Implications of Charge Ordering for Single-Particle Properties of High-$T_c$ Superconductors

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The consequences of disordered charge stripes and antiphase spin domains for the properties of the high-temperature superconductors are studied. We focus on angle-resolved photoemission spectroscopy and optical conductivity, and show that the many unusual features of the experimentally observed spectra can be understood naturally in this way. This interpretation of the data, when combined with evidence from neutron scattering and NMR, suggests that disordered and fluctuating stripe phases are a common feature of high-temperature superconductors.

Recent neutron-scattering experiments by Tranquada et al. have shown that the suppression of superconductivity in La$_{1.6-x}$Nd$_{0.4}$Sr$_{0.12}$CuO$_4$ is associated with the formation of an ordered array of charged stripes which are also antiphase domain walls between antiferromagnetically ordered spins in the CuO$_2$ planes. This observation strongly supports the idea that disordered or fluctuating stripe phases are of central importance for the physics of high-temperature superconductors. In this Letter, we show that single-particle properties of a disordered stripe phase can account for the exotic features in the spectral density measured by angle-resolved photoemission spectroscopy (ARPES) in Bi$_2$Sr$_2$CaCu$_2$O$_{8+x}$ (for which the best data is available). In particular, we compute the spectral density in a background of disordered stripes and show that it reproduces the experimentally observed shape of the Fermi surface, the existence of nearly dispersionless states at the Fermi energy ("flat bands"), and the appearance of weak additional states ("shadow bands") features which have no natural explanation within conventional band theory. Finally, we comment briefly on the implications of partially ordered spin domains for NMR experiments.

The principal signature of the antiphase spin domains in La$_{1.6-x}$Nd$_{0.4}$Sr$_x$CuO$_4$ is a set of resolution-limited peaks in the magnetic structure factor at wave vectors $(\frac{1}{2} \pm \epsilon, \frac{1}{2})$ and $(\frac{1}{2}, \frac{1}{2} \pm \epsilon)$. The associated charge stripes are indicated by peaks in the nuclear structure factor at wave vectors $(\pm 2\epsilon, 0)$ and $(0, \pm 2\epsilon)$. A posteriori, it is natural to interpret the inelastic peaks in the magnetic structure factor previously observed at similar locations in reciprocal space in superconducting samples of La$_{2-x}$Sr$_x$CuO$_4$ as evidence of "extended domains" of stripe fluctuations, in which the stripes are oriented along vertical or horizontal Cu-O bond directions respectively. Indeed, any experiment, such as ARPES, that might be sensitive to the existence of an extended domain structure should be re-examined from this point of view; this is an important feature of our interpretation of the data.

Two mechanisms for producing stripe phases have been suggested by theories of doped Mott-Hubbard insulators: a Fermi-surface instability and frustrated phase separation. The former relies on Fermi-surface nesting which leads to a reduced density of states, or a gap, at the Fermi energy. In the latter mechanism, a competition between phase separation (i.e., the tendency of an antiferromagnetic insulator to expel doped holes) and the long-range part of the Coulomb interaction leads to charge-ordered phases, and especially stripe phases, which may be either ordered, quantum melted, or disordered by quenched randomness. The charge forms an array of metallic stripes, whose period is determined by the energetics of phase separation and is unrelated to any nesting vector of the Fermi surface. The charge structures, in turn, drive the modulation of the antiferromagnetic order. The experiments on La$_{1.6-x}$Nd$_{0.4}$Sr$_x$CuO$_4$ clearly favor the latter point of view. The ordering wave vectors do not nest the Fermi surface, and the ordered system has partially-filled hole bands associated with the stripes. Moreover the magnetic peaks first develop below the charge-ordering temperature. Our interpretation of the ARPES experiments on Bi$_2$Sr$_2$CaCu$_2$O$_{8+x}$ lends further support to this conclusion: nesting would lead to a diminished density of states at the Fermi surface, whereas we find an increased density of states corresponding to the flat bands seen in the experiments.

