Phase string effect in the $t$-$J$ model: General theory

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We reexamine the problem of a hole moving in an antiferromagnetic spin background and find that the injected hole will always pick up a sequence of nontrivial phases from the spin degrees of freedom. Previously unnoticed, such a stringlike phase originates from the hidden Marshall signs which are scrambled by the hopping of the hole. We can rigorously show that this phase string is nonrepairable at low energy and give a general proof that the spectral weight $Z$ must vanish at the ground-state energy due to the phase-string effect. Thus, the quasiparticle description fails here and the quantum interference effect of the phase string dramatically affects the long-distance behavior of the injected hole. We introduce a so-called phase-string formulation of the $t$-$J$ model for a general number of holes in which the phase-string effect can be explicitly tracked. As an example, by applying this new mathematical formulation in one dimension, we reproduce the well-known Luttinger-liquid behaviors of the asymptotic single-electron Green’s function and the spin-spin correlation function. We can also use the present phase-string theory to justify previously developed spin-charge separation theory in two dimensions, which offers a systematic explanation for the transport and magnetic anomalies in the high-$T_c$ cuprates. [S0163-1829(97)09805-6]

I. INTRODUCTION

A general interest in the $t$-$J$ model is motivated by the following experimental facts in the high-$T_c$ cuprates: an antiferromagnetic (AF) long-range order of Cu spins in the CuO$_2$ layers exists in the insulating phase and a metallic phase emerges after the doped holes destroys the magnetic ordering, where superconducting condensation as well as anomalous normal-state properties are found. The $t$-$J$ model is composed of two terms: $H_{t,J}=H_J+H_t$, where $H_J$ describes the AF superexchange coupling between the nearest-neighboring spins [as defined in Eq. (2.1)] which fully explains the magnetic insulating phase in the cuprates, and $H_t$ describes the hopping of holes on such a spin background [as defined in Eq. (2.6)]. The highly nontrivial competition between the superexchange and hopping processes in the $t$-$J$ model generates strong correlations among electrons, and is believed by many people to be the key to explain the strange-metal behaviors in the cuprates. Even though such a model has been intensively studied for many years, very few properties have been reliably understood in the two-dimensional (2D) doped case, which is presumably relevant to the metallic phase of the high-$T_c$ cuprates.

To see the difficulty involved in this problem, let us take as an example one of the simplest cases: only one hole is present in the AF spin background. The motion of the hole usually creates a spin mismatch along its path. Namely, the hopping changes the spin configuration, which otherwise would have perfect antiferromagnetic correlations. For the Néel order, such a ‘‘string’’-like spin mismatch is easy to see, but it is not uniquely restricted to the case with a long-range order. It has been realized that such a spin mismatch left on the spin background by the mobile hole could cost an energy linearly proportional to its length and thus has to be ‘‘repaired’’ in order to allow the hole to move around freely. In fact, it has been well known that a spin flip process can ‘‘repair’’ the spin mismatch. With the spin mismatch generated by the hopping being repairable by spin flips, the doped hole is generally believed to be a mobile object.

However, the crucial issue is whether such a mobile hole can be described as quasiparticle characterized by a nonzero spectral weight $Z$. Physically, a finite $Z$ implies that the hole only carries a local spin distortion (‘‘spin polaron’’) as it moves. This is a picture familiar in a conventional metal, where a spin polaron is usually replaced by, say, a phonon polaron. Here a spin-polaron picture can indeed be obtained by a self-consistent Born approximation, which is also supported by the finite-size exact diagonalization calculations. However, different from the phonon-polaron picture, SU(2) spins are involved here and a U(1) phase may play an important role in shaping the long-distance part of the spin polaron with little energy cost. The question whether the spectral weight $Z$ vanishes at the ground-state energy is particularly sensitive to such long-wavelength, low-energy effects. Self-consistent perturbative approaches and numerical calculations themselves cannot provide a definite answer for it. In fact, Anderson has given a general argument that $Z$ has to vanish due to the existence of the upper-Hubbard band. A vanishing $Z$ means that each hole added to the system will cause a global change in the ground state, and thus the resulting state cannot be simply described as a quasiparticle-type excitation and treated perturbatively.

Thus a more accurate description of the long-distance effect is needed in the present system in order to resolve this issue. As the spin mismatch left on the spin background has to be restored to avoid a linear potential energy, one would expect the quasiparticle picture to be generally correct, unless the hole picks up a nontrivial phase at each hopping step. The quantum interference effect of such a phase sequence, if the latter exists, can then dramatically change the long-wavelength behavior of the hole, leading to nonquasiparticle-like properties. In fact, in the one-dimensional (1D) case such a U(1) phase string has already been demonstrated, where it plays a crucial role in shaping a
non-Fermi-liquid (i.e., Luttinger liquid) behavior. In the present paper, we will rigorously demonstrate that for general dimensionality the injected hole always has to pick up a sequence of U(1) phases from the spin background when it moves around, and the resulting phase is not repairable at low energy in contrast to the aforementioned repairable spin-mismatch string. This phase-string depends on the instant spin configuration encountered by the hole and can be determined by a simple counting. We will then be able to prove that such a phase string effect leads to a vanishing spectral weight $Z$ at the ground-state energy in low dimensions.

This nontrivial effect of the U(1) phase string at large distances is generally present even when there are many doped holes, regardless of whether the ground state possesses an AF long-range order or not. Therefore, the phase-string effect is expected to be the most crucial factor in determining the low-energy, long-wavelength physics both for the one-hole problem and the finite doping case. A perturbative method, which may well describe the spin-polaron effect surrounding the doped hole, usually fails to account for this string effect. This is because the phase-string effect is basically a nonlocal effect, but conventional approximations usually average out the effect locally and thus result in a serious problem at a long distance. The natural way to avoid this difficulty is to find a method for accurately tracking the phase-string effect at large scales. We will show that such a nonlocal effect can be explicitly "counted" by introducing "mutual statistics" between spins and holes. In fact, one can exactly map the phase string effect to a statistics transmutation problem. The latter can be further transformed into a nonlocal interacting problem if one recalls that statistics-transmutation can be realized by a composite-particle representation,11,12 with the underlying particle with conventional statistics bound to a flux tube. This is an exact reformulation of the t-J model, which is of course mathematically equivalent to the conventional slave-particle representations. It has an advantage over the other formalisms, however, due to the fact that the nonlocal phase-string effect hidden in the original Hamiltonian is now made explicitly, so that its long-distance effects can be tracked even after making a local approximation in the Hamiltonian.

The one-dimensional case can serve as a direct test of the phase-string effect. As an example, the asymptotic single-electron Green’s function and the spin-spin correlation function are calculated based on the phase-string formulation developed in this paper, and the well-known Luttinger-liquid behavior in this system is reproduced. This shows that the phase string is indeed essential in shaping the long-wavelength, long-time correlations. In the 2D case, as an example of the phase-string effect, a spin-charge separation theory previously developed based on the slave-boson formalism13 will be reproduced in the present formalism. A key feature involved in this theory is nonlocal interactions between the spin and charge degrees of freedom as mediated by the Chern-Simons-type gauge fields. We show that they arise as a consequence of the nonlocal phase-string effect in 2D, and the present phase-string formalism provides both physical and mathematical justification for these topological gauge fields, which have been shown13 to be responsible for anomalous transport and magnetic properties closely resem-
\[ \langle \phi; (n) \rangle = (-1)^{N_1} | \cdots \rangle \tag{2.4} \]

with \( n \) denoting the hole site. It is easy to check that

\[ \langle \phi' ; (n) | H_j | \phi ; (n) \rangle \leq 0. \tag{2.5} \]

This means that the Marshall sign rule is still satisfied when the hole is fixed at a given site \( n \).

Now we consider the hopping of the hole. The hopping process is governed by \( H_j \) term in the \( t-J \) model which is defined by

\[ H_j = -i \sum_{\langle ij \rangle} c_{ia}^\dagger c_{ja} + \text{H.c.}, \tag{2.6} \]

where the Hilbert space is restricted by the no-double-occupancy constraint \( \sum_{\sigma} c_{ia}^\dagger c_{ia} \leq 1 \). Suppose that the hole initially at site \( n \) hops onto a nearest-neighbor site \( m \). The corresponding matrix element in the basis (2.4) is easily found to be

\[ \langle \phi ; (m) | H_j | \phi ; (n) \rangle = -i \sigma_m, \tag{2.7} \]

where \( \sigma_m \) is the site-\( m \) spin index in the state \( | \phi ; (n) \rangle \), and \( | \phi ; (m) \rangle \) is different from \( | \phi ; (n) \rangle \) by an exchange of the spin \( \sigma_m \) with the hole at site \( n \). Since \( \sigma_m = \pm 1 \), the hopping matrix element is not sign definite. In other words, the hopping process will lead to the violation of the Marshall sign rule in the ground state. In the following, we explore in detail this phase “frustration” effect introduced by the hopping of an injected hole.

