Spin-rotationally symmetric domain flux phases in underdoped cuprates

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current correlations under doping the Mott insulator has been reported in exact diagonalizations by Leung and attributed to the formation of spin bipolarons. These findings are consistent with an early observation of staggered spin chirality, since charge degrees of freedom strongly couple to spin scalar chirality. Interestingly, spin chirality/charge currents seem to compete with hole pairing and this issue requires a further careful consideration. Simultaneously with those findings, the observation of stripes and checkerboard patterns (which also include some form of charge ordering) has also been confirmed by density matrix renormalization group (DMRG) computations for some boundary conditions.

We also note that an exotic SF phase with long-range orbital current order at half-filling (in contrast to the fully projected SF phase, see Ref. 3) was stabilized in various extended Hubbard-like models (which include some form of charge fluctuations not present in the simpler model discussed above) within ladder or bilayer geometries. It was also shown that such a long-range DW order could survive with the emergence of stripe-like features under doping.

Unfortunately, even though stripe phases seem to play important role in the physics of HTS, it is still not clear how the stripes are connected, as a competing state, to d-wave superconductivity. Therefore, in this paper we introduce a new class of wave functions with composite order in a form of filled domain flux (FDF) phases, with one doped hole per one lattice atom. In addition to capturing essential properties of the SF phases, the FDF structure accounts for the incommensurate diagonal spin peaks observed in lightly (x < 0.06) doped La2−xSrxCuO4 (LSCO) and Nd-LSCO. Thus, our phase should allow one to obtain a smooth transition from the insulating state at half-filling to the d-wave superconductor above a critical doping x_c with a concomitant change of the DW orientation into vertical stripes just at x_c, as observed experimentally in LSCO. The existence of such phases is suggested by recent variational Monte-Carlo calculations which show an instability of the SF states towards phase separation and we argue that self-organization into flux domains separated by DWs is generic in the doped t–J model. Most pronounced features of these phases shown in Fig. 1(a,b) are: (i) doped holes self-organize into diagonal DWs, (ii) DWs separate weakly doped SF domains with a smoothly modulated magnitude of the flux within them, (iii) DWs introduce a phase shift of π in the flux phase and the SF domains alternate, and finally (iv) in contrast to the so-called commensurate flux (CF) phases, the total flux vanishes, and therefore no asymmetry of the magnetic response is expected when reversing the direction of an applied magnetic field. In fact, these FDF phases have strong similarities with the solution obtained in Ref. 28 using uniform (i.e., site independent) Gutzwiller factors.

The paper is organized as follows. The t-J model and its treatment in the Gutzwiller approximation are introduced in Sec. II. The properties of locally stable domain flux phases with either bond-centered or site-centered domain walls are presented in Sec. III. The paper is concluded in Sec. IV by pointing out certain possibilities of experimental verification of the suggested type of order and by a short summary of main results.

II. MODEL AND FORMALISM

We consider the t-J model:

$$H = - \sum_{\langle ij \rangle, \sigma} t_{ij} (\hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} + \text{h.c.}) + J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j, \quad (1)$$

which is believed to describe the physics of the HTS. Here the summations include each bond $\langle ij \rangle$ only once. Next, the local constraints that restrict the hopping processes $\propto \hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma}$ to the subspace with no doubly occupied sites are replaced by statistical Gutzwiller weights while decoupling in the particle-hole channel yields the following mean field (MF) Hamiltonian,

$$H_{\text{MF}} = - \sum_{\langle ij \rangle, \sigma} t_{ij} g_{ij} (c^\dagger_{i\sigma} c_{j\sigma} + \text{h.c.}) - \mu \sum_{\sigma} n_{i\sigma}$$

$$- \frac{3}{4} J \sum_{\langle ij \rangle, \sigma} g_{ij}^2 (\chi_{ji} c^\dagger_{i\sigma} c_{j\sigma} + \text{h.c.} - |\chi_{ij}|^2), \quad (2)$$

