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 \cite{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 \cite{2}, (ii) one-dimensional (1d) fluctuations at intermediate scales leading to 1d electron fractionalization \cite{3}, (iii) 2d electron fractionalization induced by proximity to exotic 2d spin liquid states \cite{4}, and (iv) coupling to superconducting phase and vortex fluctuations \cite{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 \cite{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 \cite{6} 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 \cite{7}. The hole Green’s function, $G_h$, is controlled by a new non-zero boundary scaling dimension, $\eta_b$. 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 \cite{8,4}.

As has been discussed elsewhere \cite{6}, spin fluctuations near the magnetic quantum critical point in the superconductors or insulators of interest are described by the following continuum Hamiltonian

$$H_\phi = \int d^2x \left[ \left( \pi_\alpha^2 + c_1^2(\partial_x \phi_\alpha)^2 + c_2^2(\partial_x \phi_\alpha)^2 \right) / 2 \right.$$\n\left. + \left( r/2 \right) \phi_\alpha^2 + \left( g/24 \right) (\phi_\alpha^2)^2 \right] \quad (1)$$

Here $\phi_\alpha(x,t)$ ($\alpha = 1, 2, 3$) is the component of the magnetization at wavevector $G$ (usually $G = (\pi, \pi)$) at spatial co-ordinate $x$ and time $t$, $\pi_\alpha$ is its canonically conjugate momentum, the only non-zero equal-time commutation relation is $[\phi_\alpha(x,t), \pi_\beta(x',t')] = i\hbar \delta_{\alpha\beta} \delta^2(x - x')$, $c_{1,2}$ 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 $\phi_\alpha$ fluctuations in \cite{6} because the systems of interest do not have a gapless particle-hole continuum near the wavevector $G$ \cite{10}.

We now inject a spin $S$ hole into the system described by $H_\phi$. We inject the hole spectrum near points of higher symmetry in the Brillouin zone, with momentum $k = K_1$, where its dispersion has a vanishing $k$ derivative \textit{i.e.} near van Hove points like $K_1 = (\pi, 0)$. We denote the hole creation operator in the vicinity of $K_1$ by $\psi^\dagger_{1a}(x,t)$, 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 \( \phi_\alpha \) 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 \( \psi_{2a}^\dagger(x,t) \), and it is assumed that \( \mathbf{K}_2 \) is also a van Hove point. The hole Hamiltonian is then

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

Here \( L^\alpha \) are the familiar \((2S + 1) \times (2S + 1)\) angular momentum matrices, the \( \alpha_{mi} \) determine the band curvatures near \( \mathbf{K}_{1,2} \), and \( \gamma \) is the coupling to the \( \phi_\alpha \) fluctuations. Higher order couplings between the \( \phi_\alpha \) 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, \( \epsilon_i \) 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 \( \phi_\alpha \) fluctuations is non-singular, and direct perturbative computations of the hole spectrum are adequate. The singularity in the value of \( \epsilon_0 \) 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 \( x \rightarrow x e^{-z \ell}, \ t \rightarrow t e^{-z \ell} \) with \( z = 1 \). Applying this to \( \mathcal{H}_h \) we see immediately that the \( \alpha_{mi} \) flow as \( d\alpha_{mi}/dt = -\alpha_{mi} \); 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 \( \psi_{1a} \) and \( \psi_{2a} \) 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, \( \omega \), above this pole, there is an incoherent gapless continuum, but its spectral weight vanishes rapidly as \( \omega \) 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 \( \phi_\alpha \) 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 \( \alpha_{mi} \), the remainder of this paper will neglect this non-universal decay. We will only consider low energy \( \phi_\alpha \) 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 threshold 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 \( \nu \) is the correlation length exponent of the phase transition in \( \mathcal{H}_\phi \); \( ii \) the \( \phi_\alpha \) quanta are no longer Goldstone modes, and so the matrix element for emission of a \( \phi_\alpha \) 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 \( \phi_\alpha \) 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 \( \gamma \) 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

\[
G_h(\omega) = -\mathcal{A}(\epsilon_0 - \omega)^{-1+\eta_h},
\]

where \( \mathcal{A} \) is a non-universal amplitude, and the universal exponent \( \eta_h \) is computed below.