### B. Single-hole Green’s function

Starting with the ground state \( | \psi_0 \rangle = \sum_\phi \chi_\phi | \phi \rangle \) at half-filling, one can create a “bare” hole by removing away an electron in terms of the electron operator \( c_{ia}^\dagger \):

\[ c_{ia}^\dagger | \psi_0 \rangle = (\sigma^i)^{\sum_\phi} \chi_\phi | \phi ; (i) \rangle. \tag{2.8} \]

Here \( \chi_\phi \geq 0 \) and the sign \( (\sigma^i)^{\sum_\phi} \) is from the Marshall sign originally assigned to the spin \( \sigma \) at the site \( i \) as follows: if \( \sigma = +1 \), \( (\sigma) = 1 \) and if \( \sigma = -1 \), \( (\sigma) = (-1)^i = -1 \) at the \( A \)-sublattice site and +1 at the \( B \)-sublattice site.

One can track the evolution of such a bare hole by studying the propagator

\[ G_{\sigma}(j, i; E) = \langle \psi_0 | c_{ja} G(E) c_{ia}^\dagger | \psi_0 \rangle, \tag{2.9} \]

with

\[ G(E) = \frac{1}{E - H_j + i0^+}. \tag{2.10} \]

By using the following expansion in terms of \( H_j \),

\[ G(E) = G_j(E) + G_j(E) H_j G_j(E) + G_j(E) H_j G_j(E) H_j G_j(E) + \cdots, \tag{2.11} \]

with

\[ G_j(E) = \frac{1}{E - H_j + i0^+}. \tag{2.12} \]

\[ G_{\sigma}(j, i; E) \] can be rewritten as

\[ G_{\sigma}(j, i; E) = (\sigma)^{i-j} \sum_{\phi'} \chi_{\phi'} \chi_{\phi} \prod_{s=0}^{K_{ij}} \langle \phi'; (j) | G_j(E) (H_j G_j(E))^s | \phi; (i) \rangle. \tag{2.13} \]

Then we insert the following complete set of the basis states (2.4) into the above expansion:

\[ \sum_m \sum_{\{\phi\}} | \phi; (m) \rangle \langle \phi; (m) | = 1. \tag{2.14} \]

By using the matrix element (2.7) for the nearest-neighbor hopping, we further express the single-hole Green’s function as follows:

\[ G_{\sigma}(j, i; E) = (\sigma)^{i-j} \sum_{\text{all paths}} \sum_{\text{all states}} \chi_{\phi'} \chi_{\phi} T^\text{path} \prod_{s=0}^{K_{ij}} \langle \phi'; (j) | G_j(E) (H_j G_j(E))^s | \phi ; (i) \rangle, \tag{2.15} \]

where intermediate states \( | \phi ; (m_s) \rangle \) and \( | \phi^{s+1} ; (m_j) \rangle \) describe two different spin configurations \( \{ \phi \} \) and \( \{ \phi^{s+1} \} \) with the hole sitting at site \( m_s \) on a given path connecting sites \( i \) and \( j \) as \( m_0 = i, m_1, \ldots, m_{K_{ij}} = j \). (Here \( K_{ij} \) is the total number of links for the given path, and \( \phi^0 \), \( \phi^{s+1} \) are the instant spin states at site \( m_s \) and \( m_{s+1} \) on the given path, respectively.) \( T^\text{path} \) is a product of matrices of \( H_j \), which connects \( \{ \phi^{s+1} ; (m_s) \} \) with \( \{ \phi ; (m_{s+1}) \} \) for such a path:

\[ T^\text{path} = \prod_{s=1}^{K_{ij}} (-1) \sigma_m. \tag{2.16} \]

where \( \sigma_m \) denotes the instant spin state at site \( m_s \) right before the hole hops to it.

We can further write \( G_{\sigma}(j, i; E) \) in a more compact form, namely,

\[ G_{\sigma}(j, i; E) = (\sigma)^{i-j} \sum_{\text{all paths}} \sum_{\{\phi\}} W^\text{path}[\{\phi\}] \prod_{s=1}^{K_{ij}} \sigma_m, \tag{2.17} \]

where the summation over \( \{\phi\} \) means summing over all the possible spin configurations in the initial and final, as well as the intermediate states. Here \( W^\text{path}[\{\phi\}] \) is defined by

\[ W^\text{path}[\{\phi\}] = \prod_{s=1}^{K_{ij}} \chi_{\phi} \langle \phi^{s+1} ; (m_s) | G_j(E) | \phi ; (m_s) \rangle. \tag{2.18} \]

In the following, we prove that \( W^\text{path}[\{\phi\}] \) is always positive definite near the ground-state energy. To determine the sign of \( \langle \phi^{s+1} ; (m_s) | G_j(E) | \phi ; (m_s) \rangle \), one may expand \( G_j \) as follows

\[ G_j(E) = \frac{1}{E - \sum_{E_n} H_j n}. \tag{2.19} \]
Note that
\[ \langle \phi^{+1};(m_f)|H_f^n|\phi^*(m_i) \rangle 
= (-1)^n \langle \phi^{+1};(m_f)|H_f^n|\phi^*(m_i) \rangle \]

[one may easily show it by writing $H_f^m = H_f - H_f^m - \cdots$ and inserting the complete set of Eq. (2.4) in between and using condition (2.5)]. Then one finds
\[ \langle \phi^{+1};(m_f)|G_f(E)|\phi^*(m_i) \rangle 
= \frac{1}{E} \sum_k \left| \langle \phi^{+1};(m_f)|H_f^m|\phi^{+1};(m_i) \rangle \right| 
< 0, \quad (2.20) \]
if $E < 0$. Of course one still needs to determine the convergence range of the expansion. By inserting a complete set of eigenstates of $H_f$ [denoted as $\{ |M_i(m_f)\rangle \}$] as intermediate states, $\langle \phi^{+1};(m_f)|G_f(E)|\phi^*(m_i) \rangle$ can be also written in the form
\[ \langle \phi^{+1};(m_f)|G_f(E)|\phi^*(m_i) \rangle 
= \sum_M \frac{\langle \phi^{+1};(m_f)|M_i(m_f)|M_j(m_i)|\phi^*(m_i) \rangle}{E - E_M^0 + i0^+}, \quad (2.21) \]
which is an analytic function of $E$ except for a branch cut on the real axis covered by the eigenvalues $\{ E_M^0 \}$ of $H_f$ (with a hole fixed at site $m_f$). This analytic property will guarantee the convergence of the expansion (2.20) in the whole region of $E < E_G^0 < 0$ on the real axis, where $E_G^0$ is the lowest-energy eigenvalue of $H_f$ with a hole fixed on a lattice site. We note that $E_G^0$ is always higher than the true ground-state energy $E_G$ of $H_{f+1}$, where the hole is allowed to move around to gain its kinetic energy. Therefore, near the ground-state energy $E_G$, one always has $W_{\text{path}}(\{ \phi \}) > 0$.

Since $W_{\text{path}}(\{ \phi \})$ is sign definite, one may introduce the following weighting function for each path and an arbitrary spin configuration $\{ \phi \}$:
\[ \rho_{\text{path}}(\{ \phi \}) = \frac{W_{\text{path}}(\{ \phi \})}{\sum_{(\text{all paths})} W_{\text{path}}(\{ \phi \})}, \quad (2.22) \]
which satisfies the normalized condition
\[ \sum_{(\text{all paths})} \rho_{\text{path}}(\{ \phi \}) = 1. \quad (2.23) \]
Then the propagator $G_\sigma$ in Eq. (2.17) can be reexpressed as follows:
\[ G_\sigma(j,i;E) = \bar{G}_\sigma(j,i;E)(-1)^{N^*_{\text{path}}}, \quad (2.24) \]
where
\[ \bar{G}_\sigma(j,i;E) = - (\sigma)^{i-j} \sum_{(\text{all paths})} \sum_{\{ \phi \}} W_{\text{path}}(\{ \phi \}), \quad (2.25) \]
and
\[ (-1)^{N^*_{\text{path}}} = \sum_{(\text{all paths})} \sum_{\{ \phi \}} \rho_{\text{path}}(\{ \phi \})(-1)^{N^*_{\text{path}}}, \quad (2.26) \]

Here
\[ (-1)^{N^*_{\text{path}}} = \prod_{j=1}^{N^*_{\text{path}}} \sigma_{m_f}, \quad (2.27) \]
with $N^*_{\text{path}}$ denoting the total number of $\downarrow$ spins “exchanged” with the hole as it moves from $i$ to $j$. Notice that
\[ (-1)^{N^*_{\text{path}}} = (-1)^{i-j} \]
which is independent of the path and thus the system is symmetric about $\uparrow$ and $\downarrow$ spins. $G_\sigma(j,i;E)$ defined in Eq. (2.25) may be regarded as the single-hole propagator under a new Hamiltonian $\bar{H}_{f+1}$ obtained by replacing the hopping term $H_f$ in the $t$-J model with $\bar{H}_f$, whose matrix element is negative definite without the extra sign problem shown in Eq. (2.7), namely,
\[ \langle \phi^*(m)|\bar{H}_f|\phi(n) \rangle = -t. \quad (2.28) \]

One can see from the propagator (2.24) that a sequence of signs $\Pi_{j=1}^{N^*_{\text{path}}} \sigma_{m_f} = (\pm 1) \times (\pm 1) \times \cdots \times (\pm 1) = (-1)^{N^*_{\text{path}}}$ is picked up by the hole from the spin background. A sign definite $W_{\text{path}}$ or $\rho_{\text{path}}$ means that such a phase string cannot be “repaired,” since there does not exist another source of “phases” at low energy to compensate it. In particular, if one chooses $i = j$, then all the paths become closed loops on the lattice, and the gauge-invariant phase $(-1)^{N^*_{\text{path}}}$ (which is independent of the ways in which one accounts for the Marshall sign) can be regarded as a Berry phase (see Sec. III A). This Berry phase is incompatible with a quasiparticle picture, in which the whole system should simply get back to the original state without picking up a Berry phase each time the quasiparticle returns to its original position. Due to the superposition of such phases from different paths and spin configurations as shown in Eq. (2.24), it is expected that the long-distance behavior of the hole will be dramatically modified by the quantum interference effect of the phase-strings. In the following we give a general proof that the spectral weight which measures the quasiparticle weight of the injected hole must vanish at the ground-state energy as a direct consequence of such a phase-string effect.

