PHOTOEMISSION FROM ORDERED STRIPE PHASES

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A phase separation model for stripes has found good agreement with photoemission experiments and with other studies which suggest a termination of the striped phase in the slightly overdoped regime. Here the model is extended in a number of respects. In particular, a discussion of the nature of the charged stripes is presented, suggesting how density waves, superconductivity, and strong correlations can compete with the quantum size effects inherent in narrow stripes. The anomalous doping dependence of the chemical potential is explained.

1. Photoemission from Stripe Arrays

Generically, any phase separation model of stripes has three characteristic features: (i) \textit{termination of the stripe phase} at some finite doping, \(x_0\); (ii) a \textit{crossover} at a lower doping, \(x_{cr} \sim x_0/2\) from magnetic-dominated \((x < x_{cr})\) to charge-dominated \((x > x_{cr})\) stripe arrays; (iii) some \textit{interaction} on the charged stripes which stabilizes the particular doping \(x_0\). Recent evidence suggests that the stripes and pseudogap terminate at the same doping, while superconductivity persists\cite{1}. A consistent picture yields \(x_0 \simeq 0.25\), so the crossover can be identified with the 1/8 anomaly, where both charged and magnetic stripes have their minimal width (2 Cu atoms). Then, at optimal doping in, e.g., YBa\(_2\)Cu\(_3\)O\(_{7-\delta}\) (YBCO), \(x_{opt} = 16/19 \times 0.25 = 0.21\)\cite{2} while the width of the charged stripes \(N\) satisfies \(N/(N+2) = 16/19\), or \(N = 32/3 \sim 10\) Cu wide.

Hence, models of isolated quasi-one-dimensional charged stripes are likely to be valid only in the far underdoped regime. To study the doping dependence of stripes, and particularly of the wider stripes present near optimal doping, we developed a model of ordered stripe arrays (tight-binding calculations including Coulomb charging effects) and applied it to the study of photoemission (PE)\cite{3}. (Earlier studies of the effects of stripes on PE\cite{4,5} were limited to a single doping.) We found (1) the PE consists of separate components for the magnetic stripes (upper and lower Hubbard bands) and charged stripes (filling in midgap states with doping); (2) the charged stripe PE consists of several subbands associated with quantum size effects (QSE) on the finite width stripes. The two PE components are clearly resolved in La\(_{2-x}\)Sr\(_x\)CuO\(_4\) (LSCO)\cite{6} and constitute the peak (charged stripes) and...
Figure 1: Constant energy cuts of PE dispersion for a 1/8 doping stripe array, within (a) 30 (b) 100, (c) 200, or (d) 500 meV of the Fermi level. The calculation includes a matrix element, \( M = |c_x - c_y| \), which suppresses intensity along the zone diagonal. Lines = Fermi surface of bulk (or very wide) charged stripes. Relative intensity increases with darker shading.

hump (magnetic stripes) features in superconducting \( \text{Ba}_2\text{Sr}_2\text{CaCu}_2\text{O}_8 \) (BSCCO). The main difference between the two materials is that the lower Hubbard band in BSCCO is considerably closer to the Fermi level, presumably an effect of stronger stripe fluctuations. The doping dependence of the QSE is consistent with that of the pseudogap, while the intensity of the peak feature is found to scale with doping \( x \), maximizing at the point where the stripe phase terminates, confirming that the peak is a property of the charged stripes. A map of the intensity distribution near the Fermi level, Fig. 1, is in qualitatively good agreement with experiment.

2. Nature of Charged Stripes

For the stripe phase to exist, the doping \( x_0 \) must be particularly stable. This can arise via an electronic instability, which opens up a gap over much of the Fermi surface, making the electronic phase nearly incompressible. This ‘Stability from Instability’ is a fairly general feature, underlying, e.g., Hume-Rothery alloys. [This is a modification of an argument due to Anderson.] Here, we explore a number of candidates for the predominant electronic instability. To simplify the calculation, we note that the PE from the charged stripes in an array is well modelled by the PE from an isolated charged ladder of the same width, Fig. 2. [Note from the dos that the Van Hove singularity remains well defined on a stripe.] Hence, we need only study instabilities on ladders.

