Curie and non-Curie behavior of impurity spins in quantum antiferromagnets

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We investigate a number of cases of an impurity spin S coupled to a D-dimensional antiferromagnetic (AFM) background. The qualitative behavior of the impurity susceptibility depends upon the sublattice symmetry of the coupling, whether S is integer or half-integer, and the spectral density of the low-lying AFM excitations. When the AFM background is ordered we show that the appropriate model to consider is a non-Abelian spin-boson model. Within this model, we argue that the symmetrically coupled half-integer spin impurity retains the Curie divergence of its susceptibility for $D \geq 2$. In the case of a $D=1$ spin-$\frac{1}{2}$ AFM chain the sublattice symmetric impurity behaves in the same way as the Kondo spin in the two-channel Kondo model and thus has a non-Curie $\ln(T_*/T)$ divergent susceptibility. This latter case is investigated via bosonization at the Emery-Kivelson strong-coupling line.

I. INTRODUCTION

We shall concern ourselves here with the low-frequency and low-temperature behavior of an "impurity" spin coupled to an antiferromagnetic (AFM) background. This situation arises naturally in a Mott-Hubbard insulator, where the low-energy degrees of freedom are localized spins coupled antiferromagnetically via the Anderson superexchange mechanism. Experimentally it is realized in the weakly doped cuprate insulators (the parent compounds of high-temperature superconducting materials[1]) in which the carriers introduced into the CuO planes by the dopant (e.g., O vacancies) are localized by the Coulomb potential (of the dopant). These localized states are "observable" through their contribution to optical conductivity,[2] magnetic susceptibility, and electron spin resonance (ESR).[3]

While CuO systems are quasi-two-dimensional, there also exist quasi-one-dimensional materials such as $CuSO_4 \cdot 5H_2O$ and $CuCl_2 \cdot 2NC_5H_5$ which are to a good approximation Heisenberg spin-$\frac{1}{2}$ quantum antiferromagnetic chains.[4] The behavior of magnetic impurities in this system could in principle be looked at using ESR and other techniques as it was done in another quasi-1D material, NENP,[5] which is a spin-1 antiferromagnet.

We shall explore the possibility of nontrivial ground states of the impurity spin interacting with an AFM background. It is easy to see that the qualitative behavior depends on the sublattice symmetry of the coupling and whether the impurity spin is integer or half-integer. For sublattice *asymmetric* coupling or integer spin the impurity ground state becomes nondegenerate because of the local field in the former case (when local magnetic order exists) and fluctuation-induced xy anisotropy in the latter. The most interesting case is that of a *half-integer* impurity spin where, provided that the coupling to the background is sublattice *symmetric,* the ground state can retain its double degeneracy. Because of the coupling to the low-frequency background modes[6] the behavior of the impurity spin can be nontrivial, and its description represents a problem of non-Abelian spin-boson type.[7]

We find that while for a two- (2D) and higher-dimensional AFM background (described in the spin-wave approximation) the Curie divergence of the impurity spin susceptibility remains, at least in weak coupling, albeit renormalized, this is not true in the one-dimensional (1D) case. As spin-wave theory is not appropriate in 1D, we solve the problem for a spin-$\frac{1}{2}$ AFM chain using the bosonization method.[8] We find that the sublattice symmetric impurity problem is equivalent, in a certain sense, to the two-channel Kondo model[9] while the asymmetric coupling leads to a problem similar to the single-channel Kondo model. In the former case the spin-$\frac{1}{2}$ impurity forms a collective state by "pulling in" spin one pairs of spinons to form renormalized spin-$\frac{1}{2}$ states, resulting in an *orthogonal* pair of degenerate ground states. Below we will argue that the impurity spin spectral function has finite width and the impurity susceptibility has a non-Curie divergence, $\chi \sim T_*^{-1}\ln(T_*/T)$, with energy scale $T_* \sim Je^{-\mathrm{const}J/g}$ for $g \ll J$.

A closely related problem of a spin-$\frac{1}{2}$ chain with bond defects, an adjacent pair of bonds with exchange energy differing from that in the bulk, has recently been studied by Eggert and Affleck[10] using a combination of conformal field theory and finite-size scaling. These authors conclude that the system is governed by a "healed" spin chain fixed point, with the leading irrelevant operator contributing a log-divergent impurity susceptibility.

We shall begin by discussing the problem within spin-wave theory and then proceed to the 1D spin-$\frac{1}{2}$ chain. The latter will be reduced by bosonization to the two-channel Kondo model (without the charge fields) and then analyzed explicitly at a special strong coupling line found recently by Emery and Kivelson.[11] We shall show

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that near this line the impurity spin susceptibility has a logarithmic divergence, consistent with the exact result known for the two-channel Kondo model. The explicit calculation on this special line provides further insight into the correlations between the impurity and the background. In particular, we shall show that a logarithmic divergence also appears in the *uniform* static magnetic susceptibility.