Before going to the next section, we remark that the origin of this phase string can be traced back to a highly non-trivial competition between the exchange and hopping processes represented by Eq. (2.5) and (2.7). Recall that each hopping of the hole displaces a spin, leading to a spin mismatch. Since there are three components for each $SU(2)$ spin which do not commute with each other, the induced spin mismatch string has three components in spin space which must be repaired simultaneously after the hole moves away as pointed out in the Introduction. The phase-string effect revealed in Eq. (2.24), however, implies that the spin mismatch induced by hopping cannot relax back completely, and there is always a residual $U(1)$ phase-string left behind, which is not repairable by low-lying spin fluctuations. This subtle phase string effect has been overlooked before, especially in the 2D case.

C. Phase-string effect: Vanishing spectral weight $Z(E_G)$

First, in momentum space the imaginary part of $G_\sigma(k,E)$ can be shown to be
Im$G_{\sigma}(k,E) = -\pi \sum_{M} Z_k(E_M) \delta(E-E_M)$,

where the spectral weight $Z_k$ is defined as

$$Z_k(E_M) = |\langle \psi_M | c_{k\alpha} | \psi_0 \rangle|^2,$$

with $|\psi_M \rangle$ and $E_M$ denoting the eigenstate and energy of $H_{i,j}$ in the one-hole case.

The corresponding real-space form of Eq. (2.29) is

$$G_{\sigma}^\alpha(j,i;E) = -\pi \sum_{k} e^{-ik \cdot (x_j-x_i)} Z_k(E) \rho(E),$$

where $\rho(E) = \sum_{\delta} \delta(E - E_{\delta})$ is the density of states, and $Z_k(E)$ is understood here as being averaged over $M$ at the same energy $E_{M} = E$. If low-lying excitations can be classified as quasiparticle-like, one must have a finite spectral weight at the ground state and its vicinity. Correspondingly, $G_{\sigma}^\alpha$ should generally be finite when $E \rightarrow E_G$ from $E > E_G$ side in two dimensions. 16 On the other hand, $G_{\sigma}^\alpha \equiv 0$ at $E < E_G$.

The real part of $G_{\sigma}(k,E)$ in the real space can be expressed in terms of $G_{\sigma}^\alpha$ by the following Kramers-Kronig relation:

$$G_{\sigma}'(j,i;E) = -P \int \frac{dE'}{\pi} G_{\sigma}^\alpha(j,i;E') E - E'.$$

where $P$ denotes taking the principal value of the integral. It is straightforward to check that $G_{\sigma}'(j,i;E)$ diverges logarithmically at $E \rightarrow E_G$ if $G_{\sigma}^\alpha(j,i;E)$ remains finite at $E = E_G^+$:

$$G_{\sigma}'(j,i;E) \sim -\frac{1}{\pi} G_{\sigma}^\alpha(j,i;E_G) \ln|E-E_G|.$$

On the other hand, by using the spectral expression

$$G_{\sigma}(j,i;E+i0^+) = -\int \frac{dE'}{\pi} G_{\sigma}^\alpha(j,i;E') E - E' + i0^+,$$

one finds the analytic continuation of $G_{\sigma}(j,i;E)$ from the upper-half complex plane to the real axis at $E > E_G$ to be generally well-defined except at $E = E_G$.

Now we discuss the phase-string effect. For this purpose, we introduce the following quantities

$$G_{\sigma}^{\perp}(j,i;E) = -\langle \sigma \rangle^{-i} \sum_{\langle \text{paths} \rangle} W_{\text{path}}[\{ \vec{\phi} \}] \langle \delta_{\text{path}, \text{even}} \rangle,$$

with $\delta_{\text{path}, \text{even}} = 1$ if $N_{\text{path}}^\perp = \text{even}$ and $\delta_{\text{path}, \text{even}} = 0$ if $N_{\text{path}}^\perp = \text{odd}$. Similarly,

$$G_{\sigma}^{\parallel}(j,i;E) = -\langle \sigma \rangle^{-i} \sum_{\langle \text{paths} \rangle} W_{\text{path}}[\{ \vec{\phi} \}] \langle \delta_{\text{path}, \text{odd}} \rangle.$$

One may also define $G_{\sigma}^{\perp}(j,i;E)$ and $G_{\sigma}^{\parallel}(j,i;E)$ in a similar way. Physically, $G_{\sigma}^{\perp}$ and $G_{\sigma}^{\parallel}$ measure the weights for even or odd number of $\uparrow$ and $\downarrow$ spins encountered by the hole during its propagation from site $i$ to $j$. It is important to note that, according to their definition, $G_{\sigma}^{\perp}$ and $G_{\sigma}^{\parallel}$ should behave qualitatively similar in the case of a symmetric

system. $G_{\sigma}$ in Eq. (2.24) and $\tilde{G}_{\sigma}$ in Eq. (2.25) can be then rewritten as

$$G_{\sigma}(j,i;E) = G_{\sigma}^{\parallel}(j,i;E) - G_{\sigma}^{\perp}(j,i;E)$$

and

$$\tilde{G}_{\sigma}(j,i;E) = G_{\sigma}^{\parallel}(j,i;E) + G_{\sigma}^{\perp}(j,i;E).$$

Thus $G_{\sigma}^{\parallel}(E)$ and $G_{\sigma}^{\perp}(E)$ determine both $G_{\sigma}(E)$ and $
\tilde{G}_{\sigma}(E)$, and the phase-string effect is simply represented by a minus sign in front of $G_{\sigma}^{\perp}(E)$ in Eq. (2.37).

Here a crucial observation is that the ground-state energy $E_G$ of $H_{i,j}$ is always lower than the ground-state energy $E_G$ of $H_{i,j}$ since, according to the definition in Eq. (2.28), there is no sign problem in $H_{i,j}$. Suppose that the expansions (2.35) and (2.36) for $G_{\sigma}^{\perp}(E)$ and $G_{\sigma}^{\parallel}(E)$ converge below some energy $E_0$. By increasing $E$ the expansions (2.35) and (2.36) will eventually diverge at $E_0$ with the same sign because $W_{\text{path}} \geq 0$. Correspondingly $\tilde{G}_{\sigma}(E)$ also has to diverge at the same energy $E_0$ according to Eq. (2.38). It means that $E_0 = E_G$ as $\tilde{G}_{\sigma}(E)$ is analytic at $E < E_G$. In contrast, $G_{\sigma}(E)$ should be still well defined at $E_G$ (note that $E_G > E_G$). Thus the divergent parts in $G_{\sigma}^{\perp}(E_G)$ and $G_{\sigma}^{\parallel}(E_G)$ have to cancel out exactly in Eq. (2.37). This cancellation is easily understandable, since there is no qualitative difference between $G_{\sigma}^{\perp}(E)$ and $G_{\sigma}^{\parallel}(E)$. Note that the divergence in Eqs. (2.35) and (2.36) is contributed to by all of those paths connecting the fixed $i$ and $j$ whose lengths approach infinity. In this limit, the effects of the even or odd total number of $\downarrow$ spins on the hole’s path become indistinguishable.

