Doped carrier formulation of the *t-J* model: Projection constraint and the effective Kondo-Heisenberg lattice representation

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We show that the recently proposed doped carrier Hamiltonian formulation of the *t-J* model should be complemented with the constraint that projects out the unphysical states. With this important ingredient, the previously used and seemingly different spin-fermion representations of the *t-J* model are shown to be gauge related to each other. This constraint can be treated in a controlled way close to half-filling, suggesting that the doped carrier representation provides an appropriate theoretical framework to address the *t-J* model in this region. This constraint also suggests that the *t-J* model can be mapped onto a Kondo-Heisenberg lattice model. Such a mapping highlights important physical similarities between the quasi-two-dimensional heavy fermions and the high-T_c superconductors. Finally, we discuss the physical implications of our model representation relating, in particular, the small versus large Fermi surface crossover to the closure of the lattice spin gap.

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I. INTRODUCTION

The high-T_c superconductors continue to be a puzzle to most researchers in the field. Notably, in the underdoped regime, the cuprates display highly anomalous physical properties. Above the superconducting temperature, T_c, those lightly doped materials are characterized by a spin gap and, by what seemed until recently, disconnected Fermi arcs around preferential directions in momenta space.[1,2] This phase is widely referred to as the pseudogap state. That such disconnected arcs are indeed integrated into one coherent Fermi surface was recently demonstrated by the experiment of Doiron-Leyraud *et al.*[3] unfolding the quantum oscillations in the electrical resistance of $YBa_2Cu_3O_{6.5}$. The pseudogap phase is in this way associated with a small Fermi surface as opposed to the overdoped cuprates which exhibit large Fermi surfaces instead.[4] The evolution of the cuprate Fermi surface as a function of doping has been monitored by several angle-resolved photoemission spectroscopy (ARPES) experiments.[5,6] Such a process has also been the object of investigation in a number of renormalization group calculations.[7] Despite that, it is fair to say that a more qualitative physical understanding of this Fermi surface crossover in the cuprates is still lacking.

Ever since Anderson's suggestion that the high-T_c cuprates are driven by strong electron correlations,[8] the Hubbard model, or its large U version, the *t-J* model, has been the center of attention of theorists. Recently, two new representations in terms of dopant particles have been proposed[9–11] for the *t-J* model. In the Hamiltonian approach put forward by Ribeiro and Wen,[9,10] the original projected electron operators are replaced by spin-1/2 objects (called "lattice spins"), while the dopant particles are represented by fermions with spin 1/2 (called "dopons"). In the path-integral representation, the spin-dopon partition function of the *t-J* model has been used to formulate a resonating valence bond mean-field theory to describe the superconducting phase in the cobaltates.[11] The motivation behind these approaches is clear: since the concentration of dopons is small close to half-filling, the no double occupancy (NDO) constraint for the dopons can be safely relaxed in that regime.

However, in the description of electrons in terms of spins and dopons, special care should be taken to avoid the inclusion of unphysical states. As pointed out by Ferraz *et al.*[12] a constraint should be imposed to eliminate the unphysical states. Within the doped carrier representation, the conventional no double occupancy constraint for the lattice electrons reasserts itself as the constraint to eliminate the unphysical states in the enlarged spin-dopon Hilbert space. Basically, it reflects the completeness relation of the physical Hilbert space for the *t-J* model.

It is important to note that in the Hamiltonian doped carrier representation of the *t-J* model, the NDO constraint takes on a form which is, in a sense, dual to that of the original one in the physical lattice electron representation. The original local NDO constraint for the physical lattice electrons, $\Sigma_\sigma c_{i\sigma}^\dagger c_{i\sigma} \leqslant 1$, cannot be relaxed at half-filling (in fact, right at half-filling, it reads $\Sigma_\sigma c_{i\sigma}^\dagger c_{i\sigma}=1$), but it can be dropped safely at a large enough doping. In contrast, the other spin-dopon constraint can be treated in a controlled way close to half-filling (right at half-filling, this constraint becomes a trivial identity), whereas it cannot be safely relaxed in the overdoped region. Since the underdoped region of the cuprate phase diagram is of primary interest as was stressed earlier on, this doped carrier formulation of the *t-J* model, accompanied with the spin-dopon constraint, is quite interesting and appealing.

Within the spin-dopon representation, the strong electron correlation manifests itself in the constraint to exclude the unphysical states. It turns out that this constraint can be treated reliably at the mean-field level close to half-filing. This occurs at the expense of having a more complicated form of the t-J Hamiltonian in this representation.

The present paper demonstrates the significance of the constraint that excludes the unphysical states in the doped carrier approach from both the physical and the computational points of view. Specifically, we show that there is a certain gauge ambiguity in choosing a particular form of the unprojected t-J dopon-spin Hamiltonian in the enlarged Hilbert space. This ambiguity is related to a redundancy of the representation of the projected electron operators in terms of the lattice spins and dopons. This ambiguity is removed by projecting the gauge-dependent Hamiltonian onto the physical subspace: upon projection, all the gauge-related Hamiltonians result in one and the same physical representation. In this way, we show that the previously used and seemingly different spin-fermion representations of the t-J model are, in fact, related to each other by this projection.

The spin-dopon constraint corresponds to a Kondo-type interaction between the lattice spins and the dopons. The dopons play the role of the "conduction electrons," while the lattice spins play the role of the "localized magnetic moments." This approach allows for a mapping of the original t-J model onto a Kondo-Heisenberg lattice model, which indicates a strong relationship between the physics of high-T_c materials and that of some of the quasi-two-dimensional heavy-fermion systems (see Secs. III and IV). We also show that this constraint, in contrast to the standard NDO condition, can be treated in a controlled way within mean-field approximation.

