Ferro-Orbitally Ordered Stripes in Systems with Alternating Orbital Order

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We establish a novel mechanism of stripe formation in doped systems with alternating t_{2g} orbital order—the stripe takes the form of a ferro-orbitally ordered domain wall separating domains with staggered order and allowing for deconfined motion of holes along the stripe. At a finite level of hole concentration this gives rise to the stability of this solitonic type of stripes, while we show that the phase change of the staggered order by π plays a minor role in orbitally ordered systems. These results shed new light on the physics of doped materials in which orbital degeneracy is present.

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In the context of superconductivity in cuprates, both experimental and theoretical aspects of stripes have been the subjects of intensive research [1]. At least in the low doping range, these systems can be viewed as an antiferromagnetic (AFM) phase into which holes have been injected. When a hole hops in an AFM background, it interchanges position with a single spin in each step and creates a "string" of flipped spins along its path [2], which accumulates energy cost and thus confines the hole in the system with classical (Ising-type) interaction. At finite doping spin and charge density modulations (stripes) develop, which is a way to find compromise between two opposite tendencies: (i) to delocalize holes and gain hopping energy $\propto t$ and (ii) let AFM correlations develop, which optimize the superexchange energy $\propto J$. It seems that, due to the presence of quantum spin fluctuations, stripes in cuprates show bond order, i.e., take the form of ladders with dominating singlet correlations on the rungs [3]. In addition, stripe formation has been demonstrated to exist in a model with classical AFM exchange interaction [4], the so-called t-J_z model, outlined in Figs. 1(a) and 1(b). While the t-J_z model is hard to realize in spin systems, we show in this Letter that a related mechanism of stripe generation would work in t_{2g} orbital systems.

Some previous theoretical analyses of stripe formation in orbitally degenerate systems led to the conclusion that lattice distortions are essential for this kind of ordering in systems with e_g orbital degrees of freedom [5]. Stripes in pnictides with active t_{2g} orbitals were suggested only very recently [6]. We will demonstrate that in systems with t_{2g} degeneracy and for large on-site Coulomb interaction U merely the interplay between hopping and the orbital superexchange interaction gives rise to the formation of ferro-orbitally (FO) ordered stripes as domain walls (DWs) between regions with the alternating orbital (AO) order. With the goal of analyzing this phenomenon in detail, we concentrate on the recently introduced strong-coupling version of the multiorbital Hubbard model for spinless fermions [7] on the square lattice (when the spins form a ferromagnetic order). This model is applicable either to transition metal oxides with active t_{2g} orbitals (when the tetragonal crystal field splits off the xy orbital from the $\{yz, zx\}$ doublet filled by one electron at each site, as for instance in Sr_2VO_4 [8]) or to cold-atom systems [9] with active p orbitals [10].

The strong-correlation limit of the model reads:

$$\mathcal{H}_{t_{2g}} = \mathcal{P}\,(\mathcal{H}_t + \mathcal{H}_J + \mathcal{H}_{3s}^{(l)} + \mathcal{H}_{3s}^{(d)})\,\mathcal{P}, \tag{1}$$

$$\mathcal{H}_t = -t\sum_i (b_i^\dagger b_{i+\hat{\mathbf{a}}} + a_i^\dagger a_{i+\hat{\mathbf{b}}} + \text{H.c.}), \tag{2}$$

$$\mathcal{H}_J = \frac{1}{2}J\sum_{\langle ij\rangle}\left(T_i^z T_j^z - \frac{1}{4}n_i n_j\right), \tag{3}$$

$$\mathcal{H}_{3s}^{(l)} = -\tau\sum_i (b_{i-\hat{\mathbf{a}}}^\dagger n_{ia} b_{i+\hat{\mathbf{a}}} + \text{H.c.}) - \tau\sum_i (a_{i-\hat{\mathbf{b}}}^\dagger n_{ib} a_{i+\hat{\mathbf{b}}} + \text{H.c.}), \tag{4}$$

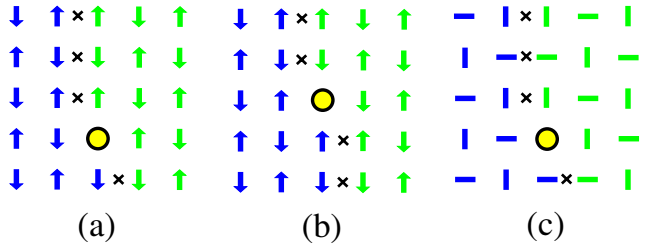

FIG. 1 (color online). The mechanism of stripe formation in the spin Ising model: a hole doped at the DW kink (a) moves together with the kink (b). In contrast, a hole doped at the DW kink in the orbital t_{2g} system (c) is confined to two sites. Two domains with AFM (AO) order are shown by arrows (boxes); broken bonds are marked by ×.

