Singular non-ordering susceptibility at a Pomeranchuk instability

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(Dated: September 22, 2010)

We study magnetic susceptibilities of two-dimensional itinerant electron systems exhibiting symmetry-breaking Fermi surface distortions, the so-called $d$-wave Pomeranchuk instability, in a magnetic field. In a pure forward scattering model, the longitudinal susceptibility $\chi_{zz}$ is found to exhibit a jump at a critical point. The magnitude of this jump diverges at a tricritical point. When scattering processes involving finite momentum transfers are allowed for, $\chi_{zz}$ is expected to diverge also at a critical point. The system displays multiple critical fluctuations. We argue that the features of $\chi_{zz}$ are general properties associated with singularities of a non-ordering susceptibility, leading to implications for a variety of materials including Sr$_2$Ru$_2$O$_7$.

PACS numbers: 75.40.-s, 71.18.+y, 05.50.+q, 64.60.F-

I. INTRODUCTION

The electronic nematic is currently among the most intriguing and intensely investigated states of quantum matter. Unlike its classical counterpart\textsuperscript{1} this phase originates from interactions between structureless, point-like particles (electrons). On the other hand, just like in the case of classical nematics, these systems exhibit orientational symmetry breaking while preserving translational invariance. The electronic nematic state is reached via a phase transition from either the electronic smectic state corresponding to the so-called charge-stripe order\textsuperscript{2} or the uniform state as found in the $t$-$J$\textsuperscript{3} and Hubbard\textsuperscript{4, 5} models. The latter route is accompanied by spontaneous Fermi surface symmetry breaking with a $d$-wave order parameter, and is often referred to as the $d$-wave Pomeranchuk instability\textsuperscript{6}.

The occurrence of the electronic nematic was indicated in a number of correlated electron systems. In two-dimensional electron gases, the electronic nematic is signaled by the strong anisotropy of magnetotransport at low temperature in half-filled higher Landau levels\textsuperscript{7}. For cuprate superconductors, there exists a strong tendency toward the nematic state despite competition with cooper pairing formation, as seen in the pronounced anisotropy of magnetic excitation spectra\textsuperscript{8}. The bilayer ruthenate Sr$_2$Ru$_2$O$_7$ displays the evidence of the nematic state\textsuperscript{9, 10}, which is realized in a certain range of a magnetic field bounded by first order transition lines at low temperature and a second order transition line at high temperature; the end points of the second order transition line are tricritical points\textsuperscript{11}.

Motivated by experiments performed for Sr$_2$Ru$_2$O$_7$, we consider the nematic instability from a uniform state, namely the Pomeranchuk instability (PI), in the presence of a magnetic field. We find that the PI is accompanied by peculiar singularities of the uniform spin susceptibility, which can be observed in real materials like Sr$_2$Ru$_2$O$_7$.

Our results are not specific to the PI and can be understood as universal singular behavior of a non-ordering susceptibility. The concept of a non-ordering susceptibility appears in the theory of tricriticality developed for helium mixtures and some metamagnetic materials\textsuperscript{12, 13}. At the tricritical point three different phases become identical\textsuperscript{14} and the full phase diagram is described by temperature ($T$), a control parameter called a non-ordering field, and an ordering field which is conjugate to the order parameter\textsuperscript{15}. The framework naturally involves two different kinds of susceptibilities, the ordering and non-ordering ones. The former is given by the second derivative of the free energy with respect to the ordering field, whereas the latter is the second derivative with respect to the non-ordering field; the non-ordering susceptibility is thus defined uniquely in the system in question. In the context of Sr$_2$Ru$_2$O$_7$, the ordering susceptibility corresponds to the $d$-wave charge compressibility\textsuperscript{16} and the non-ordering one to the longitudinal magnetic susceptibility.

