Determinant Quantum Monte Carlo Study of a Multi-Orbital Model

Interplay of Nematic and Superconducting Orders

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Phys. Rev. B **94**, 155127 (2016) [arxiv:1512.08523]

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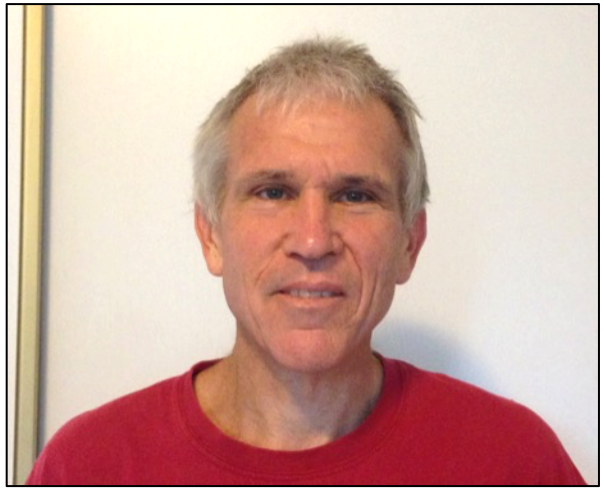

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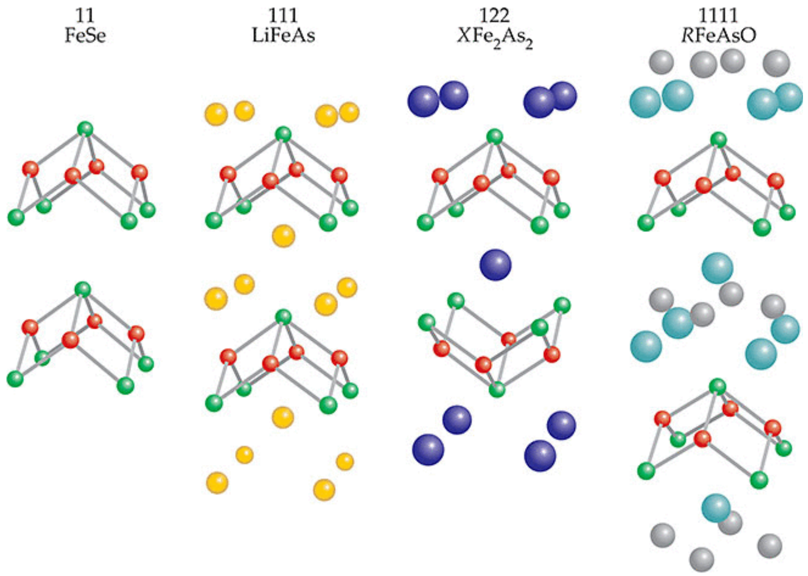
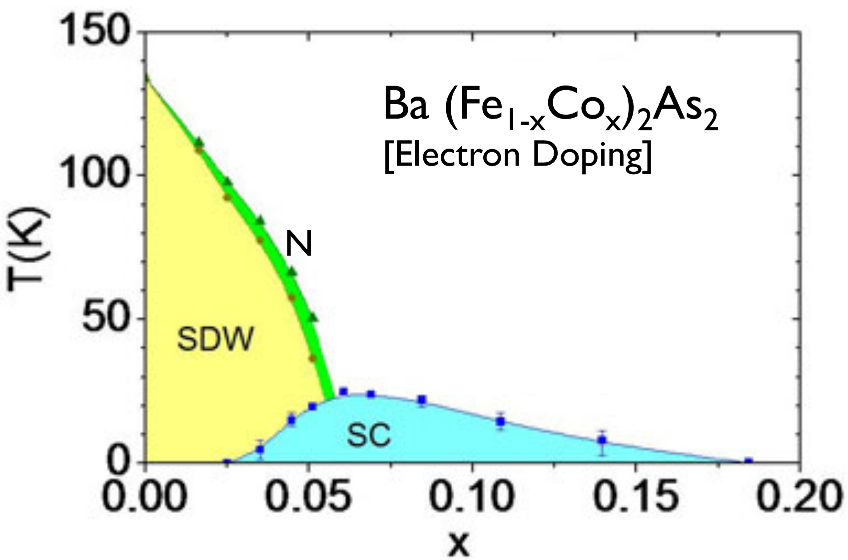
Iron Based Superconductors

- Quasi-2D Materials
- Ordered Phases
  - Nematic
  - Spin-Density Wave
  - Superconductor
- Quantum Criticality?
- Competing vs Intertwined Order?

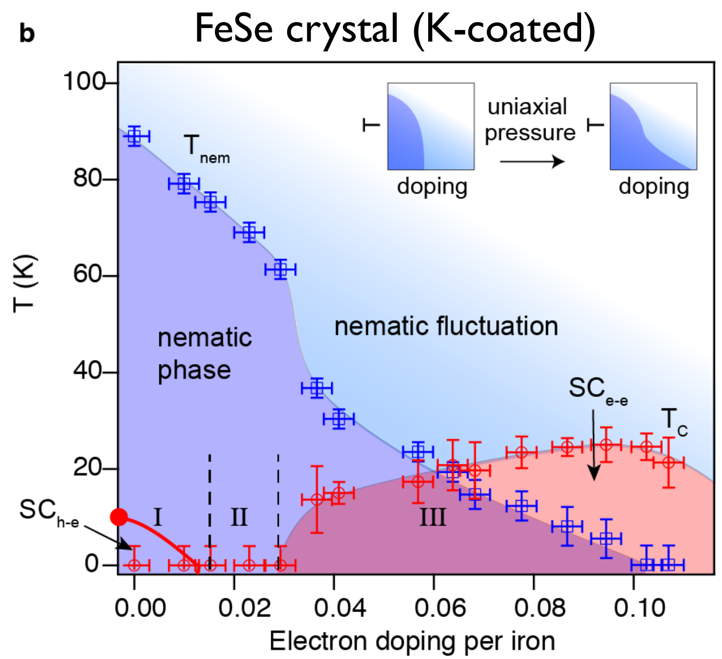


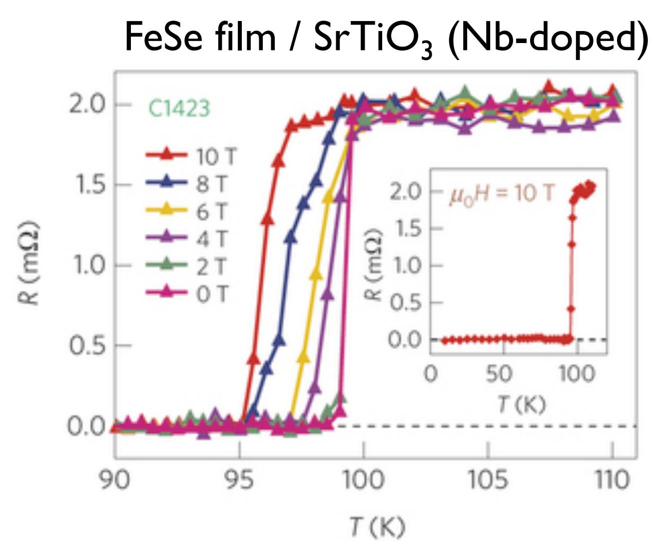


[Chu et. al. Phys. Rev. B 79, 014506 (2009)]

