

Spin rotational symmetry breaking by orbital current patterns in two-leg laddersP. Chudzinski,¹ M. Gabay,² and T. Giamarchi¹¹*DPMC-MaNEP, University of Geneva, 24 Quai Ernest-Ansermet, CH-1211 Geneva, Switzerland*²*Laboratoire de Physique des Solides, Bat. 510, Centre d'Orsay, Université Paris-Sud 11, 91405 Orsay Cedex, France*

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We investigate the physical consequences of orbital current patterns (OCP) in doped two-leg Cu-O Hubbard ladders. The internal symmetry of the pattern, in the case of the ladder structure, differs slightly from that suggested so far for cuprates. We focus on this OCP and look for measurable signatures of its existence. We compute the magnetic field produced by the OCP at each lattice site and estimate its value in view of a possible experimental detection. Using a renormalization-group (RG) analysis, we determine the changes that are caused by the SU(2) spin rotational symmetry breaking which occurs when the OCP is present in the ground-state phase diagram. The most significant one is an in-plane spin-density wave gap opening in an otherwise critical phase, at intermediate dopings. We estimate the value of this gap, give an analytic expression for the correlation functions and examine some of the magnetic properties of this new phase which can be revealed in measurements. We compute the conductance in the presence of a single impurity using an RG analysis. A discussion of the various sources of SU(2) symmetry breaking underscores the specificity of the OCP-induced effects.

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I. INTRODUCTION

More than two decades after the experimental discovery of a pseudogap in the phase diagram of high-temperature superconductors (HTSC),¹ a microscopic explanation of its origin still remains elusive. Many scenarios have been proposed²⁻⁹ but so far no consensus has emerged on any particular one. Among the contenders are proposals that the pseudogap might be linked to current formation. It was suggested that staggered current patterns [*d*-density wave (DDW) phase] (Ref. 5) would lead to a pseudogap due to the doubling of the unit cell. An alternative uniform current pattern was proposed by Varma.^{10,11} In this latter case the three-band nature of the system is crucial, since currents flow along closed loops formed by Cu-O bonds in such a way that translational symmetry is preserved, while time-reversal symmetry is broken. On the experimental front specific signatures compatible with uniform currents were observed¹²⁻¹⁵ even if the issue is still controversial.^{16,17} On the theoretical side significant efforts were made to probe the possible existence of such a phase, either using numerical approaches¹⁸⁻²⁰ or starting from Mott insulating side.²¹

As a way of investigating the physics of these states in a more controlled way and also in view of possible connections with experimental systems,²²⁻²⁶ phases exhibiting orbital current patterns (OCP) were also considered in the context of two-leg ladders.^{27,28} Indeed for this essentially one-dimensional (1D) case, various analytical tools allow one to explore the consequences of such an unusual phase. In previous work^{29,30} we established that in the weak-coupling limit of Cu-O Hubbard ladders there exists a range of doping with a quasilong-range ordering of orbital currents, such that the pattern is symmetric with respect to the exchange of the two legs (*o*-OCP). In these studies, however, possible changes in the symmetry of the system caused by the formation of the orbital currents was not taken into account. Our analysis of the two-leg ladder problem was based on the

assumption that the spin degrees of freedom were totally decoupled from the motions of the carriers in real space. Although this is a very good starting point when the order parameter is small, it is interesting to investigate the consequences of such a coupling. In particular, in the presence of a static pattern of currents, it is natural to expect that the spin of the electrons will couple to the generated moment, and lead to interesting spin-orbit effects.

The aim of the present paper is to explore and to discuss physical effects which are occurring in response to the *o*-OCP. Anticipating the results presented below, the main consequence of the *o*-OCP is the appearance of magnetic moments which break SU(2) spin rotational symmetry. While measuring the primary (first-order) response of the system to the *o*-OCP is expected to be experimentally challenging, these collateral effects constitute clear fingerprints of the existence of such a phase. We also check the stability of the *o*-OCP itself with respect to the second-order perturbation which couples the order parameter with the spin of the electrons. We argue that SU(2) symmetry is fairly well protected (in the absence of crystalline anisotropies) and that its breaking is a telltale of the existence of the *o*-OCP.

The paper is organized as follows: at the beginning of Sec. II we introduce the Hubbard model for two-leg Cu-O ladders and we review the main results that were obtained for this model in the weak-coupling renormalization-group (RG) approach. Next we derive the additional terms that arise in the presence of the *o*-OCP. The magnetic moments that they induce in the ladder are calculated and the first-order effect that they generate are also discussed there. New terms in the Hamiltonian will be derived. Section III is devoted to an RG analysis of the generalized ladder model obtained in the previous section. Experimental consequences entailed by these results are described in Sec. IV. Lastly, in Appendix, we discuss other possible sources of SU(2) symmetry breaking in two-leg Cu-O ladders (such as Rashba effect).

II. MODEL

Let us begin with a brief review of two-leg Cu-O ladder physics. We consider a two-leg Cu-O ladder with local interactions. The Hamiltonian of this system contains two parts: the kinetic energy of electrons moving on the lattice H_T and electron interactions H_{int} ,

$$H = H_T + H_{int}. \quad (1)$$

In the SU(2) invariant case, the physics of this Hamiltonian is known (assuming that H_{int} is treated as a perturbation of the kinetic term).^{29,30} In the first part of this section, we recall its main characteristics, we show the condition required for the o -OCP to exist, and we also introduce relevant notations. In the second part, we explain how the o -OCP breaks spin rotational symmetry and we derive new terms in the Hamiltonian that arise because of the broken symmetry. In principle, these terms affect both H_T and H_{int} . This secondary effect is caused by the presence of the o -OCP.

A. Cu-O Hubbard ladder

Including two Cu and five O atoms in the unit cell, the tight-binding kinetic-energy part H_T reads

$$\begin{aligned} H_T = \sum_{j\sigma} \left\{ \sum_{m \in \text{Cu}} \epsilon_{\text{Cu}} n_{mj\sigma} + \sum_{m \in \text{O}} \epsilon_{\text{O}} n_{mj\sigma} \right. \\ - \sum_{m \in \text{Cu}} t [a_{mj\sigma}^\dagger (b_{mj\sigma} + b_{mj-1,\sigma}) + \text{H.c.}] \\ - \sum_{m \in \text{Cu}} t_\perp [a_{mj\sigma}^\dagger (b_{m+1,j\sigma} + b_{m-1,j\sigma}) + \text{H.c.}] \left. \right\} \\ - \sum_{m \in \text{O}(leg)} t_{pp} [b_{mj\sigma}^\dagger (b_{m+1,j\sigma} + b_{m-1,j\sigma} + b_{m+1,j-1\sigma} \\ + b_{m-1,j-1\sigma}) + \text{H.c.}], \quad (2) \end{aligned}$$

where $a_{mj\sigma}$ ($b_{mj\sigma}$) is the creation operator of holes with spin σ on a copper (oxygen) site (j is a site along chain and m labels the atoms in each cell); $n_{mj\sigma}^{\text{Cu}} = a_{mj\sigma}^\dagger \cdot a_{mj\sigma}$. We use hole notation such that t , t_\perp , t_{pp} are all positive. $\epsilon = \epsilon_{\text{O}} - \epsilon_{\text{Cu}}$ is the difference between the oxygen and copper on-site energies.

