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Angle-resolved photoemission spectra of the stripe phase in the two-dimensional *t-J* model

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The two-dimensional t-J model with and without t' and t'' hopping-terms is studied by exact diagonalization on a 5×4 cluster, which realizes a hole stripe in y direction in a spin-Peierls phase. Next nearest hopping terms with a sign appropriate for hole-doped cuprates enhance the stripe formation. The dispersion of the quasiparticle peaks in the single-particle spectrum is in good agreement with bond operator theory for hole motion in the spin-Peierls phase, particularly so for realistic values of t' and t''. The resulting spectral weight distribution and Fermi surface agree well with experimental angle-resolved photoemission spectra on $La_{1.28}Nd_{0.6}Sr_{0.12}CuO_4$.

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The prediction of charged stripes[1] and their subsequent experimental verification[2] stand out as one of the rare instances, where a nontrivial theoretical prediction for cuprate superconductors was found consistent with experiment. Accordingly, there is currently considerable interest in the mechanism leading to the formation and the physical implications of stripes.[3–10] On the other hand few experimental techniques provide such direct experimental insight into the electronic structure of a given compound as angle-resolved photoemission spectroscopy (ARPES). It is therefore quite natural to look for the fingerprints of stripes in ARPES spectra and indeed the results of Zhou *et al.* on $La_{1.28}Nd_{0.6}Sr_{0.12}CuO_4$ (Ref. 11) are widely considered as strong evidence for stripes. It is the purpose of the present manuscript to present single-particle spectra obtained by ‘‘computer spectroscopy’’ on the stripe phase of the two-dimensional (2D) t-J model, presumably the simplest theoretical description of the CuO_2 planes in cuprate superconductors. As will be seen below these results combined with a relatively crude theory for hole motion in a spin-Peierls ‘‘background’’ already give a quite satisfactory description of most of the experimental results.

The t-J model reads

$$H=-\sum_{i,j}\sum_{\sigma} t_{i,j}\hat{c}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma}+J\sum_{\langle i,j\rangle}\left(\vec{S}_i\cdot\vec{S}_j-\frac{n_in_j}{4}\right).$$

Thereby $\langle i,j\rangle$ denotes summation over pairs of nearest-neighbor sites, $\hat{c}_{i,\sigma}=c_{i,\sigma}(1-n_{i,\bar{\sigma}})$ and $\vec{S}_i$ and n_i denote the operators of electron spin and density at site i, respectively. We denote the hopping matrix elements $t_{i,j}$ between (1,0)-like neighbors by t, between (1,1)-like neighbors by t' and between (2,0)-like neighbors t'', all other $t_{i,j}$ are zero. Throughout we will assume that $t'/t''=-2$, as would be appropriate if the physical origin of these terms is hopping via the apex oxygen $2p_z$ orbital,[12,13] and $t'/t<0$, as is the case for hole-doped compounds.

The method we apply to study this model is exact diagonalization of finite clusters by means of the Lanczos algorithm.[14] In a preceding paper[15] we have shown that by changing the geometry of the cluster from the standard tilted square form to a rectangular one (more precisely: to a 5×4 cluster) a ground state with a pronounced stripelike such as charge inhomogeneity emerges. Here we want to discuss the single-particle spectra of this state.

A question to worry about first is, whether the stripes survive the additional hopping terms $\propto t',t''$. Intuitively this is not what one would expect, because additional hopping terms increase the mobility of the holes, so that any spatial inhomogeneity should be washed out more efficiently. Surprisingly enough, the numerics show that exactly the opposite is happening: the additional hopping terms even slightly enhance the charge inhomogeneity. This is demonstrated in Table I, which compares the static density correlation function $g_D(\mathbf{R})=\Sigma_j\langle n_jn_{j+\mathbf{R}}\rangle$ for vanishing and finite t' and t''. Switching on t' and t'' separately shows that it is predominantly the t'' term which leads to ‘‘pairing in y direction’’ and thus is responsible for this behavior. Next nearest-neighbor hopping terms with the proper sign for hole-doped cuprates thus seem to have a stabilizing effect on stripes—if any.