Using our approach, the pseudogap phase can be simply interpreted as a state in which the lattice spins are paired, and the low density dopons are the quasiparticles solely responsible for generating the small Fermi surface. If the dopon concentration increases, so does the lattice spin-dopon coupling. As a result, in the normal state above T_c, there is a critical dopon concentration at which this coupling starts to dominate over the corresponding lattice spins self-interaction, finally breaking the remaining spin pairs. When this takes place, both spins and dopons integrate the large Fermi surface and the physical system crosses over to a metallic phase with no pseudogap behavior.

II. DOPED CARRIER REPRESENTATION

The t-J model Hamiltonian in terms of the Gutzwiller projected lattice electron operators takes the form

$$H_{tJ} = -\sum_{ij\sigma} t_{ij}\tilde{c}^{\dagger}_{i\sigma}\tilde{c}_{j\sigma} + J\sum_{ij}\left(\vec{Q}_i\cdot\vec{Q}_j - \frac{1}{4}\tilde{n}_i\tilde{n}_j\right), \tag{1}$$

where $\tilde{c}_{i\sigma}=c_{i\sigma}(1-n_{i,-\sigma})$ is the projected electron operator (to avoid the on-site double occupancy), $\vec{Q}_i=\Sigma_{\sigma,\sigma}\tilde{c}^{\dagger}_{i\sigma}\vec{\tau}_{\sigma\sigma}\tilde{c}_{i\sigma}$, $\vec{\tau}^2=3/4$, is the electron spin operator, and $\tilde{n}_i=n_{i\uparrow}+n_{i\downarrow}-2n_{i\uparrow}n_{i\downarrow}$.

Following Ribeiro and Wen, we consider an enlarged Hilbert space for each site i. This enlarged space is characterized by the state vectors $|\sigma a\rangle$, with $\sigma=\uparrow,\downarrow$ labeling the spin projection and $a=0,\uparrow,\downarrow$ labeling the dopon state (double occupancy is not allowed). In this way, the enlarged Hilbert space becomes

$$\mathcal{H}^{enl} = \{|\uparrow 0\rangle_i, |\downarrow 0\rangle_i, |\uparrow\downarrow\rangle_i, |\downarrow\uparrow\rangle_i, |\uparrow\uparrow\rangle_i, |\downarrow\downarrow\rangle_i\}, \tag{2}$$

while in the original Hilbert space, we can either have one electron with spin σ or a vacancy:

$$\mathcal{H} = \{|\uparrow\rangle_i, |\downarrow\rangle_i, |0\rangle_i\}. \tag{3}$$

The following mapping between the two spaces is then defined:

$$|\uparrow\rangle_i \leftrightarrow |\uparrow 0\rangle_i, \tag{4a}$$

$$|\downarrow\rangle_i \leftrightarrow |\downarrow 0\rangle_i, \tag{4b}$$

$$|0\rangle_i \leftrightarrow \frac{|\uparrow\downarrow\rangle_i - |\downarrow\uparrow\rangle_i}{\sqrt{2}}. \tag{4c}$$

The remaining states in the enlarged Hilbert space, $\frac{|\uparrow\downarrow\rangle_i+|\downarrow\uparrow\rangle_i}{\sqrt{2}}$, $|\uparrow\uparrow\rangle_i$, $|\downarrow\downarrow\rangle_i$, are unphysical and should be excluded in practical calculations. In this mapping, a vacancy in the electronic system corresponds to a singlet pair of a lattice spin and a dopon, whereas the presence of an electron is related to the absence of a dopon.

Let us call $\vec{S}_i$ the operator associated with the lattice spin on site i, and $d^{\dagger}_{i\sigma}$ the creation operator for dopons. Then under this mapping, it is not difficult to find relations between the original projected electronic operators and the new operators, such as

$$\tilde{c}_{i\uparrow} = \frac{1}{\sqrt{2}}[S^{+}_i S^{-}_i \tilde{d}^{\dagger}_{i\downarrow} - S^{-}_i \tilde{d}^{\dagger}_{i\uparrow}], \tag{5}$$

where $\tilde{d}_{i\sigma}=d_{i\sigma}(1-d^{\dagger}_{i,-\sigma}d_{i,-\sigma})$ is a projected dopon operator. Although $\vec{S}_i$ and $\tilde{d}_{i\sigma}$ act in the whole enlarged Hilbert space, specific combinations like the one given in Eq. (5) nullify the unphysical states. It is then possible to write the original t-J Hamiltonian in terms of the new operators in such a way that it vanishes when acting on the unphysical states.[10] The reason for this construction is now obvious: close to half-filling, there is a small amount of dopons in the system and, as a result, the local constraint of no double dopon occupancy can be safely dropped.

However, as soon as some mean-field approximations are performed, the unphysical states reappear in the theory *regardless of whether projected or unprojected dopon operators are used*. A constraint should, therefore, be imposed in order to eliminate the unphysical states. This constraint was proposed in Ref. 12 and it reads

$$\hat{\Upsilon}_i = \vec{S}_i\cdot\vec{M}_i + \frac{3}{4}(\tilde{d}^{\dagger}_{i\uparrow}\tilde{d}_{i\uparrow} + \tilde{d}^{\dagger}_{i\downarrow}\tilde{d}_{i\downarrow}) = 0, \tag{6}$$

where $\vec{M}_i=\Sigma_{\sigma,\sigma}\tilde{d}^{\dagger}_{i\sigma}\vec{\tau}_{\sigma\sigma}\tilde{d}_{i\sigma}$ is the spin associated with the dopon. Acting on the physical states, $\hat{\Upsilon}_i$ gives zero, while $\hat{\Upsilon}_i|\text{unphys}\rangle_i = |\text{unphys}\rangle_i$.

Since for spin 1/2, $\vec{S}_i^2=3/4$ and $\vec{M}_i^2=(3/4)\tilde{n}_i^d$, this constraint can also be recast into the form

$$\vec{J}_i^2 - 3/4(1-\tilde{n}_i^d)=0.$$

Here, $\vec{J}_i=\vec{M}_i+\vec{S}_i$ is the total spin on each lattice site. In this form, the constraint tells us that the on-site total spin can be either $j=0$ (vacancy) or $j=1/2$ (lattice spin).

