Physica C357 (2001) 78

PC-17/ISS 2000 ; October 16, 2000

Static hole in a critical antiferromagnet: field-theoretic renormalization group

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Abstract

We consider the quantum field theory of a single, immobile, spin S hole coupled to a two-dimensional antiferromagnet at a bulk quantum critical point between phases with and without magnetic long-range order. We present an alternative derivation of its two-loop beta function; the results agree completely with earlier work (M. Vojta *et al*, Phys. Rev. B **61**, 15152 (2000)), and also determine a new anomalous dimension of the hole creation operator.

Keywords: Kondo spin, critical antiferromagnet, field theory (subject index); high temperature superconductor (materials index).

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Proceedings of the 13th International Symposium on Superconductivity, October 14-16, 2000, Tokyo, Japan. To appear in Physica C.

PACS numbers: 71.27.+a, 75.20.Hr, 75.10.Jm

Recent papers [1, 2] have introduced the following model Hamiltonian for a single non-magnetic (Zn or Li) impurity in a two-dimensional d-wave superconductor or spin-gap insulator (see [3] for a review and experimental motivation):

$$\begin{aligned} \mathcal{H} &= \mathcal{H}_\phi - \gamma_0 \hat{S}_\alpha \phi_\alpha(x=0) \\ \mathcal{H}_\phi &= \int d^d x \left[\frac{\pi_\alpha^2 + c^2(\nabla \phi_\alpha)^2 + s\phi_\alpha^2}{2} + \frac{g_0}{4!}(\phi_\alpha^2)^2 \right]. \end{aligned} \tag{1}$$

We have written the Hamiltonian in d spatial dimensions, and $\hat{S}_\alpha$ ($\alpha = 1,2,3$) are spin S operators of a magnetic moment that is postulated to be present near the impurity (the case of physical interest has $S = 1/2$); these operators obey the SU(2) commutation relations

$$[\hat{S}_\alpha, \hat{S}_\beta] = i\epsilon_{\alpha\beta\gamma}\hat{S}_\gamma \tag{2}$$

and $\hat{S}_\alpha \hat{S}_\alpha = S(S+1)$. The field $\phi_\alpha(x,t)$ represents the local orientation of the antiferromagnetic order parameter at spatial position x and time t; its canonically conjugate momentum is $\pi_\alpha(x,t)$, and hence

$$[\phi_\alpha(x,t), \pi_\beta(x',t)] = i\delta_{\alpha\beta}\delta^d(x-x') \tag{3}$$

This theory has a bulk quantum critical point at $s = s_c$ between a phase with magnetic order ($s < s_c$, $\langle \phi_\alpha \rangle \neq 0$), and a symmetric phase with a spin gap ($s > s_c$, $\langle \phi_\alpha \rangle = 0$). We are interested in the spin correlations of $\mathcal{H}$ for s close to s_c, and in the vicinity of the impurity at $x = 0$. As discussed in [1, 2], universal aspects of these correlations are associated with a renormalized continuum theory of $\mathcal{H}$ defined in an expansion in $\epsilon = 3 - d$. This renormalization involves the familiar bulk renormalizations which are insensitive to the impurity degree of freedom

$$\phi_\alpha = \sqrt{Z}\phi_{R\alpha} \quad ; \quad g_0 = \frac{\mu^\epsilon Z_4}{Z^2 S_{d+1}} g \tag{4}$$

and new 'boundary' renormalizations associated with the impurity spin

$$\hat{S}_\alpha = \sqrt{Z'}\hat{S}_{R\alpha} \quad ; \quad \gamma_0 = \frac{\mu^{\epsilon/2} Z_\gamma}{\sqrt{Z Z' \widetilde{S}_{d+1}}}\gamma. \tag{5}$$

Here μ is a renormalization momentum scale (we set the velocity $c = 1$), $S_d = 2/[\Gamma(d/2)(4\pi)^{d/2}]$, and $\widetilde{S}_d = \Gamma(d/2-1)/[4\pi^{d/2}]$. The renormalization constants Z, Z_4 were computed long ago [4]; their values in the minimal subtraction scheme to order g^2 are

$$Z = 1 - \frac{5g^2}{144\epsilon} \quad ; \quad Z_4 = 1 + \frac{11g}{6\epsilon} + \left(\frac{121}{36\epsilon^2} - \frac{37}{36\epsilon}\right) g^2. \tag{6}$$

