Spin-Charge Interplay in Electronic Liquid Crystals: Fluctuating Spin Stripe Driven by Charge Nematic Ordering

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We study the interplay between charge and spin ordering in electronic liquid crystalline states with a particular emphasis on fluctuating spin stripe phenomena observed in recent neutron scattering experiments. Based on a phenomenological model, we propose that charge nematic ordering is indeed behind the formation of temperature dependent incommensurate inelastic peaks near wave vector (π, π) in the dynamic structure factor of $YBa_2Cu_3O_{6+y}$. We strengthen this claim by providing a compelling fit to the experimental data.

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The variety of competing ordering tendencies is both a hallmark of correlated electron fluids, such as cuprate and Fe-based superconductors [1,2], and a theoretical challenge. As such, a clear identification of a broken symmetry offers a valuable guiding principle. Recent observations of temperature, energy, and doping dependent onset of anisotropy in inelastic neutron scattering (INS) by Hinkov *et al.* [3] provides an opportunity for just such identification.

The symmetry of the "fluctuating spin stripe" phenomena (one-dimensional incommensurate spin modulation at finite energy) observed in Ref. [4] is consistent with that of a nematic phase [5] (a metallic state that breaks rotational symmetry without breaking translational symmetry). Furthermore, the qualitative departure in the magnetic response of underdoped $YBa_2Cu_3O_{6+y}$ in Ref. [4] from that of optimally and overdoped regimes $y \gtrsim 0.5$ [6–9] indicates the possible existence of a quantum critical point at around $y \sim 0.5$ as we sketch in Fig. 1. In specific, low-energy features are enhanced in INS of $y = 0.45$ while the high energy "hour-glass" dispersion which is prominent at higher doping is suppressed [6–10]. However, despite the reported temperature dependence of the finite-frequency incommensurability being suggestive of an order parameter [3], it has not been clear how this quantity can be related to a specific order parameter.

A number of theoretical studies considered possible signatures of electronic liquid crystal physics in the magnetic response [11–13]. While these studies shed light on the hour-glass dispersion observed in $y \gtrsim 0.5$ at high energies, their connection with the low-energy phenomena in the underdoped regime with $y < 0.5$ is unclear. Moreover, they focused on the superconducting phase while the observed onset of fluctuating spin stripe behavior is at $T_N \sim 150$ K, well above the superconducting ordering temperature $T_c = 35$ K.

In this Letter we propose that charge nematic ordering drives the fluctuating spin stripe phenomena observed in underdoped $YBa_2Cu_3O_{6+y}$. We consider a metallic system proximate to antiferromagnetic (AFM) ordering and show that charge nematic ordering quite uniquely can induce fluctuating and even static spin stripes thus providing a concrete connection between the charge [14] and spin aspects of liquid crystalline behavior in underdoped $YBa_2Cu_3O_{6+y}$. Our claims are supplemented by a successful fit with available INS data [4].

Phenomenological model.—Hinkov *et al.* [4] detect the dynamic onset of anisotropy through incommensurate inelastic peaks near the AFM wave vector $\mathbf{Q} = (\pi, \pi)$ in a metallic system (see Fig. 2). Given a microscopic theory of itinerant magnetism being an open question, we take a phenomenological approach as a first pass through the problem. In the presence of long-range AFM ordering, low-energy excitation in the particle-hole channel is dominated by gapless spin waves near $\mathbf{Q}$ with infinite lifetime:

$$\vec{\phi}(\mathbf{q}, \omega) = \int \frac{d^2\mathbf{k}\, d\Omega}{2(2\pi)^3} \psi^\dagger_\alpha(\mathbf{k} + \mathbf{Q} + \mathbf{q}, \Omega + \omega) \vec{\sigma}_{\alpha\beta} \psi_\beta(\mathbf{k}, \Omega).$$

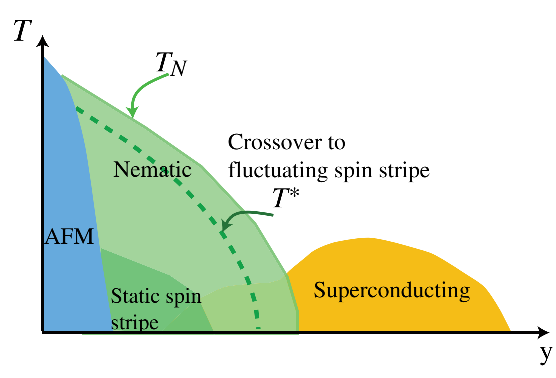

FIG. 1 (color online). Schematic phase diagram of $YBa_2Cu_3O_{6+y}$.