In this paper, we first study the uniform magnetic susceptibilities in a mean-field model of the PI on a square lattice in the presence of a magnetic field. We show that the longitudinal susceptibility $\chi_{zz}$ exhibits a jump at a critical point (CP) and a power-law divergence at a tricritical point (TCP), while the transverse susceptibility $\chi_{\perp}$ exhibits a cusp. In two-dimensional systems, the mean-field theory breaks down in a critical regime. We then argue that beyond the mean-field theory $\chi_{zz}$ diverges at both CP and TCP, which is associated with multiple critical fluctuations, i.e., soft Fermi surface fluctuations and magnetic fluctuations. The singular behavior of $\chi_{zz}$ is interpreted as a general feature associated with singularities of a non-ordering susceptibility at a phase transition, leading to implications for a variety of materials including Sr$_2$Ru$_2$O$_7$.

II. MODEL AND FORMALISM

We consider the following Hamiltonian for the PI\textsuperscript{17, 18}

\begin{equation}
H = \sum_{\mathbf{k},\sigma} (\epsilon^d_{\mathbf{k}} - \mu) n_{\mathbf{k}\sigma} + \frac{1}{2N} \sum_{\mathbf{k},\mathbf{k}',\sigma,\sigma'} f_{\mathbf{k}\mathbf{k}'} n_{\mathbf{k}\sigma} n_{\mathbf{k}'\sigma'} - \frac{h}{2} \sum_{\mathbf{k},\sigma} n_{\mathbf{k}\sigma} n_{\mathbf{k}\sigma} + \frac{1}{2N} \sum_{\mathbf{k},\mathbf{k}',\sigma,\sigma'} f_{\mathbf{k}\mathbf{k}'} n_{\mathbf{k}\sigma} n_{\mathbf{k}'\sigma'} - \frac{h}{2} \sum_{\mathbf{k},\sigma} n_{\mathbf{k}\sigma} n_{\mathbf{k}\sigma} ,
\end{equation}

describing tight-binding electrons on a square lattice, interacting via a forward scattering interaction and subject to an external magnetic field $h$. The dispersion $\epsilon^d_{\mathbf{k}} = -2t[c\cos k_x + \cos k_y + 2t' \cos k_x \cos k_y]$ retains the nearest and next-nearest neighbor hopping amplitudes; $\mu$ is the chemical potential; $n_{\mathbf{k}\sigma}$ is the electron number operator with momentum $\mathbf{k}$ and spin $\sigma$.
$N$ is the total number of lattice sites; the effective interaction

$$f_{k,k'} = -gd_k d_{k'}$$  \(2\)

involves the $d$-wave form factor $d_k = \cos k_x - \cos k_y$ and drives the PI. This interaction mimics the actual structural of the effective charge interactions in the forward scattering channel as obtained within more fundamental models \[3,4\]. The order parameter corresponding to the PI is given by

$$\eta = -\frac{g}{N} \sum_{k,\sigma} d_k \langle n_{k\sigma} \rangle .$$  \(3\)

The transition can be tuned along an isotherm either by varying the chemical potential $\mu$ or the magnetic field $h$ in the Hamiltonian \(H\). The latter mimics the actual experimental setup in Sr$_{2}$Ru$_2$O$_7$. In fact, the model (1) and different versions of it turned out to capture numerous aspects possibly associated with the Sr$_{2}$Ru$_2$O$_7$ compound \[14,20\]. We fix the band parameters $\gamma = 0.35$, $g = 1$, and $\mu = 1$ in units set by $t$ \[17,18\]. The theoretical phase diagram is shown in Fig. 1.\(1\)

The PI is realized in a region around the van Hove energy ($h = 0.8$) of the up-spin band. A second-order phase transition occurs at high $T$, but terminates at a TCP, below which the transition becomes first order.

