Superconductivity and charge density wave physics near an antiferromagnetic quantum critical point: insights from Quantum Monte Carlo studies

Xiaoyu Wang

James Frank Institute

University of Chicago

ICTP Talk, Thursday 11/16/2017

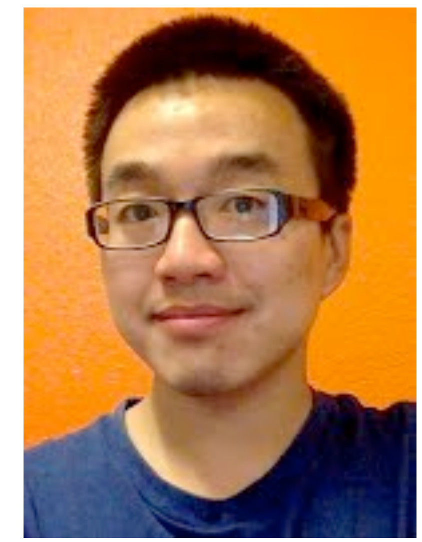
Phys. Rev. B 95, 174520 (2017)
arXiv:1710.02158

Collaborators

Rafael Fernandes
(U. Minnesota)

Erez Berg
(U. Chicago)

Yoni Schattner
(Stanford)



Yuxuan Wang
(U. Illinois)

DEPARTMENT OF ENERGY · UNITED STATES OF AMERICA

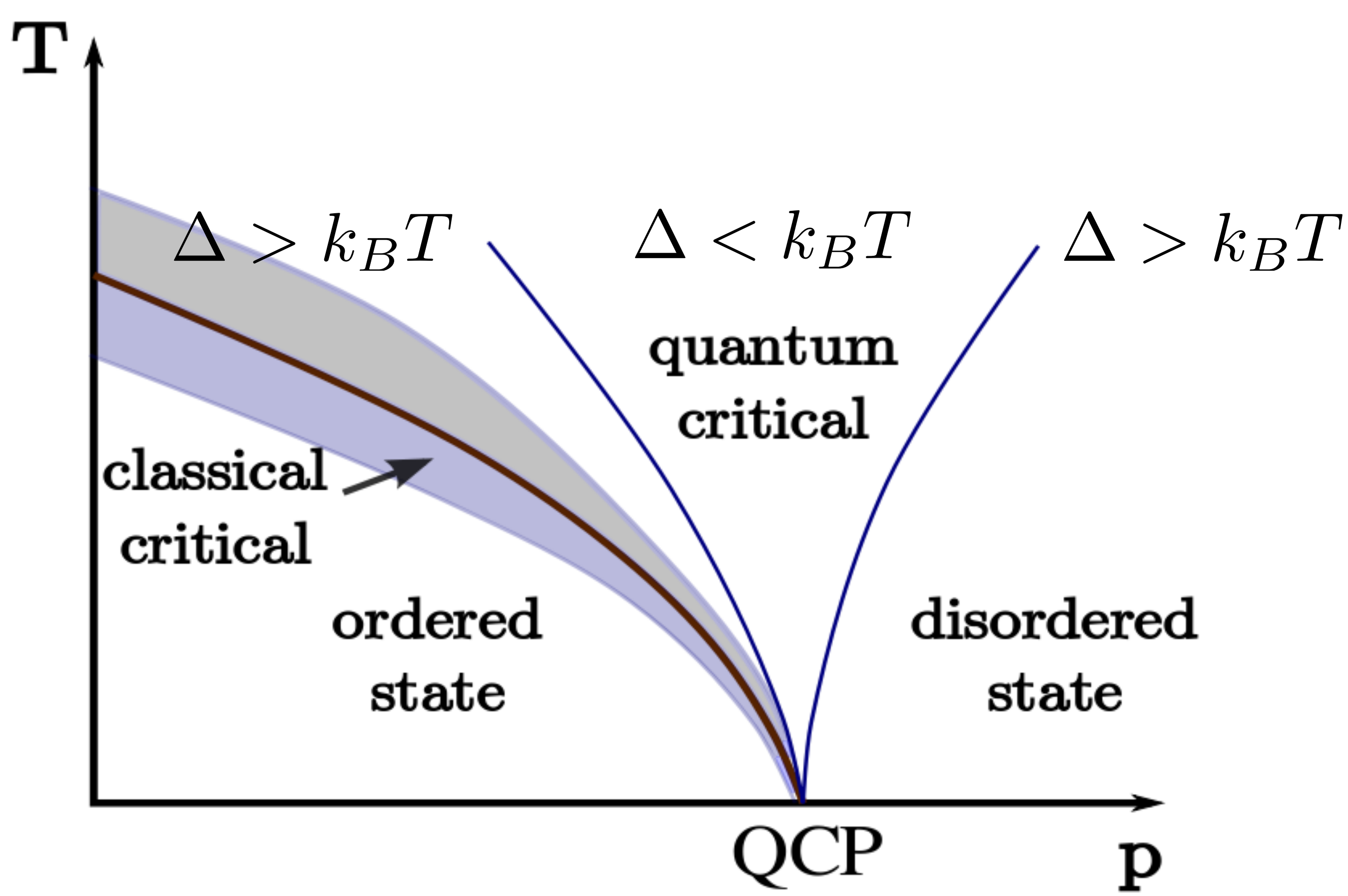
Minnesota Supercomputing Institute
UNIVERSITY OF MINNESOTA
Driven to Discover℠

