Electronic structure and string tension of stripes in high-$T_c$
superconductors

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Abstract

We present a simple, material-specific model Hamiltonian for stripes and use it to explain the observed differences between the angle-resolved photoemission spectra of La$_{2-x}$Sr$_x$CuO$_4$ and Bi$_2$Sr$_2$CaCu$_2$O$_{8+x}$, e.g, along the nodal line and around $(3\pi/4,0)$. Next we compute the string tension for stripes and find it to be smallest in the materials with the highest observed $T_{c_{\text{max}}}$.

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Information about the electronic structure of the high-temperature superconducting cuprates (HTSC) is needed for a detailed understanding of their thermodynamic and transport properties, and of the superconductivity itself. Elastic neutron scattering experiments on La$_{2-0.4-1/8}$Nd$_{0.4}$Sr$_{1/8}$CuO$_4$ have demonstrated that the CuO$_2$ layers are unstable against the formation of one-dimensional (1D) “charge stripes” which act as domain walls separating $\pi$-shifted antiferromagnetic regions [1]. These findings have triggered an intense research on models in which the spin and charge degrees of freedom of the electrons are viewed as inhomogeneous in real space [2-4].

The electronic structure of 1D domain walls in the two-dimensional (2D) CuO$_2$ layers of HTSCs has recently attracted a lot of interest in connection with angle resolved photoemission spectroscopy (ARPES) on La$_{2-x}$Sr$_x$CuO$_4$ (LSCO) [5], La$_{2-x-y}$Nd$_y$Sr$_x$CuO$_4$ (Nd-LSCO) [6,7], and Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ (BSCCO) [8,9]. A characteristic feature of the measured Fermi surfaces (FSs) in the 2D Brillouin zone (BZ) is that they possess straight segments running parallel to the (0,0)-(\pi,0) and (0,0)-(0,\pi) directions [5,6,11]. Such fingerprints of a 1D band structure can be explained successfully within the half-filled stripe model [12-16]. According to this model, the FS is a straight line, |$k_y$| = $\pi$/4, in the case of stripes running in the $y$-direction. The stripe direction, $x$- or $y$-, alternates from one CuO$_2$-layer to the next and between domains within the same layer. However, the ARPES observation of a strong dependence on the momentum $k_x$ perpendicular to the stripe, in particular the 0.2 eV-dispersion along $k_y \approx 0$ for $\pi/2 < k_x \leq \pi$ not only in Nd-LSCO [6,7], but also in underdoped LSCO [5,6], and in BSCCO [8,9] even for $0 < k_x \leq \pi$, poses a serious problem for the model. In addition, the observations of nodal quasi-particles (with momentum along the diagonal of the 2D BZ) in optimally doped LSCO [7] and BSCCO [11], but not in underdoped LSCO [5] and Nd-LSCO [6], are in direct conflict with the simple stripe picture [4,13]. Thus, 1D confinement of spectral weight appears not to be a generic feature of the stripe phase.

In this Letter we present the electronic structure of 1D domain walls in a CuO$_2$ layer, calculated with a material-specific model Hamiltonian. The resulting band structure for an electron moving in an effective stripe-potential provides a simple explanation for the observed
differences in the ARPES data between Nd-LSCO and BSCCO \[10,11\]. In addition, we shall calculate kink-excitation energies and see that they tend to zero for materials with higher observed $T_c$ at optimal doping.

We start from the 2D Hubbard model:

\[
H = \sum_{k,\sigma} \varepsilon_k a^\dagger_{k\sigma} a_{k\sigma} + U \sum_{\mathbf{R}} n_{\mathbf{R}\uparrow} n_{\mathbf{R}\downarrow},
\]

where $\varepsilon_k$ is the bare conduction band, which is periodic with primitive translation vectors $\mathbf{G}_1 = (2\pi, 0)$ and $\mathbf{G}_2 = (0, 2\pi)$, and $a_{k\sigma}$ [$a_{\mathbf{R}\sigma}$] annihilates an electron with momentum $k$ [at site $\mathbf{R} = (l, m)$] and spin $\sigma$. This model, with $\varepsilon_k = -2t (\cos k_x + \cos k_y)$ and $U = 12t$, has recently been solved numerically using the dynamical mean-field (DMF) approximation and a supercell approach \[14\]. For doping levels $0.05 < x < 0.2$, $y$-oriented half-filled stripes were found to be stable. Such a band with only nearest-neighbor hopping ($t$) is a reasonable approximation for LSCO, but for materials with higher $T_{c\text{max}}$ such as BSCCO, further hopping integrals ($t', t'', ...$) are needed to describe both the FSs observed with ARPES in overdoped samples and also the energy bands calculated with the local density approximation (LDA) \[17,18\]. In the present letter, we study the effect of using such material-specific band shapes. The self-energy in the DMF approximation, $\Sigma_{\mathbf{R}\sigma}(\omega)$, defined in terms of the one-electron Green function by:

