Quantum Magnetic Impurities in Magnetically Ordered Systems

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We discuss the problem of a spin 1/2 impurity immersed in a spin S magnetically ordered background. We show that the problem maps onto a generalization of the dissipative two level system with two independent heat baths, associated with the Goldstone modes of the magnet, that couple to different components of the impurity spin operator. Using analytical perturbative renormalization group methods and accurate numerical renormalization group we show that contrary to other dissipative models there is quantum frustration of decoherence and quasiscaling even in the strong coupling regime. We make predictions for the behavior of the impurity magnetic susceptibility. Our results may also have relevance to quantum computation.

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Quantum impurity problems are characterized by a single quantum mechanical degree of freedom coupled to a reservoir. These are the simplest problems in physics that exhibit nontrivial many-body effects. Among them, the dissipative two level system (DTLS) [1] plays a central role because it is related to a variety of different physical processes such as the dissipative tunneling of a particle in a double well or the coupling of an Ising spin to a gapless fermionic environment, i.e., the anisotropic Kondo problem (AKP). The Kondo problem is one of the best understood impurity problems and has been studied by a large variety of methods. Its thermodynamic properties can be studied exactly via Bethe ansatz [2] and renormalization group (RG) [3], its dynamic properties at low energies can be calculated via conformal field theory [4], and many of its correlation functions can be obtained exactly [5]. The problem of quantum impurities immersed in magnetic media close to a quantum phase transition has also attracted a lot of attention recently due to its possible relevance to cuprates, heavy fermions, and organic materials [6]. While most of the recent works focus on the paramagnetic phase, we concentrate on magnetically ordered phases [7,8].

We study a quantum impurity problem of a different nature, namely, the problem of a single spin 1/2 coupled to a d-dimensional magnetically ordered system with spin S. A possible application of our results can be found, for instance, in $KMn_{1-x}Cu_xF_3$ with $x \ll 1$(Cu has spin 1/2 and Mn has $S = 5/2$). $KMnF_3$ is a three-dimensional ($d = 3$) cubic quantum Heisenberg antiferromagnet (QHAF) with exchange coupling J between the Mn spins. This material orders in a Néel state and has well defined gapless magnon modes [9]. The Mn spins interact with the Cu spin via an exchange J'. In the past this problem was studied by a series of different theoretical techniques that usually assume the impurity spin to be aligned with the surrounding Néel state and/or $J' \approx J$ [9,10]. As we are going to show, while this kind of approach is warranted at low temperatures, it fails to describe the full quantum behavior of the impurity at energy scales intermediate between J' and J ($J' \ll J$) where the impurity spin fluctuates strongly and gets mixed with the quantum fluctuations of the magnetic environment. The problem at hand is similar to the Kondo effect of magnetic impurities in metals where there is a many-body crossover from weak to strong coupling as the temperature is lowered below the Kondo temperature. In our case, the screened state occurs when the impurity spin fully aligns with the surrounding background below an energy T_A. We are interested in the relaxation of the Cu spins. In particular, we calculate the frequency and temperature dependence of the imaginary part of the transverse impurity susceptibility for the QHAF in $d = 3$, $\chi_\perp(\omega, T)$.

At long wavelengths and low energies the magnetic problem can be described by a spin coherent state path integral in terms of the Euclidean action S_E (we use units such that $\hbar = k_B = 1$) with $S_E = S_{WZ} + S_M$ where S_{WZ} is the Wess-Zumino term that describes the quantum dynamics for the impurity spin $\mathbf{S}$ and

$$S_M = \int d^{d+1}x_\mu \left\{ \frac{1}{2g}[(\partial_0 \mathbf{n}(x_\mu))^2 + c^2(\partial_i \mathbf{n}(x_\mu))^2] + \delta^d(x_i)\mathbf{n}(x_\mu) \cdot \lambda \cdot \mathbf{S}(x_0) \right\}, \quad (1)$$

