Effect of Short-Range Fluctuations on Thermodynamic and Resistive Properties: The case of Ising Order

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We consider the effects of the non-local Ising-like “core spin” correlations on the order-parameter fluctuation contribution to the resistivity and thermodynamics of metals showing Ising-like order at finite temperature. We employ the well-known cluster-variation method, and present explicit results in the pair approximation for short-range order. Our calculation generalizes earlier works, where such effects were considered in the mean-field (Ornstein-Zernicke) approximation. The mean-field (MF) transition temperature $T_{c}^{MF}$, is corrected to $O(1/d)$, and the effect of the Ising spin fluctuations on the dc resistivity and magnetothermal responses is analyzed in detail. The method can be applied straightforwardly to lattices in arbitrary $d$, and, as an appealing feature, it reproduces the exact correlation length and $T_{c}^{1d}$ = 0 for the 1$d$ Ising model. We apply our results for two interesting physical cases: (i) the double-exchange model with $J_H > t$, where the core-spins can be approximated quite well by Ising spins, and (ii) a model of band electrons coupled to a localized subsystem which undergoes a nematic ordering transition coupled to an appropriate structural transition.

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I. INTRODUCTION

Finite temperature ($T$) order in solid state systems leave their imprint on thermodynamic and transport responses across the order-disorder transition. The steady enhancement of the correlation length of the system as $T$ is lowered toward $T_c$ from above directly impinges, in particular, on the $T$-dependent carrier scattering rate, and manifests itself as changes in thermal and transport behavior as the phase transition is approached. For a classical transition from a ferromagnetic metal to a paramagnet, such effects on the dc resistivity for the Heisenberg universality class were considered more than forty years ago. This estimation has been invaluable in interpreting a large body of data on band ferromagnets.

Many real compounds, however, show pronounced effects of short-range order (SRO) on carrier properties. Devising computational schemes capable of incorporating such SRO effects into realistic microscopic calculations has long been the goal in the field of electronic systems. However, to date, it has proved to be extremely demanding to go beyond the single-site approximation: in disordered transition-metal alloys, the coherent potential approximation (CPA) has long been used with great success, while for strongly correlated electronic systems, dynamical-mean-field-theory (DMFT) in conjunction with ab initio (LDA) band structure also holds a lot of promise. However, by construction, such a single-site approach cannot capture the full effects of SRO on carrier scattering rates. This requires extending DMFT(CPA) to capture SRO effects via proper cluster extensions, a formidable task realizable currently only for one-orbital models. Moreover, details of such SRO induced effects on carrier scattering rates and transport properties remain unexplored avenues for study, to our best knowledge.

Motivated by the above, we focus on a much “simpler” version of the above problem that nevertheless bears on a number of interesting issues in modern condensed matter physics. Specifically, we consider physical systems with an Ising like phase transition to an ordered phase (either rigorously or to a very good approximation). It turns out that, for this particular case, a controlled estimation of corresponding order parameter fluctuations to $O(1/d)$ (with $d$ the system dimensionality) and their feedback on band-like carriers can indeed be carried out under restricted conditions (see below).

To emphasize the relevance of our “simple” theory for physical problems of great current interest, we consider two explicit cases: (i) the double exchange (DE) model with $J_H >> t$, in which case, the spin correlations can be well approximated by an effective Ising model. This is believed to be an appropriate low-energy model for certain colossal magnetoresistance manganites in a limited doping region corresponding to a well-ordered low $T$ ferromagnet. (ii) the problem of an electronic system undergoing an electronic nematic transition, coupled, by symmetry, to an appropriate lattice distortion. This ordering rigorously belongs to the universality class of an Ising model in an external zeeman field. Evidence for electronic nematicity appears in various cases of great current interest, like bilayer Sr$_3$Ru$_2$O$_7$, underdoped Fe arsenides and underdoped high-$T_c$ cuprates.
II. FORMALISM

A. Boundaries of Validity

In this section, we describe the well-known cluster variation method (CVM) for the simple DE model (ii) above. But obviously, the formalism applies equally well for case (ii) with replacement of the real Ising spin by a $S = 1/2$ pseudospin corresponding to Ising nematic order.

