



Interplay between nematicity and superconductivity in bulk and thin films of FeSe

Jian Kang

University of Minnesota

KITP 2017



Collaborators



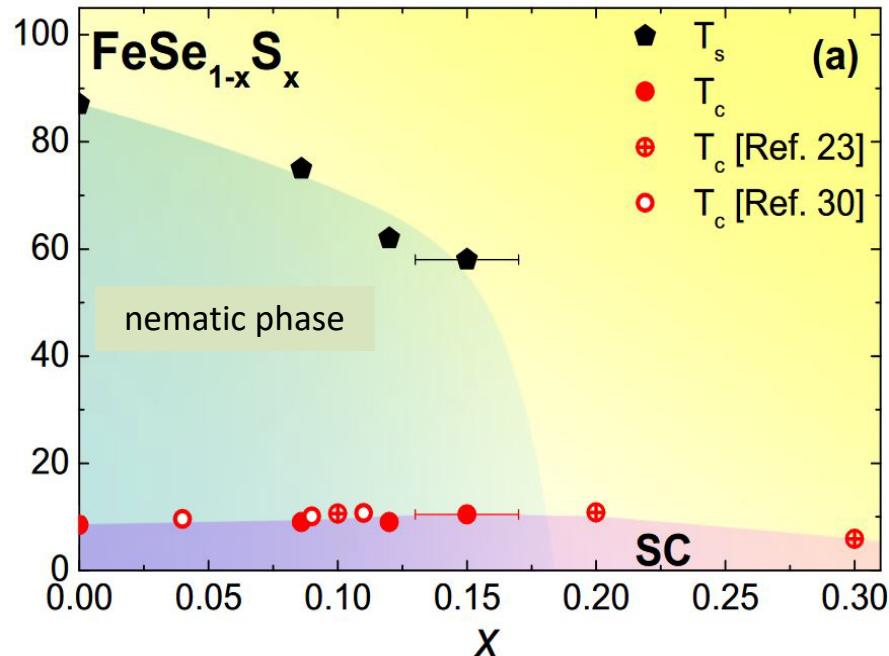
Rafael M. Fernandes
University of Minnesota



Andrey V. Chubukov
University of Minnesota



Debanjan Chowdhury
Massachusetts Institute of Technology



A. I. Coldea, Phys. Rev. B 92, 121108 (2015)

- No magnetic or charge orders
- Provide an ideal platform to study the impact of nematicity on superconductivity.

Thin Films

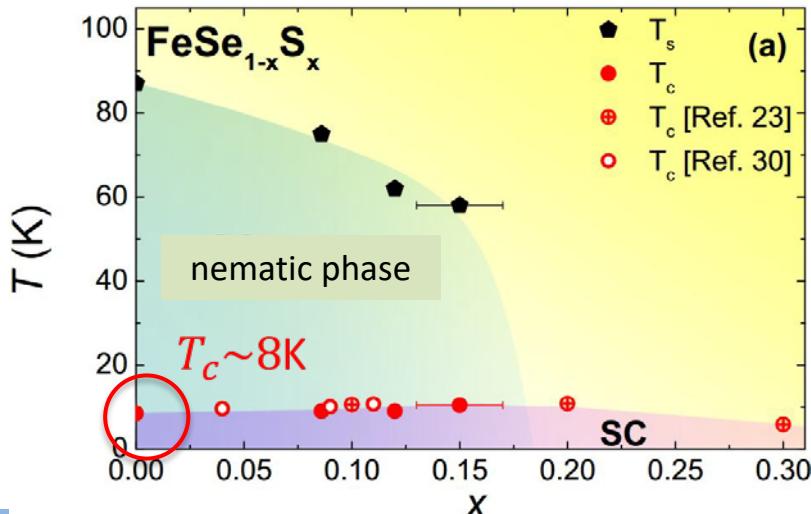
Superconductivity above 100 K in single-layer FeSe films on doped SrTiO₃

Science Bulletin

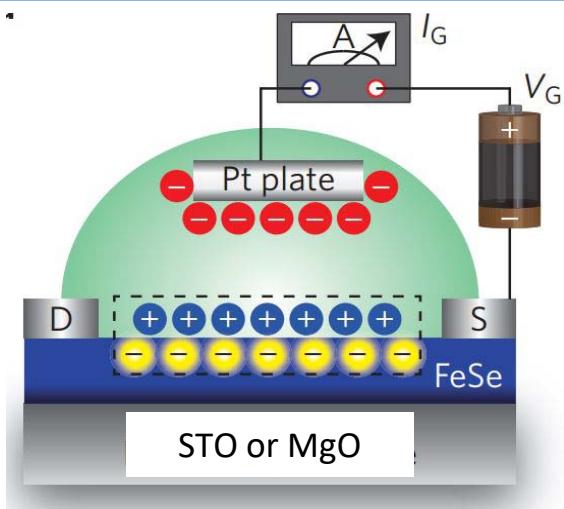
July 2015, Volume 60, Issue 14, pp 1301–1304

Onset of the Meissner effect at 65 K in FeSe thin film grown on Nb-doped SrTiO₃ substrate

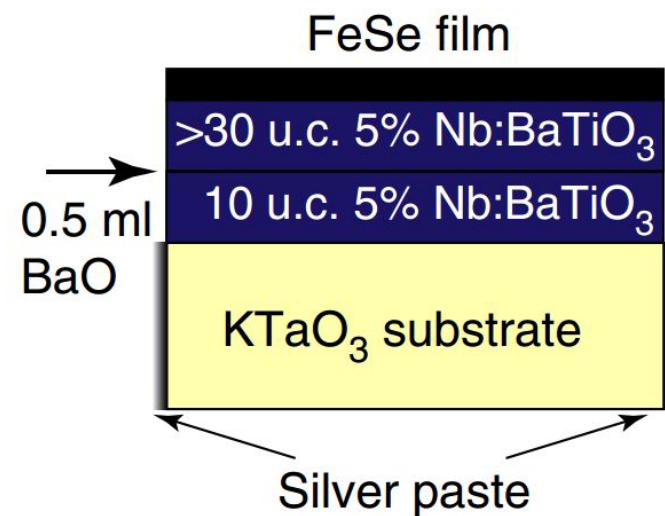
65-75 K for monolayer on the substrate of SrTiO₃ (001)



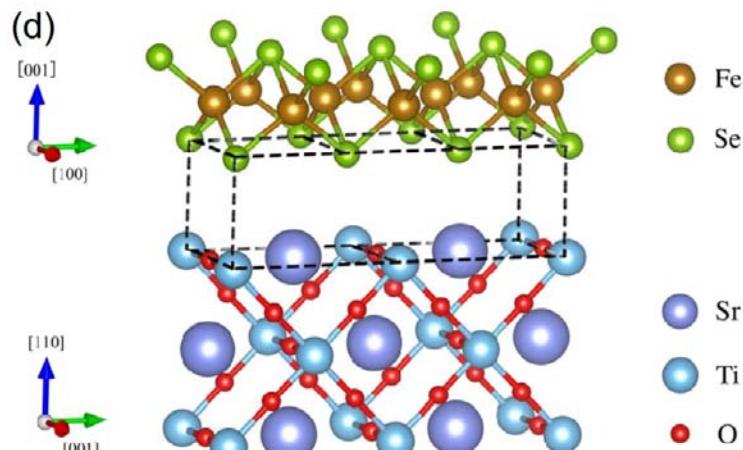
- Role of substrate?
- Mechanism of SC in FeSe thin film?



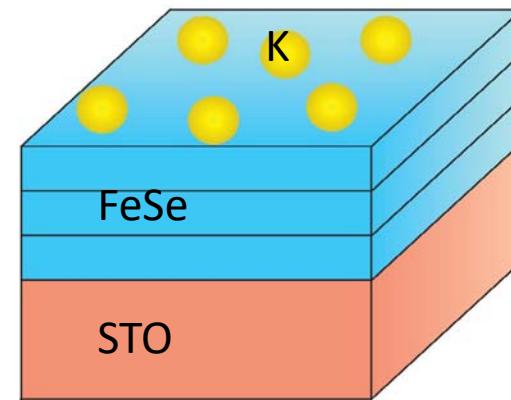
J. Shiogai, *et al.*, Nat. Phys. 12 42 (2016)



