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Bruce Normand, Arno P. Kampf

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Suppression of static stripe formation by next-neighbor hopping

B. Normand and A. P. Kampf
Theoretische Physik III, Elektronische Korrelationen und Magnetismus, Institut für Physik, Universität Augsburg, D-86135 Augsburg, Germany

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We show from real-space Hartree-Fock calculations within the extended Hubbard model that next-nearest neighbor (t') hopping processes act to suppress the formation of static charge stripes. This result is confirmed by investigating the evolution of charge-inhomogeneous corral and stripe phases with increasing t' of both signs. We propose that large t' values in YBCO prevent static stripe formation, while anomalously small t' in LSCO provides an additional reason for the appearance of static stripes only in these systems.

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The presence of charge-inhomogeneous and striped phases as candidate ground states for the cuprates continues to be one of the most contentious issues in high-temperature superconductivity (for a review and references see Ref. 1). Static stripes have been observed experimentally, but to date only in rare-earth-doped $La_{2-x}Sr_xCuO_4$ (LSCO) systems with the low-temperature tetragonal (LTT) structural distortion. Theoretical explanations for stripes fall into three categories: (i) they are a true ground state intrinsic to short-ranged models of the CuO_2 planes, (ii) they are a competing excited state stabilized by anisotropy, or (iii) they emerge when long-ranged interactions are invoked (generally to frustrate phase separation). We have recently subscribed to the second viewpoint, motivated by the direct experimental connection of lattice structure with stripe formation and suppression of superconductivity.[1]

However, the interpretation of striped phases as a consequence of lattice-induced hopping and superexchange anisotropy in the CuO_2 plane leaves some open questions. On the qualitative level, these include the absence of static stripes in orthorhombic $YBa_2Cu_3O_{7-\delta}$ (YBCO) systems, while quantitatively they include the value of the relative anisotropies required to stabilize a stripe phase. A key issue long recognized as a source of major differences between cuprate compounds is the shape of the Fermi surface.[2] This has been measured by angle-resolved photoemission (ARPES) for $Bi_2Sr_2CaCu_2O_{8+\delta}$ (BSCCO),[3] LSCO,[4] and $Nd_{2-x}Ce_xCuO_4$ (NCCO)[5] systems, and is most easily modeled by extended tight-binding band structures.[2] The primary influence of an extended band structure may be encapsulated in the single parameter t' governing the next-nearest-neighbor hopping on the square lattice. An investigation of t' effects is required in context of stripes, and is provided here within the real-space Hartree-Fock (RSHF) technique.[1]

The effects of next-neighbor hopping on stripes have been considered in the extended t-J model by exact diagonalization (ED)[6] and by density-matrix renormalization group (DMRG) calculations.[7] Both sets of authors reported a suppression of horizontal (or vertical) stripe order with increasing $|t'|$ of both signs, but detailed features of the results were not fully consistent. The authors of Ref. 7 also made a systematic comparison of stripe and pairing instabilities, finding a strong anticorrelation. A t' opposite in sign to t was included in a more general study of the extended (t-t') Hubbard model by RSHF,[8] which confirmed the tendency towards stripe suppression. The influence of t' on stripes has been considered in the context of Fermi-surface geometry,[9] and in terms of its effects on stripe filling.[10] Finally, extended hopping integrals were used in an ED study of doped stripes,[11] primarily to avoid phase separation.

The extended, anisotropic Hubbard model is given by

$$H = -\sum_{i,\eta=x,y,\sigma} t_\eta (c^\dagger_{i\pm\eta\sigma} c_{i\sigma} + \text{H.c.}) + U\sum_i n_{i\uparrow} n_{i\downarrow},$$

$$-\sum_{i,\eta=x\pm y,\sigma} t'_\eta (c^\dagger_{i\pm\eta\sigma} c_{i\sigma} + \text{H.c.}), \qquad (1)$$

where $n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$. We retain in Eq. (1) the possibility of anisotropic nearest-neighbor[1] and next-neighbor hopping, $t_x \neq t_y$ and $t'_{x+y} \neq t'_{x-y}$. However, the symmetry of next-neighbor terms in this one-band model is maintained in the LTT phase of LSCO, and for most of the study to follow. We apply the HF decomposition of the Hubbard term in Eq. (1) and seek self-consistent solutions for the static charge and spin configurations.