Our objective is to determine a phenomenological band structure for electrons moving in an effective potential generated by charge stripes and antiphase spin domains. We do not propose to solve a particular many-body model by Hartree-Fock theory; indeed, we have found that this approximation seems to favor insulating stripes, even if the long-range part of the Coulomb interaction is included. Rather we assume a phenomenological one-body Hamiltonian:

$$H = -t \sum_{\langle ll \prime \rangle \sigma} \langle c_{l \sigma}^\dagger c_{l \prime \sigma} + H.c. \rangle + \sum_{l \sigma} V_{\sigma}(R_l)a_{l \sigma},$$

(1)
where the first term is the nearest-neighbor hopping on a square lattice and the second one describes the interaction with the effective stripe potential. Here, $c_{\sigma}$ annihilates an electron of spin $\sigma = \pm$ at site $\mathbf{R}_I$ and $n_{\alpha} = c^\dagger_{\alpha} c_{\alpha}$. The effective potential is given by:

$$V_x(\mathbf{R}) = \rho(\mathbf{R}) + \sigma S(\mathbf{R}) e^{i \mathbf{Q} \cdot \mathbf{R}},$$

where $\mathbf{Q} = (\frac{x}{a}, \frac{y}{a})$ and $a$ is the lattice spacing. Specifically, for vertical stripes, we use the forms $\rho(x, y) = \rho_0 \sum \text{sech}[(x - x_n) / \xi]$, and $S(x, y) = S_0 \prod \tanh[(x - x_n) / \xi]$, where $\mathbf{R} = (x, y)$, $x_n$ are fixed centers of the stripes, and the parameters $\rho_0$, $S_0$, $\xi$, and $\xi_s$ determine the amplitude of the charge and spin modulation and whether the stripes are narrow or broad.

According to the usual interpretation, the measured photo-current in a photoemission experiment is the product of the electronic spectral density $A_\sigma(\mathbf{k}, \epsilon)$ for the removal of one electron from the system and a slowly varying matrix element which reflects the photon-polarization selection rules. This spectral density can be written as $A_\sigma(\mathbf{k}, \epsilon) = f(\epsilon) A(\mathbf{k}, \epsilon)$, where $f(\epsilon) = 1/[\text{exp}(\epsilon - \epsilon_F) / kT + 1]$ is the Fermi function, $\epsilon_F$ is the Fermi energy, and $A(\mathbf{k}, \epsilon) = -(1/\pi) \text{Im} G(\mathbf{k}, \epsilon + i0^+)$ is the spectral function of the one-electron Green’s function $G(\mathbf{k}, \epsilon) = -i(T_\sigma c_{\sigma}(t) c^\dagger_{\sigma}(0))$.

First, consider vertical stripes condensed into a regular array: $\rho(x + \ell) = \rho(x)$ and $s(x + 2\ell) = s(x)$, where $\ell$ is the separation between vertical stripes. Results will be presented for bond-centered stripes, $x_n = n\ell + a/2$ with $\ell/a$ integer, but they are largely insensitive to this assumption. For even $\ell/a$, the unit cell size is $(2\ell/a) \times 2$ so the band-structure is computed by diagonalizing a $(4\ell/a) \times (4\ell/a)$ matrix for each $\mathbf{k}$-vector. For illustrative purposes, we have used the parameters $\rho_0 = -t/2$, $S_0 = 2t$, $\xi_s = a$, and $\xi_a = 2a$, for which the ground-state of the Hamiltonian in Eq. 1 solves Hartree-Fock self-consistency conditions at small doping for the Hubbard model with $U/t = 4 - 5$. However, to make contact with the structure observed by Tranquada et al. at $\frac{1}{4}$ doping, we choose $\ell/a = 4$, which does not minimize the Hartree-Fock energy. The results are not very sensitive to the choice of parameters, so long as the stripes are not too narrow.

Figure 1 shows the spectral density $A_-$ (integrated over an energy window $\Delta \epsilon = t/30$ about $\epsilon_F$) as a function of $\mathbf{k}$. Clearly the general shape of the calculated Fermi surface is quite different from that of the noninteracting system (which circles the $\Gamma$ point) $\mathbf{[10]}$. The fine features of the Fermi surface reflect the energy gaps at points spanned by the wave vectors $(\frac{1}{2} \pm \epsilon / \ell)$ of the spin order and $(\pm 2\epsilon, 0)$ of the charge order, where $\epsilon = a/2\ell$: they are generated by the multiple foldings of the energy band in the first Brillouin zone by the effective stripe potential $V_x(\mathbf{R})$. Figure 1 also shows shadow bands — weak copies of the Fermi surface created by the local doubling of the unit cell in the regions between the stripes.

