Electronic Liquid Crystal Phases in Hole Doped Mott Insulators

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Abstract

Theoretical, numerical, and experimental studies have suggested the existence of 'striped' electronic phases in doped antiferromagnets such as the high temperature superconductors. We survey the literature and summarize the results.

1 Introduction

It has been suggested that high temperature superconductivity in the cuprates is closely related to the existence of an electronic liquid crystal phase [1]. Others suggest that these striped phases exist as a competing order to superconductivity[2]. Whichever the case may be, these states are theoretically interesting in their own right. These states represent electronic groundstates with broken symmetries similar to those found in liquid crystals and incommensurate systems.

The electronic liquid crystal phase is thought to emerge as a system is tuned to the quantum disordered side of a quantum critical point. In these materials, the cuprates and nickelates, the quantum ordered phase is a Mott insulator. By doping the system with holes, one is able to tune the system to either the ordered side, a Mott insulator, or the disordered side, an electronic liquid crystal phase. It is thought that the order parameter fluctuations expanded in a small parameter, the distance from the quantum critical point, physically manifest themselves as states with a locally broken symmetry (isotropic liquid crystal states). These order parameter fluctuations are dynamic and thus time evolve but can be pinned into place using boundaries, weak disorder, vortices, etc.[3]. This can also give rise to nematic, smectic, or crystalline phases.

Numerical studies typically study the Hubbard model or some variant thereof. These simplified Hamiltonians are chosen to reflect the most fundamental parts of Mott insulator physics and determine the effect of additional doped holes. The Hubbard model is a lattice model that can take into account interactions between neighboring spins (J), hopping between neighboring sites (t), an external potential (V), and any other components dictated by some specific problem. In this case, the cuprates and nickelates are well modelled by a two dimensional square lattice corresponding to the Cu-O or Ni-O plane. In the absence of an external potential, a two dimensional t-J model where nearest neighbor hopping and spin interaction are taken into account is often used as the model Hamiltonian of choice.

Experimental evidence for electronic liquid crystal states have been collected using a variety of techniques [3] including neutron and x-ray scattering, nuclear quadrapole resonance [7], and scanning tunneling microscopy [8]. It is generally agreed that static electronic liquid crystal phases have been observed in some nickelates and cuprates. The existence of quantum liquid crystal states, more closely associated with superconductivity, has yet to be conclusively confirmed but is suspected.

In this paper we will start with a short description of the spin and charge density wave. Then review numerical and experimental data supporting the existence of stripes. We will give a brief qualitative explanation for the mechanism of stripe formation. In conclusion we will mention possible future directions for research, and connections to other problems.

2 Spin and Charge Density Waves

Much of the following work relies on the spin density wave (SDW) and the charge density wave (CDW). Peierls predicted the existence of the CDW in one dimension in 1955. A particularly good review of CDW and their dynamics is given by ref. [9] and another. The SDW was predicted by Overhauser in 1960. A review of SDW and their dynamics is given by [11] and one on Cr in particular is [10]. Here we will define and briefly justify these collective modes.

Originally Peierls observed that a one dimensional array of ions and electrons could lower its free energy through periodic modulations in the ion and electron displacements[1]. If the periodicity of these modulations is $\lambda = \frac{\pi}{k_F}$ and the amplitude is u, it can be shown that the increase in the elastic energy of the system due to the lattice distortions goes as u^2 while the decrease in the electronic kinetic energy (for small u) goes as $u\ \log(u)$. So that for small lattice distortions the total energy of the system is decreased. This result is generally true for all 1-D systems, although the Peierls instability can be too small to observe in some materials, or at high temperatures. This result generalizes to higher dimensions in the obvious fashion.

The SDW can be shown to be a stable groundstate for an electron gas confined to one translational dimension interacting by a repulsive delta function potential. In this simplified system The energy of the SDW state as compared to the normal state is $W = NE_F[1 + b^2 - 2b\text{coth}(2nb)]$ where n is a dimensionless quantity proportional to the electronic density, $b = q/2k_F$, and q and g are parameters from the self consistant Hartree-Fock potential for this problem, $U(z) = 2gE_F(\sigma_x\text{cos}(qz) + \sigma_y\text{sin}(qz))$. Overhauser calculated this analytically using a variational argument by solving for the exact one particle spin up and spin down states, then used them to get the kinetic and potential energy terms, and finally inspecting the parameters in $U(z)$ yielding the lowest energy state.

