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Spin orthogonality catastrophe in two-dimensional antiferromagnets and superconductors

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We compute the spectral function of a spin S hole injected into a two-dimensional antiferromagnet or superconductor in the vicinity of a magnetic quantum critical point. We show that, near van Hove singularities, the problem maps onto that of a static vacancy carrying excess spin S. The hole creation operator is characterized by a new *boundary* anomalous dimension and a vanishing quasiparticle residue at the critical point. We discuss possible relevance to photoemission spectra of cuprate superconductors near the anti-nodal points.

A vigorous debate has been stimulated by photoemission experiments [1] showing that the gapped *anti-nodal* quasiparticle excitations of the high temperature superconductors have a broad energy distribution curve (EDC). The many proposals for this anomalous behavior include (*i*) electron scattering by antiferromagnetic fluctuations [2], (*ii*) one-dimensional (1d) fluctuations at intermediate scales leading to 1d electron fractionalization [3], (*iii*) 2d electron fractionalization induced by proximity to exotic 2d spin liquid states [4], and (*iv*) coupling to superconducting phase and vortex fluctuations [5].

The studies of this paper fall into category (*i*); however, our results also extend into a quasi 1d regime, and offer a different perspective on category (*ii*). We will examine the spectral function (or EDC) of the gapped anti-nodal quasiparticles [6] in the vicinity of a quantum critical point between a d-wave superconductor and a state with co-existing superconducting and antiferromagnetic order. Our results will also apply to insulators in the vicinity of a quantum transition between states with antiferromagnetic order and a spin gap: the spectral functions are then those of holes (and electrons) near van Hove singularities in the band structure of the spin gap state. Our perspective on the superconducting case differs from that of [2] in that we depart from ground states in which pairing correlations have already induced a gap to fermionic excitations in the anti-nodal regions, rather than from states with a Fermi surface. Appealing to the proximity of a magnetic quantum critical point between the former states allows us to make controlled statements in a regime with strong coupling between the fermionic quasiparticles (henceforth referred to generically as holes) and the antiferromagnetic fluctuations.

Our primary result is that the proper characterization of the damping of the holes by low energy spin fluctuations is provided by the framework of "boundary" critical phenomena [7]. The hole Green's function, G_h, is controlled by a new non-zero boundary scaling dimension, η_h. Consequently, the hole quasiparticle residue vanishes at the zero temperature (T) quantum critical point due to an "orthogonality catastrophe" induced by a cloud of low energy spin excitations around the hole. The motion of the hole charge does not play a dominant role: this may be viewed as a form a "spin-charge separation", but is not 2d electron fractionalization in the sense of [8,4].

As has been discussed elsewhere [9], spin fluctuations near the magnetic quantum critical point in the superconductors or insulators of interest are described by the following continuum Hamiltonian

$$\mathcal{H}_\phi = \int d^2x \left[\left(\pi_\alpha^2 + c_1^2 (\partial_{x_1} \phi_\alpha)^2 + c_2^2 (\partial_{x_2} \phi_\alpha)^2 \right)/2 + (r/2)\phi_\alpha^2 + (g/24)(\phi_\alpha^2)^2 \right] \quad (1)$$

Here $\phi_\alpha(x,t)$ ($\alpha = 1,2,3$) is the component of the magnetization at wavevector $\mathbf{G}$ (usually $\mathbf{G} = (\pi,\pi)$) at spatial co-ordinate x and time t, π_α is its canonically conjugate momentum, the only non-zero equal-time commutation relation is $[\phi_\alpha(x,t), \pi_\beta(x',t)] = i\delta_{\alpha\beta}\delta^2(x-x')$, $c_{1,2}$ are velocities (possibly unequal to account for a quasi 1d spatial anisotropy), r is the parameter which tunes the system across the quantum critical point ($\langle \phi_\alpha \rangle \neq 0$ in the magnetically ordered phase for $r < r_c$, and $\langle \phi_\alpha \rangle = 0$ otherwise), and g is the crucial quartic self interaction which is relevant below 3d and is responsible for the non-trivial universal scaling properties of the quantum critical point. There are no explicit damping terms for ϕ_α fluctuations in (1) because the systems of interest do not have a gapless particle-hole continuum near the wavevector $\mathbf{G}$ [10].

