Marginal Quantum Criticality at the Lifshitz Transition in Electron-Doped Iron Arsenides

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The twin issues of the nature of the “normal” state and competing order(s) in the iron arsenides are central to understanding their unconventional, high-$T_c$ superconductivity. We use a combination of transport anisotropy measurements on detwinned SrFe$_{2-x}$Co$_x$As$_2$ single crystals and LDA+DMFT calculations to revisit these issues. The peculiar resistivity anisotropy and its evolution with $x$ are naturally interpreted in terms of an underlying orbital-selective Mott transition (OSMT) that gaps out the $d_{zx}$ or $d_{yz}$ states. Further, we use a Landau-Ginzburg approach using LDA+DMFT input to rationalize a wide range of anomalies seen up to optimal doping, providing strong evidence that an electronic nematic order may be the main competitor to superconductivity. These findings suggest that strong dynamical fluctuations linked to a marginal quantum-critical point associated with this OSMT and a secondary electronic nematic order constitute a novel and intrinsically electronic glue for superconductivity in Fe-arsenides.

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Understanding the normal phase of the iron arsenide (FeAs) superconductors holds the key to unraveling the microscopic mechanism of their superconductivity. In theoretical approaches based on a weakly-correlated view of these materials, itinerant magnetic fluctuations play an important role in the emergence of spin density wave (SDW) and superconducting (SC) orders in Fe-arsenides\cite{1}. The alternative intermediate-to-strong coupling view accords preeminence to quasi-local spin fluctuations associated with Mott physics\cite{2}. A large body of experiments, especially in the extensively studied 122-FeAs family, are now poised to constrain theory. Approaching the AFM/SC boundary from the overdoped and/or high-$T_c$ side, observation of electronic nematic (EN) correlations with an onset significantly above the structural ($T_s$) and antiferromagnetic (AFM) Neel ($T_N$) temperatures together with the opposite sign of resistivity anisotropy to that expected point toward the possibility of orbital-driven EN order\cite{3} as the primary order parameter. Subsequent ARPES\cite{1} and STM\cite{5} studies performed significantly above $T_s, T_N$ provide additional support for such a view. Careful elastic studies\cite{6} on Co-doped BaFe$_2$As$_2$ strongly suggest that SC peaks at a hitherto enigmatic quantum critical point, identified as the $T = 0$ endpoint of the orthorhombic-tetragonal (O-T) structural transition. A remarkable finding is the close analogy between the $T - x$ phase diagram with the $T - P$ phase diagrams in $f$-electron systems\cite{7} exhibiting Kondo-destroying QCP at the border of AFM: in particular, the lattice coherence scale ($T_{\text{max}}$) vanishes and the effective mass ($m^*$) diverges precisely at the critical doping ($x_{\text{QCP}}$) where SC maximizes. The Fermi surface reconstruction that this implies is also consistent with a dHvA study for SrFe$_2$P$_2$\cite{8,9}. Earlier corroborating evidence for a QCP, tacitly assumed to be an AF-QCP based on a weak-correlation analysis, is also provided by transport and NMR\cite{10}, and by electronic Raman scattering\cite{11} data.

Both orbital-driven and spin-driven nematic orders have been proposed as the primary order parameter of the normal phase. However, distinguishing between these views in FeAs systems is complicated by the close proximity of structural (related to $T_s, T_c$) and AFM transitions ($T_N$): they either occur simultaneously\cite{12} or very close together, with $T_s \geq T_N$ (thus AFM always occurs in the orthorhombic phase). It is impossible to distinguish between them on purely symmetry grounds: both views involve breaking of the same (discrete rotational) $C_{4v}$ symmetry. While more tests are needed to resolve this issue, a microscopic approach can be very useful here.