with the self-consistency conditions for the bond-order parameters

$$\chi_{ji} = \langle c^\dagger_{j\sigma} c_{i\sigma} \rangle. \quad (3)$$

In principle, simultaneous decoupling in the particle-particle channel is also possible but since we are interested in the diagonal DWs similar to the ones observed in the underdoped LSCO family we focus here on nonsuperconducting solutions. In particular we choose $x = 1/16$, one of the magic doping fractions at which low-temperature in-plane resistivity of LSCO is weakly enhanced suggesting a tendency towards charge order. Here, to allow for small non-uniform charge modulations, the Gutzwiller weights have been expressed in terms of local doped hole densities

$$n_{hi} = 1 - \sum_{\sigma} \langle c^\dagger_{i\sigma} c_{i\sigma} \rangle \quad (4)$$

as follows:

$$g_{ij}^\dagger = \sqrt{z_i z_j}, \quad g_{ij} = (2 - z_i)(2 - z_j), \quad (5)$$

with $z_i = 2n_{hi}/(1 + n_{hi})$. For simplicity, results shown below correspond to nearest neighbor hopping $t_{ij} = t$ only. Thanks to developing an efficient reciprocal space scheme by making use of the symmetry the calculations were carried out on a large 256 x 256 cluster at low temperature $\beta J = 500$, which eliminates the finite size effects.
Our starting point is the CF phase, a wave function which, away from half-filling, displays remarkable commensurability effects at special fillings and fulfills the self-consistency condition at $t = 0$. Indeed, in the limit $xt/J \to 0$, the magnetic (superexchange) energy in the CF phase exhibits a minimum when the fictitious flux (in unit of the flux quantum), flowing through each plaquette and defined by a sum over the four bonds of the plaquette

$$\Phi_\square = \frac{1}{2\pi} \sum_{\langle ij \rangle \in \square} \Theta_{ij}, \quad (6)$$

where $\Theta_{ij}$ is the phase of $\chi_{ij}$, follows exactly the filling fraction, i.e., $\Phi_\square = \frac{1}{2}(1 - x)$. In this case, Hamiltonian (2) reduces to the Hofstadter Hamiltonian describing the motion of an electron in a uniform magnetic flux assumed to be rational $\Phi_\square = p/q$. Therefore, the peculiar property of the superexchange energy follows from the CF phase band structure with $q$ bands and the Fermi level lying in the largest gap above the $p$th subband. As a result, the modulus of the bond-order parameter $\chi_{ij}$, the spin correlation and the hole density are all spatially uniform [see Fig. 1(c)]. However, infinitesimally small $xt/J$ selects a special arrangement of the phases $\{\Theta_{ij}\}$ so as to optimize the kinetic energy term $\propto \sum_{ij} \cos \Theta_{ij}$ and should produce an inhomogeneous structure.

Within this class of singlet (nonmagnetic) wave functions, competing with possible inhomogeneous solutions (see later), the uniform SF phase also offers a very good compromise between the magnetic ($E_J$) and kinetic ($E_t$) energy. For small $t$ and $x$, the kinetic energy is minimized (within the MF approach) when all phases of $\chi_{ij}$ are set to a constant $\Theta_{ij} = \pm \pi/4$, corresponding to alternating fluxes $\Phi_\square = \pm 0.5$ (SF phase). Increasing $xt/J$ gradually reduces $|\Phi_\square|$ and drives the system towards a Fermi liquid state (with real $\chi_{ij}$) in a continuous way.

### III. Domain Flux Phases

Starting with initial parameters corresponding to a uniform CF phase, the self-consistent procedure leads to new FDF solutions which could explain a diagonal spin modulation observed experimentally in the insulating regime of LSCO and Nd-LSCO usually interpreted in terms of diagonal stripes, even though no signatures of any charge modulation were observed yet. This conjecture is also supported by the recent neutron scattering studies of the Ni impurity effect on the diagonal incommensurability in LSCO. Indeed, doping by Ni quickly suppresses the incommensurability and restores the Néel state. This indicates a strong effect on hole localization and thus favors the presence of charge stripes with mobile holes rather than the spiral order with localized hole spins.