But we are mainly interested in the behavior of $G_{\sigma}(E)$ near $E \rightarrow E_G$. According to the previous discussion, for a finite spectral weight $Z_k(E_G)$ the real part of $G_{\sigma}(E)$ has to diverge at $E = E_G$. On the other hand, the analytic continuation of $\tilde{G}_{\sigma}(E)$ to $E_G+i0^+$ should remain well defined in terms of the spectral expression similar to Eq. (2.34). In other words, if $Z_k(E_G) \neq 0$, one should find that $G_{\sigma}^{\perp}(E)$ and $G_{\sigma}^{\parallel}(E)$ (after an analytic continuation across the upper half plane to the real axis at $E \rightarrow E_G$) have to diverge again at $E = E_G$ in the following way:

$$G_{\sigma}^{\perp}(E_G) - G_{\sigma}^{\parallel}(E_G) \rightarrow \infty,$$

whereas

$$G_{\sigma}^{\perp}(E_G) + G_{\sigma}^{\parallel}(E_G) = \text{finite}.$$

However, this would mean that $G_{\sigma}^{\perp}(E_G)$ and $G_{\sigma}^{\parallel}(E_G)$ have to diverge with opposite signs, which is contrary to the intuitive observations [recall that both of them have the same sign at $E < E_G$ as defined in Eqs. (2.35) and (2.36) and diverge with the same sign at $E_G$ as discussed earlier on]. Such behavior also means a violation of spin symmetries of the system. Let us consider $G_{\sigma}^{\perp}$ and $G_{\sigma}^{\parallel}$ characterizing the contributions from $\uparrow$ spins, whose definitions are similar to Eqs. (2.35) and (2.36). Suppose that $i$ and $j$ belong to different sublattice sites. A simple counting then shows that $N_{\text{path}}^\perp + N_{\text{path}}^\parallel = \text{odd integer}$, and one finds that
$G_{\sigma}^{\uparrow}(E) = G_{\sigma}^{\downarrow}(E)$ and $G_{\sigma}^{\uparrow}(E) = G_{\sigma}^{\downarrow}(E)$. In terms of Eqs. (2.39) and (2.40), then, they should diverge with opposite signs too, namely, $G_{\sigma}^{\uparrow}(E) \rightarrow -\infty$ and $G_{\sigma}^{\downarrow}(E) \rightarrow -\infty$ at $E \rightarrow E_G$. However, according to their definitions, this indicates a violation of spin symmetries at $E \rightarrow E_G$, with contributions from $\uparrow$ and $\downarrow$ spins behaving drastically different in contrast to their symmetric definition at $E \approx E_G$. Therefore, one has to conclude that $G_{\sigma}^{\uparrow}(j; i; E)$ cannot diverge at $E_G$ due to the phase string effect, which indicates that the spectral weight $Z(E_G)$ has to vanish at low dimensions where the density of states $\rho(E) \neq 0$ at $E = E_G$.

The way that the phase-string effect leads to the vanishing of $Z(E_G)$ can be also intuitively understood in another way. Notice that the phase-string factor defined in Eq. (2.27) is quite singular as it changes sign each time when the total number $N_{\text{path}}$ increases or decreases by one, no matter how long the path is. But it would become meaningless to distinguish even and odd number of $\downarrow$ spins encountered by the hole when the path is infinitely long. Consequently, the average $\langle (-1)^{N_{\text{path}}^i} \rangle$ will vanish at $|i-j| \rightarrow \infty$, (since $(-1)^{N_{\text{path}}^i} = +1$ for even $N_{\text{path}}^i$ and $(-1)^{N_{\text{path}}^i} = -1$ for odd $N_{\text{path}}^i$ will have equal probability at this limit). Due to such phase-string frustration, the propagator (2.37) will always decay faster than a regular quasiparticle-like one (i.e., $\tilde{G}$) at large distance, and in particular, it has to keep decaying even at the ground-state energy $E_G$ which then requires a vanishing $Z(E)$ at $E = E_G$ as can be shown in terms of Eq. (2.31).

$Z(E_G) = 0$ means that there is no direct overlap between the “bare” hole state $c_i \psi_0$ and the true ground state. Thus the behavior of a hole injected into the undoped ground state is indeed dramatically modified by the phase-string effect, as compared to its quasiparticle-like bare-hole state. It implies the failure of a conventional perturbative approach to this problem which generally requires a zeroth-order overlap of the bare state with the true ground state. We would like to note that even though exact diagonalization calculations on small lattices$^{16}$ have indicated a quasiparticle peak at the energy bottom of the spectral function, when the lattice size goes to infinity, it is hard to tell from the small-size numerics whether such a quasiparticle peak would still stay at the lower end of the spectra or there could be some weight (e.g., a tail) emerging below the peak which vanishes at the ground-state energy [such that $Z(E_G) = 0$]. The present analysis suggests that the large-scale effect is really important in this system due to the phase-string effect. Therefore, finite-size numerical calculations as well as various analytical approaches should be under scrutiny with regard to the long-wavelength, low-energy properties.

Conditions (2.5) and (2.7) are crucially responsible for producing the nonrepairable phase-string effect in the above discussion. These are the intrinsic properties of the $t$-$J$ Hamiltonian itself. On the other hand, the condition that $|\psi_0\rangle$ is the ground state of the undoped antiferromagnet actually does not play a crucial role in the demonstration of $Z(E_G) = 0$. In other words, the whole argument about $Z(E_G) = 0$ should still remain robust even when $|\psi_0\rangle$ is replaced by a general ground state at finite doping. Of course, at finite doping some additional phase effect due to the fermionic statistics among holes will appear in the matrix (2.7), but such a sign problem should not invalidate the phase-string effect at least at small doping concentrations.

### III. Phase-String Effect at Finite Doping

The nonrepairable phase-string effect exhibited in the single-hole propagator (2.24) reveals a remarkable competition between the superexchange and hopping processes in the $t$-$J$ model. This effect leads to the breakdown of conventional perturbative methods as discussed in the one-hole case. We have also pointed out that such a phase-string effect is generally present even at finite doping. In this section, we will introduce a useful mathematical formalism to describe this effect in the presence of a finite amount of holes.

#### A. Phase-string effect and the Berry phase

The phase string is defined as a product of a sequence of signs

$$\begin{vmatrix} (\pm 1) \end{vmatrix} \times \begin{vmatrix} (\pm 1) \end{vmatrix} \times \cdots \begin{vmatrix} (\pm 1) \end{vmatrix} ,$$

where $(\pm 1) = \sigma_m$ is decided by the instant spin $\sigma_m$ at a site $m$ at the moment when the hole hops to that site. So the phase string depends on both the hole path as well as the instant spin configurations. As shown in the propagator (2.24), such a phase string is always picked up by the hopping of the hole from the quantum spin background. In particular, if the hole moves through a closed-path $C$ on the lattice back to its original position, it will get a phase $(-1)^{N_C}$, where $N_C$ is the total number of $\downarrow$ spins “encountered” by the hole on the closed path $C$. [It is noted that $(-1)^{N_C} = (-1)^{N_C}$ as a closed path $C$ always involves an even number of lattice sites. So there is no symmetry violation even though we will focus on $(-1)^{N_C}$ below.] If one lets the hole move slowly enough on the path $C$ such that the spin displacement created by its motion is able to relax back, then after the hole returns to its original position, the whole system will restore back to the original one except for an additional phase $(-1)^{N_C}$. Thus, the closed-path phase string $(-1)^{N_C}$ may be regarded as a Berry phase. Of course, here $(-1)^{N_C}$ is not simply a geometric phase which is only path-dependent, but also depends on the spin configurations along its path.

To keep track of such a Berry phase in the ground-state wave function, we may introduce the following quantity

$$e^{i\theta} = \exp \left( -i \sum_{i,l} \text{Im} \ln(z_i^{(h)} - z_i^{(b)}) \right),$$

where $z = x + iy$ with superscripts $(h)$ and $(b)$ refer to hole and $\downarrow$ spin, respectively, and the subscripts $i$ and $l$ denote their lattice sites. Here the definition is not restricted to the one-hole case, and $z_i^{(h)}$ is guaranteed by the no-double-occupancy constraint. Let us consider the evolution of $e^{i\theta}$ under a closed-loop motion for a given hole on the lattice. Recall that at each step of hole hopping, the spin originally located at the new hole site has to be transferred back to the original hole site. If it is a $\downarrow$ spin, then $\text{Im} \ln(z_i^{(h)} - z_i^{(b)})$ in Eq. (3.2) will give rise to a phase shift $\pm \pi$ due to such an “exchange” and thus a $(-1)$ factor in...
$e^{i\theta}$. After the hole returns to its original position through the closed-path $C$ and all the displacement of spins on the path is restored (which can be realized through spin flips as discussed before), one finds

$$e^{i\theta} \rightarrow (-1)^{N_1^h} \times e^{i\theta}. \quad (3.3)$$

(Each ↓ spin inside the closed-path $C$ contributes a phase $e^{\pm i2\pi} = 1$.) Thus, the phase factor $e^{i\theta}$ reproduces the aforementioned Berry phase due to the phase-string effect.