where $x_\mu = (x_0 = \tau, x_i)$ with $\mu = 0, 1, \ldots, d$ is the space-time coordinate, $c = 2\sqrt{d}JaS$ is the spin-wave velocity, $g = c^2/\rho_s$ is the coupling constant, $\rho_s = JS^2a^{2-d}$ is the spin stiffness for the nonlinear sigma model [11] described by the vector field $\mathbf{n}$ (a is the lattice spacing), and $\lambda \propto J'$ is the matrix coupling between the impurity spin and the spin environment. The action (1) has to be supplemented by the local constraint $\mathbf{n}^2(x_\mu) = 1$. In the ordered phase, we can write $\mathbf{n} \approx (\varphi_1, \varphi_2, 1)$ with $|\varphi_a| \ll 1$. We will assume $\lambda = (\lambda_1, \lambda_2, \Delta)$ and that $\Delta, \lambda_{1,2} \ll D_0 \approx J$ where D_0 is the bare cutoff of the problem. The action reduces to

$$S_M \approx \int d^{d+1}x_\mu \left\{ \frac{1}{2g}[(\partial_0 \vec{\varphi}(x_\mu))^2 + c^2(\partial_i \vec{\varphi}(x_\mu))^2] + \delta^d(x_i)\left[\Delta S_3 + \sum_{a=1,2} \lambda_a \varphi_a(x_\mu) S_a \right] \right\}, \tag{2}$$

where $\vec{\varphi} = (\varphi_1, \varphi_2)$ represents the two Goldstone modes of the QHAF. Equation (2) describes a problem of two free bosonic modes coupled to an impurity via its different spin components. Notice that the Δ coupling describes the molecular Weiss field applied by the QHAF. The other two terms represent the quantum fluctuations of the impurity due to the coupling to the Goldstone modes. Since the operators S_a obey the spin algebra, they affect the impurity spin by inducing transitions between the eigenstates of S_3. The problem can be reduced to a one-dimensional (1D) problem using an s-wave expansion [1] with a Hamiltonian, $H = H_0 + H_I \delta(x)$, where

$$H_0 = \frac{1}{2}\sum_{a=1,2}\int_0^\infty dx[\Pi_a^2(x) + c^2(\partial_x \Phi_a(x))^2],$$
$$H_I = \Delta S_3 + \sqrt{\frac{g}{(2\pi)^d}}\sum_a \lambda_a \int_0^\infty dk k^{(d-1)/2}\Phi_a(k) S_a, \tag{3}$$

where $\Phi_a(x)$ and $\Pi_a(x)$ $(a = 1, 2)$ are conjugate real scalar fields on the half line [$\Phi_a(k)$ is the Fourier transform of $\Phi_a(x)$ where k is the momentum]. It is convenient to further decompose the fields into right, $\Phi_{a,R}(x)$, and left, $\Phi_{a,L}(x)$, moving components associated with outgoing and incoming waves out of the impurity, respectively. Notice that the coupling of the impurity spin to the bosonic reservoir depends on the dimensionality. This should be contrasted with the Kondo problem where the coupling to fermions with a Fermi surface make the problem insensitive to d. To make contact with the Kondo problem we return to the path integral language and trace over the bosonic modes obtaining an effective action $S_{\text{eff}} = S_{\text{WZ}} + S_I$ for the impurity alone, where

$$S_I = \int d\tau \Delta S_3(\tau) - \sum_{a=1,2}\gamma_a \int d\tau \int d\tau' \frac{S_a(\tau) S_a(\tau')}{|\tau - \tau'|^\alpha}, \tag{4}$$

where $\gamma_a = [\lambda_a^2 g S_d \Gamma(d-1)]/[4(2\pi)^d c^d]$ [S_d is the area of the hypersphere in d dimensions and $\Gamma(x)$ is the Gamma function] and $\alpha = d - 1$ (for a ferromagnet $\alpha = d/2$).