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

\[
\mathcal{H}_S = \gamma \hat{S}_\alpha \phi_\alpha(x = 0),
\]

\(
[\hat{S}_\alpha, \hat{S}_\beta] = i\epsilon_{\alpha\beta\gamma} \hat{S}_\gamma, \ \text{and} \ \hat{S}_\alpha \hat{S}_\alpha = S(S+1).
\)
rotation invariant $\phi_0^2(x = 0)$, and such a term is irrelevant under the RG.

The properties of $H_\phi + H_S$ have already been studied in detail in the different physical context of Zn/Li impurities in the cuprate superconductors; in this earlier case the $\hat{\cal S}_a$ spin was permanently confined near the impurity, while in the present situation there is no impurity and $\hat{\cal S}_a$ is the spin of the injected hole. Indeed, the relationship between $H_\phi + H_S$ and $H_\phi + H_h$ 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 density to the fermionic bath. Here, the spin exchange with the $\phi_0$ quanta is paramount in both cases.

The critical point of $H_\phi$ defines a 2+1 dimensional, conformally invariant field theory, and $H_S$ 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 $\hat{\cal S}_a$ are characterized by its boundary anomalous dimension $\eta'/2$, which was computed to two-loop order in an expansion in $\varepsilon = 3 - d$ in $[9,14]$.

We are interested here in the $H_\phi$ 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 $\bar{\gamma}$ 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: $\eta_h$ changes from 0.375 to 0.875, while $\eta'$ changes from 1 to 0.232.

We also computed $\eta_h$ from a continuous time world-line quantum Monte Carlo $[16]$ simulation of a double layer Heisenberg antiferromagnet at its quantum critical point $[21]$. We measured $G_h(\tau)$ ($\tau$ 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 $\tau$. We obtained the estimate $\eta_h = 0.087 \pm 0.040$ from simulations on a $64 \times 64$ system by fitting to $G_h(\tau) \sim \tau^{-\eta_h} \exp(-r_0\tau)$, in the range $2 \leq \mu \tau \leq 6$ ($\mu$ 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 $[21]$.

In the $r \geq r_c, T \geq T_c$ vicinity of the critical point, $[21]$ generalizes to

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

where $A$ and $\epsilon_0$ are the same constants appearing in $[21]$ (they have absorbed a non-universal renormalization from the coupling to $\phi_0$ modes), while $\Phi_h$ is a completely universal function. We obtained numerical results for $\Phi_h$ using the large $N$ method discussed in $[21]$ and the results are shown in Fig $[21]$. The $k$ dependence of $G_h$ arises only from the irrelevant $\alpha_{mi}$ couplings, and their main effect is to replace $\epsilon_0$ 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 $[21]$ that $[21]$ 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 $[21]$ 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 $H_\phi$. Below $T_c$, the measured anti-nodal spectrum $[22]$ is similar to the $r > r_c$ spectrum in Fig $[21]$: 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 $\eta_h$, with a non-universal amplitude determined by $A$. However, our estimate of the value of $\eta_h$ 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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[6] It is important to distinguish the present work on anti-nodal quasiparticles from earlier, distinct theories of damping of nodal quasiparticles in M. Vojta, Y. Zhang, and S. Sachdev, Phys. Rev. Lett. 85, 4940 (2000).
[10] In $d$-wave superconductors, there is a gapless particle hole continuum arising from the nodal Fermi points, but this is at the wavevector, $K$, separating two nodal points, and it is assumed that $K \neq G$. The case $K = G$ can also be analyzed by the methods of this paper: the results are very similar $\eta$, and the value of $\eta_h$ is modified only at the two loop level.
FIG. 3. Large $N$ results for the imaginary part of the scaling function $\Phi_h$ in (3). At large $N$ $\eta_h = 1/2$. We used an interpolation form for the $\phi_\alpha$ propagator $1/(k^2 - \omega^2 + m^2 - 2i\Gamma\omega)$, where $m/T$ and $\Gamma/T$ are universal functions of $\Delta/T$ [9]. Both $m$ and the damping, $\Gamma$, are non-zero even at $r = r_c$ because the thermally excited $\phi_\alpha$ 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 $\Gamma = m/5 = T$. 