We start with the double exchange (DE) model in the limit $J_H \gg t$ with a nearest neighbor ferromagnetic (FM) coupling between core spins. This model is believed to be applicable to doped Europium oxide (EuO) and is an effective low-energy model for well-doped magnetanes. It reads

$$H = \sum_{\langle ij \rangle} t_{ij}(S)(c^{\dagger}_{i\sigma}c_{j\sigma}+h.c)-J' \sum_{\langle ij \rangle} S^z_i S^z_j-h_{ext} \sum_i S^z_i. \tag{1}$$

In the above, we have included only the Ising part of the intersite FM coupling, because the transverse spin fluctuations make a negligible contribution when $J_H \gg t$. In this limit, the spin correlations are well approximated by that of an effective Ising model, with an effective intersite coupling $J' = (t^2/J_H)x(1-x)$ for the well-doped FM metal. Also, $t_{ij}(S) = t[1+<S^z_i S^z_j>/2S^2]^{1/2}$ and $h_{ext}$ is the external magnetic field. We emphasize that $t_{ij}$ is to be understood as a renormalized carrier hopping integral, reduced from its bare band structure value by strong local Hubbard correlations in the real system.

In the case of the nematic order, the “core spin” above is replaced by a nematic pseudospin, $N^z$, which quantifies the degree of electronic anisotropy, reflecting spontaneous breaking of (discrete) lattice rotational symmetry. In an Ising nematic, this is defined simply as $N^z = \frac{n_a-n_{a+\pi,n_b}}{n_{a+\pi,n_b}+n_{a,n_b}}$, where $n_a$ is the average fermion occupation number along $a(= x,y)$. Physically, this can arise from multi-orbital effects (as probably the case in $Sr_2RuO_4$ and underdoped Fe arsenides) or from anisotropic (effective) two-body interactions (as possibly in underdoped cuprates). We will assume that electronic nematic (e-nematic) order has occurred, without specifying its microscopic origin in this work. By symmetry, $N^z$ directly couples to the lattice strain, which acts as a field term conjugate to the order parameter. The Hamiltonian is

$$H = \sum_{\langle ij \rangle} t_{ij}(c^{\dagger}_{i\sigma}c_{j\sigma}+h.c)-J' \sum_{\langle ij \rangle} N^z_i N^z_j-\delta(T) \sum_i N_i^z, \tag{2}$$

where $\delta(T)$ is the lattice strain, simplified here to a single $T$-dependent function to illustrate its dominant role. The intersite exchange is “ferro”, since the e-nematic state involves a $q = 0$ instability. Again, $t_{ij}$ is to be understood as an effective hopping of (substantially) renormalised band carriers in reality.

Effects of arbitrary SRO on carrier dynamics in real materials has hitherto relied on heavy-duty numerical approaches. Ideally, one would like to extend the local approximation in a way that is amenable to treatment of the problem in any dimension, and is computationally tractable. In what follows, we present an analytical version of the cluster-variation method (CVM), which has been widely used in studies of alloy formation and stability. This scheme satisfies the above requirements, is physically transparent and amenable to easy numerical implementation. We emphasize that, as a first step, we look at these effects within effective models, and our approach is only valid in the cases where SRO arises from (electronic) degrees of freedom that are effectively decoupled from the band-like carriers at low energy. This is also the reason why we cannot describe the microscopics of the ordering mechanisms: we take this as given.

B. Cluster Variation Method

As a first step, we realize that the core (Ising) spins can be thought of as an alloy system of $S^z = -1/2, +1/2$. A perfect FM order (low $T$) corresponds to a pure system of either $S^z = -1/2$ or $+1/2$. At sufficiently high $T$, the system is non-magnetic and corresponds to a completely random alloy of $S^z = -1/2, +1/2$, where the CPA should be a very good approximation. At intermediate $T$, however, SRO effects are dominant. In this situation, we map our problem to that of a short-range ordered binary alloy, which has been extensively studied in the field of magnetism of disordered transition metals. In particular, we employ the CVM, which has been very successfully used in this context. The CVM gives analytical expressions for the correlation functions of the system within the so-called pair and square approximations. In addition, it satisfies the “diffuse intensity sum rule” exactly in $d = 1$, a feature that is not shared by other, less sophisticated approximations. We make the identification $S^z_i = -1/2 \rightarrow n_i = 0$ and $S^z_i = 1/2 \rightarrow n_i = 1$. We start by writing down the functional:

$$F[\sigma] = \sum_{\sigma} E(\sigma)X(\sigma) + k_B T \sum_{\sigma} X(\sigma)lnX(\sigma), \tag{3}$$

where (for a binary system such as the one we consider) for $N$ lattice sites, the sum runs over $2^N$ configurations. Here, $E(\sigma)$ and $X(\sigma)$ denote the energy and probability of a configuration $\sigma$. The system free energy is just the minimum of $F[\sigma]$, where the minimization is carried out over all density matrices $X(\sigma)$ subject to normalization: $\sum_{\sigma} X(\sigma) = 1$.