Interestingly, we found two types of topologically different but nearly degenerate solutions which both have the same size of the unit cell (see Fig. 1): (i) a bond-centered FDF phase, very similar to the original CF one,
where each DW is characterized by a zero current, and by a maximum of the hole density spread over the related bonds [Fig. 1(a)], as well as (ii) a site-centered FDF phase, where the DWs are characterized by zero flux plaquettes ordered along a diagonal line and by a maximum of the hole density centered at two of their corner sites [Fig. 1(b)]. Apart from local doped hole densities \( n_{hi} \), bond quantities are needed for a full characterization of both phases (here we use a short-hand notation):

- the spin correlation

\[
S_i = -\frac{3}{2} g^J_{i,i+x} |\chi_{i,i+x}|^2 ;
\]

- the bond charge hopping

\[
T_i = 2 g^J_{i,i+x} \text{Re}\{\chi_{i,i+x}\},
\]

- the charge current

\[
I_i = 2 g^J_{i,i+x} \text{Im}\{\chi_{i,i+x}\},
\]

- as well as the modulated flux

\[
\Phi_{pi} = (-1)^{i_x+i_y} \Phi_{i,i+x},
\]

with a phase factor \((-1)^{i_x+i_y}\) compensating the modulation of the flux within a single domain of the SF phase. Typical profiles of the above defined observables at low doping are depicted in Fig. 2.

The stability of the FDF phases originates from a subtle competition between the magnetic \( E_J \) and kinetic energies \( E_t \). Let us first focus on the \( t/J \to 0 \) limit where the site-centered SF phase is stable and very competitive (among the nonmagnetic states), in contrast to the bond-centered one. This extreme case corresponds to the localization of doped holes at DWs and the superexchange energy in the SF domains is best optimized. Indeed, by expelling holes from the SF domains one reinforces locally the AF correlations with a concomitant reduction of both bond charge and current correlations. On the contrary, due to a large hole density, both these tendencies are reversed around the DWs. However, increasing \( t/J \) leads to a much broader charge spatial distribution in the unit cell as a larger fraction of holes enters the SF domains (see Fig. 3). Nevertheless, both FDF phases remain competitive even in the regime of large (realistic) values of \( t/J \approx 3 \) due to: (i) enhanced short-range AF correlations deep in the SF domains \( S_i \approx -0.33 \) compared to \( S \approx -0.28 \) in the uniform phase), where the fictitious flux approaches the special value \( \Phi = \frac{1}{2} \) (local minimum of the kinetic energy in the limit \( xt/J \to 0 \)), and (ii) strongly enhanced bond charge accumulated around the DWs, typically three times larger than that in the SF phase, due to both amplification of the \( g^J_{i,j} \) factors and reduced (vanishing) fictitious flux flowing through the bond-centered (site-centered) plaquettes at the DWs.

Of particular interest is whether one can also stabilize within the present formalism the so-called half-filled domain flux (HDF) phases, analogous to half-filled stripes with one hole per two atoms in a DW as observed in the cuprates around \( x = 1/8 \).

On the one hand, both self-consistent bond- and site-centered HDF phases found at \( x = 1/16 \) and \( t/J = 3 \) have a somewhat higher total energy per site \( F \approx -1.07J \) than those obtained for both degenerate FDF ones \( F \approx -1.03J \), and for the uniform SF phase \( (-1.09J) \). However, Table II shows that all domain flux phases become very competitive at \( x = 1/8 \), not only with respect to the SF phase but also with respect to a recently proposed nonuniform 4 x 4 superstructure. Note also that while the FDF phases optimize mainly \( E_J \), the HDF ones are characterized by rather low \( E_t \). Therefore, we predict that large \( t/J \) rather favors the domain flux phases with partially filled DWs. We argue that quantum fluctuations are likely to stabi-