Here the operators $\psi_\alpha^\dagger$ (ψ_α) are the fermion creation (annihilation) operators with spin $\alpha = \uparrow, \downarrow$. $\vec{\phi}$ and $\vec{\sigma}$ are vectors in spin space with $\sigma^i_{\alpha\beta}$ representing (α, β) component of Pauli matrix σ^i for $i = x$, y, z. $\mathbf{q}$ denotes the wave vector of the spin waves measured from $\mathbf{Q}$ and ω denotes their frequency. For underdoped cuprates outside of but close to the AFM phase (see Fig. 1), this spin wave can be either damped or gapped and well defined. To quadratic order in $\vec{\phi}$, the appropriate effective action takes the form [15]

$$S = \frac{1}{g}\int \frac{d^2\mathbf{q}d\omega}{(2\pi)^3}(i\Gamma|\omega| + \omega^2 - \Delta^2(\mathbf{q}))|\vec{\phi}(\mathbf{q}, \omega)|^2, \quad (1)$$

where g is an overall scale and $\Delta(\mathbf{q})$ is the momentum $\mathbf{q}$ dependent spin-wave gap in the absence of damping and Γ is the damping energy scale. Here we assume Landau damping form [16] but most of our conclusions below are insensitive to the details of the damping dynamics.

The dynamic structure factor measured by INS experiments will be proportional to the spectral function

$$\chi''(\omega, \mathbf{q}) = g\frac{\Gamma\omega}{(\Gamma\omega)^2 + (\omega^2 - \Delta(\mathbf{q})^2)^2}, \quad (2)$$

for the action of Eq. (1). The uniform component of the gap $\Delta(\mathbf{q} = \mathbf{0})$ sets the energy scale above which INS intensity is significant and the $\mathbf{q}$ dependence of $\Delta(\mathbf{q})$ determine the distribution of intensity in the Fourier space. In the absence of other symmetry breaking tendencies, $\Delta(\mathbf{q})$ will be a minimum at $\mathbf{q} = \mathbf{0}$ and respect the point group symmetry of the system. Hence the INS intensity above $\Delta(\mathbf{q} = \mathbf{0})$ will be C_4 symmetric (modulo orthorhombicity due to chain layer) and peaked at $\mathbf{q} = \mathbf{0}$. Temperature and energy dependent anisotropic incommensurability observed in Ref. [4] indicates additional ordering tendencies at play. We first study the effect of charge nematic ordering motivated by transport anisotropy observed in the nearby regime [14].

In a nematic fluid, charge degrees of freedom collectively break rotational symmetry of space while preserving

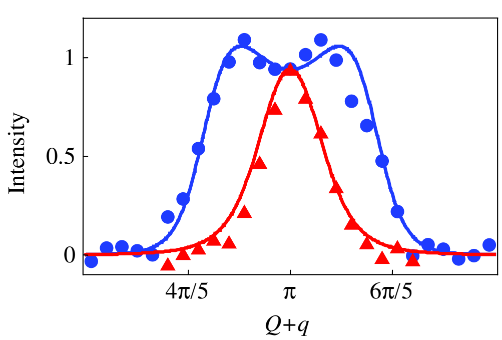

FIG. 2 (color online). Fit to momentum dependence of INS intensity along a (blue dots) and b (red triangles) axes. Data obtained from Ref. [4] taken at $T = 5$ K and $\omega = 3$ meV. Note: any slight asymmetry observed in the data is not accounted for in the phenomenological model presented here.

the translational symmetry (hence remains metallic) [5]. A nematic order parameter in a continuum system has the symmetry of charge quadrupole moment, which can either be written as a symmetric traceless tensor of rank two or as a complex field [17,18].