In general, the average configurational energy of the spin subsystem can be written down as a linear combination of many-body correlations. For a binary system, $E(\sigma) = 1/2 \sum_{ij} J^z_i S^z_i S^z_j + \sum_i h_i S^z_i, \tag{4}$
\[ F[\sigma] = E(\sigma) + \frac{k_B T}{2} \sum_{ij \sigma' \sigma} y_{\sigma \sigma'}(i,j) \ln y_{\sigma \sigma'}(i,j) \]
\[ + k_B T (1 - z) \sum_{i, \sigma} x_{\sigma}(i) \ln x_{\sigma}(i), \]
where \( x_{\sigma}(i) = [1 + \sigma \xi(i)] \) is the single-site occupation probability and \( y_{\sigma \sigma'}(i,j) = (1/4)[1 + \sigma \xi(i) + \sigma' \xi(i + j) + \sigma \sigma' \xi_2(i,j)] \) is the pair probability. The quantities \( \xi_i \) with \( i = 1, 2 \) are given by derivatives of the free energy w.r.t. the inhomogeneous field: \( \xi_i(i) = \langle S_i^z \rangle \), \( i, j \), and \( \alpha_{ij} = \xi_2(i,j) = \langle S_i^z S_j^z \rangle > -\langle S_i^z \rangle < \langle S_j^z \rangle > \frac{\alpha^2}{d \chi_{\alpha}} \),
\[
\alpha_{ij} = \xi_2(i,j) = \langle S_i^z S_j^z \rangle > -\langle S_i^z \rangle < \langle S_j^z \rangle > \frac{\alpha^2}{d \chi_{\alpha}} \tag{6}
\]
and the spin susceptibility including SRO contributions is calculated as the Fourier transform of \( \alpha_{ij} \).

In what follows, we will consider only the pair approximation as a first step, so that \( R_1 - R_2 = a \), the lattice constant. To compute the thermodynamic response and carrier scattering rate, we need the free energy of an effective Ising model in a Zeeman field: interestingly, in the pair approximation, we show that these can be obtained analytically. We find the free energy of the “core-spin” subsystem in the pair approximation as
\[ F(m, \alpha) = N(-z J' m^2/2 - m h_{ext}) - z J'(1-m^2)\alpha + F[S], \]
where
\[ F[S] = k_B T \left( \frac{1 + m}{2} \ln \frac{1 + m}{2} + \frac{1 - m}{2} \ln \frac{1 - m}{2} \right) \]
\[ + k_B T z \frac{\alpha^2}{4}. \tag{8}\]

The magnetization, \( m(T) \), is computed as the first field-derivative of the free energy:
\[ m(T) = \frac{\beta}{k_B T} \frac{\partial F}{\partial h} = \frac{z J' m (1 - \alpha) + h}{k_B T}, \tag{9}\]
where \( \alpha = \alpha_{ij} = \langle S_i^z S_j^z \rangle > -m^2(T) \). Notice the difference from the Weiss mean-field (MF) result; the non-local spin correlation function explicitly enters the transcendental equation for \( m(T) \).

The \( q \)-dependent core-spin correlation function is derived from the second field-derivative of the free energy:
\[ \chi(q, T) = \frac{-1}{N} \sum_{i,j} e^{i q (\mathbf{R}_i - \mathbf{R}_j)} \langle [S_i^z S_j^z] > m^2(T) \rangle \tag{10}\]
\[ \chi(q, T) = \frac{1 - \xi_2^2(T)}{1 + (z-1)\xi_2^2(T) - 2\xi_2^2(T)c_q^2}, \tag{11}\]
in \( d \) dimensions and \( c_q^2 \equiv \sum_{a=1}^d \cos[q_a (R_{ia} - R_{ia})]. \)
In general, \( T^F_c \) is determined from the solution of \( \chi^{-1}(q, T) = 0 \) for \( q = 0 \): i.e., as the solution of \( 1 - (z-1)\tanh(J'/\kappa) = 0 \). In \( d = 1 \), this gives \( T^F_c = 0 \), and the correlation length, \( \xi(T) = \tanh(J'/\kappa) \), which coincides with the result known from the exact solution. It is easy to see that for small \( q \) around \( q = 0 \), \( \chi(q, T) \simeq A(T)/(\xi^{-2} + q^2) \) in \( d = 3 \), which is the classical Ornstein-Zernike behavior with the FM spin correlation length given by \( \xi_2^2(T) = 2 \tanh^2(J'/\kappa)[1 - (z-1)\tanh^2(J'/\kappa)] \), again noticeably different from the MF result. Comparing with the MF result, we see that inclusion of non-local FM spin correlations within the pair approximation (CVM) depresses the transition temperature: \( T^F_c = T_{c,F}^F(z - 1) \), where \( T_{c,F}^F = 2 J'/kB \) is the Weiss MF result, as expected. The \( q = 0 \) susceptibility is directly written as,
\[ \chi(0, T) = (\gamma_B)^2 \frac{1 + \tanh(J'/\kappa)}{1 - (z-1)\tanh(J'/\kappa)} \tag{12}\]
which deviates noticeably from the MF-Curie-Weiss form at intermediate \( T \).

