Title: Determinant Quantum Monte Carlo Study of a Multi-orbital Electronic Model: Application to Nematic and Superconducting Order in FeSe

Date: Nov 30, 2015 03:30 PM

URL: http://pirsa.org/15110097

Abstract: <p>The iron chalcogenide FeSe has attracted much recent interest due to a high superconducting transition in monolayer samples. In bulk samples, nematic order is seen without the presence of magnetic order, hinting at the importance of nematic order in determining the monolayer properties. More generally, there has been growing evidence of the importance of nematic fluctuations in a variety of strongly correlated high-temperature superconductors. We study an effective two band model of the iron-pnictides with interactions that capture the nematic ordering arising from spontaneous symmetry breaking between the two orbitals. These models are sign-problem free and can be simulated in an unbiased fashion using Determinant Quantum Monte Carlo. We find a variety of unexpected orders and consider the effects of the nematic fluctuations on superconductivity. </p>

Determinant Quantum Monte Carlo Study of a Multi-orbital Electronic Model

Application to Nematic and Superconducting Order in FeSe

Philipp T. Dumitrescu
UC Berkeley

Perimeter Seminar, 30th Nov. 2015

Maksym Serbyn
(Berkeley)

Richard Scalettar
(Davis)

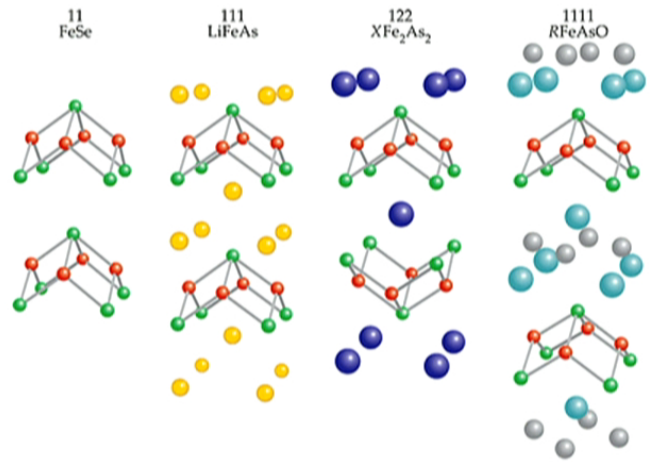
Ashvin Vishwanath
(Berkeley)

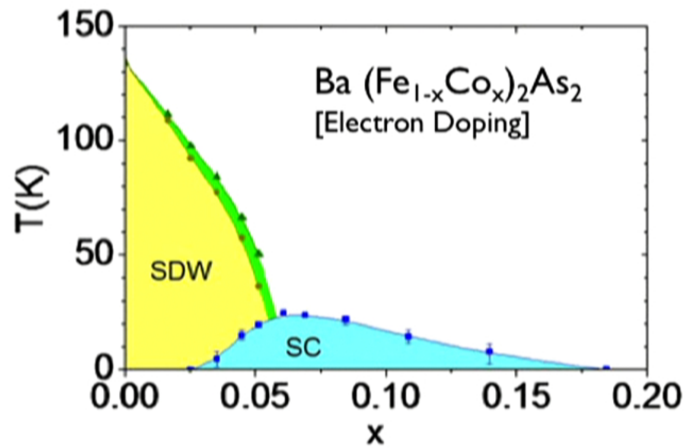
Outline

- Iron based High-Temperature Superconductors
- Nematic Quantum Criticality
- Two Band Model for Nematic Order
- Determinant Monte Carlo Study

Iron Based Superconductors

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



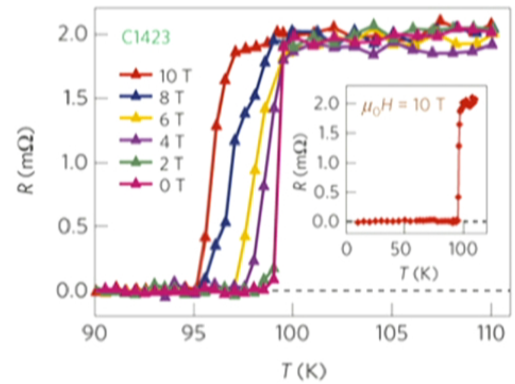


[Chu et. al. Phys. Rev. B 79, 014506 (2009)]

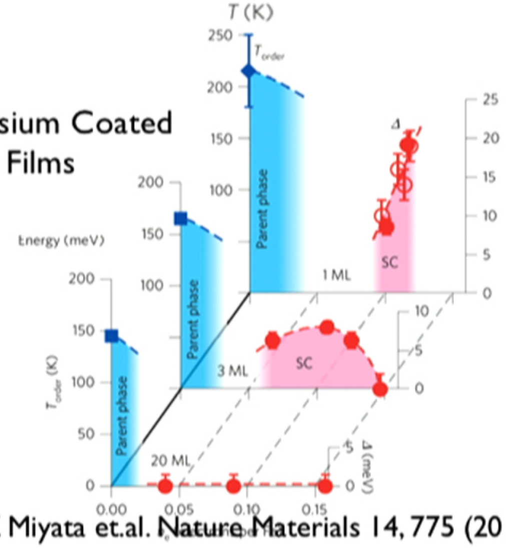
FeSe

- Undoped Bulk Properties:
  - Nematic order
  - No magnetic order without external pressure
  - Superconducting T_c ~ 8K
- Highly Doped Bulk
  - e.g. K intercalation
  - Enhanced T_c ~ 40-50 K
- Monolayer on $SrTiO_3$
  - Enhanced T_c ~ 65 K to 109 K
- Many explanations:
  - Exotic Mechanisms
  - Substrate Effects

FeSe / $SrTiO_3$ (Nb-doped)



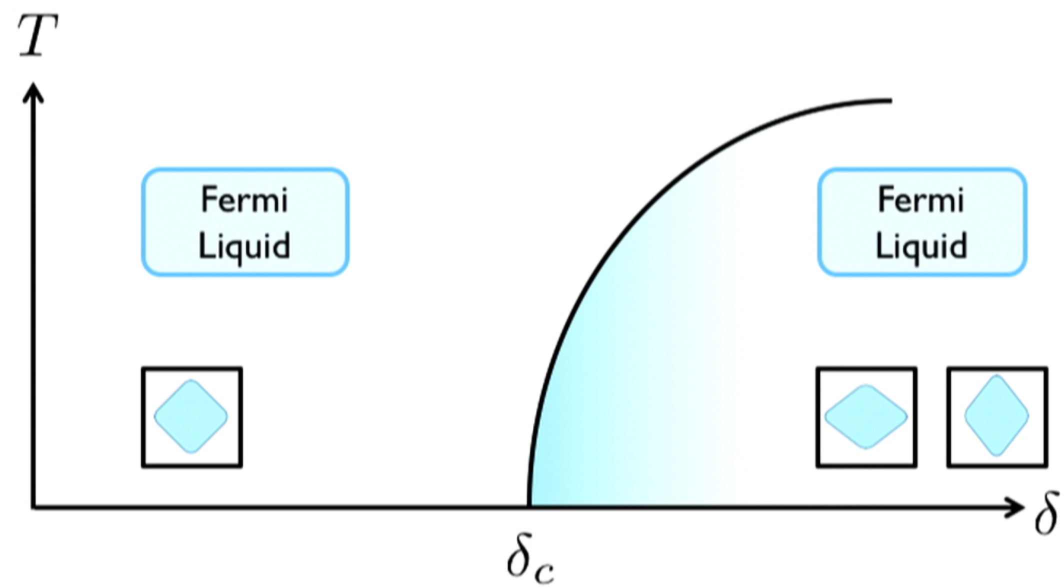
Potassium Coated FeSe Films



[Y. Miyata et.al. Nature Materials 14, 775 (2015)]

