Journal Club for Condensed Matter Physics DOI:10.36471/JCCM_June_2024_02
https://www.condmatjclub.org

Spin fluctuations in the passenger seat?

1. **Pure nematic quantum critical point accompanied by a superconducting dome.**
   Authors: K. Ishida, Y. Onishi, M. Tsujii, K. Mukasa, M. Qiu, M. Saito, Y. Sugimura, K. Matsuura, Y. Mizukami, K. Hashimoto, and T. Shibauchi
   PNAS 119 (18) e2110501119 (2022)

2. **Lifting of gap nodes by disorder in ultranodal superconductor candidate $\mathbf{FeSe_{1-x}S_x}$.**
   Authors: T. Nagashima, K. Ishihara, K. Imamura, M. Kobayashi, M. Roppongi, K. Matsuura, Y. Mizukami, R. Grasset, M. Konczykowski, K. Hashimoto, T. Shibauchi
   arXiv:2405.06320

3. **Superconductivity Mediated by Nematic Fluctuations in Tetragonal $\mathbf{FeSe_{1-x}S_x}$.**
   Authors: P.K. Nag, K. Scott, V. S. Carvalho, J. K Byland, X. Yang, M. Walker, A. G. Greenberg, P. Klavins, E. Miranda, A. Gozar, V. Taufour, R.M. Fernandes, E. H. da Silva Neto
   arXiv:2403.00615

Recommended with a Commentary by Andrey V Chubukov, School of Physics and Astronomy and FTPI, University of Minnesota

The three experimental papers, which I recommend here, collectively change the perception, shared by many, that an electronic mechanism of superconductivity must involve spin-fluctuations. Ferromagnetic spin fluctuations were long ago suggested as the glue for $p-$wave pairing in 3He, and antiferromagnetic spin fluctuations have been considered as the driving force for $d-$wave superconductivity in optimally doped and overdoped cuprates, and for s^{+-} superconductivity in Fe-pnictides [1]. Pairing by a nominally repulsive spin-mediated electron-electron interaction occurs when a pair hopping from $(k, -k)$ to $k + Q, -k - Q$, where Q is an antiferromagnetic momentum, exceeds a repulsion at small momentum transfer. In this case, a simple analysis shows [1] that superconductivity does develop, but with a sign-changing gap between $\mathbf{k}$ and $\mathbf{k} + \mathbf{Q}$ (this yields d-wave pairing for cuprates, where Q is between patches on the same Fermi surface and s^{+-} pairing for Fe-pnictides, where Q separates hole and electron pockets). For both systems, spin-fluctuation scenario is consistent with, e.g., an observation of a spin resonance peak below T_c (see [2, 3] and references