There is a yet another representation of this constraint, namely,

$$\hat{\Upsilon}_i=-\frac{1}{2}D_i^\dagger D_i+\tilde{n}_i^d, \tag{7}$$

where $D_i^\dagger=f_{\uparrow i}^\dagger \tilde{d}_{\downarrow i}^\dagger - f_{\downarrow i}^\dagger \tilde{d}_{\uparrow i}^\dagger$ creates an on-site vacancy. Here, we represent the spin degrees of freedom in terms of chargeless fermions (spinons), $\vec{S}_i=f_i^\dagger \vec{\tau} f_i, f_i=(f_{\uparrow i}, f_{\downarrow i})^t$, and $f_i^\dagger f_i=1$. In this form, the constraint $\Sigma_i \hat{\Upsilon}=0$ tells us that the total number of vacancies must be equal to the total number of dopons.[13]

Right at half-filling ($\tilde{n}_i^d=0$), the spin-dopon constraint becomes a trivial identity, $0=0$. It can, thus, be safely treated close to half-filling at a mean-field level. In contrast, in the overdoped regime ($\tilde{n}_i^d \approx 1$), it reduces to the equation $\vec{S}_i \cdot \vec{M}_i \approx -3/4$. Exactly the opposite situation is realized for the lattice electron NDO constraint: it cannot be relaxed close to half-filling, but it can be totally ignored for a low enough density of the lattice electrons. It is precisely because of this that a different dopon-spin *t-J* model representation becomes, indeed, quite appealing.

It is convenient to define the operator $\hat{\mathcal{P}}_i=1-\hat{\Upsilon}_i$. Since $\hat{\Upsilon}_i^2=\hat{\Upsilon}_i$, it is clear that $\hat{\mathcal{P}}_i$ is a projection operator which eliminates unphysical states on the site i.[15] We show now that by means of this projection operator, we can, indeed, establish alternative ways of expressing the electron operators in terms of the lattice spins and dopons. Let us consider, for example, the action of $\tilde{d}_{i\downarrow}$ on the physical states—it is simply $\tilde{d}_{i\downarrow}|\uparrow 0\rangle_i=0$, $\tilde{d}_{i\downarrow}|\downarrow 0\rangle_i=0$, and $\tilde{d}_{i\downarrow}\frac{|\uparrow\downarrow\rangle_i-|\downarrow\uparrow\rangle_i}{\sqrt{2}}=\frac{|\uparrow 0\rangle_i}{\sqrt{2}}$. Clearly, in the physical subspace, this is equivalent to the action of $\tilde{c}_{i\uparrow}^\dagger/\sqrt{2}$. Thus, we can readily write

$$\tilde{c}_{i\uparrow}^\dagger=\sqrt{2}\hat{\mathcal{P}}_i \tilde{d}_{i\downarrow}\hat{\mathcal{P}}_i. \tag{8}$$

Alternatively, we can use the projection operator $\hat{\mathcal{P}}_i$ to perform explicit calculations, resulting in

$$\sqrt{2}\hat{\mathcal{P}}_i\tilde{d}_{i\downarrow}\hat{\mathcal{P}}_i=\frac{1}{\sqrt{2}}[S_i^+S_i^-\tilde{d}_{i\downarrow}-S_i^+\tilde{d}_{i\uparrow}],$$

which when combined with the adjoint of Eq. (5) results again in our Eq. (8). In the same way, one can show that

$$\tilde{c}_{i\downarrow}^\dagger=-\sqrt{2}\hat{\mathcal{P}}_i\tilde{d}_{i\uparrow}\hat{\mathcal{P}}_i. \tag{9}$$

Consider now the action of $S_i^+\tilde{d}_{i\uparrow}$ on the physical states, namely, $S_i^+\tilde{d}_{i\uparrow}|\uparrow 0\rangle_i=0$, $S_i^+\tilde{d}_{i\uparrow}|\downarrow 0\rangle_i=0$, and $S_i^+\tilde{d}_{i\uparrow}\frac{|\uparrow\downarrow\rangle_i-|\downarrow\uparrow\rangle_i}{\sqrt{2}}=-\frac{|\uparrow 0\rangle_i}{\sqrt{2}}$. Comparing with the action of $\tilde{c}_{i\uparrow}^\dagger/\sqrt{2}$ or carrying out the explicit calculations with the $\mathcal{P}$ projection, we get yet another operator identity:

$$\tilde{c}_{i\uparrow}^\dagger \equiv -\sqrt{2}\hat{\mathcal{P}}_i S_i^+\tilde{d}_{i\uparrow}\hat{\mathcal{P}}_i, \tag{10}$$

whereas from the action of $S_i^-\tilde{d}_{i\downarrow}$, we immediately find

$$\tilde{c}_{i\downarrow}^\dagger=\sqrt{2}\hat{\mathcal{P}}_i S_i^-\tilde{d}_{i\downarrow}\hat{\mathcal{P}}_i. \tag{11}$$

Note that a few attempts have also been made at decoupling the physical electron as the spinful fermion and spinon. However, they can only be justified within some approximation scheme (see, e.g., Ref. 16). In contrast, here we display the exact form of the spin-fermion decoupling of the projected lattice electron operator in Eqs. (10) and (11). In the next section, we show that the seemingly different representations for one and the same lattice electron operator [e.g., given by Eqs. (9) and (11)] are, in fact, identical since the $\mathcal{P}$ projections of gauge-related objects coincide with each other.

