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

M. I. Salkola,[1] V. J. Emery,[2] and S. A. Kivelson[3,*]

[1]*Department of Physics and Astronomy, McMaster University, Hamilton, Ontario, Canada L8S 4M1*
[2]*Department of Physics, Brookhaven National Laboratory, Upton, New York 11973-5000*
[3]*Institute for Theoretical Physics, University of California, Santa Barbara, California 93106*

(Received 15 November 1995)

The consequences of disordered charge stripes and antiphase spin domains for the properties of the high-temperature superconductors are studied. We give a semiphenomenological description of angle-resolved photoemission experiments 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, suggests that disordered and fluctuating stripe phases are a common feature of high-temperature superconductors. [S0031-9007(96)00557-1]

PACS numbers: 74.25.Jb, 71.45.Lr

Recent neutron-scattering experiments by Tranquada *et al.* [1] 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 explains the peculiar behavior [2] of the La_2CuO_4 family of compounds near to $\frac{1}{8}$ doping and strongly supports the idea that disordered or fluctuating stripe phases are of central importance for the physics of high-temperature superconductors [3]. 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 $Bi_2Sr_2CaCu_2O_{8+x}$ (for which the best data are 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") [4–7], features which have no natural explanation within conventional band theory.

The principal signature of the antiphase spin domains in $La_{1.6-x}Nd_{0.4}Sr_xCuO_4$ is a set of resolution-limited peaks in the magnetic structure factor at wave vectors $(\frac{1}{2} \pm \epsilon, \frac{1}{2})$ and $(\frac{1}{2}, \frac{1}{2} \pm \epsilon)$ [1,8]. 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 observed [9] at similar locations in reciprocal space in superconducting samples of $La_{2-x}Sr_xCuO_4$ as evidence of "extended domains" [10] 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 reexamined 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 [11] and frustrated phase separation [12]. 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 [13]. 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 [1] on $La_{1.6-x}Nd_{0.4}Sr_xCuO_4$ 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 [1,14]. Our interpretation of the ARPES experiments on $Bi_2Sr_2CaCu_2O_{8+x}$ 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,

$$H = -t \sum_{\langle ll' \rangle \sigma} (c^\dagger_{l\sigma} c_{l'\sigma} + \text{H.c.}) + \sum_{l\sigma} V_\sigma(\mathbf{R}_l) n_{l\sigma}\,, \quad (1)$$

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, $c_{l\sigma}$ annihilates an electron of spin $\sigma = \pm$ at site $\mathbf{R}_l$ and $n_{l\sigma} = c^\dagger_{l\sigma} c_{l\sigma}$. The effective potential is given by

$$V_\sigma(\mathbf{R}) = \rho(\mathbf{R}) + \sigma S(\mathbf{R}) e^{i\mathbf{Q}\cdot\mathbf{R}}, \qquad (2)$$

where $\mathbf{Q} = (\frac{\pi}{a}, \frac{\pi}{a})$ and a is the lattice spacing. Specifically, for vertical stripes, we use the forms $\rho(x, y) = \rho_0 \sum_n \mathrm{sech}[(x - x_n)/\xi_c]$ and $S(x, y) = S_0 \times \prod_n \tanh[(x - x_n)/\xi_s]$, where $\mathbf{R} = (x, y)$, x_n are fixed centers of the stripes, and the parameters ρ_0, S_0, ξ_c, and ξ_s determine the amplitude of the charge and spin modulation and whether the stripes are narrow or broad. The hopping-matrix element t is an effective parameter which has been renormalized by high-energy fluctuations, so that $t = \mathcal{O}(J)$, the antiferromagnetic exchange interaction.

According to the usual interpretation [15], the measured photocurrent in a photoemission experiment is the product of the electronic spectral density $A_-(\mathbf{k}, \epsilon)$ 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 $A_-(\mathbf{k}, \epsilon) = f(\epsilon) A(\mathbf{k}, \epsilon)$, where $f(\epsilon) = 1/[e^{(\epsilon-\epsilon_F)/k_B T} + 1]$ is the Fermi function, ϵ_F is the Fermi energy, and $A(\mathbf{k}, \epsilon) = -(1/\pi)\,\mathrm{Im} G(\mathbf{k}, \epsilon + i0^+)$ is the spectral function of the one-electron Green's function $G(\mathbf{k}, t) = -i\langle T c_{\mathbf{k}\sigma}(t) c^\dagger_{\mathbf{k}\sigma}(0)\rangle$.