Therefore, it is natural to incorporate the phase factor $e^{i\theta}$ explicitly in the wave function to track the Berry phase, or define the following new spin-hole basis:

$$|\tilde{\phi}\rangle = e^{i\theta} |\phi\rangle, \quad (3.4)$$

where $e^{i\theta}$ is the operator form of $e^{i\theta}$ in Eq. (3.2):

$$e^{i\theta} = \exp \left[ -i \sum_{\ell} n^b_{\ell} \theta_{\ell}(l) n^\dagger_{\ell} \right], \quad (3.5)$$

in which $n^b_{\ell}$ and $n^\dagger_{\ell}$ are defined as the hole and ↓-spin occupation number operators, respectively, with $\theta_{\ell}(l)$ defined by

$$\theta_{\ell}(l) = \text{Im} \ln(z_{\ell} - z_{\ell}). \quad (3.6)$$

By using the no-double-occupancy constraint, one may also rewrite $n^b_{\ell}$ as $n^b_{\ell} = H[1 - n^b_{\ell} - \sum_\sigma \sigma n^\dagger_{\sigma \ell}]$ and thus express $e^{i\theta}$ in a symmetric form with regard to ↑ and ↓ spins:

$$e^{i\theta} = \exp \left[ -i \frac{1}{2} \sum_{\ell} n^b_{\ell} \theta_{\ell}(l) \left( 1 - n^b_{\ell} - \sum_\sigma \sigma n^\dagger_{\sigma \ell} \right) \right]. \quad (3.7)$$

According to previous discussions, this new basis should be more appropriate for expanding the true ground state $|\phi_G\rangle$ as well as the low-lying states because the hidden Berry phase due to the phase-string effect is explicitly tracked. In other words, the wave function $\tilde{\phi}$ defined in $|\phi_G\rangle = \sum_{\ell} \tilde{\phi}_{\ell} |\phi\rangle$ should become more or less “conventional” as the singular phase-string effect is now sorted out into $|\tilde{\phi}\rangle$. Correspondingly, the Hamiltonian in this new representation is expected to be perturbatively treatable as the phase-string effect is “gauged away” by the singular gauge transformation in Eq. (3.4). In the following section, we reformulate the $t$-$J$ model in this new representation for an arbitrary number of holes.

### B. “Phase-string” representation of the $t$-$J$ model

We start by generalizing the spin-hole basis (2.4) to an arbitrary hole number $N_h$ in the Schwinger-boson, slave-fermion representation:

$$|\phi\rangle = (-1)^{N_A} \{b_{11}^\dagger \cdots b_{M}^\dagger \} \{b_{M+1}^\dagger \cdots b_{N}^\dagger \} \times \{f_1^\dagger \cdots f_N^\dagger \} |0\rangle, \quad (3.8)$$

where $N_\alpha$ is the total electron (spin) number, and the fermionic “holon” creation operator $f_1^\dagger$ and the bosonic “spinon” annihilation operator $b_{\sigma \ell}$ commute with each other, satisfying the no-double-occupancy constraint

$$f_1^\dagger f_1 + \sum_\sigma b_{\sigma \ell}^\dagger b_{\sigma \ell} = 1. \quad (3.9)$$

The electron operator is written in this formalism as $c_{\sigma \ell} = f_{\sigma \ell} b_{\sigma \ell}$. Now if we redefine the spinon operator as $b_{\sigma \ell} \rightarrow (-\sigma)^i b_{\sigma \ell}$ such that

$$c_{\sigma \ell} = f_{\sigma \ell} b_{\sigma \ell} (-\sigma)^i, \quad (3.10)$$

then the Marshall sign in Eq. (3.8) can be absorbed into the spinon creation operators:

$$|\phi\rangle = (-1)^{N_A} \{b_{11}^\dagger \cdots b_{M}^\dagger \} \{b_{M+1}^\dagger \cdots b_{N}^\dagger \} \times \{f_1^\dagger \cdots f_N^\dagger \} |0\rangle, \quad (3.11)$$

with $(-1)^{N_A}$ being a trivial phase factor left for a later convenience (here $N_A$ denotes the total spin number on the $A$ sublattice site). In terms of Eq. (3.10), the superexchange term (2.1) in the $t$-$J$ model can be rewritten in the following form after using the no-double-occupancy constraint:

$$H_j = -J \sum_{(ij)\sigma\sigma'} b_{i\sigma}^\dagger b_{j\sigma'}^\dagger \sigma^\sigma. \quad (3.12)$$

It is easy to check that the matrix element $\langle \phi | H_j | \phi \rangle = 0$ for the basis defined in Eq. (3.11). Namely, the Marshall sign rule is explicitly built-in here. The hopping term $H_j$ in Eq. (2.6) becomes

$$H_j = -t \sum_{(ij)\sigma} (\sigma) f_{i\sigma}^\dagger f_{j\sigma}^\dagger b_{i\sigma} + \text{H.c.}, \quad (3.13)$$

where the spin index $\sigma$ describing the sign source generating the phase string in Eq. (3.1) is explicitly shown. Besides the sign source due to $\sigma$, the fermionic statistics of $f_{\sigma}$ in Eq. (3.13) at many-hole cases will also contribute a sign for each exchange of two fermions.

Now we introduce the new spin-hole basis (3.4) and (3.7). The phase-shift factor $e^{i\theta}$ in Eq. (3.7) can be regarded as a unitary transformation and any operator $\tilde{O}$ should be expressed in the new representation by a canonical transformation $\tilde{O} \rightarrow e^{i\theta} \tilde{O} e^{-i\theta}$. Then, the hopping term $H_j$ and the superexchange term $H_j$ of the $t$-$J$ model in the slave-fermion representation can be expressed under this transformation as follows:

$$H_j = -t \sum_{(ij)\sigma} \langle e^{i\theta} f_{i\sigma}^\dagger b_{j\sigma}^\dagger (e^{i\theta} f_{j\sigma}^\dagger) b_{i\sigma} + \text{H.c.} \rangle, \quad (3.14)$$

and

$$H_j = -\frac{J}{2} \sum_{(ij)\sigma\sigma'} \langle e^{i\theta} f_{i\sigma}^\dagger b_{j\sigma'}^\dagger (e^{i\theta} f_{j\sigma'}^\dagger) b_{i\sigma'} - \sigma. \quad (3.15)$$

in which gauge phases $A_{ij}^f$ and $A_{ij}^b$ are defined by

$$A_{ij}^f = \frac{1}{2} \sum_{\ell \neq i,j} \left[ \theta_{\ell}(l) - \theta_{\ell}(l) \right] \sum_{\sigma} \sigma n_{\sigma \ell}, \quad (3.16)$$

and

$$A_{ij}^b = \frac{1}{2} \sum_{\ell \neq i,j} \left[ \theta_{\ell}(l) - \theta_{\ell}(l) \right] n_{\ell}^b. \quad (3.17)$$
Here \( h_i \) is defined by

\[
h_i^\dagger = f_i^{\dagger} \exp \left[ -i \sum_{l \in C} \theta_l(l)n^b_{l \sigma} \right]. \tag{3.18}
\]

Equation (3.18) actually represents a Jordan-Wigner transformation\(^{18} \) which changes the fermionic statistics of \( f_i^\dagger \) into the bosonic operator \( h_i^\dagger \). So both \( h_i \) and \( b_{i \sigma} \) now are bosonic operators in this new representation. Note that the sign factor \( \sigma \) appearing in the slave-fermion formalism of \( H_f \) in Eq. (3.13) no longer shows up in Eq. (3.14), which means that the phase string is indeed “gauged away.” Nevertheless, one gets nonlocal gauge fields \( A_{ij}^f \) and \( A_{ij}^b \) in the new representation. In the one-dimensional case, \( A_{ij}^f = A_{ij}^b = 0 \) (see Sec. IV A), but they are nontrivial in two dimensions. For example, for a counterclockwise-direction closed-path \( C \) on a 2D lattice, one finds

\[
\sum_C A_{ij}^f = \pi \sum_{l \in C} \left( \sum_{\sigma} \sigma n^b_{l \sigma} - 1 \right) + \Sigma^f_C \tag{3.19}
\]

and

\[
\sum_C A_{ij}^b = \pi \sum_{l \in C} n^b_{l \sigma} + \Sigma^b_C, \tag{3.20}
\]

where the notation \( l \in C \) on the right-hand side means that the summations are over the sites inside the path \( C \), while \( \Sigma^f_C \) and \( \Sigma^b_C \) denote the contributions from the sites right on the path \( C \), the latter being different from those inside the path \( C \) by a numerical factor \( \frac{1}{2} \) or \( \frac{1}{4} \) depending on whether they are at the corner or along the edge of the closed path \( C \). Nonzero (3.19) and (3.20) show that \( A_{ij}^f \) and \( A_{ij}^b \), which cannot be gauged away in 2D, describe vortices (quantized flux tubes) centered on spinons [in fact, \( A_{ij}^f \) also includes an additional lattice \( \pi \) flux per plaquette as represented by the second term in the first summation on the right-hand side of Eq. (3.19)] and holons, respectively. Physically, this suggests the existence of nonlocal correlations between the charge and spin degrees of freedom in 2D. For instance, in \( H_J \) (3.15) spins can always feel the effect of holes nonlocally through the gauge field \( A_{ij}^b \). It is a direct consequence of the phase-string effect, which depends on both the hole path as well as the instant spin configurations on the path.

