Nematic Domains and Resistivity in an Itinerant Metamagnet Coupled to a Lattice

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The nature of the emergent phase near a putative quantum critical point in the bilayer ruthenate $Sr_3Ru_2O_7$ has been a recent subject of intensive research. It has been suggested that this phase may possess electronic nematic order (ENO). In this work, we investigate the possibility of nematic domain formation in the emergent phase, using a phenomenological model of electrons with ENO and its coupling to lattice degrees of freedom. The resistivity due to the scattering off the domain walls is shown to closely follow the ENO parameter. Our results provide qualitative explanations for the dependence of the resistivity on external magnetic fields in $Sr_3Ru_2O_7$.

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Quantum critical behavior in metamagnetism represents the most unusual critical phenomenon in itinerant electron systems. It was shown in a series of remarkable experiments that the critical end point associated with the metamagnetic transition (MMT) can be driven to zero temperature in the bilayer ruthenate $Sr_3Ru_2O_7$ by changing the angle between the external magnetic field and the c axis of the material [1,2]. The transport and thermodynamic measurements reveal unusual temperature dependence near the putative *quantum* critical end point, indicating that the underlying itinerant electrons are strongly interacting with the quantum critical fluctuations of the magnetization [1–4].

Later experiments on the ultrapure samples, however, have shown that the quantum critical end point is eventually avoided when the finite temperature critical point is pushed further down to zero temperature, and is replaced by two consecutive MMTs [5–7]. The phase bounded by two MMTs exhibits unusually high resistivity and its nature has been a recent subject of intensive research.

Currently there exist two competing proposals for the nature of this *emergent* phase. Binz *et al.* [8] proposed a phenomenological Ginzburg-Landau theory of magnetic Condon domains and suggested that the high resistivity may come from the scattering of electrons off the magnetic domains. Another proposal involves the formation of electronic nematic order (ENO) in the emergent phase; namely, the Fermi surface of the electrons spontaneously breaks the lattice rotational symmetry [5,9]. Two possible orientations of the ENO may lead to domain formation and may indeed lead to high resistivity due to domain wall scattering.

Very recently it has been reported that the high resistivity seen in the emergent phase is insensitive to demagnetization factor or shapes of the samples [10]. This is at odds with a key prediction of the magnetic Condon domain theory; the system is supposed to be very sensitive to the demagnetization factor [8]. This may leave only the theory of ENO as an alternative proposal.

In this Letter, we offer a theory of the nematic domain formation and the resulting high resistivity in the emergent phase. The possibility of the nematic domains has not been studied theoretically even though such possibility was briefly discussed in the literature [5,9]. Our objective in the current work is to provide a minimal theoretical description that can explain key experimental observations at qualitatively level.

In search for a concise description, we start with an effective electronic Hamiltonian that captures the essential physics of ENO, namely, we consider the quadrupolar interaction between electrons [9,11]. This interaction can be regarded as the angular-momentum-two channel of some general interaction or the Landau quasiparticle interaction. In real materials, the interaction in all angular momentum channels may exist, not just in the quadrupolar channel. The dominance of the quadrupolar channel is an assumption of our phenomenological theory and its validity should be tested by comparing the results with the experimental data. While it has not been proven, it is conceivable that such an instability or a dominant interaction is more likely to happen near an itinerant quantum critical point because the Fermi surface would be very soft due to strong critical fluctuations.

In view of the magnetostriction data indicating a close relationship between the lattice and the emergent phase [5], we also consider the electron-lattice interaction. Since we are studying an effective Hamiltonian, we are only interested in general properties of this Hamiltonian and the precise values of the parameters should not be taken seriously. Remarkably this simplified model contains essential ingredients of the nematic domain formation and the resulting high resistivity. It is found that the electron-lattice interaction makes the formation of the nematic domains (at finite temperatures) much more likely by offering a large number of metastable domain configurations. Another key result of our work is that the magnetic field dependence of the resistivity in the nematic domain phase closely follows the field dependence of the ENO parame-

ter. Thus the resistivity can be regarded as a measurement of the ENO.