We now inject a spin S hole into the system described by $\mathcal{H}_\phi$. We consider the hole spectrum near points of higher symmetry in the Brillouin zone, with momentum $\mathbf{k} = \mathbf{K}_1$, where its dispersion has a vanishing $\mathbf{k}$ derivative *i.e.* near van Hove points like $\mathbf{K}_1 = (\pi, 0)$. We denote the hole creation operator in the vicinity of $\mathbf{K}_1$ by $\psi_{1a}^\dagger(x,t)$, with $a = -S, \ldots, S$ a spin index (for the case where the ground states are superconductors, $\psi_{1a}^\dagger$ is the creation operator for the Bogoliubov quasiparticles). Coupling to ϕ_α fluctuations will scatter the hole to momenta near $\mathbf{K}_2 = \mathbf{K}_1 + \mathbf{G}$: we denote the hole creation operator near $\mathbf{K}_2$ by $\psi^\dagger_{2a}(x,t)$, and it is assumed that $\mathbf{K}_2$ is also a van Hove point. The hole Hamiltonian is then

$$\mathcal{H}_h = \int d^2x \left[\sum_{i=1,2} \left(\epsilon_i \psi^\dagger_{ia}\psi_{ia} + \sum_{m=1,2} \alpha_{mi}\psi^\dagger_{ia}\partial^2_{x_m}\psi_{ia} \right) + \gamma\phi_\alpha \left(\psi^\dagger_{1a} L^\alpha_{ab}\psi_{2b} + \psi^\dagger_{2a} L^\alpha_{ab}\psi_{1b} \right) \right]. \quad (2)$$

Here L^α are the familiar $(2S+1)\times(2S+1)$ angular momentum matrices, the α_{mi} determine the band curvatures near $\mathbf{K}_{1,2}$, and γ is the coupling to the ϕ_α fluctuations. Higher order couplings between the ϕ_α and $\psi_{1,2}$ are also possible, but are easily shown to be irrelevant under the renormalization group (RG) discussed below. We assume that the hole energies, ϵ_i satisfy $\epsilon_1 = \epsilon_2 \equiv \epsilon_0 > 0$ (equality holds with $\mathbf{K}_1 = (\pi, 0)$, $\mathbf{K}_2 = (0, \pi)$, and square symmetry), for otherwise the hole scattering by ϕ_α fluctuations is non-singular, and direct perturbative computations of the hole spectrum are adequate. The singularity in the value of ϵ_0 at the magnetic transition at $r = r_c$ is weak and subdominant, and can be safely neglected.

A key observation follows from a simple, tree-level, RG analysis of $\mathcal{H}_\phi + \mathcal{H}_h$. We know that $\mathcal{H}_\phi$ at $r = r_c$ is invariant under the rescaling transformation $x \to xe^{-\ell}$, $t \to te^{-z\ell}$ with $z = 1$. Applying this to $\mathcal{H}_h$ we see immediately that the α_{mi} flow as $d\alpha_{mi}/d\ell = -\alpha_{mi}$: so the band curvatures are irrelevant for the low-energy theory, and the hole may be viewed as dispersionless.

Before embarking on a complete RG analysis of $\mathcal{H}_\phi + \mathcal{H}_h$, we make some qualitative observations on the hole spectrum for $r < r_c$, $r > r_c$, and $r = r_c$.

For $r < r_c$, hole motion in the magnetically ordered state has been studied earlier [11]. Because $\langle\phi_\alpha\rangle \neq 0$, there is a non-zero mean matrix element between the ψ_{1a} and ψ_{2a} states, and we have to rediagonalize $\mathcal{H}_h$ to obtain the bare hole dispersion. Simple considerations of energy and momentum conservation show that there is an infinitely sharp quasiparticle pole in the vicinity of the absolute band minimum: the slow quadratic dispersion of the hole prevents decay by emission of linearly dispersing spin waves. At frequencies, ω, above this pole, there is an incoherent gapless continuum, but its spectral weight vanishes rapidly as ω approaches the quasiparticle pole: after the rediagonalization of $\mathcal{H}_h$ required by a nonzero $\langle\phi_\alpha\rangle$, it is easy to see that the matrix element for emission of small momentum, Goldstone, spin wave modes is suppressed by powers of the momentum. Similar considerations also apply at other van Hove points which are not global minima. However, depending upon non-universal details of the band structure, in some cases it may be possible for the hole to emit large wavevector, high energy ϕ_α quanta, and this would broaden the quasiparticle pole; for $\mathcal{H}_h$ such processes occur if one of the $\alpha_{mi} < 0$, and require momenta of order $c_{1,2}/\alpha_{mi}$ or larger (assuming $\mathcal{H}_h$ still applies at such momenta). Given the irrelevance of the α_{mi}, the remainder of this paper will neglect this non-universal decay. We will only consider low energy ϕ_α quanta, and assume that the high energy processes are either not present, or contribute a small, background, quasiparticle decay rate. If the latter were not true, there would be no sharp quasiparticle-like peak or threshhold in the hole spectrum, and the analysis of this paper would not be necessary.