### III. SOME PHYSICAL OBSERVABLES: RESISTIVITY AND THERMODYNAMICS

Given the spin correlation function, the spin disorder contribution to the dc resistivity is evaluated using Fermi’s golden rule from the equation, extended to an Ising transition.
\[ \rho_{dc}(T) = \frac{m^*}{e^2} \int_{FBZ} \chi(q, T)(1 - \cos \theta) d\theta \tag{13} \]
for \( D \) dimensions. Here, \( \sin(\theta/2) = q/2k_F \), with \( \tau^{-1}(T) = \int_{FBZ} \chi(q, T)(1 - \cos \theta) d\theta \) again involving the non-local spin correlations via \( \chi(q, T) \). We expect the detailed nature of the field induced changes in \( \rho_{dc}(T) \) to be determined by the field-induced changes in the thermal order parameter fluctuations. An external field will increase carrier mobility via \( \alpha_{ij} \), reducing \( \tau^{-1}(T) \), and resulting in increased itinerance above \( T_c \).

Calculation of the thermal expansion and magnetovolume effects requires a bit more work. In a system with Ising-like local moments (magnetic or nematic), which are stable as \( T \) is raised, one invokes the same localized picture as for insulators, where any magnetovolume term is due to the volume dependence of inter-site interactions. Following, the order parameter fluctuation contribution to the thermal expansion coefficient is,
\[ \alpha_\gamma(T) = K \frac{\gamma_m}{V} \frac{d}{dT} \left( -\sum_{i,j} J[S_i^z S_j^z] > m^2(T) \right) \tag{14} \]
where \( \gamma_m = -d\ln j/d\ln V \) is the magnetic or lattice Grüneisen parameter. The integrated magnetovolume is
then,
\[
\frac{\Delta V}{V} = K \gamma_m \int_0^\infty dh \frac{dM}{dT} \left( \sum_{ij} J[<S_i^z S_j^z > -m^2(T)] \right).
\]  
(15)

Using Maxwell’s thermodynamic relation, the entropy change in a field can be directly computed from,
\[
\Delta S_M(T, h) = S_M(T, h) - S_M(T, 0) = \int_0^h \left( \frac{dM}{dT} \right)_h dh,
\]  
(16)

using the equation for the order parameter in the pair approximation derived above. (A large change in \(\Delta S_M(T, h)\) is expected near \(T_{cFM}\) in DE ferromagnets, as also in disordered local moment ferromagnets and would be interesting in the context of applications to magnetic refrigeration).

The above equations show how short-range order directly influences various transport and thermodynamic quantities in metallic systems showing an Ising-like semiclassical order via coupling of band carriers to order parameter thermal fluctuations. Obviously, our scheme is only valid when the Ising-like order arises from microscopic (electronic) degrees of freedom that are effectively decoupled from the band-like carriers, but, once established, affects carrier dynamics as shown above.

IV. RESULTS

We now discuss how the above “simple” formalism captures, surprisingly, a wide range of interesting features in the cases (i) and (ii) mentioned in the Introduction.

A. Colossal Magnetoresistance Manganites

We note that the Langer-Fisher formulation has been applied with good success by Majumdar and Littlewood. They considered a variety of doped magnetic semiconductors. However, effects of magnetic short-range order have received scantier attention in this context, and this is the issue we will address here.

In this section, we show the results of our calculation and discuss them in some detail. In Fig. 1, we show the core-spin magnetization as a function of temperature, \(T\). Notice the difference from the MF result, where \(m(T)\) vanishes at \(T_{cFM}\) (the MF curve is shown by the dotted curve in Fig. 1). Magnetic SRO (\(J' > 0\)) smears the MF transition, as shown in Fig. 1; the tail showing persistent FM SRO above \(T_{cFM}\). A small magnetic field, \(h_{ext} = 0.05t\), aligns these short-range-ordered regions, giving an appreciable \(M(T)\) well above \(T_{cFM}\). Obviously, pre-existing SRO, in conjunction with a small \(J' \sim t^2/J_M\) makes it easier for a small \(h_{ext}\) to polarize the high-\(T\) phase. Similar behavior is seen for \(h_{ext} = 0.1t\). We also clearly see emergence of hysteresis in \(m(T)\), a feature expected in an Ising model in a zeeman field. The static \((q = 0)\) spin susceptibility, \(\chi(0, T)\) shows a distinctly non-Curie-Weiss behavior below \(T \simeq 2T_{cFM}\), as indeed observed experimentally, showing the persistence of magnetic SRO to rather high temperatures.