$$H_{3s}^{(d)} = -\tau \sum_i (a^\dagger_{i\pm\hat{\mathbf{b}}} a_i b_i^\dagger b_{i\pm\hat{\mathbf{a}}} + \text{H.c.}) - \tau \sum_i (a^\dagger_{i\mp\hat{\mathbf{b}}} a_i b_i^\dagger b_{i\pm\hat{\mathbf{a}}} + \text{H.c.}). \quad (5)$$

Here a and b refer to two t_{2g} orbital flavors [7], $yz \equiv a$ and $zx \equiv b$, and the summations are carried over $i \in ab$ sites in the ab plane. The orbital superexchange $J = 4t^2/U$ and the effective next nearest neighbor hopping $\tau = t^2/U$ apply when $U \gg t$ [11]. The pseudospin operator is $T_i^z = \frac{1}{2}(n_{ia} - n_{ib})$, while the projection operator $\mathcal{P}$ removes from the Hilbert space states in which any site is doubly occupied; for more details see Ref. [7].

Single hole motion is in principle confined in the spin t-J_z model due to the potential well effect caused by the formation of strings. An effective way to avoid the string effect is to form an antiphase DW between two AFM domains, consisting of two semilines separated by a transversal kink, and to create a hole at one of two sites nearest to the kink in that DW; see Figs. 1(a) and 1(b). The hole may be shifted along the wall without increasing the number of broken bonds. As the energy gain of $-t$ is typically larger than the energy loss $J_z/2$ due to a broken bond, at a certain level of hole doping the energy decrease induced by free hopping of holes along the stripe will compensate the increase of the magnetic energy caused by the creation of the DW [4].

Despite the similarity between the spin t-J_z model [4] and the t_{2g} orbital model given by Eqs. (1)–(5), the mechanism of stripe formation based on solitonlike motion of the kink-hole complex is not applicable to orbitally degenerate systems. This can be understood by analyzing the DW shown in Fig. 1(c). Boxes aligned along the $\hat{\mathbf{a}}$ ($\hat{\mathbf{b}}$) direction represent b (a) orbital flavors in two domains with opposite phases of the AO order. Again, similarly to the Ising AFM state, we have created an antiphase DW with a kink, and we have removed an electron from one of two sites nearest to the kink center. The downward shift of the hole by one lattice spacing is blocked by the b orbital below it. This follows directly from the form of the hopping (2), which is one dimensional (1D) in ordered ab planes [7]. The upward shift of the hole by one lattice spacing is allowed, but after that move the hole will be blocked again from above. Therefore, the hole and kink motion are confined in the orbitally degenerate system with the straight antiphase DW and a single kink in it [Fig. 1(c)]. Nevertheless, since the term (2) brings the biggest energy scale ($t \gg J$), we may expect that it will modify the form of the ground state above a certain filling level. The mechanism of hole deconfinement, however, is different, as we show below by a detailed stability analysis.

The DW depicted in Fig. 1 is the most favorable one in terms of the minimal number of broken bonds per one DW site. For an orbitally degenerate system, however, the hole motion by hopping t is allowed along the chain only when orbitals reorient, similarly to the 1D e_g systems [12]. Such a FO ordered vertical chain of a orbitals in Fig. 2(a) provides a DW between AO domains, and makes it possible to deconfine the hole motion along it. The price one has to pay is two (not one) broken bonds per site. After replacing one electron (orbital) in the chain by a hole [Fig. 2(b)], the hole can move due to $\mathcal{H}_t$ (2) by one step [Fig. 2(c)], and two broken bonds are removed and two other ones are created—hence the total number of broken bonds remains unchanged. In this way the hole motion occurs in both directions, leaving behind the undisturbed zigzag pattern of broken bonds.