Nematic Quantum Criticality

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



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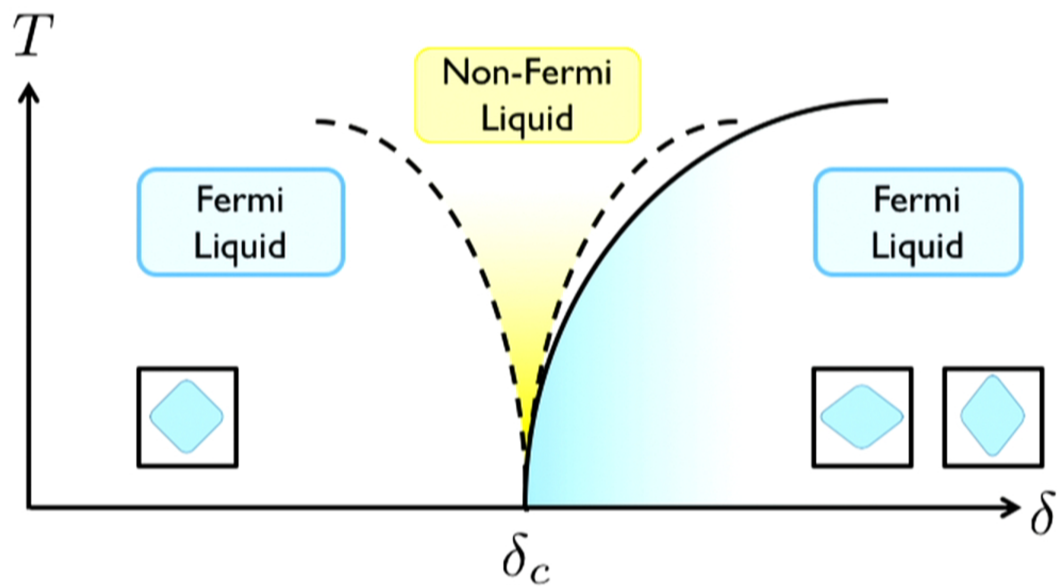

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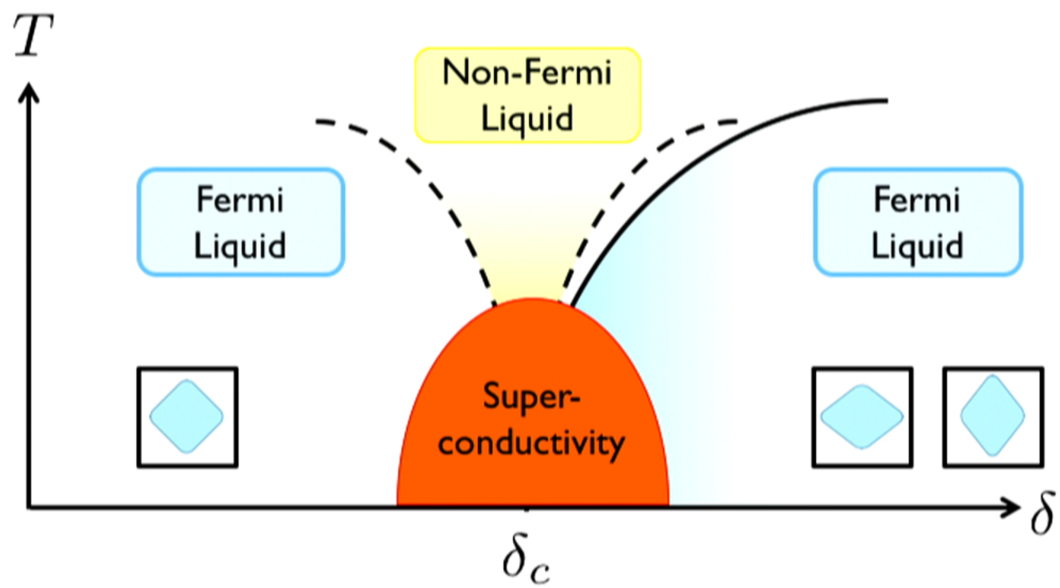
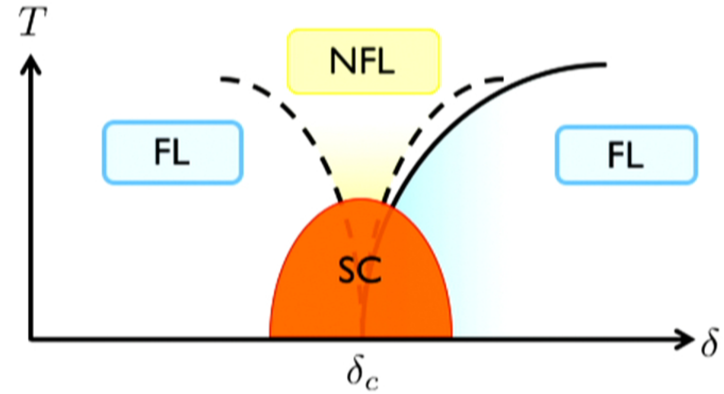
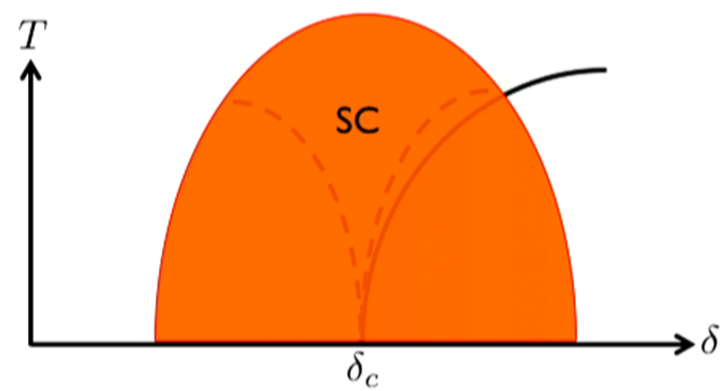


Pairing vs. Quasiparticle Destruction

- Nematic Fluctuations:
  - Enhance Pairing (SC) in all channels
  - Destroy Fermion Quasiparticles
- Open Questions
  - Does Incoherent Critical Region Survive?
  - Universal exponents above dome?

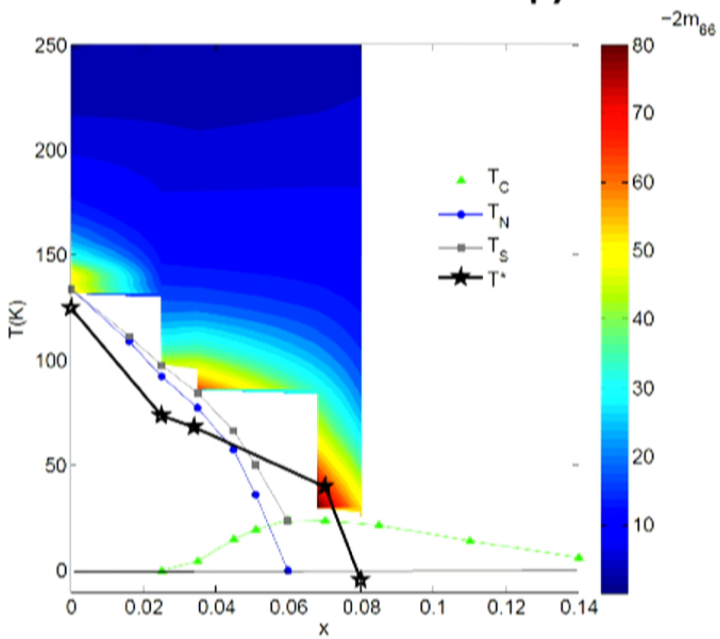




[Metlitski, Mross, Sachdev, Senthil (2014); Schattner, Lederer, Kivelson, Berg (2015); ...]

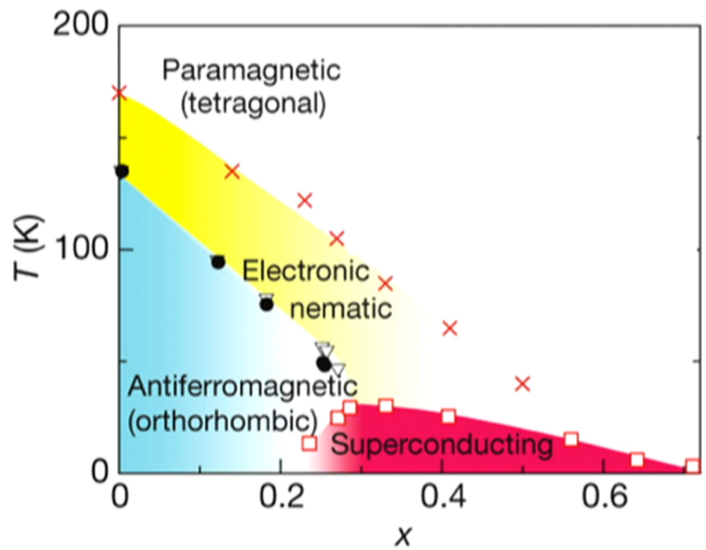
Experimental Evidence of Nematicity

- $Ba(Fe_{1-x}Co_x)_2As_2$
  Nematic susceptibility
  via resistance anisotropy



[Fisher Group: arXiv:1503.00402 &
Chu et.al. Science 337, 710 (2012)]

- $BaFe(As_{1-x}P_x)_2$
  Nematic fluctuations
  via torque magnetometry



[S. Kasahara et. al. Nature 486, 382 (2012)]