The model is reduced to two low-lying bands crossing the Fermi energy. They are denoted o (symmetric under the exchange of the two legs) and π (antisymmetric under the exchange of the two legs). With α ($=0, \pi$) and σ denoting the band and the spin index, respectively, the Hamiltonian reads

$$H_T = \sum_{k\alpha\sigma} e_\alpha(k) n_{k\alpha\sigma}, \quad (3)$$

where

$$a_{mk\sigma} = \sum_\alpha \lambda_{m\alpha} a_{\alpha k\sigma} \quad (4)$$

and $e_\alpha(k)$ and $\lambda_{m\alpha}$ are the eigenvalues and components of the eigenvectors of the Hamiltonian matrix (see Ref. 29).

In the low-energy limit one may linearize the dispersion relation in the vicinity of the Fermi energy,

$$H_T = \sum_{|q| < Q} \sum_{r\alpha\sigma} r q V_{F\alpha} a_{\alpha r q\sigma}^\dagger a_{\alpha r q\sigma} \quad (5)$$

and it is easy to bosonize this free fermion theory.^{31,32} Two charge (c) and spin (s) boson phase fields $\phi(x)$ are introduced for each fermion species (x is the spatial coordinate along the ladder).

We also introduce the phase fields θ ; their spatial derivative $\Pi(x) = \pi \nabla \theta(x)$ is canonically conjugated to $\phi(x)$. Now the Hamiltonian may be rewritten using the above phase fields. The kinetic part and those pieces in H_{int} which can be expressed as density-density terms give rise to the following quadratic form:

$$H_0 = \sum_\lambda \int \frac{dx}{2\pi} \left[(u_\lambda K_\lambda) (\pi \Pi_\lambda)^2 + \left(\frac{u_\lambda}{K_\lambda} \right) (\partial_x \phi_\lambda)^2 \right] \quad (6)$$

in the diagonal basis B_0 . $\lambda=1,2,3,4$ labels the eigenmodes (1, 2 are spin modes and 3, 4 are charge modes²⁹) For the noninteracting system one has $K_\lambda=1$ for all modes; the diagonal density basis is then the bonding/antibonding one $B_{o\pi}$ (the momentum k_\perp associated with the rungs is either 0 or π). The other basis which is commonly used in the literature is the total/transverse one, B_{+-} . It is related to $B_{o\pi}$ by,

$$\phi_{\nu+(-)} = \frac{\phi_{\nu o} \pm \phi_{\nu \pi}}{\sqrt{2}}, \quad (7)$$

where $\nu=c$ or s , depending on which particular density one considers.

The interaction part, in fermionic language, is given by

$$\begin{aligned} H_{int} = \sum_j \left(\sum_{m \in \text{Cu}} U_{\text{Cu}} n_{mj\uparrow} n_{mj\downarrow} + \sum_{m \in \text{O}} U_{\text{O}} n_{mj\uparrow} n_{mj\downarrow} \right. \\ \left. + \sum_{m \in \text{Cu}, n \in \text{O}} \sum_{\sigma, \sigma'} V_{\text{Cu-O}} n_{mj\sigma} n_{nj\sigma'} \right). \quad (8) \end{aligned}$$

Equation (8) gives rise to two types of terms: the first ones are of the forward scattering type and they can be cast in a quadratic form $[\sim \nabla \phi(x)]^2$ in bosonization language. These terms are then incorporated in the above-mentioned matrix \hat{K} of Luttinger liquid (LL) parameters, and hence they are treated exactly in this procedure. Since the form of \hat{K} depends on the basis in which the densities are expressed, the Hamiltonian will take the simple form Eq. (6) in the eigenbasis of the matrix \hat{K} . The remaining interaction terms yield nonlinear cosines and these are the ones for which the RG procedure is required. In Refs. 29 and 30 we showed that the eigenbasis for the spin and for the charge modes rotate during the RG flow. Two fixed points were found, namely, B_{+-} and $B_{o\pi}$. Interband physics dominates in the former case (mixing of the o and π bands) and intraband physics, in the latter case. Close to half filling (low-doping regime), B_{+-} is the fixed point basis for the spin and the charge modes. Both spin modes are gapped and so is one of the charge modes. Using the notation of Balents and Fisher³³ the ladder is in the $C1S0$ state [$CnSm$ denotes n (m) gapless charge (C) (spin S modes)]. For an intermediate range of dopings, B_{+-} is the fixed point basis for the spin variables and $B_{o\pi}$ the fixed point basis for the charge variables. This is the $C2S2$ regime

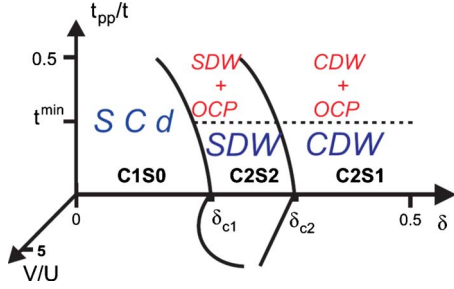


FIG. 1. (Color online) The phase diagram of two-leg Cu-O Hubbard ladders versus doping for $U_{\text{Cu}} > 0$. Zero doping corresponds to the half-filled case. Umklapp terms which open a gap in the charge symmetric mode are not included here (Ref. 29). SCd, CDW, and SDW denote, respectively, d -wave superconductivity, charge-density wave and spin-density wave states. OCP indicates that an orbital current pattern is present on top of a density wave instability.

when all modes are gapless. The decoupling of the spin and of the charge eigenbasis is responsible for this quantum critical state. For higher dopings, $B_{o\pi}$ is the fixed-point basis for the spin and the charge modes. The ladder is in the C2S1 phase where the o spin mode is gapped. The corresponding phase diagram, which was established in Refs. 29 and 30, is shown in Fig. 1.

A noteworthy result that came out of our analysis was that the symmetry of the OCP is that of the o band, for the Cu-O ladder. What is more, there exists a range of values of t_{pp} , above some critical hopping where this phase is dominant. In the following, we present a detailed discussion of experimentally accessible effects caused by the presence of this unusual phase.

B. Primary effect induced by the o -OCP: Magnetic moments

When the o -OCP is present, its current pattern $I(x)$ generates a local magnetic field $B(\mathbf{x})$ at each site \mathbf{x} of the lattice. This is the quantity that we are interested in. The value of the field can be obtained from the Biot-Savart law

$$B(\mathbf{x}) = \frac{\mu_0}{4\pi} \oint I(x) \frac{d\mathbf{l} \times \mathbf{r}}{r^3} = \frac{\mu_0}{4\pi} \sum_n I_n \oint_n' \frac{d\mathbf{l} \times \mathbf{r}}{r^3}. \quad (9)$$

\mathbf{r} is the vector joining the center of an infinitesimal element of current $I d\mathbf{l}$ to the lattice site \mathbf{x} . In the second equality, the prime on the integral means that we are integrating over an elementary Cu-O loop (triangle)—denoted by n —on the ladder; we sum over all triangles and we use the fact that current is conserved for each loop n of the lattice.

To perform the summation in Eq. (9), we first single out those triangles that belong to the particular unit cell that contains the lattice site \mathbf{x} ; we immediately notice that we get a zero net contribution whenever (1) the current flows in a direction that passes through the lattice site \mathbf{x} (the cross product $d\mathbf{l} \times \mathbf{r}$ gives zero), (2) the high symmetry of the OCP causes a cancellation of the fields due to currents connected by mirror symmetry (for that reason, the field on the on-rung oxygen is equal to zero)

These properties can easily be accounted for if one rewrites the magnetic field using a multipole expansion of the vector potential

$$A(x) = \frac{\mu_0}{4\pi} \sum_n I_n \sum_m \frac{1}{r_n^{m+1}} \oint (r')^m P_m(\cos \bar{\theta}) dl. \quad (10)$$

There are no magnetic monopoles, dipole contributions vanish because of the cancellations described above and so do quadrupole contributions inside each cell. Symmetry allows us to conclude that octupoles are the lowest-order nonvanishing terms. The above formula can be significantly simplified thanks to the fact that all atoms lie in the same plane from which we have $\cos \bar{\theta} = 1$; we can also assume that the approximate distance between the moments r' is equal to unit-cell size a .