![FIG. 1: The phase diagram in the plane of $h$ and $T$ for $\gamma = 0.35$, $g = 1$, and $\mu = 1$. $T_c$ (solid line) denotes a second (first) order transition and $T_{ni}$ is a tricritical point. The dashed line represents the position of the van Hove energy.](image)

We now analyze the uniform longitudinal magnetic susceptibility $\chi^{zz}$ within the model \(H\). The standard linear response theory yields

$$\chi^{zz} = \lim_{\eta \to 0} \left[ \sum_{q=0}^{2\pi} \int_{0}^{\infty} d\epsilon e^{-\epsilon t} \langle [S^z(q, t), S^{-z}(-q, 0)] \rangle \right].$$  \(4\)

Here $\langle \cdots \rangle$ denotes the equilibrium expectation value with the Hamiltonian $H$, $[\cdot, \cdot]$ is the commutator; $\sigma$ is a positive infinitesimal; $S(q, t) = e^{iHt}S(q)e^{-iHt}$ and $S(q)$ is the spin operator in momentum space. In the random phase approximation (RPA), $\chi^{zz}$ is given graphically by Fig. 2 and calculated as

$$\chi^{zz} = \frac{1}{4} \left[ \frac{1}{N} \sum_{k,\sigma} f'(\xi_{k\sigma}) + \frac{g}{2} \sum_{k,\sigma} \sigma d_k f'(\xi_{k\sigma}) \right]^2,$$  \(5\)

where $\xi_{k\sigma} = \epsilon_k - \mu + \eta d_k - \frac{\epsilon}{h}$; $f(x)$ is the Fermi-Dirac distribution and its first derivative is denoted by $f'$. The presence of the second term in Eq. (5) is crucial to the present study and was overlooked in Ref. \[17\]. On the other hand, the uniform transverse susceptibility is expressed by a simple bubble (Fig. 2) in the RPA, that is,

$$\chi^{\pm} = \lim_{\eta \to 0} \left[ \sum_{q=0}^{2\pi} \int_{0}^{\infty} d\epsilon e^{-\epsilon t} \langle [S^+(-q, t), S^-(-q, 0)] \rangle \right] = -\frac{1}{N} \sum_{k} f'(\xi_{k}) - f'(\xi_{k})$$  

where $\xi_{k\sigma} = \epsilon_k - \mu + \eta d_k - \frac{\epsilon}{h}$ and $\eta = \frac{1}{2N} \sum_{k,\sigma} \sigma f(\xi_{k\sigma})$ is the magnetization.

### III. RESULTS

We plot the susceptibility $\chi^{zz}$ versus temperature in Fig. 3(a) as the second-order transition line is crossed at fixed $h$. The quantity $\chi^{zz}$ exhibits a discontinuity at $T = T_c(h)$. The magnitude of the jump diverges as the field $h$ is varied toward the tricritical value $h_{ni} = 0.983$ [Fig. 3(b)]. It follows the power law $\chi^{zz} \propto |T - T_{ni}|^{-1/2}$ \[27\]. The exponent $1/2$ is visible only sufficiently close to the TCP and very high numerical accuracy is required. The divergence of $\chi^{zz}$ is observed only in the symmetry-broken phase, while in the disordered phase it remains finite and smooth. In Fig. 3(c), the jump of $\chi^{zz}$ ($\Delta \chi^{zz}$) is plotted along the transition line (solid line). The magnitude of the jump is strongly suppressed around $h$ where $T_c$ becomes maximal (see also Fig. 1) and is gradually enhanced away from it. While $\chi^{zz}$ necessarily shows a jump upon crossing a first order transition line, we also plot its magnitude in Fig. 3(c) with open circles. It is interesting to note that the magnitude of the jump of $\chi^{zz}$ at a CP is typically comparable to that at a first order transition. In contrast to the results for $\chi^{zz}$, the transverse susceptibility $\chi^\pm$ [Fig. 3(d)] exhibits a cusp upon crossing the $T_c$ line at both CP and TCP. Although $\chi^\pm$ can be enhanced below $T_c$ for a different choice of parameters, its non-analyticity at $T_c$ is always a cusp.