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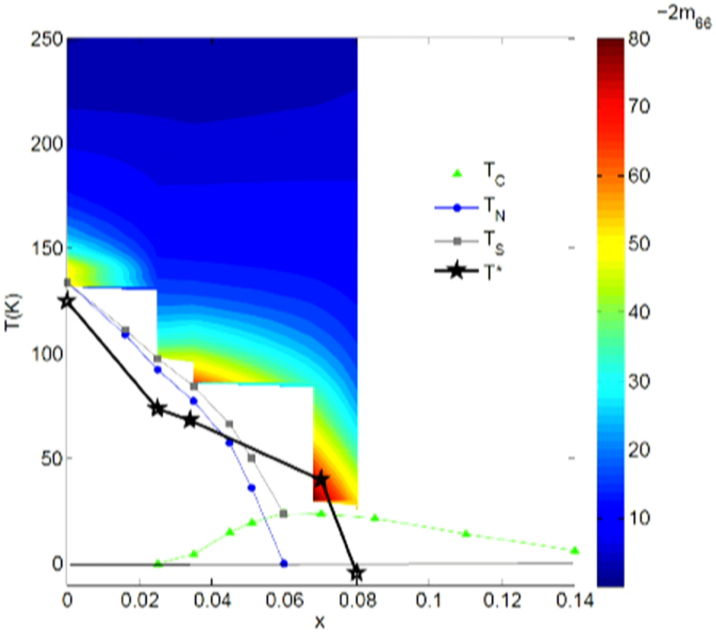

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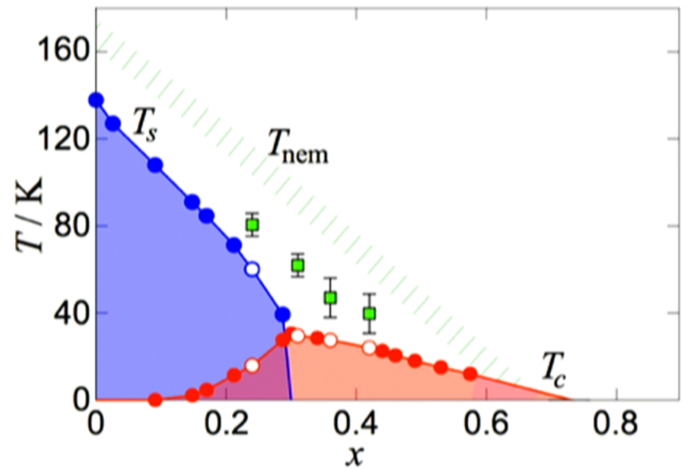
- $BaFe(As_{1-x}P_x)_2$
  Nematic fluctuations
  via reflectivity (pump-probe)

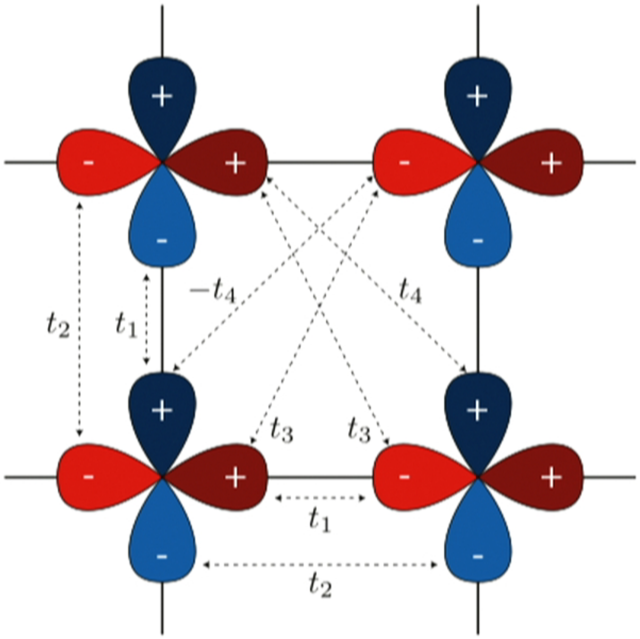


[Orenstein Group: arXiv:1507.03981]

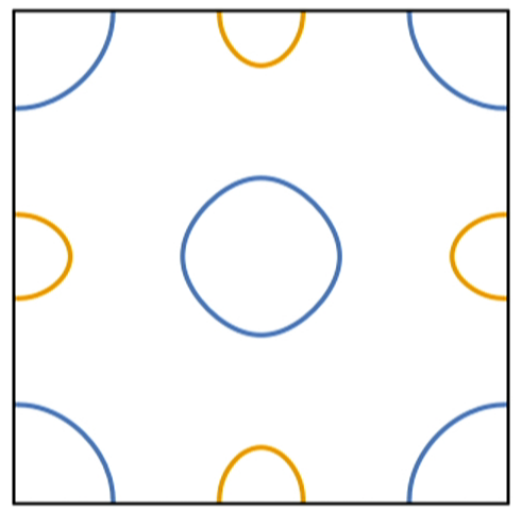
Two Band Model

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

d_{xz}, d_{yz} orbitals

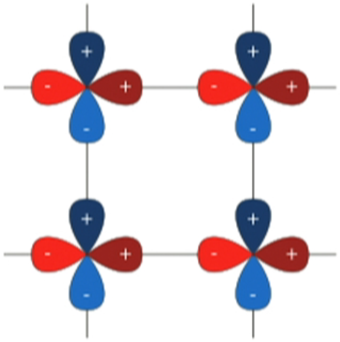


Fermi Surface: Electron & Hole Pockets



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:

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

$$(g < 0)$$

- Nematicity: Orbital Symmetry Breaking

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

- Both attractive and repulsive Hubbard-like terms

Numerical Simulations

- Challenges:
  - Quantum Fluctuations
  - Metallic: Many Energy Scales
  - Sign Problem for Fermions
- Determinant Quantum Monte Carlo
  - Unbiased Sampling of the Fermions
  - Engineer physics in sign problem free model

    [cf. Schattner, Lederer, Kivelson, Berg; arXiv:1511.03282]

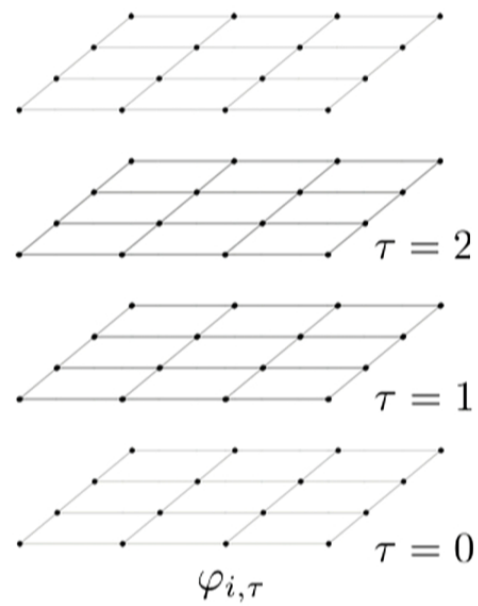
Determinant Quantum Monte Carlo

- Sample Full Path Integral
  - Integrate out Fermions for Hubbard–Stratonovich Fields

$$Z \sim \int D[c^*, c] e^{-S_f}$$

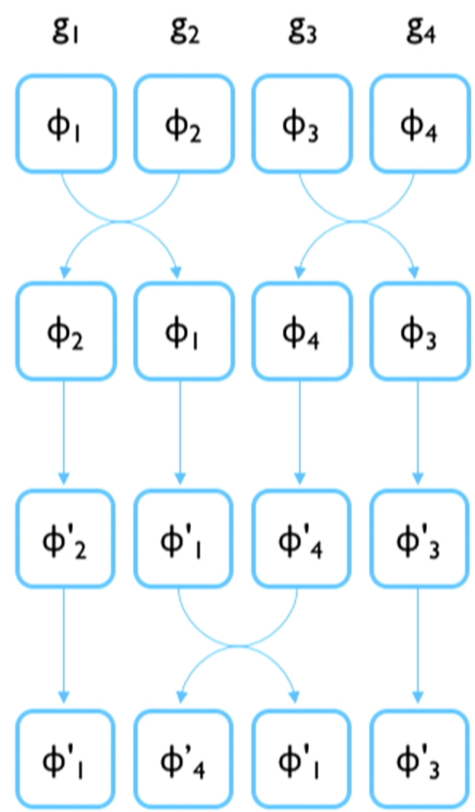
$$Z \sim \int D[\varphi]\ e^{-S_b(\varphi)} \det\left[G_\uparrow^{-1}(\varphi) G_\downarrow^{-1}(\varphi)\right]$$

- Spin Symmetry avoids Fermion Sign Problem
- Lattice sizes < 2 x 12 x 12



Code & Parallel Tempering

- New Code
- Parallel Tempering
  - No global updates
  - Improved ergodicity
  - Feedback Optimization
- Some technical values
  - $\Delta\tau = 1/16$
  - Stabilizing SVDs: every 2 $\Delta\tau$
  - min. 10,000 Sweeps