Mean-field theory of the nematic order.—The simplest model for the ENO on the square lattice can be written by keeping only the interactions in the quadrupolar channel [11] or the lattice equivalent of the angular momentum $l = 2$ channel in the continuum [12].

$$H_{\rm el} = \sum_{\mathbf{k}} \xi_{\mathbf{k}} c^{\dagger}_{\mathbf{k}} c_{\mathbf{k}} + \sum_{\mathbf{k},\mathbf{k}',\mathbf{q},\alpha} F(\mathbf{q}) f_{\mathbf{k}\alpha} f_{\mathbf{k}'\alpha} c^{\dagger}_{\mathbf{k}+\mathbf{q}} c^{\dagger}_{\mathbf{k}'-\mathbf{q}} c_{\mathbf{k}'} c_{\mathbf{k}}, \tag{1}$$

where $\xi_{\mathbf{k}} = -t(\cos k_x + \cos k_y) - 2t' \cos k_x \cos k_y - \mu$ is the single-particle dispersion and $\alpha = 1, 2$. $f_{\mathbf{k}1} = \cos k_x - \cos k_y$ and $f_{\mathbf{k}2} = \sin k_x \sin k_y$ are the form factors in the quadrupolar channels. $F(\mathbf{q})$ represents a short range interaction in real space with $F(\mathbf{q} \to 0) = F = \text{const}$. Here we suppress the spin indices and it should be understood that the interaction terms exist in both spin channels with possibly different interaction strength.

The ENO parameter is $Q(\mathbf{q}) = F \sum_{\mathbf{k}} f_{\mathbf{k}1} \langle c^{\dagger}_{\mathbf{k}+\mathbf{q}} c_{\mathbf{k}} \rangle$. In the uniform state $\mathbf{q} \to 0$, this order parameter leads to the renormalized dispersion in the mean-field theory, $\xi^{\rm ren}_{\mathbf{k}} = -[t + Q(0)] \cos k_x - [t - Q(0)] \cos k_y - 2t' \cos k_x \cos k_y - \mu$. Clearly, the resulting Fermi surface would break the $\pi/2$ rotation symmetry of the lattice. An alternative ENO parameter with $f_{\mathbf{k}2}$ vanishes for the interaction form chosen here [12].

In the presence of a magnetic field, the Zeeman energy leads to different chemical potentials for the spin-up and -down electrons, $\mu_{\uparrow,\downarrow} = \mu \pm \mu_B H$, where μ_B is the Bohr magneton and H is the external magnetic field. As the magnetic field increases, the Fermi surface volume of the majority (minority) spin increases (decreases). When the Fermi surface of the majority or minority spin touches the van Hove singularity, a first order phase transition to a nematic phase occurs with a sudden opening and elongation of Fermi surface along a or b axis [9]. Here the Fermi surface volume of the majority or minority spin jumps, leading to a MMT. When the magnetic field increases further, the other side of Fermi surface touches the van Hove singularity again. This leads to another first order transition and the lattice rotational symmetry is restored afterwards [9].

In the uniform nematic state, the spontaneously chosen nematic direction can be either the a or b axis. On the other hand, nonuniform solutions can arise as metastable states in the mean-field theory, In particular, the nematic domains with different orientations can coexist. These static domain structures, however, may not be favorable even as metastable states in two and one dimensions because of large quantum fluctuations. Thus if the nematic domains were to arise, there should be additional degrees of freedom.

Normal modes of lattice distortions.—The magnetostriction effect observed in $Sr_3Ru_2O_7$ suggests that the electron-lattice interaction is a natural degree of freedom to consider. In the uniform nematic-ordered state, the electron-lattice interaction would induce a tetragonal lattice distortion. This systemwide shape change, however, is energetically very costly and the system may rather prefer to have twin boundaries between the phases with different nematic orientations so that the overall shape is preserved. Thus the electron-lattice interaction may indeed prefer the formation of the nematic domains.

We treat the lattice classically assuming slow lattice dynamics. For simplicity, we will only consider two-dimensional lattice distortions even though the full analysis of the electron-lattice coupling may require a three-dimensional lattice structure. Implications to the distortions out of plane will be discussed later.

It is useful to write the lattice Hamiltonian in terms of distortion modes of a lattice plaquette. Apart from the rotational and two translational modes of the entire plaquette, there are five normal modes described in Fig. 1. These normal modes are, however, not independent in the lattice and three constraints between the normal modes are necessary [13]. Using the classical approximation, we can write the harmonic part of the lattice Hamiltonian as follows.

$$H^0_{\rm lat} = \frac{1}{2} \sum_i \Big\{ \sum_{n=1,2,3} A_n [e_n(i)]^2 + \sum_{m=+,-} B[s_m(i)]^2 \Big\}, \tag{2}$$

where it should be understood that only two of the normal modes are independent.

It is easy to have a grip on the physical meaning of the parameters in this Hamiltonian. The normal modes $s_{\pm}$ appear at the domain walls so that B is related to the domain wall energy. It is also clear that the e_3 mode couples directly to the ENO; the domain boundaries of the lattice distortions related to the e_3 modes will coincide with those of the ENO. It is expected that the e_3 mode is particularly affected and will be soft. Thus we assume that A_3 is small while all the A_n and B are positive.