The boundary renormalizations were computed to the same order in [1, 2]:

$$Z' = 1 - \frac{2\gamma^2}{\epsilon} + \frac{\gamma^4}{\epsilon} \quad ; \quad Z_\gamma = 1 + \frac{\pi^2[S(S+1)-1/3]}{6\epsilon}\gamma^2 g \tag{7}$$

This paper will rederive the above results by a new method which also yields a renormalization constant for the hole creation operator. Furthermore, the present approach, unlike that of [2], has the advantage of being formulated entirely in terms of perturbation expansion which has a Wick theorem, and can thus be presented in conventional time-ordered Feynman diagrams.

We will identify the spin $\hat{S}_\alpha$ with that of a hole, with creation operator $\psi_a^\dagger$, that has been injected into the antiferromagnet. So

$$\hat{S}_\alpha = \psi_a^\dagger L^\alpha_{ab} \psi_b \tag{8}$$

where a, b take the $2S+1$ values $-S, \ldots S$, and the L^α are the $(2S+1) \times (2S+1)$ angular momentum matrices associated with the spin S representation. The hole operators obey the anticommutation relation

$$\psi_a^\dagger \psi_b + \psi_b \psi_a^\dagger = \delta_{ab} \tag{9}$$

So the remainder of this paper will consider the Hamiltonian

$$\mathcal{H}_\psi = \lambda \psi_a^\dagger \psi_a + \mathcal{H}_\phi - \gamma_0 \psi_a^\dagger L^\alpha_{ab} \psi_b \phi_\alpha(x=0) \tag{10}$$

We will only look at the Hilbert space with a single hole, and λ, the energy of this hole is an arbitrary positive number.

We now consider the renormalization of $\mathcal{H}_\psi$. The standard procedure suggests the parameterization

$$\psi_a = \sqrt{Z_h}\,\psi_{Ra} \quad ; \quad \gamma_0 = \frac{\mu^{\epsilon/2}\widetilde{Z}_\gamma}{Z_h\sqrt{Z\widetilde{S}_{d+1}}}\gamma. \tag{11}$$

It is important to note that despite the relation (8), the renormalization of the spin $\hat{S}_\alpha$ is not the square of the renormalization of ψ_a, $Z' \neq Z_h^2$; bringing the two Fermi operators to the same spacetime point introduces a composite operator renormalization which invalidates such a relation. Instead, the relationship between the two renormalization schemes emerges by comparing the renormalization of γ_0 in (5) and (11); consistency of these relations demands

$$Z_h^2 Z_\gamma^2 = \widetilde{Z}_\gamma^2 Z' \tag{12}$$

We will now compute Z_h and $\widetilde{Z}_\gamma$ by completely standard field theoretic methods, and verify that their values and (7) satisfy (12).

The Feynman diagrams for the renormalization of two-point ψ Green's function are shown in Fig 1. As an explicit example, we display the computation of the simplest one-loop graph in Fig 1a:

$$\begin{aligned}
(1a) &= \gamma_0^2 S(S+1) \int \frac{d^d k}{(2\pi)^d} \int \frac{d\omega'}{2\pi} \frac{1}{(\omega'^2 + k^2)} \frac{1}{(-i(\omega+\omega')+\lambda)} \\
&= \gamma_0^2 S(S+1) \frac{S_d}{2} \int_0^\infty \frac{k^{d-2} dk}{(-i\omega + k + \lambda)} \\
&= A_\mu (-i\omega+\lambda) \gamma^2 S(S+1) \left[-\frac{1}{\epsilon} + \aleph/2 + \mathcal{O}(\epsilon) \right],
\end{aligned} \tag{13}$$

where $A_\mu \equiv \mu^\epsilon (-i\omega+\lambda)^{-\epsilon} \widetilde{Z}_\gamma^2 / (Z_h^2 Z)$. In the last step, the integral was evaluated in dimensional regularization. The constant $\aleph = -0.8455686701969\ldots$ is a consequence of phase space factors and will eventually cancel out of our final results. The remaining diagrams can be evaluated in a very similar manner: the frequency integrals are performed first, followed by integrals over the radial momenta. The results for the two-loop diagrams in Fig 1 are