We explored the competition between a charge-density wave (CDW) and d-wave superconductivity on a ladder in a weak coupling calculation similar to Ref. 12, 13. For wide stripes, the bulk results are recovered. As the stripe width decreases,
Figure 2: (a) Dispersion of a stripe array with charged stripes 6 Cu wide (magnetic stripes 2 Cu wide). Data from Fig. 7d of Ref. 3; triangles (diamonds) = predominantly from charged (magnetic) stripes, while circles = mixed origin; dashed line = Mott bands of magnetic stripes; solid line = single (charged) stripe model, with \( k_x \) approximated by nearest quantized value. (b) Density of states for a single stripe 6 Cu wide.

Quantum confinement rapidly eliminates the CDW gap, by \( N \sim 8 \). Superconductivity is less affected, but is still suppressed by \( N = 2 \). [If the doping on the stripe were not fixed, there would be a large superconducting gap when the Fermi level coincides with the one-dimensional VHS of a stripe subband.]

Strong correlations can be included by incorporating some kind of spin ordering on the stripes. At the mean-field level, we have found a low-energy, phase separated solution to the Hubbard model \(^{14}\) which closely resembles a White-Scalapino (WS) stripe \(^{15}\). In a one-band Hubbard model with mean-field magnetization \( m_q \), the quasiparticle dispersion is

\[
E_{\pm} = \frac{\epsilon_k + \epsilon_{k+q}}{2} \pm \sqrt{\left(\frac{\epsilon_k - \epsilon_{k+q}}{2}\right)^2 + U^2 m_q^2},
\]

(1)

with

\[
\epsilon_k = -2t(c_x + c_y) - 4t'c_xc_y,
\]

(2)

and \( c_i = \cos k_i a \). For the cuprates, we expect \( t \approx 325 \text{ meV}, U/t \approx 6 \) and \( t'/t \approx -0.276 \). For \( q = \bar{Q} \equiv (\pi, \pi) \), this is the dispersion we assumed for the antiferromagnetic (AFM) stripes. A linear antiferromagnetic (LAF) phase arises when \( q = (\pi, 0) \); in general its properties closely resemble those of the WS stripes. For instance, 2-Cu wide LAF stripes act as antiphase boundaries for AFM stripes, a finite \( t' \) destabilizes the LAF phase, and the hole doping on an LAF stripe is close to that on a WS stripe \(^{14}\). The Fermi surfaces for AFM-LAF stripe arrays are even closer to experiment \(^{14}\) than those of Fig. 1.

Ordered phases are much more stable on LAF ladders. For instance, near \( x = 0.5 \) there is a CDW phase stabilized by near neighbor Coulomb repulsion \( V \), which is
highly stable, essentially independent of ladder width. For this strongly correlated CDW, the hole density varies from 0 to 1, not 2, Fig. 3. An attractive V can stabilize a d-wave-like superconductor on a ladder, with an anisotropic gap Fig. 4 which actually increases for the narrowest stripes. The optimum superconducting gap corresponds to the Fermi level at the LAF saddle point.

3. Chemical Potential Shifts in a Stripe Phase

While stripes persist up to $x_0 = 0.25$ in LSCO, the chemical potential is independent of doping only between half filling ($x = 0$) and $x = 0.125$, Fig. 5a. Actually, the same anomaly is found in La$_{2-x}$Sr$_x$NiO$_4$ (LSNO) Fig. 5b, which has long-range charge order up to at least $x = 0.5$, although $\mu(x)$ is constant only up to $x_c = 0.33$. By rescaling the LSNO $x_c$ to that of the cuprates (circles in Fig. 5b),
Figure 5: Doping dependence of chemical potential $\mu$ for (a) LSCO (triangles) and (b) LSNO. In (a), the circles are the scaled data of LSNO, while the diamonds are calculated from stripe band shifts associated with charging effects (see text).