R. Peng, *et al.*, Nat. Commun. 5 5044 (2014)



P. Zhang, *et al.*, Phys. Rev. B 94 104510 (2016)



Y. Miyata, *et al.*, Nat. Mater. 14 775 (2015)

$T_c \sim 40\text{K}$ for thin films with different substrates

bulk FeSe
 $T_c = 8K$



FeSe thin film
 $T_c \sim 40K$

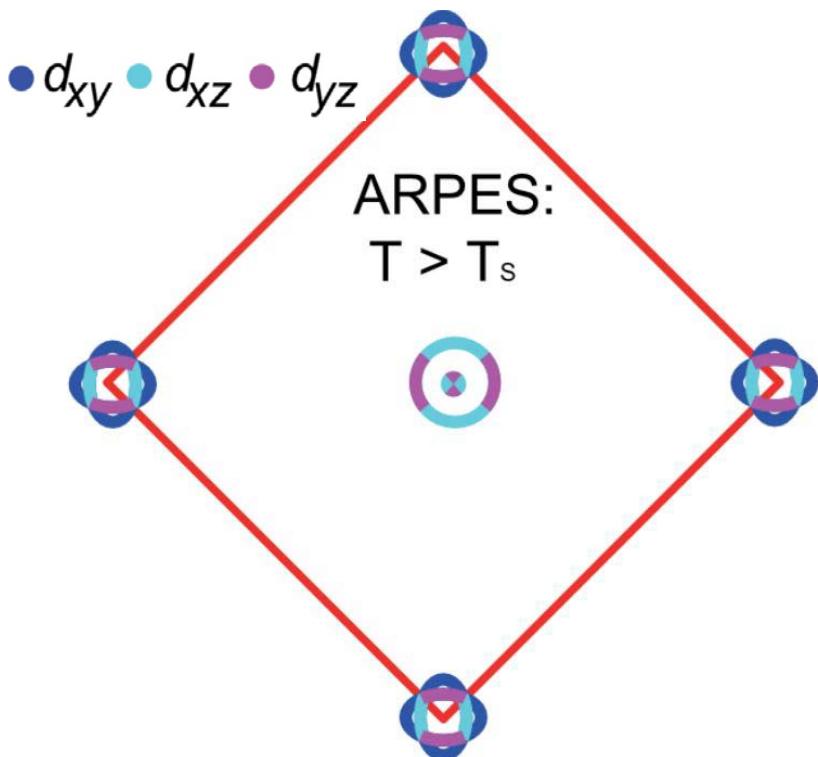
Take home: SC induced by
nematic fluctuations with
spin orbital coupling.

interfacial
phonon

J. J. Lee, *et al.*, Nature 515, 245 (2014).
V. Mishra, *et al.*, Sci. Rep. 6, 32078 (2016).
L. Rademaker, *et al.*, New J. Phys. 18, 022001 (2016).
Y. Zhou and A. J. Millis, Phys. Rev. 93, 224506 (2016).
.....

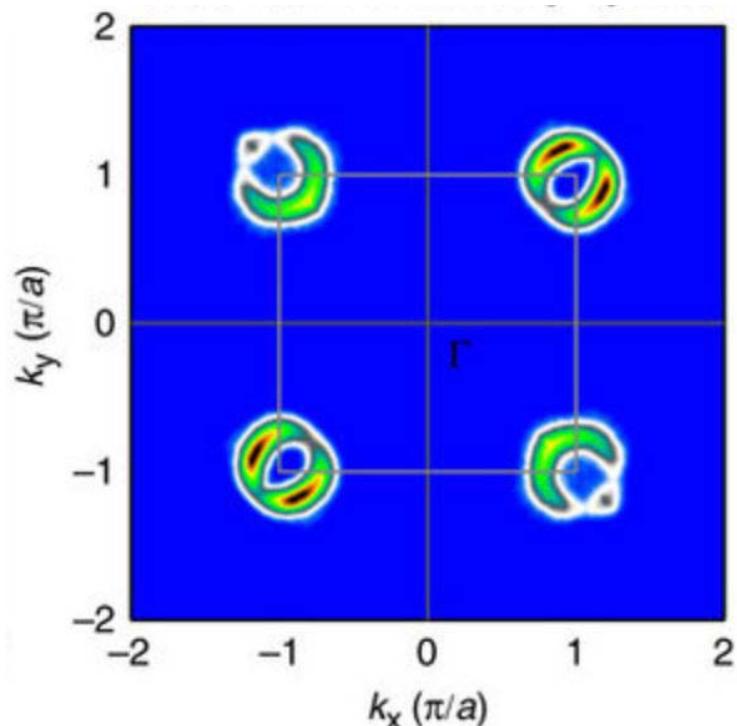
monolayer FeSe
on STO (001)
 $T_c \sim 70K$

bulk FeSe



M. D. Watson *et al.*, Phys. Rev. B 91, 155106 (2015)

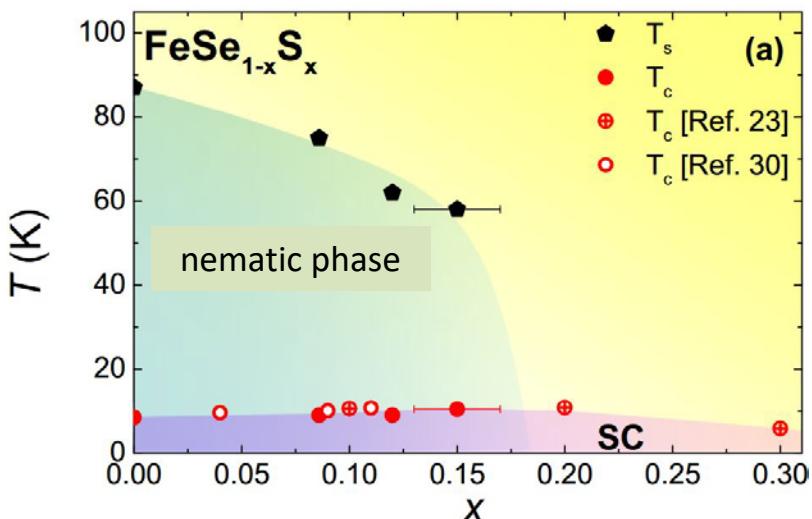
FeSe thin film



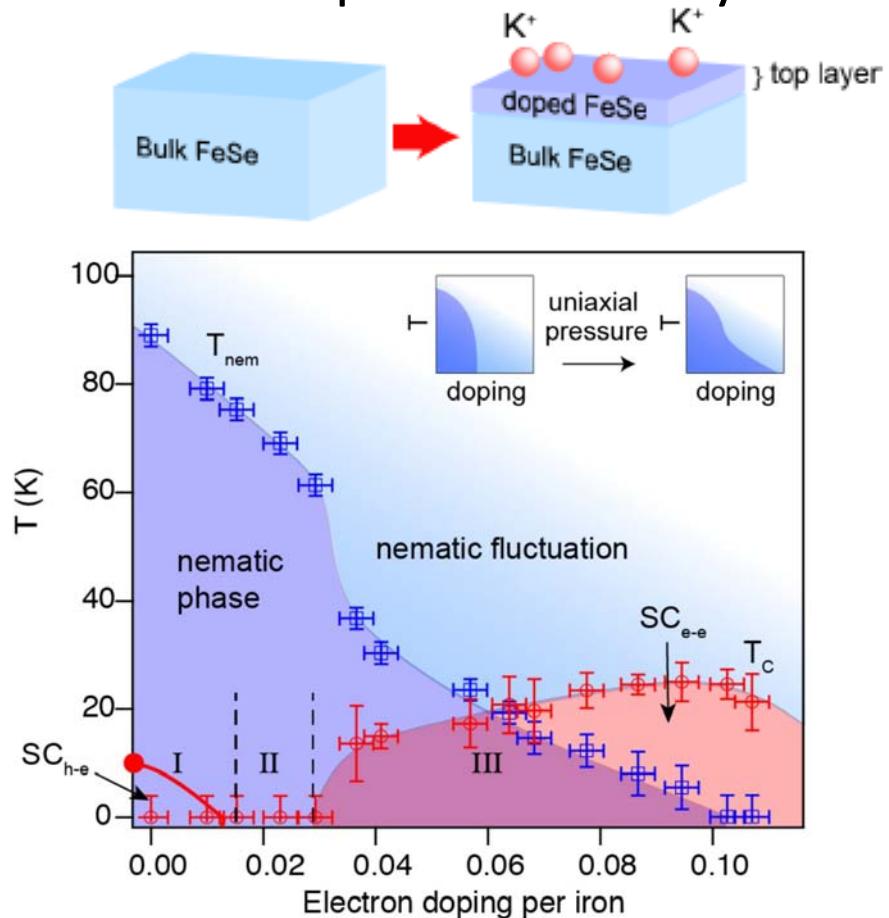
D. F. Liu, *et al.*, Nat. Comm. 3 931 (2012)

heavily electron doped in FeSe thin film

any critical, soft, bosonic mode to induce superconductivity?