II. THE MODEL HAMILTONIAN AND SPIN-WAVE CONSIDERATIONS

The impurity spin coupled to an AFM background is described in general by

$$H=H_0+H_I=J\sum_{\langle i,j\rangle}\mathbf{s}_i\cdot\mathbf{s}_j+\mathbf{S}\cdot\sum_i g_i\mathbf{s}_i \tag{1}$$

with spins $\mathbf{s}_i$ on a bipartite lattice, AFM exchange constant J, impurity spin $\mathbf{S}$, and couplings $g_i \neq 0$ for i in the neighborhood of the impurity. The continuum limit of (1) can be written in terms of a nonlinear σ model Hamiltonian

$$\begin{aligned}H_c&=H_{\mathrm{NL}\sigma}+H_I\\&=\frac{1}{2}\int d^D\mathbf{x}[\chi^{-1}\mathbf{m}^2(\mathbf{x})+\rho(\partial\mathbf{\Omega})^2(\mathbf{x})]\\&\quad+a^Dg_m\mathbf{S}\cdot\mathbf{m}(0)+g_\Omega\mathbf{S}\cdot\mathbf{\Omega}(0)\ ,\end{aligned} \tag{2}$$

where $\mathbf{m}(\mathbf{x})$ is the local magnetization and $\Omega(\mathbf{x})$ the staggered magnetization unit vector satisfying

$$\begin{aligned}&[m_\alpha(\mathbf{x}),\Omega_\beta(\mathbf{y})]=i\epsilon_{\alpha\beta\gamma}\Omega_\gamma(x)\delta(\mathbf{x}-\mathbf{y})\ ,\\&[m_\alpha(\mathbf{x}),m_\beta(\mathbf{y})]=i\epsilon_{\alpha\beta\gamma}m_\gamma(\mathbf{x})\delta(\mathbf{x}-\mathbf{y})\ ,\\&[\Omega_\alpha(\mathbf{x}),\Omega_\beta(\mathbf{y})]=0\ ,\end{aligned} \tag{3}$$

χ and ρ are the uniform susceptibility and stiffness, respectively, $\chi^{-1}\sim Ja^D, \rho\sim\zeta^2Ja^{2-D}$, with ζ being the background spin modulus and a the lattice constant. The impurity part of (2) contains the coupling g_m of $\mathbf{S}$ to $\mathbf{m}$ arising from the part of g_i even under sublattice interchange and the coupling g_Ω of $\mathbf{S}$ to $\mathbf{\Omega}$ which is odd under sublattice interchange. Clearly, in the broken symmetry state (as would be the case for $T<T_N$ in $D>2$ and at $T=0$ in $D=2$), $\langle\mathbf{\Omega}\rangle\neq0$, the g_Ω coupling would induce a Zeeman splitting of the impurity spin states. Let us consider the $g_\Omega=0$ case where the impurity remains unpolarized in the AFM ordered state.

Within spin-wave theory we expand in large ζ about the $\langle\Omega_z(\mathbf{x})\rangle=1+O(\zeta^{-1})$ ordered ground state. Since $\rho\sim O(\zeta^2)$ the transverse fields $\mathbf{m}_\perp$ and $\Omega_\perp$ are actually $O(\zeta^{1/2})$ and $O(\zeta^{-1/2})$, respectively, so that if we rescale to new fields which are $O(\zeta^0)$, i.e., $O(1)$, we have

$$[m_x(\mathbf{x}),\Omega_y(\mathbf{y})]=-[m_y(\mathbf{x}),\Omega_x(\mathbf{y})]=i\delta(\mathbf{x}-\mathbf{y})$$

and

$$\begin{aligned}H_c&=\frac{1}{2}\int d^D\mathbf{x}[\chi^{-1}\zeta\mathbf{m}_\perp^2(\mathbf{x})+\rho\zeta^{-1}(\partial\Omega_\perp)^2(\mathbf{x})]\\&\quad+a^Dg\zeta^{1/2}\mathbf{S}_\perp\cdot\mathbf{m}_\perp(0)+a^DgS_zm_z(0)\ ,\end{aligned} \tag{4}$$

where spin-wave interaction terms which are of order ζ^0 have been omitted and the dependence on ζ is now explicit. The $O(\zeta^{1/2})$ coupling of the impurity spin to the transverse fluctuations of the magnetization can be removed by a canonical transformation

$$H_c\to\tilde{H}=e^{iQ}H_ce^{-iQ}\ ,$$

$$Q=-\frac{g\chi a^D}{\zeta^{1/2}}\{S_x\Omega_y(0)-S_y\Omega_x(0)\}\ .$$

The terms in $\tilde{H}$ coupling to the impurity spin are then

$$\begin{aligned}\tilde{H}_I=&-\tfrac{1}{2}g^2\chi a^D\mathbf{S}_\perp^2-ga^D(1-\tfrac{1}{2}a^D\chi)S_z\mathbf{m}_\perp(0)\cdot\mathbf{\Omega}_\perp(0)\\&+O(\zeta^{-1/2})\ .\end{aligned} \tag{5}$$

