

# Supplemental Material for Resistive anisotropy due to spin-fluctuation scattering in the nematic phase of iron pnictides

Maxim Breitzkreis,<sup>1,\*</sup> P. M. R. Brydon,<sup>2</sup> and Carsten Timm<sup>1,†</sup>

<sup>1</sup>*Institute of Theoretical Physics, Technische Universität Dresden, 01062 Dresden, Germany*

<sup>2</sup>*Condensed Matter Theory Center, Department of Physics,  
University of Maryland, College Park, USA 20742*

(Dated: July 23, 2014)

In the main text we calculate the resistive anisotropy due to scattering off nematic spin fluctuations for a  $C_4$ -symmetric band structure. The degeneracy of the iron  $d_{yz}$  and  $d_{xz}$  orbitals is lifted in the nematic phase [1, 2], however, lowering the symmetry of the band structure to  $C_2$ . In this supplemental material we consider the effect of this orthorhombic distortion in the band structure on the resistive anisotropy.

The increased (decreased) iron-iron separation along the  $x$  ( $y$ ) axis in the orthorhombic state decreases (increases) the onsite energy of the iron  $d_{xz}$  ( $d_{yz}$ ) orbital. To model the resulting changes in our band structure, we follow Ref. [3] and decrease the size of the  $eX$  pocket, increase the size of the  $eY$  pocket, and elongate the hole pocket along the  $x$  direction, see Fig. S1(a). This distortion is motivated by the orbital composition of the Fermi pockets [4]. We implement the distortion by introducing a parameter  $\delta > 0$  in the dispersion relations for the two bands  $h$  and  $e$ :

$$\varepsilon_{hk} = \varepsilon_h - \mu + 2t_h [(1 - \delta) \cos k_x + (1 + \delta) \cos k_y], \quad (1)$$

$$\varepsilon_{ek} = \varepsilon_e - \mu + t_{e,1} \cos k_x \cos k_y - t_{e,2} \xi [(1 + \delta) \cos k_x + (1 - \delta) \cos k_y], \quad (2)$$

where length is measured in units of the iron-iron separation. We choose a relatively large orthorhombic distortion of the band structure with  $\delta = 0.03$ , for which the relative difference of the electron-pocket areas is about 21%. All other band parameters are as in the main text.

For a nonzero orthorhombic distortion, the model displays a resistive anisotropy  $\Delta\rho$  even when the nematic parameter in the susceptibility vanishes,  $\phi = 0$ . We present results for this case in Fig. S1. The calculated  $\Delta\rho$  is in rather poor agreement with experimental findings: neither the minimum near optimal doping nor the significant extent of negative values is observed. Note that while the magnitude of  $\Delta\rho$  scales with  $\delta$ , its qualitative behavior does not change significantly.

Figure S2 shows the result for the combined effect of orbital splitting ( $\delta = 0.03$ ) and the nematicity in the spin susceptibility ( $\phi = 0.017$ ). The effect of the two sources of anisotropy appear to be additive and the characteristic signatures of the nematic spin fluctuations are still conspicuous. In particular, the large positive anisotropy in electron-doped samples and the much smaller anisotropy in hole-doped samples for  $W_{sf}/W_{imp} \lesssim 1$  is still present, as is the reduction of the anisotropy in electron-doped samples for  $W_{sf}/W_{imp} \gtrsim 1$ . On the other hand, for  $W_{sf}/W_{imp} \gg 1$ , the weak contribution of the spin fluctuations in the case of electron doping means that the resistive anisotropy is controlled by the distortion of the band structure and becomes negative, as in Fig. S1.

In summary, the effect of orbital splitting alone cannot account for the observed resistive anisotropy. Better agreement might be achieved for a more sophisticated model of the band structure, although this would be at the expense of fine tuning. In contrast, including the nematicity in the spin fluctuation spectrum gives much better agreement with experimental results, is robust against the distortion of the band structure, and dominates the contribution of the distorted band structure to the resistive anisotropy over a large parameter range.

---

\* maxim.breitzkreis@tu-dresden.de

† carsten.timm@tu-dresden.de

- [1] M. Yi, D. Lu, J.-H. Chu, J. G. Analytis, A. P. Sorini, A. F. Kemper, B. Moritz, S.-K. Mo, M. G. Moore, M. Hashimoto, W.-S. Lee, Z. Hussain, T. P. Devereaux, I. R. Fisher, and Z.-X. Shen, *Proc. Natl. Acad. Sciences* **108**, 6878 (2011).
- [2] K. Nakayama, Y. Miyata, G. N. Phan, T. Sato, Y. Tanabe, T. Urata, K. Tanigaki, and T. Takahashi, arXiv:1404.0857.
- [3] R. M. Fernandes, A. V. Chubukov, and J. Schmalian, *Nature Phys.* **10**, 97 (2014).
- [4] S. Graser, T. A. Maier, P. J. Hirschfeld, and D. J. Scalapino, *New J. Phys.* **11**, 025016 (2009).

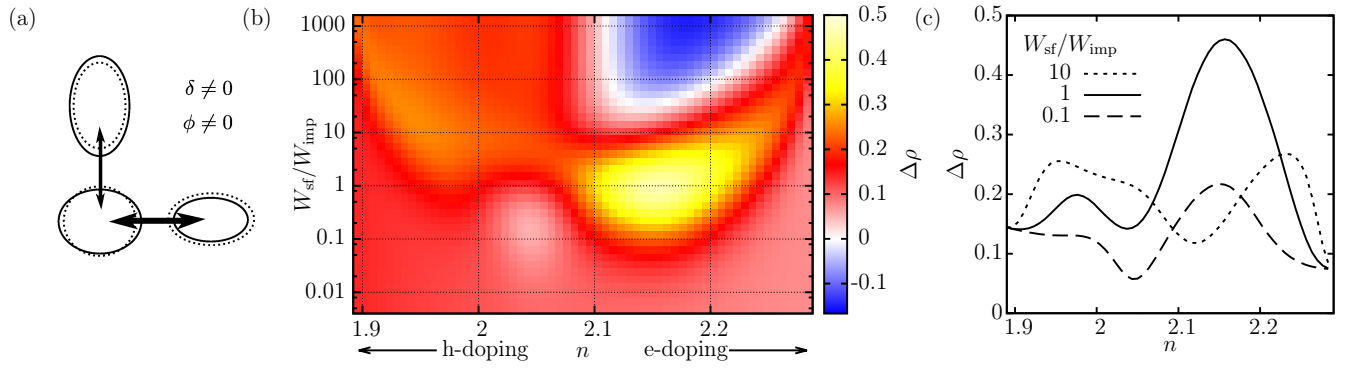


Figure S1. (Color online) (a) Sketch of the Fermi pocket distortion and the scattering strength between the hole and the electron pockets. (b), (c) Resistive anisotropy in the presence of orbital splitting ( $\delta = 0.03$ ) and a paramagnetic spin susceptibility ( $\phi = 0$ ).

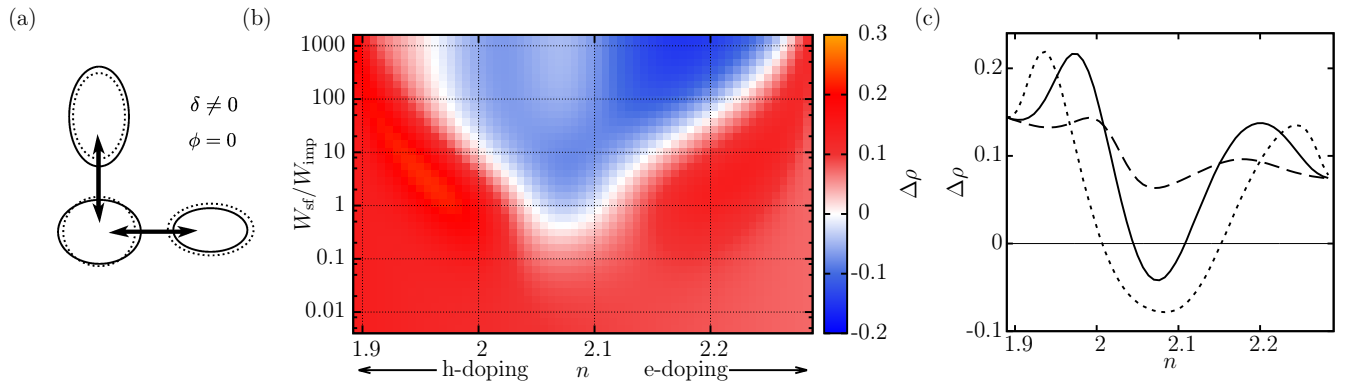


Figure S2. (Color online) (a) Sketch of the Fermi pocket distortion and the scattering strength between the hole and the electron pockets. (b), (c) Resistive anisotropy in the presence of orbital splitting ( $\delta = 0.03$ ) and nematic spin susceptibility ( $\phi = 0.017$ ).