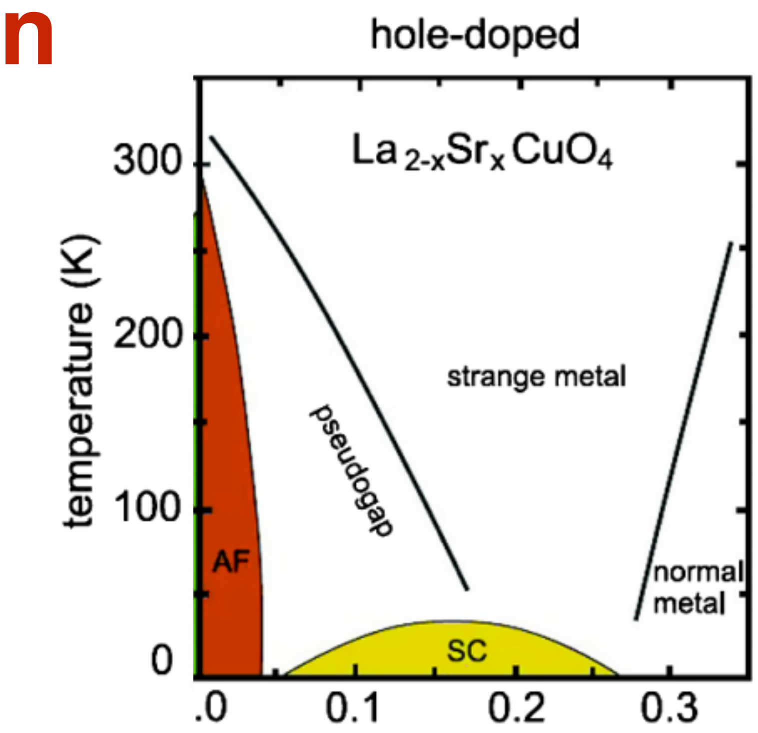
Contents

- Quantum critical phenomena
- Sign-problem free determinant QMC
- Nearly antiferromagnetic metal
    - Spin-fermion model
    - Previous analytical works
- What do we learn from numerics?
    - Superconductivity
    - Emergent symmetry