Closely related considerations apply in the spin-gap phase with $r > r_c$ [12,13], but with some important differences: (i) the incoherent continuum is separated from the quasiparticle pole by at least the spin gap energy, $\Delta \sim (r - r_c)^\nu$, where ν is the correlation length exponent of the phase transition in $\mathcal{H}_\phi$; (ii) the ϕ_α quanta are no longer Goldstone modes, and so the matrix element for emission of a ϕ_α quantum by the hole does not vanish at zero momentum transfer.

The main purpose of this paper is to understand the nature of the hole spectrum at the $T = 0$ quantum critical point at $r = r_c$, and its associated $T > 0$ quantum-critical region. The ϕ_α are now gapless critical excitations, but not Goldstone modes. Consequently, there is no factor of a small momentum suppressing their emission by the hole, and perturbative corrections in γ are infrared singular, as has also been noted by Sushkov [13]. Our RG analysis will identify the scale-invariant quantum field theory which permits a resummation of the perturbative expansion, and shows that there is no quasiparticle pole at $T = 0$ and $r = r_c$; instead

$$G_h(\omega) = -\mathcal{A}(\epsilon_0 - \omega)^{-1+\eta_h}, \quad (3)$$

where $\mathcal{A}$ is a non-universal amplitude, and the universal exponent η_h is computed below.

For the critical theory, we can set $\alpha_{mi} = 0$. Further, examination of the perturbation theory in γ shows that the presence of two hole flavors, $i = 1, 2$, makes no material difference to the critical singularities: the $\phi_\alpha \to -\phi_\alpha$ symmetry of $\mathcal{H}_\phi$ ensures that the hole self-energy has terms only in even powers of γ for which the hole flavor returns to its original value. Consequently we can drop the i index, and refer to a generic dispersionless hole ψ_a. After injection into the antiferromagnet at $x = 0$ (say), the ψ_a charge will remain localized at $x = 0$, and its spin will couple to the ϕ_α fluctuations. So we are led to consider the Bose-Kondo-like model [14,15,9], $\mathcal{H}_\phi + \mathcal{H}_S$ of a single quantum spin, $\hat{S}_\alpha$, coupled to the bosonic ϕ_α fluctuations where

$$\mathcal{H}_S = \gamma \hat{S}_\alpha \phi_\alpha(x = 0), \quad (4)$$

$[\hat{S}_\alpha, \hat{S}_\beta] = i\epsilon_{\alpha\beta\gamma}\hat{S}_\gamma$, and $\hat{S}_\alpha\hat{S}_\alpha = S(S+1)$. The charge density of the injected hole can couple only to the spinrotation invariant $\phi_\alpha^2(x=0)$, and such a term is irrelevant under the RG [9].

The properties of $\mathcal{H}_\phi + \mathcal{H}_S$ have already been studied in detail [9] in the different physical context of Zn/Li impurities in the cuprate superconductors; in this earlier case the $\hat{S}_\alpha$ spin was permanently confined near the impurity, while in the present situation there is no impurity and $\hat{S}_\alpha$ is the spin of the injected hole. Indeed, the relationship between $\mathcal{H}_\phi + \mathcal{H}_S$ and $\mathcal{H}_\phi + \mathcal{H}_h$ is similar to that between the familiar fermionic Kondo and X-ray edge problems. However, the analogy is not perfect: it is conventional in the X-ray edge problem to neglect the spin of the injected hole, and merely couple its charge density to the fermionic bath. Here, the spin exchange with the ϕ_α quanta is paramount in both cases.

The critical point of $\mathcal{H}_\phi$ defines a 2+1 dimensional, conformally invariant field theory, and $\mathcal{H}_S$ is a "boundary" perturbation along the line in spacetime at $x=0$. This perturbation flows to a fixed point which is invariant under conformal transformations which leave $x=0$ fixed. Correlations of $\hat{S}_\alpha$ are characterized by its boundary anomalous dimension $\eta'/2$, which was computed to two-loop order in an expansion in $\varepsilon = 3-d$ in [9].