The hole may also penetrate into the orbitally ordered domains, as for instance when the term (2) interchanges the hole with b orbital in Fig. 2(b), leading to the state depicted in Fig. 2(d). Now the hole can hop further to a nearest neighbor site either downwards or upwards, but when it enters "deeper" into the AO domain, the number of broken bonds increases (now by one) and the string effect [2] occurs [Fig. 2(e)]. This mechanism efficiently confines the hole motion to the stripe DW. The expected energy gain due to hole motion over a homogenous AO state is realized by the parallel alignment of a orbitals in the chain, while the phase change by π between two AO domains is irrelevant to achieve that gain. A similar FO ordered chain deconfining the hole motion and having the same energy cost can also be created by reversing every second orbital along a vertical polaronic line within a single domain of the AO order, see Fig. 2(f)—it generates a polaronic wall (PW) by a mechanism similar to that which operates in the 1D e_g orbital model [12]. The main difference between stripes depicted in Figs. 2(b) and 2(f) is that the hole in the DW stripe may penetrate one domain from each stripe site, while in the PW stripe it can enter both domains from every second site [the hole in Fig. 2(f) can move horizontally only from site j (not from l) either to site i or to site k].

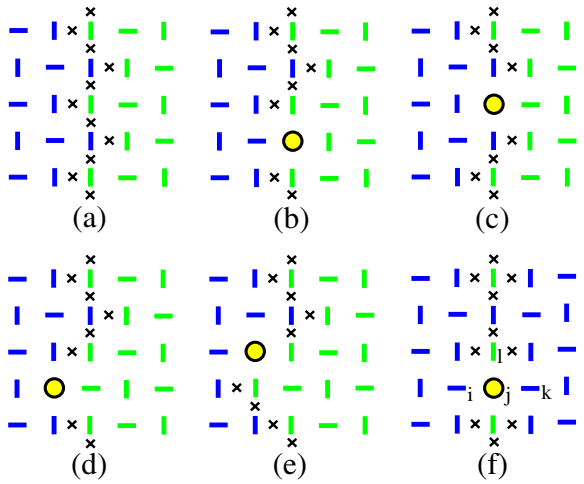

FIG. 2 (color online). Processes governing hole propagation in the stripe formed as a DW between two domains of the AO order (a): a doped hole may hop either along the DW (b),(c) or sidewards (d),(e); (f) shows the PW of a orbitals formed within a single AO domain; broken bonds are marked by ×.

The explicit analysis presented below will demonstrate that it is energetically somewhat more favorable to create the antiphase DW stripe.

In order to discuss stripe stability we must first analyze single hole propagation in the homogenous AO phase by means of the same method which will be used later for stripes. We begin with a hole replacing a orbital, as shown in Fig. 3(a)—the hopping term $\propto t$ can shift a hole only horizontally to its neighboring sites which are occupied by b orbitals [Fig. 3(b)]. The hole motion can be continued, and after the second and the third hop the number of broken bonds increases; see Figs. 3(c) and 3(d). In general, the energy rise $\propto J$, growing with the number of broken bonds, confines the hole motion (here initiated by the hop in the direction $\hat{\mathbf{a}}$) [7]. The number of defected bonds can be easily evaluated explicitly for paths up to length of seven steps, as we have done in our analysis. For longer paths reasonable approximations can be developed. They follow from the relation between the number of broken bonds and the number of bends in the path, see Fig. 3(d), and on the number of zigzags, such as that arising if the hole in Fig. 3(c) has moved left.

The action of the term (5) does not give rise to hole deconfinement, as it moves a hole generating several broken bonds, cf. Figs. 3(a) and 3(c). In contrast, weak hole deconfinement ($\tau \ll t$) occurs due to the term (4) which shifts a hole by two lattice spacings. This takes place without bringing about any additional defects in the AO order and is allowed provided that the opposite orbital (here b) occupies the intermediate site [Figs. 3(a) and 3(e)].

We are now going to cast the insights which have been outlined above into the framework of the recursion method [13] applied to the Green's function, and to determine the self-energy. The starting point is the bare Green's function $G_0(k_b, \omega)$ related with hole deconfined movement in the