Consider first the case where $\gamma_1 \neq 0$ but $\gamma_2 = 0$ and $\alpha = 2$ $(d = 3)$. In this case the action (4) can be mapped onto the AKP [3] and is equivalent to the problem of a classical 1D spin chain with long-range interactions in a magnetic field. There is a Kosterlitz-Thouless (KT) phase transition at $\gamma_1 = 1$: for $\gamma_1 < 1$, Δ scales to infinity indicating that the impurity aligns with the bulk—in the Kondo language this is equivalent to the formation of the Kondo singlet; for $\gamma_1 > 1$, Δ is irrelevant under the RG and scales to zero—this is the equivalent of the Kondo problem with ferromagnetic coupling. The second case is $1 < \alpha < 2$ and $\gamma_1 = \gamma_2 = \gamma$. Notice, on the one hand, that in terms of its Fourier transform the second term in (4) behaves like $|\omega|^{\alpha-1}|S_a(\omega)|^2$ where ω is the frequency. On the other hand, S_{WZ} describes the area of the unit sphere bounded by the trajectory parametrized by $\mathbf{S}(\tau)$. For a variation of $\mathbf{S}$ by $\delta\mathbf{S}$ the variation in this term is simply $\delta S_{\text{WZ}} = \delta\mathbf{S} \cdot (\mathbf{S} \times \partial_\tau \mathbf{S})$, and therefore S_{WZ} scales like ω. Thus, for $\alpha < 2$ $(d < 3)$ the long-range interaction is relevant at low energies and one can disregard S_{WZ}; that is, the impurity behaves classically. It may be surprising that as one lowers the dimensionality (decreases α) the magnetic impurity behaves classically but it results from the fact that the interactions in imaginary time become longer ranged. By disregarding S_{WZ} the problem reduces to a classical XY chain with long-range interactions [12] in the presence of a field in the Z direction (proportional to Δ) where γ plays the role of the inverse of the temperature. Δ is a relevant perturbation and the spin always orders with the bulk without quantum effects. For the $d = 2$ QHAF this problem has been studied via spin-wave T-matrix scattering [13], field theoretical methods [10], and quantum Monte Carlo [14]. Finally, when $\alpha > 2$ $(d > 3)$ the second term in (4) is irrelevant and the spin effectively decouples from the fluctuations of the environment at low energies; that is, the problem can be described in terms of a quantum spin in the Weiss molecular field alone.

It is clear that the case of most interest is when $\alpha = 2$ and $\gamma_1, \gamma_2 \neq 0$. Notice that for a QHAF this implies $d = 3$ which is also the case of experimental interest. Returning to (3), it is convenient to work with a single field on the entire real line by the unfolding transformation: $\phi_L(x) = \Phi_{1,L}(x)$, $\phi_R(x) = \Phi_{2,R}(x)$, and $\phi_L(-x) = \Phi_{1,R}(x)$, $\phi_R(-x) = \Phi_{2,L}(x)$, all for $x > 0$. In this case the Hamiltonian can be written as (we set $c = 1$)

$$H = \int_{-\infty}^{+\infty} dx \sum_{\alpha=R,L} (\partial_x \phi_\alpha(x))^2 + \delta(x) \times [\Delta S_3 - \sqrt{8\pi}\kappa_1 \partial_x \phi_R(x=0) S_1 - \sqrt{8\pi}\kappa_2 \partial_y \phi_L(x=0) S_2], \tag{5}$$

where $\phi_R(x)$ and $\phi_L(x)$ are right and left moving fields, and $\kappa_{1,2} = g^{1/2}\lambda_{1,2}/(4\pi^{7/2})$ are the new couplings. Similar problems to the one described by (5) have been studied in the past. In one case, a single heat bath is coupled to different spin components but in the absence of the Weiss field [6,15]; in another, the Weiss field is considered only in first order [16]. In our case it is not only important to have two independent heat baths but we also consider the strong renormalization of the Weiss field.