In order to compare with ARPES experiments on superconducting materials, the stripes must be disordered $\mathbf{[11]}$. Since the slow collective stripe motion is not strongly influenced by the single-particle dynamics, we consider a quenched random distribution of stripes, which we expect to give essentially the correct band structure $\mathbf{[10]}$. Specifically, with Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ in mind, we chose 15% doping and a mean stripe separation $\ell/a = 4$. The ensemble of stripe locations was constructed by taking $x_{n+1} - x_n = \ell + \delta$, where the random variable $\delta$ is uniformly distributed between $-3\sigma$ and $3\sigma$. The spectral density was averaged over five realizations, and we assumed a non-zero temperature, $k_B T = t/10$, which further diminished finite size effects. We have found that the results do not depend markedly on the choice of ensemble, or the parameters in the effective potential and that the large lattices used in the calculation (linear dimension 184 sites) are essentially self-averaging. In other words, our results are robust consequences of a disordered stripe array, and are largely independent of other details. (We have not investigated the effects of orientational disorder.)

Figure 2 summarizes the results by showing the $\mathbf{k}$-dependence of the spectral density at the Fermi energy, and the quasi-electron dispersion along the line $\Gamma$-$\mathbf{M}_1$-$\mathbf{X}/\mathbf{Y}$ for a single, extended domain, with disordered vertical stripes (running in the $\Gamma$-$\mathbf{M}_2$ direction). Disordering the stripes has removed the fine details from the Fermi surface leaving only one sheet which closely resembles the Fermi surface of Refs. $\mathbf{[11]}$ and $\mathbf{[12]}$. In particular, near $\mathbf{M}_1$, there is a high density of states and a truly flat “band” at the Fermi energy, extending towards the $\Gamma$ and $\mathbf{X}/\mathbf{Y}$ points. The flatness along the $\Gamma$-$\mathbf{M}_1$ line is a consequence of both the smearing of the energy gap structure seen in the ordered system, and the localization of the electronic wave functions in the direction perpendicular to the stripes. The spectral density of the shadow band is reduced so much that it no longer shows up on a linear scale, although it would reappear on a logarithmic scale. In fact, plotted on such a scale, $A_-$ looks qualitatively like that of Ref. $\mathbf{[10]}$. The effect of vertical stripes at $\mathbf{M}_2$ is completely different: band narrowing in a direction parallel to the stripes leads to an open Fermi surface.

A stripe phase, even a disordered one, breaks the four-fold rotational symmetry of the ideal CuO$_2$ plane and reflection symmetry through a plane at 45° to the Cu-O bond. However reflection symmetry through planes parallel and perpendicular to the stripes, and the associated selection rules on the polarization dependence of the matrix elements are still obeyed. Extended domains with horizontal stripes give rise to the same structures, but rotated through 90°. With the electric field polarized along the $\mathbf{M}_1$ direction, the photoelectron intensity vanishes by symmetry in the $\mathbf{M}_2$ direction, and hence the observed spectrum will de-emphasize the horizontal stripes, for which there are no Fermi-surface crossings near $\mathbf{M}_1$.  

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The photoemission experiments of Dessau et al. were performed in this geometry, so it is reasonable to compare them directly with the results for an extended domain of vertical stripes shown in Fig. 2(a); indeed, the theoretical and experimental results look remarkably similar.

For a Fermi liquid, the signature of well-defined quasiparticles is a spectral density $A_\epsilon(k,\epsilon)$ which approximates a $\delta$-function of energy as the energy $\epsilon$ approaches $\epsilon_F$. In the present calculation, it is clear from the energy-dependence of the spectral density that there are no well-defined quasiparticle features near the $M_1$ point. One consequence is that the optical conductivity, shown in Fig. 3, has a rather small weight in the Drude component, with most of the oscillator strength appearing in a broad, "midgap" peak centered in the neighborhood of $\hbar\omega \approx t$, which merges into a weak, high-energy continuum. Although the stripe-induced electronic structure can appear to be an asymmetric dispersionless quasiparticle band, as shown in Fig. 2(b), the lack of well-defined quasiparticles is consistent with a widely held view of the normal-state properties of the high-temperature superconductors. This has profound implications for d.c. transport and other low-energy two-particle properties.