Thus, we notice that we may get an accurate estimate of the contribution of all the other cells, if we assimilate them to octupole moments. Basically this approximation amounts to replacing the primed integrals within each triangle by a number (the magnetic moment at the center of each elementary triangle). The current creates a dipole moment perpendicular to the plane of the triangle (and proportional to the current flowing around it). Four neighboring current triangles, centered at a single, n th Cu site, define an elementary octupole $\zeta(n)$ (with a shape of a square). Then the magnetic field is approximated as a sum of octupoles along the ladder,

$$B = \frac{\mu_0}{4\pi} \left[\frac{\zeta(x)}{a^5} + \sum_n \left\{ \frac{\zeta(n) - \zeta(-n)}{r(x_n)^5} + \frac{\zeta(n) - \zeta(-n)}{[r(x_n)^2 + a^2]^{5/2}} \right\} \right]. \quad (11)$$

The first term comes from octupoles on opposite legs, the sum runs along the rungs of the ladder, with the first piece arising from same leg contributions and the second piece from opposite leg contributions. A crucial point is how to estimate the value of $\zeta(n) \sim I_n$. This work pertains to physical systems quite similar to cuprates. Experimental magnitudes of the local magnetic (dipolar) moments, which are tilted 45° out of the Cu-O plane, are of order $0.1 \mu_B$.¹² Thus we assume that our maximal octupolar momentum [on top of the density wave (DW)] is equal to $\zeta(I_{\text{max}}) \approx 4 \frac{\sqrt{2}}{2} 0.1 \mu_B a^2$ and we will use that value in our estimates. The case of on-leg oxygen, which lie at the boundary of each cell, is special because then the quadrupolar contribution does not vanish, and it will be discussed below.

One has to remember that the periodicity along the ladder plays an important role in the computation of such a sum; specifically, if the o -OCP were uniform along the ladder, all the different contributions would cancel out, because then $\zeta(n) = \zeta(-n)$, and the total magnetic field would be zero on each atom. In our case we have an o -OCP on top of a DW with a real-space periodicity $(2k_{F_o})^{-1}$, hence a magnetic field with the same periodicity appears.

As a result one finds that, depending on the nature of the lattice site \mathbf{x} , the magnetic field contains either only octupolar or both quadrupolar and octupolar contributions. (1) For each on-leg oxygen atom, there are quadrupolar contributions coming from the currents flowing along the neighbor-

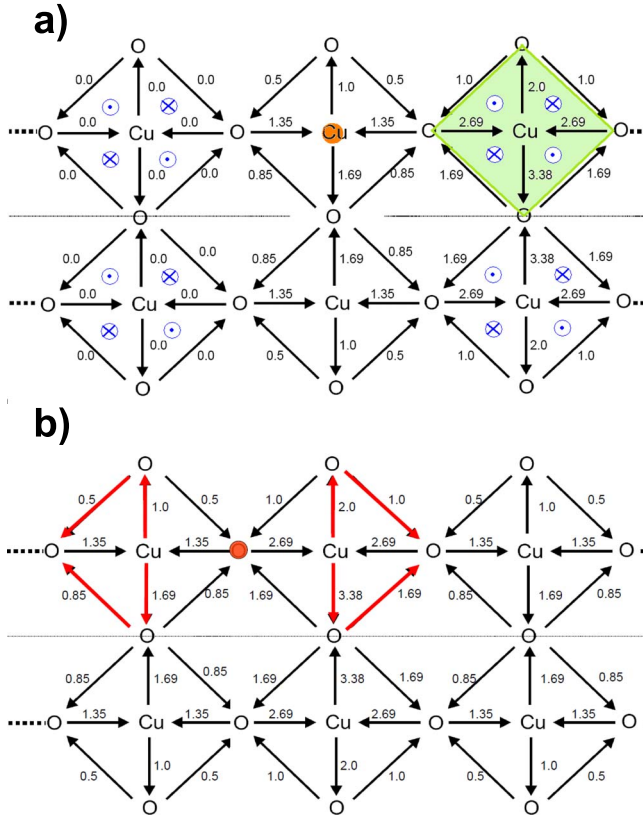


FIG. 2. (Color online) The two main contributions to the amplitude of the magnetic field at lattice site x (orange circle) as a result of the o -OCP flow: (a) the octupole moments (single octupole = green square) which should be summed up for all elementary unit (squares) along the ladder (except the one which contains lattice site x) and (b) the quadrupole magnetic moment that is present only if x is one of the on-leg oxygen; the field comes from the asymmetry of OCP amplitudes in two neighboring unit cells (nonzero contribution indicated in red); crosses (dots) correspond to single magnetic dipoles pointing into (out of) the page.

ing elementary cells which are not pointing out to this atom (the intensities of the currents are different in the two neighboring cells); see Fig. 2(b) numerically, we get a value of 50 Oe for the field. (2) For all other atoms (except the on-rung oxygen) we get octupolar contributions [as shown in Fig. 2(a)] coming from currents flowing through unit cells other than that of the atom: one piece stems from the single octupole on the leg opposite to where site x resides and the other from a sum of double octupoles along the ladder [a series oscillating with a $(2k_{F0})^{-1}$ periodicity and decreasing as $1/r^5$]; numerically, we get a value of 10/20 (Oe) for the field.

We note that both types of contributions produce a staggered field pointing in a direction perpendicular to the plane of the ladder, which possesses the periodicity of the o -OCP. The dipolar component and one of the terms in the octupolar series are illustrated in the figure below.

This local magnetic field $\vec{B}(x)$ break $SU(2)$ spin rotational symmetry. Usually, such symmetry breaking may occur in the presence of spin orbit, which adds a $\vec{L}_{eff}(x) \cdot \vec{S}(x)$ term to our Hamiltonian (it should be emphasized that both vectors are taken at the same point). Tools required to deal with such

a perturbation are readily available. We simply need to tailor these to our case. Both operators are two o -band fermion combinations, which, when coupled, will give four fermion products (to first order). Detailed analysis shows that such $\vec{L}_{eff}(x) \cdot \vec{S}(x)$ terms indeed cover the presence of magnetic field provided that hypothetical (periodic along x axis) field $\vec{B}(x)$ would have had only z component. For example, we may check the form (in bosonization language) of four fermion operators describing the coupling of the spin-density wave (SDW) with the spin degree of freedom of carriers {an example of this type of coupling is: $\psi_{oL\uparrow}^\dagger(x)\psi_{oR\downarrow}(x)[\psi_{oL/R,\sigma}^\dagger(x)\hat{\sigma}\psi_{oL/R,\sigma}(x)]$ } Thus, one can use the theory of spin-orbit coupling (as a perturbation) to solve our problem. The z -axis orientation of our perturbation is a consequence of the high symmetry of the lattice, a point which we emphasize in the next section.