As the nematic ordering involves spatial symmetry breaking, the nature of the order parameter itself is affected by crystal fields due to the lattice which lowers the spatial rotational symmetry to a discrete group. For instance, in a square lattice with C_{4v} symmetry, the ordering can occur in one of two channels $d_{x^2-y^2}$ or d_{xy} reducing the order parameter symmetry to Ising-like (a single component real field) in either case [19]. Because of this discretization of the order parameter symmetry, the nematic fluctuation below the transition temperature T_N will be massive. In $YBa_2Cu_3O_{6+y}$, the weak external field imposed by the chain layer will likely pick the nematic to occur in the $d_{x^2-y^2}$ channel and a representative form of order parameter can therefore be written as

$$N = \int \frac{d^2\mathbf{k}}{2(2\pi)^2}\bar{N}(\cos k_x - \cos k_y)\psi_\alpha^\dagger(\mathbf{k})\psi_\alpha(\mathbf{k}), \quad (3)$$

although any electronic quantity that is odd under 90° spatial rotation can serve as the order parameter [17]. In fact, nematic phases so far have been mostly detected through temperature dependent in-plane transport anisotropy in quasi-2D systems [20,21].

In $YBa_2Cu_3O_{6+y}$, Ando *et al.* [14] observed that transport anisotropy increases upon under doping below $y \sim 0.5$ while the effect of CuO chains diminishes. Its electronic origin is further supported by the fact that this anisotropy only sets in below a doping dependent onset temperatures T_N (180 K for $y = 0.45$) making nematic ordering a compelling candidate for broken symmetry in underdoped $YBa_2Cu_3O_{6+y}$ as advanced in Ref. [4] without a theoretical model.

Consider the effect of $d_{x^2-y^2}$ nematic ordering below T_N on the spin fluctuations in Fig. 1. The effective action now depends on both $\vec{\phi}$ and N. Away from the classical critical region near T_N, the gapped nematic fluctuations can be integrated out and the effect of finite N can be represented by N-dependent coefficients in the gradient expansion of $S[\vec{\phi}, N]$. We represent such N dependence of $S[\vec{\phi}, N]$ using the N dependent "gap" $\Delta(\mathbf{q}; N)$. On symmetry grounds $\Delta(\mathbf{q}; N)$ in the long distance limit takes the following form to the quadratic order in q:

$$\Delta^2(\mathbf{q}; N) = \Delta_0^2(N) + c_0^2(N)q^2 - c_2^2(N)N(q_x^2 - q_y^2) + \cdots, \quad (4)$$

where all momenta are in units of the lattice constant (i.e., $q_x \equiv k_x a$). Assuming tetragonal symmetry of underlying lattice, all the functions Δ_0, c_0, c_2 should be even functions of N since $N \to -N$ under 90° spatial rotation. For small N, we expand $\Delta(\mathbf{q}; N)$ in powers of N and treat Δ_0, c_0, c_2 as constants to lowest order in N [22]. (This approach would be only valid up to the nematic gap scale ~18 meV based on the onset temperature for transport anisotropy $T_N \approx 180$ K.)

Notice that the nematic ordering allows for anisotropic flattening of the momentum dependence of $\Delta(\mathbf{q}; N)$ in Eq. (4) which will elongate the inelastic (π, π) peak in the x direction. For $N > N^*$, with $N^* = c_0^2/c_2^2$, this effect will further shift the peaks to incommensurate positions at $(\pi \pm \delta, \pi)$ at low energy [$\omega < \Delta(\mathbf{q})$ for any $\mathbf{q}$] due to a dip in $\Delta^2(\mathbf{q}; N)$ at $\mathbf{q} = (\pm\delta(T), 0)$ with

$$\delta(T) \propto (N(T) - N^*)^{1/2}. \tag{5}$$

Such incommensurability will naturally have temperature dependence resulting from the temperature dependence of $N(T)$. We represent this crossover temperature T^* for the onset of such fluctuating spin stripe at $N(T^*) = N^*$ as a dashed line in Fig. 1. Note that while the form of Eq. (5) is reminiscent of an order parameter, there is no singularity in the free energy at T^* (this is a crossover).