The dc resistivity, \(\rho_{dc}(T)\), computed within the Born approximation, actually exhibits an insulator-like behavior above \(T_{cFM}\) (Fig. 2). Within simple MF theory, \(\rho_{dc}(T) = const\) above \(T_{cFM}\) (see Fig. 2); in the case of classical (or Ising) spins, since these act like non-magnetic scatterers, giving a resistivity characteristic of impurity scattering. With \(J' = 0\), we thus obtain a result resembling that obtained from MF theory, as seen in Fig. 2. With \(J' \neq 0\), this behavior is drastically modified: a sharp peak, reflecting coupling of carriers to the increasingly singular \(\chi(q, T)\), is clearly seen in the inset of Fig. 1. We thus conclude that it is precisely the intersite correlations, and, in particular, the dominant FM SRO above \(T_{cFM}\) which drives the insulator-like resistivity in the PM state. The effect of the external magnetic field is striking: \(h_{ext} = 0.05t\) drives the high \(T\) resistivity metallic. This is directly related to the field-dependent suppression of the FM short-range correlations, as seen in Fig. 3, reducing the scattering rate, enhancing the carrier mobility and driving the system metallic. Similar (enhanced) metallic behavior is seen for \(h_{ext} = 0.1t\), and the dc re-
FIG. 2: $dc$ resistivity with $J' = 0$. Notice how the resistivity shows a broad and smooth change across $T_c$. This is the expected result for the Ising case, which corresponds to “potential” non-magnetic disorder, giving $\rho_{dc}(T) \simeq const$ above $T_c$. This is an artifact of the MFA and is corrected by the CVM (See Fig. 3).

We consider next the magnetic entropy change, computed from the $T$-derivative of the magnetization. In Fig. 3, we show $S_M(T, h_{ext})$ for $h_{ext} = 0, 0.05, 0.1t$. A number of interesting features are apparent; the field-induced redistribution of $S_M$ is drastic, the sharp peak around $T^{FM}$ changes to a broad peak like feature in an external field. The quantity $\Delta S_M = [S_M(T, H) - S_M(T, 0)]/S_M(T, 0)$, which measures field induced entropy change shows very encouraging behavior, attaining values up to 6 in $h_{ext} = 0.15t$. We also notice that the overall shape of the curve (shown in the inset of Fig. 4) is in good qualitative agreement with observations. In this context, we notice that $Gd$ metal, widely used as a magnetic refrigerant, shows $\Delta S_M = 4.0$ near room temperature. Thus, $J_H >> t$ (small $J$) is one of the conditions favoring a large $\Delta S_M$, and possible application of such systems to magnetic refrigeration. Further, the manganites exhibit considerably small magnetic hysteresis with a coercivity of 50 Oe near $T^{FM}_c$, which should enhance their magnetic cooling efficiency. Finally, interestingly, we remark that the $\Delta S_M(T)$ we extract qualitatively resembles that found for ternary CoMnGe$_{1-x}$Sn$_x$ ferromagnetic alloys by Hamer et al. Our formalism, based on magnetic SRO, can also be readily extended to include structural/chemical SRO in disordered ferromagnetic alloys. This entails incorporation of specific electronic structure details, and lies out of scope of the present phenomenological theory.

Finally, we consider the magnetic contribution to the volume expansion, $\Delta V_M(T)/V$. Before presenting our results, we present a brief physical picture of magnetovolume effects in magnetic systems. At high-$T$, with completely disordered local moments, one has as many $\uparrow$-spins as $\downarrow$-spins, so the magnetovolume interactions average to zero. As $T$ decreases, short-range local moment correlations begin to develop, and the magnetovolume interaction is determined by the spatial dependence of the spin correlation function. Obviously, the MF approximation would give incorrect estimates of magnetovolume effects in manganites, since, as we have seen, the FM spin correlations are very different from those expected from MF approaches. In view of the ability of the CVM to yield a more consistent description of these correlations, one expects that it is able to better describe magnetovolume effects in such systems.