III. LOCAL GAUGE SYMMETRY

Let us now define the global projection operator $\hat{\mathcal{P}}=\Pi_i\hat{\mathcal{P}}_i$. The *t-J* Hamiltonian can be generally written as $H_{tJ}=\hat{\mathcal{P}}\tilde{H}\hat{\mathcal{P}}$, where $\tilde{H}$ acts on the enlarged Hilbert space. From the discussion above, it is clear that there are different choices of $\tilde{H}$ that after being projected onto the physical subspace result in the *t-J* model Hamiltonian. This is related to the gauge ambiguity of the unprojected $\tilde{H}$ with respect to the local U(1) gauge transformations generated by the constraint $\hat{\Upsilon}_i$. Under this transformation,

$$\begin{aligned}\tilde{d}_{\uparrow i} &\to \tilde{d}_{\uparrow i}(\theta_i)\\ &=\exp(-i\theta_i\hat{\Upsilon}_i)\tilde{d}_{\uparrow i}\exp(i\theta_i\hat{\Upsilon}_i)\\ &=\frac{1}{2}\left[S_i^-\tilde{d}_{\downarrow i}+\left(\frac{3}{2}+S_i^z\right)\tilde{d}_{\uparrow i}\right](e^{i\theta_i}-1)+\tilde{d}_{\uparrow i},\end{aligned} \tag{12}$$

$$\tilde{d}_{\downarrow i}(\theta_i)=\frac{1}{2}\left[S_i^+\tilde{d}_{\uparrow i}+\left(\frac{3}{2}-S_i^z\right)\tilde{d}_{\downarrow i}\right](e^{i\theta_i}-1)+\tilde{d}_{\downarrow i}. \tag{13}$$

The explicit form of the gauge-dependent operator $\vec{S}_i(\theta)$ is given by

$$\vec{S}_i(\theta_i)=[\vec{S}_i\times\vec{M}_i]\sin\theta_i+\frac{\vec{S}_i\tilde{n}_i^d-\vec{M}_i}{2}(\cos\theta_i-1)+\vec{S}_i. \tag{14}$$

Here, $\tilde{d}_{\sigma i}\equiv\tilde{d}_{\sigma i}(\theta=0)$ and $\vec{S}_i\equiv\vec{S}_i(\theta=0)$. The U(1) gauge symmetry is realized on the spin-dopon multiplet in a nontrivial way. Note also that the total on-site electron spin operator $\vec{J}_i=\vec{S}_i+\vec{M}_i$ as well as the dopon number operator are gauge invariant quantities, $\vec{J}_i(\theta)=\vec{J}_i(\theta=0)$ and $\tilde{n}_i^d(\theta)=\tilde{n}_i^d(\theta=0)$.

The $\hat{\mathcal{P}}$ projection of the different gauge equivalent operators results in the same gauge invariant representation. For instance, for any polynomial on-site operator $\hat{f}_i=\hat{f}_i(\tilde{d}_{\sigma i}, S_i)$, we get

$$\hat{\mathcal{P}}_i \hat{f}_i(\theta)\hat{\mathcal{P}}_i = \hat{\mathcal{P}}_i \exp(-i\theta_i \hat{\Upsilon}_i)\hat{f}_i \exp(i\theta_i \hat{\Upsilon}_i)\hat{\mathcal{P}}_i$$
$$= \hat{\mathcal{P}}_i[1 + \hat{\mathcal{P}}_i(e^{i\theta_i} - 1)]\hat{f}_i[1 + \hat{\mathcal{P}}_i(e^{-i\theta_i} - 1)]\hat{\mathcal{P}}_i$$
$$= \hat{\mathcal{P}}_i \hat{f}_i \hat{\mathcal{P}}_i.$$

In this way, the representation (11) follows from the equations

$$\hat{\mathcal{P}}_i \tilde{d}_{\uparrow i}\hat{\mathcal{P}}_i = \hat{\mathcal{P}}_i \tilde{d}_{\uparrow i}(\theta = \pi)\hat{\mathcal{P}}_i$$
$$= -\hat{\mathcal{P}}_i(S_i^- \tilde{d}_{\downarrow i})\hat{\mathcal{P}}_i$$
$$= \frac{1}{2}[S_i^- S_i^+ \tilde{d}_{i\uparrow} - S_i^- \tilde{d}_{i\downarrow}].$$

Notice that, in general,

$$\hat{\mathcal{P}} \sum_{ij\sigma} t_{ij} \tilde{d}_{i\sigma}^\dagger(\theta_i)\tilde{d}_{j\sigma}(\theta_j)\hat{\mathcal{P}} = \hat{\mathcal{P}} \sum_{ij\sigma} t_{ij} \tilde{d}_{i\sigma}^\dagger \tilde{d}_{j\sigma}\hat{\mathcal{P}}.$$

It can also be checked by an explicit computation that the projected electron operators, e.g., the ones given by Eqs. (8)–(11) are all gauge invariant objects. In analogy with the gauge theories from quantum field theory, we can say that essentially the choice of a given representation for $\tilde{H}$ corresponds to the fixing of a particular gauge.

The existence of the local gauge symmetry reflects a degree of redundancy in the parametrization of the Gutzwiller projected lattice electrons in terms of the lattice spins and dopons, as displayed in our Eq. (5). In principle, one can formulate a mean-field theory in this representation that respects the local U(1) gauge symmetry. In this way, one arrives at a local gauge theory that describes quantum fluctuations around the mean-field solution.

It should be kept in mind that the lattice spins and dopons are, in general, not gauge invariant and couple to the gauge field. Because of this, the dopons and lattice spins, away from half-filling, do not represent real excitations and they are introduced as an intermediate step to calculate the physical (gauge invariant) quantities such as given, e.g., by Eqs. (5) and (8)–(11). Note, however, that right at half-filling, $\vec{S}_i \rightarrow \vec{S}_i$. In other words, the lattice spins represent, in this limit, real excitations. It is, therefore, natural to assume that close to half-filling, the lattice spins and dopons can be viewed as well-defined excitations weakly coupled to the gauge field. This indicates that the mean-field spin-dopon theory[17] is presumably stable close to half-filling with respect to quantum gauge fluctuations. However, an explicit estimation of the strength of the gauge interaction can be made only after the full gauge theory is derived. The explicit form of that theory is still not available because of a rather complicated form of the U(1) group action on the spin-dopon multipletes [see Eqs. (12)–(14)].