Furthermore, the slave-fermion decomposition of electron operator in Eq. (3.10) is transformed in terms of \( c_{i \sigma} \rightarrow e^{i \theta_i} c_{i \sigma} e^{-i \theta_i} \) as follows:\(^{19} \)

\[
c_{i \sigma} = h_i^\dagger \tilde{b}_{i \sigma} (-\sigma)^j, \tag{3.21}
\]

in which

\[
\tilde{b}_{i \sigma} = b_{i \sigma} \exp \left[ -i \frac{\sigma}{2} \sum_{l \neq i} \theta_l(l)n^b_{l \sigma} \right] \tag{3.22}
\]

and

\[
\tilde{h}_i^\dagger = h_i^\dagger \exp \left[ i \frac{1}{2} \sum_{l \neq i} \theta_l(l) \left( \sum_{\sigma} \sigma n^b_{l \sigma} - 1 \right) \right]. \tag{3.23}
\]

This new decomposition form is quite nonconventional as it involves nonlocal Jordan-Wigner-type phase factors in the “spinon” annihilation operator \( \tilde{b}_{i \sigma} \) and “holon” creation operator \( \tilde{h}_i^\dagger \). One can easily check that \( \tilde{b}_{i \sigma} \) and \( \tilde{h}_i^\dagger \) satisfy the following mutual statistics

\[
\tilde{b}_{i \sigma} \tilde{h}_j^\dagger = (\pm i \sigma) \tilde{h}_j^\dagger \tilde{b}_{i \sigma}, \tag{3.24}
\]

etc., for \( l \neq j \). Here signs \( \pm \) denote two different ways (clockwise and counterclockwise) by which the spinon and holon operators are exchanged. Because of the phase \( \pm i \), spinons and holons defined here obey “semion”-like mutual statistics, and \( \uparrow \) and \( \downarrow \) spinons show opposite signs in the commutation relation (3.24). Thus the present “phase-string” representation may also be properly regarded as a “mutual-statistics” decomposition. The physical origin of the mutual statistics may be understood based on the phase-string effect. As defined in Eq. (3.1), a phase-string factor changes when and only when hopping, i.e., an exchange of a spin and a hole, takes place. Thus, it can be described as a counting problem. One may keep track of such a phase string exactly by letting the hole and spin satisfy a mutual statistics relation, such that an exchange of a hole with a spin \( \sigma_m \) should produce an extra phase depending on \( \sigma_m \), as shown in Eq. (3.1). The role of the phase-string effect may be then regarded as to simply induce a mutual statistics between the spin and charge degrees of freedom. In this way, the phase string itself may be “gauged away” from the Hamiltonian, but at the price of dealing with a mutual statistics problem.

Furthermore, Eqs. (3.22) and (3.23) can be understood as composite-particle expressions\(^{11} \) for the mutual-statistics spimon and holon (\( \tilde{b}_{i \sigma} \) and \( \tilde{h}_i \)), in terms of conventional bosons (\( b_{i \sigma} \) and \( h_i \)) carrying flux tubes. In other words, we still work in a conventional bosonic representation of spinon and holon where the mutual statistics effect is transformed to an interaction problem, which is similar to a fractional-statistics system.\(^{11,12} \) This may be seen from the corresponding Hamiltonians of Eqs. (3.14) and (3.15) in the new representation, with the gauge fields \( A_{ij}^b \) and \( A_{ij}^b \) representing mutual statistics effect.

Therefore, after explicitly sorting out the phase-string effect, the \( t-J \) Hamiltonian is reformulated in Eqs. (3.14) and (3.15), where the original singular phase-string effect is “gauged away” in 1D, while its residual effect is represented by nonlocal gauge fields \( A_{ij}^b \) and \( A_{ij}^b \) in 2D. As far as long-distance physics is concerned, fluctuations of \( A_{ij}^b \) and \( A_{ij}^b \) are presumably small for \( (ij) \in \) the nearest neighbors, as compared to the original singular phase-string effect. Physically, this is due to the fact that only a quantum superposition effect of all the phase strings from different paths contributes to the energy, which behaves relatively “mildly” as described by \( A_{ij}^b \) and \( A_{ij}^b \). Then a generalized local mean-field-type approximation (examples are to be given in the next section) may become applicable to this new formalism. On the other hand, the singular part of the phase-string effect is now kept in the electron \( c \) operator expression (3.21). Thus, in drastic contrast to the conventional picture, the “test”’ particles created by physical operators (as combinations of the electron \( c \) operators) on the ground state will not simply “decay” into internal elementary charge and spin excitations (known as holons and spinons here). The nonlocal phase in the decomposition (3.21) will change their na-
ture in a fundamental way, as will be illustrated by the 1D example given below. The relation of “test” particles to internal elementary excitations in Fermi-liquid systems is completely changed here by the phase-string effect. Thus, knowing internal holon and spinon excitations no longer means that various electron correlation functions can be automatically determined, to leading order, from a simple convolution of their propagators.

IV. EXAMPLES

In the last section, a mathematical formalism was established for a general doping concentration, in which the phase-string effect was explicitly tracked. In the following we apply this formalism to some examples in both 1D and 2D which reveal highly nontrivial consequences of the phase-string effect in the low-energy, long-wavelength regime.

A. 1D example: Asymptotic correlation functions

It is well known that the Luttinger-liquid behavior exhibited in this 1D system is difficult to describe by conventional many-body theories. The success of the bosonization approach 20–24 to this problem relies heavily on the Bethe ansatz solution 25 of the model. An alternative path-integral approach 9 without using the Bethe ansatz solution can also provide a systematic understanding of the Luttinger-liquid behavior at $J \ll t$. In this latter approach, some U(1) nonlocal phase is found to play the key role. This nonlocal U(1) phase, which originated from the coupling of doped holes with the SU(2) spins, has been also shown to be related 25 to the Marshall sign hidden in the spin background, and is thus directly connected to the phase-string effect discussed in the present paper.

In this section, we use this 1D system as a nontrivial example and outline how the phase-string effect can straightforwardly lead to the correct leading-order Luttinger-liquid behavior of correlation functions, without involving a complicated mathematical description usually associated with this 1D problem.

Let us start with the decomposition (3.21). In the 1D case, $\theta_i(l)$ defined in Eq. (3.6) is reduced to

$$\theta_i(l) = \begin{cases} \pm \pi & \text{if } i < l, \\ 0 & \text{if } i > l. \end{cases}$$

(4.1)

According to Eqs. (3.22) and (3.23), the decomposition (3.21) can be then written as

$$c_{ia} = h_i^b b_{ia} e^{\pm i (\sigma \Theta^b_i + \Theta^h_i)},$$

(4.2)

where

$$\Theta^h_i = \frac{\pi}{2} \sum_{j \geq i} (1 - n_j^h),$$

(4.3)

and

$$\Theta^b_i = \frac{\pi}{2} \sum_{j > i, a} \alpha n_{ja}^b.$$  

(4.4)

[Note that in Eq. (4.2) a phase factor $(-\alpha)^{\frac{n_i}{2}}$ is omitted which can be easily shown to be equal to 1 for a bipartite lattice.]

In terms of Eq. (4.1), it is straightforward to show that $A^h_{ij} = A^b_{ij} = 0$, and thus Eqs. (3.14) and (3.15) reduce to

$$H_i = -t \sum_{i \neq j, \sigma} h_i^b h_j^b \gamma_{a\sigma} b_{ia} \gamma_{a\sigma} + \text{H.c.}$$

(4.5)

and

$$H_j = -\frac{J}{2} \sum_{i \neq j, \sigma, a} b^\dagger_{ia} b^\dagger_{ja} \gamma_{a\sigma} b_{ja} \gamma_{a\sigma}.$$  

(4.6)

Therefore, there is no sign problem (phase frustration) present in the Hamiltonian since both holon and spinon are bosonic here. All of the important phases are exactly tracked by the phase $e^{\pm i (\sigma \Theta^b_i + \Theta^h_i)}$ in the decomposition (4.2) which is the explicit expression for the nonlocal phase string in the 1D many-hole case. Without the presence of the nonlocal phase effect, a conventional mean-field type of approximation may become applicable to the Hamiltonians in the new representation. In the following we outline a simple mean-field theory for Eqs. (4.5) and (4.6).

One may rewrite Eq. (4.6) in the following form:

$$H_j = -\frac{J}{2} \sum_{i \neq j, \sigma, a} b^\dagger_{ia} b^\dagger_{ja} \gamma_{a\sigma} b_{ja} \gamma_{a\sigma},$$

(4.7)

after using $b^\dagger_{j-a} b_{j-a} = b_{j+a} b^\dagger_{j+a}$ at an occupied site $j$ where a hard-core condition of $(b_{j+a})^2 = 0$ is employed. Then by introducing the mean fields $\chi_0 = \frac{1}{2} \sum_{\sigma} \langle b^\dagger_{j+a} b_{j+a} \rangle$ and $H_0 = \langle h_i h_j \rangle$ with $i$ and $j$ being the nearest-neighbor sites, a mean-field version of the $t$-$J$ Hamiltonian $H_{\text{eff}} = H_h + H_s$ can be obtained with

$$H_h = -t_h \sum_{ij} h_i^b h_j + \text{H.c.},$$

(4.8)

and

$$H_s = -J_s \sum_{i \neq j, \sigma} b_{ia} b_{ja} + \text{H.c.},$$

(4.9)

with $t_h = 2t \chi_0$ and $J_s = J \chi_0 + tH_0$. Such a mean-field solution has been derived before (Ref. 12). A more accurate mean-field version may be obtained 9 with the same structure as in Eqs. (4.8) and (4.9), but the summation $\Sigma$ in $H_h$ now should be understood as over a “squeezed spin chain” defined by removing hole sites away at any given instant at $J \ll t$ limit. In this way the “hard-core” constraint between the holon and spinon can be automatically satisfied.

