Vanishing spectral weight in a one-hole-doped antiferromagnet:
A rigorous result

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Abstract

By explicitly tracking the Marshall sign, a phase string induced by hopping is revealed in the one-hole-doped $t - J$ model. It is rigorously shown that such a phase string cannot be eliminated through low-lying spin excitations, and it either causes the spectral weight $Z = 0$, or leads to the localization of the doped hole. Implications for finite doping are also discussed.

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Whether the strongly-correlated $t - J$ model can be meaningfully treated in terms of a conventional perturbative method is still controversial. The key issue involves the spectral weight $Z$. If $Z = 0$ in an interested regime, it means that each particle (or hole) added to the system cannot be described as a quasi-particle-type excitation. Instead, each injected particle would cause a global change in the original ground state, which may not be tractable perturbatively. In particular, the issue whether $Z = 0$ for a one-hole doped antiferromagnet is crucial for establishing a workable method at weak doping: a finite $Z$ would mean that at least in dilute doping the low-lying state may be described by some quasiparticle-type holes on the top of an antiferromagnetic (AF) background, with weak interaction among themselves. However, $Z = 0$ would simply suggest the breakdown of this perturbative connection between the weakly-doped system and the parental antiferromagnet.

The discussions about the spectral weight $Z$ for a one-hole problem in various analytical approaches and finite-size numerical calculations have given conflicting conclusions in the two-dimensional (2D) case. The main difficulty involved in this problem arises from the competing superexchange and hopping processes, which usually result in a strong spin-polaron distortion around the doped hole. Such a spin distortion effect constitutes a dominant part in the energy spectrum of the renormalized hole. Most importantly, the spin-polaron is different from the usual phonon-polaron as $SU(2)$ spins are involved in the former, where $U(1)$ phase may play an important role in shaping the long-distance part of spin-polaron with little energy cost. In a finite-size calculation and truncated self-consistent approximation, there is no accurate way to distinguish the contributions from the coherent bare-hole part and the rest “spin-polaron” part in a sufficiently low-energy and long-wavelength regime. Therefore, a more accurate approach would be desirable in order to get access to such a regime. In this Letter, we introduce a spin-hole basis in which the Marshall sign as the sole source of sign problem hidden in the spin background can be exactly tracked. A new phase string induced by the doped hole is then revealed in this representation. Due to such a phase string, one either has $Z = 0$, or the doped hole is localized in the ground state of the one-hole doped $t - J$ model.
Let us start with the undoped antiferromagnet. It is described by the superexchange Hamiltonian

\[ H_J = J \sum_{<ij>} \left[ S_i \cdot S_j - \frac{n_i n_j}{4} \right], \quad (1) \]

which is equivalent to the Heisenberg model at half-filling as the occupation number \( n_i = n_j = 1 \). According to Marshall [4], the ground-state wavefunction of the Heisenberg Hamiltonian for a bipartite lattice is real and satisfies a sign rule. This sign rule can be uniquely determined by requiring that a flip of two antiparallel spins at nearest-neighboring sites always involves a sign change: \( \uparrow \downarrow \rightarrow (−1) \downarrow \uparrow \) in the wave-function. The meaning of the Marshall sign may be understood as follows: under a spin basis \( |\phi> \) with the Marshall sign included, the matrix element of the superexchange Hamiltonian \( (1) \) becomes negative-definite, i.e., \( <\phi'|H_J|\phi> \leq 0 \). Then it is easy to see that the ground-state \( |\psi_0> = \sum_\phi c_\phi^0 |\phi> \) always has real, positive coefficient (or wave-function) \( c_\phi^0 \), so that the aforementioned Marshall sign is indeed the only sign to appear in the ground state \( |\psi_0> \) (through \( |\phi> \)). And there is no additional sign problem in this new representation.