In Fig. 5, we show the magnetovolume changes for different field values. Note that it tends to zero for sufficiently high-$T$, consistent with the picture above. Interestingly, at temperatures much higher than $T^{FM}_c$, the effect of short-ranged FM spin correlations is manifested.
be switched in sign by an applied field above $V_{\text{ext}}$. Sensitively affected by chemical disorder is the field-induced suppression of spin fluctuations above $T_c$. The consequence for technological applications. The change is clearly seen from Fig. 5. This fact might be potentially maximum. Hence, it can only be accessed in a theory which describes SRO in a consistent way beyond the single-site limit.

The fractional change in $\alpha_M(T)$, which is negative and decreases with decreasing $T$ up to about $T_c^{FM}$. It is interesting to observe that a negative $\Delta S_M(T)/V$ (thermal expansion coefficient) is characteristic of invar alloys\textsuperscript{15}, and is observed both in the chemically disordered and ordered cases, demonstrating that chemical disorder is not the driving force of invar effects. But thermal spin fluctuations introduce spin disorder which could produce such effects. In our case, the magnetovolume changes sign at $T_c^{FM}$, so more work is needed to describe such systems, which may include cases where there is no correlation between $T_c^{FM}$ and the sign change in $\alpha_M(T)$.

The field-dependence of $\Delta V_M(T)/V$ shows how it is sensitively affected by $h_{\text{ext}}$. The fractional change in $\Delta V_M(T, h_{\text{ext}})/V$ is large, and can decrease by as much as 175 percent in $h_{\text{ext}} = 0.1t$. More interestingly, it can be switched in sign by an applied field above $T_c^{FM}$, as is clearly seen from Fig. 5. This fact might be potentially useful for technological applications. The change is maximum just around $T_c^{FM}$, and is thus intimately related to the field-induced suppression of spin fluctuations above $T_c^{FM}$. Hence, it can only be accessed in a theory which describes SRO in a consistent way beyond the single-site limit.

Here, we will show that, remarkably enough, our “simple” technique also provides a simple qualitative explanation for a variety of ill-understood fluctuation effects in physical cases where an electronic nematic (e-nematic) instability arises in metals at low $T$. The whole structure of the theory remains intact upon re-identifying the $S^z$ as nematic pseudospin variables, $N^z$. Moreover the electronic nematic transition rigorously falls into the universality class of an Ising ferromagnet in a zeeman field\textsuperscript{5}. Obviously, we want to emphasize that, in our effective approach, deeper questions relating to microscopic origin of such nematic state(s) cannot be answered: our main focus is to try to understand its consequences for thermodynamic and transport responses. To this end, we will also drastically simplify the more complicated situation in real systems of interest (like $Sr_3Ru_2O_7$ and underdoped Fe arsenides\textsuperscript{12, 24}) by replacing their undoubtedly strongly correlated (multi) bands by a single free-electron like band. In such systems, the $N^z$ may microscopically arise via orbital selective Mott localization of a subset of the $d$ orbital band states in the real correlated system, and, in our effective model, we assume that this has already occurred. Thus, our analysis cannot hold for studying nematic correlations in underdoped cuprates, where the possible nematic order and the “itinerant” carriers arise from a same single band\textsuperscript{22, 23}.

(i) First, $1/d$ (classical) order parameter fluctuations

\begin{figure}[h]
\centering
\includegraphics[width=0.45\textwidth]{fig4}
\caption{Order parameter fluctuation contribution to the entropy as a function of $T$. Significant improvement over the mean-field estimate is clear. The field-induced entropy change, $\Delta S_M(T)$, attains its maximum in a range of field values where $m(T, h)$ vs $h$ shows hysteretic behavior. For “local moment” metallic ferromagnets, combination with a coercivity of $O(50)$ Oe would make them attractive candidates for magnetic cooling applications. Similar features have recently been reported across the T-O structural transition in underdoped Fe arsenides.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=0.45\textwidth]{fig5}
\caption{Volume change as a function of $T$. There is a sign change at the ordering temperature ($T_c$). Notice the negative sign of ($\Delta V(T)/V$) below $T_c$, followed by a non-linear variation and hysteresis above $T_c$ when $J' > 0$. Similar features are characteristic of some Invar materials. They have also been reported recently across the T-O structural transition in underdoped Fe arsenides.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=0.45\textwidth]{fig3}
\caption{B. e-NEMATIC ORDER IN METALS}
\end{figure}
depress $T_{nem}$ by about 30 percent compared to the Weiss MF result. Without coupling to strain, the transition is continuous, but turns into a first-order one with a finite (not too large) $h_{ext} = \delta(T)$, with hysteretic behavior. This is clearly seen in Fig. 3 where $m(T)$ is now the nematic order parameter. The lattice constants will directly react to the onset of nematic order, inducing a structural transition (tetragonal-orthorhombic in the Fe arsenides). With reference to underdoped Fe arsenides, this describes the tetragonal-orthorhombic (T-O) phase transition: this can be either a first- or second order transition as we traverse the families of real Fe arsenides.