Next we address a special feature of the 5×4 cluster, which will be essential to understand the hole dynamics, namely the presence of spin-Peierls dimerization even at half filling. Table II shows that the static spin correlation function is strongly anisotropic, with singlet-bonds predominantly in y direction. Since the boundary conditions in 5×4 frustrate the Néel order, they apparently stabilize the energetically close spin-Peierls phase. In fact, the ground-state (g.s.) energy of the 5×4 cluster is only marginally higher than that of the square-shaped $\sqrt{20}\times\sqrt{20}$ cluster ($-1.165J$/site vs $-1.191J$/site). Clearly, this is a confirmation of the proposal

TABLE I. Static density correlation function $g_D(\mathbf{R})$, 5×4 cluster with two holes, $J/t=0.5$. Other parameters are $t'=t''=0$ (left panel) and $t'/t=-0.4$, $t''/t=0.2$ (right panel).

	2	0.298	0.139	0.035	0.303	0.151	0.037
$R_y\uparrow$	1	0.239	0.144	0.041	0.261	0.144	0.043
	0	2.000	0.049	0.018	2.000	0.016	0.010
		0	1	2	0	1	2
			$R_x\rightarrow$			$R_x\rightarrow$	

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TABLE II. Static spin correlation function for the half-filled 5 ×4 cluster.

	2	0.222	−0.162	0.052
$R_y\uparrow$	1	−0.389	0.173	−0.059
	0	0.750	−0.276	0.061
		0	1	2
			$R_x\rightarrow$	

by Read and Sachdev[16] that the transition to a spin-Peierls phase is a likely instability of the $S=\frac{1}{2}$ 2D Heisenberg antiferromagnet.

Clear evidence for the spin-Peierls nature of the half-filled ground state can be seen in the single-particle spectral function $A(\mathbf{k},\omega)$ (see Ref. 14 for a definition), which is shown in Fig. 1. It is immediately obvious that this differs markedly from the familiar dispersion for a hole in an antiferromagnet. Whereas for hole motion in a Néel state the top of the ARPES spectrum is at $(\pi/2,\pi/2)$,[17,18] the dispersion seen in the half-filled 5×4 cluster has its maximum at $(4\pi/5,\pi/2)$, which probably means $(\pi,\pi/2)$ in the infinite system. Another notable feature is the symmetry of the dispersion under the exchange $(k_x,0)\rightarrow(k_x,\pi)$—which is exactly what one would expect from the doubling of the unit cell by spin-Peierls order with dimers in y direction. To be more quantitative, let us discuss the single-hole dispersion in the spin-Peierls phase. Starting from a product state of singlets, which cover the bonds of the lattice in the form of a columnar pattern, we derive a Hamiltonian for the motion of singly occupied dimers. The singlet state on a bond formed by the sites (1,2) is $|s\rangle=1/\sqrt{2}(\hat{c}^\dagger_{1,\uparrow}\hat{c}^\dagger_{2,\downarrow}-\hat{c}^\dagger_{1,\downarrow}\hat{c}^\dagger_{2,\uparrow})|0\rangle$. A dimer with a single hole can be in either the bonding or antibonding state: $|\pm,\sigma\rangle=\mathrm{sgn}(\sigma)\sqrt{2}(\hat{c}^\dagger_{1,\sigma}\pm\hat{c}^\dagger_{2,\sigma})|0\rangle$. Introducing the "creation operator" $h^\dagger_{\pm,\sigma}=|\pm,\sigma\rangle\langle s|$ we can—by straightforward generalization of Refs. 19–21—write down the following Hamiltonian describing the motion of these effective Fermions:

$$H=\sum_{\mathbf{k},\sigma}\epsilon_+(\mathbf{k})h^\dagger_{+,\mathbf{k},\sigma}h_{+,\mathbf{k},\sigma}+\epsilon_-(\mathbf{k})h^\dagger_{-,\mathbf{k},\sigma}h_{-,\mathbf{k},\sigma}$$