Motivated thus, we undertake a joint theoretical-experimental study to illuminate these issues. We adopt a strong-correlation perspective constrained by the above observations. We perform dynamical mean field theory (DMFT) calculations on a multiband Hubbard model with first-principles bandstructures for the 122-iron arsenides. Experimentally, we focus on transport anisotropy in SrFe$_{2-x}$Co$_x$As$_2$ (Sr-Co-122) as the system is tuned through a simultaneous O-T and magnetic transitions at $T(x_{\text{QCP}}) \to 0$ (both of which coincide with each other here, in contrast to BaFe$_{2-x}$Co$_x$As$_2$, where structural criticality precedes the AF one). Wherever applicable, we also analyze extant results for BaFe$_{2-x}$Co$_x$As$_2$ in this picture. Our main finding is an onset of an orbital selective Mott transition (OSMT) near optimal doping, signaled by the appearance of a pole...
FIG. 1. (Color online) Measurements showing the variation of resistivity along the orthogonal $a$ and $b$ directions, with temperature, for various Co dopings. For the undoped SrFe$_2$As$_2$, although the resistivities are different along the two directions below the SDW transition, they are both still metallic. With doping the transition is shifted to lower temperatures and vanishes beyond a doping of 8.1 %, whereas superconductivity appears around 7.6 %. The resistivity along the $b$ direction shows an insulating temperature dependence for intermediate dopings. See SI for details of theoretical analysis.

Experimental details: We use single crystals of Sr-Co-122 grown from FeAs self-flux to study the evolution of transport anisotropy (see Supplemental Information (SI)) similar to experiments by Chu et al. [3]. The $T$-dependence of $\rho_a$ and $\rho_b$ for six Co dopings is shown in Fig. 1. From resistivity data we construct a phase diagram (see Fig. 2), where we show the resistivity anisotropy $\rho_b/\rho_a$ as a function of $T$ and doping $x$.

Several features stand out: (i) the resistivity anisotropy $\delta \rho = (\rho_b/\rho_a) > 0$ is in the opposite direction to the lattice anisotropy $b/a - 1 < 0$, (ii) $\delta \rho$ evolves non-monotonically, peaking in the vicinity of 6% doping and disappearing beyond 8% doping (i.e.) close to $x_{QCP}$. (iii) $\delta \rho$ acquires a finite value significantly above $T_a, T_N$, in accord with earlier finding, and (iv) anomalous transport (bad-metallic $\rho_{a,b}(T) \simeq 0.25$ ohm-cm at low $T$ even for $x = 0$) is enhanced with doping, with $\rho_b(T, x)$ even showing insulator-like $T$-dependence below 120 – 150 K, depending on $x$, while $\rho_a(T)$ exhibits enhanced bad-metallicity. This trend is quite intriguing, as a naive expectation mandates enhanced (“good”) metallicity upon doping.

Taken together with earlier data for BaFe$_{2-x}$Co$_x$As$_2$, the intriguing features are indicative of an unusual QCP involving electronic nematic (EN) order, situated around $x_{QCP}$ where SC is maximized. However, the insulating temperature-dependence of $\rho_b$ also indicates an orbital-selective Mott transition (of electronic states contributing to $\rho_b$) at work, and the loss of both these features in the overdoped regime suggests localization physics in a possible EN QCP scenario. We posit that this localization is not a disorder effect but rather an indicator of an OSMT, a view supported by recent analysis that finds transport anisotropy to be an intrinsic feature of the renormalized electronic structure [13]. In addition, criticality associated with divergence of the nematic susceptibility shows “clean” critical exponents [14], suggesting irrelevance of disorder. While a correct sign of $\delta \rho$ can apparently be rationalized within both spin-nematic [15] and ferro-orbital EN [16] scenarios, the insulator-like behavior of $\rho_b(T)$ over a wide range of $x$ can be very naturally understood from an OSMT view. Given that a unified view of the data suggests an intrinsic band- (orbital) selective localization tendency at work [2] [15], we consider this possibility in more detail as well as its ramifications for an EN QCP scenario in 122-FeAs systems. We note that the even more strongly correlated features visible in FeSe$_{1-x}$Te$_x$ [18] also make it a good candidate for our proposal.
Theoretical microscopic treatment: To substantiate the link between OSMT and an electronic nematic QCP, we have performed first-principles LDA+DMFT calculations following earlier work by two of us [19]. The five- $d$ bands of Fe, computed by the LMTO method, were used as inputs in a multi-orbital DMFT formalism. The multi-orbital iterated perturbation theory (MO-IPT) was used as an impurity solver in DMFT: though not exact, it is a computationally fast and effective solver, and has been shown to work quantitatively in a variety of contexts [19-21]. We chose $U = 4.5\ eV$, $J_H = 0.7\ eV$ and $U' \simeq (U - 2J_H)$ as interaction parameters for the 5-band Hubbard model, in accord with values extracted from screened LDA+GW estimates [17]. As in earlier work [22], ferro-orbital order (FOO) and EN arise via residual intersite and inter-orbital two-particle interactions in the incoherent “normal” state found in DMFT calculations.