C. Side effect of the o -OCP: New terms in the Hamiltonian

1. First-order term: Spin-dependent hopping

Because of the local magnetic fields that are generated by the o -OCP, the on-site energies of each atom (except for the on-rung oxygen), will be different for carriers with spin up and spin down. This can be viewed as local Zeeman splittings, which also affect overlap integrals for different spin rotations. The d - p orbital overlaps, and thus the hopping amplitudes, will depend on S_z . This suggests that spin-dependent hopping will be present. The additional hopping term is defined by $t_{\sigma\sigma'} = \vec{t} \cdot \vec{\sigma}$, where $\vec{\sigma}$ are Pauli matrices. Our argument implies that \vec{t} has only z components. In general there can be also other sources of \vec{t} such as coupling of electrons orbital momentum \hat{L} with magnetic moment of each triangle.

For Cu-O lattices, we can make generic statements regarding the possible spin-dependent hoppings caused by interactions with finite out-of-plane moments (the treatment is similar to a crystal-field splitting with a specific direction in space),

$$\vec{t} = \iota\lambda(B) \sum_n \frac{\langle d_{x^2-y^2} | \hat{L} | d_n \rangle}{\epsilon_{x^2-y^2} - \epsilon_n} t_{p_\gamma d_n}. \quad (12)$$

Here $d_{x^2-y^2}$ is the ground-state d orbital of the Cu atom located at some site i ; $|d_n\rangle$ is an excited d state of that atom; $t_{p_\gamma d_n}$ is the hopping amplitude between the Cu atom in the state $|d_n\rangle$ and a neighboring O atom in one of the p orbitals represented by the state $|p_\gamma\rangle$; \hat{L} is the orbital moment. One has to remember that symmetry requires some of the hopping integrals to vanish (for instance, $t_{p_y d_{xz}} = 0$ and similarly $\hat{L}|d_{3z^2-r^2}\rangle = 0$). Thus lattice symmetry implies that \vec{t} has always only a z component.

Taking this extra term into consideration, first-order effects can be easily incorporated in our tight-binding model: the problem can still be factorized in the spin variables (\vec{t} has only a z component). The magnetic field has o -band wavefunction symmetry, thus Zeeman splittings (and also overlap integrals variations) will have the same intracell symmetry.

For the OCP case, the splitting is purely vertical and it oscillates with k_{Fo} periodicity from unit cell to unit cell (whereas in the more frequently discussed Rashba case it is horizontal and the same for all the unit cells), which gives constructive interference within that band. The result is that the o band is split—the hopping parameters of spin up and down are slightly different.

There are three consequences of this type of splitting: (1) the Fermi velocities of spin-up and -down states are not equal anymore. (2) There is a mismatch of their Fermi vectors. (3) The two bands may contain different amounts of d and p orbitals

We do not need to discuss the last item because the eigenvectors of bands pairs are very similar. Let us instead focus on the first two. The difference in the velocities, translated into boson field language, yields terms of the form $\phi_{c+}\Pi_{s+}$, which affect the values of the parameters $K_{c,s+}$ and the form of correlation functions. The modification of $K_{c,s+}$ has to be taken into account in the initial condition of the RG flow; the impact on correlation functions will be described in detail in Sec. IV. The Fermi vector mismatch has an adverse impact on perpendicular (OCP case) spin scattering, because momentum is not conserved during that process, any longer. This effect will be accounted for much in the same way as one treats slight departures from commensurability with doping in Mott transitions.

In our case, we may estimate $|\vec{r}|/t < 10^{-4}$ (considering that the magnetic moment of a single loop is $\lambda \sim 0.1\mu_B$). This value gives $\delta k_{Fi}/k_{Fi}$ of the same order, so all these effects can indeed be treated as a perturbations.

2. Second-order terms: Spin-flip scattering channels

Let us turn to the next order in perturbation, which yields four fermion operators. In general these can be written in a Dzyaloshinskii-Moryia (D-M) form

$$H_{D-M} = \vec{D}_{ij} \cdot (\vec{S}_i \times \vec{S}_j). \quad (13)$$

The value of the D-M interaction between two Cu sites i and j separated by an O site l can be computed from the third-order spin-dependent hopping perturbation. The general expression is (where in the limit of small interactions ϵ is equal to the difference in the O and Cu on-site energies)

$$\vec{D}_{ij} = \frac{8}{\epsilon^3} \sum_l (t_{il}t_{lj} + \vec{t}_{il}\vec{t}_{lj}) \sum_l (t_{ij}\vec{t}_{lj} - t_{jl}\vec{t}_{il} + \vec{t}_{il} \times \vec{t}_{lj}). \quad (14)$$

The nonzero value of \vec{D}_{ij} comes from spatial inhomogeneity of (by its definition periodic) OCP pattern, which implies $\vec{t}_{ij} \neq \vec{t}_{ji}$. Taking into account $\vec{t} \sim 10^{-6}$ eV and using the fact that $\epsilon \leq t$ in Cu-based ladders (and when $U \rightarrow 0$ as for the $C2S2$ phase, ϵ determines interlevel distances), we can estimate $D \sim 10^{-5}$ eV [it is of order $\sim \vec{t}(\frac{t}{\epsilon})^3$]. This value is one order of magnitude larger than magnetic dipole-dipole interactions expected for such compounds (see Appendix).

We see that in the OCP case, where $\vec{t} \parallel z$, the crossterm in the second parenthesis of Eq. (14) is zero, and hence \vec{D} is perpendicular to the plane of the ladder. It also implies that this four-fermion operator will be proportional to the asym-

metry between neighboring Cu-Cu links (il th and lj th). We note that if the local magnetic moments were constant along the ladder, $\vec{D} = 0$.

Thus, the periodicity of the symmetry-breaking perturbation plays a critical role here. The OCP is superimposed on a DW with a $(2k_{Fo})^{-1}$ periodicity in real space, and the Fourier transform of $D(\mathbf{x})$ —which originates from the local magnetic fields—has components at $|q| = 2k_{Fo}$ only, i.e., corresponds to a backward scattering vertex. This mirrors the fact that the spin rotational symmetry-breaking physics brought about by currents is due to the o band and can only involve carriers scattering in this band.

When $\vec{D}_{ij} \parallel z$ one may deduce that the processes which explicitly break spin rotational symmetry are of the form $\hat{S}_x \hat{S}_y$. Using spin-flip operators we have terms such as $S_+^\dagger S_- + \text{H.c.}$. Physically this indicates that spin is not a conserved quantity anymore and that new instabilities may arise as a result of the additional scattering channels. The new term in the Hamiltonian is

$$H_{D-M} = g_{fo} \int \psi_{Lo\sigma}^\dagger \psi_{Ro\sigma}^\dagger \psi_{Lo\bar{\sigma}} \psi_{Ro\bar{\sigma}}, \quad (15)$$

where g_{fo} is the $2k_{Fo}$ component of the Fourier transform of D_{ij} . This can be bosonized in the standard way,

$$H_{D-M} = g_{fo} \int dr \cos(2\theta_{so}) = g_{fo} \int dr \cos(\theta_{+s} + \theta_{-s}). \quad (16)$$

Since spin-flip terms are involved in the fermionic operators, none of these will give simple density-density contributions to the bosonized expression of the Hamiltonian; instead they produce nonlinear interaction terms which require RG perturbative treatment. They may thus open a gap in the spectrum and cause new types of orderings in the ladder [which were previously forbidden as they explicitly break SU(2) symmetry]. We investigate this possibility in the next section.

III. ANALYSIS OF THE SU(2) SYMMETRY-BREAKING TERMS USING BOSONIZATION AND RG ARGUMENTS

The standard way to deal with four fermion operators, which produce cosine terms in bosonization language, is to follow an RG approach. This was extensively discussed in the context of SU(2) symmetric two-leg ladders (see, for example, Sec. III in Ref. 29) and we transpose it to the present situation.

