Quantum impurity in a magnetic environment

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Abstract

A unified perspective is given on a number of different problems involving the coupling of a localized quantum spin degree of freedom to the low energy excitations of an antiferromagnet, a spin glass, or a Kondo insulator. The problems are related to those in the class often referred to as "Bose Kondo".

I. INTRODUCTION

The Kondo problem has played a central role in the development of the theory of correlated electron systems. At its simplest it consists of a single quantum spin, $\hat{S}_\alpha$ ($\alpha = x, y, z$), interacting with the *fermionic* excitations in a metallic environment. In a modern perspective, many aspects of the Kondo problem can be understood in the framework of boundary conformal field theory: the fermionic excitations in the environment are represented by a $1+1$ dimensional, free, conformal field theory with central charge $c = 1$, and this interacts with the quantum spin degree of freedom located at spatial co-ordinate $x = 0$.

More recently, attention has focused on a new type quantum impurity problem. Here, we again consider a quantum spin $\hat{S}_\alpha$, but it now interacts with *bosonic* excitations in the environment. Such models become appropriate when the environment is in the vicinity of a magnetic ordering transition, and there are low energy spin excitations in the bulk; the latter may be viewed as excitonic particle-hole bound states of a metal/insulator/superconductor which peel off below the continuum of a pair of fermionic particles or holes.

We begin by describing the simplest 'Bose Kondo' problem, and postpone a discussion of specific physical motivations till later, when we consider more realistic models. The simplest model[1] has the Hamiltonian

$$\mathcal{H}_1 = -\lambda \phi_\alpha \hat{S}_\alpha \tag{1}$$

where λ is a coupling constant, and the $\hat{S}_\alpha$ obey the usual relations of a Heisenberg spin with angular momentum S,

$$[\hat{S}_\alpha, \hat{S}_\beta] = i\epsilon_{\alpha\beta\gamma}\hat{S}_\gamma \quad ; \quad \hat{S}_\alpha \hat{S}_\alpha = S(S+1). \tag{2}$$

The Bose field ϕ_α has Gaussian correlations in the absence of its coupling to $\hat{S}_\alpha$, with the two-point correlation obeying

$$\langle \phi_\alpha(\tau)\phi_\alpha(0)\rangle_{\lambda=0} \sim \frac{1}{|\tau|^\mu}, \tag{3}$$

for large $|\tau|$ with $\mu > 0$, where τ is imaginary time.

It is important to distinguish the above Bose Kondo problem, from the 'spin boson' problem which had been the focus of much earlier attention [2]. The latter deals with a two-level system coupled to a bath of harmonic oscillators. Upon interpreting the two-level system as a spin, the splitting between the energy levels behaves like a magnetic field on the spin. In this situation, the spin-inversion symmetry, $\hat{S}_\alpha \to -\hat{S}_\alpha$ for any 2 of the 3 α values, is explicitly broken by the Hamiltonian. In contrast, in the Bose Kondo problem of interest here, this spin inversion symmetry is preserved (when combined with the transformation $\phi_\alpha \to -\phi_\alpha$).

Despite the simple form of the Hamiltonian $\mathcal{H}_1$ and of the correlator (3), the spin commutation relations (2) make this a problem of some complexity which cannot be solved exactly. This is also evident from its path integral formulation, in which we integrate over $\phi_\alpha(\tau)$ and over a unit length field $n_\alpha(\tau)$, where $\hat{S}_\alpha = S n_\alpha$:

$$\begin{aligned}
\mathcal{Z}_1 &= \int \mathcal{D}\phi_\alpha(\tau)\mathcal{D}n_\alpha(\tau)\delta\left(n_\alpha^2 - 1\right)\exp\left(-\mathcal{S}_{\rm b}[\phi_\alpha] - \mathcal{S}_{\rm imp}\right) \\
\mathcal{S}_{\rm imp} &= \int d\tau \left[iSA_\alpha(n)\frac{dn_\alpha(\tau)}{d\tau} - \lambda S\phi_\alpha(\tau)n_\alpha(\tau)\right] \\
\mathcal{S}_{\rm b}[\phi_\alpha] &= \frac{1}{2}\int d\tau d\tau' \phi_\alpha(\tau)Q^{-1}(\tau-\tau')\phi_\alpha(\tau'). \qquad (4)
\end{aligned}$$

In this formulation, all the non-linearities are in the first Berry phase term, which involves the vector potential of a unit Dirac monopole at the origin of spin space obeying

$$\epsilon_{\alpha\beta\gamma}\frac{\partial A_\gamma(n)}{\partial n_\beta} = n_\alpha. \qquad (5)$$

Also, $Q(\tau)$ is the two-point ϕ_α correlator at $\lambda = 0$, and (3) implies that its Fourier transform, $Q(i\omega)$, has the spectral density $\text{Im}Q(\omega) \sim \text{sgn}(\omega)|\omega|^{\mu-1}$ at small frequencies.