it can be seen that the dependence $\mu(x/x_c)$ is quite similar in the two compounds. This also suggests an explanation: the break in slope for $\mu$ above $x_c$ is associated with commensurability effects. Each commensurate configuration has a well defined Madelung energy due to charge inhomogeneity. Between two commensurate configurations this charging energy changes linearly with doping (the intermediate states are presumed to be mixtures of the commensurate phases), but crossing over a commensurate phase leads to a different mixed phase, and a change in slope of the charging energy. In a layered compound, this charging energy contributes to the chemical potential of the layer involved. Thus, in the nickelates, the break is near 1/3 doping, and the 1/3 stripes are found to be stable over an extended doping range. In the cuprates, a similar effect at 1/8 is very plausible, since the charging energy is minimized at that doping. In fact, we can estimate the charging energy, since this Coulomb interaction also raises the chemical potential of the charged stripes with respect to the magnetic stripes, as found in our earlier calculation. These two charging effects should be proportional. The diamonds in Fig. 5a plot the calculated band-edge shift of the charged stripes with respect to the magnetic stripes, showing a reasonable agreement with the CuO$_2$ plane chemical potential shift.

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References
1. J.L. Tallon, cond-mat/9911422, J.L. Tallon, J.W. Loram, and G.V.M. Williams, cond-mat/9911423.
2. Consistent with $x_{opt} = 0.21$ [Y. Tokura, J.B. Torrance, T.C. Huang, and A.I. Nazabal, Phys. Rev. B38, 7156 (1988)], 0.24 [U. Tutsch, P. Schweiss, R. Hauff, B. Obst, Th. Wolf, and H. Wühl, cond-mat/9912361], 0.2 [M. Merz, N. Nücker, P. Schweiss, S. Schuppler, C.T. Chen, V. Chakarian, J. Freeland, Y.U. Idzerta, M. Kläser, G. Müller-Vogt, and Th. Wolf, Phys. Rev. Lett. 80, 5192 (1998)].
3. R.S. Markiewicz, to be published, Phys. Rev. B (cond-mat/9911108).
4. M.I. Salkola, V.J. Emery, and S.A. Kivelson, Phys. Rev. Lett. 77, 155 (1996).
5. G. Seibold, F. Becca, F. Bucci, C. Castellani, C. di Castro, and M. Grilli, cond-mat/9906108.
6. A. Ino, C. Kim, M. Nakamura, T. Mizokawa, Z.-X. Shen, A. Fujimori, T. Kakeshita, H. Eisaki, and S. Uchida, cond-mat/9902048.
7. Z.X. Shen, presented at M$^{2}$S-HTSC-VI, Houston, TX, Feb. 20-25, 2000; D.L. Feng, D.H. Lu, K.M. Shen, C. Kim, H. Eisaki, A. Damascelli, R. Yoshizaki, J.-i. Shimoyama, K. Kishio, G. Gu, S. Oh, A. Andrus, J. O’Donnell, J.N. Eckstein, and Z.-X. Shen, unpublished.
8. H. Ding, J.R. Engelbrecht, Z. Wang, J.C. Campuzano, S.-C. Wang, H.-B. Yang, R. Rogan, T. Takahashi, K. Kadowaki, and D.G. Hinks, cond-mat/0006143.
9. X.J. Zhou, P. Bogdanov, S.A. Kellar, T. Noda, H. Eisaki, S. Uchida, Z. Hussain, and Z.-X. Shen, Science 286, 268 (1999).
10. J. Hafner, “From Hamiltonians to Phase Diagrams” (Springer, Berlin, 1987).
11. P.W. Anderson, “Van Hove singularities as a source of anomalies in the cuprates”, PUP preprint 414 (1994), and “The Theory of High-$T_c$ Superconductivity”, (Princeton, University Press, 1997).
12. R.S. Markiewicz, C. Kusko and V. Kidambi, Phys. Rev. B60, 627 (1999).
13. C. Balseiro and L. Falicov, Phys. Rev. B20, 4457 (1979).
14. R.S. Markiewicz and C. Kusko, unpublished.
15. S.R. White and D.J. Scalapino, Phys. Rev. Lett. 80, 1272 (1998), ibid. 81, 3227 (1998).
16. A. Ino, T. Mizokawa, A. Fujimori, K. Tamasaku, H. Eisaki, S. Uchida, T. Kimura, T. Sasagawa, and K. Kishio, Phys. Rev. Lett. 79, 2101 (1997).
17. M. Satake, K. Kobayashi, T. Mizokawa, A. Fujimori, T. Tanabe, T. Katsufuji, and Y. Tokura, Phys. Rev. B61, 15515 (2000).