As shown in Fig. 2, $\chi^{zz}$ involves contributions from two diagrams. Its peculiar behavior originates from the second diagram, which is evaluated as the second term in Eq. (5). This
FIG. 3: (a) and (b) The longitudinal susceptibility $\chi_{zz}$ plotted versus temperature as the second order transition is approached at $h = 0.88$ (a) and at the tricritical field $h_{tri} = 0.983$ (b). The dashed line is the result for $g = 0$. (c) The jump of $\chi_{zz}^2$ along a second order transition line (solid line) and at a first order transition (circle) on the side of the symmetry-broken phase. The magnitude of the jump is scaled by $\chi_{zz}$ on the side of the normal phase ($\chi_{zz}^n$). (d) $\chi^\pm$ is plotted for $h = 0.88$ and 0.983 in a similar fashion to (a).

A. Comparison with a jump of the specific heat

It is instructive to compare the jump of $\chi_{zz}$ with a jump of the specific heat coefficient ($C/T$) [12], which is plotted along the transition line with a solid line in Fig. 4. The jump is pronounced around the van Hove energy ($h = 0.8$) and is suppressed monotonously away from it. The quantity $C/T$ rapidly increases and ultimately diverges upon approaching the vicinity of the TCP; the singularity is given by $C/T \sim |T - T_{tri}|^{-1/2}$ at $T = T_{tri}$ or $C/T \sim |h - h_{tri}|^{-1/2}$ at $T = T_{tri}$ sufficiently close to the TCP, displaying the same exponent as in the case of $\chi_{zz}$. A crucial difference from Fig. 3(c) is that while the specific heat exhibits the same singularities even for $h = 0$ if the PI is tuned, e.g., by the chemical potential [16], the jump of $\chi_{zz}$ at a CP and its divergence at a TCP occur only for $h \neq 0$. This feature can be checked by observing that the second term in Eq. (5) vanishes for $h = 0$. Therefore the singular behavior of $\chi_{zz}$ is a field-induced anomaly. As we shall show below, it is a manifestation of a general feature of a non-ordering susceptibility and hence the presence of a finite non-ordering field (a magnetic field here) is necessary.

B. Scaling analysis and criticality beyond the RPA

So far we have considered the forward scattering model. Its universal features in the vicinity of CP and TCP are well described by mean-field theory, and are correctly captured also...
by a Landau-type $\phi^d$ theory \cite{12}. By allowing a small momentum transfer in Eq. (2), we can incorporate order parameter fluctuations. The obtained singularities of $\chi^z$ and $C/T$ are expected to be modified in a critical regime. By virtue of universality, the character of the non-analyticities and the exact values of critical exponents can be deduced without performing explicit calculations. The order parameter describing the PI [Eq. (3)] is characterized by the Ising symmetry. The exact critical exponents of the Ising universality class are well known for ordering quantities. The clue to obtain the exact exponents of non-ordering quantities is seen in theory of tricritical points \cite{12}. The scaling hypothesis allows one to write the singular part of the Gibbs potential around a TCP as

$$G_{\text{sing}}(t, g, s) = |g|^{2-\alpha} G \left( t/|g|^\alpha, s/|g|^\kappa \right),$$

where $t = (T - T_\text{c})/T_\text{c}$ and $s$ is an ordering field which is conjugate to the order parameter; the scaling field $g$ is chosen as $g = (h - h_\text{eq}) - at$ where $h$ is a non-ordering field and $\alpha^{-1}$ is a slope of the transition line at the TCP. We focus on a situation where the transition line is approached with a finite angle.