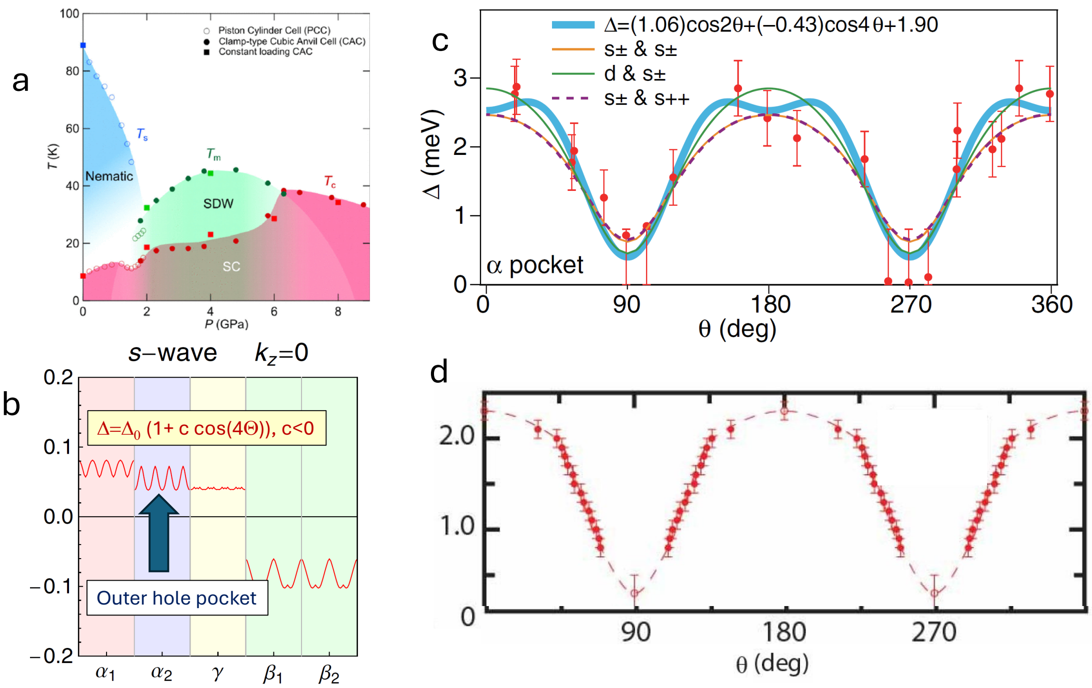

Figure 1: The results for FeSe, consistent with superconductivity due to spin fluctuations. a)P–T phase diagram with the magnetic phase bordering the nematic phase [5]; (b) s^{+-} gap anisotropy within the spin-fluctuation scenario [6]. The gap on the outer hole pocket has maxima at 45^0. (c) and (d) gap anisotropy extracted from ARPES (top) and STM data [7, 8]. This gap anisotropy is in line with (b), after adjusting for co-existence with nematicity.

therein). For Fe-pnictides, a composite spin order, generated by soft antiferromagnetic spin fluctuations, was suggested [4] as the origin of a spontaneous breaking of lattice rotational symmetry (nematicity), which develops there very near the onset of antiferromagnetism.

The situation is somewhat different in bulk Fe-chalcogenide FeSe, which has been extensively studied in the last few years using various techniques [5, 9–12]. This material has a hole pocket, constructed out of d_{xz} and d_{yz} orbitals, and a d_{xz}/d_{yz} (inner) electron pocket, like in Fe-pnictides. Yet, a nematic order in pure FeSe develops at $T_p \sim 90K$, without a magnetic order nearby. This fueled speculations that nematicity in FeSe may be a spontaneous $d-$wave Pomeranchuk order rather than a composite spin order. Still, antiferromagnetism is nearby, as evidenced by its appearance under pressure [5], and the angular dependence of the superconducting gap, extracted from ARPES [7] and STM [8], is consistent with the spin fluctuation scenario (Fig. 1).

The three recommended papers report the results of careful and detailed studies of superconductivity in FeSe doped by S or Te ($FeSe_{1-x}S_x$ and $FeSe_{1-x}Te_x$) near x_c – the end point of the nematic order ($x_c = 0.17$ for S and 0.55 for Te). They all argue that near x_c a spin-mediated interaction is likely not the driving force for superconductivity. Two papers are from the Shibauchi group at the University of Tokyo. The first one (by Ishida et al) presents the results of their measurements of T_c as a function of S and Te doping. They

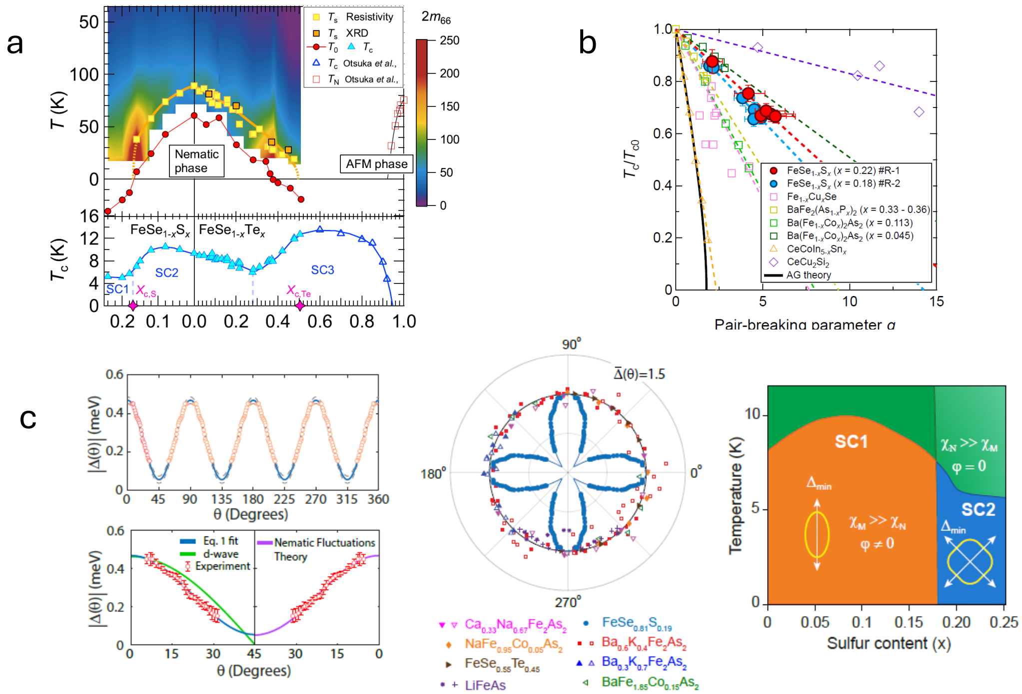

Figure 2: The results for doped FeSe. (a) The phase diagram under S and Te doping with three different superconducting regions (from Paper 1), (b) Behavior of T_c under irradiation (from Paper 2), (c) Gap anisotropy, extracted from STM data for $FeSe_{0.81}S_{0.19}$, and comparison of these data with the earlier ones for pure FeSe and for Fe-pnictides (from Paper 3).