Fig. 3 and Fig. 4 clearly mark out the OSMT in our LDA+DMFT calculations. Im$\Sigma_x(\omega)$ with $a = xz, yz$ in Fig. 3 clearly testify to this as a sharp pole in Im$\Sigma_x(\omega = E_F)$. However, Im$\Sigma_y(\omega)$ reveals bad-metallicity for all $x$: an evident fingerprint of the OSMT. The OSMT directly implies insulator-like resistivity along $b$. In Fig. 4 we show the calculated resistivities along $a, b$, computed from the full DMFT Green functions at finite-$T$. The $T$ and $x$-dependence of the calculated resistivity is in very good qualitative agreement with resistivity data in Figs. 1 and 2. In particular, (i) at $x = 0$, bad metallic resistivity at low $T$ and maximal anisotropy at $T_s$ persists above $T_s$, as found before [22], and (ii) $\delta \rho$ increases at low $T$ as $x$ increases. $\rho_0(T)$ shows insulator features, even as $\rho_a(T)$ shows enhanced bad-metallic conductivity, in full accord with data, and (iii) $\delta \rho > 0$ for $x > x_c \simeq 0.1$, where we define $x = (6+n)/5$ [23] reflecting gradual disappearance of the EN state and transport anisotropy: this compares favorably with $x_{QCP} \simeq 0.11$. In the Supplemental Information, we present additional evidence for an insulating normal state for the $b$ direction and a superconductor-insulator transition driven by phase fluctuations based on a Halperin-Nelson fit of the resistivity data of Fig. 2.

Along with recent diamagnetism study [24], this supports an OSMT picture, since phase fluctuations are expected to be implicated in inter-orbital, intersite pairing (involving $xz, yz$ states) once partial Mott localization of $xz$-states occurs.

Landau-Ginzburg-Wilson phenomenology: The existence of the putative electron-nematic QCP, now linked to an OSMT, at $x_{QCP}$ corresponding to maximum $T_c$, naturally leads us to ask: What role do these coupled criticalities play in near-optimally doped Fe-arsenides? Since both electronic nematicity and superconducting instabilities result from the same residual interaction, how do we describe the competition between the two phases?

Clearer physical insight into these issues is gained by constructing a Landau-Ginzburg-Wilson (LGW) functional for the competing “normal”-SC and “normal” metal-EN metal transitions. In contrast to earlier attempts [25, 26], a novel feature of our phenomenology is that LGW parameters for different $x$ are computed from the LDA+DMFT incoherent spectral functions (see Supplemental Information) rather than from LDA [27]. The OSMT in the $xz$ sector corresponds to a pocket-vanishing Lifshitz transition with consequent ferro-orbital and electronic nematic instabilities (for which ARPES evidence indeed exists), whence we define the EN order parameter $N = \frac{n_{xz} - n_{yz}}{2(n_{yz} + n_{xz})}$, with the free energy expansion [27].
\[ F_{EN}[N] = aN + b_\mu N^2 + c_\mu N^3 + d_\mu N^4. \]

Here, following Yamaji \textit{et al.}, the suffix \( \mu = p \) refers to the case where there is no selective-Mott transition (and associated spontaneous breaking of four-fold rotational symmetry) in the \( xx \) orbital and \( \mu = m \) refers to the symmetry-broken phase \( (N < 0) \) brought about by the opening of a Mott gap and vanishing of the \( xx \) pocket across the pocket vanishing Lifshitz point. Since spontaneous symmetry breaking is only on the \( N < 0 \) side, we assume \( b_\mu, c_\mu, d_\mu > 0 \). On the \( N < 0 \) side, \( b_m \) can change sign. Thus \( F[N] \) is not a usual LGW functional since the coefficients are non-analytic. We incorporate Jahn-Teller orbital-lattice coupling and/or uniaxial strain through the renormalization \( b_m \to (b_m - g^2/K) \) (see S.I.).