The first term introduces an easy plane anisotropy for the impurity spin which for *integer* impurity spin S leads immediately to a nondegenerate ground state. For a half-integer spin the lowest energy state, with minimal S_z^2, remains degenerate, $S_z=\pm\frac{1}{2}$. Thus the interesting case is that of half-integer S. Since the low-energy manifold is doubly degenerate we can without loss of generality consider directly the $S=\frac{1}{2}$ case. The remaining interaction term in $\tilde{H}_I$ which couples S_z to the *longitudinal* component of $\mathbf{m}$ (recall $\mathbf{m}\cdot\mathbf{\Omega}=0$ and $m_z(\mathbf{x})=-[\mathbf{m}_\perp(\mathbf{x})\cdot\Omega_\perp(\mathbf{x})]$) is of the same order, ζ^0, as the spin-wave interaction terms and so will not be considered here.[12]

We thus arrive at the problem of a spin-$\frac{1}{2}$ impurity coupled to a magnon bath and governed by the Hamiltonian (4) without the final S_zm_z (0) term. In contrast to the (Abelian) spin-boson model discussed in Ref. 7 our problem involves the coupling of *two* polarizations of the spin impurity, which do not commute, to a bath of gapless bosons, which we therefore refer to as a *non-Abelian* spin-boson problem.

Let us compute the susceptibility of the impurity spin. We have just found perturbatively that for a sublattice symmetric coupling and half-integer impurity spin the ground state remains doubly degenerate. Does this necessarily imply a Curie divergence of the static susceptibility of the impurity spin?

Within spin-wave theory we have

$$\begin{aligned}\chi^{+-}(i\omega_n)&=\int_0^\beta d\tau\, e^{i\omega_n\tau}\langle S^+(\tau)S^-(0)\rangle\\&=\int_0^\beta d\tau\, e^{i\omega_n\tau}\frac{1}{Z}\mathrm{Tr}\{e^{-(\beta-\tau)\tilde{H}}e^{iQ}S^+e^{-iQ}\\&\qquad\times e^{-\tau\tilde{H}}e^{iQ}S^-e^{-iQ}\}\ .\end{aligned}$$

Since

$$\begin{aligned}e^{iQ}S^\pm e^{-iQ}=&S^\pm+\frac{g\chi a^D}{\zeta^{1/2}}S_z\Omega^\pm(0)\\&-\frac{1}{2}\left[\frac{g\chi a^D}{\zeta^{1/2}}\right]^2[\mathbf{S}\cdot\mathbf{\Omega}_\perp(0)]\Omega^\pm(0)\end{aligned}$$

we find perturbatively

$$\chi^{+-}(i\omega_n)=\int_0^\beta d\tau\, e^{i\omega_n\tau} \times\left\{1-\frac{(g\chi a^D)^2}{2\xi}[G_\Omega(0,\tau)-G_\Omega(0,0)]\right\} .$$

We thus observe that the correction to Curie behavior involves *temporal* fluctuations of the staggered magnetization at the impurity site. Explicitly,

$$\delta\chi^{+-}(i\omega_n)=\frac{2c}{\rho}(g\chi a^D)^2 \times\int_0^\Lambda \frac{d^Dk}{(2\pi)^D}\left\{\frac{2c}{\omega_n^2+c^2k^2}-\frac{\beta}{k\tanh(\beta ck/2)}\right\} \quad (6)$$

so that

$$\lim_{\omega\to 0}\delta\chi^{+-}(\omega)=\frac{2c}{\rho}(g\chi a^D)^2 \times\int_0^\Lambda \frac{d^Dk}{(2\pi)^D}\left\{\frac{2\tanh(\beta ck/2)-\beta ck}{ck^2\tanh(\beta ck/2)}\right\} . \quad (7)$$