$H_h$ and $H_s$ are the tight-binding Hamiltonians for hard-core bosons which can be easily diagonalized. For example, one may introduce the Jordan-Wigner transformation

$$h_i = f_i \exp \left( \frac{\pi}{2} i \sum_{l > i} n_l^b \right).$$

(4.10)
where $f_i$ is a fermionic operator, and correspondingly $H_h$ becomes

$$H_h = -t_h \sum_{\langle i, j \rangle} f_i^\dagger f_j + \text{H.c.}, \quad (4.11)$$

which describes the tight-binding model of free fermions and can be diagonalized in the momentum space. The solution for $H_s$ is similarly known after using the Jordan-Wigner transformation $b_{i\sigma} = f_{i\sigma} \exp(\mp i \pi \sum_{\langle j, \alpha \rangle} a_{i\alpha}^\dagger)$. Thus, in principle one can use the decomposition (4.2) to determine various correlation functions.

Let us consider the single-electron Green's function

$$\langle c_{i_1}^\dagger(t) c_{i_1}(0) \rangle = \langle h_{j}(t) b_{j}^\dagger(t) e^{-i(\Theta^{(t)}_{i_1} + \Theta^{(t)}_{i_1})} e^{\mp i(\Theta^{(0)}_{i_1} + \Theta^{(0)}_{i_1})} b_{i_1}(0) h_{i_1}(0) \rangle = \langle h_{j}(t) e^{-i(\Theta^{(t)}_{i_1})} e^{\mp i(\Theta^{(0)}_{i_1})} h_{i_1}(0) \rangle \langle b_{j}^\dagger(t) e^{-i(\Theta^{(t)}_{i_1})} e^{\mp i(\Theta^{(0)}_{i_1})} b_{i_1}(0) \rangle,$$

where a spin-charge separation condition in the ground state of $H_{	ext{eff}} = H_h \mp H_s$ is used. Since both $H_h$ and $H_s$ can be expressed in terms of free-fermion solutions, one may use the bosonization * to describe the quantities involved on the right-hand side of Eq. (4.12) in the long-distance and long-time limit. For example, to leading order, one finds

$$\langle h_{j}(t) e^{-i(\Theta^{(t)}_{i_1})} e^{\mp i(\Theta^{(0)}_{i_1})} h_{i_1}(0) \rangle = \left\langle f_j(t) \exp \left( \mp i \frac{\pi}{2} \sum_{j \neq i} [1 + n_{i_1}^b(t)] \right) \exp \left( \pm i \frac{\pi}{2} \sum_{j \neq i} [1 + n_{i_1}^b(0)] \right) f_i^\dagger(0) \right\rangle \approx \frac{1}{(x \pm v_{\text{F}} t)^2} \exp \left( \mp i \frac{\pi}{2} \sum_{j \neq i} :n_{i_1}^b(t): \right) \exp \left( \pm i \frac{\pi}{2} \sum_{j \neq i} :n_{i_1}^b(0): \right),$$

where the normal ordering $:n_{i_1}^b:$ is defined as $n_{i_1}^b - \langle n_{i_1}^b \rangle$. The spinon part can be similarly evaluated based on the bosonization technique:

$$\langle b_{j}^\dagger(t) e^{-i(\Theta^{(t)}_{i_1})} e^{\mp i(\Theta^{(0)}_{i_1})} b_{i_1}(0) \rangle = \left\langle f_j^\dagger(t) \exp \left( \pm i \frac{\pi}{2} \sum_{j, \alpha} n_{i_1}^b(t) \right) \exp \left( \mp i \frac{\pi}{2} \sum_{j, \alpha} n_{i_1}^b(0) \right) f_i(0) \right\rangle \approx \frac{1}{(x \pm v_{\text{F}} t)^2} \exp \left( \pm i \frac{\pi}{2} \sum_{j, \alpha} :n_{i_1}^b(t): \right) \exp \left( \mp i \frac{\pi}{2} \sum_{j, \alpha} :n_{i_1}^b(0): \right),$$

which can be easily shown to give a momentum distribution near $k_f$ as

$$n(k) \sim n(k_f) - c |k - k_f|^{1/8} \text{sgn}(k - k_f). \quad (4.18)$$

The lack of a finite jump at $k = k_f$ implies the vanishing spectral weight, i.e., $Z(E) = 0$ at the Fermi points.

One may also calculate the asymptotic spin-spin correlation function. For example,

$$\langle S_j^-(t) S_i^- (0) \rangle = \langle b_{j}^\dagger(t) b_{i}^\dagger(0) b_i(0) b_{j}(0) \rangle \times \langle e^{-i2\Theta^{(t)}_{i_1}} e^{\mp i2\Theta^{(0)}_{i_1}} \rangle,$$

The averages on the right-hand side are also easily determined for the ground state of $H_{\text{eff}}$.
\[ \langle b_{\tau j}^+(t)b_{\tau j}(0)b_{\tau j}^+(t)b_{\tau j}(0) \rangle \approx \frac{1}{(x^2 - v_f^2 t^2)^{1/2}} \] (4.20)

and

\[ \langle e^{i2\theta^h_j(t)}e^{-i2\theta^h_j(0)} \rangle \approx \cos \left[ (\pi/2a)(1 - \delta)\chi \right] \frac{3}{(x^2 - v_f^2 t^2)^{1/2}}. \] (4.21)

As similar asymptotic form can be found for \( \langle S^+_\tau(t)S^-\tau(0) \rangle \) if the "squeezed spin chain" effect is considered. Then,

\[ \langle S^+_\tau(t)S^-\tau(0) \rangle \approx \cos(2k_F t) \frac{3}{(x^2 - v_F^2 t^2)^{1/2}}. \] (4.22)

Therefore, the well-known asymptotic behavior of the single-electron Green's function and the spin-spin correlation function at \( J \ll t \) is easily and correctly reproduced here. The phase-string contribution plays an essential role in Eqs. (4.12) and (4.19). A lesson which we can learn from this is that even though the decomposition (4.2) is mathematically equivalent to the conventional slave-fermion and slave-boson formalisms, it has the advantage of explicitly tracking the phase-string effect, so that such a nonlocal singular phase is not lost when one makes some mean-field-type approximation to the Hamiltonian. Such a phase-string effect is really crucial, due to its nonrepairable nature, to the long-time and long-distance Luttinger-liquid behavior studied here. Thus if one were to start from a conventional slave-particle scheme, a nonperturbative method beyond the mean-field theory must be employed in order to deal with the nonlocal phase-string effect hidden in the Hamiltonian. In contrast, in the present phase-string formulation, a mean-field-type treatment of the Hamiltonian gives reasonable results.

Finally, we make a remark about the physical meaning of the decomposition (4.2). For a usual slave-particle decomposition, the quantum number (momentum) of the electron is a simple sum of the momenta of "spinon" and "holon" constituents (due to the convolution relation). Here in the decomposition (4.2) the phase-string factor will "shift" the relation of the electron momentum to those of true spinon and holon excitations in a nontrivial way, which is actually equivalent to the information provided by the Bethe ansatz solution. In fact, Ren and Anderson\(^{22}\) have identified a similar effect (called a "phase shift" by them) based on the Bethe ansatz solution.

### B. 2D example: Nonlocal interactions

In the last section, the phase-string effect has been shown on the 1D example to modify the long-distance and long-time electron correlations in a dramatic way. The 1D system is special in that the phase string only appears in correlation functions through the decomposition (3.21), but it does not show any direct effect in the Hamiltonian. Namely, the phase-string effect can be "gauged away" in the Hamiltonian for an open-boundary 1D chain. This is consistent with the picture that spinon and holon as elementary excitations are decoupled, as indicated by either the exact solution\(^{29}\) or the analytic considerations in the \( J \to 0 \) limit.\(^{9}\) However, for a 2D system such phase-string effect can no longer be simply gauged away in the Hamiltonian. It is described by the lattice gauge fields \( A^s_{ij} \) and \( A^h_{ij} \) in the Hamiltonians (3.14) and (3.15), which are the Chern-Simons-type gauge fields satisfying conditions (3.19) and (3.20), respectively. Therefore, even if there exists a spin-charge separation in the 2D case, one still expects to see nonlocal interactions between the spin and charge degrees of freedom, which may lead to anomalous transport and magnetic phenomena.