Introducing now the superconducting (SC) free energy, \( F_S[\Psi] = \alpha|\Psi|^2 + \beta|\Psi|^4 \), and the superconductor-EN coupling \( F_{NS}[N, \Psi] = uN^2|\Psi|^2 \), \((u > 0)\) the total free energy is \( F = F_{EN} + F_S + F_{NS} \). Microscopically, \( F_{NS} \) arises from a mean-field decoupling of the intersite residual interactions with coupled charge-orbital-spin character \cite{10}. For weak coupling of EN and SC order parameters, \( u^2 < 4\beta d_m \), the mean-field phase diagram consists of four phases: (i) disordered, \( \Psi = N = 0 \), (ii) EN, \( \Psi = 0, N \neq 0 \), (iii) SC, \( \Psi \neq 0, N = 0 \), and (iv) coexisting \( \Psi \neq 0, N \neq 0 \). Experimental observation of coexistence of EN and SC phases in underdoped samples would imply a small-\( u \) regime in the iron pnictides. For larger \( u \), the coexistence phase is preempted by a first order line separating the EN and SC phases, which is not seen in experiment. The phase diagram in the \( \alpha - b_m \) plane with \( c_m > 0 \), (the sign calculated from DMFT) is shown in Fig. 5 and details of the mean-field analysis are in the Supp. Information.

The sign of \( c_m \) has a significant effect on the nature of phase transitions in our model. For \( c_m < 0 \), one would have a line of Lifshitz transitions at \( b_m = 0 \) in the absence of SC and \( b_m = b_m - u_4/2\beta = 0 \) in its presence. However, for \( c_m > 0 \) that we find in our calculations, a first order transition (line \( NOBXA \) in Fig. 5) preempts the Lifshitz transition (line \( N'O'B'X'A' \)) which is also the limit of metastability. The first-order character of the disordered-EN transition drives an electronically phase-separated (EPS) state, that one finds in the case of the pnictides. Electronic phase separation is generally expected in the region between the phase transition and limit of metastability (see for e.g. Ref. \cite{28}). We find \( c_m > 0(x < x_L) \) and \( c_m < 0(x \geq x_L) \) from LDA+DMFT calculations (\( x_L \) is the value of doping \( x \) at which the OSMT takes place), which implies that only underdoped samples should exhibit EPS. This finding is supported by STM studies on underdoped CaFe\(_2\)As\(_2\)P\(_x\) \cite{29}.