For $D\geq 3$, approximation of the integral in (7) yields

$$\chi_{D\geq 3}(T)\sim\left[1-\lambda_D\frac{1}{\xi}\left[\frac{g}{J}\right]^2\right]\frac{1}{T} \quad (8)$$

with additive corrections which are $O(1)$ and $O(T^{D-2})$, and λ_D is a D-dependent $O(1)$ (positive) numerical factor. For $D=2$ there is a logarithmic correction to Curie susceptibility

$$\chi_{D=2}\sim\left[1-\lambda_2\frac{1}{\xi}\left[\frac{g}{J}\right]^2\right]\frac{1}{T} +\left[\mu_2\frac{1}{\xi^2}\left[\frac{g}{J}\right]^2\right]\frac{1}{J}\log\left[\frac{\xi J}{T}\right] , \quad (9)$$

where μ_2 is another $O(1)$ (positive) numerical factor. Note that although for $D=2$ we should cut off the k integral in (7) at a momentum of the order of the inverse correlation length, the result (9) is insensitive to this.

We therefore conclude that for $D\geq 2$, in weak coupling and within the framework of noninteracting spin-wave theory, the impurity spin susceptibility has a (renormalized) Curie form at low temperature and/or low frequency.

On the other hand for $D=1$, (7) yields a contribution to $\delta_\chi(T)$ proportional to $-(1/T)\log(J/T)$ which is analogous to the divergence encountered in perturbative treatments of the Kondo and x-ray edge problems.[13] One may therefore expect that in $D=1$ the Curie divergence will disappear altogether. In the next section we shall study this phenomenon in detail.

III. IMPURITY SPIN IN A SPIN-$\frac{1}{2}$ CHAIN AND THE TWO-CHANNEL KONDO MODEL

We return to (1) (but generalized to the anisotropic case) retaining only the sublattice symmetric coupling

$$H=H_J+H_I$$

$$H_J=\sum_i\left[\frac{J_\perp}{2}[s^+(i)s^-(i+1)+s^-(i)s^+(i+1)] +J_z s^z(i)s^z(i+1)\right] \quad (10)$$

$$H_I=\tfrac{1}{2}g_\perp\{S^+[s^-(0)+s^-(1)]+S^-[s^+(0)+s^+(1)]\} +g_zS_z[s^z(0)+s^z(1)] .$$

We shall now show, using bosonization techniques, that this problem is equivalent, in a sense to be made precise, to the two-channel Kondo problem. We can then use the known results for the latter, which tell us about the impurity susceptibility and specific heat. We will also compute the spin susceptibility explicitly at a special strong-coupling line (corresponding to the Emery-Kivelson line of the two-channel Kondo model[11]).

In order to solve (10) we apply a Jordan-Wigner transformation to the spins in the chain, and then bosonize.[8] In the continuum limit the bosonized form of H_J is

$$H_B=u\int\frac{dx}{\pi}\{\kappa[\nabla\theta(x)]^2+\kappa^{-1}[\nabla\phi(x)]^2\} \quad (11)$$

$u=J\alpha$ is the "spin-wave" velocity, α a short-distance cutoff and $\phi(x),\theta(x)$ are "Bose" fields obeying the commutation rules

$$[\phi(x),\phi(y)]=[\theta(x),\theta(y)]=0 , \quad (12)$$
$$[\phi(x),\theta(y)]=i\pi\Theta(x-y) ,$$

where $\Theta(x)$ is the Heaviside step function. [N.B. $\Pi_\phi(x)=\nabla\theta(x)/\pi$ is the canonical momentum conjugate to $\phi(x)$.] We take $\kappa=\frac{1}{2}$ corresponding to the isotropic fixed point of H_J, with appropriately renormalized u and we have omitted from H_B the marginally relevant $\cos 4\phi$ term. By doing so we will neglect the logarithmic corrections that appear in some correlation functions of the spin-$\frac{1}{2}$ chain at the fixed point. The continuum spin field is related to the bose fields by

$$s^+(x)=\frac{1}{\sqrt{2\pi}}[2e^{-i\pi x}e^{-i\theta(x)} +(e^{-i[2\phi(x)+\theta(x)]}+e^{+i[2\phi(x)-\theta(x)]})] ,$$

$$s^z(x)=\frac{\alpha}{\pi}\frac{\partial\phi(x)}{\partial x}+\frac{1}{\pi}e^{i\pi x}\cos 2\phi(x) \quad (13)$$

so that the sublattice symmetric coupling to the impurity spin has the form[14]

$$H_I=\frac{g_\perp}{\sqrt{2\pi}}[S^+(e^{i(2\phi+\theta)(0)}+e^{-i(2\phi-\theta)(0)})+\text{H.c.}] +\frac{g_z\alpha}{\pi}S_z\frac{\partial\phi(0)}{\partial x} . \quad (14)$$