$$\begin{aligned}
(1b) &= A_\mu^2 (-i\omega+\lambda) \gamma^4 S^2 (S+1)^2 \left[\frac{1}{2\epsilon^2} + \frac{1-\aleph}{2\epsilon} + \mathcal{O}(\epsilon^0) \right] \\
(1c) &= A_\mu^2 (-i\omega+\lambda) \gamma^4 S(S+1)(S^2+S-1) \left[-\frac{1}{\epsilon^2} + \frac{-1+2\aleph}{2\epsilon} + \mathcal{O}(\epsilon^0) \right]
\end{aligned} \tag{14}$$

Turning to the renormalization of the vertex γ_0, the Feynman diagrams are shown in Fig 2. Evaluating these as above we obtain

$$(2a) = \gamma_0 A_\mu \gamma^2 (S^2+S-1) \left[\frac{1}{\epsilon} - 1 - \aleph/2 + \mathcal{O}(\epsilon) \right]$$

$$
\begin{aligned}
(2b) &= \gamma_0 A_\mu^2 \gamma^4 (S^2+S-1)^2 \left[\frac{1}{2\epsilon^2} - \frac{3+\aleph}{2\epsilon} + \mathcal{O}(\epsilon^0)\right] \\
(2c) &= \gamma_0 A_\mu^2 \gamma^4 (S-1)(S+2)(S^2+S-1) \left[\frac{1}{2\epsilon} + \mathcal{O}(\epsilon^0)\right] \\
(2d) &= \gamma_0 A_\mu^2 \gamma^4 (S^2+S-1)^2 \left[\frac{1}{\epsilon^2} - \frac{2+\aleph}{2\epsilon} + \mathcal{O}(\epsilon^0)\right] \\
(2e) &= \gamma_0 A_\mu^2 \gamma^4 S(S+1)(S^2+S-1) \left[-\frac{1}{\epsilon^2} + \frac{2+\aleph}{2\epsilon} + \mathcal{O}(\epsilon^0)\right] \\
(2f) &= -\gamma_0 \frac{A_\mu^2 Z_h^2 Z_4}{\widetilde{Z}_\gamma^2 Z} \gamma^2 g (S^2+S-1/3) \left[\frac{\pi^2}{6\epsilon} + \mathcal{O}(\epsilon^0)\right]
\end{aligned}
\tag{15}
$$

The two-loop expression for the boundary renormalization constants follows immediately from the results (13,14,15). Demanding cancellation of poles in ϵ in the expressions for the renormalized vertex and ψ Green's function at external frequency $-i\omega + \lambda = \mu$ we obtain

$$
\begin{aligned}
Z_h &= 1 - \gamma^2 \frac{S(S+1)}{\epsilon} + \gamma^4 \left[\frac{(S-1)S(S+1)(S+2)}{2\epsilon^2} + \frac{S(S+1)}{2\epsilon}\right] \\
\widetilde{Z}_\gamma &= 1 - \gamma^2 \frac{(S^2+S-1)}{\epsilon} + \gamma^4 \left[\frac{(S^2+S-3)(S^2+S-1)}{2\epsilon^2} + \frac{(S^2+S-1)}{2\epsilon}\right] \\
&\quad + g\gamma^2 \frac{\pi^2 (S^2+S-1/3)}{6\epsilon}
\end{aligned}
\tag{16}
$$

It can be checked that (16) and (7) satisfy (12).

The validity of (12) implies that the beta function for the coupling γ is the same as that in [2]. Using either (5,6,7) or (11,6,16) we obtain

$$
\beta(\gamma) = -\frac{\epsilon\gamma}{2} + \gamma^3 - \gamma^5 + \frac{5g^2\gamma}{144} + \frac{g\gamma^3\pi^2}{3}(S^2+S-1/3). \tag{17}
$$