First, consider vertical stripes condensed into a regular array, $\rho(x + \ell) = \rho(x)$ and $S(x + 2\ell) = S(x)$, where ℓ is the separation between vertical stripes. Results will be presented for bond-centered stripes, $x_n = n\ell + a/2$ with ℓ/a integer, but they are largely insensitive to this assumption. For even ℓ/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 $\rho_0 = -t/2$, $S_0 = 2t$, $\xi_c = a$, and $\xi_s = 2a$, 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.* [1] at $\frac{1}{8}$ 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 ϵ_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 Γ point) [16]. The fine features are a consequence of the fact that energy gaps are generated at points on the original Fermi surface ($V_\sigma \equiv 0$) that are spanned by the wave vectors $(\frac{1}{2} \pm \epsilon, \frac{1}{2})$ of the spin order and $(\pm 2\epsilon, 0)$ of the charge order, where $\epsilon = a/2\ell$. They are a consequence of the multiple foldings of the energy band in the first Brillouin zone by the effective stripe potential V_σ. 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.

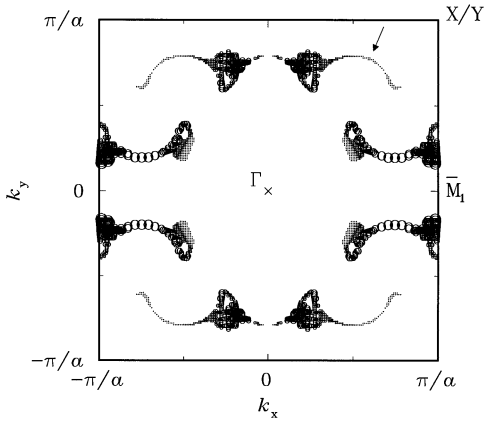

FIG. 1. The spectral density A_- in the first Brillouin zone integrated over an energy window $\Delta\epsilon = t/30$ about ϵ_F for an ordered array of vertical stripes of period $\ell = 4a$ with $\frac{1}{8}$ doping. The size of a circle, denoting a Fermi-surface crossing at a given value of $\mathbf{k}$,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

In order to compare with ARPES experiments on superconducting materials, the stripes must be disordered [17]. Since the system is not far from a stripe-ordered phase, the collective stripe motion is slow, and, moreover, it is not strongly influenced by the single-particle dynamics. Consequently, we consider a quenched random distribution of stripes, which we expect to give essentially the correct band structure [18]. Specifically, with $Bi_2Sr_2CaCu_2O_{8+x}$ 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 δ is uniformly distributed between $-3a$ and $3a$. The spectral density was averaged over five realizations, and we assumed a nonzero 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 quasielectron dispersion along the line Γ-$\bar{M}_1$-X/Y for a single, extended domain, with disordered vertical stripes (running in the Γ-$\bar{M}_2$ direction). Disordering the stripes has removed the fine details from the Fermi surface