$$+(V(\mathbf{k})h^\dagger_{+,\mathbf{k},\sigma}h_{-,\mathbf{k},\sigma}+\mathrm{H.c.}),$$

$$\epsilon_\pm(\mathbf{k})=\mp t+t\left(\cos(k_x)\pm\frac{\cos(2k_y)}{2}\right)\pm t'\cos(k_x)$$

$$\times(1+\cos(2k_y))+t''(\cos(2k_x)+\cos(2k_y)),$$

$$V(\mathbf{k})=-\frac{it}{2}\sin(2k_y)-it'\cos(k_x)\sin(2k_y). \qquad (1)$$

Diagonalizing the Hamiltonian (1) we obtain the dispersion relation $\epsilon_\alpha(\mathbf{k})$ and the quasiparticles $\gamma^\dagger_{\alpha,\mathbf{k},\sigma}=u_{\alpha,\mathbf{k}}h^\dagger_{+,\mathbf{q},\sigma}+v_{\alpha,\mathbf{k}}h^\dagger_{-,\mathbf{q},\sigma}$, where $\alpha\in\{1,2\}$. Figure 1 shows that there is good agreement between the numerical peak dispersion in the 5×4 cluster and our simple theory. The main differences are the flattening of the cluster dispersion near the band maximum at $(4\pi/5,\pi/2)$ and the smaller bandwidth in the numerical spectra. Taking into account the simplicity of our calculation, however, the agreement is quite satisfactory, and is clear evidence for the spin-Peierls nature of the half-filled ground state.

While this dimerization clearly renders the 5×4 cluster unsuitable to describe undoped compounds such as $Sr_2CuO_2Cl_2$[17], it makes the interpretation of the spectra for the striped ground state at finite doping a lot easier—as will be seen now. Ignoring for the moment the formation of a hole stripe as well as the fact that the dimer-Fermions $h^\dagger_{\pm,\mathbf{q},\sigma}$ actually obey a hard-core constraint, one would expect that the doped holes accumulate near the top of the single-hole dispersion, thus forming to simplest approximation a cigar-shaped hole pocket[20,21] centered at $(4\pi/5,\pi/2)$ [or rather $(\pi,\pi/2)$ in the thermodynamical limit]. Figure 2, which shows the single-particle spectrum for the two-hole g.s. for different t' and t'', demonstrates that this is indeed exactly what happens. For most momenta there is a clear analogy between the PES for the doped case and half filling, with the dispersion of the quasiparticle peak being essentially unchanged. Whereas peaks with a higher binding energy become more diffuse, the low energy peaks at $(4\pi/5,\pi/2)$ and (to a lesser extent) at $(2\pi/5,\pi/2)$ clearly cross to the inverse photoemission spectrum (IPES). Due to finite-size effects there is always a substantial gap between PES and IPES of finite clusters—after all the electron numbers of initial and final states differ by a finite fraction (10% in the present case). It is therefore impossible to decide, whether the present gap is simply a finite-size effect or due