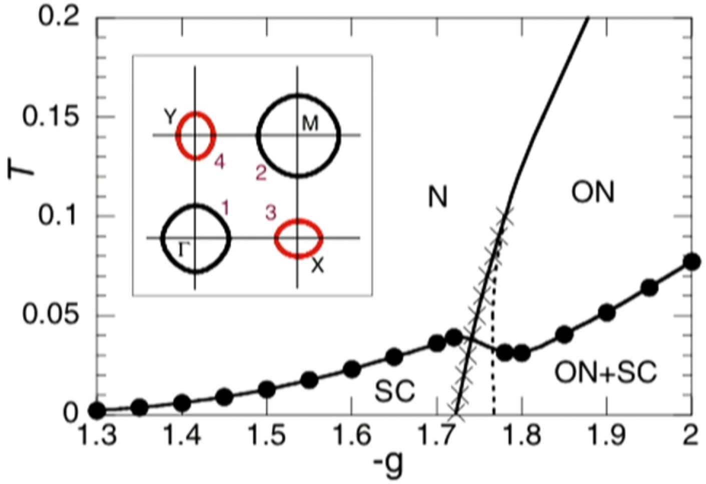


Weak Coupling Expectations

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

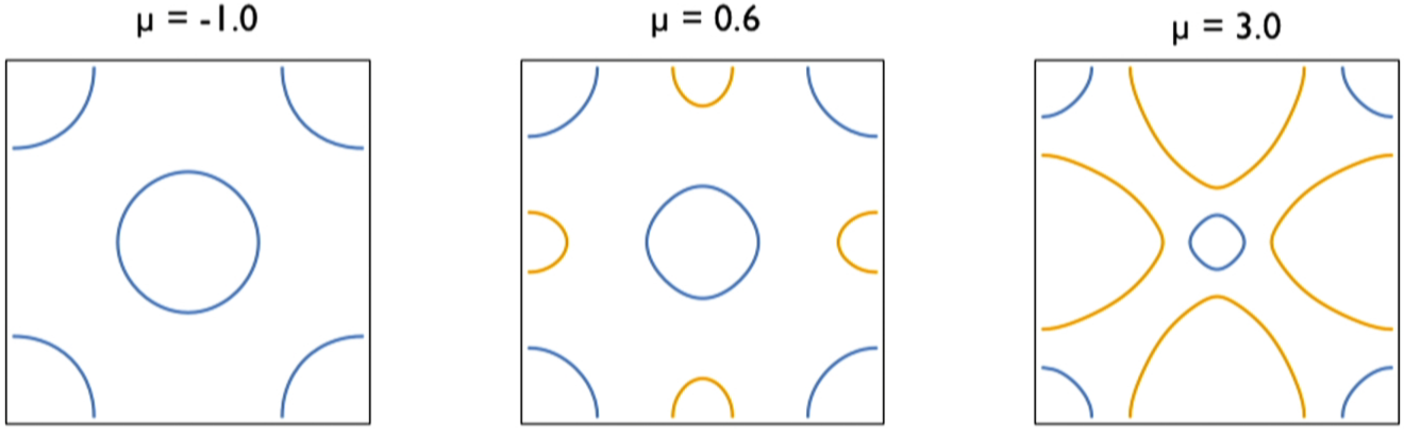
$$H_I = \frac{g}{2}\sum_i \delta n_i \delta n_i$$

- Weak Coupling (RPA)
  - Finite g transition to uniform nematic order
  - Supercondutivity Peak in Eliashberg Theory

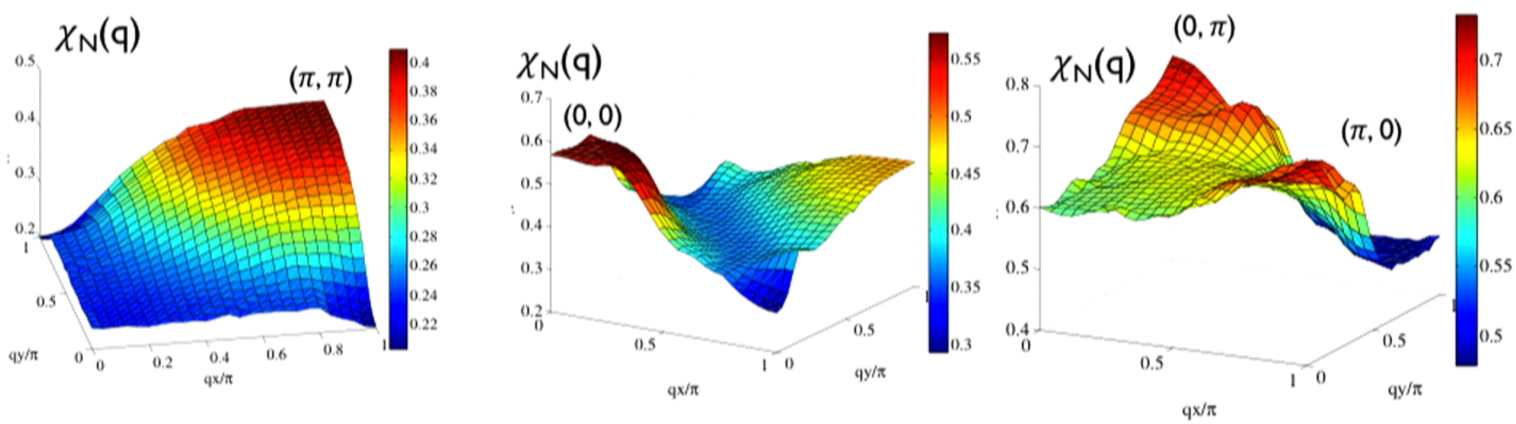


[Yamase & Zeyher PRB, 88, 180502 (2013)]

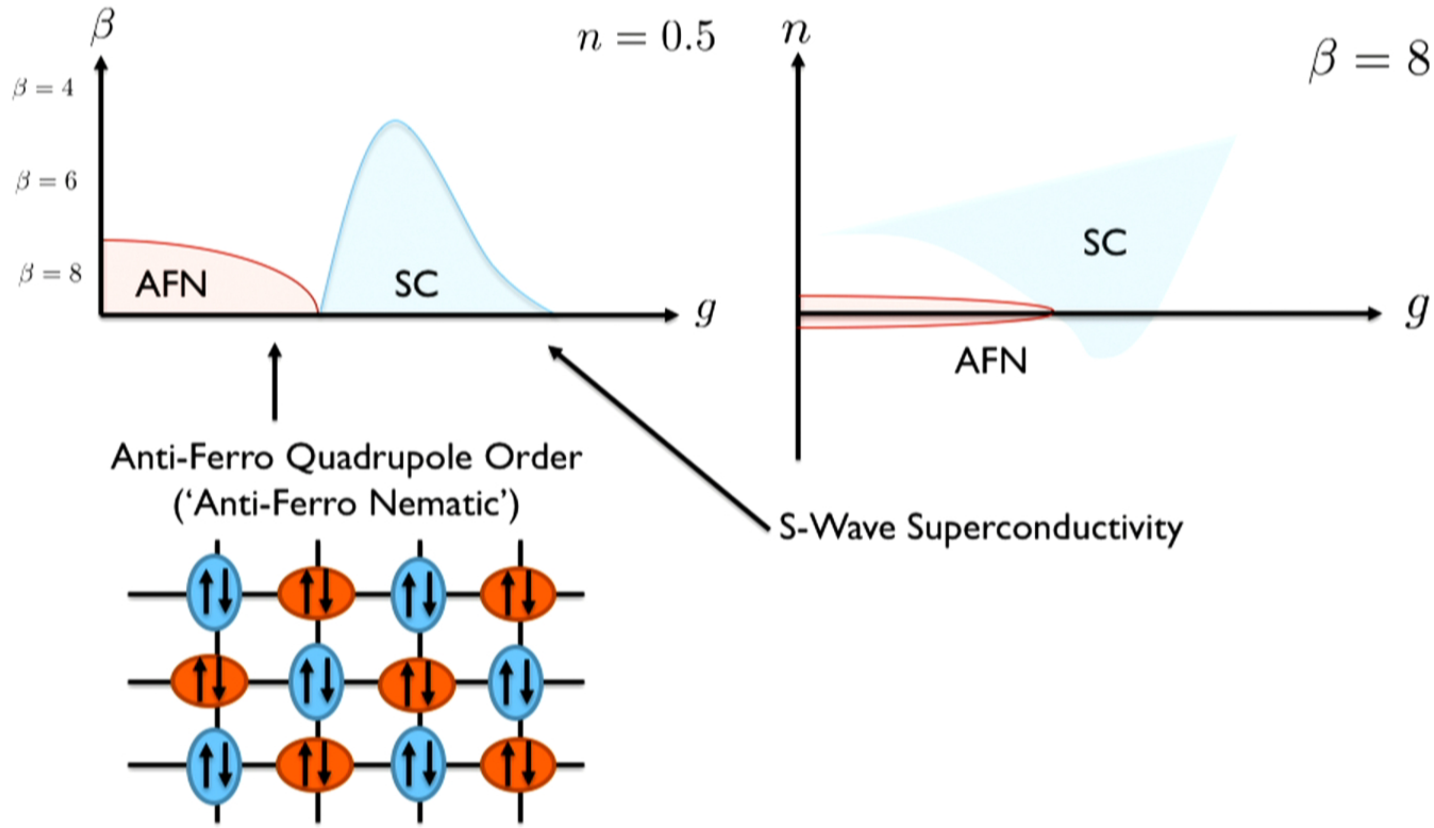
RPA Ordering Sensitive to Doping



RPA Onsite Nematic Susceptibility $\chi_N(q)$ at $\beta = 16\ t_1$



Proposed Phase Diagram



Measured Quantities

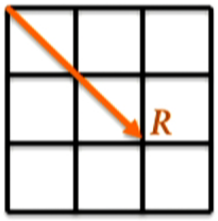
- Nematic Correlation Function:

$$\langle \delta n \delta n \rangle_{(q,\tau=0)}/L^2$$

- Binder Ratio for Nematic Order

$$B = 1 - \frac{1}{3} \frac{\langle \phi^4 \rangle}{\langle \phi^2 \rangle^2}$$

- Superconducting Correlation Function
  - Maximum Diagonal: $\langle \Delta_s \Delta_s \rangle (R, \tau = 0)$
  - Fourier Q = 0: $\langle \Delta_s \Delta_s \rangle (q = 0, \tau = 0)/L^2$



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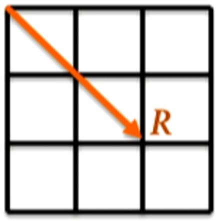
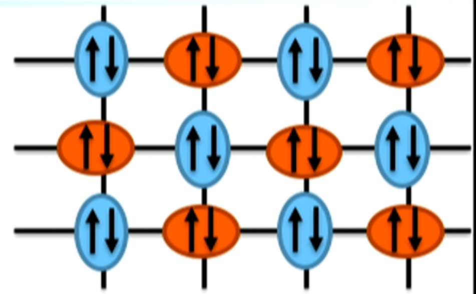
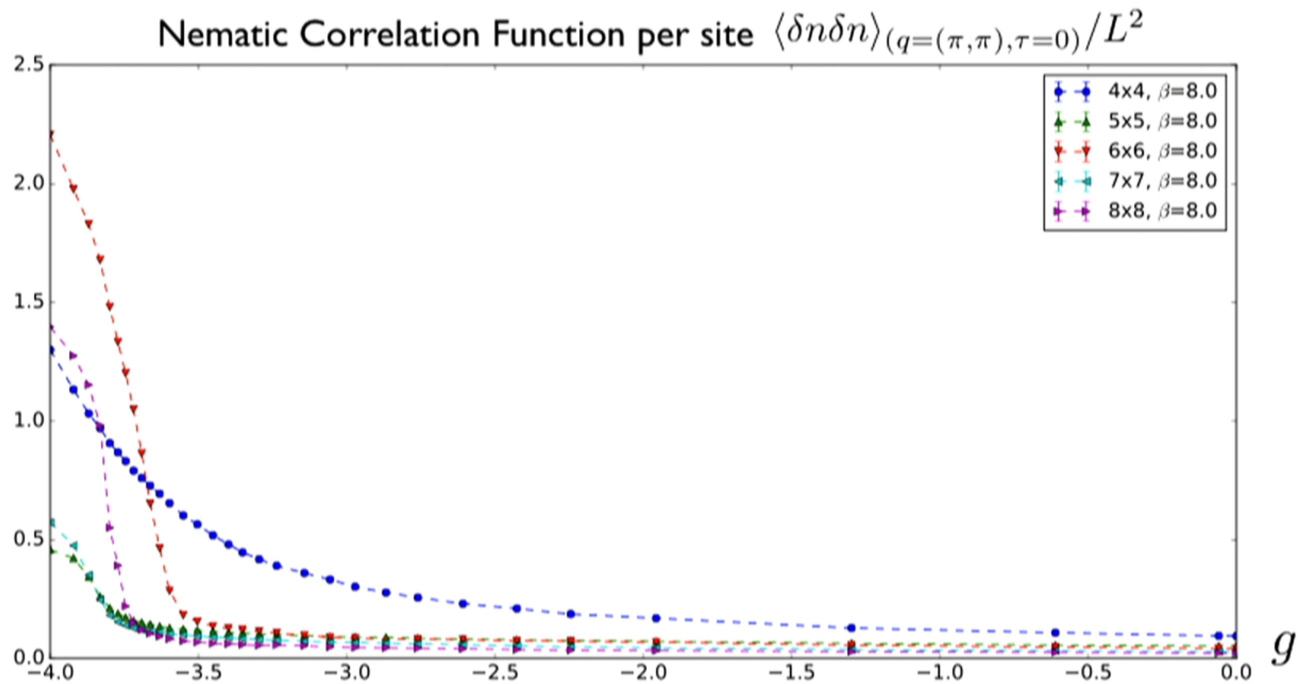


'Anti-Ferro Nematic' Order

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

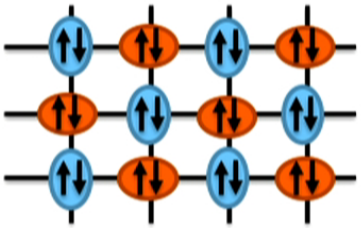




Binder Ratio Fingerprints Transition

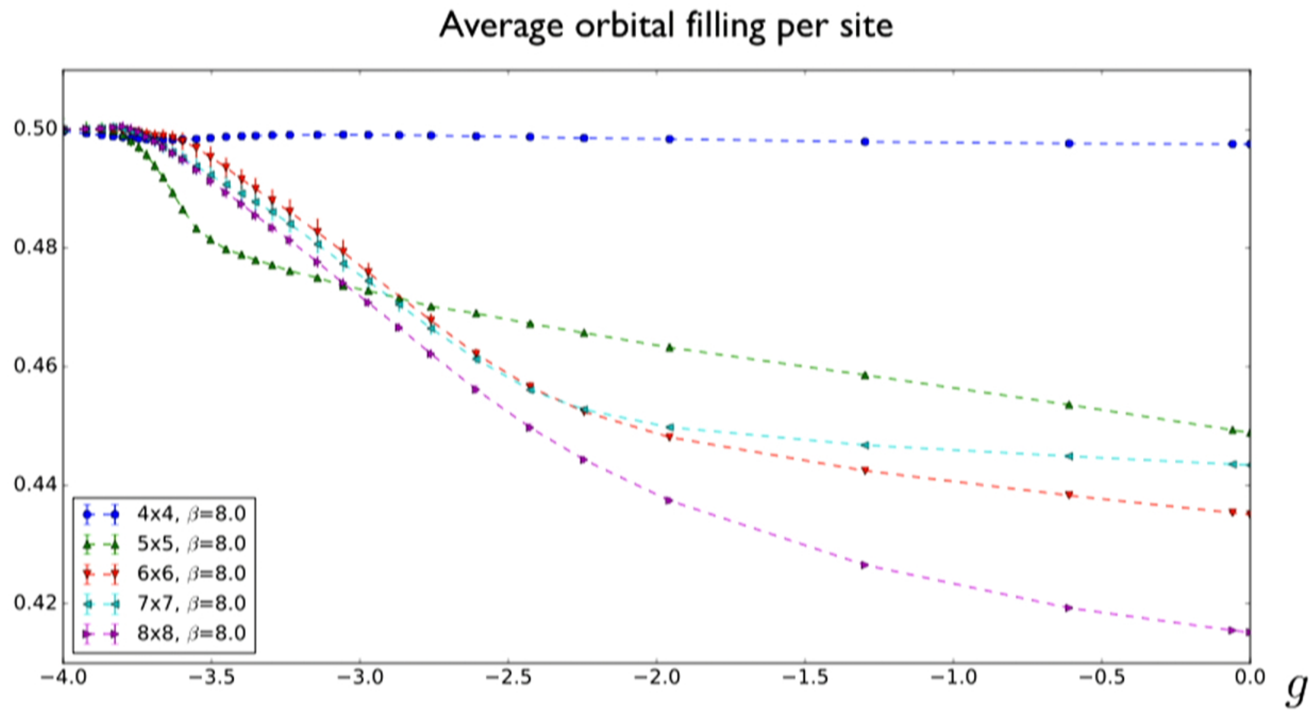
- Binder Ratio for Nematic order at q = (π, π). :

$$= 1 - \frac{1}{3} \left. \frac{\langle \phi^4 \rangle}{\langle \phi^2 \rangle^2} \right|_{q=(\pi,\pi),\omega=0}$$