found three regions of superconductivity with different functional forms of $T_c(x)$ (Fig.2a) and clear evidence for a two-dome structure, at least for Te-doping. In the subsequent study [13] these authors extracted T_c in the presence of an applied magnetic field and found a clear tendency towards shrinking of the superconducting regions to two domes, each centered at a finite x. The second paper (by Nagashima et al) presents the results of their study of how superconductivity in $FeSe_{1-x}S_x$ at $x > x_c$ is affected by defects, which they introduced by electron irradiation. I show a representative of their results in Fig.2b. The results still await full interpretation, but they clearly point to the presence of low-lying fermionic excitations both near T_c and deep in the superconducting state. The existence of such excitations is consistent with the observation by the same group [5] of highly unconventional behavior of the specific heat in $FeSe_{0.8}S_{0.2}$ with no jump at T_c and a finite offset of $C(T)/T$ at $T \to 0$, when extrapolated from $T \leq T_c$. This is complimented by STM measurements [14], which show a finite residual density of states below T_c. In the third paper, from the da Silva Neto group at Yale, Nag et al show the angular dependence of the superconducting gap in $FeSe_{0.81}S_{0.19}$, extracted from their STM data. The results show (Fig. 2c) that the gap maxima are shifted by 45^0 compared to pure FeSe. The gap is highly anisotropic and nearly vanishes in some angular range in between the maxima. This angular dependence is much stronger than in Fe-pnictides and in pure FeSe, after adjusting for co-existence with nematicity.

There is more. Recent μSR experiments [15, 16] presented evidence for time-reversal symmetry breaking in doped FeSe. The μSR signal is present below T_c for all x, however in

$FeSe_{1-x}Te_x$ it clearly increases above x_c. This raises a possibility that the superconducting state at $x > x_c$ breaks time-reversal symmetry. Additionally, ARPES measurements of $FeSe_{0.78}S_{0.22}$ with polarized light (Ref. [17]) presented evidence for C_4 symmetry breaking in the nematic state (the superconducting gap has been detected for the polarization of light which covers momenta near the X direction in the 1Fe zone, but no gap has been detected for the polarization selecting momenta near Y).

Where does this leave us? The results of all three recommended papers show that superconductivity near and above the end point of the nematic phase is qualitatively different from that in pure FeSe. Does this imply that spin fluctuations are no longer in the driving seat? There are two arguments that this well may be the case. One comes from the data — the measurements of the phase diagram as a function of pressure [18] show a clear difference between $x = 0$ and $x \approx x_c$. At $x = 0$, a magnetic phase emerges already at small deviations from ambient pressure. At $x \approx x_c$, it emerges only at rather strong pressure and occupies a much smaller portion of the phase diagram. Another argument is theoretical: to obtain spin-mediated superconductivity, the repulsion at momentum transfer Q must exceed the repulsion at small momentum transfer. A nematic order parameter has zero momentum transfer, and near its onset, a repulsion at small momentum transfer gets enhanced, acting against spin-mediated pairing.

There are two theoretical proposals about superconductivity in doped FeSe. One is that the pairing is mediated by nematic fluctuations, in line with the titles of the recommended papers. This proposal has been put forward in Refs. [19, 20], by assuming phenomenologically that the nematic-mediated pairing interaction is attractive. This is not guaranteed, however, because a nematic order develops in a density (charge) channel. In a single band system, the pairing interaction, mediated by charge fluctuations, remains repulsive, like the original Coulomb interaction. It was later argued by K. Islam and me [21] that in a two-orbital/two-band lattice system, the nematic pairing interaction $V(\mathbf{k}, -\mathbf{k}; \mathbf{p}, -\mathbf{p})$ does acquire an attractive component, proportional to the nematic susceptibility and peaked at $\mathbf{k} = \mathbf{p}$. However, the magnitude of the attraction depends on the position of $\mathbf{k}$ on the Fermi surface as $\cos^2 2\theta_k$ This leads to highly unconventional gap function, which above a nematic critical point opens up at T_c only at points $\theta_k = \pi n/2$, $n = 0, 1, 2, 3$, and extends to arcs at smaller T. In between the arcs, the original Fermi surface survives. This is consistent with the gap anisotropy, observed by the da Silva Neto group, and with the absence of the jump of the specific heat at T_c. The other proposal [22] does not specify the pairing mechanism, but explores the idea that the presence of low-lying excitations and reported breaking of the time-reversal symmetry below T_c may imply the existence of a set of zero energy excitations in the superconducting state, dubbed Bogoliubov Fermi surface (BFS) [23]. Recent experiments on doped FeSe from the Shibauchi group, e.g., the recommended paper by T. Nagashima et al, have been interpreted in terms of a BFS.