The Marshall sign described above can be easily built into the \( S^z \)-spin representation even in the presence of a hole. The bipartite lattice can be divided into even (\( A \)) and odd (\( B \)) sublattices. For each down spin at \( A \) site or up spin at \( B \) site, one may assign an extra phase \( i \) to the basis. In this way, a flip of two nearest-neighboring spins will always involve a sign change (i.e., the Marshall sign): \( \uparrow \downarrow \rightarrow (i^2) \downarrow \uparrow = (−1) \downarrow \uparrow \). Of course, this is not a unique way to incorporate the Marshall sign in the spin basis, but it will be quite a useful bookkeeping once hole is introduced into the system. Generally speaking, the spin basis with one hole may be defined as

\[ |\phi(n)> = i^{N_A^− + N_B^+} | \uparrow \ldots \downarrow \uparrow \downarrow \ldots \downarrow >, \quad (2) \]

with \( N_A^− \) and \( N_B^+ \) as total numbers of down and up spins at \( A \)- and \( B \)-sublattices, respectively, and the subscript \( (n) \) specifying the hole’s site. It is straightforward to verify that the matrix element
\[ < \phi'_{(n)} | H_J | \phi_{(n)} > \leq 0, \]  

under this new basis. Namely, even in the presence of a hole, the superexchange term \( H_J \) still does not have sign problem in the representation (2).

Now we consider the hopping of the hole. The hopping process is governed by \( H_t \) defined by

\[
H_t = -t \sum_{<ij>} c^\dagger_{i\sigma} c_{j\sigma} + H.c.,
\]

where the Hilbert space is restricted by the no-double-occupancy constraint \( \sum_{\sigma} c^\dagger_{i\sigma} c_{i\sigma} \leq 1 \).

Suppose the hole initially sitting at site \( n \) hops onto a nearest-neighboring site \( m \). The corresponding matrix element in the basis (2) can be easily obtained:

\[
< \phi_{(m)} | H_t | \phi_{(n)} > = -t \times (\pm i),
\]

where the sign \( \pm \) is determined by the original site-\( m \) spin state \( \sigma_m = \pm 1 \) in the following way:

\[
(\pm i) \equiv (-1)^m e^{i\pi \sigma_m}.
\]

Here \((-1)^m\) is the staggered factor: \((-1)^A = +1\) and \((-1)^B = -1\). Thus, in terms of the representation (2), it is revealed that the hole will always leave behind a trace of phases (phase string) \((\pm i) \times (\pm i) \times \ldots\) when it moves around. On the other hand, if there exists a long-range AF ordering in the ground state, the hopping process in (3) also creates a well-recognized “string” defect [3,5], namely, a line of mismatched spins along the polarization direction left by the moving hole. However, this latter type of string can be dynamically eliminated through spin-flip process described in (3). Instead of causing the localization of the hole, it merely leads to a reduction of the spectral weight \( Z \) by \( J/t \) [2] (or to some power of \( J/t \) [2,3]). In contrast, the phase string induced by hopping (3) cannot be repaired through the spin process (3) at low energy (see below). Therefore, one expects such a phase string to be essential in determining the long-wavelength behavior of the hole. This phase problem is closely related to a \( U(1) \) subgroup of the \( SU(2) \) spins, whose importance has been
already revealed in the one dimensional (1D) case [6]. In the following, we will investigate its crucial role for a general dimensionality.

We define a “bare” hole to be described by $c_{i\sigma}|\psi_0>$. One can track its evolution by studying the propagator $G_{1\sigma}(i,j;E) = <\psi_0|c^\dagger_{j\sigma}(E - H_{t-J} + i\eta)^{-1}c_{i\sigma}|\psi_0>$, with $H_{t-J} = H_t + H_J$ and $\eta = 0^+$. In momentum space, the imaginary part of $G_{1\sigma}(k,E)$ is given by

$$\text{Im}G_{1\sigma}(k,E) = -\pi\sum_M Z_k(E_M)\delta(E - E_M),$$

(7)

where the spectral weight $Z_k$ is defined as

$$Z_k(E_M) = |<\psi_M|c_{k\sigma}|\psi_0>|^2,$$

(8)

with $|\psi_M>$ and $E_M$ denoting the eigenstate and energy of $H_{t-J}$ in the one hole case. The corresponding real-space form of (7) may be rewritten as

$$G''_{1\sigma}(j,i;E) = -\pi\sum_k e^{-ik\cdot(x_j-x_i)}Z_k(E)\rho(E),$$

(9)

where $\rho(E) = \sum_M \delta(E - E_M)$ is the density of states, and here $Z_k$ is understood as being averaged over $M$ at the same energy $E$.