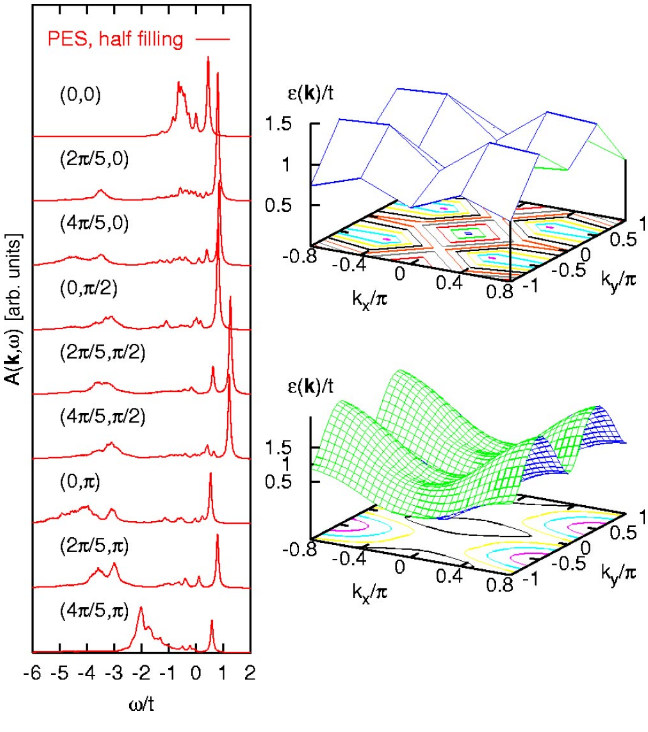

FIG. 1. (Color online) Left: Photoemission spectrum (PES) for the half-filled 5×4 cluster, $J/t=0.5$., $t'/t=-0.2$, $t''/t=0.1$. Right: Dispersion of the quasiparticle peak as extracted from the numerical spectra (top) compared to the theoretical single-hole dispersion $\epsilon_1(\mathbf{k})$ in the spin-Peierls phase (bottom).

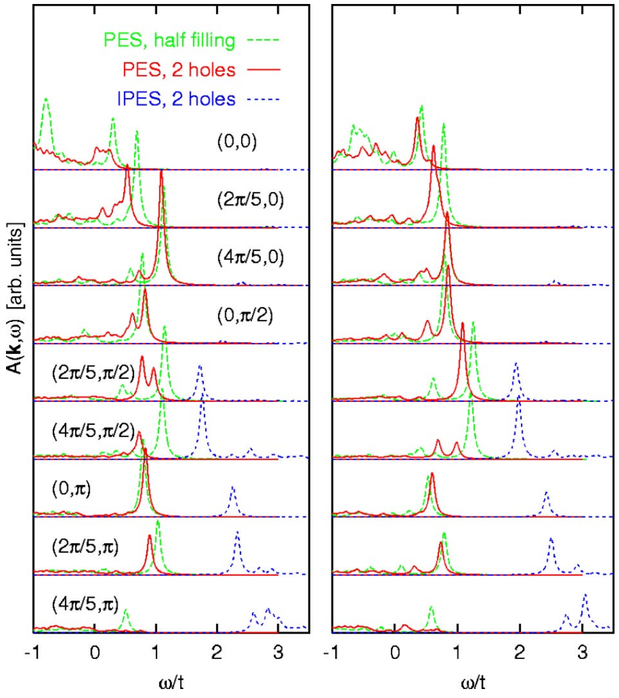

FIG. 2. (Color online) Single-particle spectrum for the 5×4 cluster with two holes. Parameter values are $J/t=0.5$, $t'=t''=0$ (left) and $J/t=0.5$, $t'/t=-0.2$, $t''/t=0.1$ (right). Only the parts near the Fermi energy $E_F/t\approx 1.5$ are shown.

to the stripe formation. The only deviation from this ideal rigid-band behavior is the appearance of high-energy IPES peaks along $(0,\pi)\rightarrow(4\pi/5,\pi)$. The interpretation of these peaks, however, is straightforward: in inverse photoemission, an electron is necessarily inserted into a dimer occupied by a single electron. The spins of the two electrons then can couple either to a singlet—which means the IPES process leads back to the spin-Peierls ‘‘vacuum’’—or to a triplet—which means the IPES process leaves the system in a spin-excited state. The IPES peaks along $(0,\pi)\rightarrow(\pi,\pi)$ presumably originate from the latter process (we note that exactly the same holds true also for the ‘‘usual’’ ground state of the t-J model, see Ref. 22). Taken together, the data presented so far demonstrate that the spin-Peierls order in the striped phase is the key to understand its single-particle spectra.