\[
G^{-1}_{\mathbf{R}\mathbf{R}'\sigma}(\omega) = [\omega + \mu - \Sigma_{\mathbf{R}\sigma}(\omega)] \delta_{\mathbf{R}\mathbf{R}'} - \sum_k \varepsilon_k e^{i\mathbf{k} \cdot (\mathbf{R} - \mathbf{R}')} = \omega + \Sigma_{\mathbf{R}\sigma}(\omega) \delta_{\mathbf{R}\mathbf{R}'},
\]

was found in Ref. \[14\] to have a spin, site, and energy dependence which, for low energies and for the doping levels $x \equiv 1/(4N) = 1/8$ and $1/12$, we now model by:

\[
\Sigma_{\mathbf{R}\sigma}(\omega) \approx -\frac{1}{2} \sigma V \sin (\mathbf{Q} \cdot \mathbf{R}) - \omega \lambda - i\delta, \quad |\omega| < 1.5t,
\]

\[
\mathbf{Q} = \pi \left(1 - \frac{1}{2N}, 1\right) = (2N - 1) \mathbf{g}_1 + N \mathbf{g}_2.
\]

This yields a low-energy electronic structure which is the bare band, $\varepsilon_k$, subject to a magnetic stripe potential of width $V$ and a mass renormalization $1 + \lambda$. In the $t$-$J$ model, the latter is due to the formation of spin polarons. From the DMF calculations we obtain: $V = 3t$.
and $\lambda = 2$, for $x = 1/8$. The spin-periodicity of the stripe potential is $4N$ so that the primitive translation vectors are $T_1 = (4N,0)$ and $T_2 = (2N,1)$ in real space, and $g_1 = \pi \left(\frac{1}{2N},-1\right)$ and $g_2 = \pi (0,2)$ in reciprocal space. The observed magnetic (charge) Bragg peak is $Q (-2Q)$. The values of $\sin [Q \cdot (l,0)]$ for $l$ running from 0 to respectively 7 and 11 are: 0, $\sqrt{2}/2$, $-1$, $\sqrt{2}/2$, 0, $-\sqrt{2}/2$, 1, $-\sqrt{2}/2$ and 0, $1/2$, $-\sqrt{3}/2$, 1, $-\sqrt{3}/2$, 2, $-\sqrt{3}/2$, 1, ... . In the limit when $V \gg t$, the approximate form (1) of the self-energy yields a 1D band with energy $\sim [\pm (V/2) \sin \{Q \cdot (l,0)\} - \mu] / (1 + \lambda)$ for each row of atoms. Here and in the following, the upper (lower) sign is for a spin-up (down) electron. The zero-energy, spin-degenerate, metallic stripe bands centered at $l=0$ and $2N$ have the dispersions $\varepsilon(k_x,k_y)=\frac{\pi}{2} \frac{k_y}{(1 + \lambda)}$ and $\varepsilon(\pi/2,k_y+\pi)/ (1 + \lambda)$, respectively.

Since for the interpretation of ARPES spectra we need the $|k,\sigma\rangle$-projection and since the stripe-potential takes the simple form (1), which couples $|k,\sigma\rangle$ to just $|k - Q,\sigma\rangle$ and $|k + Q,\sigma\rangle$, it is convenient to transform to the $|k + nQ,\sigma\rangle$-representation, with the integer $n$ taking $4N$ consecutive values. As a result:

$$
\langle k+nQ,\sigma | G(\omega) | k+n'Q,\sigma' \rangle =
\delta_{\sigma\sigma'} \left\{ \{ \omega (1 + \lambda) + \mu + i\delta \} 1 - H_k \right\}^{-1}_{nn'},
$$