Let us introduce rescaled left and right bose fields $\Phi_{L,R}$ satisfying

$$[\Phi_{L,R}(x),\Phi_{L,R}(y)]=\mp\frac{i\pi}{4}\mathrm{sgn}(x-y) ,$$

$$[\Phi_L(x),\Phi_R(y)]=-\frac{i\pi}{4}$$

in terms of which

$$\theta(x)=\sqrt{2}[\Phi_R(x)-\Phi_L(x)] ,$$

$$\phi(x)=\frac{1}{\sqrt{2}}[\Phi_R(x)+\Phi_L(x)] .$$

For convenience, we transform the right moving field $\Phi_R(x)$ into a left mover $\Phi_L'(x)$ via $\Phi_L'(x)=-\Phi_R(-x)$ to obtain

$$H_B=\frac{2u}{\pi}\int dx\{[\nabla\Phi_L(x)]^2+[\nabla\Phi_L'(x)]^2\} ,$$

$$H_I=\frac{g_\perp}{\sqrt{2\pi}}[S^+(e^{-i2\sqrt{2}\Phi_L'(0)}+e^{-i2\sqrt{2}\Phi_L(0)})+\mathrm{H.c.}]$$

$$+\frac{g_z\alpha}{\sqrt{2}\pi}S_z\left[\frac{\partial\Phi_L'(0)}{\partial x}+\frac{\partial\Phi_L(0)}{\partial x}\right] . \quad (15)$$

We shall now sketch the bosonization of the two-channel Kondo model and in so doing we show how it is related to the bosonized Hamiltonian, (15), of our impurity model. The two-channel Kondo Hamiltonian is

$$H=v_F\left[\int_{-\infty}^{\infty}dx\, H_0(x)+H_K\right] ,$$

$$H_0=i\psi_i^{\alpha\dagger}(x)\frac{\partial}{\partial x}\psi_{i\alpha}(x) , \quad (16)$$

$$H_K=\lambda\psi_i^{\alpha\dagger}(0)\frac{\sigma_\alpha^\beta}{2}\psi_{i\beta}(0)\cdot\mathbf{S} .$$

Here λ is the (dimensionless) Kondo coupling of the Kondo spin $\mathbf{S}$ to the two channels of conduction electrons, ψ_i, which are both left-moving fermions, α, β are spin indices, $i=1,2$ is the channel index, and σ are Pauli matrices. Bosonizing via

$$\psi_{i\alpha}(x)=\frac{e^{-i2\phi_{i\alpha}(x)}}{\sqrt{2\pi\alpha}}$$

introducing charge and spin fields for each channel,

$$\phi_{ic,\sigma}=\frac{1}{\sqrt{2}}(\phi_{i\uparrow}\pm\phi_{i\downarrow})$$

and generalizing (16) to anisotropic coupling we obtain

$$H_0=\frac{2}{\pi}\sum_i\{[\nabla\phi_{ic}(x)]^2+[\nabla\phi_{i\sigma}(x)]^2\} ,$$

$$H_K=\frac{\lambda_\perp}{2\pi\alpha}[S^+(e^{-i2\sqrt{2}\phi_{1\sigma}(0)}+e^{-i2\sqrt{2}\phi_{2\sigma}(0)})+\mathrm{H.c.}]$$

$$+\frac{\lambda_z}{2\pi}\left[\frac{\partial\phi_{1\sigma}}{\partial x}(0)+\frac{\partial\phi_{2\sigma}}{\partial x}(0)\right] . \quad (17)$$

The Kondo spin is decoupled from the charge degrees of freedom of the conduction electrons, and is therefore governed by the same Hamiltonian as (15) which is the bosonized form of our impurity spin model. Note that the role of the "flavor" in the latter is taken up by the parity. Insofar as the Kondo spin is unaffected by the charge degrees of freedom, its properties will be identical to that of our impurity spin.[15] In particular, we may take over the known exact results[16] for the impurity spin susceptibility and specific heat:

$$\chi^{\mathrm{imp}}(\omega,T)\sim\frac{1}{T_*}\ln\left[\frac{T_*}{\max(\omega,T)}\right] ; \quad (\omega,T\ll T_*) , \quad (18)$$

$$C^{\mathrm{imp}}(T)\sim\frac{T}{T_*}\ln\frac{T_*}{T} ; \quad (T\ll T_*) \quad (19)$$

where the characteristic temperature $T_*\sim Je^{-\mathrm{const}J/g}$ in weak coupling.[17]