(ii) Correspondingly, the dc resistivity shows a clear, sharp anomaly at $T_{nem}$ for $\delta = 0$, and a “rounding off” of this sharp feature for a finite $\delta$, with a hysteresis in $\rho_{dc}(T)$ above $T_{nem}$, as shown in Fig. 3.

(iii) The entropy change, $\Delta S_{nem}$, now interpreted as the entropy loss across the e-nematic transition, also exhibits a clear, relatively sharp, maximum precisely at $T_{nem}$, as shown in Fig. 3.

(iv) Finally, the nematic fluctuation contribution to the thermal expansion co-efficient, $\alpha(T)$, shows a clear SRO-induced decrease above $T_{nem}$, and a sharp peak at $T_{nem}$, as shown in Fig. 3.

Let us now see to what extent these results square up with experimental data on underdoped Fe arsenides, where recent work on the so-called 122-systems reveals tantalizing signs of an orbital nematic state coupled to the tetragonal-orthorhombic (T-O) transition. Surprisingly, we find that effects of fluctuations of such an e-nematic order (with Ising symmetry) on the carriers, reflected in thermodynamic and transport data, seem to be qualitatively rationalizable in our “simple” model.

(i) the resistivity, $\rho_{dc}(T)$, shows a maximum at the T-O transition, not at the antiferromagnetic (AF-SDW) transition with $Q = (\pi, 0)$. It also exhibits remarkable hysteretic behavior above $T_{T-O} = 150$ K. This goes hand-in-hand with the disappearance of the orthorhombicity, defined as $\langle O \rangle = \frac{a-b}{c+2c}$, where $a, b$ are unit-cell constants (Fe-Fe nearest neighbor distances) in the FeAs plane. Interestingly, setting $J' = 0$, i.e., neglecting nematic ordering tendency, kills the prominent peak as well as the hysteresis (above $T_{T-O}$) in our results, in disagreement with experiment (see also below). If we assume that a mean field nematic expectation value, $\langle N^z \rangle = (n/2) > 0$, develops at the T-O transition (though it must be kept in mind that, because the coupling of the e-nematic order to strain, the e-nematic order cannot be separated from the T-O distortion, and the e-nematic transition will be smeared), one can address the issue of the in-plane resistivity anisotropy above the T-O distortion in our phenomenological approach. Namely, one can now identify the “external” zeeman field value $\delta(T) = h_z = n$ with the $N^z = 1/2$ state with $\langle O \rangle > 0$ and the value $\delta(T) = h_z = 0$ with the $N^z = -1/2$ state with $\langle O \rangle < 0$ in Ising nematic language. From our theoretical resistivity curves (Fig. 3), we clearly see the development of a clear resistivity anisotropy: interestingly, it extends to temperatures significantly higher than $T_{T-O}$, and achieves its maximum precisely around $T_{T-O}$, where the nematic susceptibility is maximal. These findings are broadly consistent with experiment, and constitute phenomenological explication in terms of an electronic nematic order coupled, by symmetry, to the T-O distortion.

To the extent that the above e-nematic-plus T-O transition is intimately tied to a finite $\langle O \rangle$, its stabilization prepares the ground, via anisotropic electronic structure changes, for striped antiferromagnetic spin-density-wave (AF-SDW) state with $Q = (\pi, 0)$ to emerge in a natural way. This program, within the context of a proposal for ferro-orbital order, has been carried out in Ref. $^7$, and the resulting $J_{1a} - J_{1b} - J_2$ model with large $J_2/J_{1a,b}$ indeed achieves a satisfying description of spin-wave dispersion in the AF-SDW state in the O-structure. Electronic nematicity has hitherto not been considered within such a program. In view of the fact that e-nematic and T-O transitions are strongly coupled (the former is smeared), it follows that a similar instability to an AF-SDW state can be worked out in the present case as well. We do not do it here, and only mention that, once the T-O distortion occurs, the scenario of Ref $^7$ can take over.