We can see that the energy difference between SDW and normal state normal state, corresponding to $b = 1$, is less than zero and therefore represents a state of higher energy than the energy minimizing choice for b. Physically, the lowered energy corresponds to a lowering of the exchange energy at the price of increased kinetic energy. However, Overhauser states that "this increase is sufficiently small for the exchange energy to dominate" [12]. The potential $U(z)$ has the property that only electron states with $k = k, \uparrow$ and $k' = k + q, \downarrow$ are mixed. The resulting energy gaps in the free electron spectrum lower the energy of the system if $q = k_F$ so that occupied states have their energy lowered and unoccupied states have their energy raised[10]. Later the author generalized this work to three dimensions with realistic electron interactions in 1962 with similar results.

[1] This is a CDW.

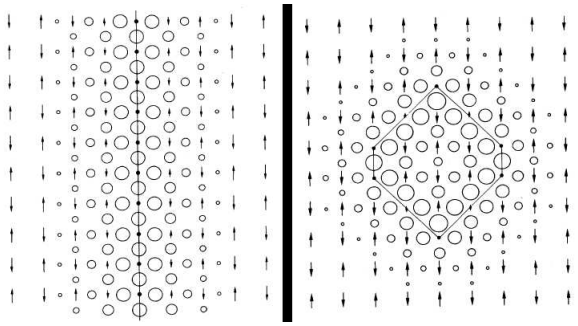

Figure 1: Results for numerical calculations of holes on antiferromagnetic perovskite ($Cu0_2$) planes. Excess hole density on O is illustrates by circle radius while spin on Cu sites is illustrates by arrows. On left, ten holes in a 9x10 supercell. On right, ten holes in a 10x10 supercell.

3 Theoretical and Numerical Results

In 1989 Zaanen and Gunnarsson [4] numerically studied a model cuprate system using the two band Hamiltonian,

$$H = H_0 + H_1 \tag{1}$$

$$H_0 = \sum_{j,\sigma}(\epsilon_p p^\dagger_{j,\sigma} p_{j,\sigma}) + \sum_{i,\sigma}(\epsilon_d d^\dagger_{i,\sigma} d_{i,\sigma}) + \sum_{\langle i,j\rangle,\sigma} V_{ij}(d^\dagger_{i,\sigma} p_{j,\sigma} + H.c.) \tag{2}$$

$$H_1 = \sum_i U n_{d,i,\uparrow} n_{d,i,\downarrow} \tag{3}$$

within the Hartree-Fock approximation where H_1 is replaced with a mean field approximation. The subscripts p, d refer to the shell the electron resides in, σ represents the Pauli matrices. The full order parameter symmetry is taken into account by including the magnitude of the spin along the quantization axis as well as the canting angle from it. The parameters they used in the Hamiltonian $(\epsilon_p, \epsilon_d, V_{ij}, U)$ for this calculation were fit from data obtained using both electron spectroscopy data and the local-density-approximation.

The authors found two different charge structures, a charge ring and a charged stripe. The charge ring structure was shown to be of higher energy than the stripe due to curvature. The conclusions are that the ground state of the model Hamiltonian they studied in the low doping regime (less than ten percent hole concentration) was a broken symmetry state consisting of parallel charge stripes, the CDW, which may or may not be accompanied by a SDW, and that in this context the strong coupling t-J model would make sense.