To gain some further insight into the problem, we shall follow the approach which Emery and Kivelson used to study the two-channel Kondo problem.[11] Consider (15) and introduce the fields

$$\Phi_{S,A}(x)=\frac{1}{\sqrt{2}}[\Phi_L(x)\pm\Phi_L'(x)] .$$

Then

$$H_B=\frac{2u}{\pi}\int dx\{[\nabla\Phi_S(x)]^2+[\nabla\Phi_A(x)]^2\} ,$$

$$H_I=\frac{g_\perp}{\sqrt{2\pi}}[S^+(e^{-i2(\Phi_S-\Phi_A)(0)}+e^{-i2(\Phi_S+\Phi_A)(0)})+\mathrm{H.c.}]$$

$$+\frac{g_z\alpha}{\pi}S_z\frac{\partial\Phi_S(0)}{\partial x} .$$

The transverse coupling of the impurity spin to the Φ_S field can be removed by a canonical transformation (a rotation about the z axis in spin space) $H\to\tilde{H}=UHU^{-1}, U=e^{i2\Phi_S(0)S_z}$ to yield

$$H_I=\frac{g_\perp}{\sqrt{2\pi}}[S^+(e^{i2\Phi_A(0)}+e^{-i2\Phi_A(0)})+\mathrm{H.c.}]$$

$$+\left[\frac{g_z\alpha}{\pi}-4u\right]S_z\frac{\partial\Phi_S(0)}{\partial x} . \quad (20)$$

Introducing a Majorana fermion representation for the impurity spin

$$S^+=d^\dagger\eta ,$$

$$S_z=d^\dagger d-\tfrac{1}{2} ,$$

where d is a fermion and $\eta=c+c^\dagger$ is a Majorana fermion ($\eta^2=1$), we can define a left moving fermion

$$\Psi_A(x)=\eta\frac{e^{-i2\Phi_A(x)}}{\sqrt{2\pi\alpha}} \quad (21)$$

and make a similar definition (without the Majorana field) for $\Psi_S(x)$ so that along the "Emery-Kivelson line," $g_z\alpha=4\pi u$ the model is quadratic in fermion fields and therefore exactly solvable:

$$\tilde{H}=iu\int_{-\infty}^{\infty}\left[\Psi_S^\dagger(x)\frac{\partial}{\partial x}\Psi_S(x)+\Psi_A^\dagger(x)\frac{\partial}{\partial x}\Psi_A(x)\right]$$

$$+g_\perp\sqrt{\alpha}[\Psi_A(0)+\Psi_A^\dagger(0)](d^\dagger-d) . \quad (22)$$

We now calculate some correlation functions within this framework. Particularly simple is the calculation of the transverse impurity spin susceptibility. Using $\tilde{S}^- = US^-U^{-1} = \sqrt{2\pi\alpha}\Psi_S(0)\eta d$ and the conjugate for $\tilde{S}^+$ we have

$$\begin{aligned}\chi^{-+}(\tau) &= \langle T_\tau S^-(\tau)S^+(0)\rangle_H \\ &= \langle T_\tau \tilde{S}^-(\tau)\tilde{S}^+(0)\rangle_{\tilde{H}} \\ &= 2\pi\alpha\langle T_\tau \Psi_S(0,\tau)\Psi_S^\dagger(0,0)\rangle\langle T_\tau d(\tau)d^\dagger(0)\rangle \end{aligned} \quad (23)$$

the final line coming from the fact that the d-on and the Ψ_S fermion are noninteracting on the Emery-Kivelson line. As seen from the explicit solution of (22) the d-on propagator has a piece which is free, a result of the fact that the Ψ_A field couples to only "half" of the impurity spin, viz. $(d^\dagger - d)$ in (22). This dominates the large-τ behavior of $\chi^{-+}(\tau)$. We therefore have

$$\chi^{-+}(\tau) = 2\pi\alpha[\theta(\tau)\langle\Psi_S(0,\tau)\Psi_S^\dagger(0,0)\rangle + \theta(-\tau)\langle\Psi_S^\dagger(0,0)\Psi_S(0,\tau)\rangle]$$

[note the crucial sign change, central to Kondo-type problems, of $\chi^{-+}(\tau)$ relative to $\langle T_\tau\Psi_S(0,\tau)\Psi_S^\dagger(0,0)\rangle$] so that

$$\chi^{-+}(\omega,T) \sim -\frac{\alpha}{4}\int_{-1/\alpha}^{1/\alpha} dk \frac{\tanh[uk/2T]}{\omega - uk + i\delta} . \quad (24)$$