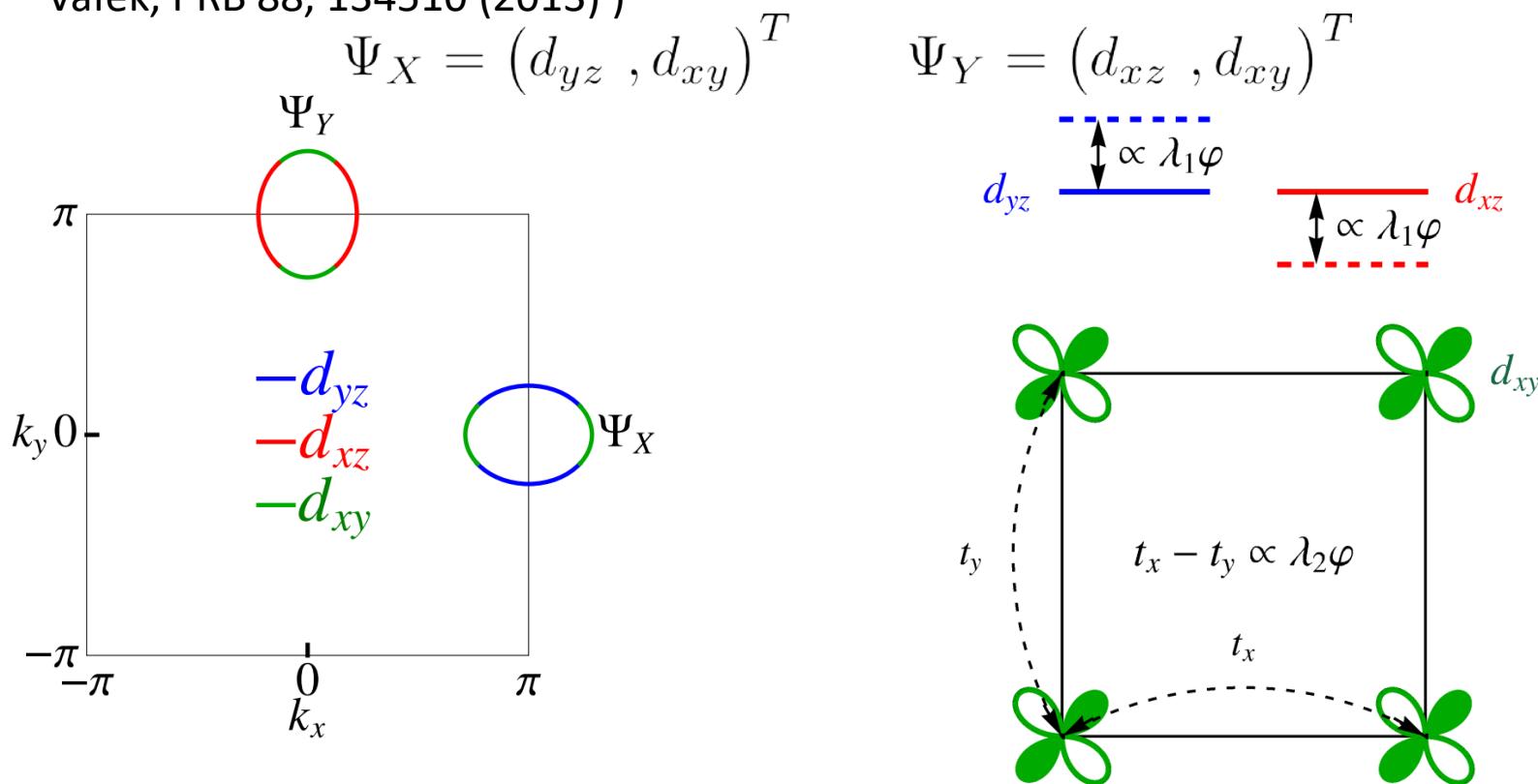
A. I. Coldea, Phys. Rev. B 92, 121108 (2015)



Z. R. Ye, et al., arXiv 1512.02526 (2015).

nematic fluctuation

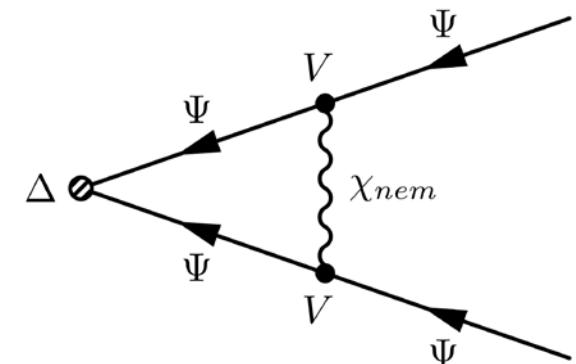
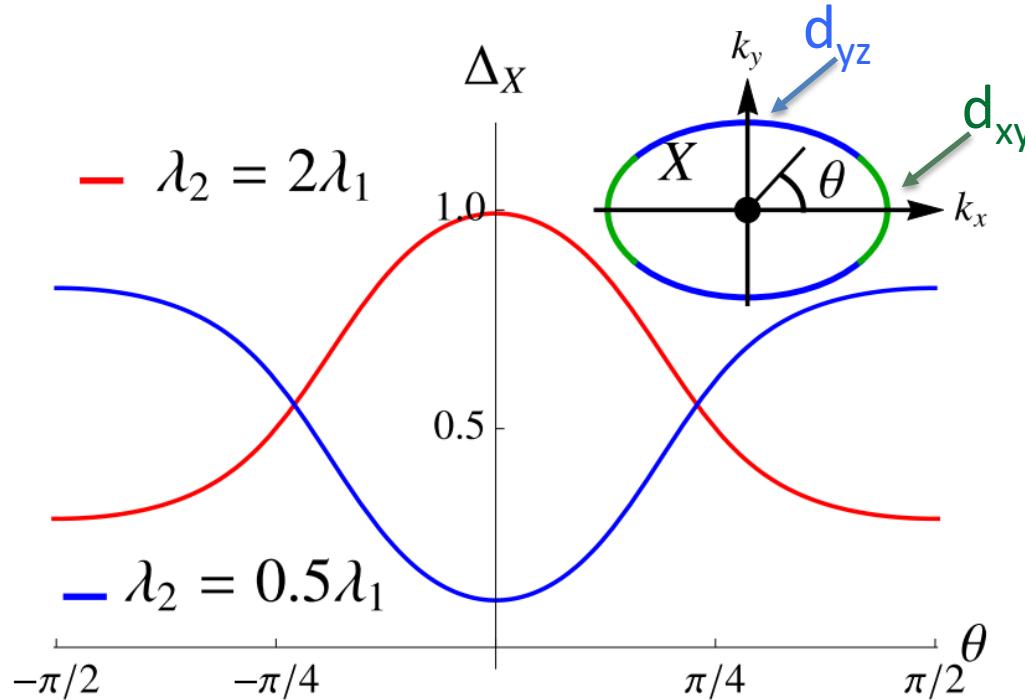
Introduce spinors to describe the low energy model: (V. Cvetkovic and O. Vafek, PRB 88, 134510 (2013))



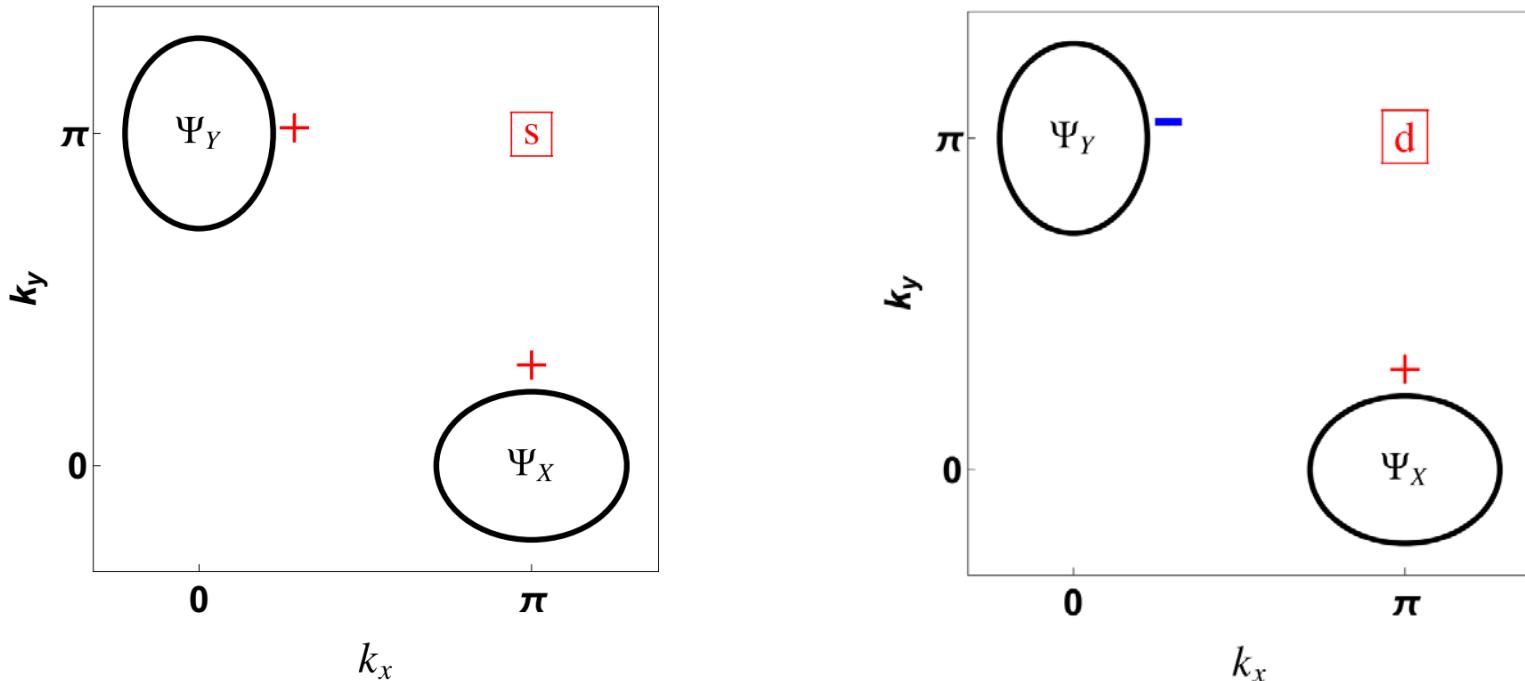
- Two coupling constants λ_1 and λ_2 (R. Fernandes and O. Vafek, PRB 90, 214514 (2014))