A detailed analysis of the RSHF technique was provided in a recent study of anisotropy effects on stripe formation.[1] The solutions were characterized as functions of the "intrinsic" system parameters, by which is meant the ratio U/t, the (hole) filling x, the temperature T, and the hopping anisotropy $t_x \neq t_y$, and for their dependence on the "extrinsic" parameters system size and geometry, boundary conditions (BCs), and commensuration of x with system size. As a result of this investigation, we have chosen two parameter sets representative of inhomogeneous spin and charge configurations whose evolution we will follow on varying t' in the extended Hubbard model. Hereafter we take the energy unit to be $t = 1$.

We focus on 12×12 systems with open BCs, and take $U/t = 5$ to give line-like charge structures. The cases we consider are: I—isotropic hopping, $t_x = t_y = 1$, with hole doping $x = 1/8$, where the ground state is a corral, or closed loop of diagonal, antiphase domain walls; II—anisotropic hopping, $t_x = 0.9$, $t_y = 1.1$, with hole doping $x = 1/6$, where the ground state consists of uniform, filled, antiphase stripes. The charge configurations with $t' = 0$ are reproduced[1] in Figs. 1(a) and (b) respectively for cases I and II. The site- or bond-centered

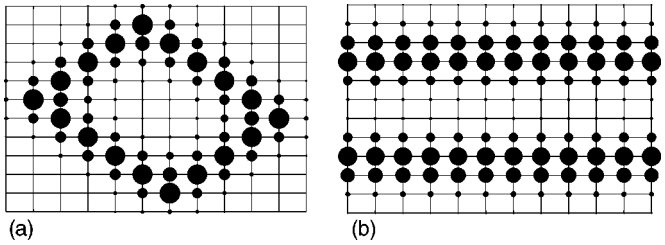

FIG. 1. Ground-state charge distributions for Hubbard model on a 12×12 cluster with $U=5$ and open BCs. In (a) $x=1/8$, $t_x=t_y=1$, and $t'=0$, while in (b) $x=1/6$, $t_x=0.9$, $t_y=1.1$, and $t'=0$. The hole density is scaled by radius, the largest circles corresponding to $\langle n_i\rangle=0.644$, or 35.6% doping of the site.

nature of the charge structures is not important for studying the influence of t'. With regard to stability against small changes in t', both corral and stripe solutions are found to have only minor, quantitative alterations when $|t'|\leq0.05$ for both signs.

Figure 2 illustrates the effects of increasing t' with the same sign as t. This changes the shape of the Fermi surface, which remains closed around the Γ point but expands in the directions $(k,\pm k)$ while contracting along $(\pm k,0)$ and $(0,\pm k)$. For the corral solution we see at $t'=0.1$ [Fig. 2(a)] a trend towards breaking of the domain line into small clusters, followed before $t'=0.2$ [Fig. 2(b)] by a complete evaporation of the inhomogeneous charge structure. The solution here and for higher $|t'|$ is a charge-uniform, "metallic" phase. The stripe solution shows similar behavior, in that the

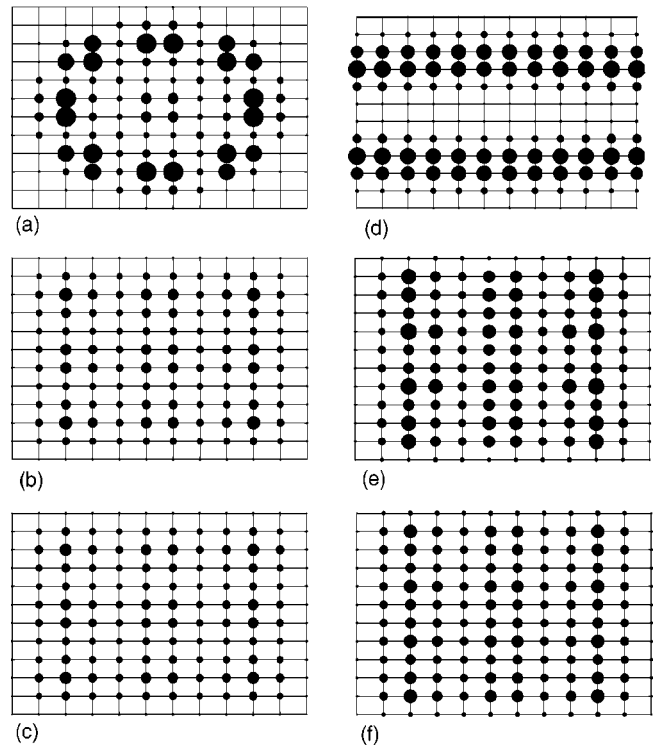

FIG. 2. As in Fig. 1. In (a)–(c) $x=1/8$ and $t_x=t_y=1$, while in (d)–(f) $x=1/6$, $t_x=0.9$, and $t_y=1.1$. $t'=0.1$ in (a) and (d), $t'=0.2$ in (b) and (e), and $t'=0.3$ in (c) and (f).