Neglecting subtleties such as the possible formation of a Luttinger liquid along the stripes,[5] the possible condensation of d-like hole pairs along the stripes[23] or the formation of various kinds of order parameter,[21] the spectra show that the system can be described by the dispersion for a single hole in a spin-Peierls background being filled up with holes.

We now want to use this (rather oversimplified) scenario to discuss the experimental ARPES spectra on $\mathrm{La_{1.28}Nd_{0.6}Sr_{0.12}CuO_4}$.[11] Using the following representation of the electron annihilation operator:

$$c_{\mathbf{k},\sigma}=\frac{1}{\sqrt{2}}\left[\cos\left(\frac{k_y}{2}\right)h^{\dagger}_{+,-\mathbf{q},\bar{\sigma}}-i\sin\left(\frac{k_y}{2}\right)h^{\dagger}_{-,-\mathbf{q},\bar{\sigma}}\right] \qquad (2)$$

we can obtain the full ARPES spectrum from bond-operator theory. Thereby $\mathbf{q}$ is the ‘‘backfolded version’’ of $\mathbf{k}$, so as to take into account that the Brillouin zone of the spin-Peierls phase is $[-\pi,\pi]\times[-\pi/2,\pi/2]$. Equation (2) is readily verified by taking matrix elements of both sides between $|s\rangle$ and $|\pm,\sigma\rangle$. The spectral weight of a given quasiparticle branch then is $w=|u^{*}_{\alpha,\mathbf{k}}\cos(k_y/2)+iv^{*}_{\alpha,\mathbf{k}}\sin(k_y/2)|^2$. In Fig. 3 the resulting spectra for the symmetric momenta (k_x,k_y) and (k_y,k_x) have been averaged, as would be appropriate for an ARPES experiment on a compound with domains of different singlet direction.[11] The experimental ARPES spectrum should be compared to the parts of the spectrum below the Fermi energy, indicated as the vertical line in Fig. 3. Along the (1,1) direction there is a band dispersing upwards and disappearing halfway between (0,0) and (π,π). This is actually not a Fermi level crossing—the *dispersion* of the band actually bends downwards again after passing through $(\pi/2,\pi/2)$—but rather a vanishing of the spectral weight of the dimer fermions. The situation along (1,1) thus is similar to the ‘‘remnant Fermi surface’’ in the half-filled compounds.[24] The minimum distance from the Fermi energy along (1,1) depends on t' and t'': bond-operator theory predicts that $\epsilon_1(\pi,0)-\epsilon_1(\pi/2,\pi/2)=4t''-2t'$. For decreasing $|t'|$ and $|t''|$ the band maximum near $(\pi/2,\pi/2)$ approaches $(\pi,0)$, and thus moves away from E_F—see Fig. 3. This may explain, why the depletion of low-energy spectral weight along (1,1) is most pronounced for the $\mathrm{La_{1.28}Nd_{0.6}Sr_{0.12}CuO_4}$ system, which has relatively small values of t' and t''.[13] Actually the situation in this compound is slightly more involved in that Zhou *et al.* could show subsequently[25] that by