As discussed in the previous section, we add the $g_{fo} \sim D(2k_{Fo})$ -type contributions to the Hubbard-type interactions and, following the standard procedure for cosine terms in the bosonization representation, we perform an RG analysis of the set of four fermions operators. Because spin-flip processes are now allowed, we have to add scattering events where—for instance—two incoming fermions are in a spin-up state and the two outgoing particles are in the spin-down state.

A. Extended system of RG equations

We proceed along the same lines as in our previous studies of two-leg Cu-O ladders; however additional subtle factors have to be taken into consideration. The fact that $D(q)$ has always just one component in momentum space simplifies the analysis and enables us to exclude some processes

One should take the system of RG equations derived for two-leg Cu-O Hubbard ladders [Eqs. (17)–(31) in Ref. 29] and add to it two equations describing the renormalization of the g_{fo} terms (intra o -band spin-flip scattering),

$$\frac{dg_{f1}}{dl} = g_{f1}[2 - (K_2^{-1} + K_1^{-1})] + P_1 Q_1 (K_2^{-1} - K_1^{-1}) g_{f2}, \quad (17)$$

$$\frac{dg_{f2}}{dl} = -g_{f2}[2 - (K_2^{-1} + K_1^{-1})] + P_1 Q_1 (K_2^{-1} - K_1^{-1}) g_{f1}, \quad (18)$$

where $g_{f1} = \frac{g_{fo} + g_{f\pi}}{2}$, $g_{f2} = \frac{g_{fo} - g_{f\pi}}{2}$, and by definition, in our case, $g_{f\pi} \equiv 0$ initially. We are using the same notation as in Ref. 29: $K_{1,2}$ are the LL parameters of the eigenmodes in the spin sector, i.e., linear combinations of $K_{s\pm}$ such that $K_1 = P_1^2 K_{s-} + Q_1^2 K_{s+}$ and $K_2 = P_1^2 K_{s+} - Q_1^2 K_{s-}$. The initial values of $K_{s\pm}$, P , and Q are determined from the Fermi velocities in the two bands and interactions of the forward type which are included in the LL matrix \hat{K} (note that $P_1^2 + Q_1^2 = 1$). Since g_{fo} has a cosine form in bosonization language, it does not change the initial values of the entries of the LL matrix \hat{K} .

Basically the new couplings g_{f1} and g_{f2} can be treated in a way similar to g_1, g_2 ; as they pertain to the θ_{+s} field, these cannot couple with other interactions g_i . The second-order g_{fo}^2 terms will enter the renormalization equations of the LL parameters K_i and $\cot 2\alpha$ (eigenbasis angle) in the spin sector,

$$\Delta \frac{dK_1}{dl} = \frac{1}{2}(g_{f1}^2 + g_{f2}^2) + f(P_1)(g_{f1}g_{f2}), \quad (19)$$

$$\Delta \frac{dK_2}{dl} = \frac{1}{2}(g_{f1}^2 + g_{f2}^2) - f(P_1)(g_{f1}g_{f2}), \quad (20)$$

$$\Delta \frac{dB_{12}}{dl} = h(P_1)g_{f1}g_{f2}, \quad (21)$$

where, as before

$$f(P_1) = \left(P_1 Q_1 + \frac{1}{4} \frac{P_1^2 - Q_1^2}{P_1 Q_1} \right)^{-1}, \quad (22)$$

$$h(P_1) = [(P_1 Q_1)^2 + 0.25(P_1^2 - Q_1^2)]^{-1}. \quad (23)$$

We notice that, as one might have expected, only the spin sector is affected by the new nonlinear terms. The modifications that these terms cause to the RG flow (in particular, as far as the eigenbasis rotation is concerned) are not easy to evaluate, because—as we argue below—several effects play a role. A qualitative analysis of the RG equations only allows

one to predict that the evolution of $\cot 2\alpha$ during the flow will be much slower than in the standard case.

The initial values of the K_i parameters will be different from what they are in the standard case, if only because of spin-charge mixing (following our discussion in Sec. II C 1, spin up and down are not degenerate any longer). This effect was partially accounted for by Moroz *et al.*:³⁴ they found that it can be implemented through a proper change in the scaling dimension of $\cos(\phi)$ [Eq. (38) in Ref. 34]. More explicitly, K_{s+} and K_{c+} will mix (just as $K_{s\pm}$ do, in response to particle-hole symmetry breaking) with a mixing parameter proportional to $\tilde{\epsilon} = (V_{F\uparrow} - V_{F\downarrow})/V_F$.

Assuming that the o band is decoupled from the π band, we can easily carry over Moroz's results to the ladder case and conclude that the mixing of spin and charge generated by the spin-orbit coupling is irrelevant in the o -OCP case, because here $\tilde{\epsilon} \ll \tilde{\epsilon}_{crit} = \frac{V_{s+}^0}{V_{Fo}}$.

Yet, another effect does play a role. As we pointed out in the band-structure discussion, because of the Fermi vector mismatch, perpendicular spin scattering is reduced compared to parallel spin scattering (as is the case with umklapp scattering, slightly away from $k_F = \pi/2$). This causes a shift of the phase boundaries in the ground-state phase diagram but it does not generate any new phases. To demonstrate this explicitly requires a full blown RG treatment but heuristic arguments pertaining to the RG flow in the $C2S2$ phase—presented in the next section—give clear indications of this trend.

B. Relevance of the g_f terms

The overall structure of the phase diagram that emerges from the RG analysis, when these additional terms are included, is similar to that obtained in our previous papers, so we discuss here the stability of the phases that were found for ladders possessing SU(2) symmetry. Let us start from the half-filled case when there is on average one carrier per copper atom and move toward the highly doped regime when the π band is nearly empty.

The low-doping **C1S0** phase is not affected, since the o -OCP does not exist, and hence $D(2k_{Fo}) = 0$. However, to be on the safe side, we have checked that even if $D(2k_{Fo}) \neq 0$ interactions of the g_{fo} type are irrelevant. This can be justified by symmetry considerations regarding the eigenbasis: in the low-doping regime $B_{+/-}$ is the proper basis of LL modes, thus a small g_{fo} , which induce instability in the $B_{o\pi}$ basis cannot be relevant in this doping range. It must be interband spin-flip scattering which causes a relevant perturbation of the **C1S0** phase—the possibility of the other types of spin-flip interactions are briefly discussed in Appendix.

A significant difference, caused by g_{fo} , is found for the massless **C2S2** phase that was present in a finite, intermediate doping range of the SU(2) symmetric problem. We recall, that for this phase, $B_{o\pi}$ is the proper basis of the charge sector, thus interband instabilities are suppressed. Adding g_{fo} favors a flow toward this basis. We can simplify our analysis even further if we assume that in given range of dopings, the RG equations describing the evolution of the o band are decoupled from the rest of RG system. This allows us to

work with Eq. (17) and the equation (derived previously²⁹) describing intraband backscattering,

$$\frac{dg}{dl} = g[2 - (K_2 + K_1)] + P_1 Q_1 (K_2 - K_1) g,$$

g_o was proved to be irrelevant since the initial $K_2 > 1$ and we would need a large value of Q_1^2 in order to open a gap in ϕ_{so} . Roughly speaking K_{so} was approaching its fixed point $K_{so} \rightarrow 1$ too slowly and the flow was finally only marginal. In our extended case g_{fo} tends to increase K_{so} or at least (in the beginning) protects its constant value. The arguments given in Ref. 29 work exactly in the opposite way for the $\cos \theta_{so}$ instability, which is relevant provided $K_{so} > 1$. This can be quantified by studying an invariant of our extended RG system,

$$A^2 = (K_{so} - 1)^2 - (g_o^2 + g_{fo}^2). \quad (24)$$

We see that by adding the new terms A^2 is shifted (from $A \approx 0$) to negative values; it is known that an imaginary A in the Kosterlitz-Thouless RG flow corresponds to a divergent trajectory that is to a relevant instability destroying the LL fixed point. The only possibility corresponding to that case is that g_{fo} becomes the relevant perturbation.