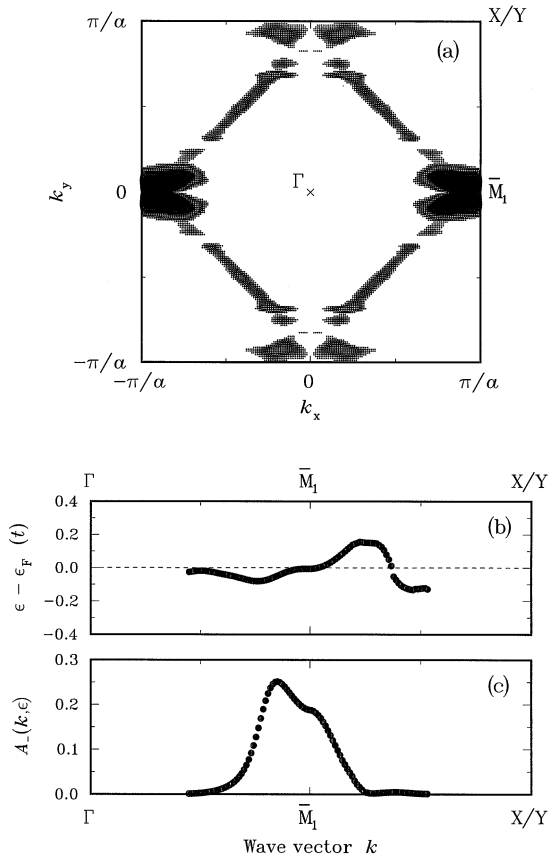

FIG. 2. (a) The spectral density A_- in the first Brillouin zone integrated over an energy window $\Delta\epsilon = t/30$ about ϵ_F, (b) the dispersion relation, and (c) the corresponding spectral density of the highest-energy occupied "band" as a function of $\mathbf{k}$ along the Γ-$\bar{M}_1$-X/Y line. The band is determined by broadening the energy δ 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 the temperature $k_BT = t/10$. The rest of the parameters are $\rho_0 = -t/2$, $S_0 = 2t$, $\xi_c = a$, and $\xi_s = 2a$.

leaving only one sheet which closely resembles the Fermi surface of Refs. [4] and [6]. In particular, near $\bar{M}_1$, there is a high density of states and a truly flat "band" at the Fermi energy, extending towards the Γ and X/Y points. The flatness along the Γ-$\bar{M}_1$ 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. There is in fact a *region* of almost degenerate states, and it appears in the vicinity of the $\bar{M}_1$ point because the energy-gap structure is most significant where the band dispersion of the undoped system is weak, i.e., near to Van Hove singularities. 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. [5]. The effect of vertical stripes at $\bar{M}_2$ 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°. Of course, an ARPES experiment averages over the two stripe orientations but, with the electric field polarized along the $\bar{M}_1$ direction, the photoelectron intensity vanishes by symmetry in the $\bar{M}_2$ direction, and hence the observed spectrum will deemphasize the horizontal stripes, for which there are no Fermi-surface crossings near $\bar{M}_1$. The experiments of Dessau *et al.* [4] were performed in this geometry, so it is reasonable to compare them directly with our results for vertical stripes shown in Fig. 2(a); indeed, the theoretical and experimental results look remarkably similar.

In a Fermi liquid, the signature of well-defined quasiparticles is a spectral density $A_-(\mathbf{k}, \epsilon)$ which approximates $\delta(\epsilon)$ as the energy ϵ approaches ϵ_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 $\bar{M}_1$ point. One consequence is that the optical conductivity has a rather small weight at low frequencies, with most of the oscillator strength appearing in a broad peak centered in the neighborhood of $\hbar\omega \sim t$. This feature, shown in Fig. 3, corresponds to the "midgap peak" deduced from a two-component analysis of the experiments. (For a brief review and list of references, see Ref. [12].) The absence of quasiparticles is consistent with a widely held view of the normal-state properties of the high-temperature superconductors [19], and has profound implications for the physical origin of

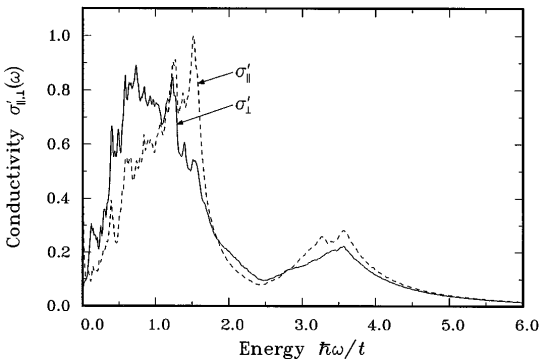

FIG. 3. The real (absorptive) part of the optical conductivity $\sigma'_{\parallel,\perp}(\omega)$ with the electric field polarized parallel (dashed line) and perpendicular (solid line) to a disordered array of vertical stripes with the mean separation of $\ell = 4a$ at 15% doping at zero temperature. The stripe ensemble and the parameters are the same as in Fig. 2.

the "Drude-like" component of the optical conductivity and for dc transport.

In summary, Bragg scattering from ordered stripe phases has been observed in neutron scattering in nonsuperconducting $La_{1.6-x}Nd_{0.4}Sr_xCuO_4$, and strong evidence for disordered and/or fluctuating stripes can be derived from the similar structures seen in the dynamic spin structure factor of $La_{2-x}Sr_xCuO_4$. The assumption that there exist disordered or slowly fluctuating stripes in $Bi_2Sr_2CaCu_2O_{8+x}$ 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. Since 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 fourfold 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.