The problem (4) appeared in Ref. 1 in the context of a mean-field theory of a quantum Heisenberg spin glass. It was solved here by generalizing the SU(2) symmetry to SU(N), and taking the large N limit. In this limit, the spin correlations obey

$$\langle \hat{S}_\alpha(\tau)\hat{S}_\alpha(0)\rangle \sim \frac{1}{|\tau|^{2-\mu}} \qquad (6)$$

for large τ and $0 < \mu < 2$, while for $\mu \geq 2$ and small λ there is a broken spin rotation symmetry[3] and the $\hat{S}_\alpha$ two-point correlator reaches a non-zero value at large $|\tau|$. The exponent in (6) was also obtained using a one-loop renormalization group analysis [3, 4], and was subsequently shown [5, 6] to hold to all orders in an expansion in $2-\mu$. The result (6) has also been found to hold in certain quantum impurity models in which the spin $\hat{S}_\alpha$ is coupled simultaneously to bosonic and fermionic excitations in its environment [3, 4, 7, 8], including cases with spin anisotropy.

It is important to note that (6) relies crucially on the presence of the Berry phase in (4). In the absence of this term, we can integrate over the Gaussian ϕ_α modes, and then

(4) becomes equivalent to a *classical* ferromagnetic spin chain at finite 'temperature', with exchange interactions which decay as $1/|\tau|^\mu$. The properties of this classical model[9] are very different and have an interesting 'dual' structure. Now, the ferromagnetic phase with broken spin rotation symmetry appears only for $\mu < 2$ and low 'temperatures' (large λ)—in contrast, with the Berry phase term, as we noted above, spin rotation invariance was broken for $\mu \geq 2$ and small λ. Furthermore, in the classical model without the Berry phase, the paramagnetic phase with preserved spin rotation symmetry (present for all 'temperatures' for $\mu \geq 2$ and in the high 'temperature' (small λ) phase for $\mu < 2$) has its two-point $\hat{S}_\alpha$ correlator decaying as $1/|\tau|^\mu$—in contrast, with the Berry phase we found a rotationally invariant phase for $\mu < 2$ and with the correlator (6).

Intriguing and interesting as the properties of $\mathcal{Z}_1$ are, their physical interpretation and application require care and must be discussed in the context of the underlying model from which $\mathcal{Z}_1$ was derived. In particular, a free Bose field with a gapless spectrum is a delicate object which can become unstable under infinitesimal perturbations (this should be contrasted from a free Fermi field, which has a robust stability). One instance of this instability is the response to an applied magnetic field, H_α; there must be a coupling which imposes a precession of ϕ_α about the direction of magnetic field, and in these conditions the action is unstable to arbitrarily large fluctuations in ϕ_α in the directions orthogonal to the field. For the initial spin glass context in which $\mathcal{Z}_1$ was studied, the 'quantum critical' state described by (6) was found to be unstable to the onset of spin glass order at low temperatures [6].

In the remainder of this paper we will review another context in which $\mathcal{Z}_1$ has appeared: the theory of quantum impurities in insulators and superconductors with low energy quantum spin fluctuations. Here, as we will see below, it is essential to include a quartic ϕ_α^4 term for proper computations of the $\hat{S}_\alpha$ correlations.

II. QUANTUM ANTIFERROMAGNETS: ϕ^4 FIELD THEORY

A concrete application of the 'Bose Kondo' theory, which is now reasonably well understood, is the problem of quantum impurities in two-dimensional antiferromagnets. For definiteness, consider the simple coupled ladder antiferromagnet, illustrated in Fig 1. As the ratio of the exchange constants is varied, two distinct types of ground states are ob-