Using the constraints, the lattice Hamiltonian with an anharmonic correction can be rewritten as follows.

$$H_{\rm lat} = \sum_{\mathbf{q},a,b=1,3} e^*_a(\mathbf{q}) \frac{M_{ab}(\mathbf{q})}{2} e_b(\mathbf{q}) + \frac{C_3}{4} \sum_i [e_3(i)]^4, \tag{3}$$

with $M_{ab} = A_a \delta_{ab} + A_2 \frac{\beta_a \beta_b}{\beta_2^2} + B \frac{\beta_4}{\beta_2^2} [\beta_1 \delta_{ab} + \beta_3 (1 - \delta_{ab})]$. C_3 is a constant and $\beta_1(\mathbf{q}) = 1 - \cos q_x \cos q_y$, $\beta_2(\mathbf{q}) = -\sin q_x \sin q_y$, $\beta_3(\mathbf{q}) = \cos q_x - \cos q_y$, and $\beta_4(\mathbf{q}) = (1 - \cos q_x)(1 - \cos q_y)$.

Electron-lattice interaction.—We consider the Su-Schrieffer-Heeger type electron-lattice interaction,

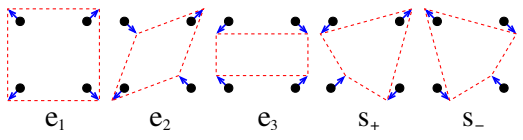

FIG. 1 (color online). Normal modes.

$$H_{\text{el-lat}} = g\sum_i [(d^x_{i+\hat{x}} - d^x_i)c^\dagger_{i+\hat{x}}c_i + (x \leftrightarrow y) + \text{H.c.}], \quad (4)$$

where d_i represents the lattice displacement. Writing this interaction in terms of the lattice normal modes, we get

$$H_{\text{el-lat}} = g\sum_{\mathbf{k},\mathbf{q}} \left[\frac{f_{\mathbf{k}0}e_1(\mathbf{q}) + f_{\mathbf{k}1}e_3(\mathbf{q})}{(1+e^{iq_x})(1+e^{iq_y})} c^\dagger_{\mathbf{k}+\mathbf{q}}c_{\mathbf{k}} + \text{H.c.} \right], \quad (5)$$

where $f_{\mathbf{k}0} = \cos k_x + \cos k_y$. Notice that the e_3 mode couples to the ENO through the form factor $f_{\mathbf{k}1}$ and the e_1 mode to the kinetic energy.

Domain structures.—We numerically determine the electronic and lattice configurations of the system described by $H = H_{\text{el}} + H_{\text{el-lat}} + H_{\text{lat}}$. The simplest domain wall solutions can be obtained by assuming that the spatial modulations exist only along the diagonal direction. This makes the numerical works easier while one can still understand the key properties of the domain wall configurations. We also assume that the e_1 mode is much stiffer than the e_3 mode so that e_1 mode is not heavily affected by the nematic transitions. We will discuss later the role of the e_1 mode in the context of the magnetostriction measurements in $Sr_3Ru_2O_7$.

The nonuniform ENO parameter and lattice configurations are determined by the self-consistent mean-field theory described below. We compute the energy of the anharmonic part of the lattice Hamiltonian in real space while the rest of the energy is computed in the reciprocal space. We use the periodic boundary condition in the reciprocal space and the fast-Fourier transform to connect the real and reciprocal space computations. Here the number of discrete $\mathbf{q}$ points in the Brillouin zone of the reciprocal space is related to the lattice size in the real space. We first consider $H_{\text{el}} + H_{\text{el-lat}}$ and determine the ENO parameter $Q(\mathbf{q}; e_3)$ of the electronic state for a given initial lattice configuration $\{e_3\}$. The resulting electronic state $|\Phi(e_3)\rangle_{\text{el}}$ is used to compute the energy $\tilde{E}_{\text{el}}(e_3) = {}_{\text{el}}\langle\Phi(e_3)|H_{\text{el}} + H_{\text{el-lat}}(e_3)|\Phi(e_3)\rangle_{\text{el}}$. Next, we minimize the total energy $E_{\text{total}}(e_3) = \tilde{E}_{\text{el}}(e_3) + H_{\text{lat}}(e_3)$ by the Euler method [13]. The resulting lattice configuration is in general different from the initial one and it is then fed back to determine a new electronic state $|\Phi(e_3)\rangle$. We update the lattice configuration $\{e_3\}$ following the maximum energy slopes with respect to $e_3(\mathbf{q})$ until $\frac{\delta E_{\text{total}}(e_3)}{\delta e_3} = 0$ is satisfied.