Many sides of FeSe Superconductivity

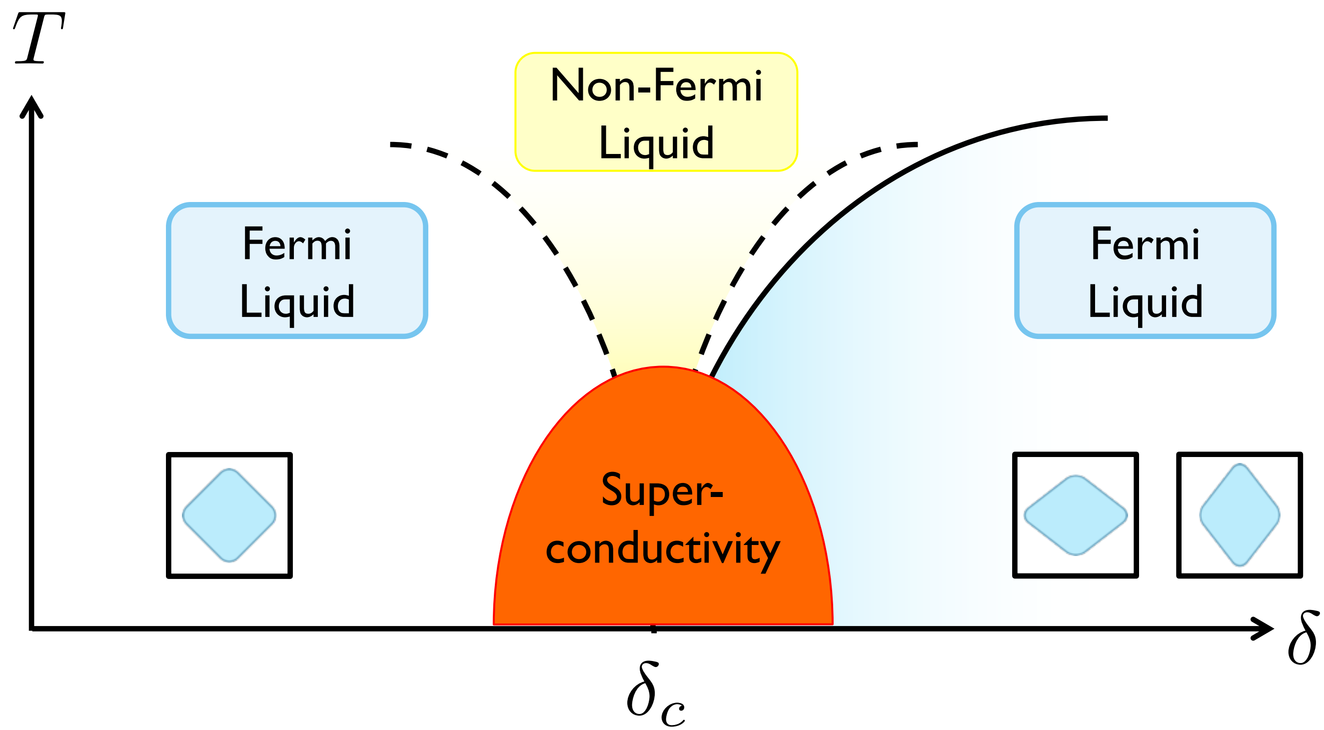
- Undoped Bulk Properties:
  - Nematic order
  - No magnetic order [without external pressure]
  - Superconducting T_c ~ 8K
- Highly Doped Bulk / Monolayers
  - e.g. K coated surface
  - Two Superconducting domes
  - T_c ~ 40 K
- Monolayer on $SrTiO_3$
  - T_c ~ 65 K to 109 K





Nematic Quantum Criticality

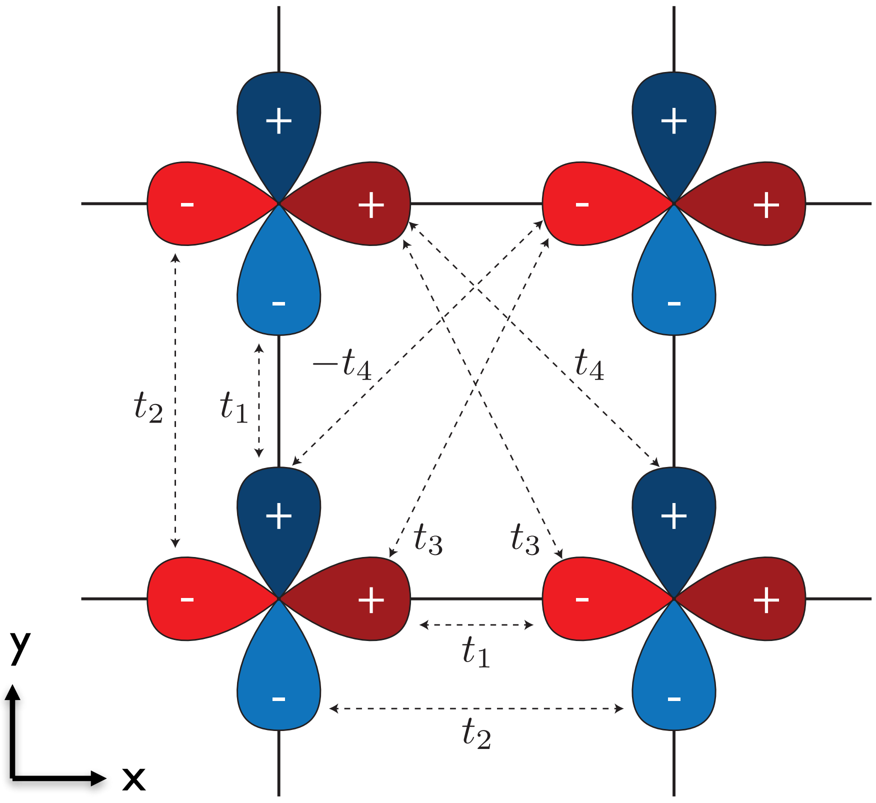
- C_4 to C_2 Symmetry Breaking
  - Electronically Driven
  - Fermi Surface Fluctuations