The anomalous dimension of the ψ_a field at the quantum critical point also follows from (16)

$$
\eta_h = \beta(\gamma) \frac{d \ln Z_h}{d\gamma} = S(S+1)(\gamma^2 - \gamma^4), \tag{18}
$$

while, as in [2], the anomalous dimension of the spin field, $\hat{S}_\alpha$, follows from (5,7):

$$
\eta' = 2(\gamma^2 - \gamma^4). \tag{19}
$$

For completeness we also note the beta function for the coupling g which follows from (6)

$$
\beta(g) = -\epsilon g + \frac{11g^2}{6} - \frac{23g^3}{12}. \tag{20}
$$

The stable fixed point of the beta functions (17,20) has $g \neq 0$ and $\gamma \neq 0$ [2]. Evaluating (18) at the fixed point of the beta functions [2], we obtain

$$\eta_h = S(S+1)\left[\frac{\epsilon}{2} - \left(\frac{5}{484} + \frac{\pi^2(S^2+S-1/3)}{11}\right)\epsilon^2 + \mathcal{O}(\epsilon^3)\right] \tag{21}$$

($\eta' = 2\eta_h/[S(S+1)]$ at this order). This anomalous dimension implies that the Green's function $G = \langle \psi_a \psi_a^\dagger \rangle$ obeys

$$G(\omega) \sim (\lambda - \omega)^{-1+\eta_h}. \tag{22}$$

The equations (16,18,21) are the main new results of this paper. Unfortunately, the order ϵ^2 corrections in (21) are rather large: this suggests that truncating the asymptotic series for η_h at order ϵ probably gives the most reasonable estimate for its numerical value.

There is also an unstable fixed point at which the bulk interactions vanish ($g = 0$). As shown in [2], $\eta' = \epsilon$ exactly at this fixed point, and here we find that $\eta_h = S(S+1)\epsilon/2 + \mathcal{O}(\epsilon^3)$. There appears to be no general reason for the higher order terms in η_h to vanish. The $g = 0$ fixed point can also be studied in a large N theory [2], and the $N = \infty$ results are $\eta' = 1$ and $\eta_h = 1/2$.

The physical motivations and implications of the above results are discussed in a separate paper [5]: there we argue that the anomalous dimension η_h characterizes photoemission spectra of *mobile* holes in two-dimensional antiferromagnets and superconductors in the vicinity of points in the Brillouin zone where their dispersion spectra are quadratic (*i.e.* near energy minima, maxima, and van Hove singularities). The intensively studied $(\pi, 0)$, $(0, \pi)$ points (the anti-nodal points) in the high temperature superconductors are prominent examples.

ACKNOWLEDGMENTS

This research was supported by US NSF Grant No DMR 96–23181.