To make this point clearer, let us contrast the properties of the gauge symmetry generated by $\hat{\Upsilon}_i$ with those of the U(1) local gauge symmetry generated by the standard NDO constraint in the frequently used slave-boson representation for the lattice electron operators. With this formalism, the projected electron operator is written as

$$\tilde{c}_{i\sigma}^\dagger = f_{i\sigma}^\dagger b_i, \tag{15}$$

with the NDO condition

$$\hat{Q}_i := \sum_\sigma f_{i\sigma}^\dagger f_{i\sigma} + b_i^\dagger b_i = 1,$$

where $f_{i\sigma}$ is a fermion (spinon) operator and b_i is a slave-boson (holon) operator. Conservation of the gauge charge $\hat{Q}_i$ can be derived by the Noether theorem starting from the local U(1) gauge transformation,[18]

$$f_{i\sigma} \rightarrow e^{i\theta_i} f_{i\sigma}, \quad b_i \rightarrow e^{i\theta_i} b_i, \tag{16}$$

which leaves the physical electron operator (15) intact. This U(1) local gauge symmetry takes care of the redundancy of the parametrization (15). In contrast to the spin-dopon charge $\hat{\Upsilon}_i$, the operator $\hat{Q}_i$ does not vanish at half-filling, $\hat{Q}_i \rightarrow \hat{Q}_i^{hf} = \Sigma_\sigma f_{i\sigma}^\dagger f_{i\sigma}$. This indicates that the spinons are strongly coupled to the bare gauge field close to half-filling. However, the auxiliary gauge field can, in general, acquire nontrivial dynamics at low energies, effectively moving the model to a weak coupling regime. Therefore, to judge whether confinement or deconfinement of slave particles really occurs in the physical low-energy excitations, one must explicitly investigate the gauge dynamics in the low-energy regime.[19]

Note also that in contrast to the NDO constraint for the lattice electrons, the set of local constraints $\hat{\Upsilon}_i = 0$ (one for each lattice site) can be replaced by the global condition $\hat{\Upsilon} = \Sigma_i \hat{\Upsilon}_i = 0$. The reason for this simplification is that the unphysical states appear as the degenerate eigenvectors of $\hat{\Upsilon}_i$ with an eigenvalue, 1. Therefore, acting on an unphysical state, $\hat{\Upsilon}$ simply produces the same state multiplied by a positive number. Acting on a physical state, $\hat{\Upsilon}$ always gives zero. Note, however, that $\hat{\Upsilon}_i$ involves a quartic power of interacting dopons and spins. The standard NDO constraint appears as a quadratic form of the electron operators. We will comment on this point further at the end of the paper.

Summing up all the above, we can write down the exact form of the *t-J* Hamiltonian in the spin-dopon representation as

$$H_{tJ} = \hat{\mathcal{P}} \sum_{ij\sigma} 2t_{ij} \tilde{d}_{i\sigma}^\dagger \tilde{d}_{j\sigma}\hat{\mathcal{P}} + J \sum_{ij} \hat{\mathcal{P}} \Big((\vec{S}_i + \vec{M}_i)(\vec{S}_j + \vec{M}_j)$$
$$- \frac{1}{4}(1 - \tilde{n}_i^d)(1 - \tilde{n}_j^d) \Big) \hat{\mathcal{P}}. \tag{17}$$

Within the path-integral approach, this representation has been used in Ref. 11 to obtain the mean-field T_c phase diagram for the cobaltates. The exact spin-dopon path-integral representation of the *t-J* partition function given in Ref. 11 is written down in terms of the classical fermion amplitudes $\psi_{i\sigma}$, which are related to the dopon amplitudes in the following way: $\psi_i = \frac{1}{\sqrt{2}}\left(\frac{1}{2} - 2\vec{S}_i^{cl}\vec{\tau}\right)\tilde{d}_i^{cl} = \sqrt{2}(\hat{\mathcal{P}}_i \tilde{d}_i \hat{\mathcal{P}}_i)^{cl}$. This relation holds provided $\Upsilon_i^{cl} = 0$. Note that in this case $(n_i^\psi)^{cl} = (\tilde{n}_i^d)^{cl}$. Within that path-integral approach, the constraint to exclude the unphysical states reasserts itself in the form of the SU(2)

invariant site product of the delta functions that singles out the physical subspace.

Since $\vec{Q}_i=\hat{\mathcal{P}}_i(\vec{S}_i+\vec{M}_i)\hat{\mathcal{P}}_i=\vec{S}_i(1-\tilde{d}^{\dagger}_{i\sigma}\tilde{d}_{i\sigma})$ and $\hat{\mathcal{P}}_i(1-\tilde{d}^{\dagger}_{i\sigma}\tilde{d}_{i\sigma})\hat{\mathcal{P}}_i=(1-\tilde{d}^{\dagger}_{i\sigma}\tilde{d}_{i\sigma})$, we can rewrite Eq. (17) in the form

$$H_{tJ}=\hat{\mathcal{P}}\sum_{ij\sigma}2t_{ij}\tilde{d}^{\dagger}_{i\sigma}\tilde{d}_{j\sigma}\hat{\mathcal{P}}+J\sum_{ij}\left(\vec{S}_i\cdot\vec{S}_j-\frac{1}{4}\right)(1-\tilde{n}^d_i)(1-\tilde{n}^d_j). \tag{18}$$

Note the important factor of 2 in front of the t term in these formulas. It originates from the fact that the vacancies are represented in this theory by the spin-dopon singlets given by Eq. (4c).