Our earlier observation that momentum mismatch reduces the initial value of the perpendicular spin-scattering interaction while leaving those of the parallel and spin-flip processes unchanged reinforces the inequality $(K_{so} - 1) > g_{\perp}$. We then study a Kosterlitz-Thouless RG flow with all the g_{\perp} terms smaller than the $g_{\parallel o}$ terms; in that case we find that we move away from the SU(2) separatrix and scale toward larger K_{so} , which favors the new intermediate phase (with the θ field ordered).

One finds that a new gap opens in the spectrum of the θ_{so} field. We find that $C2S2 \rightarrow C2S1'$ with an ordering within the o band. Using a bosonic version of order operators we find that SDW in the plane of the ladder (SDW_x in the o band) is favored. The order operator is defined as follows:

$$\begin{aligned} O_{SDW_o}^x(x) &= \psi_{oR\uparrow}^\dagger \psi_{oL\downarrow}(x) + \psi_{oR\downarrow}^\dagger \psi_{oL\uparrow}(x) \\ &\approx \exp(-2ik_{Fo}x) \exp[i\sqrt{2}\phi_{co}(x)] \cos[\sqrt{2}\theta_{so}(x)]. \end{aligned}$$

The interaction breaking spin rotational SU(2) symmetry dominates in this regime, so it is clear that the resulting phase also breaks this symmetry.

This simplified analysis is confirmed when we perform the actual RG calculation including the additional terms. Furthermore, we are able to obtain the exact boundary between the g_{fo} and g_o dominated phases [i.e., the boundary between the SU(2) symmetric and symmetry-broken phases]. We also see that the assumption $K_{so} \approx \text{const}$ is justified, so we can approximate the value of a gap by taking the following RG flow: $\frac{dK_{so}}{dl} = 0$, from which one deduces that a proper estimate of the gap value is,³¹

$$\Delta \approx \Lambda_0 g_{fo}^{1/2-2K_{so}^{-1}}. \quad (25)$$

Assuming $K_{so} \leq 2$ (strong, but local, Hubbard interaction limit) we find $\Delta \approx 0.01D$, which gives quite a small but experimentally accessible transition temperature $\in (1, 10)$ mK.

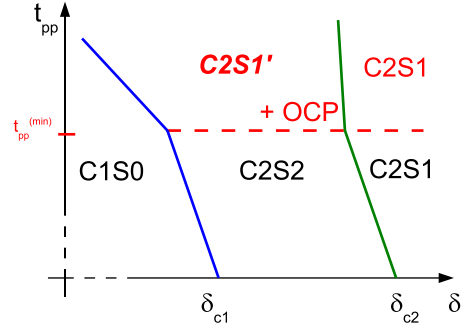


FIG. 3. (Color online) Modified phase diagram (to be compared with Fig. 1) of the two-leg Cu-O ladder when intra- o -band spin-flip processes are included: as before δ is the hole doping and t_{pp} inter-oxygen hopping. In the intermediate doping range—where a C2S2 phase was previously found in the SU(2) symmetric problem, a C2S1' state is present, which has a SDW in the plane of the ladder as a result of the opening of a spin gap.

For the C2S1 phase the additional g_{fo} terms compete with the interaction $g_o = g_1 + g_2$, so the theory of spin-flip effects in the case of a single chain applies. The reasoning is very similar to that for the C2S2 phase, except that now g_o dominates. To put it on a more quantitative level: as long as the initial g_f is smaller than g_o —which is a reasonable assumption, because g_o is a relevant perturbation dominant in this doping range—the ordering of the ϕ_{so} field overwhelms spin-flip processes. Giamarchi and Schulz³⁵ have found that the critical line for this problem is at $g_f = g_o$. This assumption can fail only close to the low-doping boundary of the C2S1 phase since the strength of g_o decreases as one reaches δ_{c2} . We can thus conclude that, except for a shift of the lower boundary, the charge-density wave (CDW) state is unaffected by the spin-orbit coupling. The new phase diagram, in the presence of g_{fo} is summarized in the figure below (Fig. 3).

IV. DISCUSSION

The breaking of SU(2) symmetry, that occurs in the presence of the OCP, opens a gap in the spin mode of the o band. In the range of dopings where previously a critical line was found, the C2S2 phase is replaced by a different ground state, namely, a phase with in-plane SDW_x denoted by C2S1'. An important question is whether this unusual phase is detectable, or if any small symmetry breaking will make it undistinguishable from the standard, high-doping C2S1 phase. To answer this question we present a discussion along three lines: the first one is devoted to high-temperature correlation functions, the second to transport properties, and the third to magnetic properties. A limitation of the discussion presented below, which affects experiments, is the energy scale: the effects will be clearly visible only in a temperatures range below the gap Δ .

One may also wonder whether the existence of the OCP is the only source of SU(2) symmetry breaking. As the Cu-O lattice forms a fairly rigid structure, it is stable both against crystal-field d levels splitting and standard L - S coupling $\sim Z^2$ on heavy Cu ions (with $Z=29$), and, insofar as we may need

glect size effects, the presence of an OCP is the source of symmetry breaking. A detailed discussion of these issues will be presented in Appendix.

A. Correlation functions for the LL phase

Correlation functions for LL with spin-orbit interactions have been evaluated both for two-³⁴ and four-fermion³⁶ operators. Let us briefly summarize here their main features. Chiral separation is still preserved and correlators can still be factorized in terms of two modes but not spin and charge anymore. Interactions and spin-orbit coupling (L-S) reinforce one another; in the presence of L-S, the density of states decays faster than for free fermions, and the difference between the velocity of the two modes $\delta V = V_{\uparrow} - V_{\downarrow}$ is proportional to \vec{l} . According to Ref. 36 the exponents are slightly changed when a term proportional to a difference of the velocities is added (we use these results slightly modified, because it was Rashba-type spin-orbit coupling treated in Ref. 36, while we are interested in Zeeman-type coupling); for example, the behavior of our dominant fluctuation is given by (at zero temperature, up to first order in δV),

$$O_{\text{SDW}_o}^x(r) \approx \cos(2k_{F_o}x)r^{-(K_{co}+1/K_{so}-\theta^s)}, \quad (26)$$

where $\theta^s \sim \delta V$. As a consequence the four fermion operators have a nonzero conformal spin proportional to δV .

In our case intra- o -band L-S coupling is quite weak (this small value enabled us to neglect some effects of spin-charge mixing during the RG flow). Accordingly, in the high-temperature LL phase, the functional (power-law) form of the correlators will be the same for the $C2S1$ and $C2S1'$ phases, and the only difference comes from small changes in the exponents. Taking into account small (and oscillating) value of δk (δV), and experimental difficulty with extracting exact value of bare LL exponent K_{io} , we doubt that $C2S1'$ existence can be shown in this way.

