Ferro-Orbitally Ordered Stripes in Systems with Alternating Orbital Order

Piotr Wróbel\textsuperscript{1,2} and Andrzej M. Oleś\textsuperscript{3,4}

\textsuperscript{1}Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187 Dresden, Germany
\textsuperscript{2}Institute for Low Temperature and Structure Research, P.O. Box 1410, 50-950 Wrocław 2, Poland
\textsuperscript{3}Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, 70569 Stuttgart, Germany
\textsuperscript{4}Marian Smoluchowski Institute of Physics, Jagellonian University, Reymonta 4, 30-059 Kraków, Poland

(Dated: 28 January 2010)

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 $\pi$ 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.

Published in: Phys. Rev. Lett. \textbf{104}, 206401 (2010).

PACS numbers: 71.10.Fd, 72.10.Di, 72.80.Ga, 75.60.Ch

In the context of superconductivity in cuprates both experimental and theoretical aspects of stripes have been the subjects of intensive research \cite{1}. At least in the low doping range, these systems can be viewed as an antiferromagnetic (AF) phase into which holes have been injected. When a hole hops in an AF background, it interchanges position with a single spin in each step and creates a “string” of flipped spins along its path \cite{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 AF correlations to 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, \ie take the form of ladders with dominating singlet correlations on the rungs \cite{3}. In addition, stripe formation has been demonstrated to exist in a model with classical AF exchange interaction \cite{4}, so called $t$-$J$ model, outlined in Figs. \textsuperscript{1}(a) and \textsuperscript{1}(b). While the $t$-$J$ 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 analyzes of stripe formation in orbitally degenerate systems lead to the conclusion that lattice distortions are essential for this kind of ordering in systems with $e_g$ orbital degrees of freedom \cite{5}. Stripes in pnictides with active $t_{2g}$ orbitals were suggested only very recently \cite{6}. We will demonstrate that in systems with $t_{2g}$ degeneracy and for large onsite 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 multi-orbital Hubbard model for spinless fermions \cite{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, \eg for instance in Sr$_2$VO$_4$ \cite{8}), or to cold-atom systems \cite{9} with active $p$ orbitals \cite{10}. The strong-correlation limit of the model reads:

\begin{align}
\mathcal{H}_{t_{2g}} &= \mathcal{P} \left( \mathcal{H}_{t} + \mathcal{H}_{J} + \mathcal{H}_{3s}^{(l)} + \mathcal{H}_{3s}^{(d)} \right) \mathcal{P}, \\
\mathcal{H}_{t} &= -t \sum_{i} \left( b_{i\uparrow} b_{i\uparrow}^\dagger + a_{i\uparrow}^\dagger a_{i\uparrow} + \text{H.c.} \right), \\
\mathcal{H}_{J} &= \frac{1}{2} J \sum_{(ij)} \left( T_{i}^{z} T_{j}^{z} - \frac{1}{4} n_{i} n_{j} \right), \\
\mathcal{H}_{3s}^{(l)} &= -\tau \sum_{i} \left( b_{i\uparrow}^\dagger a_{i\uparrow} n_{i} b_{i\uparrow} + \text{H.c.} \right), \\
\mathcal{H}_{3s}^{(d)} &= -\tau \sum_{i} \left( a_{i\uparrow}^\dagger a_{i\uparrow} n_{i} b_{i\uparrow} + \text{H.c.} \right).
\end{align}

\begin{figure}[ht]
\centering
\includegraphics[width=\textwidth]{fig1.png}
\caption{(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 AF (AO) order are shown by arrows (boxes); broken bonds are marked by $x$.}
\end{figure}

\textsuperscript{1}PACS numbers: 71.10.Fd, 72.10.Di, 72.80.Ga, 75.60.Ch

\textsuperscript{2}Published in: Phys. Rev. Lett. \textbf{104}, 206401 (2010).
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 $P$ 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 AF 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)-(b). The hole may be shifted along the wall without increasing the number of broken bonds. As the energy gain of $-\tau$ 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 soliton-like 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 $\hat{a}$ ($\hat{b}$) direction represent $b$ ($a$) orbital flavors in two domains with opposite phases of the AO order. Again, similarly to the Ising AF 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 [4], 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 deconfin e the hole motion along it. The price one has to pay are 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 $H_t$ 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 zig-zag 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 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 $\pi$ 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. 3(f) can move only from site \(j\) (not from \(l\)) either to site \(i\) or to site \(k\). 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 an orbital [Fig. 3(a)] — the hopping term \(\propto t\) can shift a hole only horizontally to its neighboring sites which are occupied by \(\text{AO}\) 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)-(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 \(\hat{a}\)) [3]. 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 [4] does not give rise to hole deconfinement, as it moves a hole generating several broken bonds, cf. Figs. 3(a)-(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), 3(e)].