We identify \( x_{QCP} \) (the doping corresponding to extrapolation of the line of nematic transition to \( T = 0 \)) in experiment with \( x_L \), the marginal quantum critical endpoint of the first-order line of the OSMT. Turning to finite-\( T \), we assume \( b_m = b_0(T - T^*(x)) \), in the mean-field spirit, where \( T^*(x) = T'(x_L - x) + O(x_L - x)^2 \). Firstly, this implies a divergent charge nematic susceptibility, \( \kappa(x) \propto b_m^{-1}(x, T) = 1/b_0(T - T^*(x)) \) (i.e. the critical exponent, \( \gamma = 1 \)) as the Lifshitz point is approached from the disordered state. Such a “Curie-Weiss” behavior has indeed been observed in strain response \cite{14} and Raman \cite{11} data. Secondly, the coupling of the nematic order to lattice strain will shift \( T_s \) above \( T^* \) (see Ref. \cite{13}). The divergence of \( \chi_{nem} \) in Raman data at \( T^* < T_s \) can be explained by this picture given that the Raman study unveils the intrinsic, strain-free nematic scale. We note that in this picture, the shift between \( T^*, T_s \) is a consequence of coupling of strain to an \textit{intrinsic} EN state (“zeeman” field on an Ising-like orbital nematic), and does not necessarily require that additional (spin nematic) mechanisms are needed. It must be emphasized, though, that onset of orbital nematicity will induce a spin-nematic purely on symmetry grounds. While both states break the same \( C_{4v} \), lattice rotational symmetry of the \( T \)-phase, an OSMT-induced EN state can naturally account for the data unlike extant spin-nematic scenarios. Our LDA+DMFT+LGW analysis explains a broad set of experimental observations and unearths the hitherto unidentified link between soft quasi-local and dualistic electronic fluctuations. Their combined occurrence at the EN-QCP is identified as a consequence of an underlying marginal quantum critical point at a Lifshitz transition, now associated with an OSMT.
Our theory naturally accounts for a range of additional unusual responses in the best-studied 122-FeAs systems. In the selective-Mott view, vanishing of a FS (now justified ipso facto from selective-Mottness induced local moments) with $J_{1a} < J_{1b}$ and $J_2 > J_{1b}/2$ \cite{H. Shishido, A. F. Bangura, A. I. Coldia, S. Tonegawa, K. Hashimoto, S. Kasahara, P. M. C. Rourke}, $H. Ikedaa, T. Terashimaa, R. Settaie, et al., Phys. Rev. Lett. 104, 057008 (2010).

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I. MEAN-FIELD ANALYSIS OF THE LGW FREE ENERGY

Consider the free energy $F = F_{EN} + F_S + ...$ associated with $\delta F/\delta N = 0$ and $\delta F/\delta \Psi = 0$. The mean field equations are

$$\alpha\Psi + 2\beta|\Psi|^2\Psi + u\Psi N^2 = 0,$$

(1)

$$a + 2(b_m + u|\Psi|^2)N + 3c_m N^2 + 4d_m N^3 = 0, \quad (N \leq 0).$$

(2)

In the following analysis we set the “Zeeman” field $a = 0$ without loss of generality. Let us first discuss the case where the superconducting order parameter is zero. Now if $c_m < 0$ (which is the case discussed in Ref. [1]), we can drop the stabilizing term $d_m N^4$. For this case, straightforward analysis (see Ref. [1]) now shows that a line of first-order transitions (for $a < 0$, $b_m < 0$, where $N$ jumps discontinuously) ends at a marginal quantum critical end-point (M-QCEP) ($a = 0 = b_m$), beyond which ($b_m > 0$) only a smooth crossover is obtained. If $c_m > 0$, the stabilizing term $d_m$ is needed and the phase diagram differs from the $c_m < 0$ case. The key difference is that a first order transition to the EN phase is possible even as $b_m > 0$. This transition takes place at $b_m = c_m^2/4d_m > 0$ where the compressibility diverges, indicating anomalously soft electronic fluctuations associated with the M-QCEP of the line of first-order transitions associated with EN order. The first order transition thus intervenes before the M-QCEP ($b_m = 0$) can be reached. However, if the first order transition is weak, proximity to the M-QCEP will still be reflected in the physical properties. In practice, this proximity is unearthed by strain-tuning as done by Fisher et al.

Consider now the coexistence phase, $\Psi \neq 0$ and $N \neq 0$. We eliminate $|\Psi|^2$ from the free energy using the mean-field solution for $|\Psi|^2$ and get

$$F[N] = \tilde{b}_m N^2 + c_m N^3 + \tilde{d}_m N^4 - \frac{\alpha^2}{4\beta}$$

(3)

where $\tilde{b}_m = b_m - u\alpha/2\beta$ and $\tilde{d}_m = d_m - u^2/4\beta$. For stability of this phase, we need $\tilde{d}_m > 0$. The non-trivial solution for $N_{ml} < 0$ is

$$N_{ml} = \frac{3c_m - \sqrt{9c_m^2 - 32\tilde{d}_m \tilde{b}_m}}{8\tilde{d}_m}.$$

(4)

This need not be the solution with the lowest free energy. However once $\tilde{b}_m$ is small enough such that $F[N_{ml}] = 0$, we get a first order transition to the coexistence phase. To find where this occurs, we note that we are essentially looking for the condition for coincident nonzero roots of Eq.3. This gives us the condition

$$c_m^2 = 4b_m \tilde{d}_m$$

(5)

for the (first order) boundary of the coexistence phase and the disordered phase.