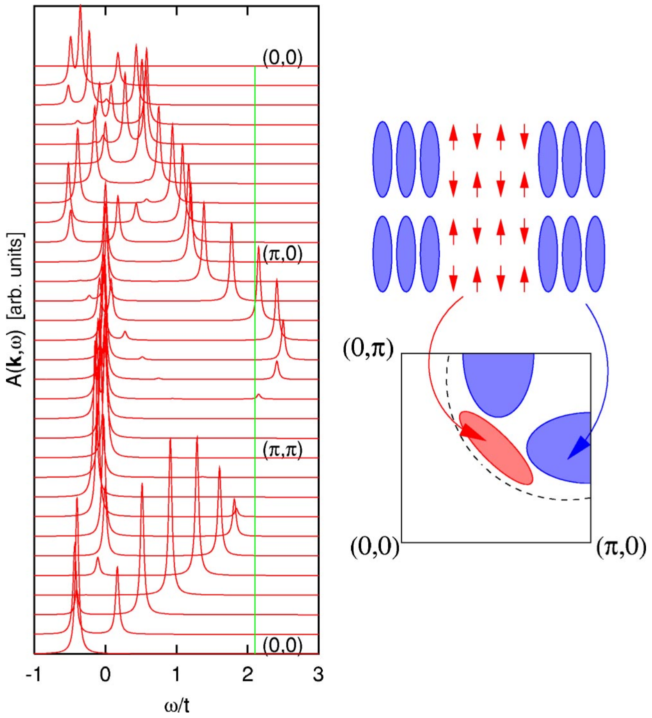

FIG. 3. (Color online) Left: Single-particle spectral function from bond-operator theory for $t'/t=-0.1$, $t''/t=0.05$, the Fermi energy (vertical line) corresponds to a hole density of 0.16. Right: In the inhomogeneous striped phase, the Fermi surfaces of the ‘‘subsystems’’ may combine to form a free-electron-like ‘‘large’’ Fermi surface.

taking special measures to enhance the ARPES intensity a Fermi level crossing along (1,1) could be made visible. As pointed out by Zhou *et al.*,[25] however, the very small spectral weight of the respective band portion suggests that this is due to disorder and/or fluctuations.

Next, along $(\pi,0)\rightarrow(\pi,\pi)$ there are two real Fermi-surface crossings, which are symmetric around $(\pi,\pi/2)$. Again due to matrix element effects, the one between $(\pi,\pi/2)$ and (π,π) has small spectral weight, which would probably render it unobservable in an ARPES experiment. ''Spectroscopically'' the system thus would look very much like having a single Fermi-surface sheet near $(\pi,0)$ running roughly parallel to (1,0) (see Fig. 3) and disappearing as $(\pi/2,\pi/2)$ is approached.

The bond-operator theory outlined above does not take into account a key feature of the striped phase, namely its spatial inhomogeneity. In the stripe phase, weakly doped regions with antiferromagnetic order alternate with higher-doped spin-Peierls stripes, see Fig. 3. The Fermi surface for the antiferromagnetic domains would be hole pockets centered on $(\pi/2,\pi/2)$, the one for the spin-Peierls domains would be (larger) pockets centered on $(\pi,\pi/2)$. Making the reasonably plausible assumption that to simplest approximation the Fermi surface observed in an ARPES experiment corresponds to a superposition of those of the two subsystems—thereby taking into account the fact that the respective backsides of the Fermi surfaces, i.e., the portions facing (π,π), have a practically no spectral weight—one might expect to see something that looks very much like a free-electron Fermi surface, as observed in Bi2212. Thereby the magnitude $|t'|$ and $|t''|$ plays a crucial role, in that it determines the energy of $(\pi/2,\pi/2)$ relative to $(\pi,0)$ and thus controls the relative size of the two ''components'' of the Fermi surface. Clearly, a more elaborate theory which takes account of the spatial inhomogeneity is necessary to describe this.

In summary, numerically exact diagonalization results show that the 2D t-J model with next-nearest-neighbor hopping terms appropriate to describe hole-doped cuprates has a spin-Peierls phase which leads to the formation of pronounced hole-stripes. The single-particle spectrum in the stripe phase then in found to be in good agreement with a simple bond-operator theory for hole motion in a spin-Peierls phase, thus providing further evidence for the intimate relationship between spin-Peierls ordering and stripe formation. Upon doping, holes accumulate near the top of the single-hole dispersion to simplest approximation forming cigar-shaped pockets centered on the corner of the spin-Pierls Brillouin zone at $(\pi,\pi/2)$—the latter in full agreement with bond-operator theory.[20,21] The notion of a Fermi surface should not be taken too literal, because close to E_F the stripe formation is likely to change this simply free-particle picture drastically, but all in all the quasiparticle dispersion and spectral weight distribution of the stripe phase as seen in the simulations are in good agreement with ARPES experiments.

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