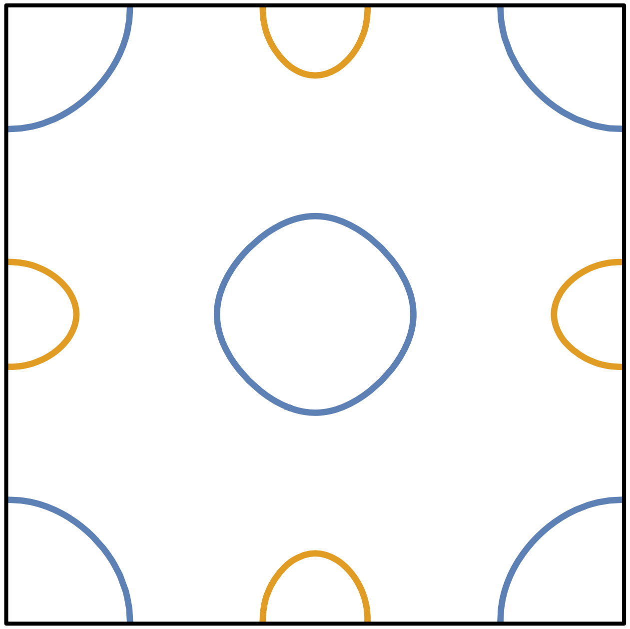
Two Band Model

$$H_0 = -\sum_{ij,ab,\sigma} t_{ij,ab}(c^\dagger_{i,a,\sigma} c_{j,b,\sigma} + \mathrm{h.c.}) - \mu \sum_{i,a,\sigma} c^\dagger_{i,a,\sigma} c_{i,a,\sigma}$$

d_{xz}, d_{yz} orbitals

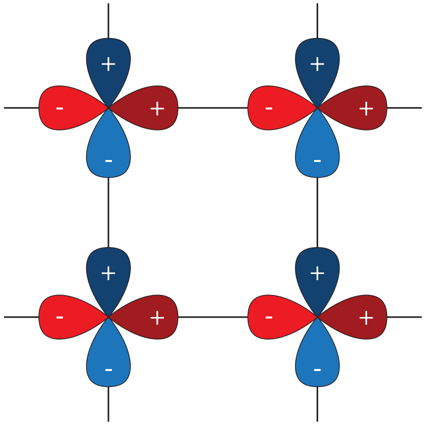


Fermi Surface: Electron & Hole Pockets



t_1 = -1.0 t_3 = -1.2 μ = 0.6
t_2 = +1.5 t_4 = -0.95

Interactions favor Nematic Order



- On-site interactions:

$$H_I = -\frac{g}{2}\sum_i \delta n_i \delta n_i$$

- Nematicity: Orbital Symmetry Breaking

$$\delta n_i = n_{i1\uparrow} + n_{i1\downarrow} - n_{i2\uparrow} - n_{i2\downarrow}$$

- Unbiased Sampling of the Fermions using DQMC; Global Updates using Parallel Tempering

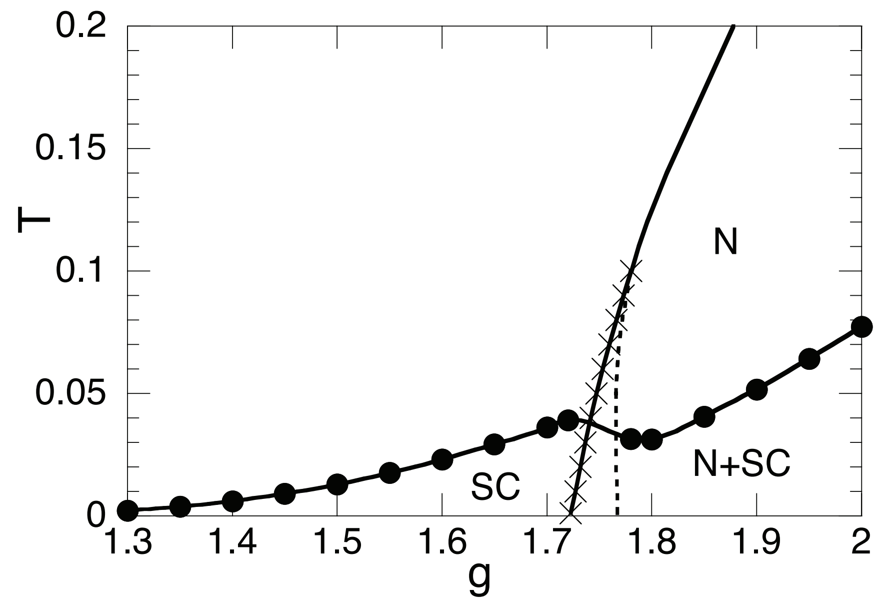
- Engineer physics in sign problem free mode
  [cf. Li, Jiang, Yao. arXiv:1601.05780,
  Schattner, Lederer, Kivelson, Berg, PRX. 6, 031028 (2016),
  Berg, Metlitski, Sachdev, Science 338, 1606 (2012).]

Weak Coupling Expectations

$$H_0 = -\sum_{ij,ab,\sigma} t_{ij,ab}(c^\dagger_{i,a,\sigma} c_{j,b,\sigma} + \mathrm{h.c.}) - \mu \sum_{i,a,\sigma} c^\dagger_{i,a,\sigma} c_{i,a,\sigma}$$