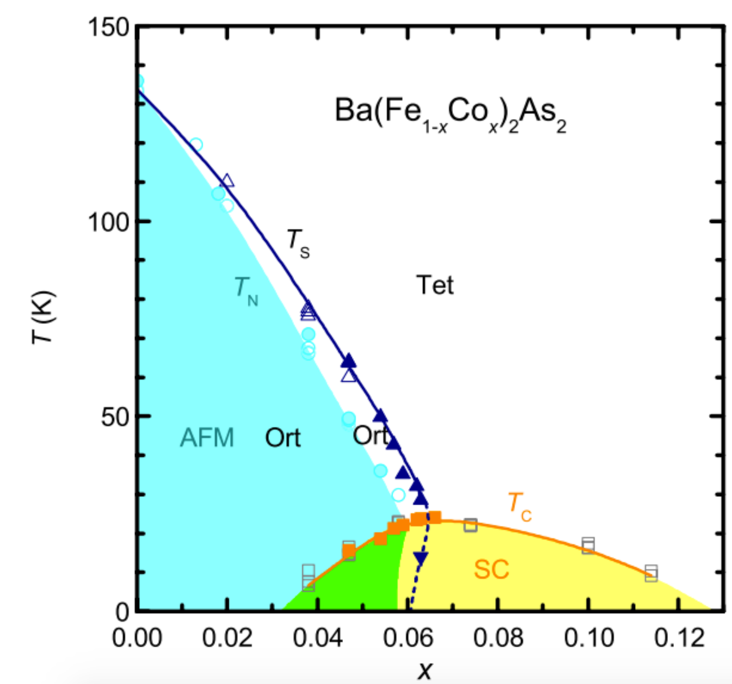
Quantum Phase Transition

- T=0 phase transition driven by an external parameter p
- Quantum critical point (QCP)
  - Divergent correlation time — quantum coherence
  - Quantum critical fan
- QCPs in metals
  - Landau damping; non-Fermi liquid; emergent orders
  - Signature in unconventional superconductors





Armitage et al, RMP (2010)



Nandi et al, PRL (2010)

Hertz, PRB 1976; Millis, PRB 1993
Sachdev, *Quantum Phase Transitions*

- QCPs not easily obtained from microscopic models
- Basic ingredients for a low-energy model
  - Quantum critical order parameter fluctuations
  - Fermi surface
  - Minimal coupling — space-time local
- What do we look for?
  - Phase diagram
  - Collective excitations
  - Scaling behavior
  - Comparison to experiments and other microscopic calculations

Even effective models are hard to solve! Need numerics!

Determinant Quantum Monte Carlo

- Partition function

$$Z_{\rm s.f} = \int \mathcal{D}\left[\bar{\psi}, \psi; \vec{\phi}\right] \exp(-S_F - S_B - S_\lambda)$$

- QCP tuned by bare boson mass

$$S_B = \frac{1}{2}\int_{\mathbf{r},\tau} \frac{1}{v_s^2}(\partial_\tau \vec{\phi})^2 + (\nabla\vec{\phi})^2 + r_0\vec{\phi}^2 + u\vec{\phi}^4$$

- Electronic action is Gaussian:

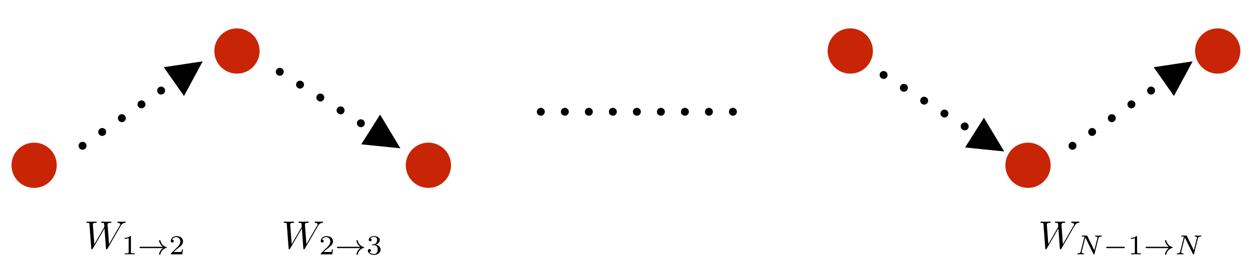
$$Z_{\rm s.f.} = \int \mathcal{D}[\vec{\phi}]\rho\{\vec{\phi}(\mathbf{r},\tau)\}$$