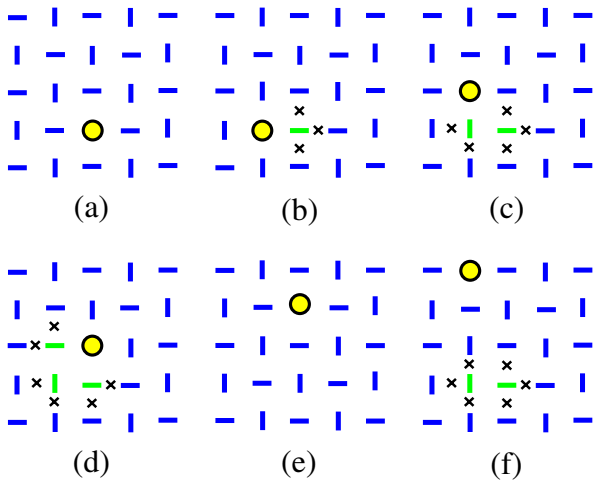

FIG. 3 (color online). Artist's view of hole propagation in the homogenous $|\mathrm{AO}\rangle$ state (a)—a hole may move due to t (2) and create broken bonds, marked by $\times$, after one (b), two c), or three (d) hops, while τ (4) does not disturb the AO order (a) and (e), but may also leave behind broken bonds (c) and (f).

$|\mathrm{AO}\rangle$ state mediated by the free propagation term (4) along the $\hat{\mathbf{b}}$ axis, with momentum k_b [Fig. 3(e)]—it is $G_0^{-1}(k_b, \omega) \equiv \omega - 2\tau\cos(2k_b) - J$. A reference energy of the $|\mathrm{AO}\rangle$ state has been subtracted in $G_0^{-1}(k_b, \omega)$, and the energy J above arises from the four bonds removed from the $|\mathrm{AO}\rangle$ state by adding a hole. The energy dispersion $\propto\tau$ in $G_0(k_b, \omega)$ is given by the matrix element of the full Hamiltonian evaluated for the propagating state $|1\rangle = \sqrt{\frac{2}{L}}\sum_n \exp(i2nk_b)a_{2n\hat{\mathbf{b}}}|\mathrm{AO}\rangle$, where L is the system length along $\hat{\mathbf{b}}$, and the hole is at the origin in Fig. 3(a).

The full Green's function contains the self-energy, $G^{-1}(k_b, \omega) = G_0^{-1}(k_b, \omega) - \Sigma(\omega)$, which stems from the confined motion initiated by the first step in the **a** direction transverse to the coherent propagation along **b**. The confined motion [Figs. 3(a)–3(d)] is accompanied by string formation and path retracement by holes. We evaluated $\Sigma(\omega)$ analytically by applying the recursion procedure, i.e., by the consecutive action with the Hamiltonian (1) on the state $|1\rangle$, which represents the hole created in the perfect AO order [Fig. 3(a)]. The only approximations consist of neglecting (i) some details in long hole paths, (ii) some processes mediated by the term (4) (such as those represented by Figs. 3(c) and 3(f); they bring about only a minor incoherent contribution [7]), and (iii) hole-hole interactions within AO domains. On the other hand, we always implement the constraint that the hole path cannot encircle a plaquette—its topological reason can be recognized by analyzing Fig. 3.

$\Sigma(\omega)$ takes the form of a continued fraction. For example, if we neglect, for demonstration purposes only, the term (5) (it is taken into account in the actual calculation but gives only minor corrections as $\tau \ll t$), one finds

$$\Sigma(\omega) = \frac{2t^2}{\omega - \frac{7}{4}J - \frac{2t^2}{\omega - 9J/4 - \cdots}}, \tag{6}$$

where prefactors 2 at t^2 refer to the number of ways by which a path can be further extended after the 1st and 2nd hop to a neighboring site. Such terms represent off-diagonal matrix elements of the Hamiltonian between consecutive states created during the recurrence procedure [13]. The prefactors 7 and 9 at $J/4$ stand for the number of bonds for which the superexchange (3) gives 0 for paths of length 1 and 2, respectively (instead of $-J/4$ as for all bonds in the $|\mathrm{AO}\rangle$ state)—they enter as diagonal matrix elements of the Hamiltonian. By searching for zeros of $G^{-1}(k_b, \omega)$ the quasiparticle dispersion $\epsilon_0(k_b)$ can be derived. For the numerical results shown in Fig. 4(a), sufficiently long paths (up to 12 steps) have been considered in order to obtain the saturation of results.