A. Free-energy Functional from LDA+DMFT Results

Here, we present details of the calculations resulting in the free-energy functional, $F(N)$, from LDA+DMFT results for the “normal” quantum paramagnetic (incoherent) metal to the EN phase transition in the main text.

Our starting point is earlier LDA+DMFT calculations on a five-orbital Hubbard model, performed by two of the authors [2]. There, a sizeably correlated limit of the five-band model was shown to give a good quantitative accord with a range of one- and two-particle responses in the “normal” state without any symmetry breaking, as well as with key features in both SC [2] and (orbital) electronic nematic (EN) [3] states. The sizably correlated view is also supported by other first-principles approaches [4] and underlies the frustrated Heisenberg model approaches [5] to magnetism in Fe arsenides.

We start by observing that EN order and associated (local) dynamical fluctuations can be incorporated into the DMFT ideology as described elsewhere [3]. The crucial point to appreciate is that this is tied to fermio-orbital order and the structural instability as a result of removal of $d_{xz,yz}$ orbital degeneracy of the tetragonal (T) phase. The upshot is that coupling to a Jahn-Teller or a uniaxial strain term, $\lambda \sum_i Q_i (n_{i,xz} - n_{i,yz})$ (spin indices are suppressed) now lowers the $d_{xz}$ band by $\lambda Q_i$ and raises the $d_{yz}$ band by the same amount. This mechanism thus offers a simple way of visualising the relative shift of the $d_{xz,yz}$ bands needed to achieve consistency with the ARPES FS well above $T_s, T_N$, and it is important to emphasise that it is intimately linked to ferro orbital order and resultant (orbital) nematicity. It is also precisely this coupling which results in terms odd in $N$ in the LGW free energy used in the main text.

Using the DMFT local spectral functions of the five-band Hubbard model, we determined the coefficients $d_{L,\pm}^{0}$ and $d_{L,\pm}^{(1)}$ needed to compute the co-efficients in $F(N)$ by following Yamaji et al. [1] and linearising the DMFT spectra around $E_F$ at and away from the Lifshitz point. Since the EN instability is primarily associated with FOO and lifting of the $d_{xz,yz}$ orbital degeneracy, we used only the DMFT results for the $xz, yz$ bands,
computed from the full five-orbital problem. The relevant formulae are similar to those appearing in Yamaji et al. [1].

The resulting $a, b_{ij}, c_{ij}$ are used in the Lifshitz free energy (Eq.(1)) in the main text and used to derive the main conclusions of the first part in this work. We emphasise that this procedure yields non-analytic co-efficients used in Eq.(1), and, in contrast to pure phenomenological works, are now derived from the correlated electronic structure (DMFT) input. In another crucial difference with other phenomenological approaches, the non-analytic co-efficients used in the LGW expansion are a non-trivial consequence of the underlying selective-Mott physics found in LDA+DMFT.

\[ H_{J-T} = \sum_i Q_i (n_{i,zz} - n_{i,zz}) \approx \lambda \sum_i Q_i N_i \] (6)

In the planar geometry of the FeAs systems, $Q_i$ is related to the orthorhombicity, $O = b_{i,j} - b_{j,i}$ (where $a_{ij}$ are unit cell lattice constants). In the LGW functional, the orbital-lattice coupling thus induces an extra term $\lambda (Q_i) N_i$, where $(Q_i)$ is determined by minimising

\[ H_{\text{el}} = H_{\text{JT}} + H_{\text{lat}} = \lambda Q N + K Q^2 / 2 \] (7)

with respect to $Q$. Here, $K$ an effective “spring constant” related to the details of the phonon spectrum. This yields $Q = (-\lambda/K) N$, and resubstituting this into $H_{J-T}$ yields the extra term $(-\lambda^2/K) N^2$ which renormalises $b \to (b - \lambda^2/K)$ as stated in the main text. The importance of this effect is seen from the fact that $b$ can now change sign, as is needed to derive a line of first-order (now nematic-plus-structural) transitions separated from the region of a smooth crossover by a quantum critical end-point where the exotic marginal quantum criticality obtains.