At even lower temperatures, large enough N may even stabilize *static* spin stripes. While our lowest order in N analysis may not be applicable in its explicit form for large N, it predicts a critical value N_c where $\Delta(\pm\delta, 0; N_c) = 0$. For $N > N_c$ the system will develop static spin stripes. Such static spin stripes were recently observed at $T = 2$ K by Haug *et al.* [23] and a similar effect was also reported in $La_{2-x}Sr_xCuO_4$ [24]

Comparison with experiments.—The model defined by Eqs. (1) and (4) provides a natural connection between transport measurements [14] and recent INS studies in $YBa_2Cu_3O_{6+y}$ [4]. One nontrivial prediction is the T dependence of the incommensurability $\delta(T)$ in the vicinity of T^*.

Equation (4) implies temperature dependence of $\delta(T)$ reminiscent of that of a mean field order parameter yet without any thermodynamic singularity at $T = T^*$. This is independent of the unknown order parameter exponent β of $N \propto (T - T_N)^\beta$ and any microscopic details. As long as N^* is small and the spin waves are gapped, so that we may use the quadratic action of Eq. (1), the $(N - N^*)^{1/2}$ dependence of δ in Eq. (5) is valid to leading order in $(N - N^*)$. By inserting $N \propto (T - T_N)^\beta$ to Eq. (5), one can show

$$\delta \propto (T - T^*)^{1/2}, \tag{6}$$

which is in good agreement with experimental observation in Ref. [4].

As a practical test of our phenomenological theory, we fit the INS data of Ref. [4] with the spectral function Eq. (2) using $\Delta(\mathbf{q}; N)$ from Eq. (4). Figure 2 shows a fit to momentum line cuts of INS data at $\omega = 3$ meV and $T = 5$ K by setting $g/\Gamma = 5.1$ meV, $[\Delta_0^2 - (3\text{ meV})^2]/\Gamma = 2.7$ meV, $c_0^2/\Gamma = 16$ meV, $c_2^2 N/\Gamma = 24$ meV. [We also include symmetry allowed quartic terms of the form $\lambda_1(q_x^4 + q_y^4) + \lambda_2 q_x^2 q_y^2 + \lambda_3 N(q_x^4 - q_y^4)$ to fit high $\mathbf{q}$ part of data [25].] Note that this fit at $\omega = 3$ meV is insensitive to the relative strength between damping and gap energy scales Γ/Δ_0. Only the ω dependence is sensitive to this ratio. Similar fits at higher temperatures ($T = 40$ K and $T = 100$ K) hint at thermal fluctuation driven damping at higher temperatures and T^* being below 100 K [26]. Note that we are using a different scheme for extracting T^* from that of Ref. [4].

Fixing most of model parameters by the $\omega = 3$ meV, $T = 5$ K data, we fit the frequency dependence of uniform susceptibility $\chi''(\omega)$ at 5 K. The energy dependence fit shown in Fig. 3 is valid up to the estimated scale of nematic fluctuation mass (≈18 meV). Both Figs. 2 and 3 show good agreement with data. While fitting is more of a check rather than the main result of this Letter, the frequency dependence allows us to estimate $\Gamma/\Delta_0 \sim 1.3$ giving a reasonable fit. Note that while one expects the spin wave to be well defined inside the superconductor, the data of Ref. [4] appear to indicate a significant amount of damping. Speculating the source of this damping is beyond the scope of our Letter but this might be consistent with the existence of the low-energy excitations reported in superconducting underdoped $Bi_2Sr_2CaCu_2O_{8+\delta}$ [27].

Effect of other ordering tendencies.—For completeness, we also consider the effect of two other competing orders possibly proximate to the regime of our interest: the charge stripe (smectic) and d wave superconductivity.