stable stripe phase is lost in the range $0.1<t'<0.2$ in favor of the uniform phase, which then persists to high values of t'. The spin configuration (not shown) in the uniform phase is commensurate antiferromagnetism, with an ordered moment suppressed in comparison to the antiferromagnetic (AF) regions of the corral and stripe solutions at $t'=0$.

This result has a straightforward interpretation in terms of the metallic state maximizing the hopping kinetic energy. Positive t' terms cause direct frustration of local charge and spin alignment by competing with the t term, resulting in a uniform distribution. One may also consider a band picture, where for this sign of t' the bandwidth of the lower Hubbard band in the spin-density wave (SDW) state at half-filling is increased, suggesting that doped hole-like carriers favor delocalization.[8] Our result and interpretation are fully consistent with DMRG studies of the t-J model,[7] which for $t'>0$ show a systematic loss of stripe charge order. These also find an enhancement of hole pairing, which is further consistent with our result because superconductivity would be expected as the leading low-temperature instability of the isotropic, metallic state. ED calculations[6] in this regime differ in that they report enhanced stripe order for $0<t'<0.2$, albeit for diagonal stripes at smaller (physical) values of J/t. The authors interpret this result in terms of the explicit next-neighbor hopping required to cancel the intra-sublattice hopping generated implicitly by the t term, and in accord with the present findings expect that carrier localization and stripe-formation are maximized when the sum of these two contributions to t' is minimized. A DMRG study[6] which tends to support this result remains in minor contradiction to Ref. 7, and the resolution is presumably to be found in commensuration effects on the differing system sizes used.

Figure 3 illustrates the effects of increasing $|t'|$ in the physical regime for the cuprates, where t' has the opposite sign to t. This results in the change from a closed to an "open" Fermi surface around the Γ point. For the corral solution we see at $t'=-0.1$ and -0.2 [Figs. 3(a,b)] a reinforcement of undisturbed AF order in the center of the system, and retention of the diagonal domain walls, until a more complex behavior sets in at $t'=-0.3$ [Fig. 3(c)]. For the stripe solution there is a definite crossover from horizontal stripes at small $|t'|$ to diagonal stripes at $t'=-0.1$ and -0.2 [Figs. 3(d,e)], again preceding a less clear structure at $t'=-0.3$ [Fig. 3(f)]. For both parameter sets, the high-t' configurations shown in Fig. 4 are rather complex in shape, only weakly inhomogeneous in charge structure and weakly but commensurately AF in spin structure.

For $t'/t<0$, the narrowing of the lower SDW Hubbard band suggests reduced carrier mobility and thus an enhanced tendency toward charge inhomogeneity. In a local hopping picture, all next-neighbor processes cost kinetic energy, and so are suppressed[1] by (i) aligning spins ferromagnetically on diagonal bonds, promoting AF order, and (ii) aligning holes on diagonal bonds, promoting diagonal domain walls. Both of these tendencies are clear in Fig. 3. At higher t' this trend cannot be sustained, as the kinetic energy cost of failure to delocalize is too great, and for $-0.4<t'<-0.3$ the kinetic energy associated with t' becomes negative despite the sign, as shown in Fig. 5. This is possible by a change in the coef-