System Pulled towards Half Filling

- Anti-Ferro Nematic arises only at Half Filling



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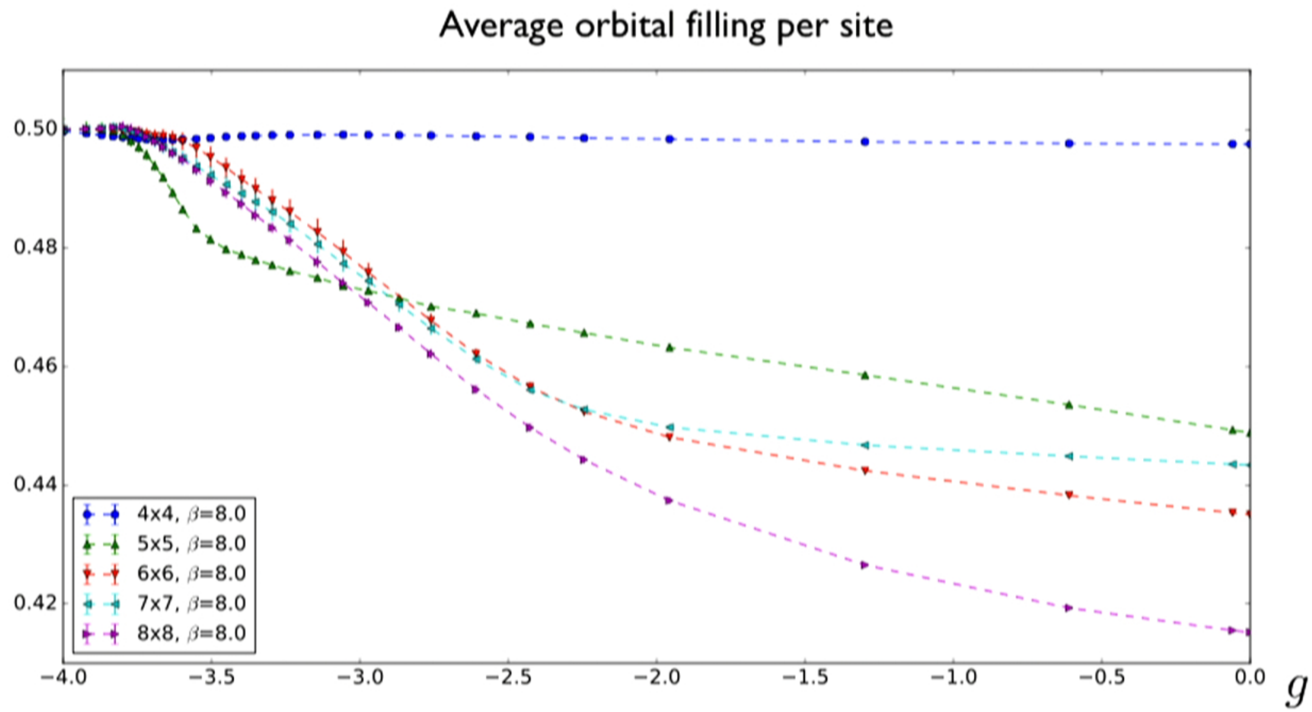
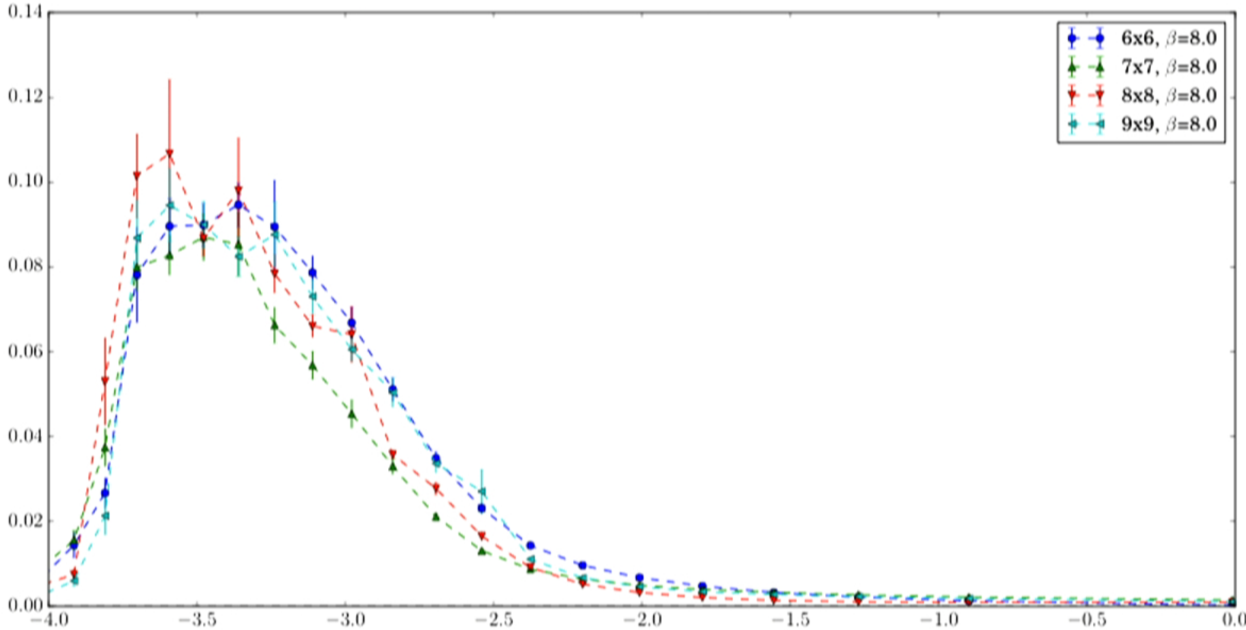


Evidence of Superconductivity

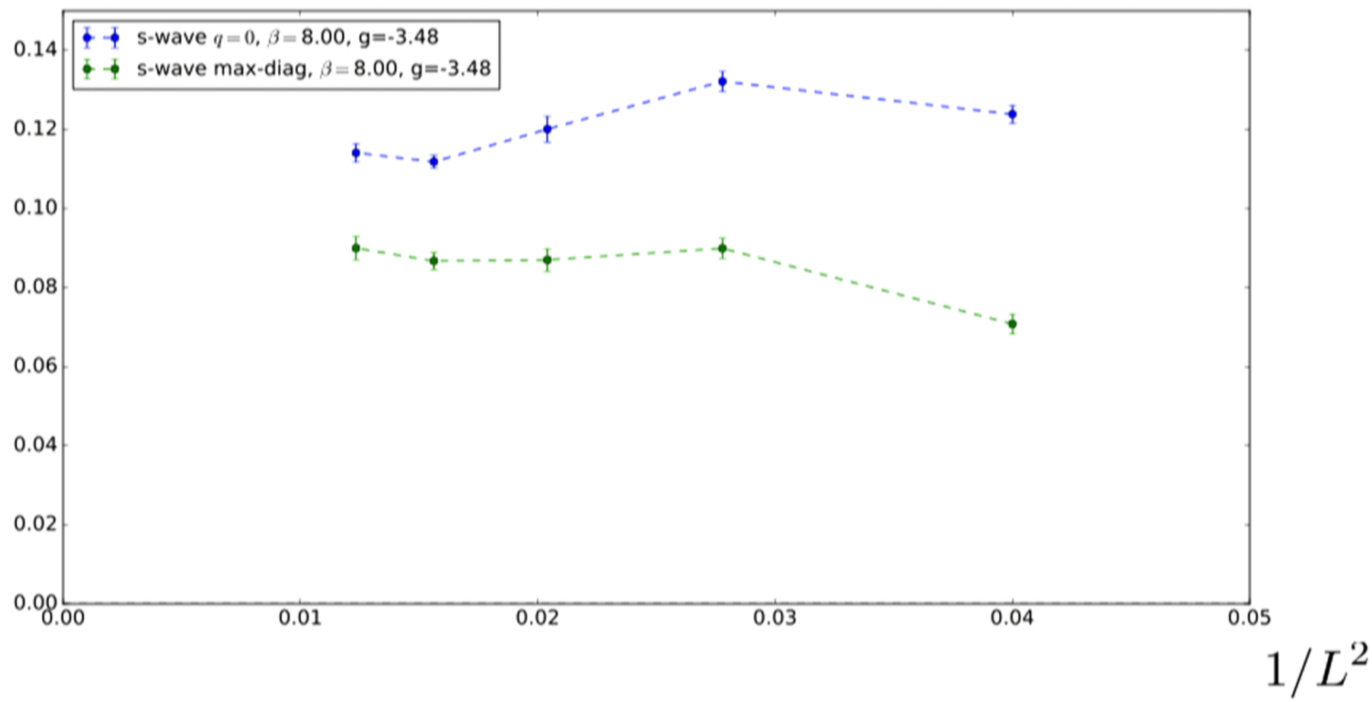
- Pair Correlation function in on-site s-wave (A_1) channel saturates with system size: $\langle \Delta_s \Delta_s \rangle (R, \tau = 0)$