More visible signatures can be expected at low temperature where the θ_{so} field is ordered, as all the observables depending on magnetic susceptibilities—such as NMR responses—are affected (notwithstanding the relatively smallness of the gap): if the θ_{so} field is locked, then averages over the ϕ_{so} field go abruptly to zero. According to Ref. 29 one expects quite abrupt suppression of the o -band electronic part of the Knight-shift K and relaxation rate ($1/T_1$) at $T < \Delta$ (for example, $K \sim \langle \cos \phi_{so} \rangle$).

B. Transport properties: Analysis of the impurity problem

Let us briefly discuss here what happens if a nonmagnetic impurity is introduced in the two-leg Cu-O ladder. This problem was discussed in detail recently;³⁷ here we focus on the consequences of spin rotational symmetry breaking. Specifically, we investigate the doping range where the $C2S2$ phase was stable in the absence of spin-orbit scattering. In the previous section we have shown that K_{so} behaves differently at the lowest temperatures because of a gap opening due to spin-orbit terms. So the temperature dependence of the transmission through a single impurity—which is connected to the renormalized backscattering $V_o[l;K]$ —will also be affected.

Spin-orbit coupling is present only inside the o band, so we may restrict our analysis to reflection (transmission) of carriers inside this band. In such a simplified case, the RG equation for backscattering on the impurity is given by

$$\frac{dV_o}{dl} = (2 - K_{so} - K_{co})V_o \quad (27)$$

instead of Eq. (15a) in Ref. 37, where it was assumed that $K_{so} = 1$. From this, it is clear that increasing K_{so} (which promotes an ordering of the θ_{so} field) can cause V_o to become irrelevant. More precisely, this operator is always relevant at the beginning of its flow, because $K_{co} < 1$ (and this value is constant in the absence of umklapp terms), but this trend may change as the energy is decreased. This would give rise to an unusual temperature dependence of the conductivity.

On the other hand, if the initial value of K_{co} is sufficiently small (strongly interacting case), we would arrive at an open boundary problem (V_o relevant). In our previous paper,³⁷ intraband Kondo physics was suggested for this case. The following RG equation describes this regime [assuming open boundary conditions (OBC)]

$$\frac{dJ_o}{dl} = J_o(1 - K_{so}^{-1}). \quad (28)$$

We see here that if $SU(2)$ symmetry is broken by the o -OCP, this coupling becomes relevant, which confirms our previous predictions. In the limit of quite strong Hubbard interactions $K_{co} \rightarrow 1/2$ —which is the case when $K_{so} \gg 1$ —it can give rise to the unusual regime predicted many years ago by Furusaki and Nagaosa³⁸ who took second-order tunneling processes into account, showing that double spinon tunneling events may dominate the physics around the impurity. The competition between OBC Kondo physics and spinon transmission will take place in the strong interaction limit (the barrier asymmetry will also play a significant role) but this is beyond the scope of the present paper.

An experimental consequence of this effect, is that in the phase where spin-orbit coupling dominates, the usual line broadening caused by impurities that is expected in an NMR measurement, will not be seen. This is because spinons can be transmitted through nonmagnetic impurities (and hence the backscattering in the spin sector is expected to be weak).

C. Magnetic properties

Obviously, the local magnetic field will affect the Knight shifts of the NMR lines. The magnetic field is alternating and incommensurate with the lattice: as a result of such local magnetic field variation NMR lines will not have standard (thermal broadened) shape but it will depend on the number of atoms feeling a given value of the field $N(B_{loc})$. The incommensurability with the lattice allows us to rephrase this question and ask what is the density of states for a cosine curve. Thus the NMR line shape resemble 1D density of states with two peaks line shape (1D density of states has $1/\omega$ singularity coming from the bottom of the cosine band). The splitting is equal to $2B_{\max}$ and, because the effective field is different at each atom inside unit cell, thus different

line shapes are expected: the widest on on-leg oxygen atom, and nonperturbed (zero split) on the on-rung, central oxygen. This effect should be distinguished from the one described in the previous paragraph, in total OCP modifies NMR lines in two ways: it suppress the amplitude of the satellites, of the impurity at the origin, and splits the central peak. Unfortunately estimated values of this splitting are at the limit of the current experimental resolution, so this primary effect might be difficult to detect. One can alternatively detect anisotropic g factors through Zeeman effect.

There will also be a signal coming from the magnetic ordering itself. We predict that there is a magnetic moment component perpendicular to the ladder plane due to B_{eff} induced by the o -OCP (primary effect) but there is also a secondary effect: from our RG procedure we have found an in-plane component corresponding to a SDW_x with the same periodicity as for the staggered moments along z . The fact that both components have the same periodicity in k space, $2k_{Fo}$, is quite important: they can add up creating a moment tilted out of plane. The tilting angle will be determined by their relative amplitudes. We have started with $\mu_x=0.1\mu_B$ which induce an ordering gap Δ . The value of μ_x is connected with the average $\mu_x \sim \langle \cos \theta_{so} \rangle$ so it will be reduced with increasing temperature. Even at zero-temperature quantum fluctuations cause $\langle \cos \theta_{so} \rangle \neq 1$. In order to estimate the average at zero temperature we compare the values of the gap we found in Sec. III with the one found when the LL velocity (kinetic energy) goes to zero Δ_∞ . It is known that $\Delta_\infty \approx |\vec{D}|$. The ratio $\Delta/\Delta_\infty=0.01$ is proportional to $\langle \cos \theta_{so} \rangle$ and allows us to estimate $\mu_x \approx 0.01\mu_B$, from which we deduce a tilting angle on the order of $\vartheta \sim 6^\circ$ (counted from vertical axis). This kind of modulated (in space) magnetic moments composition should be detectable using elastic neutron scattering but quite low temperature (~ 10 mK) would be required for this experiment.

V. CONCLUSIONS

The main question which we addressed in this work was: what is the feedback effect of an OCP on the properties of the ladder, if one takes into account the coupling between the electrons and the induced orbital moment? Such feedback can in fact potentially provide an additional method to probe the existence of the OCP; it does not require a direct measurement of the induced—and quite tiny—magnetic field. Detecting such feedback can however prove challenging due to two important constraints. First, one would need to obtain highly doped ($\sim 25\%$) two-leg ladders; second, experiment have to be performed at temperatures below Δ . Still, we hope that our present detailed insight into the low-energy properties of the intermediate phase will invite experimental and numerical investigations.

A nontrivial issue is how reliable our value of Δ is. We have used a weak-coupling RG approach which is reasonable in the case of the otherwise gapless $C2S2$ phase: the statement $\Delta < |\vec{D}|$ is justified. Thus, in our framework the only way to increase Δ , assuming a given amplitude of the OCP ($\sim \mu_z$) is by taking larger λ coefficient in Eq. (12) (this would give larger $|\vec{D}|$). This may arise because of particular,

unknown property of copper oxides and/or constructive interference of L-S couplings defined on the top of the DW. Larger gap value will push the tilt angle ϑ toward larger values.

Beyond the experimental manifestations, which we have discussed in Sec. IV, the magnetic moment pattern should be detectable using elastic neutron scattering. Such experiments were recently performed in the pseudogap phase of two-dimensional (2D) HTSC.^{12,15} The data was interpreted as evidence for out-of-plane magnetic moments with an alternating tilt. There is a similarity with our prediction but one must not forget that there are several important differences between the OCP that we have discussed and the one that could serve to interpret the experiments in cuprates: in our 1D case the pattern is modulated in space with a k_{Fo} periodicity (this modulation was in fact critical to obtain a nonzero coupling with the spin degree of freedom) and has a different internal symmetry: θ_1 instead of θ_2 in Varma's notation.¹¹ One must keep in mind these caveats, nonetheless our result invites one to look for similar effects in two-leg ladders.