The $\hat{\mathcal{P}}$-projected dopons describe the physical doped carriers. Calculating explicitly the $\hat{\mathcal{P}}$-projected dopon operators, we get

$$H_{tJ}=\sum_{ij\sigma}\frac{t_{ij}}{2}\tilde{d}^{\dagger}_i\left(\frac{1}{2}-2\vec{S}_i\vec{\tau}\right)\left(\frac{1}{2}-2\vec{S}_j\vec{\tau}\right)\tilde{d}_j+J\sum_{ij}\left(\vec{S}_i\cdot\vec{S}_j-\frac{1}{4}\right)(1-\tilde{n}^d_i)(1-\tilde{n}^d_j). \tag{19}$$

The representation (19) has been used by Ribeiro and Wen within the mean-field approximation. However, they oversimplified the magnetic term in the following way:

$$J\sum_{ij}\left(\vec{S}_i\cdot\vec{S}_j-\frac{1}{4}\right)(1-\tilde{n}^d_i)(1-\tilde{n}^d_j)\rightarrow\tilde{J}\sum_{ij}\left(\vec{S}_i\cdot\vec{S}_j-\frac{1}{4}\right), \tag{20}$$

where $\tilde{J}=J(1-x)^2$ and x is a density of dopons. It is clear that the representation (20) totally ignores the dynamically induced doping changes in the underlying spin correlations. The authors instead introduce phenomenological x-dependent hopping parameters to take into account the feedback of the dopons on the spin dynamics. To take into account the actual J dependent spin-dopon interaction, one should use the constraint $\hat{\Upsilon}_i=0$. It is satisfied provided $\vec{M}_i+\tilde{n}_i\vec{S}_i=0$. This yields (up to unessential constant factors)

$$H_{tJ}=\sum_{ij\sigma}\frac{t_{ij}}{2}\tilde{d}^{\dagger}_i\left(\frac{1}{2}-2\vec{S}_i\vec{\tau}\right)\left(\frac{1}{2}-2\vec{S}_j\vec{\tau}\right)\tilde{d}_j+J\sum_{ij}\left[\left(\vec{S}_i\cdot\vec{S}_j-\frac{1}{4}\right)+(\vec{S}_i\vec{M}_j+\vec{S}_j\vec{M}_i)+\left(\vec{M}_i\vec{M}_j-\frac{\tilde{n}_i\tilde{n}_j}{4}\right)\right]. \tag{21}$$

The magnetic term in this representation explicitly accounts for the spin-dopon interaction as produced by the magnetic moment-moment interactions. In general, it is the representation (21) that should be used as a starting point to apply a mean-field approximation. In this way, a complete dynamical mean-field phase diagram to describe hole and/or electron doped cuprates emerges in contrast to the semiphenomenological one previously derived.[9,10]

Close to half-filling, an alternative way of dealing with the constraint can be proposed. First, we can drop the projection operator and add the constraint with an appropriate Lagrange multiplier. That is, we now write

$$H_{tJ}=\sum_{ij\sigma}2t_{ij}\tilde{d}^{\dagger}_{i\sigma}\tilde{d}_{j\sigma}+J\sum_{ij}\left(\vec{S}_i\cdot\vec{S}_j-\frac{1}{4}\right)(1-\tilde{n}^d_i)(1-\tilde{n}^d_j)+\lambda\hat{\Upsilon}, \tag{22}$$

where λ is to be sent to $+\infty$ at the end of calculations. Second, since the dynamics is now restricted to the physical subspace, we can, close to half-filling, make the change $J\rightarrow\tilde{J}$ to get

$$H_{tJ}=\sum_{ij\sigma}2t_{ij}d^{\dagger}_{i\sigma}d_{j\sigma}+\tilde{J}\sum_{ij}\left(\vec{S}_i\cdot\vec{S}_j-\frac{1}{4}\right)+\lambda\hat{\Upsilon}. \tag{23}$$

By writing the Hamiltonian in this way, we see the decisive role played by the constraint which incorporates the interaction between dopons and lattice spins, while the nonconstrained Hamiltonian simply corresponds to noninteracting dopons and lattice spins.

The large-λ limit eliminates unphysical states with the total spin $j=1$ and, at the same time, dynamically generates a vacancy on a lattice site in the form of a spin-dopon singlet.[12] An analogy of this result can be drawn with the dynamical formation of the Zhang-Rice singlet produced by the hybridization effects that strongly bind a hole and a Cu^{2+} ion together to form a local singlet state associated with such a vacancy.[20] The important point here being again the fact that such an empty site (vacancy) can be physically interpreted as a spin singlet.

We now introduce the chemical potential for dopons and use the explicit representation of the constraint, Eq. (6), to get the Hamiltonian:

$$H_{tJ}=\sum_{ij\sigma}t^{\mathrm{eff}}_{ij}d^{\dagger}_{i\sigma}d_{j\sigma}+\tilde{J}\sum_{ij}\left(\vec{S}_i\cdot\vec{S}_j-\frac{1}{4}\right)+\lambda\sum_i\vec{S}_i\cdot\vec{M}_i, \tag{24}$$

where $t^{\mathrm{eff}}_{ij}=2t_{ij}+\left(\frac{3}{4}\lambda-\mu\right)\delta_{ij}$. The parameter λ must be sent to $+\infty$ at the end of calculations.[21–24]

Finally, we can safely treat the constraint close to half-filling at the mean-field level. In this case, λ is determined self-consistently from the ground-state average

$$\left\langle\sum_i\left(\vec{S}_i\cdot\vec{M}_i+\frac{3}{4}\tilde{n}_i\right)\right\rangle=0$$

and becomes doping dependent. The mean-field Hamiltonian obtained in this way is that of a Kondo-Heisenberg lattice problem, where the lattice spins play the role of localized magnetic moments, while the dopons take the role of conduction electrons.