Singualr contributions to non-ordering quantities are obtained by taking derivatives of $G_{\text{sing}}$ with respect to $h$ at $h = h_\text{eq}$ and $s = 0$ with $t \to 0$:

$$m = -\frac{\partial G_{\text{sing}}}{\partial h} \sim |t|^\beta_2,$$

with $\beta_2 = 1 - \alpha$ and

$$\chi = -\frac{\partial^2 G_{\text{sing}}}{\partial h^2} \sim |t|^{-\gamma_2},$$

with $\gamma_2 = \alpha$, where the additional subscript ”2” indicates the exponents corresponding to non-ordering quantities. In the present case, the non-ordering field $h$ corresponds to a magnetic field and thus $m$ ($\chi$) is the magnetization (longitudinal magnetic susceptibility). Since the specific heat coefficient $C/T$ at $h = h_\text{eq}$ is given by

$$C/T = -\frac{\partial^2 G_{\text{sing}}}{\partial T^2} \sim |t|^{-\alpha},$$

$\gamma_2$ is the same as the specific heat exponent. Hence we obtain the following scaling laws:

$$\alpha + 2\beta_2 + \gamma_2 = 2, \quad \alpha = \gamma_2.$$

For an ordinary CP, replacing a TCP with a CP and employing the standard form

$$G_{\text{sing}}(g, s) = |g|^{2-\alpha} G \left( s/|g|^\alpha \right),$$

we obtain the same scaling laws. Therefore Eq. (13) holds for both CP and TCP. This is worth emphasizing that even the existence of TCP is not necessary for the fulfillment of the relation Eq. (13).

Since the exact value of $\alpha$ is known both at CP and TCP \cite{12}, Eq. (13) gives the exact values of $\beta_2$ and $\gamma_2$ (Table I). That is, $\chi^z$ exhibits a divergence in a critical regime at both CP and TCP, indicating that the PI in a magnetic field is accompanied not only by soft Fermi surface fluctuations but also by sizable ferromagnetic fluctuations. It should be noted that the singularity of $\chi^z$ seen in Fig. 3(d) is expected to remain the same even in the presence of fluctuations, because the relation $\chi^z = 2m/h$ [Eq. (8)] still holds beyond the RPA as long as the effective interaction between electrons retains the spin-rotational invariance \cite{29}, and $m/h$ is continuous at both CP and TCP.

| \(\alpha\) | CP Mean field | CP Exact | TCP Mean field | TCP Exact |
|---|---|---|---|---|
| 0 (jump) | 0 (log) | 1/2 | 8/9 |
| 1 | 1 | 1/2 | 1/9 |
| 0 (jump) | 0 (log) | 1/2 | 8/9 |
| 1/2 | 1/8 | 1/4 | 1/24 |
| 1 | 7/4 | 1 | 37/36 |

### TABLE I: Critical exponents at a CP and a TCP. Mean-field values at a TCP are exponents on the symmetry-broken side. The exponents of ordering quantities are also listed for completeness: $\eta = |h|^\kappa$ and $k_\parallel \sim |h|^\kappa$, where in the present case $\eta$ corresponds to the order parameter of the PI [Eq. (3)] and $k_\parallel$ to the $d$-wave compressibility \cite{16}.

### IV. DISCUSSION

#### A. Relevance to Sr$_3$Ru$_2$O$_7$

There is growing evidence that the bilayer ruthenate Sr$_3$Ru$_2$O$_7$ exhibits the PI \cite{9–11}. Although other interactions, not included in our model (1), may exist in Sr$_3$Ru$_2$O$_7$, by virtue of universality, the present approach is sufficient to correctly capture the universal singularities (Table I) associated with the PI. Inclusion of other terms like spin-orbit coupling does not influence the order parameter symmetry [Eq. (5)] and therefore the system can be presumed to remain in the two-dimensional Ising universality class even if the microscopic model is tailored to capture more specific features of Sr$_3$Ru$_2$O$_7$.

