermi liquid and may interpolate between a local Fermi liquid and some non-Fermi liquid.[7] Some quantum critical phenomena have also been predicted in some integrable models.[8,9] Generally speaking, these findings indicate that the quantum impurity models renormalize to critical points corresponding to conformally invariant boundary conditions.[10] Another important progress is the study on the Kondo problem in Fermi systems with pseudogap,[11] i.e., the density of states $\rho(\epsilon)$ is power-law dependent on the energy, $\rho(\epsilon)\sim\epsilon^r$. With renormalization-group (RG) analysis, Withoff and Fradkin[11] showed that there is a critical value J_c for the Kondo coupling constant J. For $J>J_c$, Kondo effect occurs at low temperatures, while for $J<J_c$, the impurity decouples from the host. We note that all the quantum critical behaviors mentioned above only occur for $T\to 0$ and therefore fall into the general category of quantum phase transitions.[12]

In an earlier publication, Larkin and Mel'nikov studied the Kondo effect in an almost ferromagnetic metal.[13] With the traditional perturbation theory they showed that the impurity susceptibility is almost Curie-type with logarithmic corrections at intermediately low temperatures. However, the critical behavior of a Kondo impurity in a quantum critical ferromagnet has never been touched. The main difficulty in approaching this problem is that almost all perturbation techniques fail in the critical regime and exact results are expected. As discussed in some recent works,[14] the critical behavior of the impurity strongly depends on the host properties and seems to be nonuniversal. Typical quantum critical ferromagnet is the Heisenberg system in reduced dimensions $(d\leqslant 2)$. These systems have long-range-ordered ground states but are disordered at any finite temperatures due to the strong quantum fluctuations. In this paper, we study the critical behavior of an impurity spin coupled with a Heisenberg ferromagnetic chain. The model Hamiltonian we shall consider reads

$$H=-\frac{1}{2}\sum_{j=1}^{N-1}\boldsymbol{\sigma}_j\cdot\boldsymbol{\sigma}_{j+1}+J\boldsymbol{\sigma}_1\cdot\mathbf{S},\tag{1}$$

where $\boldsymbol{\sigma}_j$ is the Pauli matrices on site j, N is the length of the chain, $\mathbf{S}$ is the impurity spin sited at one end of the chain, and J is a real constant which describes the Kondo coupling between the impurity and the host. The problem is interesting because (i) the model is not conformally invariant due to the nonlinear dispersion relation of the low-lying excitations, $\epsilon(k)\sim k^2$, and $\rho(\epsilon)\sim\epsilon^{-1/2}$, and represents a typical quantum critical system beyond the universality of the conventional Luttinger liquid; (ii) the Hamiltonian is very simple (without any superfluous term) and allows exact solution via algebraic Bethe ansatz.[15] In fact, most known methods[8,9] developed for the impurity problem in a Luttinger liquid cannot be used for the present system due to the strong quantum fluctuations.

Let us first summarize the solution of Eq. (1). Define the Lax operator $L_{j\tau}(\lambda)\equiv\lambda+i/2(1+\boldsymbol{\sigma}_j\cdot\boldsymbol{\tau})$, where $\boldsymbol{\tau}$ is the Pauli matrices acting on the auxiliary space and λ is the so-called spectral parameter. For the impurity, we define $L_{0\tau}\equiv\lambda+i(1/2+\mathbf{S}\cdot\boldsymbol{\tau})$. Obviously, $L_{j\tau}$ and $L_{0\tau}$ satisfy the Yang-Baxter equation (YBE).[16] It can be easily shown that the doubled-monodromy matrix

$$\begin{aligned}T_\tau(\lambda)\equiv{}&L_{N\tau}(\lambda)\cdots L_{1\tau}(\lambda)L_{0\tau}(\lambda-ic)\\&\times L_{0\tau}(\lambda+ic)L_{1\tau}(\lambda)\cdots L_{N\tau}(\lambda)\end{aligned}\tag{2}$$

satisfies the reflection equation

$$\begin{aligned}&L_{\tau\tau'}(\lambda-\mu)T_\tau(\lambda)L_{\tau\tau'}(\lambda+\mu)T_{\tau'}(\mu)\\&\quad=T_{\tau'}(\mu)L_{\tau\tau'}(\lambda+\mu)T_\tau(\lambda)L_{\tau\tau'}(\lambda-\mu).\end{aligned}\tag{3}$$