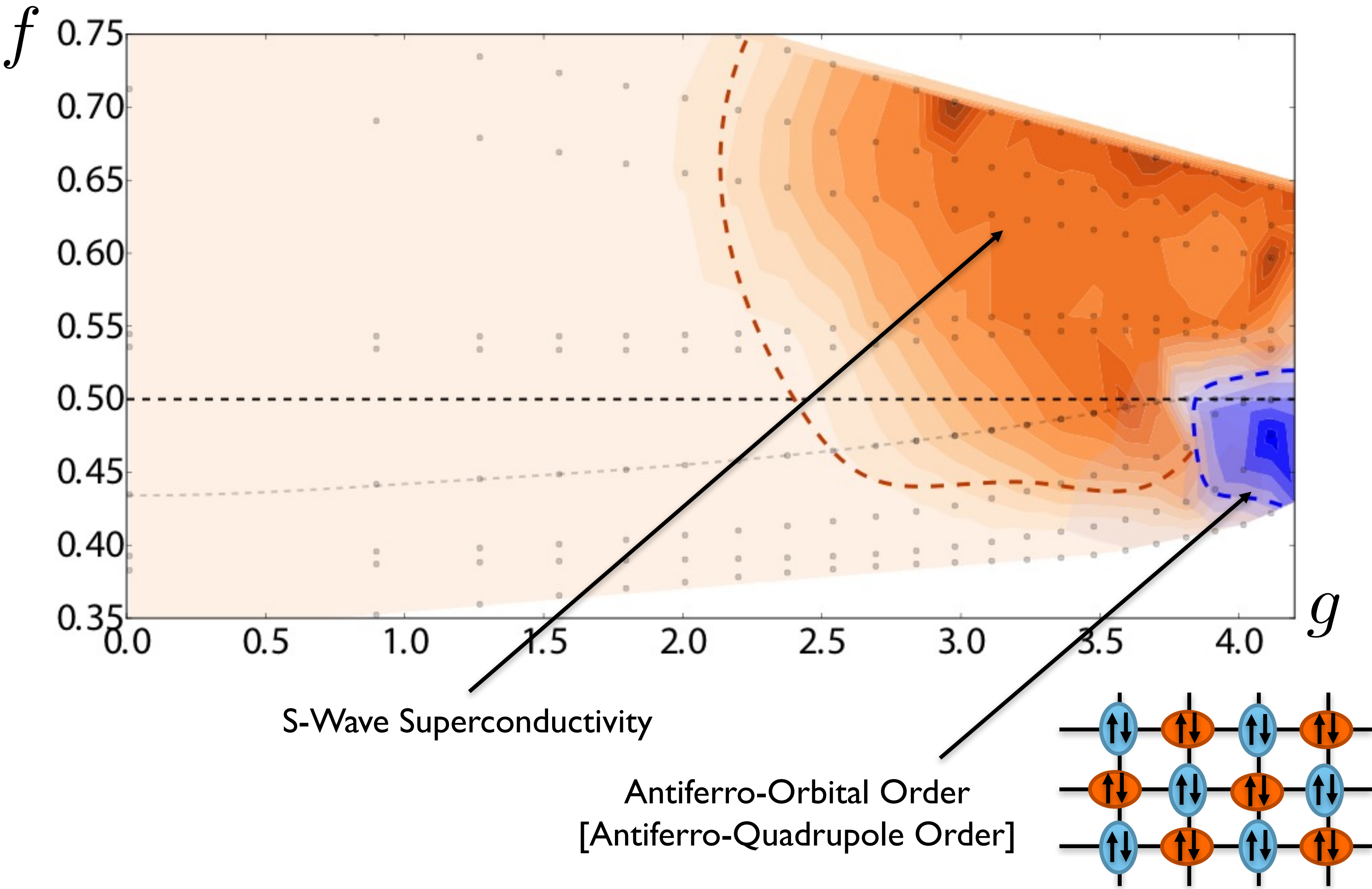
$$H_I = -\frac{g}{2}\sum_i \delta n_i \delta n_i$$

- Weak Coupling (RPA)
  - Finite g transition to nematic order
  - Superconductivity in Eliashberg Theory

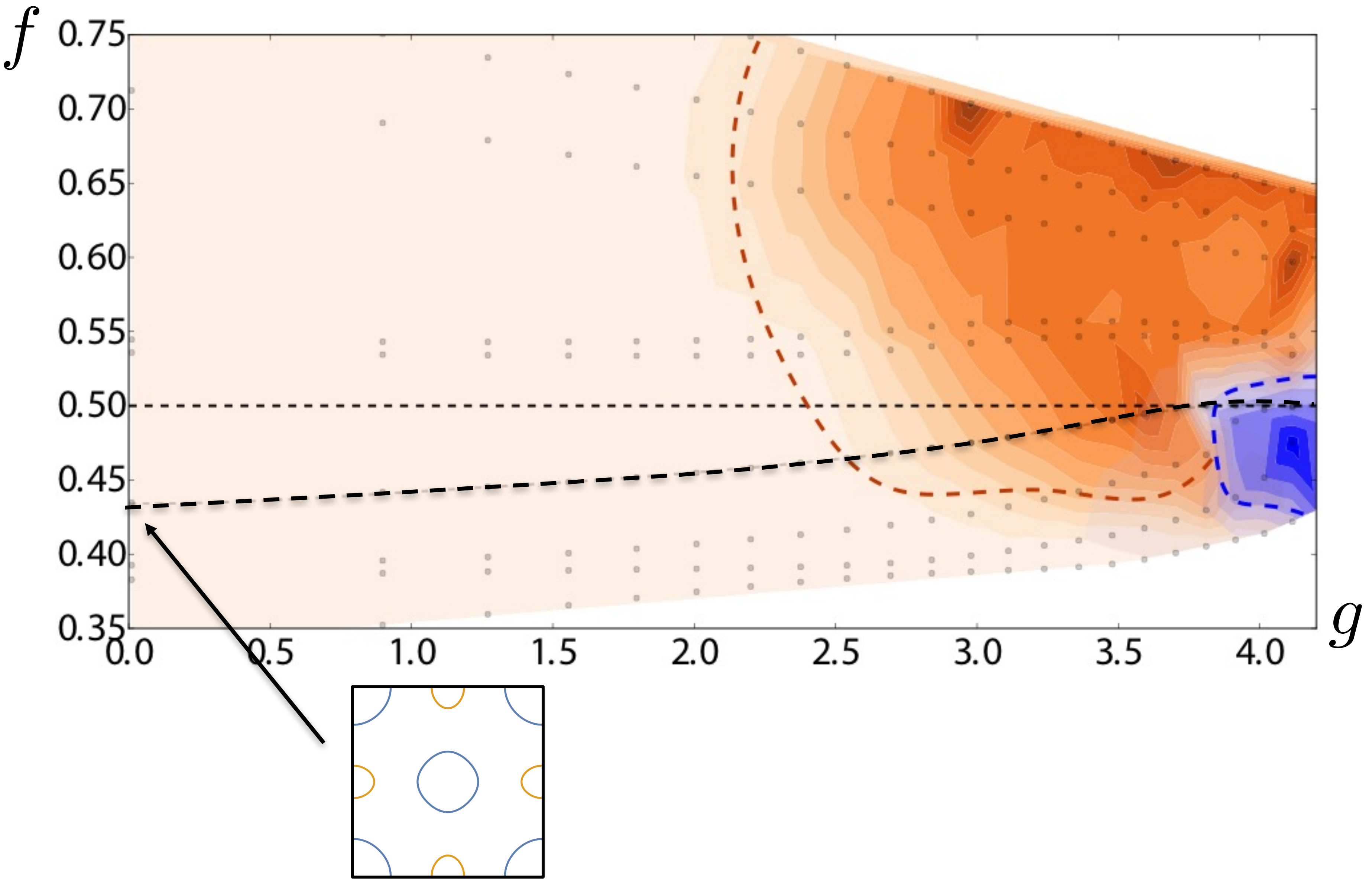


[Yamase & Zeyher PRB, 88, 180502 (2013)]