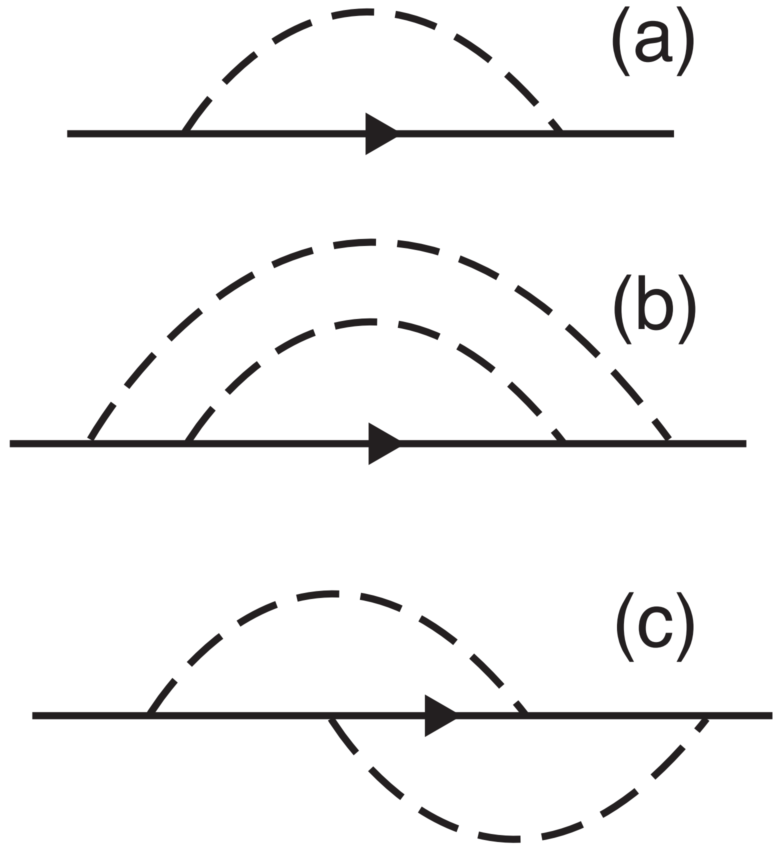

FIG. 1: Diagrams contributing to the ψ fermion self energy. The full line is the fermion propagator, while the dashed line is the ϕ_α propagator.

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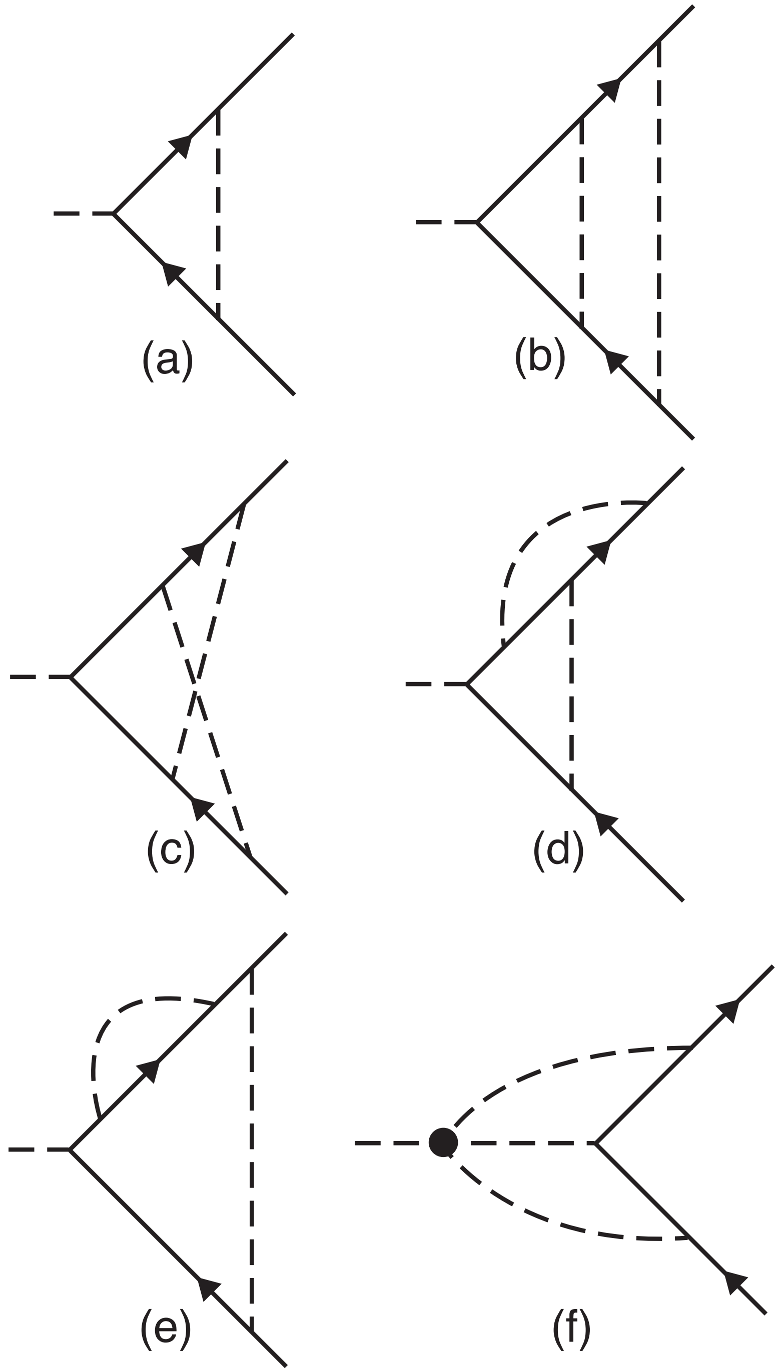

FIG. 2: Diagrams contributing to the renormalization of the coupling γ. The full circle is the interaction g