Charge stripes in the two-orbital Hubbard model for iron pnictides

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The two-orbital Hubbard model for the pnictides is studied numerically using the real-space Hartree–Fock approximation on finite clusters. Upon electron doping, states with a nonuniform distribution of charge are stabilized. The observed patterns correspond to charge stripes oriented perpendicular to the direction of the spin stripes of the undoped magnetic ground state. While these charge-striped states are robust when the undoped state has a Hubbard gap, their existence when the intermediate-coupling magnetic metallic state of pnictides is doped was also observed for particular model parameters. Results for hole doping and implications for recent experiments that reported electronic nematic states and spin incommensurability are also briefly discussed.

I. INTRODUCTION

The recent discovery of the iron-based pnictide superconductors[1] and the perception that the pairing mechanism may be triggered by antiferromagnetic fluctuations, similarly as in the cuprates, has motivated a considerable theoretical effort to understand the properties of multiorbital Hubbard models. Using a mean-field, random phase approximation, and computational techniques, several groups have addressed the nature of the undoped ground state of Hubbard models and the dominant pairing mechanisms upon doping.[2–7] Among the most robust results recently unveiled are (i) the existence of an intermediate Hubbard U coupling regime where the undoped state is simultaneously antiferromagnetic and metallic[6,7] as found in transport and neutron scattering experiments,[1] and (ii) the presence of superconducting tendencies upon charge doping mainly in the A_{1g} channel (extended $s\pm$, with nodes),[2–4,8] with the nodal pairing states B_{1g} and B_{2g} located close in energy.[3,4,8]

While the superconductivity and $(\pi,0)$ magnetism have received most of the attention, recent experiments have revealed an even more complex behavior in pnictides. For example, inelastic neutron scattering (INS) experiments reported evidence for spin incommensurability (spin IC) in the superconducting state of the hole very-overdoped pnictide KFe_2As_2.[9] This material does not have electron pockets in its band structure due to the heavy doping (50%) and, as a consequence, nesting mechanisms cannot produce the spin IC, whose origin then remains puzzling. Neutron studies for $FeSe_{0.5}Te_{0.5}$[10,11] have also reported low-energy spin IC peaks near the spin resonance.[11] Electron-doped pnictides such as $Ba(Fe,Co)_2As_2$ do not show spin IC at low energies,[12] but above 50 meV there is a splitting of the $(\pi,0)$ peak.

In parallel to these developments, scanning tunneling microscopy (STM) experiments on underdoped $Ca(Fe_{0.97}Co_{0.03})_2As_2$ reported the existence of static unidirectional electronic nanostructures of dimension 8 a_{Fe-Fe} (with a_{Fe-Fe} the interiron distance) along the a axis.[13] This electronic nematic order state is qualitatively similar to those widely discussed in other materials, such as in the high-temperature superconductors based on copper.[14,15] Note that the lines of spins that point in the same direction, namely the orientation of the $(\pi,0)$ spin stripes, is actually along the b axis, namely the nematic order and the spin-stripe order are perpendicular to one another.

The spin IC and nematic order reveal new similarities between the Cu- and Fe-based high-temperature superconductors, more than expected considering the widely accepted perception that the former are in the strongly correlated regime of Hubbard U couplings while the latter are at weak or intermediate coupling. In the Cu-oxide context, both spin IC and several electronic anisotropies in transport have been rationalized in terms of charge-*striped* states, either static or dynamic.[15] Could it be that similar states are also of relevance in the pnictides?

With this motivation, in this paper the possible existence of charge-striped states in Hubbard models for the pnictides will be explored. Within the real-space Hartree–Fock approximation, it will be shown below that the two-orbital Hubbard model indeed displays charge-striped states upon doping. The charge, spin, and orbital properties of these states will be discussed. The properties of the striped states reported below are robust when the coupling U is above the critical value needed to open a gap in the undoped limit. Considering the complex nature of multiorbital systems, it is important to document the properties of these striped states even in gapped regimes that at first sight are unrelated to undoped pnictides that are known to be (bad) metals. However, the charge amplitude of the stripes (namely the difference between the largest and smallest values of the charge at every site in the striped state) decreases with decreasing gap, and an interesting observation is that (weak) stripes are still found upon doping the intermediate coupling magnetic and *metallic* state of the undoped limit for particular hopping parameters. This result is conceptually different from the previous investigations of stripes in doped large-U Hubbard insulators.

II. MODEL AND METHOD

In this paper, the Hubbard model[3–5] based on the d_{xz} and d_{yz} Fe orbitals will be investigated. The use of these two orbitals is reasonable since they provide the largest contribution to the pnictide's Fermi surface.[16] Studies involving models

with more orbitals are certainly important, but they will be addressed only in future investigations after introducing the present findings based on two orbitals. A variety of other results that have recently been gathered for the two-orbital model[3,4,8] have already clearly shown that this model is in good agreement with experiments in several respects, including the existence of $(\pi,0)$-$(0,\pi)$ magnetic order, a Fermi surface that by construction is similar to those found in photoemission, and pairing channels that include the A_{1g} state (of which the s± pairing is a special case) as well as competitors with B_{1g} and B_{2g} symmetries. Note also that the use of five orbital models would demand a much larger computational effort than reported here, since the diagonalizations used in the iterative procedure to solve the Hartree–Fock (HF) equations scales as $(2N)^4$, with N the number of sites of the real-space cluster and 2 the number of orbitals. Thus a similar calculation for five orbitals will require $(5/2)^4 \sim 39$ times more computer time. It is for these reasons that it is reasonable to report first the analysis of the case of two orbitals, identifying the main tendencies, and then in the near future increase the number of orbitals. In the case of five orbitals, recent *ab initio* calculations supplemented by the construction of a model Hamiltonian led to predictions for the values of all the couplings that will be used in our model.[17] However, since not all pnictides have the same couplings, and since the calculation of Ref. 17 involves approximations, in this paper, and in future efforts with more orbitals, an exploration will be carried out varying the couplings in a reasonable range (mainly focusing on intermediate-U values, as suggested in Refs. 6,7), as opposed to fixing those couplings to a unique set.

As hopping amplitudes in the tight-binding portion of the model, fits to band calculations[5] as well as Slater–Koster (SK) hoppings[3,4] will be used. The electronic interaction is given by the standard Hubbard term, which has an intraorbital repulsion U, a Hund coupling J_H, an interorbital repulsion U' (fixed as $U' = U - 2J_H$ here), and a pair-hopping term with coupling $J' = J_H$.[18] The explicit model does not need to be reproduced here since it is well known from several previous investigations.[3-5] In the standard HF approximation in real space, the first term with the intraorbital repulsion U becomes $H_1^{HF} = U \sum_{i\alpha\sigma\sigma'} (-1)^{1-\delta_{\sigma,\sigma'}} [c_{i,\alpha,\sigma}^\dagger c_{i,\alpha,\sigma'} \langle c_{i,\alpha,-\sigma}^\dagger c_{i,\alpha,-\sigma'} \rangle - \frac{1}{2} \langle c_{i,\alpha,\sigma}^\dagger c_{i,\alpha,\sigma'} \rangle \langle c_{i,\alpha,-\sigma}^\dagger c_{i,\alpha,-\sigma'} \rangle]$. The other terms involve HF expressions too long to be reproduced here, but they are standard and the reader can find the full HF Hamiltonian in the supplementary information.[19] The minimization of the HF energy with respect to the various expectation values was carried out numerically via an iterative process,[20] mainly employing 16×16 clusters, with a starting configuration for the expectation values chosen at random at every site (i.e., without biasing toward striped states). Several clusters smaller than 16×16 were also explored, and size effects do not seem large.

III. RESULTS

A. Hoppings of Refs. 3,4

Let us start the description of our main results using the SK hoppings introduced in Refs. 3,4. A wide range of electronic densities $\langle n \rangle$ were numerically explored by varying the chemical potential μ. In most cases, the results of the HF

model energy minimization were sufficiently clear that they admit a simple discussion, and the emphasis below will be on those special cases, such as $\langle n \rangle \sim 2.3$. At these densities, several starting configurations for the unknown expectation values that appear in the HF model were chosen via a random number generator, and it was observed that the iterative process leads to nearly identical solutions or, if this was not the case, to local minima solutions with a higher energy. When different types of solutions were found, of course only those with the lowest energy were kept and analyzed.

Following the energy minimization criterion, the charge patterns found in some other cases were slightly more complicated, with segments of stripes clearly formed at the local level but sometimes with these segments not properly merged together to form nearly perfectly spaced stripes. Since these states still have all the characteristics of stripe states, it may occur that for a particular set of couplings some stripe configurations do not fit properly in the cluster sizes used, and geometrical frustration effects may lead to the partial breaking of the stripes. So while the focus below is on the most clear cases, the other states found are all "stripy" in nature; thus our results seem generic for a broad range of couplings and densities.[21]

Figure 1(a) contains a typical HF state that has been observed repeatedly in our studies, even using several different starting configurations for the iterations. It is clear that the charge is not uniformly distributed but it forms vertical stripes, breaking spontaneously rotational invariance. Of course, the $\pi/2$-rotated state is also a degenerate solution (horizontal stripes) and the convergence to one or the other depends on the randomly chosen initial state for the iterative process. Note that these stripes are "weaker" than the usual Cu-oxide HF stripes in the sense that the charge difference Δn [~0.15 in Fig. 1(a)] between the maximum n_{max} and minimum n_{min} local charges is not as large as in the cuprates where Δn is of the order of 1. This simply arises from the values of the coupling U that were investigated that are smaller for pnictides than for cuprates, in units of the bandwidth. Also it is interesting to
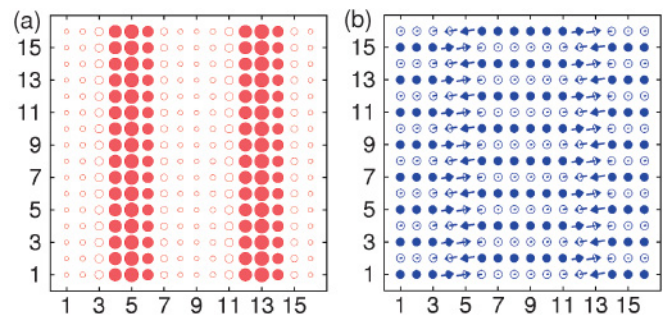

FIG. 1. (Color online) (a) Example of charge-striped state found in the HF approximation to the two-orbital model, using the hoppings of Refs. 3,4, $\langle n \rangle = 2.33$, $U = 0.8$, $J_H/U = 0.25$, and a 16×16 cluster. The size of the circles is linearly related to the charge, with the largest circles denoting $n_{max} = 2.42$ and the smallest $n_{min} = 2.27$. Here, and in the other figures, full (open) circles are used when the local density is larger (smaller) than the average. (b) Mean value of the spin in the state shown in (a). Note the presence of domain walls at the location of the charge stripes, inserted in a mainly $(0,\pi)$ background.

note that n_{min} in Fig. 1(a) is 2.27. Thus, the regions in the striped state that have the less charge still deviate from the "undoped" limit, and they are electron doped as the rest of the striped state, while in the cuprates the regions between the hole stripes have densities very close to those of the undoped insulator. From this perspective, our striped states should be metallic, in agreement with the density of states (not shown) that has a nonzero weight at the chemical potential μ.

The expectation values of the spin at each site, defined as $\vec{s}_{\mathbf{i}} = \langle \sum_{\alpha,\sigma,\sigma'} c^{\dagger}_{\mathbf{i},\alpha,\sigma} \vec{\sigma}_{\sigma\sigma'} c_{\mathbf{i},\alpha,\sigma'} \rangle$, that correspond to the striped state shown in Fig. 1(a) are given in Fig. 1(b). The spin pattern is dominated by the $(0,\pi)$ configuration, with spins parallel along one axis and antiparallel along the other. However, at the locations of the maximum electronic densities in Fig. 1(a), the $(0,\pi)$ spin order breaks locally and domain walls are formed,[22] with the spins where the local charge is maximized presenting an orientation nearly perpendicular to the rest. In a HF minimization problem, where all the expectation values are entangled, it is difficult to establish if the spin state with walls drives the charge stripes or vice versa. But by analogy with the cuprates, it can be expected that the spin state $(0,\pi)$ tries to expel the extra charge since it is disruptive to such a state, and such excess charge is located at the walls where the spin does not maintain locally the $(0,\pi)$ order. Of course, all these statements made for vertical stripes and spin $(0,\pi)$ order are the same for the rotated degenerate configuration with horizontal stripes and $(\pi,0)$ spin order.

The HF state of Figs. 1(a) and 1(b) has other interesting properties: (i) The orbital d_{yz} is more populated than d_{xz} in regions with the lowest local charge, i.e., where the spin order is locally $\sim(0,\pi)$. In our opinion, this should not be considered as indicative of long-range orbital order but instead it indicates an orbital weight "redistribution" induced by the spin order that breaks rotational invariance, as recently discussed elsewhere.[23] Where the local charge is the largest, on the other hand, both orbitals are populated approximately equally. (ii) The deviations from a perfect $(0,\pi)$ spin state induce a small shift away from $(0,\pi)$ in the spin structure factor peak position, toward (π,π). Then, the HF striped states can produce spin IC, as found in some experiments (see Sec. I). (iii) Note that the charge stripes and the spin stripes [i.e., the lines of parallel spins in the $(0,\pi)$ arrangement] are *perpendicular* to one another, as observed in the STM experiments where nematic order was reported.[13]

Figure 2(a) contains another typical HF state with charge stripes that was found in our studies, at an electronic density $\langle n \rangle$ larger than in Fig. 1(a), thus concomitantly inducing a reduction in the distance between stripes. It is interesting to observe that Δn is smaller than that in Fig. 1(a), suggesting that there must be an "optimal" doping for vertical/horizontal stripe formation, as found in cuprate's investigations, since in the undoped case $\langle n \rangle = 2.0$ there are no stripes and thus $\Delta n = 0$. Also, note that our results even farther from $\langle n \rangle = 2.0$ indicate a variety of complex patterns, with checkerboards, diagonal stripes, and other arrangements. However, since their associated spin orders are very different from the $(\pi,0)$ [or $(0,\pi)$] state prevailing in pnictides, and the doping is too large to be compared with available experimental results, those exotic states will not be described here. Presumably when the electronic density deviates substantially from the
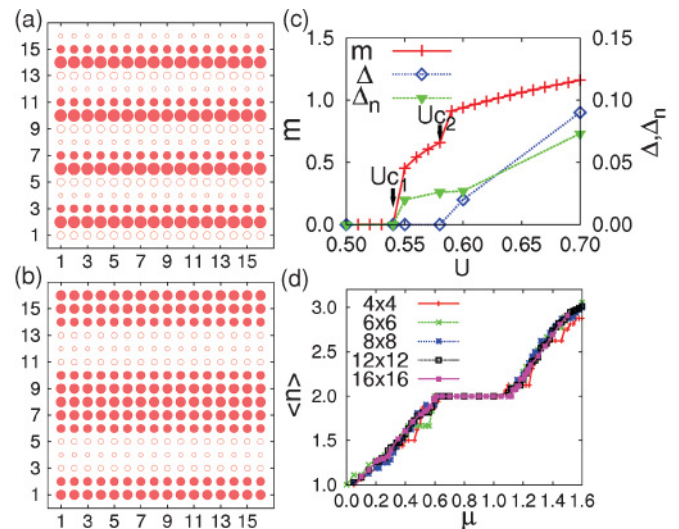

FIG. 2. (Color online) (a) HF charge-striped state using the hopping amplitudes of Refs. 3,4, at $\langle n \rangle = 2.45$, $U = 0.8$, and $J_{\rm H}/U = 0.25$. The size of the circles is proportional to the charge, with $n_{max} = 2.48$ and $n_{min} = 2.41$. (b) Same as (a) but for $\langle n \rangle = 1.83$, $U = 1.0$, with $n_{max} = 1.84$ and $n_{min} = 1.81$. (c) $(\pi,0)$ antiferromagnetic order parameter m, charge gap Δ (from $\langle n \rangle$ vs. μ), and $\Delta n = n_{max} - n_{min}$ at $\langle n \rangle \sim 2.3$, as a function of U. (d) $\langle n \rangle$ vs. μ at $U = 1.0$, $J_{\rm H}/U = 0.25$, and various lattice sizes, suggesting that size effects are small in this quantity. Results at others U's appear equally well converged.

undoped case, then our results reach a regime not yet found experimentally in these materials, or the two-orbital model breaks down.

Figure 2(b) contains results for the case of hole doping, and here the stripes are found to be weaker, with $\Delta n \sim 0.03$. At least for the hopping amplitudes of Refs. 3,4, the stripe tendencies appear stronger for electron doping than for hole doping. Also, in the hole-doped case the lines of parallel spins tend to run parallel to the charge stripes, instead of perpendicular as in the electron-doped case. This parallel vs. perpendicular relative patterns of charge and spin may depend on details and may not be universal; thus they need to be investigated in more detail in the future.

Figure 2(c) displays Δn vs. U, at $\langle n \rangle \sim 2.3$, compared with results for the undoped limit, namely the $(\pi,0)$ [or $(0,\pi)$] magnetic order parameter m and the charge gap Δ. While m rapidly grows with U at U_{c1}, Δ remains zero in a narrow region beyond U_{c1}, and only after reaching a second critical value U_{c2} it slowly increases with increasing U. This intermediate region is both metallic and magnetic, and has been emphasized before as the regime of interest for pnictides.[6,7] Δn follows Δ with decreasing U from strong coupling but it appears to survive, albeit with a small value, in the intermediate magnetic/metallic phase. If this result would survive the introduction of fluctuations beyond the HF approximation, the undoped metallic magnetic state would admit weak charge stripes upon doping, a conceptually novel result since previous stripe efforts have focused on their presence only when doping a Hubbard insulator. For those insulators the rationale for the presence of stripes was dominated by the fact that extra charges tend to disrupt the regular spin order of the undoped case.

Thus, to reduce this "damage" to spin order, the extra charge is arranged forming stripes. Such a way to understand the stripes of the cuprates can be extended to pnictides even in the magnetic and metallic regime: The extra charge may need to be accumulated in patterns, as opposed to regularly distributed, to minimize the energy damage to the spin order. Note also that size effects do not seem large here since some quantities are already converged on the 16×16 cluster [see Fig. 2(d)].

B. Hoppings of Ref. 5

The HF results obtained using another set of hopping amplitudes (Ref. 5) are presented in Fig. 3. In this case, the analysis was slightly more involved, since the convergence of the HF energy minimization was slower, with the iterative process for convergence sometimes ending in metastable states with charge inhomogeneous irregular patterns (but still displaying stripes locally). However, in many cases the convergence to a nearly perfect stripe pattern was clear. Figures 3(a) and 3(c) display the charge order in the HF states at two different $\langle n \rangle$'s and two U's with a magnetic undoped state (the hopping unit t_1 of Ref. 5 is taken as 0.2 eV here, as in Ref. 8). In both cases, charge stripes can be identified, with Δn growing with U, as in Fig. 2(c). At $U = 0.50$ the charge gap is negligible, so these (weak) charge stripes appear in the metallic magnetic state. The associated spin patterns also present a striped arrangement, and the spin and charge stripes are perpendicular. There are some differences between the stripes of Figs. 1 and 3, such as the stripe periodicity. These differences are to be expected since both sets of hopping parameters were constructed to produce similar undoped Fermi surfaces but

FIG. 4. (Color online) (a) Ground state of the HF Hamiltonian at $\langle n \rangle = 2.56$, $U = 1.0$, and $J_H/U = 0.25$, using the SK hoppings.[3,4] In the 16 sites shown in gray, there is an on-site energy $\epsilon = -0.85$ that simulates the presence of quenched disorder, such as caused by Co doping. (b) Monte Carlo results (equilibrated snapshot) obtained using the two-orbital spin-fermion model of Ref. 24 with SK hoppings,[3,4] $\langle n \rangle = 2.55$, $K = -1$, $J_{NN} = J_{NNN} = 0.05$, magnitude of the classical spins $S = 1$, temperature 0.005 eV, and 45,000 steps. The small deviation from a perfect stripe is caused by temperature.

their full band structures are different. However, it must be emphasized that, with both sets of hoppings, charge stripes are found in several cases, and, thus, their existence is a qualitative conclusion of our HF investigations.

C. Preliminary studies of the influence of Co doping on a striped state

The striped states found here could be of relevance to explain the static nematic state found via STM.[13] To test this hypothesis, a randomly-chosen set of lattice sites was selected to simulate the presence of Co-dopants via an on-site energy ϵ, and then the minimization of the HF model was again carried out in that background. A typical result is shown in Fig. 4(a). It is observed that this quenched disorder effectively cuts the long stripes into shorter segments, and the overall state qualitatively resembles those found with STM. Of course, only a tuning of couplings and electronic densities may render this agreement quantitative (for instance producing features of size 8 lattice spacings, as in experiments), and that effort is postponed for future work. Here, simply note that the charge and spin stripes found in our study tend to be perpendicular to one another, in nice agreement with the STM investigations.

D. Results for the spin-fermion model

Striped states were also studied via the two-orbital spin-fermion model recently proposed.[24] Using Monte Carlo techniques,[25] metastabilities limited the present effort to 8×8 clusters. In cases where good convergence was achieved, stripes were also found [Fig. 4(b)]. Thus, via the use of two rather different models and techniques, the presence of charge nonuniform states was confirmed.