Evidence of Superconductivity

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

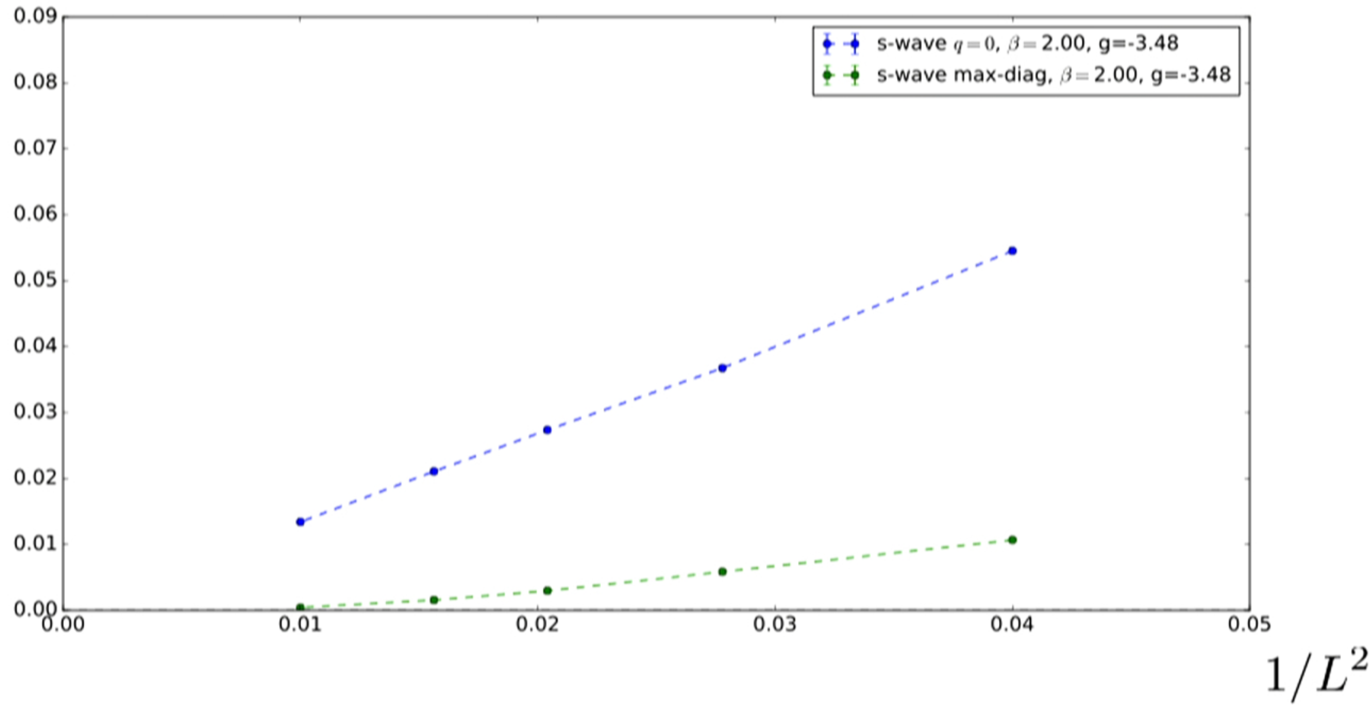
$$\langle \Delta_s \Delta_s \rangle (q=0, \tau=0)/L^2 \quad \text{vs} \quad \langle \Delta_s \Delta_s \rangle (R, \tau=0)$$



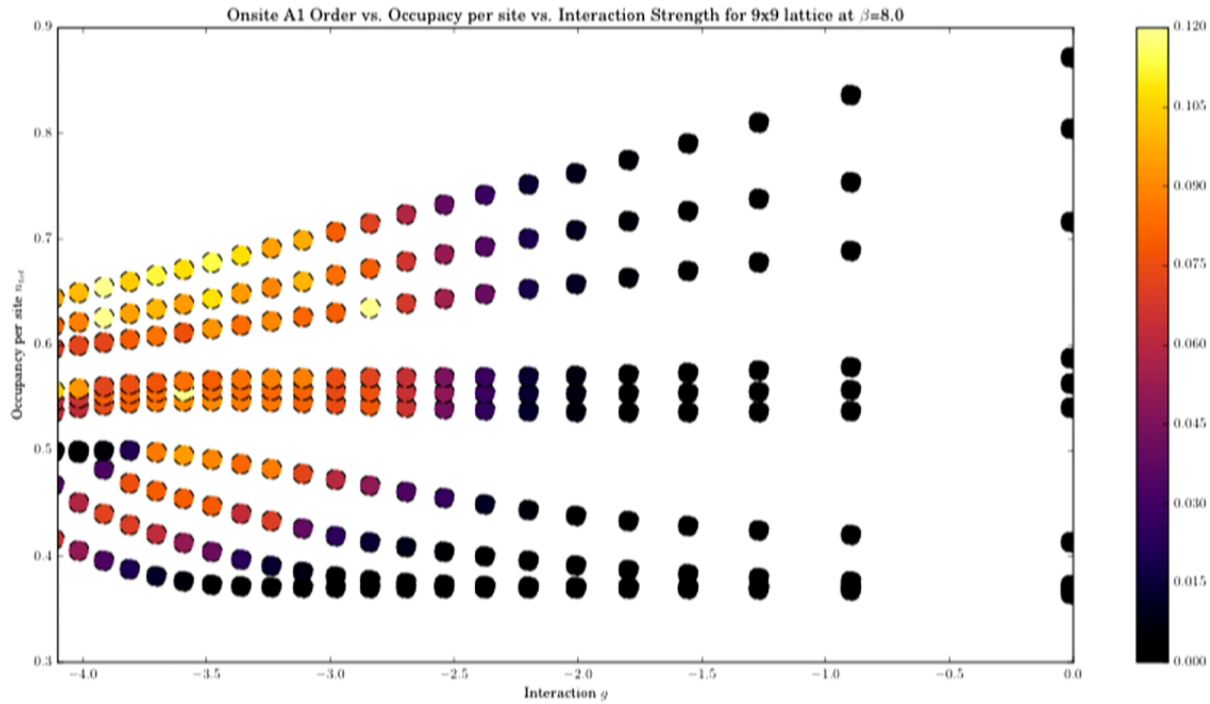
Evidence of Superconductivity

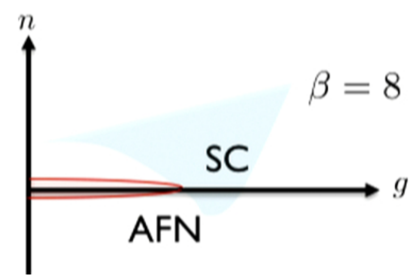
- q=0 correlation function vs max. diagonal (β = 2)

$\langle \Delta_s \Delta_s \rangle (q=0, \tau=0)/L^2$ vs $\langle \Delta_s \Delta_s \rangle (R, \tau=0)$



Changing Doping (β = 8)