Phase Diagram



Phase Diagram

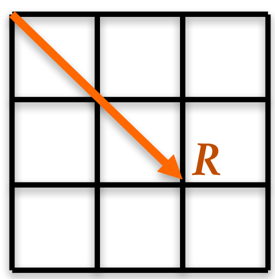


Determining the Phase Diagram

- Nematic Correlation Function:

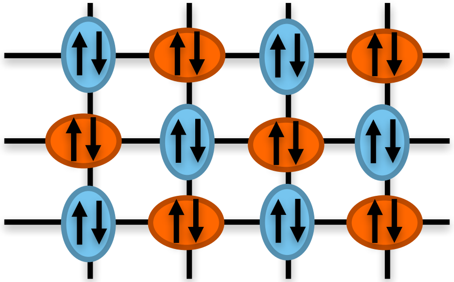
$$\langle \delta n \delta n \rangle_{(q,\tau=0)}$$

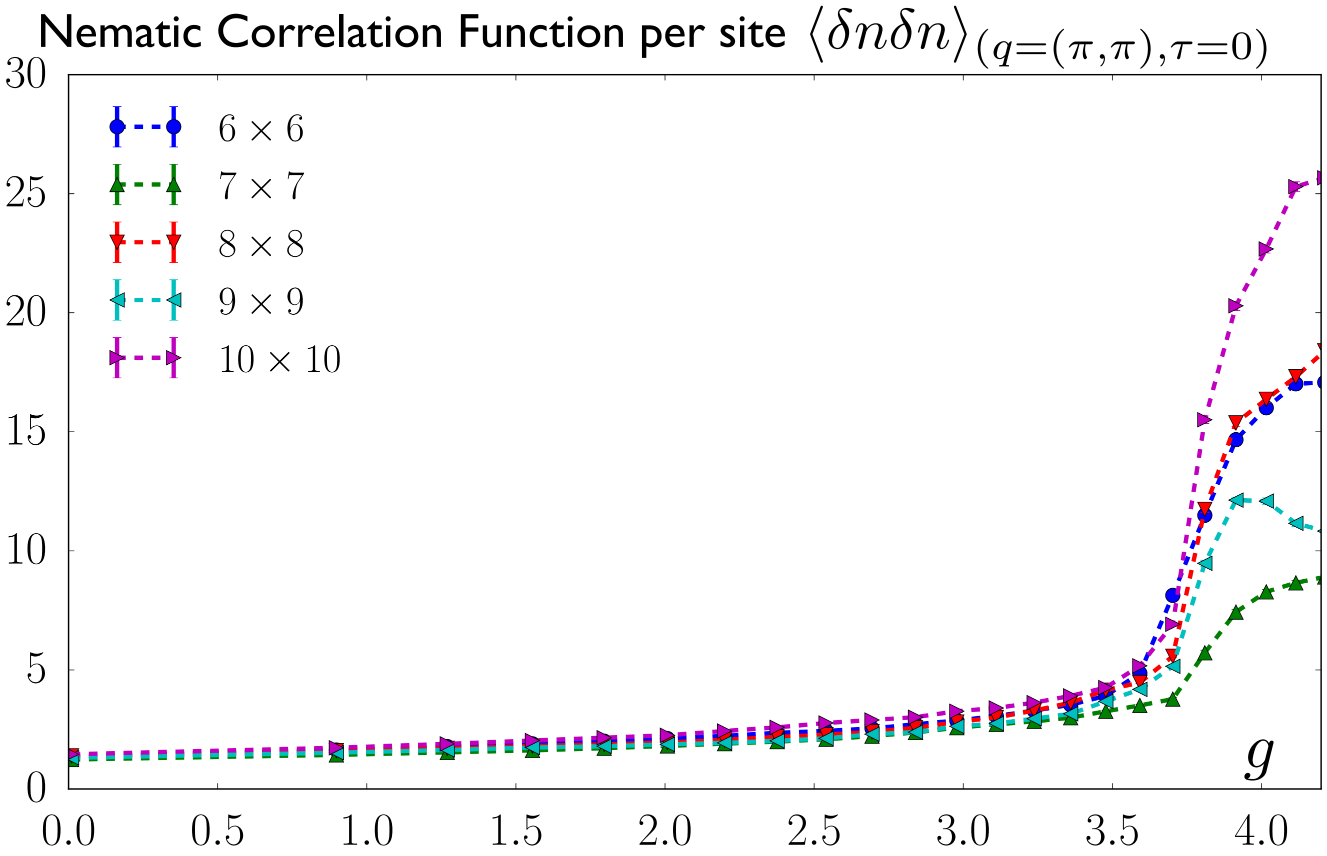
- Superconducting Correlation Function
  - Maximum Diagonal: $\langle \Delta_s \Delta_s \rangle (R, \tau = 0)$



