Stripe Disordering Transition

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\textbf{Abstract.} We have recently begun Monte Carlo simulations of the dynamics of stripe phases in the cuprates. A simple model of spinodal decomposition of the holes allows us to incorporate Coulomb repulsion and coherency strains. We find evidence for a possible stripe disordered transition, at a temperature below the pseudogap onset. Experimental searches for such a transition can provide constraints for models of stripe formation.

The relationship between stripe phases and the pseudogap in underdoped cuprates is not well understood. In our model \cite{1–3} the pseudogap is primary. It represents an instability of the hole Fermi liquid driven by Van Hove nesting \cite{4}. However, there is a competition of instabilities, with an antiferromagnet (or flux phase \cite{5–7}) at half filling and a charge-density wave (CDW) at the bare Van Hove singularity (VHS) near optimal doping. This competition leads to a classical phase separation of the holes – two minima in the free energy \cite{8,1}. This is restricted to a nanoscopic scale by long-range Coulomb effects, leading to phases similar to the experimentally observed stripe phases \cite{9}.

For such a nanoscale phase separation, the correct dispersion and pseudogap must be found by appropriate averaging over the heterogeneous, usually fluctuating stripes. Fortunately, tunneling and photoemission are sensitive mainly to the pseudogaps, and hence can be described by a simple \textit{Ansatz} of the stripe phase \cite{2,3}. For other purposes, a more detailed picture of the stripes is needed.

As a first step, we have begun Monte Carlo calculations of a classical picture of this restricted phase separation. Using the derived form of the free energy vs doping, we calculate the dynamic spinodal decomposition of the holes in the presence of Coulomb interactions. We find that there can be a stripe disordered transition, Fig. 1, at a temperature below the pseudogap onset. The disordered temperature is proportional to the free energy barrier between the two end-phases, inset, Fig. 2.

Technical details of the calculation are as follows: we work with a generic form of the free energy, $F = F_0 x(x - x_c)^2$, which approximates the calculated free energy of Ref. \cite{1}. The calculations are done on 128×128 lattices, with periodic boundary conditions. The critical doping $x_c$ is taken as 1/6, which necessitates...
a non-Markovian algorithm – a particular lattice site must retain memory of the average hole occupation over several cycles. We typically choose 30 cycles, which means that a single hole must spread out over 6 lattice sites – close to the size of a magnetic polaron [10]. The algorithm chosen is able to find the correct ground states in the low doping limit (which can be found analytically). The stripes are not topological, and the stripe-like domains are produced by coherency strains [11]. In the absence of such strains, the domains would be irregular shaped, approximately equiaxed, as found by Veillette, et al. [12] The coherency strains produce a mixture of stripes along both $x$ and $y$ axes; to get single-axis stripes, as in the figure, it is assumed that there are local martensitic domains.

The phase separation can be most clearly seen in a plot of the distribution of site occupancies by holes, Fig. 2. At low temperatures, this is a two-peaked structure, with one peak (off scale in the figure) at zero doping, and the other near $x_c$ (it is actually at a doping below $x_c$, due to charging effects). As the temperature increases, the two-peak structure is gradually smeared out, and at high temperatures there is only a monotonic distribution. This finite system has a crossover rather than a sharp transition. For the parameters chosen, the transition
is centered near $k_BT_m \sim 30\text{meV}$, which is approximately the barrier height of the free energy (inset). This result is not very sensitive to the value of dielectric constant, $\epsilon$.

Thus, as the underdoped cuprate cools from high temperatures, there can be a series of phase transitions. At high temperatures, there will be the pseudogap onset. In our simplified mean field Ansatz [3], this appears as a long-range ordered CDW phase, but the inclusion of two-dimensional fluctuations [13,14] leads to appropriate pseudogap behavior. The stripe phase ordering temperature found here could in principle fall at a lower temperature. The stripes in our simulations continue to fluctuate, and the long-range stripe order phase seen by Tranquada [9] may be yet another transition. The two-branched transition to a stripe phase bears some resemblance to the phase diagram of Emery, Kivelson, and Zakhar [15], but is in fact different. Their upper transition ($T_1^*$) corresponds to the onset of stripe order, their lower ($T_2^*$) to the onset of a spin gap on the hole doped stripes.

There is not much experimental evidence for the onset of short-range stripe order, although phase separation in La$_2$CuO$_{4+\delta}$ starts near 400K [16], much lower than the pseudogap onset temperature, $\sim 800K$ [17]. In most materials, the incommensurate magnetic modulations near ($\pi, \pi$) broaden out and disappear near the pseudogap $T^*$, which is a lower temperature ($\sim\leq150K$ for the compositions studied) [18]. The best place to look would be in the extremely underdoped regime, where $T^*$ is highest.

While the above calculations reproduce the general properties of the stripes, there are a number of features which are not well reproduced. First, for the elastic constants of LSCO [19], the stripes lie along the orthorhombic axes – i.e., they are diagonal stripes. Further, for the parameters assumed, the charged stripes tend to grow wider with increased doping, maintaining a constant interstripe spacing, whereas experiment [20] suggests that the stripe shape stays constant, but the stripes move closer, as doping increases, at least for $x \leq 0.12$. This suggests that some important feature has been omitted from the model, most probably the topological nature of the stripes as magnetic antiphase boundaries.

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