Spectral weight $Z_k(E)$ describes the overlap of the bare-hole state $c_{k\sigma}|\psi_0>$ with the real eigenstates at energy $E$. If the low-lying excitation can be classified as quasiparticle-like, $Z_k(E)$ must be finite and peaked at a lower-bound energy $E_k$ near the ground-state energy $E_G$, with a well-defined dispersion relation with regard to the momentum $k$. Particularly, at the band bottom $Z_k(E_G)$ should be finite at some discrete $k$’s determined by $E_k = E_G$. In terms of (9), then, $G_{1\sigma}$ must become sufficiently extended in a large scale $|x_j-x_i|$ when $E$ is close enough to $E_G$. In other words, if one finds $G_{1\sigma} \rightarrow 0$ as $|x_j-x_i| \rightarrow \infty$ even near $E = E_G$, $Z_k(E_G)$ has to be either zero [7] or involves a continuum of $k$’s to lead a decay in (9). In the latter case, $E_k$ is dispersionless near the band bottom such that the hole in the ground state has an infinite effective mass and is localized in space.

To separate the hopping and superexchange processes, one may expand $G_{1\sigma}$ in terms of $H_t$ as follows
where $G_0^J = (E - H_J + i\eta)^{-1}$. Then, by inserting intermediate states in terms of the representation of $q$, one obtains

$$G_{1\sigma}(j, i; E) = \langle \psi_0 | c^\dagger_{j\sigma} \left( G_0^J + G_0^J H_J G_0^J + \ldots \right) c_{i\sigma} | \psi_0 \rangle,$$

(10)

which involves those intermediate states $\{|\phi^s_{(m_s)}\rangle\}$ where the hole is on a path $m_0, m_1, \ldots, m_{K_{ij}}$ connecting sites $i$ and $j$. Here $m_0 = i$, $m_{K_{ij}} = j$, and $K_{ij}$ denotes the number of links for a given path. And $|\phi^0_{(m_0)}\rangle \equiv |\phi(0)\rangle$, $|\phi^{K_{ij}+1}_{(m_{K_{ij}})}\rangle \equiv |\phi(j)\rangle$. $T_{ij}$ is the contribution from $H_t$ for such a path:

$$T_{ij}(\{\phi\}) = (-i\eta)^{K_{ij}} \prod_{k=1}^{K_{ij}} (1 - \langle \sigma_{m_k} \rangle),$$

(11)

with $\sigma_{m_k}$ specifies the site-$m_k$ spin state in the state $|\phi^k_{m_{k-1}}\rangle$ where the hole is at site $m_{k-1}$. Equation (12) shows that each path connecting sites $i$ and $j$ is weighted by a spin-dependent phase string $\prod_{k=1}^{K_{ij}} (-1)^{m_k} \sigma_{m_k}$. The rest phases explicitly shown in (11) and (12) are constant for each path, and thus are trivial. (In fact, those phases lead to oscillations of the propagator corresponding to momenta, e.g., $(\pm \pi/2, \pm \pi/2)$ in 2D, which is well-known in a single-hole doped problem $q$.)