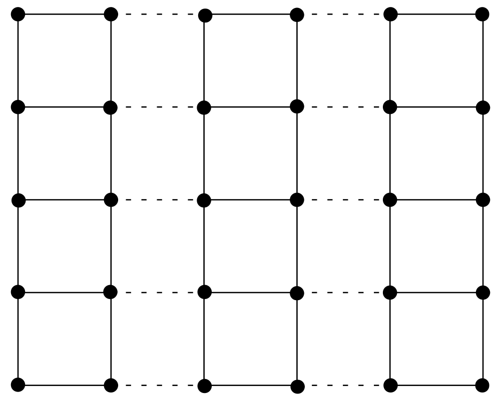

FIG. 1: The coupled ladder Hamiltonian. Quantum spins resides on the filled circles. They are coupled by two different antiferromagnetic exchange constants, indicated by the full and dashed lines.

tained. For weakly-coupled ladders, the ground state is a spin singlet and there is a gap to all excitations; the ground state is adiabatically connected to the state in which each spin is paired in a singlet with its partner across the rung of the ladder. In contrast, when the inter- and intra-ladder exchange constants are roughly equal, the model has the structure of the square lattice antiferromagnet, and so has antiferromagnetic Néel order in its ground state; in this case spin rotation symmetry is broken, and the spin operators have an average expectation value which has opposite signs on the two sublattices. Given the distinct nature of these two ground states, there must be a quantum phase transition between them. There is now quite convincing evidence [10] that there is one second-order quantum critical point, and in its vicinity the spin fluctuations are described by the ϕ^4 field theory, written here in d spatial dimensions:

$$\widetilde{\mathcal{S}}_{\rm b}[\phi_\alpha] = \int d^d x d\tau \left[\frac{1}{2} \left\{ (\partial_\tau \phi_\alpha)^2 + c^2 (\nabla_x \phi_\alpha)^2 + r \phi_\alpha^2 \right\} + \frac{u}{24} (\phi_\alpha^2)^2 \right]. \tag{7}$$

The field ϕ_α represents the staggered Néel order parameter, and the tuning parameter r moves the system from the spin gap state at large r, to the Néel state at smaller r. The spin-wave velocity is c, and u is the quartic non-linear coupling.

Now insert an arbitrary quantum impurity in the spin ladder system: two examples are shown in Fig 2. In the spin gap state, the presence of such a impurity may liberate one or more spins from their partners, and this leads to a residual Curie spin susceptibility at a

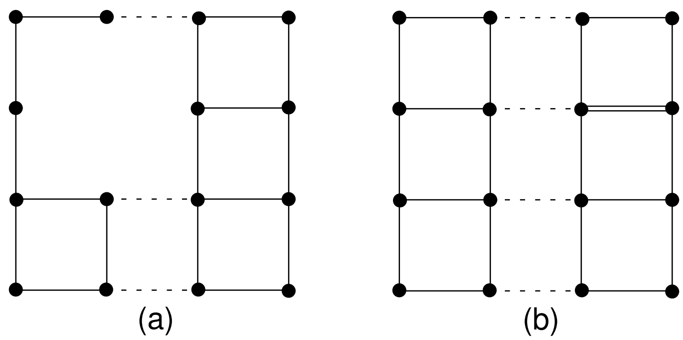

FIG. 2: Two examples of quantum impurities in the coupled ladder antiferromagnet, assumed to have spins with angular momentum S' on the filled circles. (a) A vacancy, which is characterized by $S = S'$ in (8). (b) A defect bond: the double line represents a large ferromagnetic exchange, and this is characterized by $S = 2S'$ in (8).

low temperature T:

$$\chi_{\rm imp} = \frac{S(S+1)}{3k_B T} \quad ; \text{ spin gap in bulk antiferromagnet.} \tag{8}$$

Here S is an integer or half-odd-integer which characterizes the impurity. A remarkable property [5] of the low energy dynamics of the quantum impurity is that *no other parameters* are needed to described the spin dynamics in its vicinity, provided the bulk antiferromagnet is not too far from its quantum critical point. This result emerges from an analysis of the theory coupling the impurity to the ϕ^4 field theory:

$$\begin{aligned} \mathcal{Z}_2 &= \int \mathcal{D}\phi_\alpha(x,\tau)\mathcal{D}n_\alpha(\tau)\delta\left(n_\alpha^2 - 1\right)\exp\left(-\widetilde{\mathcal{S}}_{\rm b}[\phi_\alpha] - \widetilde{\mathcal{S}}_{\rm imp}\right) \\ \widetilde{\mathcal{S}}_{\rm imp} &= \int d\tau \left[iSA_\alpha(n)\frac{dn_\alpha(\tau)}{d\tau} - \lambda S \phi_\alpha(x=0,\tau)n_\alpha(\tau)\right], \end{aligned} \tag{9}$$