Anti-Ferro Orbital Order

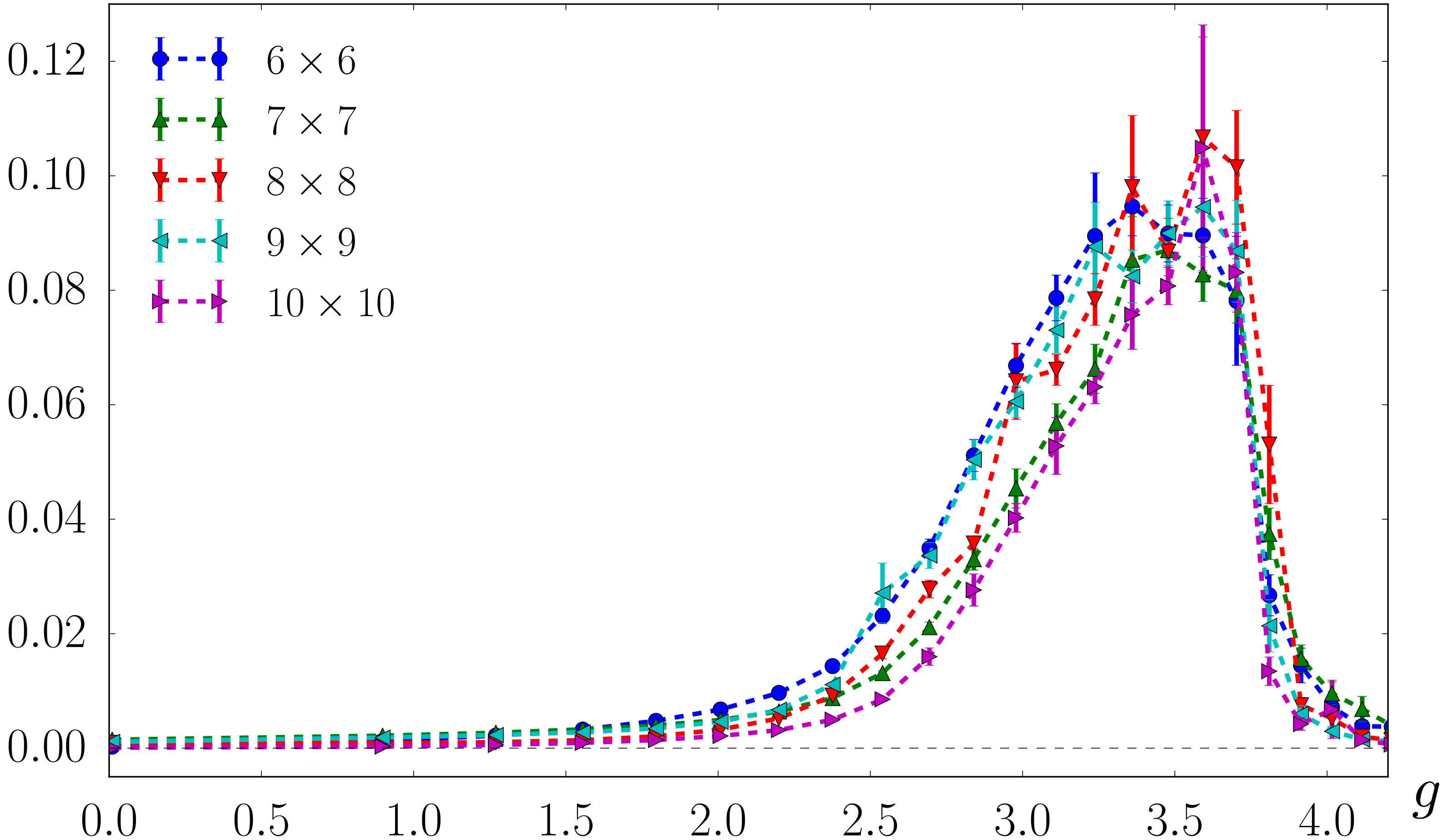
- No Uniform Nematic Order β < 8.0
- Orbital Order at q = (π, π):





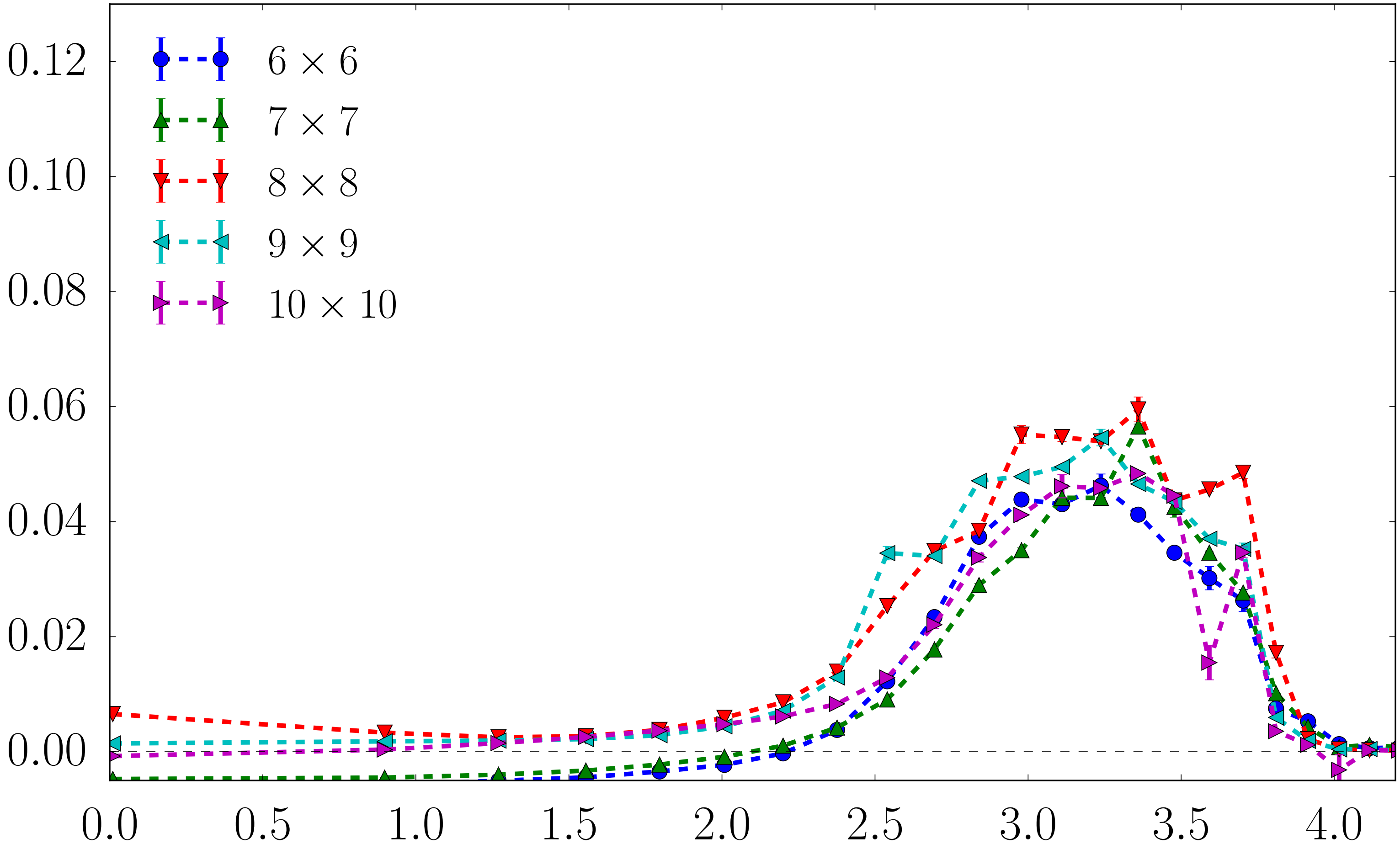
Primary Onsite A_1 Superconductivity

- Pair Correlation function on-site s-wave (A_1) saturates with system size: $\langle \Delta_s \Delta_s \rangle (R, \tau = 0)$