The relative probability of getting the metastable domain solutions is obtained by trying a large number (typically 50 in a given set) of random initial conditions. This probability is only 32% for the 8×8 lattice, it increases to 50% for the 18×18 lattice, and 63% for the 20×20 lattice with 2–3% error. Thus the number of metastable domain solutions increases as the system size increases in accord with similar computations in manganites [13]. These domain solutions imply a large number of local minima in the free energy and will be likely chosen at finite temperatures by entropic effect. Figure 2 shows a typical uniform and a metastable domain solution. The qualitative features of these solutions do not depend on the details of the parameters chosen here; for example, the electron filling factor $\frac{120}{256}$ with $t' = 0$ is chosen just to avoid the van Hove singularity and a similar result is obtained for the half-filling with a small finite t'.

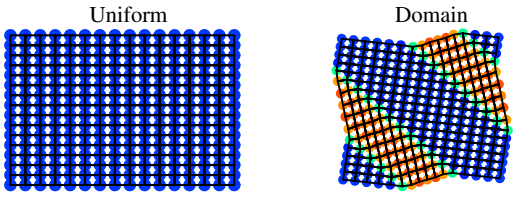

FIG. 2 (color online). The red, blue, and green represent the negative, positive, and zero ENO parameter, respectively. Here, $A_1 = 20$, $A_2 = 20$, $A_3 = 0.001$, $B = 1$, $C_3 = 100$, $t = 0.1$, $t' = 0$, $F = 0.2$, and $g = 0.2$. The electron filling is $\frac{120}{256}$ per site to be slightly away from the van Hove singularity.

The stability of domains.—The stability of the domain configurations would be determined by the barrier potential in the energy landscape and the energy difference between the uniform state and the domain structure.

Here we consider an indirect criterion of the "local" stability, $\kappa \equiv \sum_{\mathbf{q}} \frac{\delta^2}{\delta e_3(\mathbf{q})^2} E_{\text{total}}$ evaluated at the local minima corresponding to the metastable domain configurations. This quantity is the curvature of the energy topography in the hyperspace of lattice configurations. Larger κ would correspond to a deeper local minimum, implying perhaps a more stable configuration. Even though this quantity measures the stability of the domains in the lattice deformations, the nematic domains would follow because they are basically locked together.

Of particular interest is the stability with respect to the electron-lattice coupling g and the strength of the anharmonicity C_3. Figures 3(a) and 3(b) show the dependence of κ on the dimensionless coupling constants $\bar{g} = g\bar{e}_3/t$ and $\bar{C}_3 = C_3\bar{e}_3^4/t$, where $\bar{e}_3$ is the average of e_3 and about the order of 0.1 lattice constant. The increase of κ in both of the uniform and domain solutions may lead to bigger

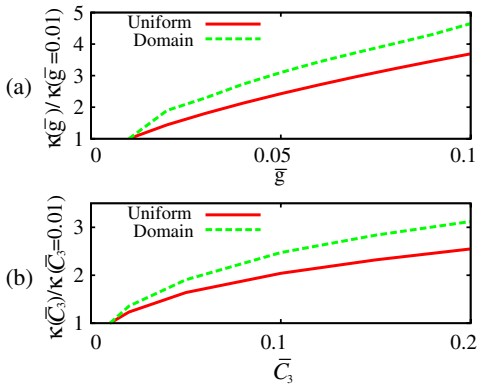

FIG. 3 (color online). κ as a function of (a) the electron-lattice coupling and (b) the anharmonicity. We use $t' = 0$, $F = 2t$, and $B = 20t$. $\bar{C}_3 = 0.05$ for (a) and $\bar{g} = 0.1$ for (b).

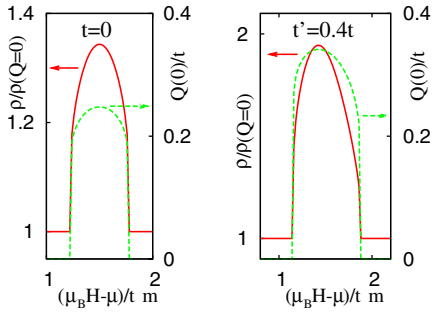

FIG. 4 (color online). The dashed line denotes the uniform ENO parameter in the mean-field theory [12]. The solid lines represent the resistivity with $t' = 0$, and $0.4t$. Here we use $\rho/\rho(Q=0) = \frac{\alpha}{\alpha - Q(0)^2}$ with $\alpha = 0.24$ and $F = 1.974t$.

barrier height and the faster increase of κ for the domain configuration may imply that the domain structure at large $\bar{g}$ and $\bar{C}_3$ would be at a relatively deeper minimum.