The same method of analysis apart from a minor modification may also be applied to the DW stripe itself. Since two states shown in Figs. 2(b) and 2(c) are not related to each other by a translation, both of them, $|1'\rangle = \sqrt{\frac{2}{L}}\sum_n \exp(i2nk_b)a_{2n\hat{\mathbf{b}}}|\mathrm{DW}\rangle$ and $|1''\rangle = \sqrt{\frac{2}{L}}\sum_n \exp\{i(2n+1)k_b\}a_{(2n+1)\hat{\mathbf{b}}}|\mathrm{DW}\rangle$, need to be chosen as a starting point in

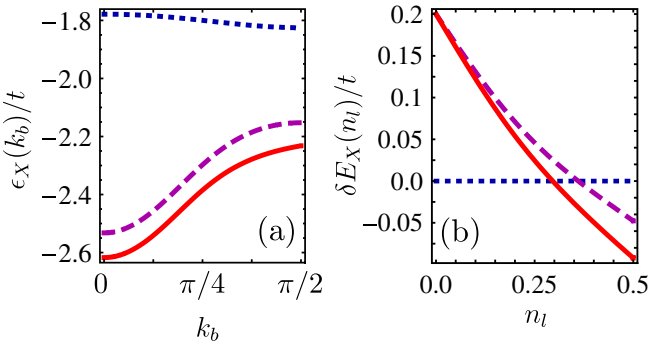

FIG. 4 (color online). (a) Quasiparticle dispersion $\epsilon_X(k_b)$ for the homogeneous AO phase ($X = 0$, dotted line) and for two kinds of stripes, $X =$ PW (dashed line) and $X =$ DW (solid line). (b) Energy gain $\delta E_X(n_l)$ per site (7) for two stripe phases for increasing stripe filling n_l. Parameters: $J = 0.4t$, $\tau = 0.1t$.

the recursion method. Here $|\mathrm{DW}\rangle$ stands for the empty stripe depicted in Fig. 2(a), and the position of the hole in Fig. 2(b) is given by the zero vector. Thus the recursion method has to be generalized to the case of several initial states. We have found this generalization, but since the procedure has turned out to be equivalent to the so-called projection-operator technique [14], we do not discuss it here in detail. The Green's function and the self-energy are given now by 2×2 matrices. The inverse bare Green's function has only off-diagonal nonvanishing matrix elements, $[G_0^{-1}(k_b, \omega)]_{1'1''} = [G_0^{-1}(k_b, \omega)]_{1''1'} = \omega - 2t\cos(k_b) - J/4$, where the reference energy due to the Ising term (3) has been subtracted again. When applying the recurrence procedure to the evaluation of $\mathbf{\Sigma}(\omega)$, we may use our previous observations regarding the matrix elements of the Hamiltonian between states representing different paths, in some cases including modifications brought about by the presence of the DW.

The PW stripe formed as a FO ordered chain within the AO order, shown in Fig. 2(f), can also be solved by using the generalized version of the recursion method. By looking for the zeros of the inverted Green's function, or of the determinant, if $G(k_b, \omega)$ is given by a matrix, we have determined and showed in Fig. 4(a) the energy dispersion $\epsilon_0(k_b)$ in the $\hat{\mathbf{b}}$ direction for the homogeneous system with AO order, $\epsilon_{\mathrm{PW}}(k_b)$ for the PW stripe and $\epsilon_{\mathrm{DW}}(k_b)$ for the antiphase DW stripe. Different dispersions confirm that the hole motion stems from t (τ) hopping in the stripe phases (homogeneous AO phase).

We investigate the stability of both types of stripe phases using the energy gain per site ($X =$ DW, PW),

$$\delta E_X(n_l) = \frac{1}{\pi}\int_0^{n_l\pi} dk_b \epsilon_X(k_b) - E_0(n_l) + \delta E_J, \qquad (7)$$

with respect to the doped homogeneous AO phase with energy $E_0(n_l) = n_l\epsilon_0(\pi/2)$, given by the band energy minimum $\epsilon_0(\pi/2)$ and proportional to the linear stripe filling n_l in the low doping regime (when the linear filling does not increase the global filling). Here $\delta E_J = J/2$ is the energy cost of two broken bonds in a stripe phase. The stripes are stabilized by increasing n_l, see Fig. 4(b), but the PW stripes are somewhat less stable, which we interpret as following from the destructive interference of hole penetration paths into left or right AO domains.

In conclusion, we have shown that a purely electronic mechanism leads to self-organization in the form of FO ordered stripes at antiphase DWs, penetrating into the AO order—this novel phase becomes more stable than the doped homogeneous AO state at the linear filling of $n_l \simeq 0.26$ ($n_l \simeq 0.25$) for $J = 0.4t$ ($J = 0.2t$). The energy gain over the PW stripes is small for all n_l, which suggests that the latter form of stripes might also be formed at finite temperature. These features are unique and can be of relevance to the behavior of doped Mott insulators with t_{2g} or p orbital order when spins may be neglected.

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