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From the above equation we can show that the transfer matrices $\theta(\lambda)\equiv Tr_\tau T_\tau(\lambda)$ with different spectral parameters are commutative, $[\theta(\lambda),\theta(\mu)]=0$. Therefore $\theta(\lambda)$ serves as a generator of a variety of conserved quantities. The Hamiltonian Eq. (1) is given by

$$H=(i/2)\,J(-1)^N(\partial/\partial\lambda)\,\theta(\lambda)|_{\lambda=0}+\tfrac{1}{2}(N+1-J), \quad (4)$$

with $J=1/[c^2-(S+1/2)^2]$. Following the standard method[15,8] we obtain the Bethe ansatz equation (BAE)

$$\left(\frac{\lambda_j-i/2}{\lambda_j+i/2}\right)^{2N}\frac{\lambda_j-i(S+c)}{\lambda_j+i(S+c)}\,\frac{\lambda_j-i(S-c)}{\lambda_j+i(S-c)}=\prod_{l\neq j}^{M}\frac{\lambda_j-\lambda_l-i}{\lambda_j-\lambda_l+i}\,\frac{\lambda_j+\lambda_l-i}{\lambda_j+\lambda_l+i}, \quad (5)$$

with the eigenvalue of Eq. (1) as

$$E(\{\lambda_j\})=\sum_{j=1}^{M}\frac{1}{\lambda_j^2+\frac{1}{4}}-\frac{1}{2}(N-1)+JS, \quad (6)$$

where λ_j represent the rapidities of the magnons and M the number of the magnons.

Ground state. In the thermodynamic limit, the bulk solutions of λ_j are described by the so-called n strings.[17] However, due to the presence of the impurity, some boundary bound states may exist for $c>S$, which are usually called the $n-k$ strings:[18]

$$\lambda_b^m=i(c-S)+im, \quad m=k,k+1,\ldots n. \quad (7)$$

In the ground state, only some $n-0$ strings may survive. We call them boundary n strings. In our case, $n\geqslant 0$ has also an upper bound $n\leqslant 2S-1$ since $\lambda_j=\pm i(c+S)$ are forbidden as we can see from Eq. (5). No bulk strings can exist at zero temperature since they carry positive energy. Boundary bound state can exist only for $c>S+1/2$ (antiferromagnetic Kondo coupling) because in this case, the boundary n strings carry negative energy. For zero external magnetic field, the most stable boundary string has the length of $2S$ with the energy $\epsilon_{2S}=2S/[S^2-(c-1/2)^2]$. Therefore the impurity contributes a magnetization of $-S$. Such a phenomenon can be understood in a simple picture. Due to the antiferromagnetic coupling between the impurity and the bulk, $2S$ bulk spins are swallowed by the impurity at zero temperature to form a $2S+1$-body singlet. This singlet does not contribute to the magnetization of the ground state. In this sense, the impurity is completely screened, no matter how large the impurity moment is. Such a situation is very different from that of the conventional Kondo problem, where the impurity moment can only be partially screened by the host when $S>S'$ (S' the spin of the host particles).[19] This difference is certainly due to the different properties of the hosts. In the antiferromagnetic spin chain or a normal metal, the spin correlation of the bulk is antiferromagnetic-type which repels more than one bulk spin or electron to screen the impurity. However, in a ferromagnetic spin chain, the bulk correlation is ferromagnetic which allows and in fact enhances some bulk spins to form a larger moment to screen the impurity. The local singlet is nothing but a bound state of $2S$ magnons. The boundary string may be broken by the external field. In fact, there are $2S$ critical fields:

$$H_c^n=\frac{1}{n}\left(\frac{2S}{(c-\frac{1}{2})^2-S^2}-\frac{2S-n}{[c-(n+1)/2]^2-(S-n/2)^2}\right),$$
$$n=1,2,\ldots,2S. \quad (8)$$

When $H_c^n<H<H_c^{n+1}$, only a boundary $(2S-n)$-string survives in the ground state and when $H>H_c^{2S}$, any boundary string becomes unstable. Notice that at $H=H_c^n$, the ground-state magnetization has a jump $\delta M=1$, which corresponds to some type of quantum phase transition. The finite value of H_c^1 indicates that the zero temperature susceptibility of the local singlet is exactly zero.

