Settling the Chicken and Egg question in iron based superconductors

Divergent nematic susceptibility in an iron arsenide superconductor

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Measurement of the elastoresistivity coefficients of the underdoped iron-arsenide $Ba(Fe_{0.975}Co_{0.025})_2As_2$

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Nematic susceptibility of hole- and electron-doped $BaFe_2As_2$ *iron-based superconductors*

Authors: A. E. Böhmer, P. Burger, F. Hardy, T. Wolf, P. Schweiss, R. Fromknecht, M. Reinecker, W. Schranz, C. Meingast, arXiv:1305.3515.

Recommended with a Commentary by Jörg Schmalian, Karlsruhe Institute of Technology

Superconductivity in the iron based systems occurs in regions of the phase-diagram that are near two phase-transitions: a structural transformation at T_0 and transition to an antiferromagnetic phase at $T_N \leq T_0$. While the former hints at an important role of the electron-phonon interaction, similar to the A-15 compounds and numerous element superconductors under pressure, the latter is more akin to what is seen in heavy electron superconductors, copper oxides, or organic charge transfer salts. Both phase-transformations occur as function of temperature, pressure or chemical composition near each other (frequently within a few degrees, while $T_0 = 134.5$K for $BaFe_2As_2$). This is strong evidence for the fact that both transitions are closely related. The vicinity of magnetic and structural order does, however, not explain whether the new crystal structure is causing the electronic order or is a consequence of a magnetic / electronic mechanism. Since the structural phase transition occurs at a slightly higher temperatures than the magnetic transition, it is tempting to conclude that fluctuations of the lattice are primary.

At first glance, it seems not even clear whether the question to search for the primary and for the secondary order parameter is well defined. The structural order parameter in the iron pnictides is the shear strain $\varepsilon_6 = 2\varepsilon_{xy}$ that behaves like a scalar order parameter. One

expects a symmetric bi-linear coupling of ε_6 to electronic degrees of freedom, characterized by an order parameter φ that transforms the same way as ε_6:

$$H_c = -\lambda \int d^d x \varepsilon_6(x)\, \varphi(x)\,. \tag{1}$$

Several proposals for the order parameter φ exist. It could be an orbital polarization (i.e. the difference in the occupation of Fe-3d$_{xz}$ and Fe-3d$_{yz}$ states) or of magnetic origin (the relative orientation of neighboring Fe-spins). In both cases φ behaves like a discrete, Ising-like variable. The chicken-and-egg question is to judge whether ε_6 or the electronic (nematic) order parameter φ is primary.

Chu *et al.* performed a measurement of a generalized nematic susceptibility (see below) analyzing the proper thermodynamic variables and concluded that the driving force of the structural instability is indeed electronic and that the structural order is secondary and induced. Their finding implies that a phase transition would occur even in the limit of a perfectly rigid lattice. The result is confirmed by Kuo *et al.* who analyze the tensor of the elastoresistivity coefficients and demonstrate that a rotational symmetry is broken at T_0, hence the name *nematic*. Finally, Böhmer *et al.* utilize the coupling in Eq.(1) and measure the nematic susceptibility in electron and hole doped systems, finding nematic quantum-criticality in the former.

Let us assume that φ is the dominant order parameter and responsible for the transition, while ε_6 is induced and secondary. In the absence of the coupling of Eq.(1), let ε_6 be characterized by a bare elastic constant C_{66}^0. If we include two external fields h and σ that couple to φ and ε respectively, the two order parameter susceptibilities are

$$\chi_\varphi = -\frac{\delta^2 F}{\delta h^2} \text{ and } \chi_\varepsilon = -\frac{\delta^2 \mathrm{F}}{\delta \sigma^2}. \tag{2}$$