with $\widetilde{\mathcal{S}}_{\rm b}[\phi_\alpha]$ given in (7). Notice the similarity of $\mathcal{Z}_2$ to $\mathcal{Z}_1$: at $r = 0$, $u = 0$, we can integrate out all the $\phi_\alpha(x \neq 0, \tau)$, and then $\mathcal{Z}_2$ reduces to $\mathcal{Z}_1$ with $\mu = d - 1$. However, it is crucial in the proper theory of $\mathcal{Z}_2$ that the non-linearity u be treated at an equal footing with λ; there is a non-trivial 'interference' between u and λ, and the interaction u significantly modifies the magnetic environment coupling to the impurity. It is not permissible to treat the environment as a Gaussian quantum noise, and focus only on its Kondo-like coupling to the impurity.

A systematic renormalization group based analysis of $\mathcal{Z}_2$ was carried out[5] in an expansion in $(3 - d)$. The couplings λ^2 and u both approach fixed point values of order $(3 - d)$, and this is the reason the coupling between the bulk and impurity spin fluctuations becomes universal, as claimed above. At the critical point, the spin correlations decay as

$$\langle \hat{S}_\alpha(x,\tau)\hat{S}_\alpha(x,0)\rangle \sim \frac{1}{|\tau|^{\eta'}} \quad ; \quad x \approx 0, \tag{10}$$

close to the impurity. The exponent $\eta' \neq 2-\mu = 3-d$, as would be implied by (6), because of the non-zero fixed point value of u. Well away from the impurity, the results are as in the absence of the impurity with

$$\langle \hat{S}_\alpha(x,\tau)\hat{S}_\alpha(x,0)\rangle \sim \frac{1}{|\tau|^{d-1+\eta}} \quad ; \quad x \to \infty, \tag{11}$$

where η is the well-known anomalous dimensions of the ϕ^4 field theory in $d+1$ spacetime dimensions. The value of η', and numerous other physical properties of the impurity on both sides of the bulk quantum critical point, were computed in Ref. [5] to second order in an expansion in $(3-d)$. Numerical studies [12, 13] have investigated some of these properties. Related theoretical results were obtained recently [11] in magnetically ordered states in the presence of spin anisotropy.

III. QUANTUM ANTIFERROMAGNETS: NON-LINEAR SIGMA MODEL

An alternative approach to the impurity dynamics discussed in Section II is provided by a different representation of the bulk spin fluctuations. It is well known that in low dimensions the ϕ^4 field theory can be represented by the non-linear sigma model: the fluctuations of the amplitude, ϕ_α^2, become irrelevant, and we need only focus on the angular fluctuations of the Néel order parameter. These are represented by a unit-length field $N_\alpha(x,\tau)$. Such a 'non-linear sigma model' representation provides an expansion in powers of $(d-1)$ for the bulk critical properties.

In the quantum impurity problems of interest here, such a fixed-length representation offers some benefits. One is that it allows systematic computation of some properties in the 'renormalized classical' regime directly in spatial dimension $d=2$. However, more importantly, in the fixed-length formulation the universal nature of the couplings between the bulk and impurity spin fluctuations can be accounted for at the outset. Indeed, it was argued[14] that in the scaling limit of the fixed-length theory, the quantum impurity behaves as if it is in the $\lambda \to \infty$ limit, and hence the impurity spin orientation align along the direction of the bulk spin order; in other words, we have $n_\alpha(\tau) = N_\alpha(x = 0, \tau)$. With these arguments, we can rewrite the model described by the partition function $\mathcal{Z}_2$ as

$$\begin{aligned}
\mathcal{Z}_3 &= \int \mathcal{D}N_\alpha(x,\tau)\delta\left(N_\alpha^2 - 1\right)\exp\left(-\mathcal{S}_{\rm b}[N_\alpha] - \overline{\mathcal{S}}_{\rm imp}\right) \\
\overline{\mathcal{S}}_{\rm imp} &= \int d\tau\left[iSA_\alpha(n)\frac{dn_\alpha(\tau)}{d\tau}\right] \quad \text{with } n_\alpha(\tau) = N_\alpha(x=0,\tau) \\
\mathcal{S}_{\rm b}[N_\alpha] &= \frac{1}{2cg}\int d^dx d\tau\left[\left(\partial_\tau N_\alpha\right)^2 + c^2\left(\nabla_x N_\alpha\right)^2\right],
\end{aligned} \tag{12}$$