Thus the static transverse impurity susceptibility is

$$\chi^{-+}(\omega=0,T) = \frac{\alpha}{2u}\ln\frac{u}{\alpha T} . \quad (25)$$

This logarithmic divergence can be thought of simply in the following way: on the Emery-Kivelson line the canonical transformation removes all coupling to S_z and "attaches" a fermion to the spin flip operators. As a result the two ground states are *orthogonal* in the sense that they are not connected by the spin flip operators. This removes the Curie divergence (which is the direct result of $S_z = \frac{1}{2}$ and $S_z = -\frac{1}{2}$ ground states being connected by a spin flip), replacing it by a weaker logarithmic one. Note that the factor u/α is just the cutoff energy scale, E_c (recall that the velocity $u \sim J\alpha$). However, the Emery-Kivelson line is at strong coupling, so that if the "bare" coupling was small, $g/J \ll 1$, one would have to apply renormalization-group scaling first until the effective coupling $g(E_c)/E_c \sim O(1)$ which means that the effective cutoff to use in $E_c \equiv T_* \sim Je^{-\text{const}J/g}$.

We can also calculate the longitudinal susceptibility $\chi^{zz}(\omega,T)$, which requires the determination of the anomalous d-on Green's functions (see Ref. 11). We find

$$\chi^{zz}(\omega,T) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega' \frac{\tanh\beta\omega'/2}{(\omega'-\omega)}\frac{\gamma}{\omega'^2+\gamma^2} , \quad (26)$$

where $\gamma = 2g_\perp^2\alpha/u$, from which the low temperature $(T \ll \gamma)$ static part is

$$\chi^{zz}(\omega=0,T) = \frac{1}{\pi\gamma}\ln\frac{\gamma}{T} + \frac{1}{\gamma}[\text{const} + O(T/\gamma)^2] . \quad (27)$$

The anisotropy, $\chi^{zz} \neq \chi^{-+}$, is to be expected at the Emery-Kivelson line. Strictly speaking, our continuum limit restricts us to $g_\perp/g_z \sim O(\alpha^{1/2})$, however we observe that for $g_\perp \sim g_z$, γ is of the order of the cutoff so that both the transverse and longitudinal impurity susceptibilities agree with the result (18) from the exact solution of the two-channel Kondo problem.

The *uniform* static susceptibility of the spin chain is also found to exhibit anomalous low-temperature behavior when in the presence of an impurity spin. In the *absence* of an impurity $\chi_0(k=0,\omega=0) \propto L/u$. If we now calculate $\chi^{zz}(k=0,\omega=0)$ in the presence of an impurity on the Emery-Kivelson line we obtain the interesting result that $\chi^{zz}(k=0,\omega=0)$ is the same as that in the absence of the impurity. This occurs because

$$Um_z(x)U^{-1} = \frac{\alpha}{\pi}\frac{\partial\phi(x)}{\partial x} - \alpha S_z\delta(x)$$

so that a uniform external magnetic field couples only to the first term which is the magnetization in a spin chain alone [see Eq. (13)]. The calculation of $\chi^{zz}(k=0,\omega=0)$ then involves correlation functions of Ψ_S which is a free field on the Emery-Kivelson line, and so the impurity spin is completely screened and there is no anomalous contribution to $\chi^{zz}(k=0,\omega=0)$.

However if we perturb in $\delta g_z \equiv g_z - 4u\pi/\alpha$ about the Emery-Kivelson line we do then find a logarithmic contribution to the longitudinal uniform susceptibility

$$\delta\chi^{zz}(k=0,\omega=0) \sim \frac{(\delta g_z)^2}{\gamma}\left[\frac{\alpha}{u}\right]^2 \ln\frac{\gamma}{T} . \quad (28)$$

One may also calculate the transverse uniform susceptibility

$$\chi^{-+}(k=0,\omega=0) = \frac{1}{\alpha^2}\int dx \int dy \int_0^\beta d\tau \langle[\alpha S^-(\tau)\delta(x) + m^-(x,\tau)][\alpha S^+(0)\delta(y) + m^+(y,0)]\rangle .$$

In this case an anomalous logarithmic contribution arises even on the Emery-Kivelson line, and comes directly from the impurity contribution (25) to $\chi^{-+}(k=0,\omega=0)$, the other pieces involving the background magnetization giving regular contributions at low T.

Further insight into the physics of the fixed point can be obtained from the equal time correlation function $\langle\Omega_z(x)\Omega_z(-x)\rangle$. Under the canonical transformation induced by $U = e^{i2\Phi_S(0)S_z}$ we find $U\Omega_z(x)U^{-1} = \text{sgn}(x)\Omega_z(x)$ so that

$$\langle\Omega_z(x)\Omega_z(-x)\rangle_{g\neq 0} = -\langle\Omega_z(x)\Omega_z(-x)\rangle_{g=0} ,$$

where $g=0$ denotes the case where the impurity spin is decoupled from the spin chain, and $g \neq 0$ denotes coupling on the Emery-Kivelson line. One may interpret this result, along with that obtained above for $\delta\chi^{zz}$ on the Emery-Kivelson line, as indicating that all the spins to the left of the impurity are flipped, a "kink" is introduced, and the impurity spin is "pulled into" the chain. It therefore appears that the original AFM coupling between the two spins on either side of the impurity has scaled to zero and that the fixed point is of the type referred to by Eggert and Affleck[10] as a "healed" spin chain, viz., all exchange couplings in the chain are of equal strength.