![FIG. 2: (color online) (a,e) Hole density \( n_{hi} \) (b,f) spin correlation \( S_i \) (c,g) bond charge \( T_i \) (d,h) modulated flux \( \Phi_{pi} \) in the bond-centered (left) and site-centered (right) FDF phases at \( x = 1/16 \) for: \( t/J = 1 \) (triangles), and \( t/J = 3 \) (squares). For comparison, circles depict the related \( t/J \to 0 \) solutions: the CF phase with uniform fictitious flux \( \Phi = 15/32 \) (left) and a two-domain \( |\Phi| = \frac{1}{2} \) SF phase (right).](image-url)
lize them, in analogy to the half-filled stripe phases or to the fully projected $4 \times 4$ checkerboard wave function which was recently shown to be more stable than the uniform SF phase. This suggests that other inhomogeneous solutions might be stable as well. Unfortunately, a direct comparison of our singlet wave functions to the original (magnetic) stripe phases is not possible yet since both are described within two entirely different formalisms. Hence further studies using more sophisticated methods (like projected wave functions as in Ref. 38) are needed.

An experimental support of the FDF phases follows from angle-resolved photoemission (ARPES) experiments on lightly doped LSCO that show a strongly suppressed spectral weight near the pseudogapped $X = (\pi, 0)$ and $Y = (0, \pi)$ points, and a quasiparticle band crossing the Fermi energy $\mu$ along the nodal $\Gamma - M$ direction, with $M = (\pi, \pi)$. Both features are qualitatively reproduced in the FDF phases – the electronic bands are almost dispersionless along the $X - Y$ direction, and a gap opens at $\omega = \mu$ (Fig. 3), indicating that transport across the DWs is suppressed. However, the most salient feature of the electronic structure in FDF phases is a relativistic cone-like dispersion around the $S = (\pi/2, \pi/2)$ point. Indeed, massless Dirac excitations are at the heart of the quantum electrodynamics in (2+1) dimensions (QED$_3$) theory of pseudogap in the cuprates. This feature is also found in the SF phase, but for the uniform flux and hole distribution it occurs away from the Fermi energy $\mu$. The shape of the electronic structure in the FDF phase depends on the actual value of $t/J$. Firstly, a strong localization of holes at DWs in the limit $t/J \to 0$ pushes the top of the lower band cone well below $\mu$. Secondly, finite $t$ weakens the stripe order so that the gap between the lower and upper band at the $S$ point is reduced. A further increase of $t$ pushes some lower band states above $\mu$ enabling transport along the DWs.

### IV. DISCUSSION AND SUMMARY

For possible experimental verification of the present proposal it is important to realize that orbital currents of the domain flux phase give rise to weak magnetic fields (that should be experimentally distinguishable from the copper spins). Muon spin rotation ($\mu$SR) technique is an extremely sensitive local probe especially suited to study small modulations of local fields. Earlier estimations give 10 to 100 Gauss corresponding roughly to 0.03 to 0.25 $\mu_B$ in cuprates. In fact, incommensurate order in the LSCO family seen in neutron scattering measurements (with a large but finite correlation length) might be attributed, at least partly, to the existence of orbital moments. Finally, note that although the phases considered here do not break SU(2) symmetry and do not exhibit AF long range order, on general principle they can still sustain AF correlations on large distances (i.e., beyond nearest neighbor sites) between copper spins.

In summary, we have introduced and investigated a new class of flux phases that unify the remarkable properties of the SF uniform phase with the incommensurate magnetic correlations established in the underdoped cuprates. Bond- and site-centered FDF phases are nearly degenerate which indicates strong fluctuations which are expected to be amplified, either for increasing $t/J$ or for increasing doping $x$. As these phases are only marginally unstable at the MF level, they might be stabilized by quantum effects and explain the low temperature physics of the cuprates in the low doping regime, where a pseudogap phase forms at higher temperature. Therefore, the solutions presented here could be viewed as a low-temperature instability of the nearby DDW pseudogap phase (stable at higher temperature but below $T^*$ in the same way as the "ordinary" stripe phases could be seen as an instability of the nearby doped AF Néel state at infinitesimal $x$). Therefore, our proposal calls for a search of experimental signatures of domain flux phases in the underdoped cuprates, especially in the LSCO family.
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