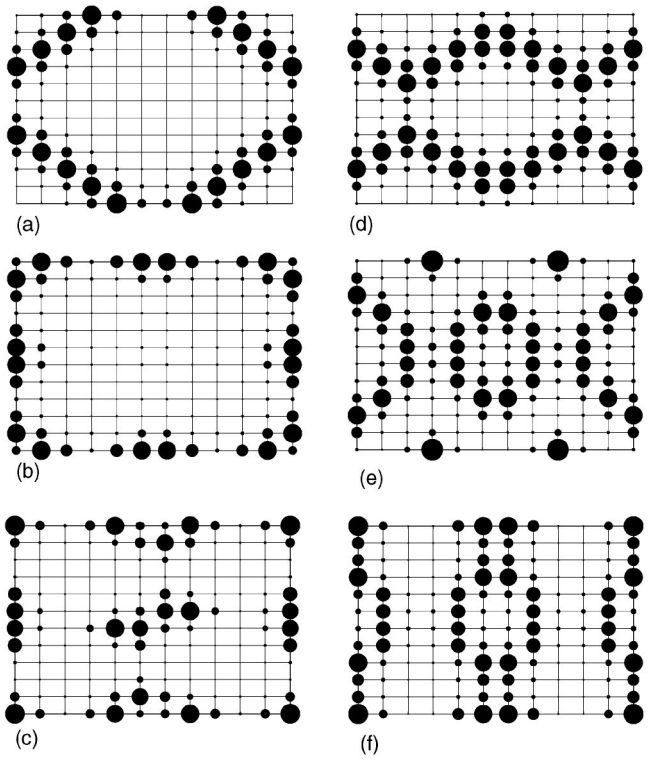

FIG. 3. As in Fig. 1. Here $x=1/8$ and $t_x=t_y=1$ in (a)–(c), while $x=1/6$, $t_x=0.9$, and $t_y=1.1$ in (d)–(f). $t'=-0.1$ in (a) and (d), $t'=-0.2$ in (b) and (e), and $t'=-0.3$ in (c) and (f).

ficients of the HF wave function such that on average the sign of the diagonal overlap is negative. While such an alteration is not readily visualized in terms of charge configurations, its consequences are the weakly inhomogeneous structures in Fig. 4. The tendency to carrier delocalization also for this sign of t' is in accord with the results of Ref. 10 for the hole filling of an isolated stripe.

In the DMRG calculations,[6,7] increasing $|t'|$ up to 0.3 introduces a doubling of the charge periodicity. From the above considerations we may offer a change from horizontal to diagonal stripes as a possible consistent explanation of this result, given the small number of holes involved. The observed suppression of pairing[7] is certainly consistent with the expectation of charge localization accompanying the formation of static, inhomogeneous charge structures. In the ED results,[6] both vertical and diagonal stripe correlations are strongly suppressed by t', whereas pairing correlations remain appreciable. Other RSHF studies of the extended Hubbard model[8] confirm a significantly reduced tendency to stripe formation in this parameter regime.

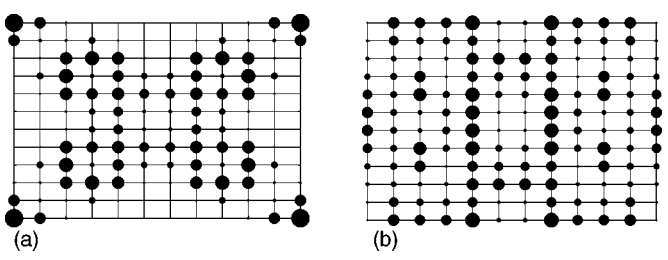

FIG. 4. As in Fig. 1, but with $t'=-0.6$.

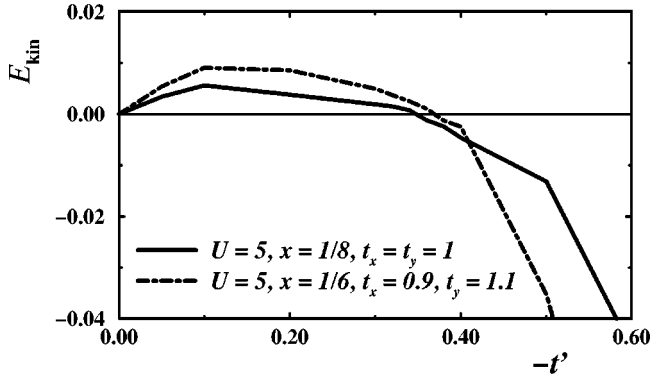

FIG. 5. Average kinetic energy $E_{\rm kin}$ per diagonal bond as a function of next-neighbor hopping t' opposite in sign to t.