An idea of the extent of the disturbance due to the impurity may be obtained from the equal time correlation function $\langle S^+(0)m^-(x,0)\rangle$. At zero temperature the asymptotic behavior at large x is $\sim 1/x^2$ which is not inconsistent with a "healed" chain fixed point. While we are unable to calculate $\langle S^+(0)\Omega^-(x,0)\rangle$, we expect that it will behave as $1/x$.

Finally, to make contact with possible experiments one needs to examine the problem of a finite density of impurities. Interactions between impurities (induced by the chain) will complicate the application of the single impurity results. A naive argument based upon length scales would suggest that for temperatures T, and impurity densities δ, satisfying $J\delta < T$ the impurities would be essentially noninteracting so that, for example, the contributions of the impurities to the uniform, static susceptibility would be simply additive and thus give rise to a logarithmic behavior for $J\delta < T < T_*$. However the validity of this argument needs to be carefully examined: the problem may be very sensitive to the nature of the probability distribution governing interimpurity spatial separations.

IV. CONCLUSION

We have considered above a number of cases of an impurity spin coupled to an AFM background. The application of spin-wave theory, appropriate as long as there is AFM order, immediately leads to the conclusion that only a half-integer impurity spin with sublattice symmetric coupling retains divergent susceptibility (at $T=0$). This can be compared to the observed presence of a Curie component in the magnetic susceptibility of O-doped La-CuO compounds[3] where the $\frac{1}{2}$ spins of the localized carrier states would have the symmetry of Cu-Cu bond and thus sublattice symmetric coupling. On the other hand, the absence of the Curie term in the Zn substitution compound[3] can also be easily understood: the nonmagnetic Zn which goes onto the Cu site can be thought of as an additional spin-$\frac{1}{2}$ with a strong AFM onsite coupling. As it sees the local field due to the staggered magnetization no Curie divergence appears. (Alternatively, one can think of an on-site spin vacancy which introduces a localized magnetic moment which is "polarized" by the staggered order.) Curiously, the Curie term scaling with Zn concentration reappears in the Sr-doped compounds[3] when the AFM order is lost.

In the interesting case of half-integer sublattice symmetric impurity we find a possibility of non-Curie divergent susceptibility which is realized in one dimension. This nontrivial behavior arises because of the effective orthogonality of the degenerate impurity spin states as they become "dressed" by background spin fluctuations (with constant spectral density at low frequency). This is the same effect as in the two-channel Kondo model. Here the role of the fermion flavor is taken up by the spatial parity of the "spinons" of the AFM chain. Since the *local* susceptibility of the spin-$\frac{1}{2}$ chain is also log-divergent one could think that the impurity susceptibility is just that of the spin in the chain. Yet, the impurity moment is localized, in the sense that it contributes the $T_*^{-1}\ln(T_*/T)$ divergence to the *uniform* susceptibility.

Finally, we remark that it would be interesting to study the magnetic impurities in spin-$\frac{1}{2}$ AFM chain compounds such as $CuCl_2\cdot 2NC_5H_5$,[4] as a possible realization of the two-channel Kondo phenomenon.

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[12]The coupling of **S** to m_z appears to be a "dangerous" one in 2D, leading to an instability of the spin-wave theory. We interpret this instability as implying a *local* suppression of the staggered magnetization $\langle\Omega_z\rangle\to 0$. To fully determine the nature of the spin background in the vicinity of the impurity spin to $O(\zeta^0)$ one would need to consider spin-wave interaction terms, which are also $O(\zeta^0)$.

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[14]Note that marginally relevant $\cos 4\phi$ term dropped from H_B

will not introduce any further the *relevant* couplings to the impurity spin; however, it will lead to renormalization of the bare $g_{\perp}$ and g_z and so the parameters in (11) should be understood as renormalized.

[15]Note however that we cannot say that our impurity spin model is *equivalent,* in the sense of a one-to-one correspondence of Hilbert spaces, to the two-channel Kondo model. The charge degrees of freedom in the latter interact in a "statistical" fashion with the spin and flavor degrees of freedom: there are selection rules involved in filling up real electron states.

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