where now g is the coupling constant that tunes the bulk antiferromagnet across the quantum critical point. Notice that there is no other coupling constant, and hence the universal nature of the coupling between the bulk and impurity is explicit. A systematic $(d-1)$ expansion of $\mathcal{Z}_3$ was performed[14], and all results were found to be consistent with those reviewed in Section II. In particular, a $(d-1)$ expansion was presented for the exponent η' in (10), associated with computation of a 'boundary' renormalization constant for the field $N_\alpha(x = 0, \tau)$. Related results were also obtained in Ref. [15].

IV. ELECTRON SPECTRAL FUNCTION IN KONDO INSULATORS

Kondo insulators are another class of physically interesting systems displaying a magnetic transition. In Kondo lattice models with a commensurate density of conduction electrons, increasing the Kondo exchange can drive the ground state from an ordered Néel state to a paramagnetic insulator in which the conduction electrons and local moments are strongly hybridized. The low energy magnetic fluctuations near such a critical point are also believed to be described by the ϕ^4 field theory (7).

Now, let us consider the photoemission spectrum of a conduction electron in such an insulator in the vicinity of the magnetic transition [16]. Away from the critical point, there will be a sharp quasiparticle/hole pole with a finite residue, and the position of this pole will disperse in the Brillouin zone. Focus on the spectral function at the minimum of this dispersion[17, 18], where the momentum dependence is quadratic. It was argued [18] that near this minimum, and in the vicinity of the magnetic ordering transition where the action (7) applies, we can safely neglect the quadratic dispersion of the hole. We are therefore left with the problem of a *static* hole interacting with the magnetic environment described by (7). This problem is clearly analogous to the X-ray edge problem, where a static hole interacts with a Fermi liquid.

This "Bose X-ray edge" problem is described by the partition function

$$\mathcal{Z}_4 = \int \mathcal{D}\phi_\alpha(x,\tau)\mathcal{D}\psi_a(\tau)\mathcal{D}\psi_a^\dagger(\tau)\exp\left(-\widetilde{\mathcal{S}}_{\rm b}[\phi_\alpha] - \mathcal{S}_\psi\right)$$
$$\mathcal{S}_\psi = \int d\tau\left[\psi_a^\dagger\left(\frac{\partial}{\partial\tau}+\varepsilon_0\right)\psi_a - \frac{\lambda}{2}\phi_\alpha(x=0,\tau)\psi_a^\dagger\sigma^\alpha_{ab}\psi_b\right], \quad (13)$$

with $\widetilde{\mathcal{S}}_{\rm b}[\phi_\alpha]$ given in (7). The ψ_a are Grassman variables representing the hole with $a,b=\uparrow,\downarrow$, and σ^α are the Pauli matrices. A complication has been ignored in our presentation here of $\mathcal{Z}_4$ here: as the field ϕ_α carrier spin fluctuations at a finite momentum, it actually couples fermionic excitations at two different points in the Brillouin zone. We have not included this effect here because keeping track of the fermionic momentum label does not modify the critical properties[18].

With the hole present, the quantum theory $\mathcal{Z}_4$ is, in fact, identical to $\mathcal{Z}_2$ (with $S=1/2$): we have simply realized the quantum spin by a single hole. Consequently, the renormalization group equations for the λ coupling in (13) are identical for those for λ in (9). However, the present formulation allows determination of a new renormalization constant associated with the insertion of a hole. This constant measures the overlap of the system wavefunctions with and without the hole; in contrast, in (9) the spin is always present and so this physics is inaccessible.

Specifically, in the paramagnetic phase, away from the critical point, the single hole Green's function G, has a quasiparticle pole given by

$$G(\omega) = \frac{Z}{\omega - \varepsilon_0} \quad (14)$$

where Z is the quasiparticle residue, and ε_0 has absorbed a renormalization from the coupling of the hole to ϕ_α. As we approach the critical point, there is an orthogonality catastrophe and $Z \to 0$. Instead, at the critical point we have[17, 18, 19]

$$G(\omega) \sim \frac{1}{(\omega-\varepsilon_0)^{1-\eta_f}}. \quad (15)$$

The exponent η_f is distinct from η', and its determination requires a separate renormalization group analysis. The value of η_f has been obtained in a two-loop expansion [19] in powers of $(3-d)$, and by a numerical simulation [18].

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