where the un-renormalized Hamiltonian matrix,

$$
H_k \equiv 
\begin{pmatrix}
\varepsilon_{k-(2N-1)Q} & 0 & 0 & 0 & \pm \frac{V}{4} \\
0 & \varepsilon_{k-Q} & \pm \frac{V}{4} & 0 & 0 \\
0 & \pm \frac{V}{4} & \varepsilon_k & \pm \frac{V}{4} & 0 \\
0 & 0 & \pm \frac{V}{4} & \varepsilon_{k+Q} & 0 \\
\pm \frac{V}{4} & 0 & 0 & 0 & \varepsilon_{k+2NQ}
\end{pmatrix},
$$

is tri-diagonal and periodic. It is isomorphic with the Hamiltonian for a $4N$-atomic ring with on-site energies $\varepsilon_{k+nQ}$ and nearest-neighbor hopping integrals $\pm V/4$. 

4
For the bare band we shall use the LDA Cu–O antibonding pdσ-band as obtained by integrating out the high-energy degrees of freedom

\[
\varepsilon_k = -\left\{ (1 - p)u_k + \frac{2rv_k^2}{1 - 2ru_k} \right\}/\delta. \tag{2}
\]

Here, \(u_k \equiv \frac{1}{2}(\cos k_x + \cos k_y), \ v_k \equiv \frac{1}{2}(\cos k_x - \cos k_y), \ 1/\delta\) is the band-width parameter, and \(r\) and \(p\) are band-shape parameters. Whereas \(1/\delta \equiv 2t_{pd}^2/\left[\mu - (\varepsilon_p + \varepsilon_d)/2\right]\) is always about 1.6 eV, \(r\) contains the essential materials dependence and was recently observed to increase with \(T_{c_{\text{max}}}\) \[18\]. It describes the conduction-band content of the axial-orbital, a hybrid between Cu 4s, Cu 3d_{3z^2-1}, apical oxygen 2pz, and farther orbitals. The axial orbital lowers the energy of the conduction band near \((\pi, 0)\), but not along the nodal line. The parameter \(p\) describes buckling-induced plane-oxygen 2pz-content and is non-zero in materials such as YBa\(_2\)Cu\(_3\)O\(_7\) and BSCCO. For a flat layer, \(p = 0\), whereas for a layer so buckled that \(p \geq (1 - 2r)^2\), the saddlepoint is bifurcated away from \((\pi, 0)\) \[17\]. If we expand \(1/(1 - 2ru_k)\) in \(2\), \(\varepsilon_k\) takes the form of a one-band Hamiltonian with \(t = (1 - p + o(r))/4\delta, \ t' = [r + o(r)]/4\delta, \ t'' = t'/2 + o(r)\), etc.. Hence, \(t/ (1 + \lambda) \approx (1 - p) \times 125\) meV is at the order of the exchange coupling \(J\), and \(r\) gives the range of the hopping. For LSCO, \(r \sim 0.1\) and \(p = 0\), while for BSCCO and YBCO, \(r \sim 0.3\) and \(p \sim 0.17\) \[17,18\].

In Fig. 1 we show for 1/8 hole-doped LSCO and BSCCO the calculated bands projected onto \(|k\rangle\) in the large BZ. The spectrum for LSCO agrees well with that obtained from the full DMF calculation with only nearest-neighbor hopping \[14\]: The two metallic stripe bands are separated by gaps from the below-lying three magnetic valence bands and from the above-lying three magnetic conduction bands. In the \(|k\rangle\)-projection, the stripe band centered at \(l=0\) and with bottom along \(\Gamma X\) is seen near \(X\), where it is \(\sim 75\) meV below the chemical potential \(\mu\). Proceeding now in the \(y\)-direction, this stripe band disperses upwards and passes \(\mu\) near \((\pi, \pi/4)\). The top of the band is seen again near \(Y\), where it is \(\sim 75\) meV above \(\mu\). From \(Y\) towards \(\Gamma\), the band initially stays flat and as it starts to disperse downwards through \(\mu\), it loses its \(|k\rangle\)-character. Finally, from \(\Gamma\) along the nodal direction towards \(M\), the stripe band picks up \(|k\rangle\)-character only when, near \((\pi/2, \pi/2)\), it is above \(\mu\); the nodal
direction therefore appears to be gapped.