We have performed RG calculations for (5) in the Coulomb gas formulation [17] in two different limits: (i) $\kappa_{1,2} \ll 1$; (ii) $\kappa_1 \ll 1$ with κ_2 arbitrary and vice versa. The RG equations are

$$\partial_\ell \kappa_1 = -\kappa_1 \kappa_2^2 - \kappa_1 \kappa_3^2, \qquad \partial_\ell \kappa_2 = -\kappa_2 \kappa_1^2 - \kappa_2 \kappa_3^2,$$
$$\partial_\ell \kappa_3 = (1 - \kappa_1^2 - \kappa_2^2)\kappa_3, \qquad (6)$$

where $\kappa_3 = \Delta/D_0$ and $\ell = \ln(D/D_0)$ where D is the renormalized cutoff. Notice that the RG equations are symmetric under the exchange of couplings κ_1 and κ_2. There are three fixed points: (1) $\kappa_1 = \kappa_2 = \kappa_3 = 0$, (2) $\kappa_1 = \kappa_3 = 0$, $\kappa_2 = 1$, and (3) $\kappa_2 = \kappa_3 = 0$, $\kappa_1 = 1$. The two nontrivial fixed points (2) and (3) are the KT transitions of the AKP model discussed previously. In the $\kappa_1 \times \kappa_2$ plane ($\kappa_3 \neq 0$) the RG flow is shown in Fig. 1.

When $1 > \kappa_1 > \kappa_2$, away from the isotropic line, the final RG flow is anisotropic ($\kappa_3 \to \infty$) and in the same universality of the AKP. When the couplings are large and anisotropic ($\kappa_1 \gg \kappa_2 > 1$) the RG indicates that one of the couplings flow a fixed value while the others flow to zero ($\kappa_3 \to 0$). In terms of (5) this indicates that the impurity spin aligns in a direction perpendicular to the molecular field which was assumed to point in the Z direction in (2). In the Kondo language this is the equivalent to the Kondo effect with ferromagnetic coupling, when the impurity decouples from the environment. A possibility that is not considered in this work is associated with the formation of a spin texture around the impurity spin. In a classical spin system a spin texture can be formed in the bulk spins due to the presence of strong and/or anisotropic interactions. The spin texture can follow the impurity as it tunnels, invalidating the methods used here (an instanton calculation is required to take into account the collective nature of the texture) [8].

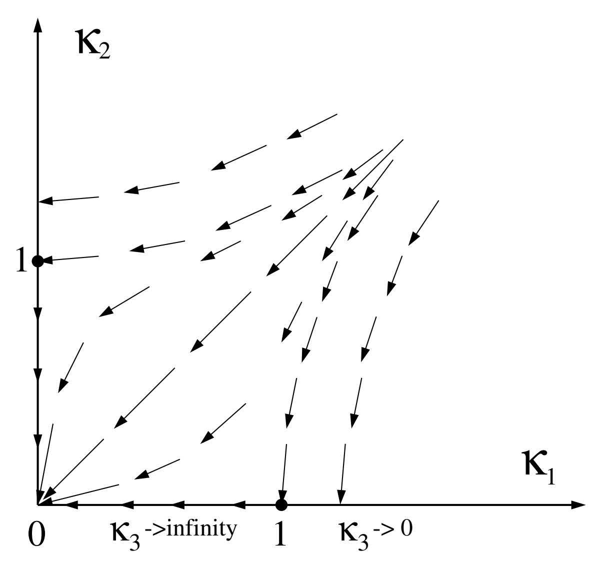

FIG. 1. RG flow in the $\kappa_1 \times \kappa_2$ plane.

Our results are valid only if no spin texture is formed around the magnetic impurity.