Gap Anisotropy

leading pairing instability: intra-orbital and intra-pocket



gap anisotropy depends on orbital weight and relative coupling strength



Small momentum transfer leads to pairing degeneracy: s- and d wave

$$F_{SC} = \frac{a}{2} (|\Delta_s|^2 + |\Delta_d|^2) + \frac{u}{4} (|\Delta_s|^2 + |\Delta_d|^2)^2 + O(\Delta^6)$$

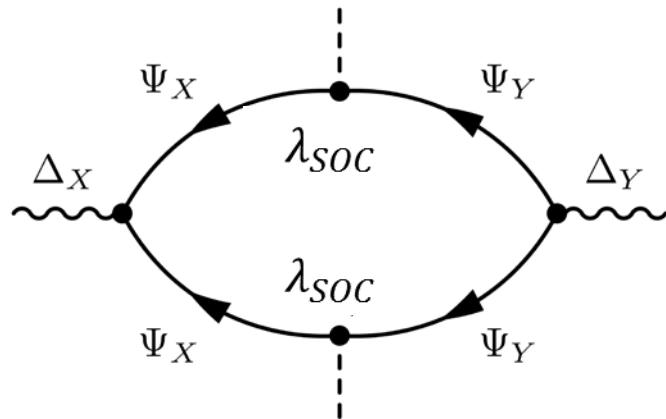
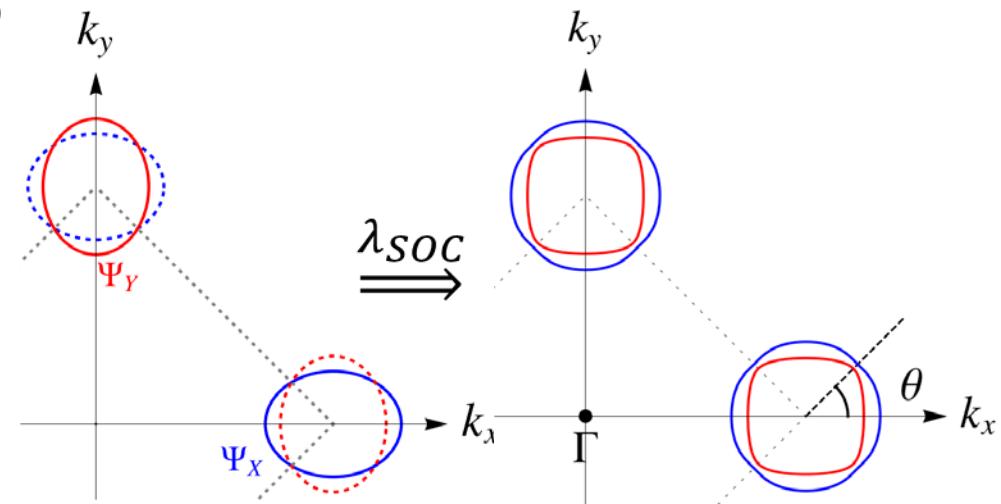
$$\frac{u}{2} |\Delta_s|^2 |\Delta_d|^2 \implies a_s \rightarrow a + u \langle |\Delta_d|^2 \rangle \quad a_d \rightarrow a + u \langle |\Delta_s|^2 \rangle$$

Pairing fluctuation suppressed T_c

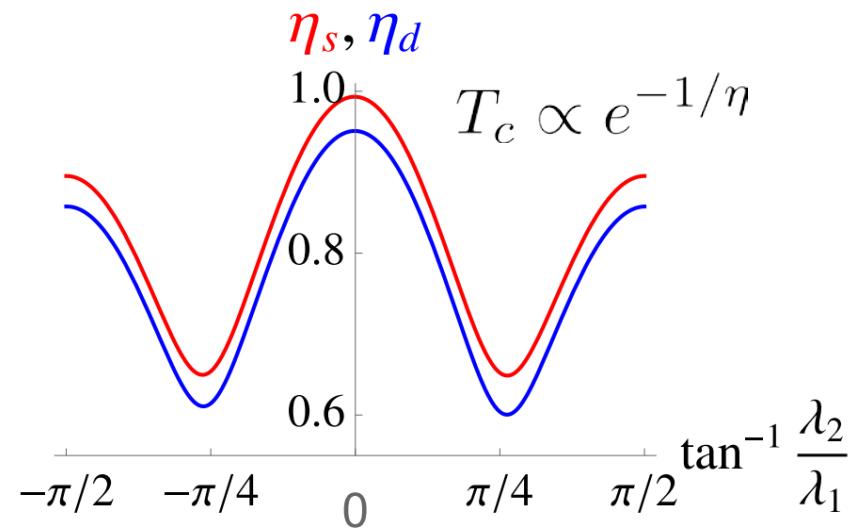
How to lift the pairing degeneracy?

Spin orbital coupling: $\lambda_{SOC} \vec{L} \cdot \vec{S}$

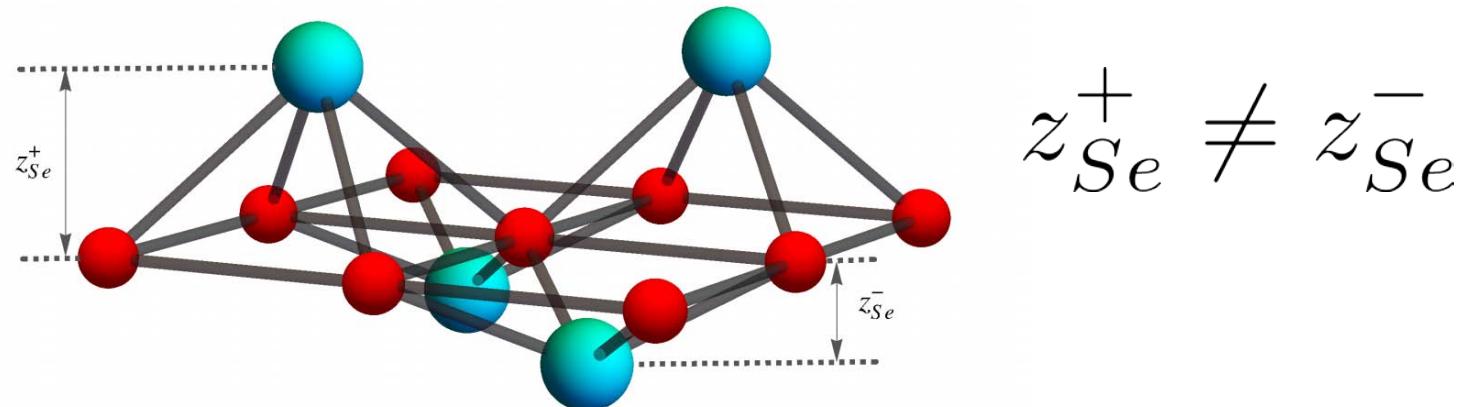
- Hybridization between two electron pockets
- Introduce spin triplet pairing.
- Lift degeneracy between s and d pairing



$$\delta F = \gamma (\Delta_X \Delta_Y^* + h.c.) \quad \text{with } \gamma < 0$$



- Another mechanism to hybridize electron pockets
 - Inversion symmetry breaking

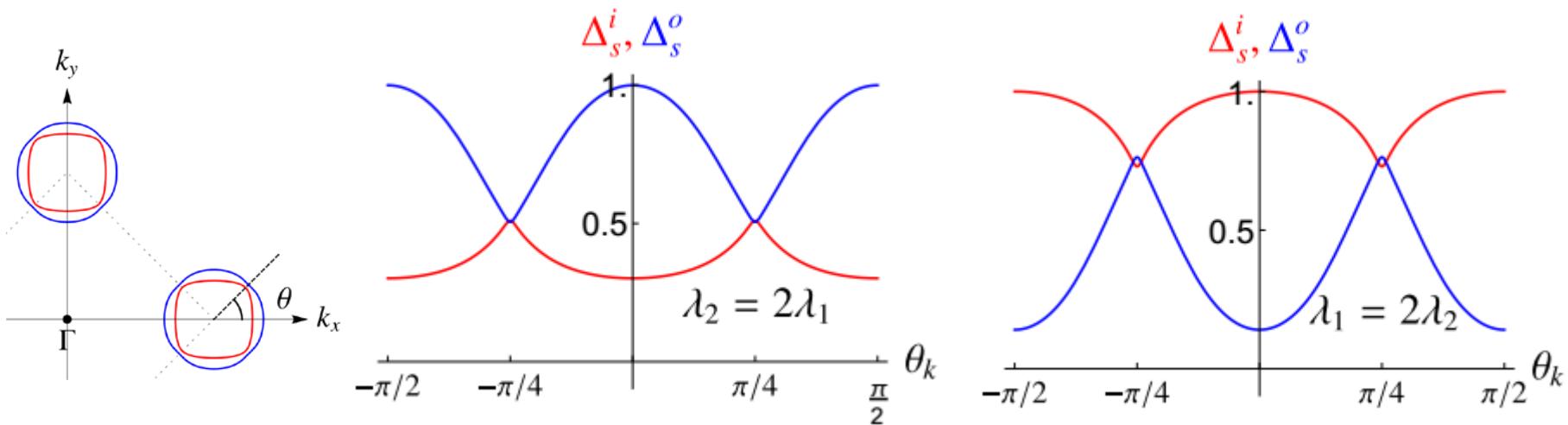


- Hybridize dxz and dyz orbitals
- Impact on SC is similar to SOC
 - s becomes leading instability

Gap anisotropy revisited

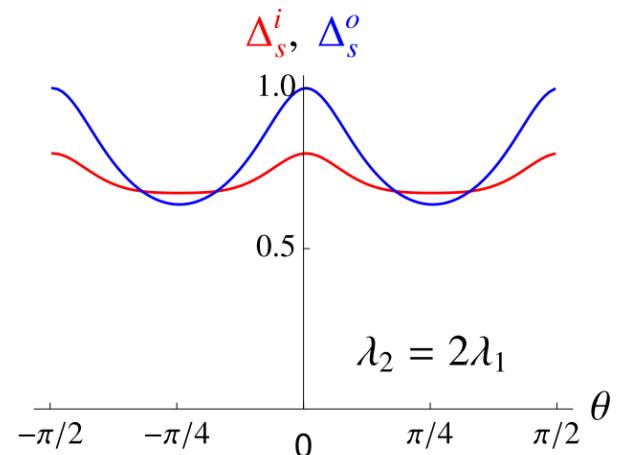
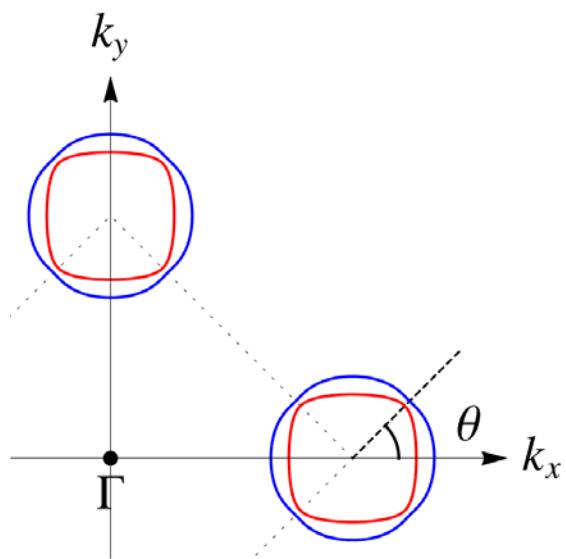
- Gap anisotropy depends on the relative strength between SOC/inv and the mismatch of electron pockets

$$\lambda_{SOC}, \lambda_{inv} \ll \delta_m$$

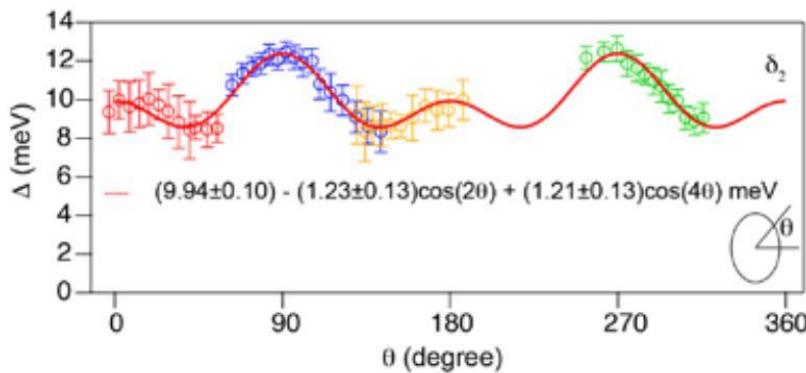


SOC has little impact on gap anisotropy

$$\lambda_{SOC}, \lambda_{inv} \gg \delta_m$$



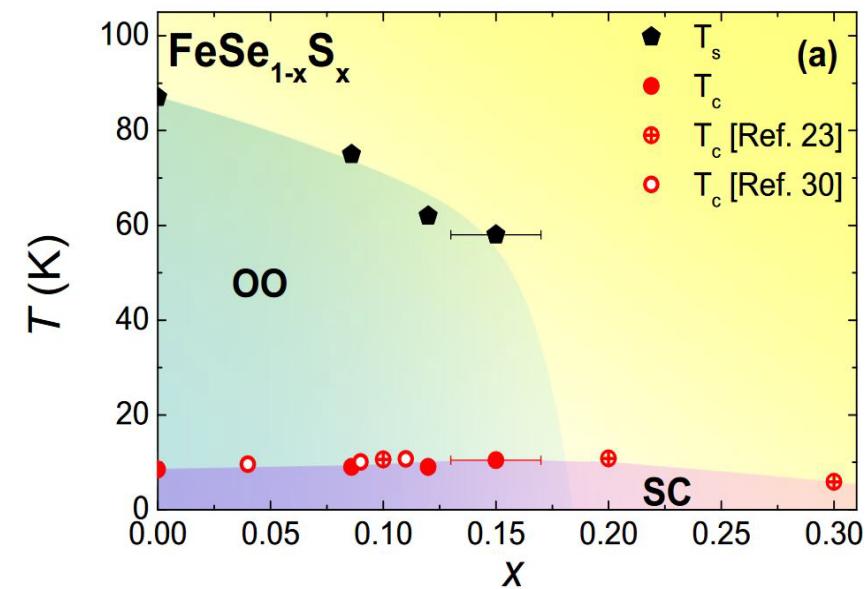
monolayer FeSe



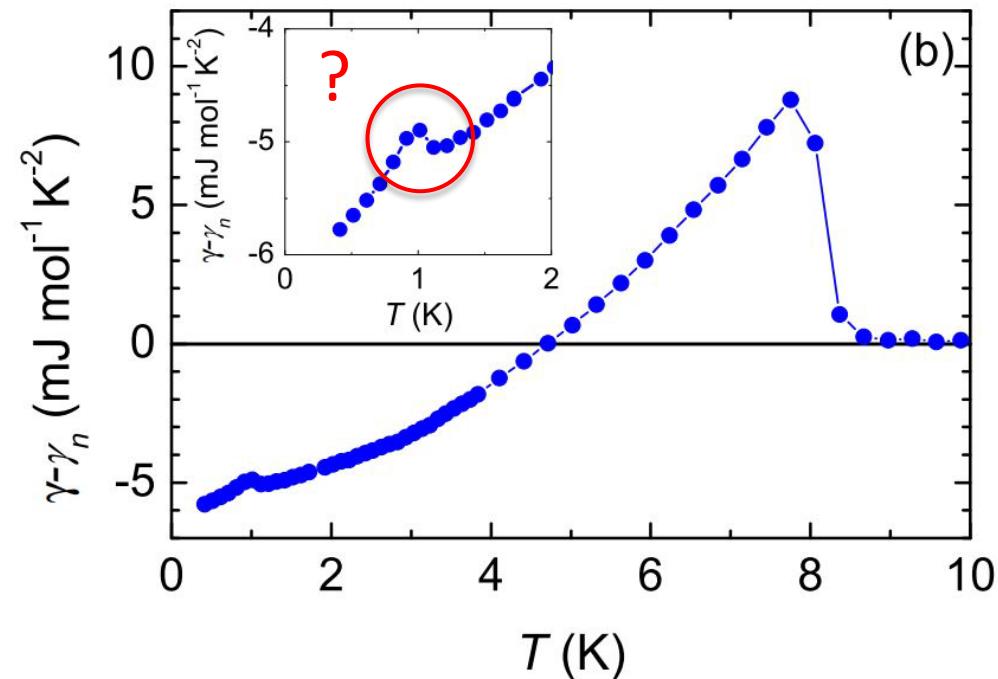
Y. Zhang, et al., Phys. Rev. Lett. 117, 117001 (2016)

Bulk FeSe

SC Phase in bulk FeSe

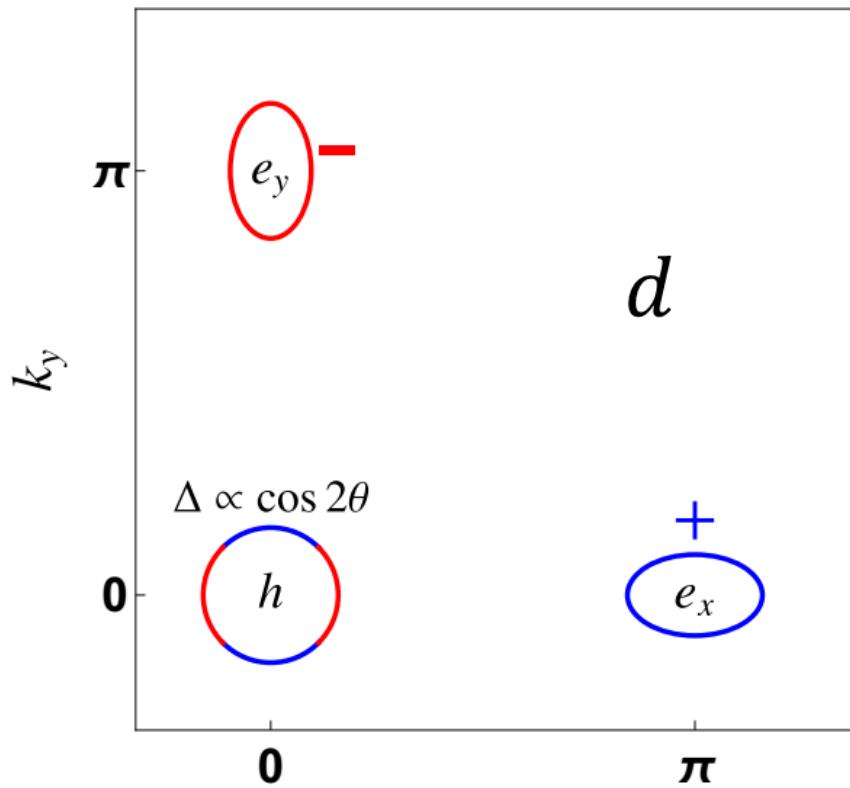
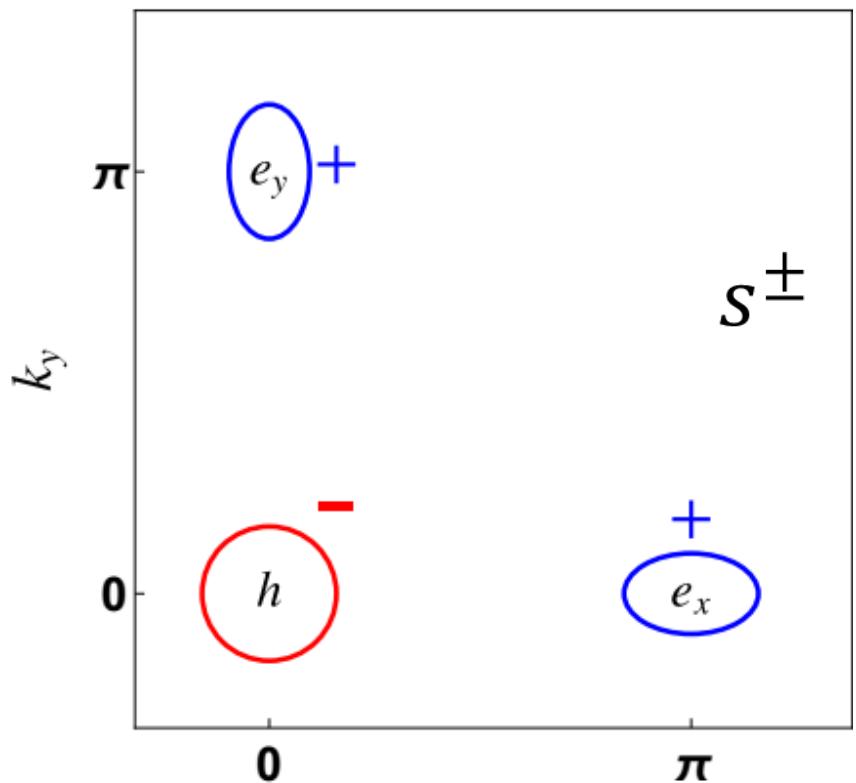


A. I. Coldea, Phys. Rev. B 92, 121108 (2015)



H.-F. Wen, et al., arXiv:1703.08680

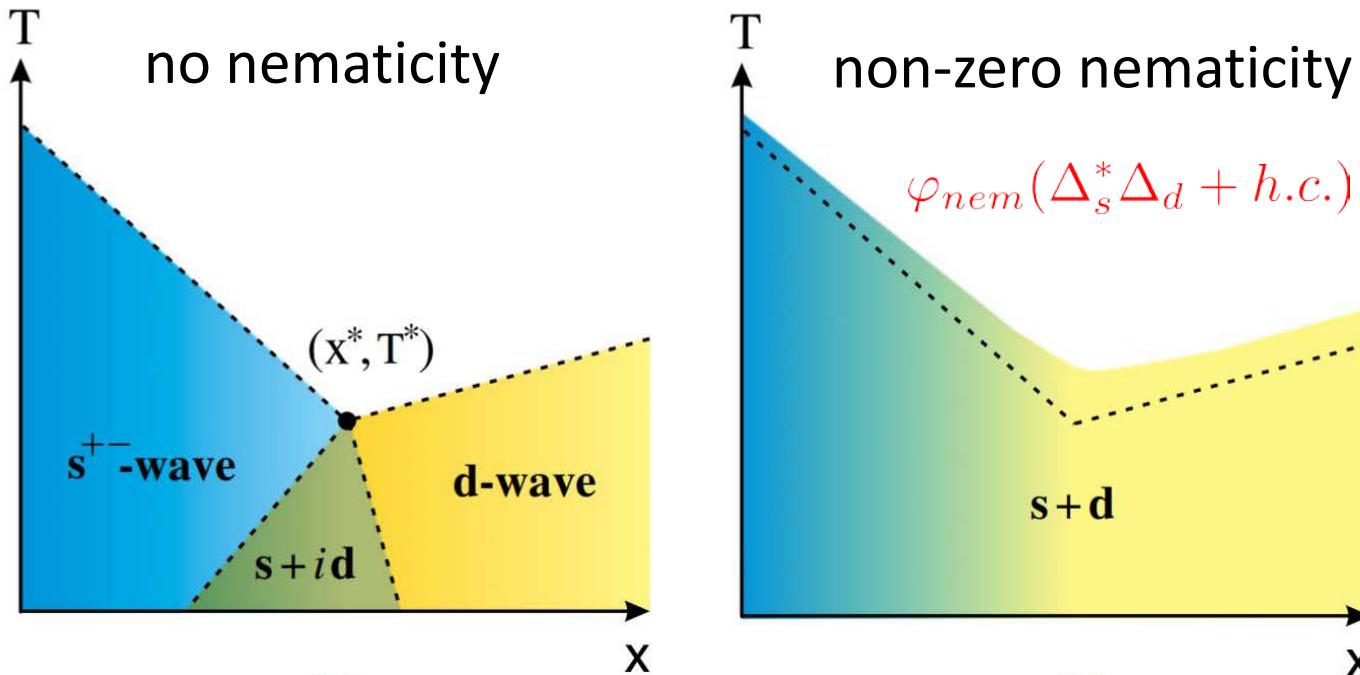
Jump in heat capacity at $T < T_c$



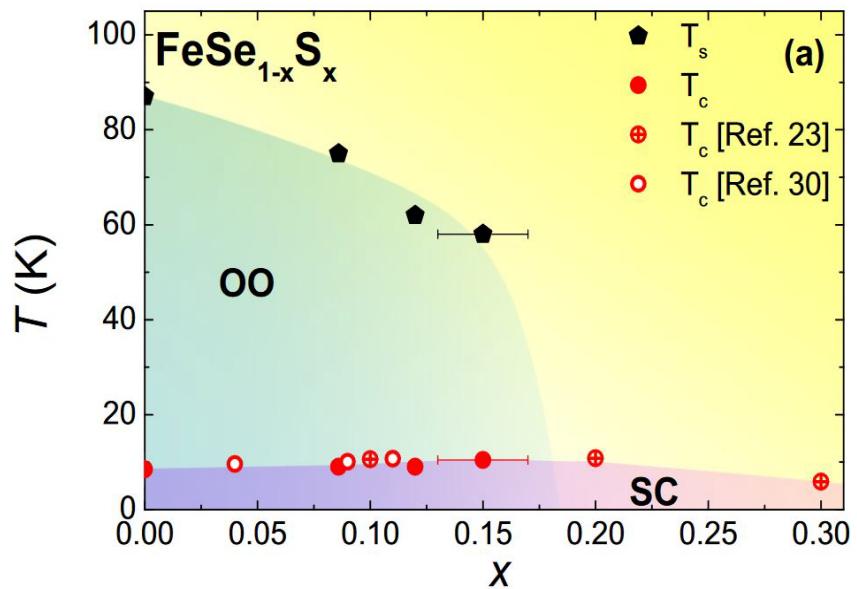
- k_x I.I. Mazin, *et al.*, Phys. Rev. Lett. 101, 057003 (2008) k_x
 K. Kuroki, *et al.*, Phys. Rev. Lett. 101, 087004 (2008)
 A.V. Chubukov, *et al.*, Phys. Rev. B 78, 134512 (2008)
 J. Zhang, *et al.*, Phys. Rev. B 79, 220502 (2009)
 F. Wang, *et al.*, EPL 85, 37005 (2009)
 S. Graser, *et al.*, New J. Phys. 11, 025016 (2009)
 S. Maiti, *et al.*, Phys. Rev. B 84, 224505 (2011)
 F. Kretzschmar, *et al.*, Phys. Rev. Lett. **110**, 187002 (2013)
-

TRSB in iron-based SC

- Near degeneracy between s and d pairing channels.
- Nematicity is generally incompatible with TRSB



R. Fernandes and A. Millis, Phys. Rev. Lett. 111, 127001 (2013)
J. Kang and R. Fernandes, Phys. Rev. Lett. 113, 217001 (2014)

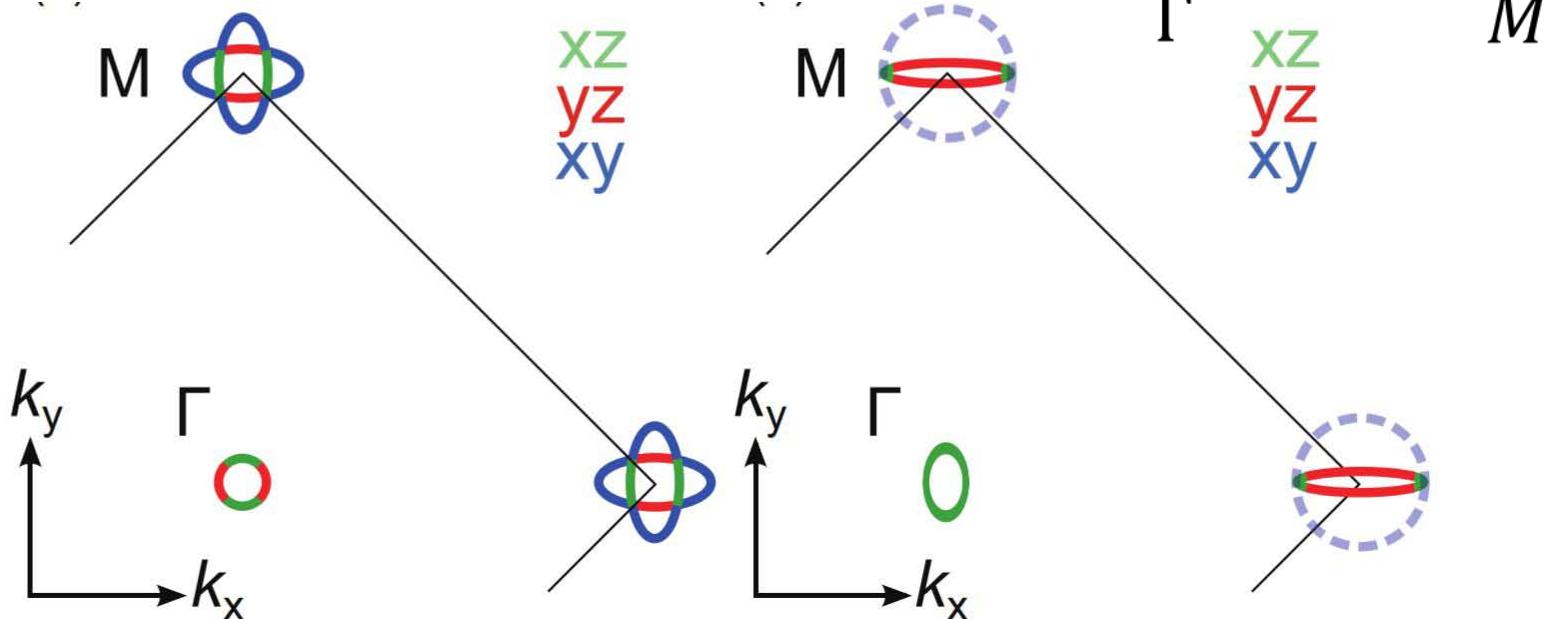
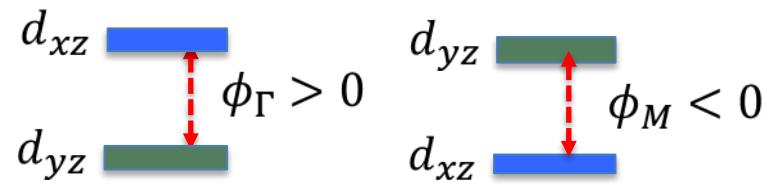


A. I. Coldea, Phys. Rev. B 92, 121108 (2015)

Momentum-dependent nematicity

- Sign inversion nematicity

$$\phi_{\mathbf{k}}(n_{xz} - n_{yz})$$



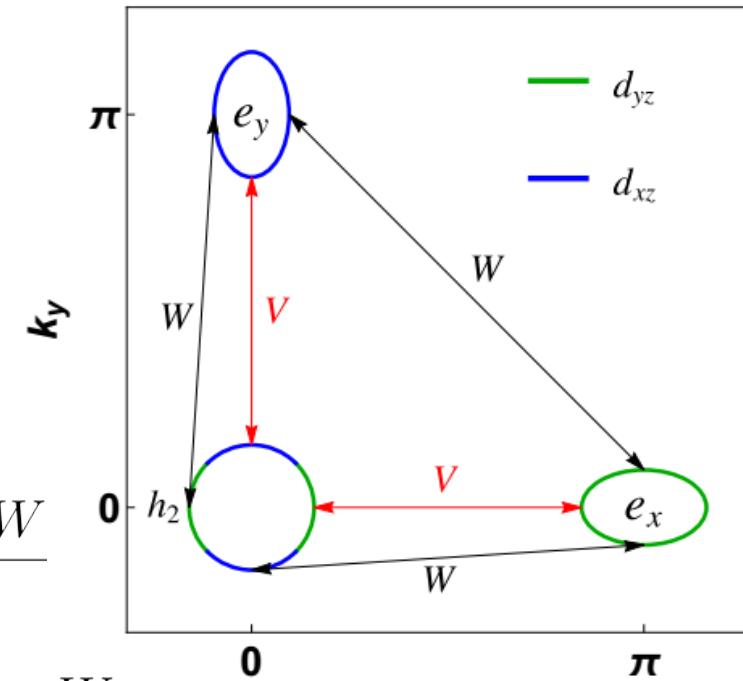
Y. Suzuki, et al., Phy. Rev. B. 92, 205117 (2015)

$$\sim (\phi_{\Gamma} + \phi_M)(\Delta_s^* \Delta_d + h.c.)$$

Does the *sign-inversion* nematicity help TRSB SC state?

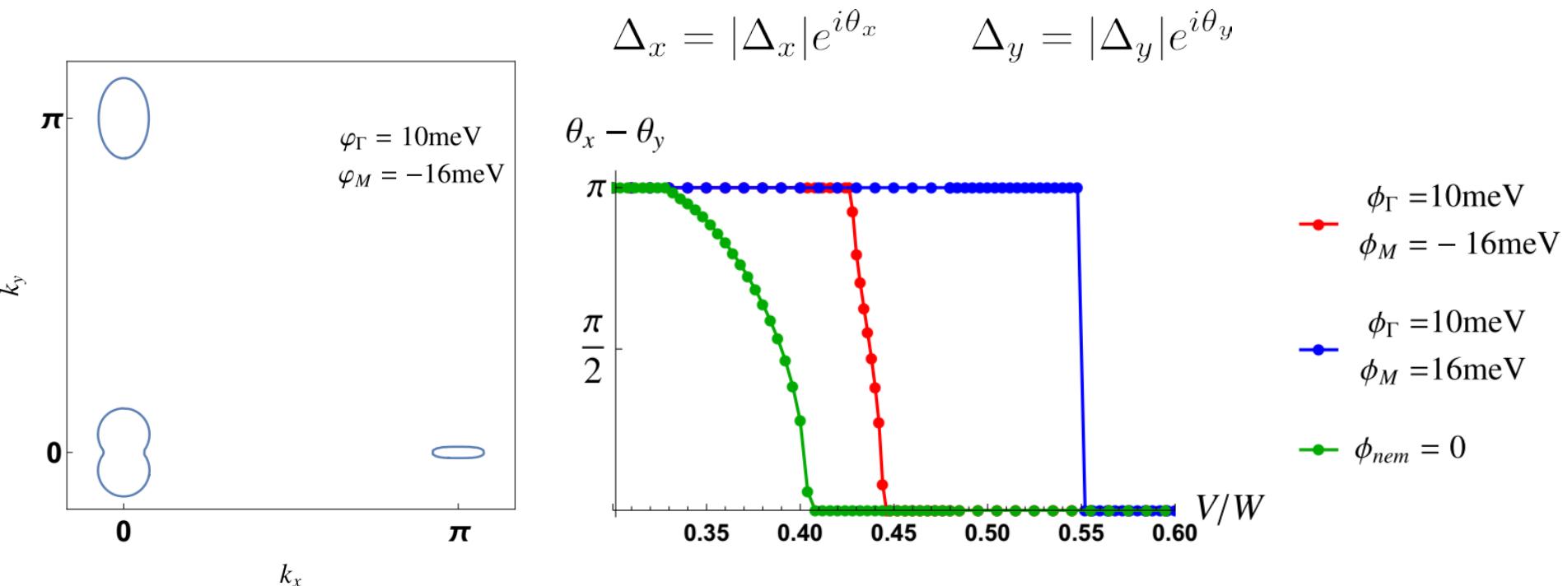
Pairing interaction

- Inter-pocket pairing interaction:
 - Intra-orbital pairing: V
 - Inter-orbital pairing: W
- SC in s and d channels:
 - s^\pm wave:
$$U_{xy}^{eff} = -W, \quad U_{hx}^{eff} = U_{hy}^{eff} = \frac{V + W}{2}$$
 - d wave:
$$U_{xy}^{eff} = W, \quad U_{hx}^{eff} = -U_{hy}^{eff} = \frac{V - W}{2}$$
 - s^\pm - d degeneracy: $V \sim W$



TRSB SC with nematicity

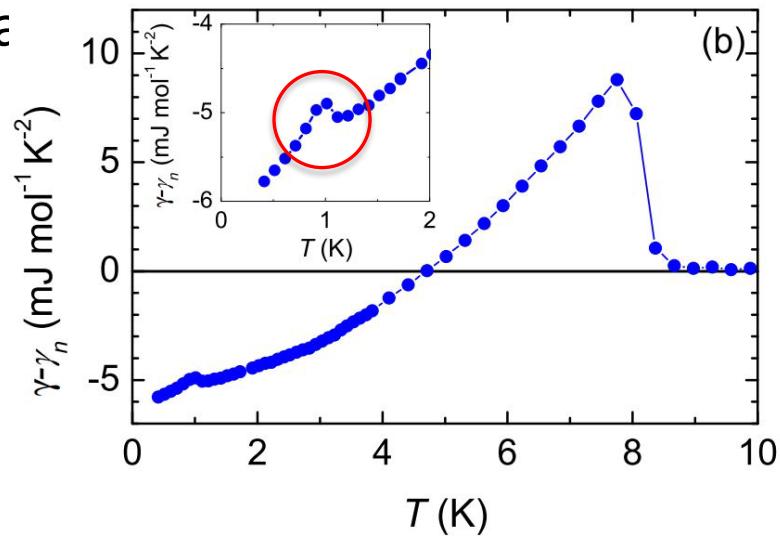
- $\phi_{nem} \sim \epsilon_f$
 - Numerical results with fitting the band structure



Sizable *sign-inversion* nematicity is compatible with
TRSB SC state.

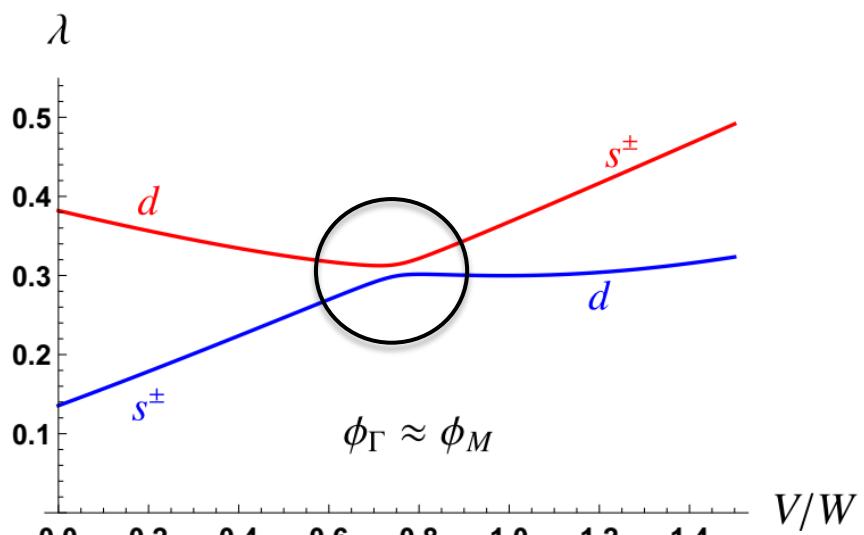
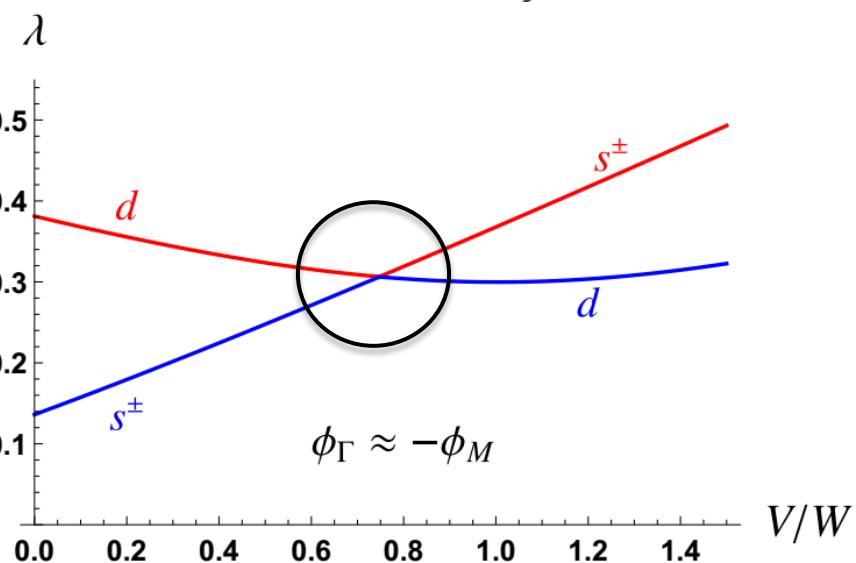
Conclusion

- Nematic fluctuations with SOC may induce SC in ultrathin FeSe film and dramatically enhance Tc.
- Sign-inversion nematicity in the bulk FeSe is compatible with TRSB SC state. It might account for the kink of the specific heat in the superconductivity phase.



Superconductivity with small nematicity

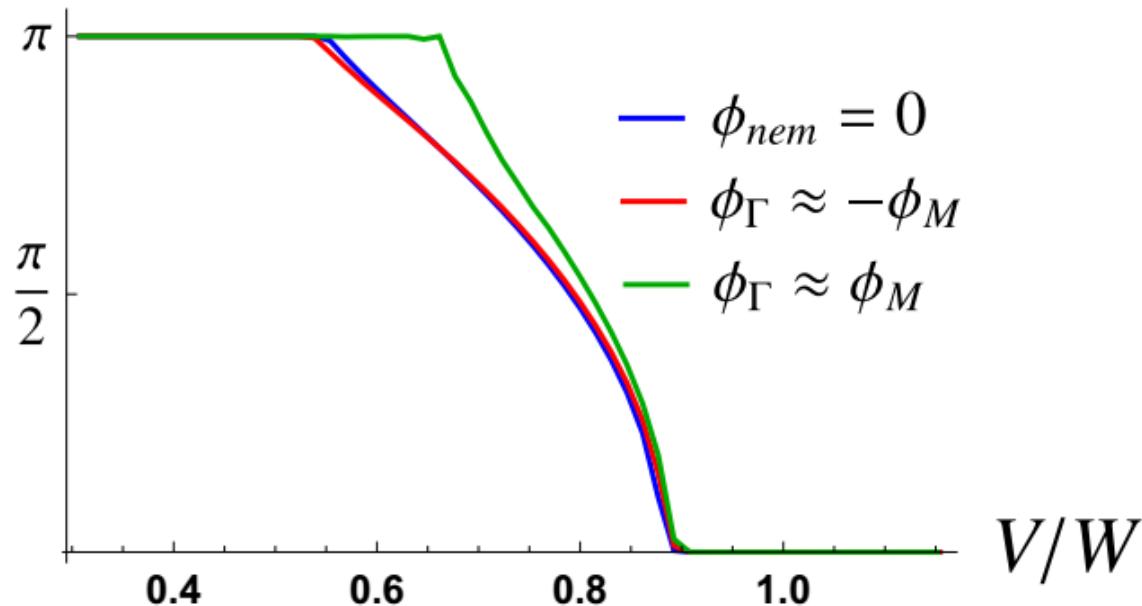
- Small $\phi_{nem} \ll \varepsilon_f$



Sign-inversion nematicity has little impact on the s-d pairing degeneracy

TRSB with small nematicity

$\theta_x - \theta_y$



Small sign-inversion nematicity has little impact on the TRSB SC state.