$$\rho\{\vec{\phi}(\mathbf{r},\tau)\} \equiv \det_{\vec{\phi}} \exp(-S_B)$$

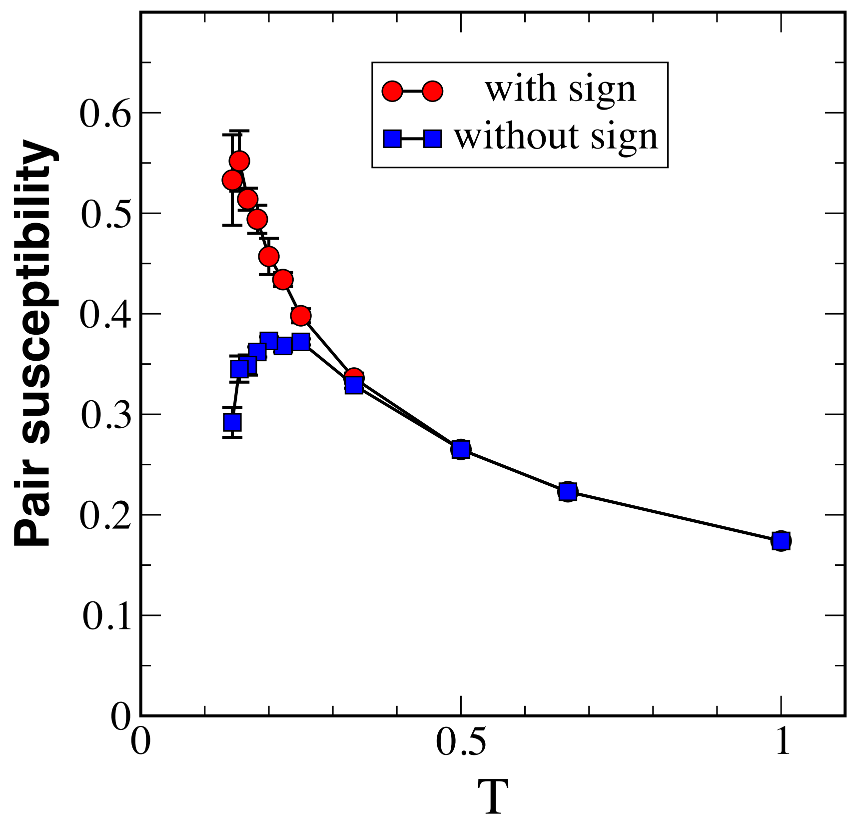
"fermion determinant"

DQMC:

- Construct a thermal ensemble by sampling;
- Unlimited by various approx. schemes
- Small system sizes; Finite size scaling



- Fermion sign problem:
  - fermion determinant is calculated from a *time-ordered product*
  - in general complex; especially severe at low-T



Scalapino, arXiv:cond-mat/0610710

Blanckenbecler, Scalapino & Sugar, PRD (1981)

- Fermion sign problem is generic

- Sign-free QMC due to Kramer's symmetry:

$$\tilde{U}^2 = -1; \text{ and } [H, \tilde{U}] = 0$$

- e.g., negative-U Hubbard model; positive-U Hubbard model at half-filling

Congjun Wu and Shou-Cheng Zhang, PRB (2005)

- Engineered models:
  - Remove sign-problematic sector of the action
  - Need to show they preserve the low-energy physics qualitatively

AFM QCP:
Berg, Metlitski & Sachdev, Science (2012)
Schattner, Gerlach, Trebst and Berg, PRL (2016)
Gerlach, Schattner, Berg and Trebst, PRB (2017)
XW, Schattner, Berg and Fernandes, PRB (2017)
XW, Wang, Schattner, Berg and Fernandes, arXiv