In the isotropic case when $\kappa_1 = \kappa_2 = \kappa$ the RG equations become

$$\partial_\ell \kappa = -\kappa^3 - \kappa\kappa_3^2, \qquad \partial_\ell \kappa_3 = (1 - 2\kappa^2)\kappa_3. \qquad (7)$$

Observe that contrary to the KT transition $\kappa_3(\ell)$ always scales towards strong coupling indicating the relevance of the molecular field (although it decreases initially under the RG if $\kappa > 1/\sqrt{2}$). However, the RG breaks down at a scale $\ell^* = \ln(D_0/T_A)$ when $\kappa_3(\ell^*) \approx 1$. T_A is the crossover energy scale from weak to strong coupling (the equivalent of the Kondo temperature). It is easy to see that the value of T_A depends on the bare value of $\kappa(\ell = 0)$. If $\kappa(0) < \kappa_3(0)$ the κ^3 term in (7) does not play a role, the flow is essentially the same as the usual KT flow and $T_A \approx D_0[\kappa_3(0)]^{1/[1-2\kappa^2(0)]} \approx \Delta[1 - 2\kappa^2(0)\ln(D_0/\Delta)]$. If, on the other hand, $\kappa(0) > \kappa_3(0)$, then the κ^3 term dominates and $\kappa_3(\ell)$ flows to strong coupling leading to $T_A \approx \Delta[1 + 2\kappa^2(0)\ln(D_0/\Delta)]^{-1}$. We immediately notice that the κ^3 term in the RG destroys the KT transition. Unlike the Kondo problem, the system retains coherence even at large coupling and is never overdamped. This is a quantum mechanical effect and comes from the fact that the spin operators do not commute. While the S_1 operator in (5) wants to orient the impurity spin in its direction, the same happens for the S_2 operator. In a classical system (large S) the spin would orient in a finite angle in the XY plane. However, for a $S = 1/2$ impurity this is not possible, and the impurity coupling is effectively *quantum frustrated* reducing the effective coupling to the environment. Another interesting feature of the RG flow is that for $1 > \kappa(0) > 1/\sqrt{2}$ the value of $\kappa^* = \kappa(\ell^*) \approx \ln(D_0/T_A)/2$ is essentially independent of $\kappa(0)$ at energy scale T_A. While T_A gives the crossover energy scale between weak and strong coupling, κ^* provides information about the dissipation rate, τ^{-1}, of the impurity dynamics. Our results indicate that for $\kappa(0)$ sufficiently large, τ^{-1} is independent of the initial coupling to the bosonic baths.

In order to investigate the dynamical correlations we study the frequency dependent impurity spin correlation function, $\chi''_\perp(\omega) = \text{Im}\{\int_0^\infty dt e^{i\omega t}\langle[S_1(t), S_1(0)]\rangle\}$. One of the great advantages of writing the problem in the form of an impurity problem as in (5) is that it can be accurately studied by numerical renormalization group (NRG) methods [18]. In order to perform the NRG calculation we transform (5) into a 1D fermionic problem and map the bosonic couplings onto fermionic coupling by studying the spectrum of both problems [8]. In Fig. 2 we plot $\chi''_\perp(\omega)/\omega$ for different values of $\gamma_1 = \gamma_2 = \gamma$ as a function of ω/T_A. We see that the curves collapse for $\gamma > 0.4$ (quasiscaling) while deviations are observed for small enough γ. This result agrees with the RG since the width of $\chi''_\perp(\omega)/\omega$ is exactly the dissipation rate, τ^{-1}, which becomes independent of γ [or $\kappa(0)$] for $\gamma > 0.4$. In Fig. 3 we compare the behavior of the correlation function

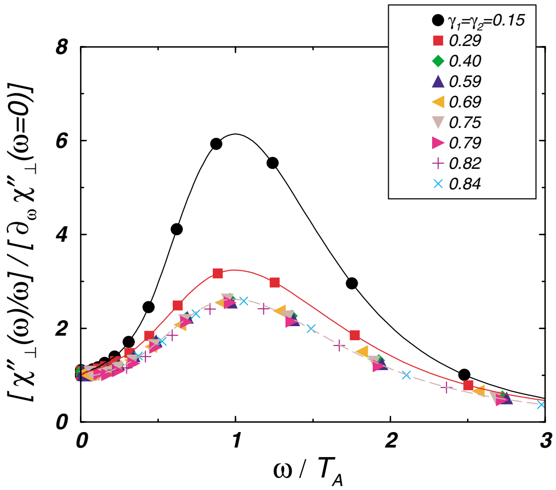

FIG. 2 (color online). $\chi''_\perp(\omega, \alpha)/\omega$ as a function of ω/T_A.