In summary, Bragg scattering from ordered stripe phases has been observed in neutron scattering in non-superconducting La$_{1.6-x}$Nd$_{0.4}$Sr$_2$CuO$_4$, and strong evidence for disordered and/or fluctuating stripes can be derived from the similar structures seen in the dynamic spin structure factor of La$_2-x$Sr$_x$CuO$_4$. The assumption that there exist disordered, or slowly fluctuating stripes in Bi$_2$Sr$_2$CaCu$_2$O$_{8+x}$ provides a natural explanation for the unusual features of the ARPES data, including the shape of the Fermi surface and the regions of flat bands. Although there are also theoretical reasons for believing that such combined charge and spin structures are the natural consequences of frustrated phase separation in a doped antiferromagnet, it is reasonable to look anew at a wide variety of experiments in the high-temperature superconductors to see whether they can be better understood in terms of the properties of extended domains with short-ranged stripe order. For instance, since stripes break the four-fold rotational symmetry of the crystal, dramatic consequences can be expected for any local experiment which is designed to determine the symmetry of the order parameter of the superconducting state. This perspective will be examined in the still broader context of a global theory of synthetic "bad metals" in a forthcoming publication. However, it is worth mentioning some of the more straightforward implications here, for concreteness focusing on La$_2-x$Sr$_x$CuO$_4$.

Since the stripes are charged, they are easily pinned by disorder. Thus, if the temperature is not too high, we can think of the system as a quenched disordered array of stripes, which divides the Cu-O plane into long thin regions, with weak antiphase coupling between the inter-vening hole-deficient regions. This picture rationalizes the observation that NMR sees two distinct species of Cu nuclei, which we would associate with those in a pinned stripe and those between the stripes. Since the antiphase coupling between regions is potentially frustrating, this picture gives a microscopic justification for the observation of a "cluster-spin-glass" phase in samples with $x < 15\%$ [21]. There is, moreover, evidence that the creation of dilute metallic stripes can account for the rapid suppression of the Néel temperature for $x < 2\%$ [22].

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Conventionally, the word "domain" is used in two distinct senses. One refers to the region of spins between the charge stripes, the other to larger regions in which one of a discrete set of degenerate ground states is realized. In this paper, we use the name "extended domain" for the second case. Such a domain might be macroscopic or mesoscopic.

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A simple argument using Ginsburg-Landau theory shows that, if the order is driven by the charge, there should be two transitions, with spin ordering occurring at the lower temperature. Recent neutron scattering experiments support this picture. (J. Tranquada, private communication.)

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In our notation, the $k$-space points are labeled as $\Gamma = (0,0)$, $X/Y = (\pi a, \pi a)$, $\bar{M}_1 = (\pi a, 0)$, and $\bar{M}_2 = (0, \pi a)$.

In principle, a superconducting material could have an ordered array of stripes. However, there is no long-range magnetic order in La$_{2-x}$Sr$_x$CuO$_4$ and no evidence of charge order in La$_{2-x}$Sr$_x$CuO$_4$ or Bi$_2$Sr$_2$CaCu$_2$O$_{8+}$x. Consequently it is appropriate to assume disordered stripes in calculating the band structure. The agreement with experiment indicates that this is a realistic assumption.

Our calculation is similar in spirit to that of A. P. Kampf and J. R. Schrieffer, Phys. Rev. B42, 967 (1990) (KS), although it differs in detail. We compute the effects of static incommensurate spin fluctuations exactly. KS carried out a perturbative treatment of the dynamics of commensurate spin fluctuations. The major physical difference is that we focus on states associated with the metallic stripes which reside in the pseudogap found by KS.

For a particularly insightful exposition of this view, see P. W. Anderson, Science 256, 1526 (1992). See also V. J. Emery and S. A. Kivelson, Phys. Rev. Lett. 74, 3253 (1995); and references therein.

FIG. 1 The spectral density $A_-$ in the first Brillouin zone integrated over an energy window $\Delta \epsilon = t/30$ about $\epsilon_F$ for an ordered array of vertical stripes of period $\ell = 4a$ with $\frac{d}{8}$ doping. The size of a circle, denoting a Fermi-surface crossing at a given value of $k$, shows the relative magnitude of $A(k, \epsilon_F)$. The parameters specifying the effective potential are $\rho_0 = -t/2$, $S_0 = 2t$, $\xi_c = a$, and $\xi_s = 2a$.

FIG. 2 (a) The spectral density $A_-$ in the first Brillouin zone integrated over an energy window $\Delta \epsilon = t/30$ about $\epsilon_F$, (b) the dispersion relation, and (c) the corresponding spectral density of the highest-energy occupied “band” as a function of $k$ along the $\Gamma$-\bar{M}_1-X/Y line. The band is determined by broadening the energy $\delta$-functions by a Lorentzian of the full width of $t/4$ at half maximum and finding the highest-energy maximum of $A_-$. The results are for a disordered array of vertical stripes with the mean separation of $\ell = 4a$ at 15 % doping at zero temperature. The stripe ensemble and the parameters are the same as in Fig. 2.