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 intervening hole-deficient regions. 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 $x < 15\%$ [20]. There is, moreover, evidence that the creation of dilute metallic stripes can account for the rapid suppression of the Néel temperature for $x < 2\%$ [21].

We are grateful to A. Loeser, Z.-X. Shen, J. Tranquada, and B. Wells for stimulating discussions. This work was supported in part by the Division of Materials Science, U.S. Department of Energy under Contract No. DE-AC02-76CH00016 (Brookhaven) and by NSF Grant No. DMR-93-12606 (UCLA). M.I.S. was supported in part by the U.S. Department of Energy, Natural Sciences and Engineering Research Council of Canada, and the Ontario Center for Materials Research.

*Permanent address: Department of Physics, University of California, Los Angeles, CA 90095.

[1] J. M. Tranquada *et al.*, Nature (London) **375**, 561 (1995).
[2] A. R. Moodenbaugh *et al.*, Phys. Rev. B **38**, 4596 (1988).
[3] S. A. Kivelson and V. J. Emery, in *Strongly Correlated Electronic Materials: The Los Alamos Symposium 1993*, edited by K. S. Bedell *et al.* (Addison-Wesley, Reading, 1994).
[4] D. S. Dessau *et al.*, Phys. Rev. Lett. **71**, 2781 (1993).
[5] P. Aebi *et al.*, Phys. Rev. Lett. **72**, 2757 (1994).
[6] J. Ma *et al.*, Phys. Rev. B **51**, 9271 (1995).
[7] H. Ding *et al.* (unpublished).
[8] Here, wave vectors are expressed in units of 2π divided by the lattice spacing.
[9] S.-W. Cheong *et al.*, Phys. Rev. Lett. **67**, 1791 (1991); T. E. Mason, G. Aeppli, and H. A. Mook, Phys. Rev. Lett. **68**, 1414 (1992); T. R. Thurston *et al.*, Phys. Rev. B **46**, 9128 (1992).
[10] 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. Here, we use "extended domain" for the second case. Such a domain might be macroscopic or mesoscopic.
[11] J. Zaanen and O. Gunnarsson, Phys. Rev. B **40**, 7391 (1989); H. Schulz, Phys. Rev. Lett. **64**, 1445 (1990); J. A. Verges *et al.*, Phys. Rev. B **43**, 6099 (1991); M. Inui and P. Littlewood, Phys. Rev. B **44**, 4415 (1991).
[12] V. J. Emery and S. A. Kivelson, Physica (Amsterdam) **209C**, 597 (1993).
[13] U. Löw, V. J. Emery, K. Fabricius, and S. A. Kivelson, Phys. Rev. Lett. **72**, 1918 (1994); L. Chayes, V. J. Emery, S. A. Kivelson, Z. Nussinov, and G. Tarjus, Physica (Amsterdam) **225A**, 129 (1996).
[14] A simple argument using Ginzburg-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).]
[15] M. Cardona and L. Levy, *Photoemission in Solids I* (Springer-Verlag, Berlin, 1978).
[16] In our notation, the **k**-space points are labeled as $\Gamma = (0,0)$, $X/Y = (\frac{\pi}{a}, \frac{\pi}{a})$, $\bar{M}_1 = (\frac{\pi}{a}, 0)$, and $\bar{M}_2 = (0, \frac{\pi}{a})$.
[17] In principle, a superconducting material could have an ordered array of stripes. However, there is no evidence of long-range stripe order in $Bi_2Sr_2CaCu_2O_{8+x}$. Consequently, it is appropriate to assume disordered stripes in calculating the band structure. The agreement with experiment indicates that this is a realistic assumption.
[18] Our calculation is similar in spirit to that of A. P. Kampf and J. R. Schrieffer, Phys. Rev. B **42**, 7967 (1990) (KS). 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.
[19] 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.
[20] J. H. Chou *et al.*, Phys. Rev. B **46**, 3179 (1992).
[21] F. Borsa *et al.*, Phys. Rev. B **52**, 7334 (1995); A. Castro-Neto and D. Hone, Phys. Rev. Lett. **76**, 2165 (1996).