In BSCCO the stripe bands indirectly overlap the magnetic valence and conduction bands. This is due to the pushing down by the axial orbital of the $\varepsilon_k$ band near X and Y. Along the nodal line, however, the $\varepsilon_k$ band is completely – and the $\varepsilon_{k-Q}$ and $\varepsilon_{k+Q}$ bands are nearly– unaffected so that the electronic structure is like in LSCO, but $\mu$ lies lower because it is dragged down with the bands near X and Y. As a consequence, $\mu$ straddles off the top of the magnetic valence band along the nodal line. Hence, if the striped phase of BSCCO exists in the superconducting state, it will have nodal quasiparticles contributed by the magnetic valence band. Near X and Y, $\mu$ lies higher with respect to the bands than in LSCO. It even touches the upper part of the stripe band at Y, as well as the equivalent part of the other ($l=4$-centered) stripe band at $(\frac{3}{4}\pi, 0)$. This behavior agrees quantitatively with the ARPES measurements on BSCCO [10,11]. In particular, our calculation identifies both the extra electronic component observed near $(\frac{\pi}{2}, \frac{\pi}{2})$, which arises from the antiferromagnetic regions separated by 1D domain walls, and also the piece of FS observed near $(\frac{3}{4}\pi, 0)$, which is part of the $l=4$-centered stripe band.

The tri-diagonal form of $H_k$, together with the smallness of $V/8t$, allows us to discuss these features analytically: As seen in Fig. [I], the shape of the $\varepsilon_k$ band is left fairly intact, except where it is crossed by the $\varepsilon_{k-Q}$ or the $\varepsilon_{k+Q}$ band, or where it is crossed by the $\varepsilon_{k-2Q}$ or the $\varepsilon_{k+2Q}$ band and the corresponding intermediate band, $\varepsilon_{k-Q}$ or $\varepsilon_{k+Q}$, is close by. At such crossing points, $H_k$ may be truncated to a $2 \times 2$ or $3 \times 3$ matrix.

Along the nodal line $\Gamma M$, the $\varepsilon_k$ band is crossed by the $\varepsilon_{k+Q}$ and $\varepsilon_{k-Q}$ bands, which are nearly parallel and have $\varepsilon_{k+Q} > \varepsilon_{k-Q}$. The gap surrounding $\mu$ in LSCO and lying just above $\mu$ in BSCCO is therefore primarily due to the interaction with the $\varepsilon_{k-Q}$ band. The (un-renormalized) energies are then: $\varepsilon_{\pm} = \left\{ \varepsilon_{\pm}^2 + (V/4)^2 \right\}^{1/2}$, where $\varepsilon_{\pm} = (\varepsilon_k \pm \varepsilon_{k-Q})/2$, and the anti-bonding state is part of the $l=0$-centered stripe band while the bonding state is part of a magnetic valence band.

Next we consider $k = (\frac{3}{4}\pi, 0)$. Since the XM line is a mirror, $\varepsilon_{k-2Q} = \varepsilon_k$ for all $k$ along
the line \((\frac{2N-1}{2N}\pi, k_y)\), and \(\varepsilon_{k-Q} \sim \varepsilon_k\) when \(k_y = 0\). The Hamiltonian is thus like that of an \(aba\) molecule: A non-bonding state, \((|k - 2Q\rangle - |k\rangle) / \sqrt{2}\), remains at \(\varepsilon_{k-2Q} = \varepsilon_k\), while the energies of the bonding and anti-bonding states are \(\varepsilon_+ \pm \left[\varepsilon_-^2 + 2(V/4)^2\right]^{1/2}\). Whereas the bonding state is part of the magnetic valence band, the non- and anti-bonding states are part of the metallic stripe bands centered at respectively \(l=0\) and \(2N\).

An important scale of energies which contribute spectral weight perpendicular to the stripes is set by the transverse stripe fluctuations [19]. We have calculated the energies of various elementary kink excitations relevant for the string tension of the stripes by displacing the stripe potential and using periodic boundary conditions with an \(8 \times 6\) cell. The smallest energies were found for the excitations shown in the top panel of Fig. 2. As shown in the bottom panel, the string tension is calculated to decrease with the range-parameter \(r\), once \(r > 0.25\), and to vanish for \(r \sim 0.4\). Hence, the energy cost of creating a kink is compensated by the energy gain due to long-range hopping which allows for coherent escape of holes sideways to the string. Since \(r\) is strongly material dependent [18], so is the string tension. Also, as may seem obvious from the two spectra in Fig. 1, the energy gained by stripe formation decreases with \(r\). It has been observed that for a large number of hole-doped HTSCs, \(r\) calculated with the LDA correlates with the measured \(T_c\) at optimal doping [18]. Specifically, as \(r\) increases from \(\sim 0.1\), to \(\sim 0.3\), and to \(\sim 0.4\), \(T_{c,max}\) increases from \(\sim 25\) K, to \(\sim 60\) K, and to \(\sim 135\) K. Needless to say, the reason for this correlation is unknown, but the present results indicate that suppression of stripes might increase \(T_c\). In addition, our results in Fig. 2 show that once \(r > 0.2\), the string tension is softened by dimpling or buckling of the CuO\(_2\) planes as it occurs in bilayered YBa\(_2\)Cu\(_3\)O\(_7\) and BSCCO. Finally, we have found that the domain-wall geometry with the shorter perpendicular distance has the lower energy. This implies that domain-wall dynamics does weaken the potential barrier for pair-tunneling between charge stripes [20].