Thermal BAE. Since we are interested mostly in the critical behavior, we consider $T,H\ll H_c^1$ and $J>0$ case in the following text. In this case, any excitations breaking the boundary string can be plausibly omitted due to the energy gap associated with them. With the standard thermal Bethe ansatz,[17] we derive the thermal BAE as

$$\ln(1+\eta_n)=\frac{2\pi a_n(\lambda)+nH}{T}+\sum_{m=1}^{\infty}\mathbf{A}_{mn}\ln[1+\eta_m^{-1}(\lambda)], \quad (9)$$

or equivalently,

$$\ln\eta_1(\lambda)=(\pi/T)\,g(\lambda)+\mathbf{G}\,\ln[1+\eta_2(\lambda)],$$
$$\ln\eta_n(\lambda)=\mathbf{G}\{\ln[1+\eta_{n+1}(\lambda)]+\ln[1+\eta_{n-1}(\lambda)]\}, \quad n>1, \quad (10)$$
$$\lim_{n\to\infty}(\ln\eta_n/n)=H/T\equiv 2x_0,$$

where $a_n(\lambda)=n/2\pi[\lambda^2+(n/2)^2]$, $\mathbf{A}_{mn}=[m+n]+2[m+n-2]+\cdots+2[|m-n|+2]+[|m-n|]$; $g(\lambda)=1/2\cosh(\pi\lambda)$; $\eta_n(\lambda)$ are some functions which determine the free energy of the system; and $[n]$ and $\mathbf{G}$ are integral operators with the kernels $a_n(\lambda)$ and $g(\lambda)$, respectively. The free energy is given by

$$F=F_{bulk}+F_{imp},$$
$$F_{bulk}=F_0-\left(N+\frac{1}{2}\right)T\int g(\lambda)\left\{\ln[1+\eta_1(\lambda)]-\frac{2\pi a_1(\lambda)+H}{T}\right\}d\lambda, \quad (11)$$
$$F_{imp}=\frac{1}{2}T\sum_{n=1}^{\infty}\int\phi_n'(\lambda)\ln[1+\eta_n^{-1}(\lambda)]d\lambda,$$

where $a_{n,m}(\lambda)=\sum_{l=1}^{min(m,n)}a_{n+m+1-2l}(\lambda)$, $\phi_n'(\lambda)=a_{n,2S}(\lambda-ic+i)+a_{n,2S}(\lambda+ic-i)$; F_0 is the ground-state energy, F_{bulk} and F_{imp} are the free energies of the bulk (including the bare boundary) and the impurity, respectively. Notice that Eqs. (9) and (10) are more difficult to handle than those of the antiferromagnetic chain,[17] since here all η_n diverge as for $T\to 0$. These equations were solved numerically[20] in studying the critical behavior of the ferromagnetic Heisenberg chain. In addition, Schlottmann gave an analytical result based on a simple correlation-length approximation[21] and the result coincides with the numerical ones very well. As we can see from Eqs. (9) and (10), when $T\to 0$, $\eta_n\to\infty$. To arrive at the asymptotic solutions of

$\eta_n(\lambda)$, we make the ansatz $\eta_n(\lambda)=\exp[2\pi a_n(\lambda)/T]\phi_n$. Substituting this ansatz into Eq. (10) we readily obtain $\phi_n\sim 1$ for finite n and λ. Therefore

$$\eta_n \approx \exp\left(\frac{2\pi a_n(\lambda)}{T}\right), \quad T\to 0. \tag{12}$$

On the other hand, when $\lambda\to\infty$ or $n\to\infty$, the driving term in Eq. (10) tends to zero. This gives another asymptotic solution of η_n for very large λ or n:[17]

$$\eta_n=\frac{\sinh^2[(n+1)x_0]}{\sinh^2 x_0}-1+O\left(\frac{1}{T}e^{-\pi|\lambda|}\right). \tag{13}$$

For intermediate λ and n we have a crossover regime. We call Eq. (12) the strong-coupling solution, while Eq. (13) is the weak-coupling solution. By equating them we obtain two types of crossover scales, $\lambda_c(n)$ for small n and $n_c(T)$:

$$\lambda_c(n)\approx\left(\frac{n}{4T\ln(1+n)}\right)^{1/2},$$

$$n_c(T)\approx\frac{1}{4T\ln(1+n_c)}\approx-\frac{1}{4T\ln T}, \tag{14}$$

which characterize the crossover of the strong-coupling regime and the weak-coupling regime. Notice that the strong-coupling solution gives the correct ground-state energy and the low-temperature thermodynamics is mainly dominated by the weak-coupling solution.[22] With such an approximation, the recursion for η_n can be performed by substituting the asymptotic solutions into the right-hand side of Eq. (9) and therefore the leading-order correction upon the asymptotic solutions can be obtained. In the following recursion process, we adopt the strong-coupling solution in the region of $\lambda<\lambda_c$ and $n<n_c$, while the weak-coupling solution is adopted in other cases. This corresponds to an abrupt crossover, which does not affect the temperature dependence of the thermodynamic quantities in leading orders but their amplitudes. For convenience, we define $\zeta_n(\lambda)\equiv\ln[1+\eta_n(\lambda)]-[2\pi a_n(\lambda)+nH]/T$, which are responsible for the temperature-dependent part of the free energy.

Low-temperature susceptibility of the impurity. For convenience, we consider $2c=integer$ case. Taking the boundary string into account, the free energy of the impurity can be rewritten as

$$F_{imp}=\frac{1}{2}T\int g(\lambda)[\zeta_{2c+2S-2}(\lambda) - \mathrm{sgn}(2c-2S-2)\zeta_{|2c-2S-2|}(\lambda)]d\lambda. \tag{15}$$

Substituting the asymptotic solutions Eqs. (12) and (13) into Eq. (9) and omitting the exponentially small terms, we obtain

$$\zeta_n(\lambda)\approx\sum_{m=1}^{n_c}\left[\ln\left(1+\frac{1}{m(m+2)}\right)-\frac{2}{3}x_0^2\right] \times\left(\int_{\lambda_c(m)}^{\infty}+\int_{-\infty}^{-\lambda_c(m)}\right)A_{mn}(\lambda-\lambda')d\lambda' +2n_c\ln[\sinh(1+n_c)x_0/\sinh n_c x_0], \tag{16}$$

where A_{mn} is the kernel of $\mathbf{A}_{mn}$. For small $n\ll n_c$, up to the leading order, we find that the x_0^2 term of $\zeta_n(\lambda)$ is exactly n times of that of $\zeta_1(\lambda)$. From Eq. (15) we easily derive

$$\chi_{imp}=-2S\chi_{bulk}+\text{subleading-order terms}, \tag{17}$$

where $\chi_{bulk}\sim T^{-2}\ln^{-1}(1/T)$ is the per-site susceptibility of the bulk.[20,21] Very interestingly, the impurity contributes a negative susceptibility, which indicates an interesting Kondo diamagnetic effect. That means the Kondo coupling dominates always over the ''molecular field'' generated by the bulk ferromagnetic fluctuations. Notice that Eq. (17) is only the contribution of the bare impurity. If we take the screening cloud ($2S$ bulk spins which form the bound state with the impurity) into account, we find that the total susceptibility of the local singlet is exactly canceled in the leading order. That means the polarization effect of the local bound state only occurs in some subleading order, which indicates a strong-coupling fixed point $J^*=\infty$. In fact, the local singlet is much more insensitive to a small external magnetic field as we discussed for the ground state. When $T\to 0$, its susceptibility must tend to zero due to the bound energy as shown in Eq. (8). We note that the present method is not reliable to derive the total susceptibility of the local singlet but the above picture must be true. The same conclusion can be achieved for arbitrary $J>0$.

Specific heat of the local composite. In the framework of the local Fermi-liquid theory,[23] the Kondo effect is nothing but the scattering effect of the rest bulk particles $(N-2S)$ off the local-spin-singlet composite or equivalently, the polarization effect of the local composite due to the scattering. Taking the boundary string into account, the BAE of the bulk modes can be rewritten as

$$\left(\frac{\lambda_j-i/2}{\lambda_j+i/2}\right)^{2(N-2S)}=e^{i\phi(\lambda_j)}\prod_{l\neq j}^{M-2S}\frac{\lambda_j-\lambda_l-i}{\lambda_j-\lambda_l+i}\,\frac{\lambda_j+\lambda_l-i}{\lambda_j+\lambda_l+i}, \tag{18}$$

$$e^{i\phi(\lambda)}=\frac{\lambda-i(c+S-1)}{\lambda+i(c+S-1)}\,\frac{\lambda+i(c-S-1)}{\lambda-i(c-S-1)}\left(\frac{\lambda+i/2}{\lambda-i/2}\right)^{4S}, \tag{19}$$

where $\phi(\lambda)$ represents the phase shift of a spin-wave scattering off the local composite (boundary bound state). When $S=1/2, c\to 1+0^+$ or $J\to+\infty, \phi(\lambda)=0$. That means one of the bulk spin is completely frozen by the impurity and the system is reduced to an $N-1$-site ferromagnetic chain. When $S=1/2, 1<c<3/2$, only $\zeta_1(\lambda)$ is relevant and the free energy of the local composite reads

$$F_{loc}=-T\int g(\lambda)[\zeta_1(\lambda)-\tfrac{1}{2}\zeta_1(\lambda-ic+i) -\tfrac{1}{2}\zeta_1(\lambda+ic-i)]d\lambda. \tag{20}$$