The t-J model justified by Zaanen and Gunnarsson,

$$\hat{H} = J \sum_{<i,j>} (\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} n_i n_j) - t \sum_{<i,j>,s} (c^\dagger_{i,s} c_{j,s} + H.c.) \tag{4}$$

is often used in the literature to model these materials. It is a Heisenberg spin model on a two dimensional square lattice with nearest neighbor hopping terms, t, and antiferromagnetic nearest neighbor spin-spin coupling constant J. A collection of results taken

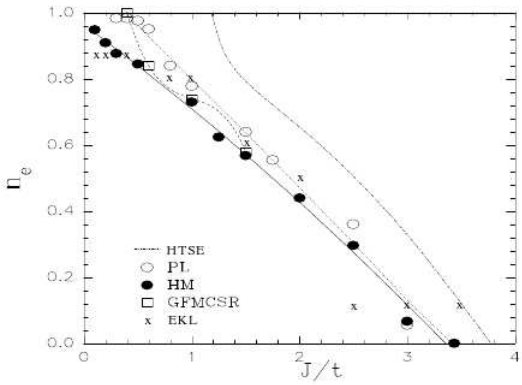

Figure 2: Several different studies results for the location of the boundary between striped and non-striped phases. n_e is the electron density, J/t is the dimensionless ratio of the spin coupling strength to that of nearest neighbor hopping. For all of these studies the boundary does exist, there is phase separation. From Carlson et al. Figure 36.

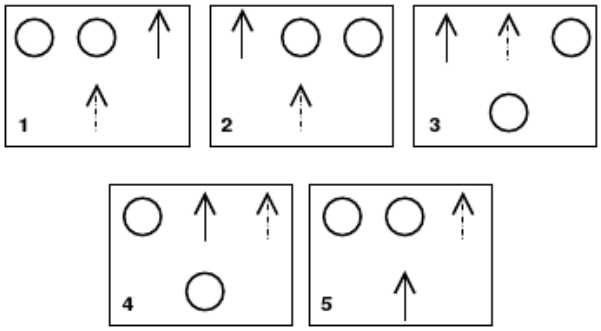

Figure 3: As the bound hole pair propagates around the lattice the spins switch place. This frustrates hole pairing.

from Carlson et al.[1] summarizes many different numerical approaches to solving this Hamiltonian (Fig. 2). The technical details of these methods are of secondary importance. The important result is that phase separation is observed in this model in some regime for many different numerical approaches.

Hole dynamics play an important role in determining the ground state structure of this Hamiltonian and the phase separation found in these studies. A single hole in an antiferromagnetic lattice experiences a strong resistance to nearest neighbor hopping because it leaves behind a frustrated series of spins as it hops between the two spin sublattices. For two holes it was initially thought that a bound state would result and that they would not experience a barrier to tunneling. All the spins would remain on the correct sublattice as the bound hole pair propagated through the antiferromagnetic lattice. However this is not the case. The fermion statistics of the spins increase the pair energy, see Fig. 3, and prohibit the kinetic energy driven pairing of the holes.

The qualitative reason for the separation of the hole rich and spin rich regions is the minimization of the hole kinetic energy and the spin potential energy. The hole kinetic

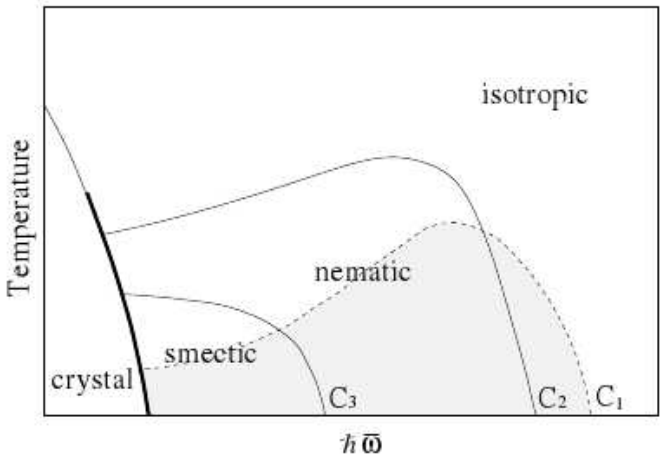

Figure 4: $\hbar\bar{\omega}$ is a measure of the magnitude of the importance of the transverse fluctuations of the CDW. The grayed region is that of suspected superconductivity, however we are interested only in the liquid crystal phases indicated by crystalline, smectic, nematic, and isotropic. From [1]

energy is minimized by allowing them to delocalize in some region where they can hop without leaving behind a frustrated spin lattice. The exchange energy between neighboring spins is minimized by expelling the holes. When the coulomb interactions between the spins (electrons) and holes are included, the strength of the coulomb interaction sets the scale for this phase separation. There is a competition between short range phase separation and long range homogeneity.

This competition between the short range and long range forces determine the length scale at which the liquid crystal phases emerge. They exist as "rivers of charge" in two dimensions [1]. These structures can be insulating, metallic, or superconducting depending on several more complicated factors. Of the different orders that are possible, as the temperature of the system goes to zero, the CDW susceptibility (static striped phase) diverges most strongly [6]. This indicates an insulating ground state since the change is locked into quasi-one dimensional configurations. Tunneling between stripes is exponentially small. However when the transverse fluctuations of the stripes are taken into account[2] the result can be metallic and/or superconductive behavior. The phase diagram as a function of temperature and transverse fluctuation strength is illustrated in Fig. 4. The basis of all these phases is the charge stripe as is illustrated in Fig. 5.

4 Experimental Observations

Neutron scattering studies of the cuprates are particularly useful for uncovering striped order. The primary reason for this is that the neutrons can scatter off of the electron spins and can image the lattice distortions caused by the CDW. However it has been

[2]They are not truly static unless pinned into place by disorder in the lattice or some other effect [3]

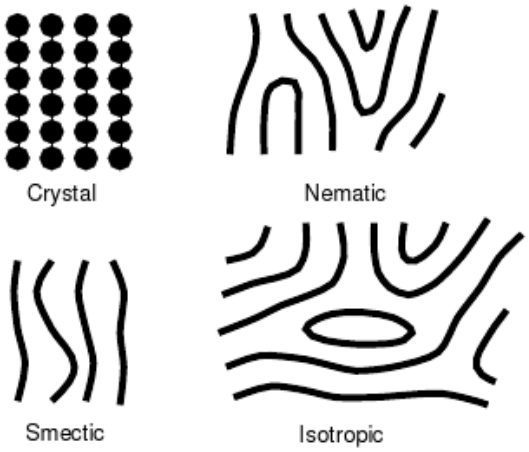

Figure 5: Cartoon illustrations of the discussed phases. Crystalline respects the discrete point symmetry of the underlying lattice. The smectic phase is translationally invariant in one direction. The nematic phase has an axis of orientation but is translationally and rotationally invariant. The isotropic phase breaks no spatially symmetries but is locally inhomogeneous. From [6]

shown that SDW implies the existence of CDW (see [4]) so evidence of the former predicts existence of the latter. Neutron scattering experiments on materials with electronic liquid crystal order should contain additional Bragg peaks corresponding to the charge stripes.

Tranquada et al.[13] found evidence for magnetic order in $La_{1.6-x}Nd_{0.4}Sr_xCuO_4$ at several doping levels. The antiferromagnetic ordering of the material is characterized through low energy neutron scattering by its wave vector $\mathbf{Q}=(\frac{1}{2},\frac{1}{2})$. In the presence of a SDW, this antiferromagnetic wave vector is shifted to $\mathbf{Q}=(\frac{1}{2}\pm\epsilon,\frac{1}{2})$ and $\mathbf{Q}=(\frac{1}{2},\frac{1}{2}\pm\epsilon)$ where $\epsilon\approx x$ where x is the hole doping concentration. The left side of Fig. 6, taken from this study, illustrates this shift. Later, a rather complete neutron scattering study on $La_{1.6-x}Nd_{0.4}Sr_xCuO_4$ by Ichikawa et al. [7] considers the existence of charge and spin stripes a foregone conclusion due to this earlier study and their own results.

Scanning tunneling microscopy/spectroscopy (STM) is another useful probe for determining the presence of striped order, and an optimal probe for detecting nematic order. A spatial modulation in the density of states with a checkerboard pattern caused by Friedel oscillations around impurities is expected in materials with striped order. In a homogeneous two dimensional state the Fourier transform of the Friedel oscillations defines a circle of radius $2k_f$. In the electronic liquid states, Friedel oscillations are expected to be checkerboard in pattern because they reflect the broken symmetry of the striped state. The Fourier transform of these oscillations would appear as four points in the power spectrum of the local density of states. The local density of states is easily probed using STM then Fourier transformed to get the power spectrum.

Howald et al. performed such a study and found stripe (and likely nematic) order in $Bi_2Sr_2CaCu_2O_{8+\delta}$ (BSSCO). The study showed that near-optimally doped BSCCO has

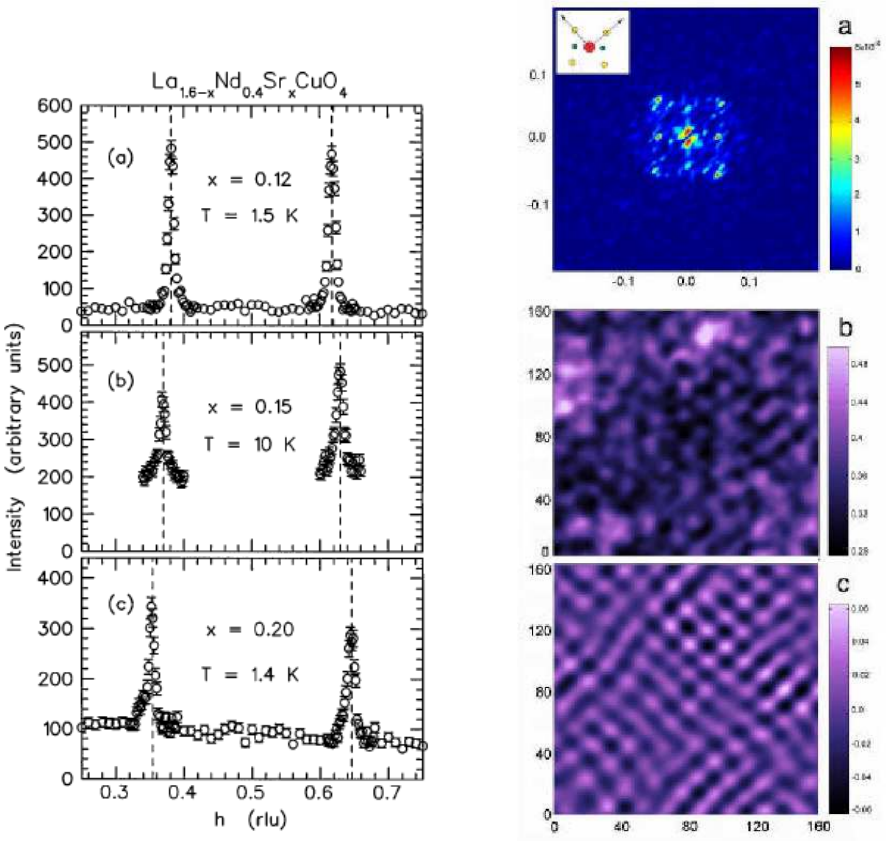

Figure 6: (Left) Scans through the magnetic peaks show pronounced spikes in the neutron scattering intensity. This is a strong indication of a SDW. From [13]. (Right) Top is the Fourier transform of the LDOS. the two points on the x axis correspond to the superlattice of the underlying material. The central point is large due to random impurities. The four points in the corners are the evidence for a CDW. The bottom LDOS map is a filtered version of the middle LDOS map, accentuating the CDW. This image can be interpreted as evidence for an electronic nematic phase. From [8].

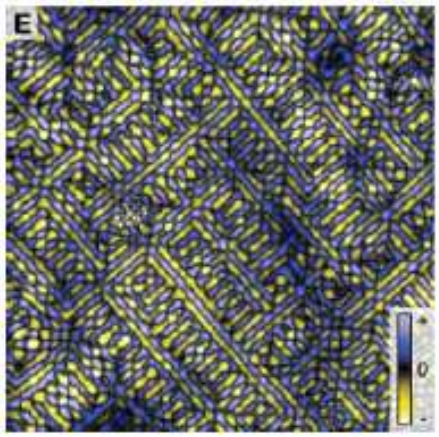

Figure 7: From [16]. Image of laplacian of tunneling anisotropy in $Ca_{1.88}Na_{0.12}CuO_2Cl_2$ at 4.2K ($T_c \approx$21K). The color indicates the relative hole concentration. The characteristic length of structures in this image is $4a_0$x$4a_0$ where a_0 is the Cu-O-Cu distance. According to the paper, this structure is a bond centered electronic glass. It appears to be a striped structure viewed through kaleidoscope eyes.

striped electronic order that lies along the Cu-O bonds. These results are illustrated in the right hand side of Fig. 6. The bottom right map is a Fourier filtered real space map of the LDOS, and supports the presence of an electronic nematic phase.

A more recent result with higher resolution of the stripes was obtained by Kohsaka et al.[16] in two different lightly hole doped materials, $Ca_{1.88}Na_{0.12}CuO_2Cl_2$ and $Bi_2Sr_2Dy_{0.2}Ca_{0.8}Cu_2O_{8+\delta}$. The technique they used was slightly different in that they used the anisotropy of the tunneling spectrum[15] to image the stripe structure.

In a system with strong repulsive interactions it is relatively easier to subtract an electron than to add one. If we denote the local hole concentration at some point $\vec{r}$, $x(\vec{r})$, then, as shown in ref. [15], the STM matrix elements can be written as a ratio of sum rules[3] to find,

$$\frac{\int_0^{\Omega_L} d\omega\, g(\vec{r};\omega)}{\int_{-\infty}^{0} d\omega\, g(\vec{r};\omega)} = \frac{2x(\vec{r})}{[1-x(r)]} + \dots \tag{5}$$

where $g(\vec{r};\omega)$ is the local tunneling conductance, $\frac{dI(\vec{r};\omega)}{dV}$, and Ω_L is the cutoff. According to the paper there are some omitted terms that are approximately 10% the fist terms magnitude. The quantity on the left can be calculated using the STM data, thereby yielding the local hole concentration $x(\vec{r})$. Plotted in Fig 7. from Kohsaka et al. is the laplacian of this quantity.

It is apparent from the image that there is some structure to this electronic configuration. Locally there is the characteristic checkerboard pattern, but there is a lack of long range order. The authors conjecture that with increased doping and a different

[3]This avoids the necessity to find some unknown factors. By using a ratio they cancel.

underlying lattice, $La_{1.875}Ba_{0.125}CuO_4$ or another La based cuprate, at doping levels of x=1/8 stripes might arise.

5 Conclusions and Future Directions

The existence of a static striped phase in the cuprates and nickelates is generally accepted. However, there is still some controversy about the interpretation of the STM data. It is possible that the checkerboard pattern in the LDOS could be interpreted as quasiparticle excitations in a d-wave superconductor [3]. This interpretation is discounted in the Review of Modern Physics article, but may not be entirely disproven. In Kohsaka et al.[16] this was avoided by using a different analytic technique to analyze the data.

Although quantum Monte Carlo lacks the accuracy required to detect superconductivity, it should be able to detect striped order if it exists. In Zaanen and Gunnarson's studies on holes, the energy scales are of order 0.01V. This is easily resolvable within quantum Monte Carlo. Some of the problems cites are choice of boundary conditions, or finite size effects[4]. The problem with ab-initio all electron quantum Monte Carlo is the large size of the system. Some simplified Hamiltonian or model system of complexity intermediate to a Hubbard model and ab-initio methods is desirable.

There is an emerging picture of strong correlations leading to hole and spin rich regions, however the connection to high temperature superconductivity is not clear. The connection suspected to exist between quantum striped phases, quantum superpositions of stripes, and superconductivity has yet to be fully elucidated. There are questions as to whether stripes are a general feature of these materials, if it is a competing order, if it causes pairing, and other issues [1]. Theoretical and experimental work is ongoing to discover this connection if it exists[17].

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