In order to take into account a possible hybridization between the localized spins and the dopons,[28] one should use the following form of the constraint:

$$\left\langle-\frac{1}{2}\sum_i D^{\dagger}_iD_i+\sum_i\tilde{n}^d_i\right\rangle=0.$$

The relevant order parameter takes the form $\sigma:=\langle D\rangle$, where we have linearized the on-site operator product in the averaged constraint in the following way: $D^{\dagger}_iD_i\approx D^{\dagger}_i\langle D\rangle+\langle D^{\dagger}\rangle D_i-\langle D^{\dagger}\rangle\langle D\rangle$. This procedure preserves the SU(2) sym-

metry, which must be present in the underdoped phase. Since $\sigma \propto \sqrt{x}$, the error produced by this simplification is at most of order $\mathcal{O}(x), x \to 0$, which does not affect the results quantitatively in that regime. The breakdown of the Kondo regime implies then $\sigma = 0$.

IV. PHYSICAL IMPLICATIONS

In the previous section, we showed that the t-J model can be mapped onto a Kondo-Heisenberg model for dopons and lattice spins. In this section, we explore some immediate physical implications of that mapping, leaving a more detailed analysis to a future work.

The Kondo-Heisenberg lattice model has attracted much attention in the context of heavy-fermion systems.[25–28] It is believed that a variety of physical phenomena could be accounted for by that model, such as non-Fermi-liquid behavior, different types of magnetic and charge orderings, and perhaps unconventional superconductivity.[29]

In fact, recent experiments have revealed striking similarities between quasi-two-dimensional heavy-fermion systems (the CeMIn$_5$ family) and the high-T_c cuprates.[30–32] The mapping discussed in the last section suggests that these similarities could be accounted for by the fact that both quasi-two-dimensional heavy fermions and high-T_c cuprates capture universal features of strongly correlated electron systems in the presence of strong antiferromagnetic (AF) correlations.

Our mapping reinforces earlier suggestions of a common magnetically mediated mechanism for superconductivity in heavy-fermion compounds and in the cuprates.[33,34] In this way, the superconductivity in the cuprates can be directly associated with the pairing of dopons induced by the Kondo-like interaction with the lattice spins. However, if this is indeed the case, a crucial question arises naturally: why are the critical superconducting transition temperatures observed in heavy fermions (low T_c) and cuprates (high T_c) so different from each other? Our explanation for that is signalled by the different charge carrier mass renormalizations and the typical coupling constant magnitudes in those two referred systems. Suppose the critical superconducting temperature is given generically by $T_c = \Delta \exp(-cm^*/\lambda)$, where c is a constant, m^* is the charge carrier effective mass, λ is the lattice spin-dopon coupling, and Δ is some typical energy scale. In heavy-fermion compounds, $\lambda = J_K$ is small and m^* is 2 or 3 orders of magnitude bigger than the bare electron mass. This leads to a very small T_c. In contrast, from infrared Hall measurements on underdoped LSCO and YBCO, m^* is of the same order of magnitude as the bare electron mass and λ is large. This is due to the fact that in the large-λ limit, for optimally doped cuprates, we arrive at a Kondo-like regime with $T_c \propto T_K \propto D$, the dopon bandwidth.

Let us now connect our result more directly to the recent experimental results of Doiron-Leyraud *et al.*[3] Right at half-filling and below Néel temperature $T_N \propto J/4$, the antiferromagnetic ordering is accounted by the Heisenberg interaction term in Eq. (24). Above T_N, thermal fluctuations destroy the long-range order. However, since the spin exchange energy J is, in fact, extraordinarily large, the system still shows strong short-range AF correlations well above T_N. This phase is accounted for by the spin liquid state of the spin-spin singlets. As the dopon concentration increases, the long-range AF order is melted by the quantum mechanical jiggling of the local spin moments induced by the small (in this regime) dopon-spin interaction, and it eventually disappears altogether. Although the Ruderman-Kittel-Kasuya-Yosida (RKKY) spin-spin interaction induced by dopons produces by itself the long-range AF ordering of the lattice spins, its strength is $\propto \lambda^2$, which is much less than the spin-spin exchange energy, J. As a result, at some finite dopon concentration, the AF long-range order gives way to short-range AF spin-spin correlations and the lattice spins become paired. As the doping increases, the individual lattice spins become less correlated with each other due to the competition between AFM fluctuations and the Kondo screening.

Suppose we are now in the pseudogap regime. The lattice spins form singlet pairs interacting with the dopons by means of a still weak λ coupling. The low density dopons are the only fermionic carriers present in the system which can be associated with the small hole pocket Fermi surface (FS) of the pseudogap state. The small volume of such a FS is accounted by the low density dopons present in the system. As the density of dopons increases, the dopon-spin coupling also increases and the dopon-spin singlets evolve continuously out of the pseudogap state into a more Kondo-like regime.[35]

Let us now estimate the critical density associated with such a crossover. The necessary energy to break the lattice spin pairs is roughly J. Since the individual spins in each pair and dopons become closely coupled to each other by means of the increase of λ, the dopon kinetic energy $2tx$, where x is dopon concentration, soon becomes of the order of J. Consequently, when $2tx > J$, the spin gap is destroyed and the resulting FS is now enlarged by the presence of the highly correlated charged spins, which together with the dopons are now counted as charge carriers. Taking simply $J/t \approx 1/3$, we arrive immediately at the lower bound estimate for the critical density $x_c \approx 0.17$, which is in very good agreement with the experimental value for the small versus large FS crossover which, for the hole doped cuprates, takes place in the doping range of 0.15–0.25, and it is associated with the complete disappearance of the pseudogap state.

It is also worthwhile at this stage to compare our scheme with the earlier mean-field slave-boson formulation. In that representation, the electron operator is decoupled into a spinon (fermion) and a holon (boson). Clearly, when the spinons are paired into singlet states and the charged bosons are not yet Bose-Einstein condensed, the resulting spin gapped state has no FS to be associated with. This is in direct disagreement with the recent experimental findings which demonstrate the metallic character of the pseudogap phase.