Resistivity.—The large enhancement of the residual resistivity in the emergent phase may be explained by the scattering at the nematic domain walls. We adopt the Landauer formula to estimate the conductance through a domain wall, namely $G_{\mathrm{DW}} = \frac{e^2}{\pi\hbar} T$, where T is the transmission coefficient [14]. In the case of a domain wall parallel to the b axis, the transmission coefficient along the a axis (or the x axis) is given by $T = \sum_{\mathbf{k}\in \mathrm{FS}} T_{\mathbf{k}}$, where $T_{\mathbf{k}} = v_{Fx}^{(+)}(\mathbf{k}) v_{Fx}^{(-)}(\mathbf{k}) / |v_{Fx}^{(+)}(\mathbf{k}) + v_{Fx}^{(-)}(\mathbf{k}) + iV_0|^2$ and $\mathbf{k} \in \mathrm{FS}$ ensures that only the $\mathbf{k}$ vectors residing on the appropriate Fermi surface are included. Here $\mathbf{v}_F^{(\pm)}(\mathbf{k}) = \frac{\partial}{\partial \mathbf{k}} \xi_{\mathbf{k}}^{\mathrm{ren},(\pm)}|_{\mathbf{k}\in \mathrm{FS}}$, V_0 is the strength of the scattering potential at the interface, and $\pm$ sign denotes the direction of the nematic-ordered Fermi surfaces in the different sides of the domain wall. If the scattering processes at different domain walls are incoherent, the resistivity due to N_{DW} domain walls would be

$$\rho_{\mathrm{DW}} \propto N_{\mathrm{DW}} G_{\mathrm{DW}}^{-1} = N_{\mathrm{DW}}/(u_0 - u_1 Q^2), \qquad (6)$$

where $u_0 = \frac{e^2}{\pi\hbar} \int_{\mathbf{k}\in \mathrm{FS}} \frac{d^2k}{(2\pi)^2} \frac{(t - 2t' \cos k_y)^2 \sin^2 k_x}{4(t - 2t' \cos k_y)^2 \sin^2 k_x + V_0^2}$, $u_1 = \frac{e^2}{\pi\hbar} \times \int_{\mathbf{k}\in \mathrm{FS}} \frac{d^2k}{(2\pi)^2} \frac{\sin^2 k_x}{4(t - 2t' \cos k_y)^2 \sin^2 k_x + V_0^2}$. The resulting resistivity is shown in Fig. 4 for $t' \neq 0$ and $t' = 0$ cases. Notice that $t' \neq 0$ case leads to an asymmetric profile of the resistivity similar to that seen in the experiment. The important point, however, is that the overall shape of the resistivity follows the behavior of the ENO and this aspect is independent of the parameters.

Summery and discussion.—The theory of ENO is consistent with several key experimental observations in $Sr_3Ru_2O_7$ [5,10]. (1) There exist two first order MMTs as the magnetic field increases, (2) the electrons are itinerant in the entire phase diagram, (3) the emergent phase exists only in a window of magnetic fields. (4) the finite temperature transition to the emergent phase seems to be continuous [5,9]. In this Letter, we have shown that this theory combined with the coupling to the lattice leads to nematic domain formation and this naturally explains the high resistivity in the emergent phase [5,10]. In particular, it is shown that the resistivity is determined by the magnetic field dependence of the ENO parameter.

Some additional remarks are in order. The magnetostriction data on $Sr_3Ru_2O_7$ show a sudden change in the c-axis lattice constant upon entering and exiting the emergent phase [5]. This may be explained by a relatively soft e_1 mode that is related to a change in the ab-plane unit-cell area. Such a change would lead to elongation of the lattice along the c axis to conserve the three dimensional unit-cell volume. The jump in the kinetic energy of the electrons with the majority or minority spin, via the coupling to the e_1 mode, would induce an abrupt change of the c-axis lattice constant at the nematic transitions.

A very recent experiment observed an interesting dependence of the resistivity on the relative orientation of the in-plane magnetic field and the current direction [10]. When they are parallel (perpendicular) to each other, the high resistivity disappears (is maintained). This is reminiscent of the situation in the nematic quantum Hall states in high Landau levels [15]. A similar mechanism [16] of the nematic domain alignment by an in-plane magnetic field may work here as well. This similarity, therefore, may make the relevance of the nematic theory even stronger. It would be an excellent subject of future study.

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