In Figs. 3 and 4 we show how the kink distortions influence the single-particle spectra calculated for LSCO and BSCCO, respectively. The gaps, say at \((\frac{2N-1}{2N}\pi, 0)\) between the
two stripe bands and between the lower stripe band and the upper magnetic valence band, tend to get filled. Even for LSCO, the parallel excursion of neighboring domain walls shown in the upper left of Fig. 2 nearly fills the charge gap and gives strong spectral intensity in the nodal direction. Our LSCO spectra shown at the bottom of Fig. 3 are in accord with the experimental observation of FS features near \((\pi, \pi)\) generated by dynamic stripes in \(\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4\). One should, however, note the difference to BSCCO where nodal spectral intensity from the magnetic valence band exists in already the ordered stripe phase. Kinks thus influence the spectrum in the nodal direction and near \(\mu\) far less for BSCCO than for LSCO. Consistent with our energy analysis we understand that transverse stripe fluctuations are weaker in LSCO due to the energy cost of losing the charge gap along the nodal direction. Figs. 3 and 4 show that dominant FS features, such as the straight, \(k_x\)-directed stripe-band segments, the magnetic valence-band sheet near the middle of the nodal line in BSCCO, and the sheet near \((\frac{2N-1}{2N}\pi, 0)\) from the 2N-centered stripe band in BSCCO, are fairly robust. This finding for the \((\frac{2N-1}{2N}\pi, 0)\)-sheet is in accord with recent experimental observations \([10,11]\) and clarifies the questions raised in the experimental papers about the origin of such quasi-particle states.

In conclusion, we have shown that the low-energy spectral properties of striped phases can be studied with a simple, material-specific model for electrons moving in an effective stripe potential. This model has allowed us to understand experimental features, such as: (i) the absence of spectral weight in the nodal direction for underdoped LSCO and 1/8-doped Nd-LSCO, (ii) the presence of spectral weight in the nodal direction for BSCCO, (iii) the low-energy photoemission states around \((\frac{3}{4}\pi, 0)\) in BSCCO, (iv) the filling of the gap along the nodal direction in the dynamic striped phase of optimally doped LSCO, and (v) the enhancement of superconducting fluctuations due to stripe dynamics. Finally, we have seen that the string tension of a stripe tends to be smallest in the HTSC materials with the highest observed \(T_{c_{\text{max}}}\).

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FIGURES

FIG. 1. Calculated single-particle spectra, $A(k, \omega)$ for $k$ along the symmetry directions of the large BZ, of the $y$-oriented striped phase for 1/8 doped LSCO (top) and BSCCO (bottom). \( \Gamma = (0, 0), \ X = (\pi, 0), \ Y = (0, \pi), \ M = (\pi, \pi), \ S = (\pi/2, \pi/2). \)

FIG. 2. Calculated energy cost for creating localized kinks in an $8 \times 6$ cell ($l = -2, \ldots, 5$ and $m = 0, \ldots, 5$) for 1/8 hole doping as a function of the range parameter $r$. Circles are for flat layers ($p = 0$) and squares are for $p = 0.17$. As illustrated in the upper panel, the open (closed) symbols refer to kinks which do (not) conserve the distance between domain walls.

FIG. 3. Calculated spectra of the $y$-oriented striped phase with kinks in 1/8 doped LSCO. The top and the lower-right (left) parts are for the kinks shown in the upper-right (left) part of Fig. 2. The figures of the lower panel show the spectral weight in the large BZ, integrated over an energy window extending from $\mu$ to 25 meV below.

FIG. 4. Spectra as in Fig. 3 but for BSCCO.