When $x_0=0$, we have

$$\zeta_1(\lambda)-\tfrac{1}{2}\zeta_1(\lambda-ic+i)-\tfrac{1}{2}\zeta_1(\lambda+ic-i) =16(c-1)^2T^{3/2}\frac{1}{\pi}\sum_{m=1}^{n_c}\ln\left[1+\frac{1}{m(m+2)}\right] \times m^{-1/2}\ln^{3/2}(1+m)+\ \ldots. \tag{21}$$

The sum in the above equation is convergent for large n_c. Therefore we can extend it to infinity, which gives the low-temperature specific heat of the local composite as

$$C_{loc} \sim T^{3/2}. \quad (22)$$

A similar conclusion can be arrived for arbitrary S and $J > 0$. As long as the Kondo coupling is antiferromagnetic ($c \geqslant S+1/2$), the low-temperature specific heat of the local composite is described by Eq. (22). There is a slight difference between the $S=1/2$ case and the $S>1/2$ case. For the former when $J \rightarrow \infty$, the local singlet is completely frozen and $C_{loc} \rightarrow 0$, while for the later even when $J \rightarrow \infty$, C_{loc} takes a finite value. This can be understood in a simple picture. For $S>1$, more than one bulk spin will be trapped by the impurity. Even for $J \rightarrow \infty$, only one bulk spin (on the nearest-neighbor site) can be completely frozen and the rest is still polarizable via the bulk fluctuation. We note the specific heat of the local singlet is much weaker than that of the Kondo impurity in a conventional metal. This still reveals the insensitivity of the local bound state to the thermal activation. Though the anomalous power law Eq. (22) looks very like that obtained in the Luttinger Kondo systems,[8,9] they are induced by different mechanisms. In the present case, this anomaly is mainly due to the strong quantum fluctuation while in the Luttinger liquid, the anomaly is in fact induced by the tunneling effect of the conduction electrons through the impurity.[6,24,25]

For the ferromagnetic coupling case ($J<0$), no boundary bound state exists. Even in the ground state, the impurity spin is completely polarized by the bulk spins. At finite temperature, the critical behavior is locked into that of the bulk $[C_{imp} \sim T^{1/2}, \chi_{imp} \sim -(T^2 \ln T)^{-1}]$.[19,20]

Similar phenomena may exist in higher dimensions. The antiferromagnetic Kondo coupling indicates a local potential well for the magnons. Therefore some bound states of the magnons may exist in the ground-state configuration, which indicates the formation of the local spin-singlet. In this sense, the impurity behaves as a diamagnetic center. When $J<0$, the Kondo coupling provides a repulsive potential to the magnons and no local bound state can exist at low-energy scales. The impurity must be locked into the bulk.

In conclusion, we solve the model of a ferromagnetic Heisenberg chain coupled with a boundary impurity with arbitrary spin. It is found that as long as the Kondo coupling is antiferromagnetic, (i) the impurity spin behaves as a diamagnetic center and is completely screened by $2S$ bulk spins in the ground state, no matter how large the impurity spin is; (ii) the specific heat of the local composite (impurity plus $2S$ bulk spins which form bound state with it) shows a simple power law $C_{loc} \sim T^{3/2}$. We note that for a finite density of impurities, the local bound states are asymptotically extended to an impurity band of the magnons, which is very similar to that of a ferrimagnetic system. The critical behavior may be different from that of the single impurity case. When the impurity density $n_i \sim 1/(2S)$, we expect a spin singlet ground state.

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[22] Notice that the leading term of the free energy upon the ground-state energy comes from the small λ corrections to the strong-coupling solution, which is mainly determined by the weak-coupling solution as shown in Eq. (9). In fact, the bulk strings serve as a variety of spin waves with generalized exclusion statistics. This may explain why the spin-wave theory gives the correct critical exponents of the ferromagnetic Heisenberg chain (Refs. 20 and 21).

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