A. Landau-Ginzburg Theory with Strain-nematic coupling

In this section, we detail the finite-$T$ GL theory for orbital-nematic order coupled to strain, to simulate the actual physical situation in experimental studies. More specifically, we couple the free energy for the pocket-vanishing Lifshitz transition,

\[ F[N] = \frac{b_2}{2} N^2 + \frac{c_3}{3} N^3 + \frac{d_4}{4} N^4 \] (8)

to the strain part, written as

\[ F(\epsilon) = \frac{\alpha}{2} \epsilon^2 + \frac{\beta}{4} \epsilon^4 \] (9)

by a coupling term, $F_{\text{coup}} = -\lambda \epsilon N$. In the presence of external stress, we follow earlier work [6] and differentiate $F = F[N] + F[\epsilon] + F_{\text{coup}}$ with respect to both $N$ and $\epsilon$ to get

\[ \frac{dN}{d\epsilon} = \frac{\lambda}{(b_m - \lambda^2/\alpha) + 2c_m N + 3d_m N^2} \] (10)

Then, in the limit $\lambda \to 0$ (zero-stress limit), $\delta N \to 0$, and we get

\[ \frac{dN}{d\epsilon} = \frac{\lambda}{b_m - \lambda^2/\alpha} \] (11)

Thus, in presence of strain the nematic susceptibility diverges at $b_m = \lambda^2/\alpha$. Also, above the structural transition, we can neglect terms $O(N^3)$, to get $N = \frac{\lambda}{b_m - \lambda^2/\alpha} \epsilon$. Finally, in our mean-field picture of the transition, we assume that $b_m$ has the usual $T$-dependence, i.e., that $b_m(T, x) = b_0(T - T^*(x))$, with $T^*(x) \approx T^*(x_L - x) + O(x_L - x)^2$. At $T = 0$, the $x$-dependence comes from LDA+DMFT results as discussed before.

Thus, the finite-$T$ nematic susceptibility is now

\[ \frac{dN}{d\epsilon} = \frac{\lambda}{(b_m(T, x) - \lambda^2/\alpha) + 2c_m N + 3d_m N^2} \] (12)

whence it follows that finite $N, \epsilon$ occur simultaneously at a renormalized temperature, $T_s = T^* + \frac{\lambda^2}{b_m} > T^*$. The intrinsic nematic mean-field transition scale is thus lower than that at which the structural transition occurs (at $T_s$). Physically, this arises because strain acts as a conjugate field to the nematic order parameter, and so enhances intrinsic nematicity. It also offers a natural explanation of the shift between the structural transition temperature ($T_s$) and the temperature where resistivity anisotropy is maximum in the normal state, as seen from the $T - x$ phase diagram. It is also consistent with the fact that, in electronic Raman scattering data [7], the extrapolated charge susceptibility diverges at a $T = T^*$ lower than $T_s$: this is now simply because there is no strain effect in Raman studies, which may consequently be unearthing the intrinsic $T^{*} = T_{nem}$. Finally, it is also
the reason for apparently different conclusions in literature, where measurements under strain-tuning find that the EN phase persists into the overdoped region in the $T-x$ phase diagram: strain stabilizes EN order but washes out nematic (quantum) criticality, while Raman measurements, not carried out under strain, reveal the intrinsic nematic scale $T_{nem}$.