We are interested here in the $G_h = \langle \psi_a \psi_a^\dagger \rangle$, and by (3) we identify $\eta_h/2$ as the boundary anomalous dimension of ψ_a, which is not simply related to η'. G_h involves an overlap between eigenstates of $\mathcal{H}_\phi + \mathcal{H}_S$ and states in which the hole has been removed (the latter are outside the Hilbert space of $\mathcal{H}_\phi + \mathcal{H}_S$). The needed results do not follow from the previous analysis of $\mathcal{H}_\phi + \mathcal{H}_S$ alone, and require extensions we describe here.

At one-loop order, we perform a standard momentum-shell RG of $\mathcal{H}_\phi + \mathcal{H}_h$ in d spatial dimensions, in which fields with momenta between Λ and $\Lambda e^{-\ell}$, and all frequencies, are integrated out. This is followed by the rescalings $x \rightarrow x e^{-\ell}$, $t \rightarrow t e^{-\ell}$, $\phi_\alpha \rightarrow \phi_\alpha e^{(d-1+\eta)\ell/2}\phi_\alpha$, $\psi_a \rightarrow \psi_a e^{(d+\eta_h)\ell/2}$. The RG flow of the bulk couplings r, g is well known: g approaches a finite fixed point value g^* at $r = r_c$, while $\eta = 0$ at one loop order. For the hole, evaluation of the one-loop graphs in Fig 1 shows that $\eta_h = S(S+1)\widetilde{\gamma}^2$, where $\widetilde{\gamma} = \gamma(c_1 c_2)^{-d/4}\Lambda^{-\varepsilon/2}(\Gamma(d/2)(4\pi)^{d/2})^{-1/2}$ obeys the same flow equation as that obtained earlier for $\mathcal{H}_\phi + \mathcal{H}_S$ [9,14] (as expected):

$$d\widetilde{\gamma}/d\ell = \varepsilon\widetilde{\gamma}/2 - \widetilde{\gamma}^3. \quad (5)$$

We observe that $\widetilde{\gamma}$ also approaches a fixed-point value, and at which we have the anomalous dimension

$$\eta_h = \varepsilon S(S+1)/2 + \mathcal{O}(\varepsilon^2). \quad (6)$$

At the same order, a closely related computation shows that $\eta' = \epsilon$ [9]. The extension of these results on the boundary exponents to two (and higher) loops requires the field-theoretic renormalization group and the results are presented elsewhere [16]: at next order there is interference between bulk and boundary interactions, and the flow equation for $\widetilde{\gamma}$ involves g. This interference is a novel feature of the present problem and is absent in the fermionic Kondo and X-ray edge problems, where the bulk degrees of freedom can be represented by free fields. Direct numerical evaluation of the two-loop corrections for the physical values $\varepsilon = 1$ and $S = 1/2$ shows significant changes from the one loop values: η_h changes from 0.375 to 0.087, while η' changes from 1 to 0.232.

We also computed η_h from a continuous time worldline quantum Monte Carlo [17] simulation of a double layer Heisenberg antiferromagnet at its quantum critical point [18]. We measured $G_h(\tau)$ (τ is imaginary time) for a single hole on a fixed site i, by relating it to correlators of spin world lines at site i which do not flip in time τ. We obtained the estimate $\eta_h = 0.087 \pm 0.040$ from simulations on a 64×64 system by fitting to $G_h(\tau) \sim \tau^{-\eta_h}\exp(-\epsilon_0\tau)$, in the range $2 \leq J\tau \leq 6$ (J is the intralayer exchange, and $\epsilon_0/J = 2.102 \pm 0.016$ was determined separately from the ground state energies of the antiferromagnet with and without a hole); the numerical data is in Fig 2.

In the $r \geq r_c$, $T \geq 0$ vicinity of the critical point, (3) generalizes to

$$G_h(\omega) = \frac{\mathcal{A}}{T^{1-\eta_h}}\Phi_h\left(\frac{\omega-\epsilon_0}{T}, \frac{\Delta}{T}\right) \quad (7)$$

where $\mathcal{A}$ and ϵ_0 are the same constants appearing in (3) (they have absorbed a non-universal renormalization from the coupling to ϕ_α modes), while Φ_h is a completely universal function. We obtained numerical results for Φ_h using the large N method discussed in [9] and the results are shown in Fig 3. The $\mathbf{k}$ dependence of G_h arises only from the irrelevant α_{mi} couplings, and their main effect is to replace ϵ_0 by the actual hole dispersion near the van-Hove point.