To summarize: despite certain similarities, the 2D cuprates studied in Refs. 12 and 15 cannot be treated as an experimental realization of our problem. A good candidate would be a doped ladder, such as the so-called telephone compound ($Sr_{14-x}Ca_xCu_{24}O_{41}$), provided sufficient doping levels can be attained (from the standpoint of solid-state chemistry, this is a highly nontrivial task). Neutron-diffraction or μ SR experiments would be desirable for such a ladder system.

An important point is the possible role of apical oxygen. In the framework of a tight-binding model the new hoppings will make the two bands (o and π) more asymmetric; this implies larger effective t_{pp} , which shifts the $C2S2$ phase toward smaller dopings δ (see Fig. 1). New conducting paths will also increase the OCP amplitude for a given value of t_{pp} , shifting the critical t_{pp}^{min} to smaller values. As a result the new phase $C2S1'$ will be easier to access experimentally in the $(\delta - \frac{t_{pp}}{t_{pd}})$ plane. The new current paths can also give rise to higher-order L-S couplings: for example, $\vec{\mu}$ can induce additional currents flowing in the loops involving the apical oxygen. We may conclude that including apical oxygen should favor the effects predicted in this paper. This statement, about a positive role of apical oxygen, is in qualitative agreement with recent work²¹ studying currents emerging because of particular spin textures.

A nontrivial outcome of this work is that it underscores the hidden connection between a phase with OCP and a pseudo (partial) gap in the spin sector. The emergence of such a gap shields the intermediate, previously marginal, phase from weak perturbations such as interladder hopping or disorder. In conclusion our work shows that a strong perturbation is caused by the presence of the OCP and validates the phase diagram for two-leg Hubbard ladders which had been obtained in Ref. 30.

APPENDIX: OTHER SU(2) SYMMETRY-BREAKING MECHANISMS

In this appendix, for the sake of completeness, we briefly discuss alternative sources of spin rotational symmetry

breaking. A few of them come readily to mind: dipole-dipole interactions, standard $\vec{L} \cdot \vec{S}$ spin-orbit coupling and Rashba mechanism.

(1) Direct spin-dipolar interactions. The value of this spin anisotropy depends on the average distance between carriers as $\sim 1/\langle r \rangle^3$. The $\langle r \rangle$ is obviously changing when one add carriers into the ladder which implies a doping dependence. We can use values found for the half-filled case in a similar compound³⁹ and simply assume that carriers are more diluted. For the most interesting phase (C2S2) there are at least two times less carriers which gives reduction by a factor 8, thus we have estimated the dipole-dipole anisotropy to be one order of magnitude smaller than OCP effects.

Besides, in the C2S2 regime, OCP effects are predominant because they possess the proper o -band symmetry, in contrast with the generic form of dipolar interactions. Thus we assume that this mechanism cannot compete nor mimic the OCP effects predicted in this paper.

(2) The spin orbit $\vec{L} \cdot \vec{S}$ coupling is a fairly typical effect for heavy atoms. Thus we should check whether it could induce much stronger effects than those predicted in our analysis.

The key point is the symmetry of the lattice: so long as copper atoms are sitting in a C_4 symmetric environment, hoppings to and from all the neighboring oxygen will conspire to give a zero net outcome. We can also invert this argument and say that if electron ordering finds a way to lower the rotational symmetry of a lattice then it would provide an efficient way to increase the λ coefficient in Eq. (12) and thus enhance effects discussed in this paper. This property does not hold if the lattice is distorted (in the Peierls or Jahn-Teller cases for instance) or warped. As the lattice is quite rigid (and we are not working at half filling) for ladders, these effects are not expected to be significant in the bulk. The situation may be different at an interface but we are not dealing with such a case in this paper. This is the reason why we focused on OCP-induced effects.

The only exception might be if the primary OCP involved apical oxygen. Let us make a *gedanken* experiment and assume that there is a current flowing through some of bonds toward these atoms. This might enhance the total amplitude of the OCP, lowering the value $t_{pp}^{(crit)}$. It can also be a higher-order perturbation induced by the in-plane SDW(x). The conducting bonds tend to be shorter which can displace apical oxygen. The emergence of such distortion will lower the lattice symmetry from C_4 to C_2 allowing for the nonzero net expectation value of the spin-orbit coupling on Cu atoms. This would cause a S^z -dependent hopping, as can be seen from Eq. (12) which shows that the displacement is equivalent to admixing $d_{x^2-y^2}$ orbitals with the apical oxygen band. Importantly, this effect is caused by the OCP, thus it should have the same periodicity and phase. This additional L-S coupling enhances the OCP induced effects discussed above.

(3) Another possible mechanism of interest in the cuprate case, giving spin-dependent hopping, arises from the Rashba effect which couples directly electron motions to their spins.

It describes the precession of carriers in the presence of a strong electric field. The Rashba Hamiltonian is

$$H_R = \alpha(\vec{k} \times \vec{n}) \cdot \vec{\sigma}, \quad (\text{A1})$$

where α is a coupling constant and \vec{n} is a unit vector in the electric field direction. Obviously, this coupling (which depends on the total momentum of the carrier) will be different for the o and π bands, because of the inequality $k_{F_o} > k_{F_\pi}$ (one should not forget that k_{F_π} has large on-rung components).

First, let us consider the bulk of a ladder material. The electric field which we expect will lie in the plane of the ladders in a direction perpendicular to the legs. It will result from the arrangements of DW in neighboring ladders (so again it will be restricted to the high-doping regime and again have a $(2k_{F_o})^{-1}$ periodicity in real space). There are two limitations here: these arrangements can only be stable for certain dopings (quarter filling) and they are expected to be quite small in amplitude.

Straightforward analysis (with again crucial element of DW modulation) of Eq. (A1) gives a spin-dependent hopping parameter $\vec{t} \sim [0, 0, t']$, so again it has only a z component. It implies that the analysis done in the core of this paper applies also in this case. Thus, this kind of Rashba (if such kind of perpendicular arrangement does exist) would enhance the effects predicted before. The only difference which would allow us to distinguish this case from that induced by an OCP is the magnetization component perpendicular to the ladder plane.

Let us finish with a brief discussion of an interface where the Rashba mechanism can induce quite new physics. In this case the electric field will be perpendicular to the ladder plane because it arises from charge-polarization effects at the interface. On the interface, when charge differences are very high (polarization catastrophe) at very small (interatomic) distances, this effect can be really huge. What is more, in contradistinction with the mechanisms that we discussed until now, the amplitude is not alternating in space (the sign of the coupling is not oscillating).

In the case of strong electric field there are only nondiagonal (spin-flip) hoppings; level splitting is induced by the Rashba term Eq. (A1) (if the electric field \vec{E} is in the z direction, H_R can be expressed as $\sim [t', 0, 0] \cdot \vec{\sigma}$ in the o band and approximately by $[0, t', 0] \cdot \vec{\sigma}$ in the π band). In this case spin and charge are strongly mixed thus spin up and spin down are not a good quantum number any longer.

Also spin-flip interactions will be highly nontrivial in such a model: we may find \vec{t}_{ij} with perpendicular orientations, for instance, when the two scattering carriers are from two different bands. Thus it is the last term in the parenthesis of Eq. (14) which is nonzero; we are then dealing with interband scattering. We note that both \vec{t} lie in the ladder plane, so that, once again, $\vec{D}_{ij} \parallel z$ (spin-flip process). We expect very different physics emerging in this case, which is out of scope of this paper. A detailed RG analysis will be postponed to a future publication devoted to surface effects.

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