(ii) thermal expansion co-efficient in underdoped Fe arsenides has been recently measured by Wang et al. $^{22}$. Marked anomalies in $\alpha(T)$ are found precisely at the T-O transition, and these also appear to survive and change with increasing doping: in particular, at doping levels close to the T-O boundary at low $T$, the “fluctuation” contribution, $\Delta \alpha(T)$, becomes negative below $T_{T-O}$, changing sign to positive for $T > T_{T-O}$. Remarkably, this is exactly the form we extract: in our approach (Fig. 3), it arises due to fluctuations associated with Ising-like e-nematic order coupled with the T-O distortion. Adding a purely phenomenological term, linear in $T$, to our $\alpha(T)$ computed above could give nice qualitative agreement with these experimental results. Closer inspection, in fact, shows that our result for $\alpha(T)$ for finite $J'$ (i.e., including nematicity) is in much closer accord with data than the one with $J' = 0$. In particular, the dip (peak) in the (total) measured $\Delta V_M(T)/V$ slightly below/above $T_{T-O}$ is nicely rationalized as arising from short-range fluctuations of an Ising-like nematic order associated with $(xz, yz)$ orbitals in real underdoped Fe arsenides. The estimated entropy change across the structural transition also bears similarities to our computed result, but, since the striped AF instability also occurs (slightly below or concurrently with) the structural instability, a direct comparison between our theory (which only focuses on nematicity and the accompanying T-O distortion) and experiment is premature.

While the above is by no means a microscopic description, the “localized” nematic pseudospins ($N^z$) can microscopically arise in physical situations where sizable multi-orbital electronic correlations selectively localize a subset of the relevant planar orbital band states, leaving others metallic. Thus, elucidation of the microscopics of the e-nematic-plus T-O transition in Fe-arsenides,
and, in particular, investigating issues like (i) how such e-nematic-plus T-O transition occurs as an instability of the bad-metal “normal” state, and (ii) its relation (competitor) to unconventional superconductivity, involves much more work, and will be reported separately.

Nevertheless, we close this section with a few remarks that may have a bearing on recent experimental data for underdoped Fe arsenides. Given that our phenomenological Hamiltonian,

\[ H = t \sum_{\langle i,j \rangle, \sigma} (c^\dagger_{i,\sigma} c_{j,\sigma} + h.c) - J' \sum_{\langle i,j \rangle} N^z_i N^x_j - h_z \sum_i N^z_i , \]

for the e-nematic transition describes (renormalized in reality) band-like electrons coupled to a ferro-“magnetic” Ising model in a zeeman field, the critical behavior falls into the liquid-gas universality class. It is then perfectly possible that an additional “tuning parameter”, say static chemical disorder, could tune the system to the \( T = 0 \) quantum critical end-point of the line of first-order transitions of this quantum liquid-gas transition. This could possibly bear a relation to signatures of quantum criticality observed in some of the Fe arsenides as a function of doping, and would not be inconsistent with the (observed) fact that maximal SC \( T_c(x) \) in Fe arsenides does not occur at the critical value \( x = x_1 \) where AF-SDW order vanishes, but rather at \( x \) where \( T_{T-O} \) would have vanished, as is clear by observation of the \( T - x \) phase diagrams where \( T_{T-O}(x) \) and \( T_{N}(x) \) are well-separated in \( T, x \). An upshot of this reasoning would be then to inquire whether, in a quantum-critical scenario, soft fluctuations associated with an underlying QCP associated with orbital e-nematic order could act as a pair glue for SC, along lines worked out by Si et al.\(^{20}\). It would be interesting to investigate this line of thinking in more detail, but this is out of scope of the present work.

V. CONCLUSION

To conclude, in this paper, we have studied how thermally induced SRO and associated order parameter fluctuations affect various thermodynamic and resistive properties in two cases: (i) the double exchange model with \( J_u >> t \), where an effective Ising-like spin model arises, and (ii) an electronic system undergoing a phase transition to an e-nematic state, coupled to a lattice distortion and shown how a careful treatment of SRO goes quite a long way toward a qualitative understanding of several striking features in correlated systems of great current interest. Our analysis should be valid as an effective phenomenological treatment in situations where the Ising-like order sets in independently of the nature of the band-like electronic state, but, once established, drastically affects thermodynamic and transport responses via coupling of carriers to the order parameter spin susceptibility. Being extremely simple to implement, it can easily be used to analyze experimental results in a wide variety of other systems, e.g., in multi-orbital systems where orbital order, generically Ising like, plays a crucial role in shaping their physical properties. It can also be used very efficiently for Ising models with competing interactions (the axial-next-nearest-neighbor Ising (ANNNI) model\(^{21}\)) in a zeeman field, which, in itself, is interesting as an effective model for complex ordering phenomena in diverse contexts. We plan to address such applications in future work.

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