All of the above results are for hole-doped systems. In the electron-doped regime, we find by RSHF an exact reproduction of the charge configurations in Figs. 1–4, with the important proviso that the sign of t' be reversed. This symmetry emerges from the band and local physics arguments invoked above, and can be seen in Fermi-surface shapes, but most importantly can be proven rigorously from the invariance of the Hamiltonian [Eq. (1)] under particle-hole transformation combined with sign reversal $c_i \rightarrow -c_i$ on one sublattice.

In summary, next-neighbor hopping terms t' lead to a rapid suppression of the $t'=0$ inhomogeneous charge structures in the Hubbard model. For hole- (electron-) doped systems the primary influence of positive (negative) t' (Fig. 2) on stripes lies in its delocalization effect, while that of negative (positive) t' (Figs. 3 and 4) is destruction of the spin registry and antiphase domain wall nature. This latter result suggests the importance of AF order in stabilizing static horizontal stripes.[14]

In cuprates ($t'/t<0$), the effective t' is intrinsically smaller for LSCO and related monolayer systems than for YBCO, BSCCO and the related mono-, bi-, and trilayer systems. This result may be obtained by simple fitting of tight-banding models to the Fermi surfaces measured by ARPES[2] and is also confirmed both by reduction (downfolding) of band structure calculations[12] and by cell perturbation techniques.[13] In addition to the number of layers, the apical oxygen atoms are seen to be an important factor contributing to the difference. Because deviations of the Cu–O–Cu bond angle from 180° reduce orbital overlap, the LTT and low-temperature orthorhombic (LTO) distortions of the LSCO structure also act to reduce $|t'|$ in comparison with unbuckled cuprate layers. At the tight-binding level, when t and t' are the only parameters in the extended hopping band structure, t' values of order $-0.5t$ are required to model the open, YBCO-like Fermi surface, while the closed LSCO surface is reproduced by values of $|t'|<0.2$.

We have considered previously the possible key role of the LTT distortion, which is the ground-state lattice structure only in Nd- and Eu-doped LSCO compounds.[1] Only the LTT distortion produces anisotropic t terms, and to the best of our

knowledge there remain no reports of static stripes in any non-LTT LSCO structures, or in any other cuprates. A natural question then arises concerning YBCO, where the presence of $\hat{b}$-axis chains leads to a planar structural anisotropy. Our results offer an explanation for the absence of static stripes in YBCO: the large effective t' values [Fig. 4] suppress the formation of charge-inhomogeneous structures which are candidate ground states at smaller t'. Further, t' is expected to be an important factor contributing to the absence of static stripes in the majority of hole-doped cuprates, where the Fermi surfaces of the CuO_2 planes are open. For electron-doped systems, we have shown these to be in the regime where stripe formation is suppressed by any value of t', which here favors a uniform, metallic phase.

We comment briefly that the LTO structure of the CuO_2 planes in LSCO and BSCCO has an asymmetrical t'. In RSHF, and for t' opposite in sign to t, a sufficiently large anisotropy $t'_{x+y} > t'_{x-y}$ yields diagonal stripes in the direction $\hat{x}+\hat{y}$. However, the required anisotropies are physically unjustified, and no effect of this nature is expected in the real material.

In conclusion, we have studied the effects of next-neighbor hopping within the extended Hubbard model on the formation of static stripes in cuprates. In a RSHF treatment, t' terms of both signs cause rapid suppression of horizontal stripe formation. When t' has the physical sign for cuprates (opposite to t), we find for hole-doped systems a window in which diagonal stripes are favored, and then a broad regime at large t' where the compromise charge configuration is only weakly inhomogeneous. For the opposite sign of t', a homogeneous, metallic phase is preferred. These properties are exactly reversed in electron-doped systems.

In contradiction to observations of superconductivity, the "physical" case is dominated by charge localization and suppression of hole pairing, whereas competition of inhomogeneous charge structures with the superconducting instability is reduced for $t'/t > 0$. However, these results are consistent with previous studies of extended Hubbard and *t-J* models. We propose that the weak t' terms characteristic of the LSCO system in comparison with other high-T_c superconductors is an important contributing factor to the appearance of static stripes only in these materials, and that stripe formation in electron-doped cuprates is suppressed for all t'.

We have recently become aware of the results of Ref. 15, which also emphasize the key role of extended hopping terms in destabilizing static stripes. The authors consider kink fluctuations in horizontal stripes at $x = 1/8$ as a function of t', and argue that extended hopping should be still more important at higher dopings, as is shown here.

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