We are going now 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 \(G_\text{0}(k_b, \omega)\) related with hole deconfined movement in the \(\text{AO}\) state mediated by the free propagation term [4] along the \(\text{b}\) axis, with momentum \(k_b\), [Fig. 3(e)] — it is \(G_\text{0}^{-1}(k_b, \omega) = \omega - 2\tau \cos(2k_b) - J\). A reference energy of the \(\text{AO}\) state has been subtracted in \(G_\text{0}^{-1}(k_b, \omega)\), and the energy \(J\) above arises from the four bonds removed from the \(\text{AO}\) state by adding a hole. The energy dispersion \(\propto \tau\) in \(G_\text{0}(k_b, \omega)\) is given by the matrix element of the full Hamiltonian evaluated for the propagating state \(|1\rangle = \sqrt{\frac{2}{L}} \sum_n \exp(i2nk_b)a_{2n\text{b}}[^{\text{AO}}\rangle\), where \(L\) is the system length along \(\text{b}\), and the hole is at the origin in Fig. 3(a).

The full Green’s function contains the selfenergy, \(G^{-1}(k_b, \omega) = G_\text{0}^{-1}(k_b, \omega) - \Sigma(\omega)\), which stems from the confined motion initiated by the first step in the \(\text{a}\) direction transverse to the coherent propagation along \(\text{b}\). The confined motion [Figs. 3(a)-(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 [4] 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) all 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 can not encircle a plaquette — its topological reason can be recognized by analyzing Fig. 4.

\[
\Sigma(\omega) = \frac{2t^4}{\omega - \frac{t}{4}J - \sqrt{\omega^2 - 9J^2/4}} \quad : (6)
\]

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 [12]. The prefactors 7 and 9 at \(J/4\) stand for the number of bonds for which the superexchange [4] gives 0 for paths of length 1 and 2 respectively (instead of \(-J/4\) as for all bonds in the \(\text{AO}\) state) — they enter as diagonal matrix elements of the Hamiltonian. By searching for zeros of \(G^{-1}(k_b, \omega)\) the quasiparticle dispersion \(\epsilon_\text{Q}(k_b)\) 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 be also applied to the DW stripe it-
We investigate the stability of both types of stripe phases using the energy gain per site \( (X = \text{DW, PW}) \),

\[
\delta E_X(n_l) = \frac{1}{\pi} \int_0^{\pi/2} dk_b \epsilon_X(k_b) - E_0(n_l) + \delta E_J, \tag{7}
\]

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/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 \( n_l \approx 0.26 \) \((n_l \approx 0.25)\) for \( J = 0.4t \,(J = 0.2t)\). The energy gain over the PW stripes is small for all \( n_l \), which suggests that also the latter form of stripes might 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.

We thank P. Fulde, S. Kirchner, and K. Wohlfeld for insightful discussions. A.M.O. was supported by the Foundation for Polish Science (FNP) and by the Polish Ministry of Science and Education Project N202 068 32/1481.

---

[1] For recent reviews and more details see: J. Zaanen, Physica C 317, 217 (1999); S. Sachdev, Rev. Mod. Phys. 75, 913 (2003); S.A. Kivelson et al., ibid. 75, 1201 (2003); M. Vojta, Adv. Phys. 58, 699 (2009).

[2] L.N. Bulaevski, E.L. Nagaev, and D.I. Khomskii, Sov. Phys. JETP 27, 836 (1967); W.F. Brinkman and T.M. Rice, Phys. Rev. B 2, 1324 (1970); S.A. Trugman, ibid. 37, 1597 (1988).

[3] J.M. Tranquada et al., Nature (London) 429, 534 (2004); R. Eder and Y. Ohta, Phys. Rev. B 69, 094433 (2004); M. Vojta and T. Ulbricht, Phys. Rev. Lett. 93, 127002 (2004); P. Wróbel, A. Maciag, and R. Eder, J. Phys.: Condens. Matter 18, 1249 (2006).

[4] A.L. Chernyshev, A.H. Castro Neto, and A.R. Bishop, Phys. Rev. Lett. 84, 4922 (2000); A.L. Chernyshev, S.R. White, and A.H. Castro Neto, Phys. Rev. B 65, 214527 (2002); J.A. Riera, ibid. 64, 104520 (2001).

[5] T. Hotta, M. Feiguin, and E. Dagotto, Phys. Rev. Lett. 86, 4922 (2001); T. Hotta and E. Dagotto, ibid. 92, 227201 (2004); S. Dong et al., ibid. 103, 107204 (2009).

[6] Frank Krüger et al., Phys. Rev. B 79, 054504 (2009).

[7] M. Daghofer et al., Phys. Rev. Lett. 110, 066403 (2008); K. Wohlfeld et al., Phys. Rev. B 78, 214423 (2008).

[8] J. Matsuno et al., Phys. Rev. Lett. 95, 176404 (2005).

[9] D. Jaksch and P. Zoller, Ann. Phys. (N.Y.) 315, 52 (2005).
[10] X. Lu and E. Arrigoni, Phys. Rev. B 79, 245109 (2009).
[11] This condition is fulfilled in transition metal oxides; here an effective interaction $U$ includes Hund’s exchange.
[12] M. Daghofer, A.M. Oleš, and W. von der Linden, Phys. Rev. B 70, 184430 (2004).
[13] R. Haydock, J. Phys. C 5, 2845 (1972); O.A. Starykh and G.F. Reiter, Phys. Rev. B 53, 2517 (1996).
[14] H. Mori, Prog. Theor. Phys. 34, 399 (1965).