III. MEASUREMENT OF TRANSPORT ANISOTROPY USING CLAMP CELL

Single crystals of $\text{SrFe}_2\text{As}_2$ were grown using self flux growth method. Crystals of dimensions of approximately 3 mm x 4 mm x 1 mm were obtained. The crystals grow naturally with the flat surface of the crystal perpendicular to the tetragonal $c$-axis. The crystals were cleaved, annealed and checked for single domain using Laue. The orthorhombic unit cell is rotated by 45° with respect to the tetragonal unit cell. The crystal was oriented and parallel cuts were made perpendicular to the [110] tetragonal direction so that a rectangular shaped crystal was obtained. A clamp capable of providing uniaxial pressure was designed for the purpose of detwinning. The clamp was made of lysol and had brass screws with a stainless steel spring which provided a force of 20 N when completely compressed, which resulted in a force of 1.75 N per pitch of the screw. This translated to a pressure of about 5-10 Mpa on the sample which was placed carefully between the front two pieces of the clamp assembly. Four probe contacts were made using 50 micron gold wire. Circuitworks CW2400 was used for making the initial contact and was heat treated for better mechanical strength. Epolead 4929 silver epoxy was then used for making good electrical connection. The contact resistance was around 2 ohms. A continuous flow cryostat was used to do the resistance measurements. An ac signal source of frequency 77 Hz supplied a current of 50 microAmps and the voltage was measured using a Princeton Instruments E G & G Lock-In Amplifier. Magneto-resistance measurements were done on electron doped crystals in a 15T magnet supplied by Oxford Instruments.

Resistivity measurements were done on first on the twinned crystal which measured $R_{Tw} = \frac{2a_1+2b_1}{3}$. Subsequently, pressure was applied using the clamps and resistance was measured again which gave $\rho_a$. The anisotropy defined as $(\frac{\rho_b}{\rho_a} - 1)$ was obtained from these two measurements.

IV. HALPERIN-NELSON FITS FOR THE RESISTIVITY DATA ALONG THE INSULATING b DIRECTION

The actual resistivity data near optimal doping is sensitive to superconducting fluctuation effects, and $\rho_b$ does not, at first sight, appear to follow an Arrhenius law we expect from a Mott insulator. This is indeed the case at intermediate $T$, but at lower $T$, this gives way to a form characteristic of strong superconducting fluctuations. To separate the effect of superconducting fluctuations, we have fitted the resistivity data near $T_c$ (see Fig. 1) to the well-known Halpern-Nelson interpolation formula, $R_N = \frac{R}{1+\frac{t}{\xi_0^2}+1} = \frac{1}{1+\frac{t}{\xi_0^2}+1}$, where $\xi_0 = \alpha \sinh \frac{t}{\sqrt{4t}}$ and $R_N \sim \exp(\Delta/T)$. Here, $t = T-T_0$ while $a$, $b$ and $\Delta$ are fitting parameters. The Halpern-Nelson behavior in the normal state and the Kosterlitz-Thouless like behavior near $T_c$ is typically seen in a superconductor-insulator transition driven by phase fluctuations. Together with recent evidence for precursor diamagnetism [8] in 122-systems, this finding further supports selective-Mottness setting in around $x_{opt}$ as a natural contender for possible quantum criticality. The key point is that from the number-phase uncertainty principle, an OSMT immediately implies a strong phase fluctuation-dominated regime for a subsequent SC instability. Since both $xz, yz$ states are macroscopically implicated in the $s_\pm$ SC pairing, Mott localization of (a subset) $xz$ carriers in the “normal” state must now necessarily implicate large phase fluctuations above $T_c$, precisely as indicated by the HN fit. In addition, we
also find that an external magnetic field leads to a positive magnetoresistance (MR) (enhances the insulator-like $\rho_b$ for all $x < x_{QCP}$), while conventional negative MR is recovered for $x > x_{QCP}$, further supporting the hypothesis of a QCEP associated with OSMT around $x_{QCP}$.

Without any additional assumptions, OSMT also stabilizes FOO and associated EN by enhancing (reducing) $n_{xz}(n_{yz})$ relative to their para-orbital values. Thus, the EN QCP is intimately tied down to the OSMT, and is thus expected to have an underlying Mott-like criticality.

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