If indeed ε_6 is secondary one obtains for the equation of state $C_{66}^0 \langle \varepsilon_6 \rangle = -\sigma + \lambda \langle \varphi \rangle$ and it follows that the two susceptibilities are related:

$$\chi_\varepsilon = C_0^{-1} + \frac{\lambda^2}{C_0^2} \chi_\varphi. \tag{3}$$

A diverging χ_φ induces a divergence of χ_ε. χ_ε^{-1} is the elastic modulus C_{66} that includes the nemato-elastic coupling Eq.(1). C_{66} was measured by Böhmer *et al.*. Using Eq.(3) they conclude that the nematic susceptibility $\chi_\varphi(T \to 0)$ diverges in the electron doped system $\mathrm{Ba}(\mathrm{Fe}_{1-x}\mathrm{Co}_x)_2\mathrm{As}_2$ at a quantum critical point, precisely where the superconducting

transition temperature is largest. In contrast, for the hole doped systems $Ba_{1-x}K_xFe_2As_2$ χ_φ grows to large values, yet does not diverge. The origin of this avoided criticality and its relation to superconductivity is unclear at the moment, yet fluctuation driven first order transitions have been predicted for the magnetic scenarios for φ. Eq.(3) again suggests that it is hard to disentangle the driving force of the transition from the induced order and fluctuations.

How to decide which degree of freedom is primary was shown by Chu *et al.* The crucial idea is to perform a Legendre transformation from the free energy $F(\sigma, h)$ to either $G(\varepsilon, h) = F + \sigma\epsilon$ or $H(\sigma, \varphi) = F + h\varphi$ and to compare the mixed derivatives

$$\widetilde{\chi}_\varphi(\varepsilon, h) = -\frac{\delta^2 G(\varepsilon, h)}{\delta\varepsilon\delta h} \text{ and } \widetilde{\chi}_\varepsilon(\varphi, \sigma) = -\frac{\delta^2 \mathrm{H}(\varphi, \sigma)}{\delta\varphi\delta\sigma}. \tag{4}$$

One finds from the above equation of state that the generalized nematic susceptibility $\widetilde{\chi}_\varphi(0,0)$ diverges while $\widetilde{\chi}_\varepsilon(0,0)$ remains constant. If φ is the fluctuating variable, fixing φ, as done in $\widetilde{\chi}_\varepsilon$, will suppress fluctuations and the susceptibility stays finite. In contrast, fixing ε, as done in $\widetilde{\chi}_\varphi$ may change the location of the transition, but will not change the fact that the system is fluctuating. In case where strain would be the primary order parameter the behavior of $\widetilde{\chi}_\varepsilon$ and $\widetilde{\chi}_\varphi$ is inverted. Chu *et al.* measured $\widetilde{\chi}_\varphi$ by varying the external strain and performed the Legendre transformation explicitly by plotting the induced anisotropy of the resistivity (as measure of φ) as function of strain ε_6. The so-obtained susceptibility $\widetilde{\chi}_\varphi$ does indeed diverge.

Going even further, Kuo *et al.* systematically controlled the strain using strain gauges glued to the surface of a piezoelectric stack and varied the strain by gluing samples with different orientations to the stack. This allowed for the determination of the elastoresistivity coefficients m_{ij} defined as:

$$(\triangle\rho/\rho)_i = \sum_{j=1}^{6} m_{ij}\varepsilon_j. \tag{5}$$

Here the forth rank tensor m_{ij} is expressed as usual in terms of a symmetric 6×6 matrix. Kuo *et al.* confirmed the finding by Chu *et al.*. In addition they demonstrate that the symmetry of the transition is fully consistent with an underlying Ising order parameter that describes two-fold symmetry in the low temperature phase. In particular it was shown that $m_{66} \propto \widetilde{\chi}_\varphi$.

The microscopic origin of φ is not settled by these experiments. However they demonstrate that such an electronic order parameter exists, that it is the primary degree of freedom,

and that it is closely tied to low temperature quantum fluctuations in the regime where superconductivity is largest. The beauty is that "simple" thermodynamic variables revealed the electronic origin of the structural distortion and utilized the coupling to the lattice to demonstrate that nematic quantum criticality is present in some iron based systems.