The specific heat jump was reported recently \cite{10} at a CP of the PI. The actual critical region seems tiny enough not to be resolved in the experiment and the observed jump corresponds to the mean-field behavior. Therefore we predict the same behavior also for $\chi^z$ [Figs. 3(a) and (c)]. To the best of our knowledge, Sr$_3$Ru$_2$O$_7$ can provide the first example of a jump of the magnetic susceptibility at a continuous phase transition in condensed matter. On the other hand, at a TCP we predict a divergence of the jump of $\chi^z$ [Figs. 3(b) and (c)] as well as that of $C/T$ (Fig. 4), although the latter becomes visible only sufficiently close to a TCP, which requires high accuracy of an experimental measurement. The quantity $\chi^z$ is not a non-ordering susceptibility and its singularity might depend on microscopic details of the system. In particular, in Sr$_3$Ru$_2$O$_7$ the spin-rotational invariance is broken due to the spin-orbit coupling. Nonetheless, as far as the underlying interaction driving the PI [Eq. (2)] does not contribute to $\chi^z$...
The system features multiple critical fluctuations. The $\gamma$ around a TCP may be more pronounced because the value of $\gamma_2$ is close to $\gamma$. Though the universality class is different from the present two-dimensional Ising type, singular behavior of a non-ordering susceptibility was indeed measured at a TCP in some metamagnetic compounds such as CsCoCl$_2$-2D$_2$O and Dy$_3$Al$_5$O$_{12}$ in 1970s [13]. A manifestation of multiple singular susceptibilities is seen also in recent literature. For example, in Ref. 30 peculiar behavior of the uniform magnetic susceptibility was invoked to propose an explanation of anomalous properties associated with singularities of a non-ordering susceptibility at a phase transition. While such properties have not been recognized well in modern condensed matter literature, it can be tested for Sr$_2$Ru$_2$O$_7$ by measuring the longitudinal magnetic susceptibility.

**B. Implications for other materials**

As seen from the derivation of Eq. (13), the singular behavior of $\chi^{zz}$ is not a specific feature of the PI in the presence of a magnetic field, but can be interpreted as a phenomenon associated with singularities of a non-ordering susceptibility at a phase transition in general. This observation provides implications for a variety of materials. In particular, when a critical region is accessed by experiments, the mean-field predictions break down. In such a region, both ordering and non-ordering susceptibilities diverge simultaneously ($\gamma$ and $\gamma_2$ in Table I). The system features multiple critical fluctuations. The effect around a TCP may be more pronounced because the value of $\gamma_2$ is close to $\gamma$. Though the universality class is different from the present two-dimensional Ising type, singular behavior of a non-ordering susceptibility was indeed measured at a TCP in some metamagnetic compounds such as CsCoCl$_2$-2D$_2$O and Dy$_3$Al$_5$O$_{12}$ in 1970s [13]. A manifestation of multiple singular susceptibilities is seen also in recent literature.

**V. SUMMARY**

We have studied the uniform magnetic susceptibility at the PI on a square lattice in the presence of a magnetic field. In a mean-field model, $\chi^{zz}$ is found to exhibit a jump at a critical point and a power-law divergence at a tricritical point, whereas $\chi^x$ exhibits a cusp. The mean-field results may be modified in a critical region. In particular, $\chi^{zz}$ is expected to diverge also at a critical point, indicating that the PI in a magnetic field is accompanied not only by soft Fermi surface fluctuations but also by sizable ferromagnetic fluctuations. Involving the scaling hypothesis we have argued that the features of $\chi^{zz}$ are not specific to the PI in a magnetic field, but are general properties associated with singularities of a non-ordering susceptibility at a phase transition. While such properties have not been recognized well in modern condensed matter literature, it can be tested for Sr$_2$Ru$_2$O$_7$ by measuring the longitudinal magnetic susceptibility.

**Acknowledgments**

We would like to acknowledge valuable discussions with A. A. Katanin, H. Kohno, W. Metzner, K. Miyake, and M. Napiórkowski, and warm hospitality of the Max-Planck-Institute for Solid State Research in Stuttgart.

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