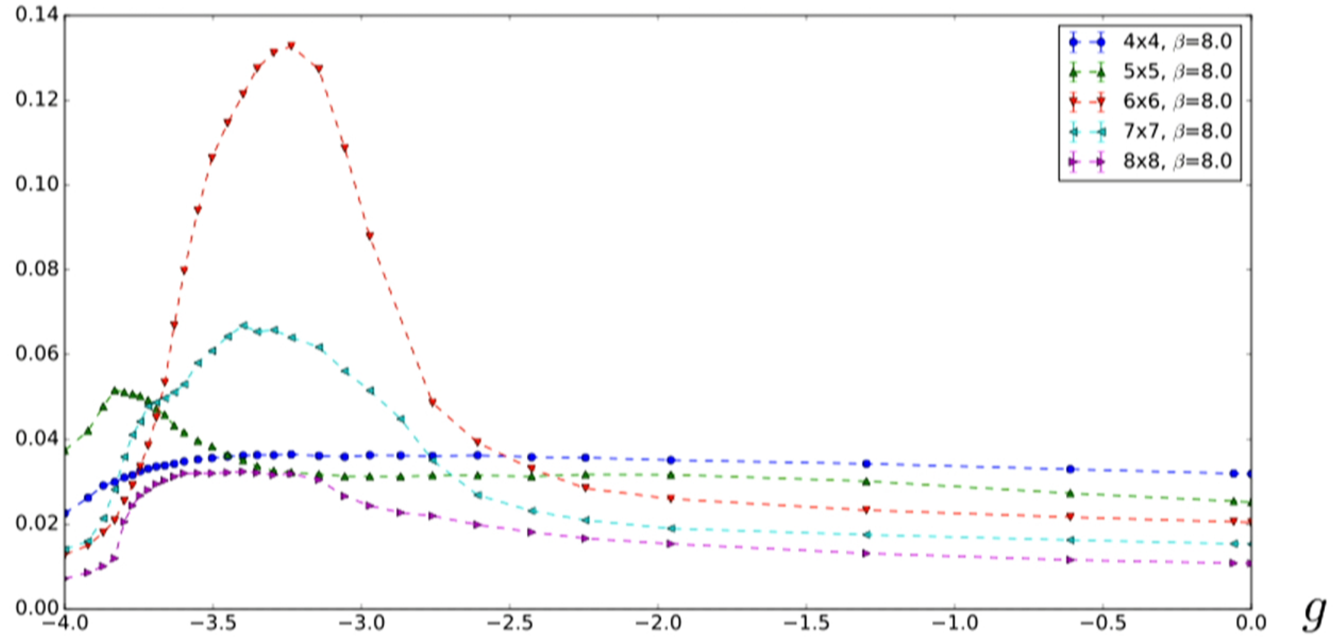




Uniform Nematic Fluctuations

- Signs of uniform Nematic fluctuations

Nematic Correlation Function per site $\langle \delta n \delta n \rangle_{(q=(0,0),\tau=0)}/L^2$

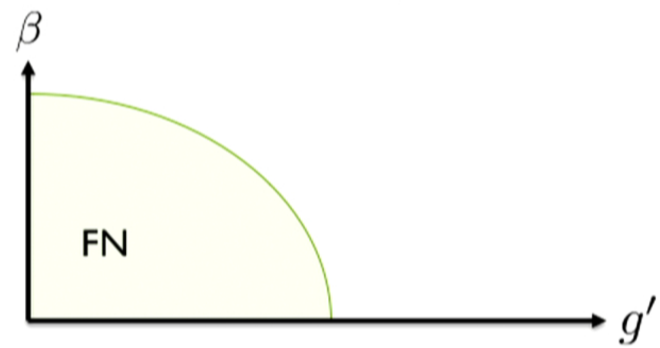


Bond Nematic Interactions

- Change Interactions to Bond Nematic

$$H_I = \frac{g'}{2} \sum_{\langle ij \rangle} [\delta n_i + \delta n_j]^2 \qquad (g' < 0)$$

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



Bond Nematic Interactions

- Model to prefer uniform (q = 0) nematic order

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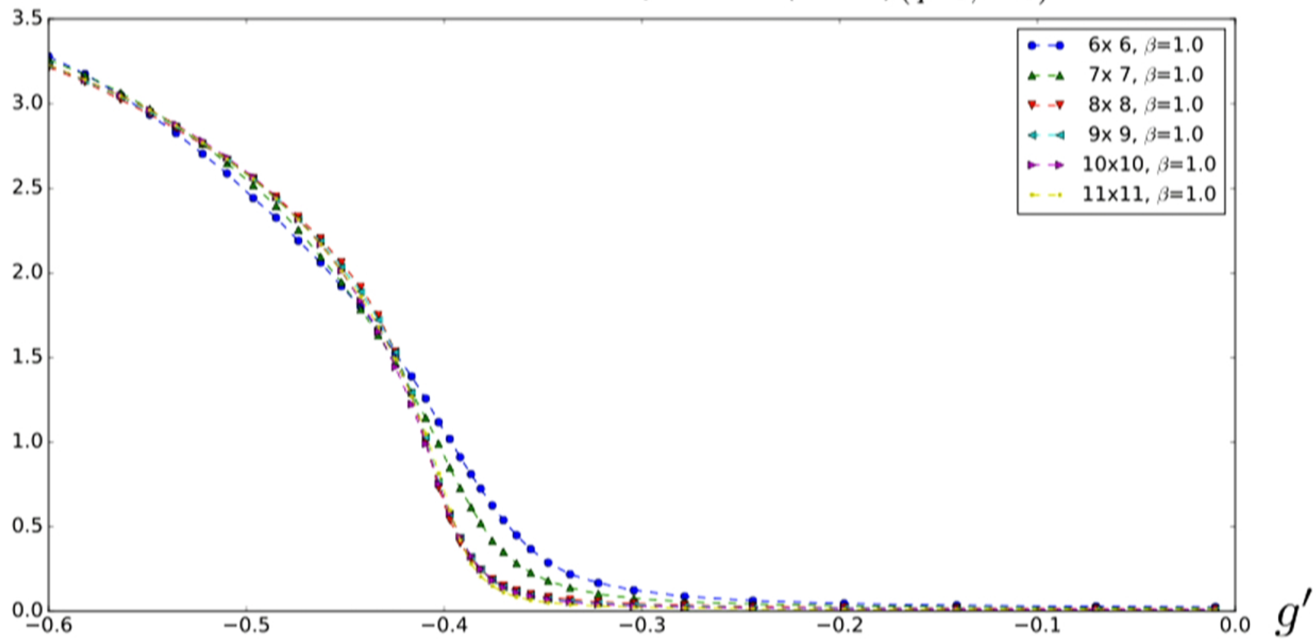
Nematic Correlation Function per site $\langle \delta n \delta n \rangle_{(q=0,\tau=0)}$



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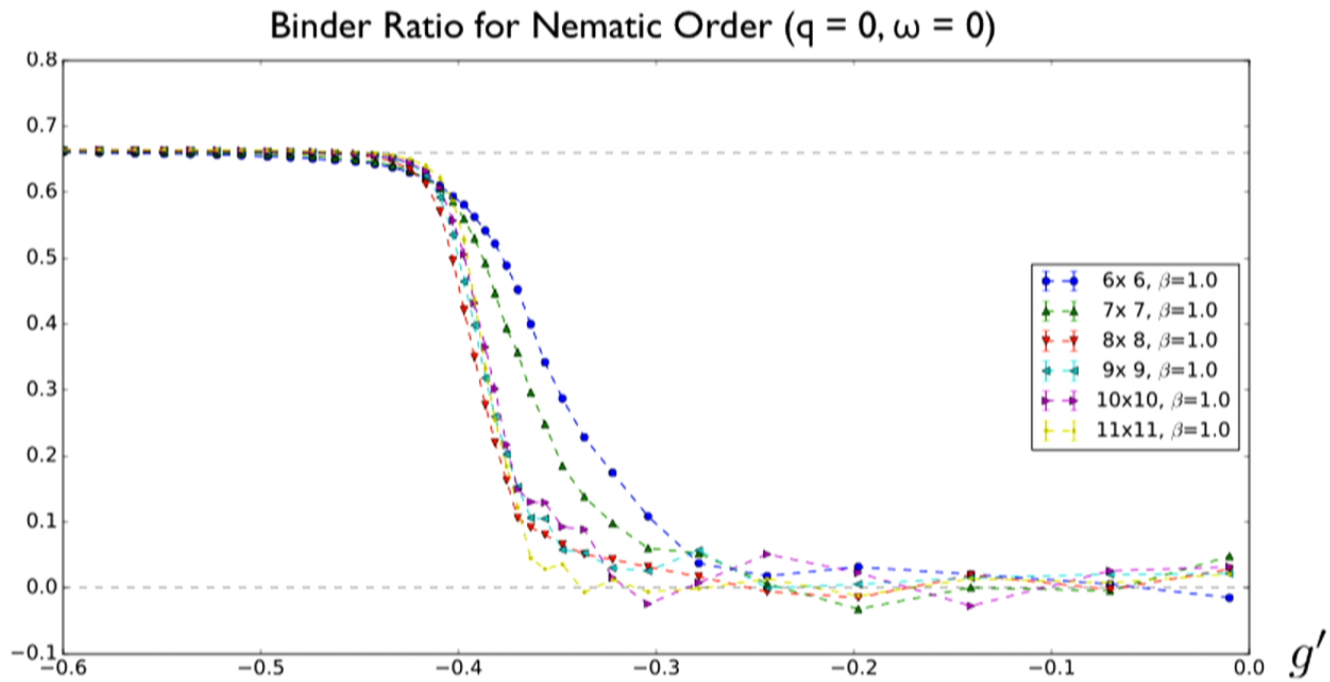

Conclusions & Open Questions

- Enhance Superconductivity in two-orbital model
- Different picture than RPA
  - No Uniform Nematic Order
  - Strongly enhanced Superconductivity
- Is there an uniform nematic *phase*?
- Details of the Superconductivity for FeSe