To determine the phase of $\langle \phi^J_{(m)} | G_0^J | \phi_{(m)} \rangle$ in (11), one may expand $G_0^J$ as follows

$$G_0^J(E) = \frac{1}{E} \sum_k \frac{H_J^k}{E^k}.$$

(13)

By using $\langle \phi^{s+1}_{(m_s)} | H_J^k | \phi^s_{(m_s)} \rangle = (-1)^k |\phi^{s+1}_{(m_s)} | H_J^k | \phi^s_{(m_s)} \rangle |$ according to (3), one finds

$$\langle \phi^{s+1}_{(m_s)} | G_0^J(E) | \phi^s_{(m_s)} \rangle = \frac{1}{E} \sum_k \left| \frac{\langle \phi^{s+1}_{(m_s)} | H_J^k | \phi^s_{(m_s)} \rangle}{(-E)^k} \right| < 0,$$

(14)

if $E < 0$. It is easy to see that $E < E^0$ (the lowest energy bound of $H_J$ with the hole localized at site $m_s$) will guarantee the convergence of (14). So the matrix element $\langle \phi^J_{(m)} | G_0^J | \phi_{(m)} \rangle$ appearing in (11) is always sign-definite at low energy. Therefore, the phase string induced
by the doped hole in (12) indeed is not “repairable” by the low-lying spin fluctuations in the energy regime $E_G^0 > E \geq E_G$. This is consistent with the previous intuitive observation, and implies important consequences for long-wavelength behaviors of a doped hole.

Now we focus on the contribution of the phase string $\hat{T}_{ij} \equiv \prod_{k=1}^{K_{ij}} (-1)^{m_k} \sigma_{m_k}$ in (11). It is convenient for one to define

$$\tilde{\sigma}_m = (-1)^k \sigma_m.$$  (15)

The physical meaning of $\tilde{\sigma}_m$ is as follows: if there is a fully-polarized Néel order in the spin background, one has $\tilde{\sigma}_m \equiv 1$ (or $-1$ by shifting the ordering by one lattice constant). Then $\tilde{\sigma}_m = -1$ represents a “spin-flip” at site $m$ with regard to such a Néel configuration. This Néel configuration is just a reference for describing various intermediate spin configurations in (11), and the phase string is contributed by all those “spin flips” in terms of $\prod_{k=1}^{K_{ij}} \tilde{\sigma}_{m_k} = (-1)^{N_{ij}^{flip}}$, where $N_{ij}^{flip}$ is the total number of zero-point “spin flips” on the given path connecting $i$ and $j$. Thus the effect of the zero-point spin fluctuations is accumulated in the phase string. In other words, with the increase of length scale, more and more spin-flips will be involved, with each of them contributing a $(-1)$. Such an effect, then, must lead to a vanishing contribution to the propagator (11) when $|i - j| \to \infty$. The proof is quite straightforward. One may define the contribution of the phase string in (11) as $\langle e^{i\pi N_{ij}^{flip}} \rangle_{\text{path}}$, where $\langle ... \rangle_{\text{path}}$ means the average over all the spin states for a given path, weighted by other sign-definite quantities shown in (11). If $\langle e^{i\pi N_{ij}^{flip}} \rangle_{\text{path}}$ would approach to a finite quantity $B_\infty < 1$ (omitting some oscillation factor) beyond a large scale $L$ ($L \gg$ the spin-fluctuational correlation length), then at a scale $\sim r \times L$ ($r > 1$), one would have $\langle e^{i\pi N_{ij}^{flip}} \rangle_{\text{path}} \sim (B_\infty)^r$ to the leading order, which should approach to zero as $r \to \infty$. This is contradictory to the original assumption of a finite saturation $B_\infty$. To be consistent, then, $B_\infty$ has to continuously vanish as $L \to \infty$. Such a conclusion holds for a general spin state, no matter whether there is a real long-range order or not. The energy $E$ lying in the regime $E_G^0 > E \geq E_G$ should not affect the decay significantly even when it is close to the ground state energy, since the detailed spin fluctuations there are not
crucial. The actual decay of $G_{1\sigma}$ could be even faster with the increase of $|x_j - x_i|$ when all the paths are summed up in (11) which contributes additional phase-frustration due to the strong-oscillation nature of those phase strings.