We conclude by discussing possible physical application of our results to photoemission measurements on the cuprate superconductors. We have already argued elsewhere [9,20] that (1) should be a reasonable description of the antiferromagnetic fluctuations in the low and moderate doping regime, both above and below the superconducting T_c. There is evidence from NMR [21] and neutron scattering experiments [22] that the quantum critical region of the $r = r_c$ critical point describes the antiferromagnetic fluctuations above T_c; so for the same systems, the $r = r_c$ spectrum in Fig 3 should apply to photoemission at the anti-nodal points. The proximity of such a magnetic quantum critical point may be associated with the onset of quasi 1d correlations, but this incidental to our theory—the anisotropy is merely reflected by changes to the couplings in $\mathcal{H}_\phi$. Below T_c, the measured anti-nodal spectrum [23] is similar to the $r > r_c$ spectrum in Fig 3: this is accounted for in our approach by the reasonable assumption that the onset of superconductivity induces the spin-gap-like correlations and so increases the value of the effective r controlling the magnetic fluctuations. The high frequency tail of the EDC both above and below T_c should decay as $1/\omega^{1-\eta_h}$. Note that this tail is present for any non-zero value of η_h, with a non-universal amplitude determined by $\mathcal{A}$. However, our estimate of the value of η_h here is quite small, and it appears that the interaction effects discussed here cannot explain the prominent tail seen in current experiments on their own. It is likely that the strong disorder in the local gap values (as seen in recent STM measurements [24]) also plays an important role.

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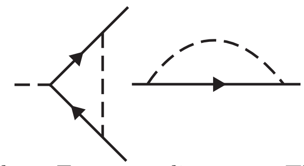

FIG. 1. One-loop Feynman diagrams. The full line is ψ_a and the dashed line is ϕ_α.

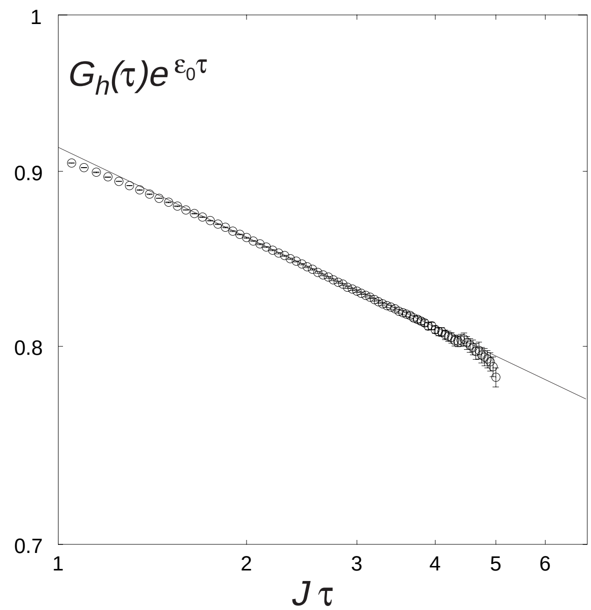

FIG. 2. Quantum Monte Carlo results for a localized hole Green's function at the quantum-critical point of a double layer Heisenberg antiferromagnet. Both axes are logarithmic.

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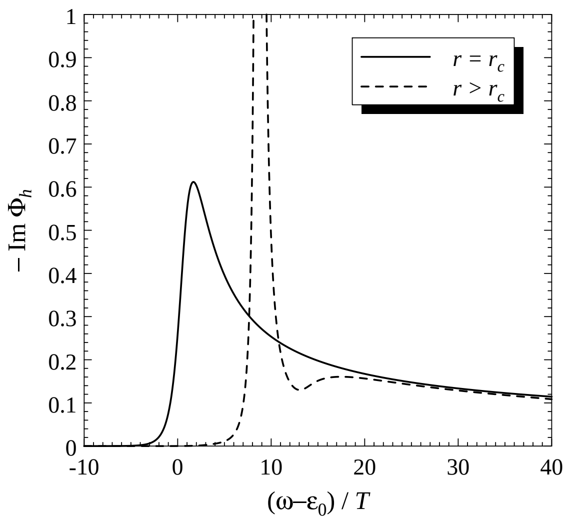

FIG. 3. Large N [9] results for the imaginary part of the scaling function Φ_h in (7). At large N $\eta_h = 1/2$. We used an interpolation form for the ϕ_α propagator $1/(k^2 - \omega^2 + m^2 - 2i\Gamma\omega)$, where m/T and Γ/T are universal functions of Δ/T [19]. Both m and the damping, Γ, are non-zero even at $r = r_c$ because the thermally excited ϕ_α quanta scatter strongly off each other by the non-zero fixed point value of the bulk interaction, g, in $\mathcal{H}_\phi$. For $r = r_c$ we used $m = \Gamma = T$, and for $r > r_c$ we used $\Gamma = m/5 = T$.