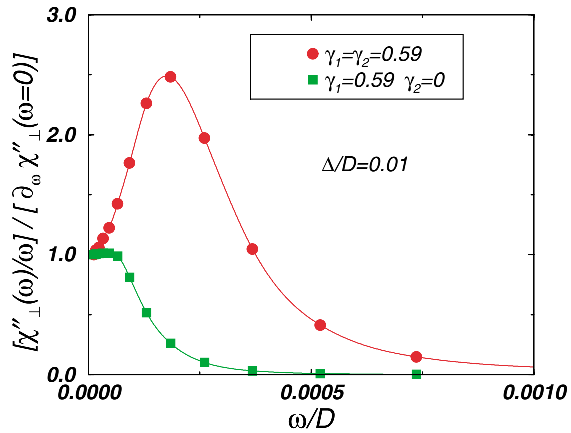

FIG. 3 (color online). $\chi''_\perp(\omega)/\omega$ as a function of ω/D.

in the isotropic case ($\gamma_1 = \gamma_2 = 0.59$) to the behavior in the strongly anisotropic case, that is, in the DTLS ($\gamma_1 = 0.59$ and $\gamma_2 = 0$). The differences are striking. While in the isotropic case the peak in the response at $\omega = T_A$ remains—that is, the system is underdamped—it has disappeared in the anisotropic case where the dynamics is overdamped.

Since the RG indicates that the transverse couplings of the impurity to the environment always flow to $\kappa \ll 1$ one could use perturbation theory to calculate $\chi''_\perp(\omega)$. However, perturbation theory in κ generates only a Dirac delta peak at $\omega = \Delta$, that is, $\tau^{-1} = 0$. In order to get a finite τ^{-1} one needs a nonperturbative calculation. The RPA with the bare parameters replaced by the renormalized ones gives [8]

$$\frac{\chi''_\perp(\omega)}{\omega} = \frac{(\pi/2)[\arctan(\Delta\tau)]^{-1}T_A/\tau}{[\omega^2 - (T_A)^2 - 1/\tau^2]^2 + 4\omega^2/\tau^2}, \qquad (8)$$

where $\tau^{-1} \approx (\kappa^*)^2 T_A$. Notice that (8) reduces to a Dirac delta function at $\omega = \Delta$ as $\kappa(0) \to 0$, as expected. We find that this approximation is good for $\omega \ll T_A$ and also describes well the NRG results for all $\omega < D_0$ when $D_0 > T_A \gg D_0\kappa^*$. In the zero frequency limit (8) reduces to $\chi''_\perp(\omega = 0) \approx (\kappa^*)^2\omega/(T_A)^2$ and the Kramers-Kronig relation immediately leads to $\chi_\perp(\omega = 0, T = 0) \approx 1/(4T_A)$. For $D_0 > \omega \gg T_A > D_0\kappa^*$ (8) agrees with the NRG results giving $\chi''_\perp(\omega) \propto 1/\omega^3$. In the case where $T_A \ll D_0\kappa^*$, in the frequency and temperature range $T_A \ll \omega, T \ll D_0$, we find $\chi''_\perp(\omega) \approx \pi/[8\kappa^2(0)\omega\ln^2(D_0/\omega)]$ and $\chi_\perp(T) \approx 1/[8\kappa^2(0)T\ln(D_0/T)]$ [8].

In summary, we have studied the problem of a spin 1/2 quantum impurity coupled to the Goldstone modes of a magnetically ordered system and found that the problem maps into a generalization of the DTLS that shows no decoherence even in strong coupling. We have calculated the frequency and temperature behavior of the impurity susceptibility that can be measured experimentally. We assign the destruction of decoherence (and the KT transition) to a quantum frustration between noncommuting spin operators. This result may have implications in quantum computation where decoherence effects are detrimental and the use of quantum frustration may be explored as a way to avoid decoherence.

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