Secondary Extended A_1 Superconductivity

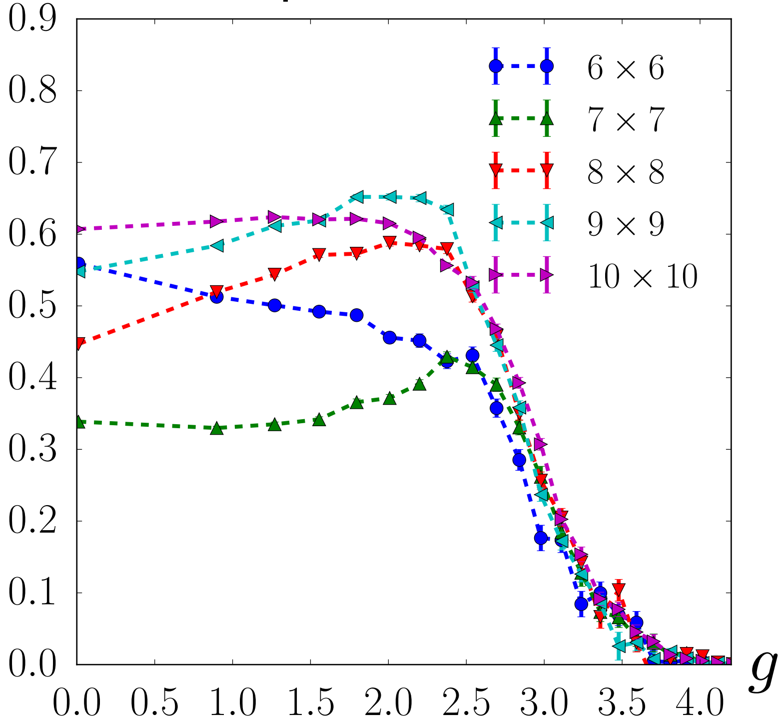
- Pair Correlation function nearest neighbor s-wave ($A_1 = B_1 \times B_1$) channel: $\langle \Delta_s \Delta_s \rangle (R, \tau = 0)$



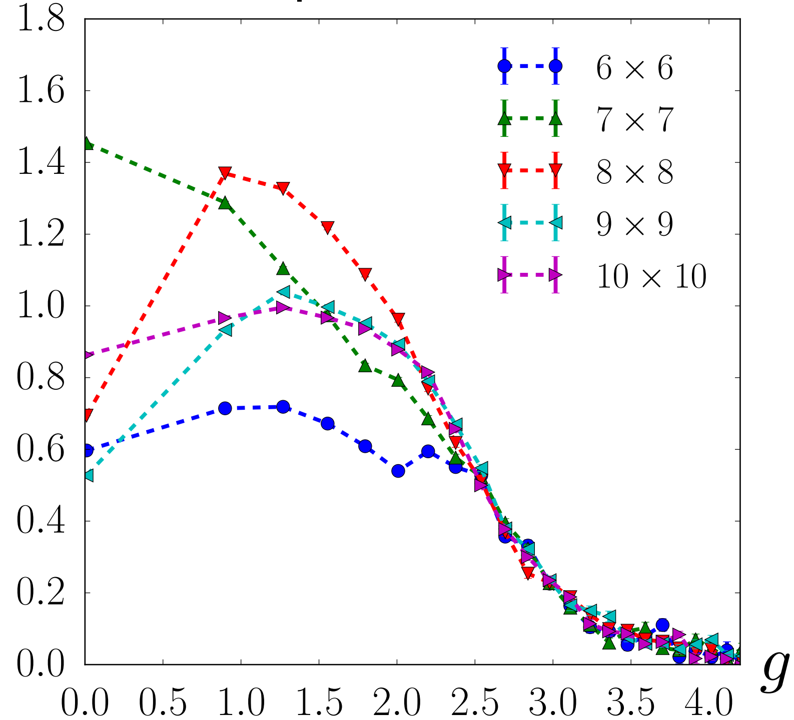
Pseudo-Density-of-States show Insulator

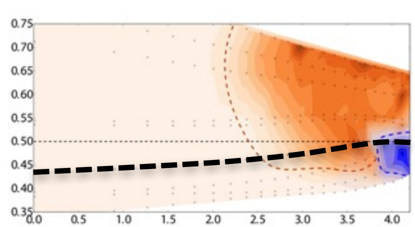
$$\widetilde{N} = \frac{1}{TL^2}\sum_{\mathbf{q}} G\left(\tau = \frac{\beta}{2}, \mathbf{q}\right) = \sum_{\mathbf{q}} \int_{-\infty}^{\infty} \frac{N(\omega, \mathbf{q})\mathrm{d}\omega}{2T\cosh(\omega/2T)}$$