For charge stripe with wave vector $\mathbf{Q}_{\rm CS}$ the order parameter is

$$\rho_{\mathbf{Q}_{\rm CS}} = \int \frac{d^2\mathbf{k}\, d\Omega}{(2\pi)^3} \langle \psi_\alpha^\dagger(\mathbf{k} + \mathbf{Q}_{\rm CS}) \psi_\alpha(\mathbf{k}) \rangle, \tag{7}$$

where the spin index α is summed over. We therefore find an additional contribution to the spin-wave action

$$\delta S_{\rm CS} = -g'_{cs} \rho_{\mathbf{Q}_{\rm CS}} \int \frac{d^2\mathbf{q}\, d\omega}{(2\pi)^3} \vec{\phi}(\mathbf{q} - \mathbf{Q}_{\rm CS}, \omega) \vec{\phi}(-\mathbf{q}, -\omega) - g_{\rm CS} |\rho_{\mathbf{Q}_{\rm CS}}|^2 \int \frac{d^2\mathbf{q}\, d\omega}{(2\pi)^3} |\vec{\phi}(\mathbf{q}, \omega)|^2. \tag{8}$$

Hence the charge stripe shifts the spin-wave gap by a constant ($g_{\rm CS}$ term) and it can also induce (fluctuating) spin stripe but with a fixed incommensurability of $\delta = Q_{\rm CS}/2$ ($g'_{\rm CS}$ term). However, incommensurability so induced will be T independent.

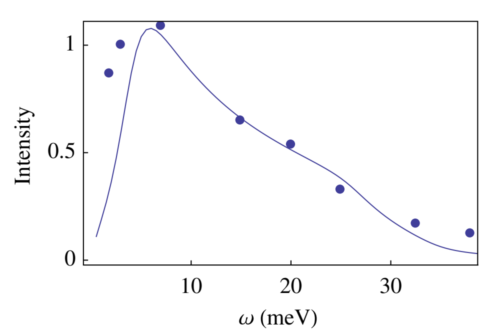

FIG. 3 (color online). The frequency dependence of the momentum integrated spectral function.

In the presence of d wave pairing Δ_d the leading additional contribution to the spin-wave action is

$$\delta S_{\rm SC} = -g_{\rm SC}|\Delta_d|^2 \int \frac{d^2\mathbf{q}d\omega}{(2\pi)^3} |\vec{\phi}(\mathbf{q}, \omega)|^2. \qquad (9)$$

Hence while d wave superconductivity can also shift the commensurate spin-wave gap $\Delta(\mathbf{q} = \mathbf{0})$ by a constant $g_{\rm SC}|\Delta_d|^2$ and enhance (for $g_{\rm SC} < 0$) or suppress (for $g_{\rm SC} > 0$) the spin fluctuations, it cannot lead to the observed T dependent incommensurability either. These conclusions can be generalized to other pairing symmetries.

Discussions.—We have shown that the existence of charge nematic ordering can take a system proximate to AFM and induce fluctuating spin stripe phenomena: incommensurate INS peaks. Within a symmetry based phenomenological approach we explained the observed $(T^* - T)^{1/2}$ dependence of the incommensurability. Hence, we established a concrete model connecting the spin and charge aspects of the electronic liquid crystalline behavior of $YBa_2Cu_3O_{6+y}$. We further argued that this is a unique feature of charge nematic ordering.

One implication of our model is the possibility that *outside* but close to the charge nematic phase, certain types of impurities could stabilize fluctuating or even static spin stripes. Since impurities break the crystal lattice symmetry, they provide a symmetry breaking field for N. In weak coupling, this would be given by $N = \chi_N h_N$ where h_N captures the orientational symmetry breaking of the impurities (see Ref. [5] for a similar argument applied to charge stripes). Since the response χ_N to this perturbation is expected to be large near a nematic phase, an $N > N^*$ or even $N > N_c$ could be induced.

Several future directions include, establishing a microscopic model which reproduces our phenomenological model in the long-wavelength limit and studying the effects of a magnetic field. This latter question is particularly important given the observations of a magnetic field stabilizing static spin stripe phase [23].

Furthermore, our analysis may provide a starting point for investigating the interplay between spin and electronic liquid crystalline ordering in other systems. By now there are a growing number of candidate correlated systems for such interplay, including Mn-doped $Sr_3Ru_2O_7$ [28] and Fe-based superconductors [29].

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