IV. CONCLUSIONS

In summary, the numerical solution of the two-orbital Hubbard model in the HF approximation away from half-filling has been here discussed. Charge stripes appear at several electronic densities and in a broad range of couplings. The associated spin and orbital properties of the HF states have
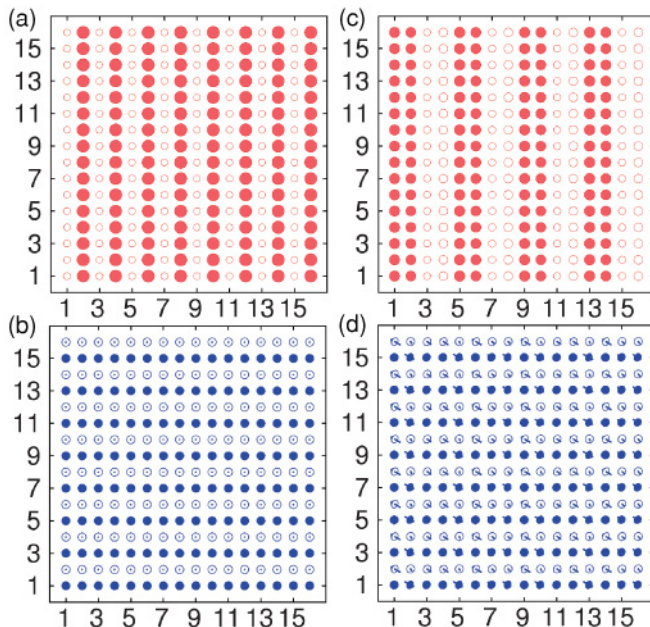

FIG. 3. (Color online) (a) Charge-striped state solution of the HF two-orbital Hubbard model, using the hoppings of Ref. 5, $\langle n \rangle = 2.36$, $U = 0.50$, and $J_H/U = 0.25$. The size of the circles is proportional to the charge, with $n_{\max} = 2.365$ and $n_{\min} = 2.361$ (a very weak charge stripe). (b) Spin state associated with (a). (c) Same as (a) but for $U = 0.90$, $\langle n \rangle = 2.14$, $n_{\max} = 2.141$, and $n_{\min} = 2.139$ (d) Spin state associated with (c).
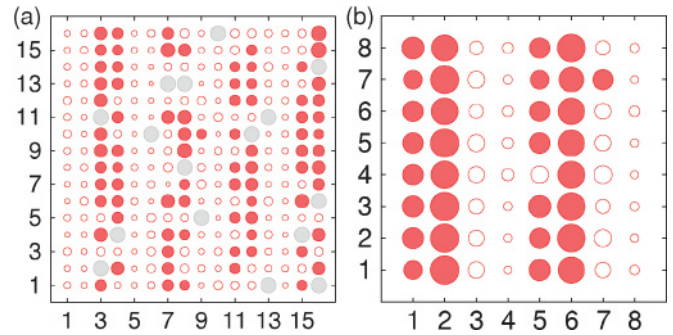
been discussed as well. However, the readers should be warned that the relevance of these states to real pnictides is a matter that still requires further work. On the one hand, the charge stripes found here appear to have an associated spin IC. Since neutron scattering results have actually unveiled a similar spin IC in cases where nesting can be excluded, then it is important to search for alternative explanations such as those presented here. In addition, the stripes discussed in this effort can also provide a qualitative rationalization of the nematic order found in STM experiments. On the other hand, the HF striped states are the more stable at couplings U where the undoped state is an insulator, albeit with a small gap. However, for the hopping sets investigated here, novel (weak) stripes were observed in the magnetic/metallic region, thus avoiding this conceptual problem. But this interesting observation must be confirmed with more refined calculations and using models with more orbitals.

In addition, it may occur that the surface of pnictides presents an effective U larger than in the bulk, due to the reduction of the carrier's bandwidth, complicating the analysis. Another issue to consider is that the use of models with more than two orbitals may lead to an effective electronic population in the d_{xz}-d_{yz} sector that is larger than 2.0, and charge stripes, magnetism, and metallicity may coexist in a single state at couplings U larger than those estimated to be realistic from the $\langle n \rangle = 2.0$ two-orbital model analysis. All these scenarios are speculative right now, and only further work can clarify the relevance of the striped states presented here to the physics of the pnictides.

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