In order to see the consequences of the gauge fields \( A^s_{ij} \) and \( A^h_{ij} \), let us consider a mean-field-type of approximation to \( H_s \) and \( H_c \) in Eqs. (3.14) and (3.15). This mean-field theory is similar to the one outlined above for the 1D case. But for the 2D case the mean-fields \( \chi_0 \) and \( H_0 \) should be defined with \( A^s_{ij} \) and \( A^h_{ij} \) incorporated as \( \chi_0 = \frac{\pi}{2} \sum_{\sigma}(e^{i\sigma A^h_{ij}}b^\dagger_{ij}b_{ij}) \) and \( H_0 = \langle e^{i\sum A^s_{ij}}b^\dagger_{ij}b_{ij} \rangle \). Correspondingly, the mean-field Hamiltonian \( H_{mf} = H_h + H_s \) can be obtained similarly to the 1D case (4.8) and (4.9) as follows:

\[ H_h = -t_2 \sum_{(ij)} (e^{iA^h_{ij}})h^\dagger_i h_j + \text{H.c.}, \] (4.23)

and

\[ H_s = -J \sum_{(ij)} (e^{i\sigma A^s_{ij}})b^\dagger_{i\sigma}b_{j\sigma} + \text{H.c.}. \] (4.24)

This mean-field solution has been previously obtained based on the slave-boson formalism,\(^{13}\) and the additional gauge fluctuations beyond the mean-field state can be shown\(^{13}\) to be suppressed (gapped) at finite doping, so that it is a real spin-charge separation state, even though there exist Chern-Simons (topological) fields \( A^s_{ij} \) and \( A^h_{ij} \) representing nonlocal scattering between the spin and charge degrees of freedom.

Let us first take a look at the charge degree of freedom. Due to the spin-charge separation (i.e., suppression of the gauge fluctuations), the charge response to external fields is entirely determined by the holon part described by \( H_h \). According to Eq. (4.23) as well as Eq. (3.19), holons always see fictitious flux tubes bound to spinons and quantized at \( \pm \pi \), besides a lattice \( \pi \)-flux per plaquette, as represented by \( A^s_{ij} \). It is important to note that the fluctuating part of \( A^s_{ij} \) not only provides a scattering source in the long wavelength, but also profoundly shapes the coherent motion of holons.\(^{13}\) The latter effect is caused by strong short-range phase interference induced by the \( \pm \pi \) flux quanta. This effect can be understood as the quantum interference of phase strings from different paths of holons. A semiclassical treatment of \( H_h \) has been given in Ref. 13, where the topological gauge field \( A^s_{ij} \) was shown to lead to anomalous transport phenomena including linear-temperature resistivity, a second scattering rate \( \sim T^2 \) in the Hall angle, a strong doping dependence of thermoelectric power, etc., which gives a systematic description of experimental measurements in the high-\( T_c \) cuprates.

The spin degree of freedom is also nontrivial here. As described by \( H_s \) in Eq. (4.24), spinons see similar fictitious flux tubes bound to holons as represented by \( A^h_{ij} \). It implies a strong frustration effect on the spin background induced by doping: each hole not only means a removal of a single spin, but also affects the rest of the spins nonlocally. This is a direct consequence of the nonlocal phase-string effect. Within this approximation, it has been found\(^{13}\) that the spin dynamics is dramatically affected by the doping effect, including the emergence of low-lying doping-dependent magnetic energy scales, non-Korringa behavior of the spin-lattice relaxation rate, etc., which qualitatively agrees with the
anomalies found in the nuclear-magnetic-resonance (NMR) and neutron-scattering measurements of the high-$T_c$ cuprates.

The above mean-field-type theory has been previously developed by using the slave-boson formalism. Here the phase-string effect and its corresponding formalism in Sec. III provide both physical and mathematical justifications for this approximate theory of the 2D $t$-$J$ model. Of course, a further improvement of the theory based on the exact formulation given in Sec. III is desirable. For example, the spin degree of freedom as described by the mean-field Hamiltonian $H_s$, is still rather rough for short-range correlations. In particular, at half-filling where the doping effect represented by $A^b_{ij}$ vanishes, $H_s$ in Eq. (4.24) reduces to a lattice model of a hard-core boson gas whose Bose condensation gives rise to the long-range AF order. However, an accurate description of the antiferromagnetism in the ground state involves a RVB-type pairing of bosonic spins, with the better mean-field solution at half-filling known as the Schwinger-boson mean-field state in which a pairing order parameter of spins is used to describe short-range spin-spin correlations. Based on the present formalism, it is not difficult to generalize the mean-field theory to incorporate such a short-range spin-spin correlation effect, which is important for quantitatively explaining the experiments. A brief description of such a generalization has been reported in Ref. 29, and a more detailed version will be presented in followup papers.

V. SUMMARY

In the present paper, we have reexamined the problem of a hole moving in an antiferromagnetic spin background and found rigorously that the hole always acquires a nontrivial phase string at low energy. This phase-string effect, particularly in 2D, has been overlooked before, but its quantum interference effect can drastically change the hole’s long-distance behavior. We have shown generally that the spectral weight must vanish at the ground-state energy due to such a phase string effect, which means that the conventional perturbative description based on a quasiparticle picture should fail at a sufficiently large distance in this system. The origin of this phase-string effect is related to the intrinsic competition between the superexchange and hopping processes. Namely, the hopping of the hole displaces the spins in such a way that the spin displacement (mismatch) cannot completely relax back via low-lying spin flips, and there is always a residual phase string left behind.

The phase-string effect is not uniquely restricted to the one-hole problem. It is also crucial at nonzero doping concentrations with or without a long-range order. The key issue is how one can mathematically describe the long-distance quantum effect of those phase strings associated with the doped holes. Such an effect is hidden in the conventional slave-boson formalism (as a kind of sign problem). And even though it shows up in a manifest way in the slave-fermion formalism after the Marshall sign rule is included, its topological role as a Berry phase at large distances is still not explicitly tracked in such a local model. Thus, any local approximation applied to those conventional formalisms can easily damage the presumably crucial long-distance phase-string effect and may result in a wrong physics in low-energy, long-wavelength regime.

As discussed in the present paper, the nonrepairable phase string on a closed path is equivalent to a Berry phase. It can be actually “counted” in terms of how many $\uparrow$ (or $\downarrow$) spins encountered by a given hole on its path. Thus such a Berry phase can be exactly tracked in the wave function. Then, based on a spin-hole basis with the built-in phase-string effect, we obtain a new mathematical formulation for the $t$-$J$ model, in which the originally hidden nonlocal phase-string effect is now explicitly represented in the Hamiltonian as interacting effects described by gauge fields with vorticities in the 2D case. On the other hand, a singular part of the phase-string effect is kept in the decomposition representation for the electron $c$ operator (i.e., in the wave functions) which is crucial when one tries to calculate electron correlation functions (as shown in the 1D example).

Another way to understand this new formulation is in terms of so-called “mutual statistics.” It has been pointed out that the phase-string effect as a “counting problem” can be also related to the “mutual statistics” between the charge and spin degrees of freedom, since each step of hole hopping may be regarded as an exchange of a hole and a spin. By using the composite representation of the “mutual statistics” holon and spinon in the conventional bosonic description, one can get the same formulation of the $t$-$J$ model in which the “mutual statistics” is described by long-range topological-type interactions (in 2D case) represented by nonlocal gauge fields. In contrast to the fractional statistics among the same species, though, no explicit $T$ and $P$ violations are present in this “mutual statistics” or phase-string description.

As an example, we have shown how the correct asymptotic behaviors of the single-electron Green’s function and spin-spin correlation function can be easily reproduced in the present scheme in the 1D finite doping case. The present phase-string formulation proves to be very powerful in dealing with this 1D problem, in contrast to difficulties associated with the conventional slave-particle formalisms. We have also discussed a 2D example by reproducing an approximate theory which gives a systematic description of the anomalous transport and magnetic properties in the high-$T_c$ cuprates. Such a theory was previously developed based on the slave-boson scheme with an optimization procedure (known as flux binding) at small doping, with the key mechanism being topological gauge-field interactions between spinons and holons. The present phase-string theory lays a solid foundation for such a mechanism, and provides a basis for the further improvement of the generalized mean-field theory and for a more quantitative comparison with the experiments. We will address these issues in followup papers.

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In a semiclassical description, the U(1) phase effect is represented by transverse spin components which exhibit a large-scale dipo larlike structure as discussed in Ref. 8.

A factor $e^{-i(1-\sigma)/2\pi N} = (\sigma)^{\pi/2}$ is omitted in Eq. (3.21) for simplicity, which has no physical effect except for maintaining anticommutation relation $\{ c_i, c_j \} = 0$ ($i \neq j$), etc., for opposite spins (Klein factor).

For a review, see E. Dagotto, Rev. Mod. Phys. 66, 763 (1994), and the references therein.


Z. Y. Weng, D. N. Sheng, Y.-C. Chen, and C. S. Ting, and the references therein.


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32. Here one should be cautious about some special cases where $\rho(E_\sigma) = 0$. For example, it occurs at a dimensionality higher than 2D for a parabolic quasiparticle spectrum, and in 2D for a massless Dirac spectrum $E_+$. 


41. Z. Y. Weng, D. N. Sheng, and C. S. Ting (unpublished).