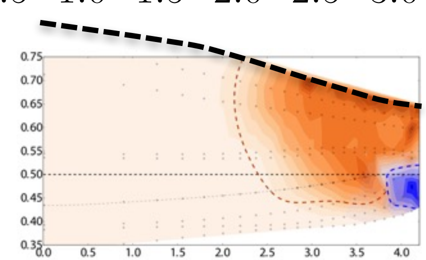
μ = 0.6



μ = 4.0

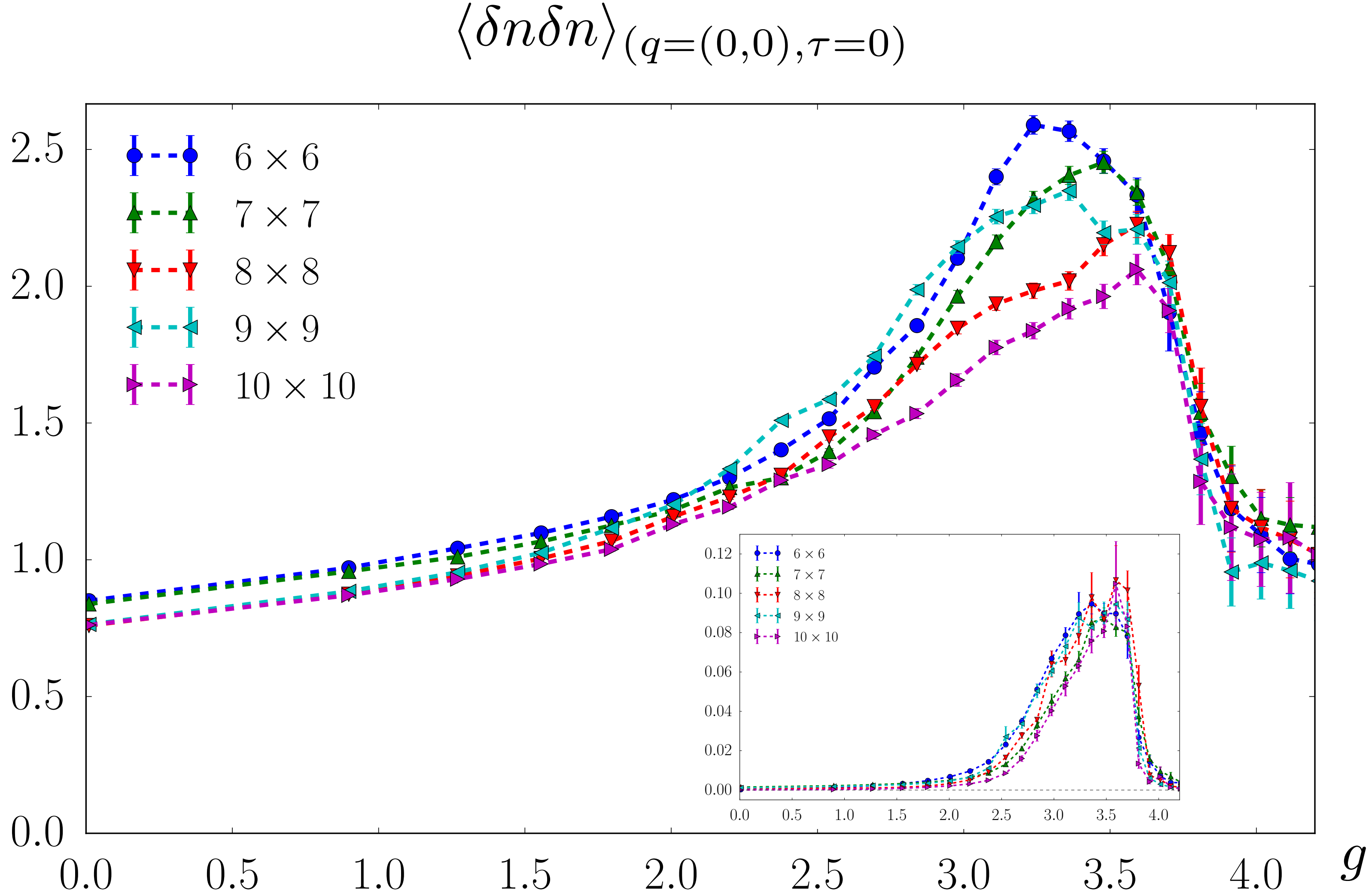






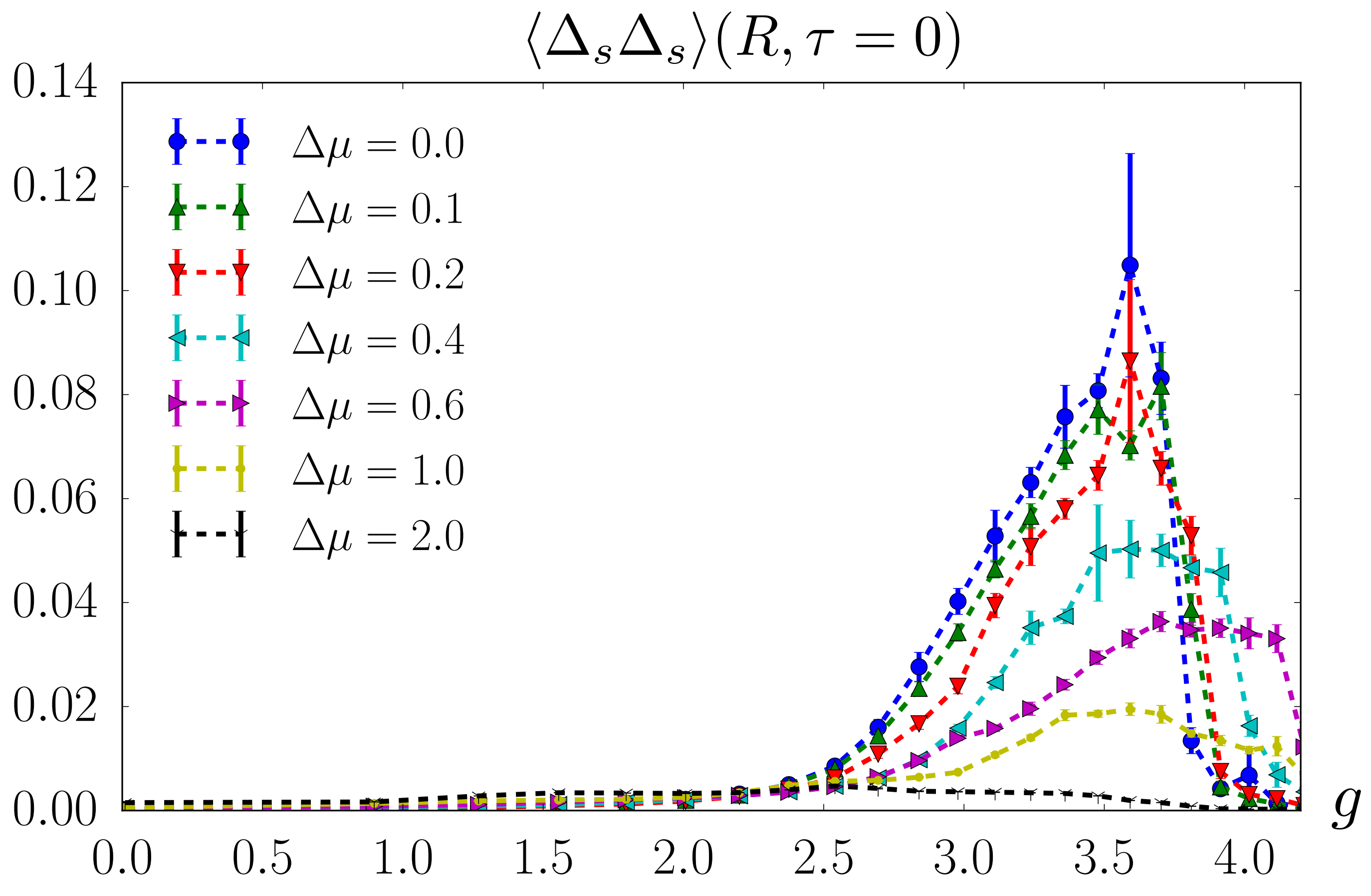
Short range Nematic Fluctuations

- q=0 correlation function vs max. diagonal (β = 8)



Uniform Orbital Ordering Suppresses SC

- Apply external chemical potential difference Δμ
- Forces nematic order; suppresses fluctuations



Conclusions & Open Questions

- Enhanced Superconductivity in two-orbital model
- Different picture than RPA: no Nematic, but SC
- Itinerant picture may hold [Chubukov, Xing PRB (2016)]
  - Small pocket limit
  - Need to extrapolate parquet approximation
- Can we make Quantitative Comparison?
- Lessons for Superconductivity in FeSe
- Ferro- & Antiferro-quadrupole Materials (TmTe, $YbRu_2Ge_2$)

Bond Interactions for Nematic Order

- Change Interactions to Nematic along Bonds

$$H_I = -\frac{g'}{2} \sum_{\langle ij \rangle} [\delta n_i + \delta n_j]^2$$

- Same model; Cross-term prefers q = 0 nematic
- Uniform Nematic, but no Superconductivity seen: