Marshall sign and the doped $t - J$ model

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Abstract

Marshall sign as a sole source of sign problem hidden in an antiferromagnet is explored under doping. By tracking the Marshall sign, a zero spectral weight $Z = 0$ is revealed in the doped antiferromagnetic system. $Z = 0$ is caused by a phase string induced by the “bare” hole. By eliminating such a phase string through nonlocal transformations, a non-perturbative scheme is obtained. It is argued that this formalism provides a unique way to get access to the real ground state of the doped $t - J$ model for both one- and two-dimensions.

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According to Marshall, 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 any two antiparallel spins at nearest-neighboring sites always involves a sign change in the wave function: $\uparrow \downarrow \rightarrow (-1) \downarrow \uparrow$. Such a Marshall sign has played a crucial role in the success of two types of approximate approaches: the resonant-valence-bond (RVB)-type variational wavefunction proposed by Liang, Doucot and Anderson, which gives one of the lowest energy bound (-0.3344 J/per bond), and the Schwinger-boson mean-field state where the Marshall sign is incorporated in the order parameter $< \sum_{\sigma} \sigma \bar{b}_{i\sigma} \bar{b}_{j-\sigma} >$ ($i$ and $j$ are the nearest-neighboring sites).

Difficulty arises when one tries to dope holes into this antiferromagnet. Doped holes are expected to mess up with the Marshall sign, and the latter becomes a crucial source of sign problem hidden in the spin background. Doping effect is described by the well-known $t-J$ model as follows

$$H_{t-J} = J \sum_{<ij>} (\mathbf{S}_i \cdot \mathbf{S}_j - \frac{n_i n_j}{4}) - t \sum_{<ij>\sigma} (c_{i\sigma}^\dagger c_{j\sigma} + H.c.)$$

$$\equiv H_J + H_t.$$ (1)

in which the Hilbert space is restricted by the no-double-occupancy constraint $\sum_{\sigma} c_{i\sigma}^\dagger c_{i\sigma} \leq 1$.

At the zero-doping limit, $H_J$ recovers the antiferromagnetic Heisenberg model. The $t-J$ model has been intensively studied in recent years due to its widely perceived connection with the high-$T_c$ problem. But very limited understandings about this model have been achieved in two dimensions (2D) because of its strongly-correlated nature.

In this paper, we shall clarify the non-perturbative characteristics of the model in terms of the Marshall sign. A new representation is proposed in which the sign problem can be totally resolved in one dimension (1D), while partially eliminated in 2D with the residual phase problem tracked exactly through some topological phases. This non-perturbative approach provides an accurate way to understand long-wavelength physics of the $t-J$ model for both 1D and 2D.

The importance of keeping the Marshall sign in the undoped Heisenberg model may
be understood as follows: under a spin basis $|\phi> \rangle$ with the aforementioned Marshall sign included, the matrix element of the Heisenberg Hamiltonian becomes negative-definite, i.e., $<\phi'|H|\phi> \leq 0$. Then the ground state $|\psi_0> = \sum_\phi c_\phi |\phi> \rangle$ will always have real, positive coefficient (or wave-function) $c_\phi$. In other words, the Marshall sign is indeed the sole source of signs in the ground state, and there is no more sign problem in this new representation. Loosely speaking, physical properties will be less sensitive to various approximations here, which is the basic reason for the success of those approaches mentioned before.

The Marshall sign described above can be easily built into the $S^z$-spin representation even in the presence of holes. 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 holes are introduced into the system. Generally, the spin-hole basis may be defined as

$$|\phi> = i^{N^\downarrow_A + N^\uparrow_B} |\uparrow \cdots \downarrow \uparrow \cdots \downarrow >,$$

with $N^\downarrow_A$ and $N^\uparrow_B$ as total numbers of down and up spins at A- and B-sublattices, respectively. It is straightforward to verify that the matrix element

$$<\phi'|H_J|\phi> \leq 0,$$

under this new basis even in the presence of holes.

However, once the holes are allowed to move around, they will cause serious sign problem. For the sake of clarity, we first consider a single hole problem, where the statistics problem among holes is absent. Suppose the hole initially sitting at site $n$ hops onto a nearest-neighboring site $m$. The corresponding matrix element can be found to be

$$<\phi(n)|H_t|\phi(m)> = -t \times (\pm i),$$
where the subscripts \((n)\) and \((m)\) denote hole’s sites in the basis \((2)\), and \((\pm i)\) is determined by the original spin state \(\sigma_m = \pm 1\) at site \(m\):

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

(5)

where \((-1)^m\) is the staggered factor: \((-1)^A = +1\) and \((-1)^B = -1\). Thus a doped hole moving around will always leave a trace of phases (phase string) \((\pm i) \times (\pm i) \times \ldots\) behind it. This phase string cannot be eliminated through spin-flip process described by (3) since the latter does not produce extra “signs”. It implies that each doped hole always creates a phase string in the spin background which is not repairable at low energy, and thus it will determine the long-distance and long-time behaviors of the hole, as to be discussed below.

In the conventional approximations, this important effect has been overlooked because the Marshall sign is not properly tracked in the doping problem.

A bare doped hole is described by \(c_{i\sigma}|\psi_0\rangle\). One may follow the evolution of the doped hole by studying its propagator \(G_1(j, i; E) = \langle \psi_0 | c^\dagger_j \sigma (E - H)^{-1} c_{i\sigma} | \psi_0 \rangle\). By using the expansion

\[
G_1 = \langle \psi_0 | c^\dagger_j \sigma \left( G^J_0 + G^J_0 H J G^J_0 + \ldots \right) c_{i\sigma} | \psi_0 \rangle,
\]

(6)

where \(G^J_0 = (E - H_J)^{-1}\), one finds the contribution to each path, connecting \(i\) and \(j\), is weighted by a corresponding phase string \((\pm i) \times (\pm i) \times \ldots = \Pi_m i(-1)^m \sigma_m\) in terms of (4) and (5). The rest factors are found to be sign-definite since each term \(\langle \phi_{(m)} | G^J_0(E) | \phi_{(m)} \rangle\) \((m\) is a hole-site on the path) is always negative, shown by using the expansion \(G^J_0 = 1/E \sum_k (H_J/E)^k\) and the condition (3). (The expansion series is converged at least when \(E\) is less than the lower energy bound \(E^0_G\) of \(H_J\) (with a hole fixed at site \(m\))). Due to the accumulated effect, the phase string \((\pm i) \times (\pm i) \times \ldots\) can be straightforwardly shown to lead to a vanishing contribution for each given path beyond the spin-fluctuational correlation length, after being averaged over the various spin configurations. Thus the bare hole will lose its coherence as it cannot travel over a large distance. In turn, it means a vanishing spectral weight \(Z(E)\) (e.g., \(Z(E_G) = | \langle \psi | c_{k\sigma} | \psi_0 \rangle |^2\), etc., where \(|\psi\rangle\) and \(E_G\) are
the ground state and its energy, respectively) at least when \( E \to E_G \). A more rigorous demonstration of \( Z = 0 \) for a one-hole doping problem will be given in a separate paper.

In the above discussion, the Hamiltonian properties (3)-(5) is crucial in leading to \( Z = 0 \) for the one-hole case. It is easy to see that even at a sufficiently small doping, where the additional sign problem due to fermionic statistics among doped holes are not important, the conclusion of \( Z = 0 \) is still robust.

\( Z = 0 \) means that there is no overlap between \( c_{i\sigma} |\psi_0> \) and the ground state (and low-lying excitation states). Each doped hole will have to induce a global adjustment of the spin background in order to reach the ground state. So one may not be able to get access to the true ground state perturbatively by starting from \( c_{i\sigma} |\psi_0> \). But \( Z = 0 \) itself does not tell how the non-perturbative approach should be pursued. Thus we have to go back to the original source which causes \( Z = 0 \). In the present case, it is due to the phase string introduced by hole, which cannot be “repaired” by spin-flip process. One may regard this as a new sign problem associated with the hopping matrix element (4) under the spin-hole basis (2), where hole is treated as a “bare” one. It is then natural to ask if such a sign problem can be eliminated through some non-perturbative transformation.

**One-dimensional case.** For a single hole case, one may define the following modified spin-hole basis in terms of (2):

\[
|\tilde{\phi}(n)> = e^{i\Theta_n} |\phi(n)>,
\]

where \( n \) specifies the hole site, and

\[
\Theta_n = \frac{\pi}{4}[1 + (-1)^n] + \frac{1}{2} \sum_l \theta_n(l)(\sigma_l - 1).
\]

In (8), the summation runs over all the spin sites on the chain and \( \sigma_l = \pm 1 \) describes the spin state at \( l \) site. And \( \theta_n(l) \) may be defined as

\[
\theta_n(l) = \text{Im} \ln(z_n - z_l),
\]

where \( z_n = x_n + iy_n \) is a 2D complex coordinate and the 1D chain is sitting on the real axis. Then one has \( \theta_n(l) - \theta_l(n) = \pm \pi \). It is straightforward to verify that

\[
<\tilde{\phi}(m)|H_t|\tilde{\phi}(n)> = -t,
\]
while the matrix element for $H_J$ remains the same as (3). In the many-hole case, $\Theta_n$ in (4) should be replaced by a total phase-shift $\Theta = \sum_n'' \Theta_n$ (the summation is over the hole sites) in addition to a fermionic-statistics factor $e^{-i \sum_n'' \theta_{n'}(n')}$, and the conclusions remain the same.

Thus, the sign problem in 1D can be completely eliminated in the new representation, and the exact ground state expanded in terms of this basis always has real, positive-definite coefficient. According to (7), then, each hole induces a nonlocal phase-shift $\Theta_n$ in the true ground state. It represents a non-perturbative change of the system and is consistent with $Z = 0$ discussed before. We note that the phase-shift idea in 1D was first proposed by Anderson, and here its accurate form is simply obtained by tracking the Marshall sign.

It is interesting to express the original electron operator in this new representation. A bare hole created by $c_{i\sigma}$ will lead to a phase-shift $e^{-i\Theta_i}$ in the new representation. Furthermore, the original spin $\sigma$ at $i$ site has a phase $e^{i\pi/4(1-\sigma(-1))}$ (Eq.(2)) and a contribution to other holes $e^{i \sum_m \Theta_m \delta_{m(i)(\sigma-1)}^1}$. One may introduce a holon creation operator $h_i^\dagger$ and a spinon annihilation operator $b_{i\sigma}$ to keep the track of charge and spin in the new representation (both are bosonic operators), then the electron annihilation operator can be determined as (up to a global constant phase)

$$ c_{i\sigma} = h_i^\dagger b_{i\sigma} \left[ e^{i \frac{1}{2} \sum_{l \neq i} \theta_{l(i)}(\sigma n_l^h - \sum_{\alpha} \alpha n_{l\alpha}^b + 1)(-\sigma)^l} \right]. \tag{10} $$

$n_l^h$ and $n_{l\alpha}^b$ in (10) are holon and spinon number operators, satisfying the no-double-occupancy constraint $n_l^h + \sum_{\sigma} n_{l\sigma}^b = 1$. It is easy to verify that $\{c_{i\sigma}, c_{j\sigma}^\dagger\} = \delta_{i,j}$ and $\{c_{i\sigma}, c_{j\sigma}\} = 0$, but for opposite spins, $\{c_{i\sigma}, c_{j-\sigma}^\dagger\} = 0$. The latter result may be a little bit surprising but is physically correct. Even though the $t - J$ model is usually formulated in terms of $c_{i\sigma}$, which satisfies anti-commutation relations for both spins, it is easy to show that the commutation relations for electrons with opposite spins are not important and one may always assign either commutation or anti-commutation relations to them without changing the physical consequences.

Two-dimensional case. In 2D, a bare hole moving through any closed path back to
its origin will always leave a phase string if the path is not a retraceable one. It suggests that the phase problem in 2D become quite different from the 1D case. In a one-hole problem, one may still use the transformations (7)-(9) to eliminate the phase string induced by the hole. Actually, this procedure is the only way to eliminate the phase strings on all paths: the spins have to know the hole’s position nonlocally to adjust themselves. But in 2D one finds

\[ < \tilde{\phi}(m) | H_t | \tilde{\phi}(n) >_M = -te^{iA_{nm}^f}, \tag{11} \]

where a phase \( A_{nm}^f \) is contributed by all the spins on the lattice other than \( n \) and \( m \) sites:

\[ A_{nm}^f = \frac{1}{2} \sum_{l \neq n,m} (\theta_n(l) - \theta_m(l)) \left[ \sum_{\alpha} \alpha n_{l\alpha}^b - 1 \right]. \tag{12} \]

\( A_{nm}^f \) (it vanishes in 1D) satisfies the following topological condition

\[ \sum_C A_{nm}^f = \pi \sum_{l \in C} \left( \sum_\alpha \alpha n_{l\alpha}^b - 1 \right), \tag{13} \]

where the l.h.s. sum is over an arbitrary closed path \( C \) on the lattice, while the r.h.s. sum is over all the sites included by the path \( C \). Hence, instead of leaving a phase string, a hole in the new representation now sees fictitious fluxes enclosed after moving through a closed path. These fluxes are composed of fictitious \( \pi \)-flux quanta (pointing at \( \hat{z} \)-direction) bound to spins on the top of a uniform lattice \( \pi \)-flux. So \( A_{nm}^f \) cannot be simply gauged away in 2D. However, critically different from the afore-discussed singular phase string, those flux quanta generally would not prevent the hole to travel across the whole system or, in other words, one can have quasiparticle-like description of the hole (holon) in this new representation. A similar topological phase can be found in the matrix element of \( H_J \) (see below).

Generalization to the many-hole case is also similar to 1D. Since we have already introduced holon and spinon operators \( h_i \) and \( b_{i\sigma} \), it is more transparent to write down \( H_{t-J} \) in the new representation in operator formalism:

\[ H_J = -\frac{J}{2} \sum_{<ij>,\sigma\sigma'} (e^{i\sigma A_{ij}^h} b_{i\sigma}^+ b_{j\sigma'}) \left( e^{i\sigma' A_{ij}^h} b_{j\sigma'}^+ b_{i\sigma'} \right) + \frac{J}{2} \sum_{<ij>} (1 - n_{i\sigma}^h) n_{j\sigma}, \tag{14} \]
\[ H_t = -t \sum_{<ij>} \left( e^{iA_{ij}^h h_i^+ h_j} \right) \left( e^{i\sigma A_{ij}^h b_{j\sigma}^+ b_{i\sigma}} \right). \]  

(15)

\( A_{ij}^h \) in (14) and (13) satisfies the following topological condition

\[ \sum_C A_{ij}^h = \pi \sum_{l \in C} n_l^h. \]  

(16)

Equations (14) and (15), together with (10), represent an exact reformulation of the \( t - J \) model. More importantly, the ground state and low-lying states may become “perturbatively” accessible in this new representation in terms of new “particles” described by \( h \) and \( b_\sigma \). In 1D, the Hamiltonians (14) and (15) becomes “trivial” without the presence of sign problem \( (A_{ij}^f = A_{ij}^h = 0, \text{ and both } h \text{ and } b_\sigma \text{ are bosonic operators}) \). All the non-trivial information about the Luttinger-liquid behaviors is now included as “phase-shift” in the \( c_{i\sigma} \) operator expression (10). Crucial asymptotic correlations can be correctly obtained in this new framework even within conventional “mean-field-type” treatment of (14) and (15). Here \( h \) and \( b_\sigma \) naturally describes the quasiparticle-like \((Z_h, Z_s \neq 0)\) holon and spinon excitations, and thus the decomposition (10) represents a “correct” spin-charge separation.

Finite \( A_{ij}^f \) and \( A_{ij}^h \) in 2D mean that holes and spins have to “feel” each other nonlocally in order to eliminate singular phase strings created by the “bare” holes. Or vice versa, those phase strings’ superposition in a large-distance, long-time scale will lead to a delicate topological effect described by \( A_{ij}^f \) and \( A_{ij}^h \). Thus charge and spin degrees of freedom are intrinsically coupled together in 2D. For example, \( A_{ij}^f \) reflects doping effect on spin background. At the zero doping limit, \( A_{ij}^h \) vanishes in (14), and \( H_J \) reduces back to a similar form as in the Schwinger boson representation with the Marshall sign being absorbed. In the latter formalism, a mean-field treatment can yield a good approximation. But in the Schwinger-boson approach, the Marshall sign is usually incorporated in the order parameter \( <\sum_\sigma \sigma \bar{b}_{i\sigma} \bar{b}_{j-\sigma}> \). When new mean-field order-parameters are introduced at finite doping, there is no systematical way to keep the track of sign. By contrast, in the present representation, the whole essential phase at finite doping is exactly tracked by \( A_{ij}^h \) and \( A_{ij}^f \) in (14) and (13). Then any approximations leaving \( A_{ij}^h \) and \( A_{ij}^f \) intact should not dramatically
affect the phase problem which is presumably crucial for the long-wavelength, low-energy physics.

In fact, the same $A^h_{ij}$ and $A^f_{ij}$ as well as the decomposition (10) have been already identified from a different approach recently. $A^h_{ij}$ in 2D has been shown there to lead to the deconfinement of spinons in (14) and of spinon-holon in (15), and introduce a finite spin-spin correlation length in a fashion of $1/\sqrt{\delta}$ ($\delta$ is the doping concentration). An anomalous transport phenomenon induced by $A^f_{ij}$ has been also studied. The gapped transverse gauge fluctuation ensures the accuracy of the topological phases $A^h_{ij}$ and $A^f_{ij}$ in long-wavelength, low-energy regime. Therefore, like in 1D, one finds 2D spin-charge separation in this formalism, and $h$ and $b_\sigma$ properly describe the elementary charge and spin excitations (holon and spinon), respectively. Strong experimental features in association with the normal state of cuprates have been found in both spin and charge channels in this approach.\[11\]

Finally, we would like to briefly discuss the slave-boson formalism $c_{i\sigma} = h^\dagger_i f_{i\sigma}$. If one writes $S^+_i S^-_j = -(f^\dagger_i f_j, f^\dagger_j f_i)$, it seems that the Marshall sign is automatically preserved here. Nonetheless, extra phase problem is introduced by the fermionic operator $f_{i\sigma}$. It is reflected in, for instance, $< f^\dagger_{i\sigma} f_{j\sigma} > = \sum_k e^{ik \cdot (x_j - x_i)} < f^\dagger_k f_k >$ where a lot of $k$’s must be involved due to the Pauli-principal. Recall that a free fermion excitation in the bosonic representation would be described as a vortex, and vice versa. Then from the present point of review, at least close to the half-filling one cannot get access to the true ground-state "perturbatively" by starting with this formalism. It is also noted that at large doping, $A^h$ in the present scheme can even split, in terms of the no-double-occupancy constraint, such that to become the statistics-transmutation phases which can turn spinons into fermionic ones to recover the usual Fermi-liquid behavior.

In conclusion, by carefully examining the Marshall sign, we have shown that a doped hole will induce a string-like phase defect in the spin background. This phase string cannot be removed by low-lying spin fluctuations, and thus causes a vanishing quasiparticle spectral weight $Z$. A nonlocal transformation is found to eliminate such a phase string in both 1D and 2D. As a result, sign problem is totally resolved in 1D, while the residual sign problem
in 2D is kept tracked through some topological phases. This is a non-perturbative scheme with regard to the original electron description where a global phase shift is present due to the superposition of phase strings caused by doped holes. We argue that in this new representation the ground-state and low-lying states can be *perturbatively* approached, and thus provide a unique way to systematically understand the weakly-doped $t - J$ model. It also lends a crucial support and justification for a recent approach\textsuperscript{[1]} based on different physical principal, which exhibits exactly the same basic structure as in the present representation. The spin-charge separation is identified there for both 1 & 2D, and the magnetic and transport anomalies are found in striking similarities with the high-$T_c$ cuprates.

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