Therefore, due to the phase string (12), the propagator $G_{1\sigma}$ has to vanish at large distance. According to the discussion at beginning, this in turn means either $Z(E) = 0$ at $E \rightarrow E_G$, or the quasiparticle spectrum $E_k$ is dispersionless near the bottom. Of course, the above discussions cannot directly distinguish whether the true ground state of a one-hole doped antiferromagnet is extended with $Z = 0$ or localized with the dispersionless $E_k$. In both cases, a “bare” hole loses its coherence in the sense that it cannot travel over a large distance near the ground-state energy. In the latter case, the quasiparticle hole would have an infinite effective mass, which could result in a divergent single-particle density of states near the ground-state energy $E_G$. In this case, finite-size numerical calculations should give a reasonable account for the density of states near the band bottom since $Z \neq 0$. However, a divergent density of states or infinite effective mass is not supported by the numerical calculations in the 2D case [3]. Furthermore, in 1D the ground state has been already known to be extended from the exact solution [9]. Thus at dimensionality $\leq 2$, we conclude $Z = 0$.

In our above demonstration, the conditions (3) and (5) are crucial in causing the unreparable phase-string defects. They are related to the intrinsic properties of the $t - J$ model. On the other hand, the property of $|\psi_0\rangle$ as the ground-state of the undoped antiferromagnet actually does not play a crucial role here. Hence, the whole argument about $Z(E_G) = 0$ should still remain robust at least in the weakly-doped case. At finite doping, additional phase due to the fermionic-statistics among holes will appear in the matrix (5), and if the density of holes is dilute enough, such a sign problem should not weaken the afore-discussed phase-string effect. On the other hand, if holes are dense enough in 2D, it is not difficult to find the strong mixing of the phase string with the statistic phase. In this case, new approach would be needed in order to clarify this issue. But there is no such a problem in 1D [6].

$Z = 0$ means that there is no overlap between the “bare” hole state $c_{i\sigma}|\psi_0\rangle$ and the true
ground state. The doped hole will have to induce a global adjustment of the spin background in order to reach the ground state. This implies that by starting from $c_{i\sigma}|\psi_0>$, one cannot get access to the ground state perturbatively, as there is no zeroth-order overlapping. Thus, in order to correctly understand the long-wavelength, low-energy physics of the weakly-doped $t-J$ model, a non-perturbative-minded approach will become necessary. Of course, $Z=0$ itself does not tell how the non-perturbative approach should be pursued. One has to go back to the original source, i.e., the phase string introduced by hole, which causes $Z=0$.

The nonlocal phase string (12) suggests that in the real ground state some nonlocal phase adjustment (i.e., phase shift) should appear. In a separate paper [8], we shall show that by eliminating the phase string (12) through some nonlocal transformation, a non-perturbative scheme can be obtained. In this new scheme, the sign problem in 1D will be totally resolved, while in 2D some residual topological phases, reflecting nonlocal coupling between spin and charge degrees of freedom, will be determined. We argue there that this formalism provides a unique way to get access to the low-lying states of the $t-J$ model perturbatively.

In conclusion, we have given a rigorous demonstration that for a one-hole doping problem in the $t-J$ model at general dimensionality, either the spectral function $Z=0$ at $E=E_G$, or the quasiparticle is localized in space with an infinite effective mass. Such a surprising result is caused by a peculiar phase string induced by the bare hole, which is revealed by explicitly tracking the Marshall sign hidden in the spin background. The present work implies that the doped $t-J$ model should not be pursued by a perturbative-minded approach in the usual spin-hole representation, and it points to the potential perturbation-applicable scheme as the one with the nonlocal phase string being eliminated.

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[7] Here one should be cautious about some special cases where $\rho(E_G) = 0$. For example, it occurs at a dimensionality higher than 2D for a parabolic spectrum, and in 2D for a massless Dirac spectrum $E_k$. But in those cases, $G_{1\sigma}/\rho(E)$ would be extended as $E \to E_G$ if $Z_k \neq 0$, and a strong energy dependence of the decay rate should be still revealed in $G_{1\sigma}$ at large $|x_j - x_i|$ when $E \sim E_G$.

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