To complete the overall discussion of the physical implications of our dopon-lattice spin system, we need to clarify the onset and disappearance of the superconducting state in both underdoped and overdoped regimes. In the underdoped limit, as emphasized earlier, the lattice spins form singlet pairs interacting weakly with the dopons through λ. This interaction λ naturally leads dopons to condense into BCS-like pairs at temperature $T \leqslant T_c$. Notice that since the coupling λ is weak at low doping, the superconducting gap resulting from BCS condensation of dopons is strongly doping

dependent and it is not directly related to the spin gap. As a result, the superconducting gap and the spin gap (pseudogap) are, in practice, two independent energy scales at very low doping. This is in agreement with recent ARPES and Raman experiments, which distinguish the roles of the nodal and antinodal gaps in the low doping superconducting phase. In contrast, in the optimal doping region for larger dopon concentration, the NDO constraint must be treated with care and, as a result, λ grows accordingly. Such a growth of λ strongly ties the spin and dopon to each other. Therefore, at sufficiently large dopings, the spin and dopon gaps should become indistinguishable from each other. The superconducting phase is well described in this regime by a single energy scale. As a result, at a sufficiently large λ, both gaps are destroyed simultaneously and we end up with a low-energy Kondo-like metal.[36] Needless to say, the projection NDO constraint is a crucial ingredient in all our arguments and it allows us to give a simple explanation of important recent results.

V. CONCLUSION

In the present paper, we discuss the physical meaning and some implications of the theory of the projection constraint in the doped carrier representation of the *t-J* model. The basic conclusions that can be drawn from our consideration are as follows. First, the complete theory that incorporates the constraint sounds quite appealing, since it allows for a controlled mean-field treatment of the *t-J* model in the most interesting region close to half-filling. This happens at the expense of having more complicated interaction terms in the spin-dopon *t-J* Hamiltonian. It would be of utmost importance to derive the complete mean-field theory in this representation, which is now under consideration. However, as a first step in that direction, we just discuss some immediate qualitative consequences of the improved spin-dopon approach.

Second, the constraint enforced by the Lagrange multiplier term allows for an explicit mapping of the *t-J* model onto the Kondo-Heisenberg lattice model in the underdoped region. This indicates that the physics behind these two models are, indeed, related to each other. This mapping is very appealing in view of recent experiments that suggest striking similarities between quasi-two-dimensional heavy-fermion systems and high-T_c cuprates. Some physical implications are briefly discussed, pointing to the unified physics of heavy-fermion and high-T_c materials. Namely, it is possible that the very same physical mechanism is responsible for the formation of Cooper pairs in those systems, with different critical temperatures related to different mass renormalizations of the charge carriers and to different magnitudes of the existing coupling constants.

We also discuss the small-large evolution of the FS with doping. We associate this crossover to the closure of the spin gap and the destruction of the pseudogap state. We estimate the lower bound density for such a crossover. We make direct contact with the recent FS experiment of Doiron-Leyraud *et al.* When the spin gap is present, the pseudogap state has a small FS with the dopons being the only available charge carriers. With the increase of the dopon concentration and with the consequent increase of the coupling λ, the dopons and the individual lattice spins become strongly correlated to each other. In this way, when the spin gap is destroyed, above the superconducting temperature T_c, both dopons and lattice spins generate the associated FS.

Making explicit use of the projection constraint, we also discuss the onset and disappearance of superconductivity in both underdoped and overdoped regimes. Further work is, however, needed to explore in a more quantitative basis our mean-field doped carrier formulation of the *t-J* model. This is already in progress and the results will be presented elsewhere.

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APPENDIX: ANALOGY WITH THE GUTZWILLER PROJECTION

The global projection operator described above is similar to that used in the $U=\infty$ Hubbard model. Let us consider the Hamiltonian $H_{Hub}=\Sigma_{ij\sigma}t_{ij}c^{\dagger}_{i\sigma}c_{j\sigma}+U\Sigma_i n_{i\uparrow}n_{i\downarrow}$. In the case $U\rightarrow\infty$, the system is subject to the constraint $n_{i\uparrow}+n_{i\downarrow}\leqslant 1$. This constraint is equivalent to $\hat{Y}^G_i=n_{i\uparrow}n_{i\downarrow}=0$. In this way, when $\hat{Y}^G_i$ acts on the unphysical state (doubly occupied), we have $\hat{Y}^G_i|\text{unphys}\rangle_i=|\text{unphys}\rangle_i$. Therefore, $\hat{P}^G_i=1-n_{i\uparrow}n_{i\downarrow}$ is a projection operator that eliminates the unphysical state at site i. The gauge transformation generated by this constraint,

$$c_{\downarrow}\rightarrow c_{\downarrow}e^{i\epsilon n_{\uparrow}},\quad c_{\uparrow}\rightarrow c_{\uparrow}e^{i\epsilon n_{\downarrow}},$$

leaves the projected electron operators $\tilde{c}_{\sigma}=c_{\sigma}(1-n_{-\sigma})$ intact. The global projection operator is the well known Gutzwiller projector $\hat{P}^G=\hat{\Pi}_i\hat{P}^G_i$. We can then implement the constraint by writing $H_{Hub}=\hat{P}^G\Sigma_{ij\sigma}t_{ij}c^{\dagger}_{i\sigma}c_{j\sigma}\hat{P}^G$, which is equivalent to $H_{Hub}=\Sigma_{ij\sigma}t_{ij}\tilde{c}^{\dagger}_{i\sigma}\tilde{c}_{j\sigma}$. From this point of view, the parameter U of the Hubbard model becomes the Lagrange multiplier which is necessary to enforce the NDO constraint.

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[36] In case the optimal doping is already large enough (i.e., for the cobaltates), one should use the full spin-dopon representation of the Heisenberg term as given by Eq. (21) instead of the simplified one used in Eq. (24). In this case, a direct dopon-dopon interaction becomes relevant, which may result in the RVB-type dopon-dopon superconducting pair state (Ref. 11).