More detailed analysis is needed to distinguish between the nematic and BFS scenarios, but the three recommended papers clearly point out that superconductivity in doped FeSe is qualitatively different from that in pure FeSe and in Fe-pnictides and requires a novel pairing mechanism, which does not involve spin-fluctuations.

References

[1] D. J. Scalapino, Rev. Mod. Phys. **84**, 1383 (2012).

[2] M. Eschrig, Advances in Physics **55**, 47 (2006).

[3] D. S. Inosov, Comptes Rendus Physique **17**, 60 (2016).

[4] R. M. Fernandes, P. P. Orth, and J. Schmalian, Annual Review of Condensed Matter Physics **10**, 133 (2019).

[5] T. Shibauchi, T. Hanaguri, and Y. Matsuda, Journal of the Physical Society of Japan **89**, 102002 (2020).

[6] S. Graser, A. F. Kemper, T. A. Maier, H.-P. Cheng, P. Hirschfeld, and D. Scalapino, Physical Review B **81**, 214503 (2010).

[7] H. Xu, X. Niu, D. Xu, J. Jiang, Q. Yao, Q. Chen, Q. Song, M. Abdel-Hafiez, D. Chareev, A. Vasiliev, *et al.*, Physical review letters **117**, 157003 (2016).

[8] P. O. Sprau, A. Kostin, A. Kreisel, A. E. Böhmer, V. Taufour, P. C. Canfield, S. Mukherjee, P. J. Hirschfeld, B. M. Andersen, and J. S. Davis, Science **357**, 75 (2017).

[9] A. I. Coldea and M. D. Watson, Annual Review of Condensed Matter Physics **9**, 125 (2018).

[10] A. E. Böhmer and A. Kreisel, J. Phys. Cond. Mat. **30**, 023001 (2017).

[11] Q. Wang, Y. Shen, B. Pan, X. Zhang, K. Ikeuchi, K. Iida, A. Christianson, H. Walker, D. Adroja, M. Abdel-Hafiez, *et al.*, Nature communications **7**, 12182 (2016).

[12] P. Wiecki, K. Rana, A. Böhmer, Y. Lee, S. L. Bud'ko, P. Canfield, and Y. Furukawa, Physical Review B **98**, 020507 (2018).

[13] K. Mukasa, K. Ishida, S. Imajo, M. Qiu, M. Saito, K. Matsuura, Y. Sugimura, S. Liu, Y. Uezono, T. Otsuka, *et al.*, Physical Review X **13**, 011032 (2023).

[14] T. Hanaguri, K. Iwaya, Y. Kohsaka, T. Machida, T. Watashige, S. Kasahara, T. Shibauchi, and Y. Matsuda, Science Advances **4**, 6419 (2018).

[15] K. Matsuura, M. Roppongi, M. Qiu, Q. Sheng, Y. Cai, K. Yamakawa, Z. Guguchia, R. P. Day, K. M. Kojima, A. Damascelli, *et al.*, Proceedings of the National Academy of Sciences **120**, e2208276120 (2023).

[16] M. Roppongi et al, preprint.

[17] T. Nagashima, T. Hashimoto, S. Najafzadeh, S.-i. Ouchi, T. Suzuki, A. Fukushima, S. Kasahara, K. Matsuura, M. Qiu, Y. Mizukami, *et al.*, preprint, https://doi.org/10.21203/rs.3.rs-2224728/v1 (2022).

[18] K. Matsuura, Y. Mizukami, Y. Arai, Y. Sugimura, N. Maejima, A. Machida, T. Watanuki, T. Fukuda, T. Yajima, Z. Hiroi, K. Y. Yip, Y. C. Chan, Q. Niu, S. Hosoi, K. Ishida, K. Mukasa, S. Kasahara, J.-G. Cheng, S. K. Goh, Y. Matsuda, Y. Uwatoko, and T. Shibauchi, Nature Communications **8**, 1143 (2017).

[19] S. Lederer, Y. Schattner, E. Berg, and S. A. Kivelson, Proceedings of the National Academy of Sciences **114**, 4905 (2017).

[20] A. Klein and A. Chubukov, Physical Review B **98**, 220501 (2018).

[21] K. R. Islam and A. Chubukov, npj Quantum Materials **9**, 28 (2024).

[22] C. Setty, S. Bhattacharyya, Y. Cao, A. Kreisel, and P. Hirschfeld, Nature communications **11**, 523 (2020).

[23] D. Agterberg, P. Brydon, and C. Timm, Physical review letters **118**, 127001 (2017).