Ising-nematic QCP:
Schattner, Lederer, Kivelson and Berg, PRX (2016)
Lederer, Schattner, Kivelson and Berg, PRL (2017)

Many others:
Li, Jiang and Yao, PRL (2016)
Dumitrescu, Serbyn, Scalettar, Vishwanath, PRB (2017)
Xu, Sun, Schattner, Berg and Meng, PRX (2017) …

AFM QCP and Spin-fermion model

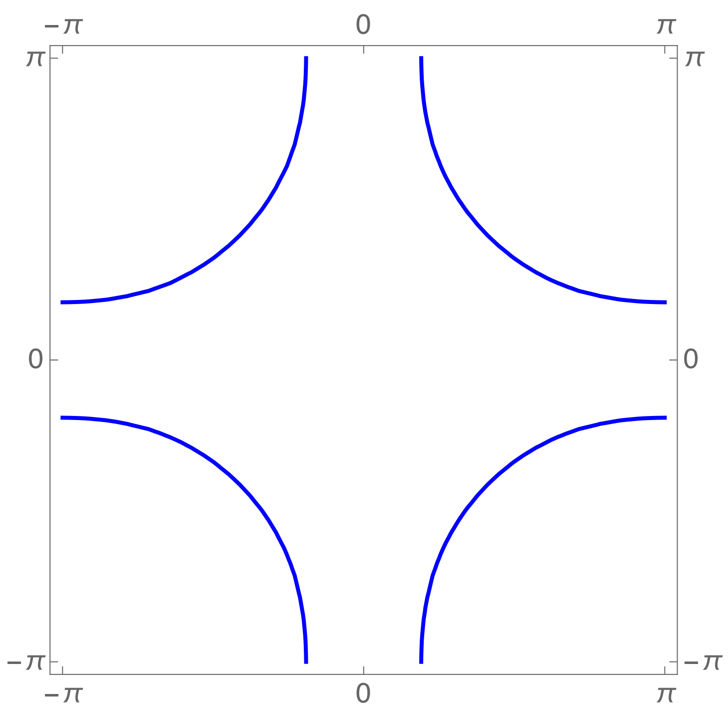
Spin-fermion model

Abanov, Chubukov & Schmalian, Adv. in Phys. (2003)
Metlitski & Sachdev, PRB (2010) …

- Electrons near the Fermi surface coupled to quantum critical antiferromagnetic fluctuations

$$S_F = \int_\tau \sum_{\mathbf{k}\alpha} \bar{\psi}_{\mathbf{k}\alpha}(\partial_\tau + \varepsilon_{\mathbf{k}-\mu})\psi_{\mathbf{k}\alpha}$$

- Fermi surface



Spin-fermion coupling:

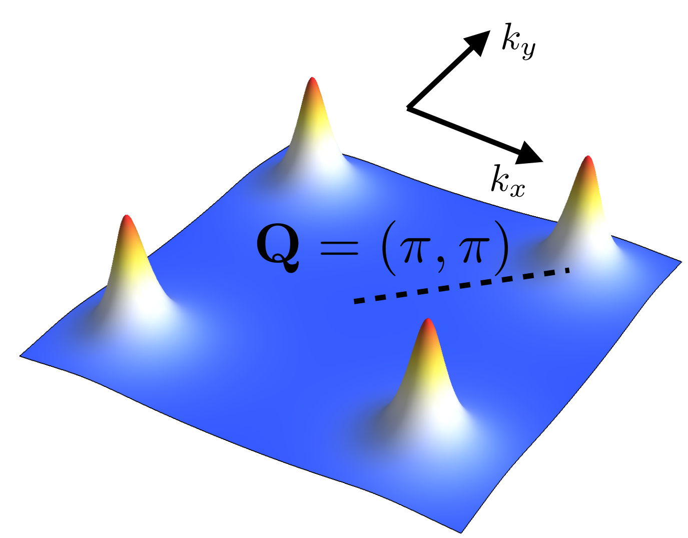
$$S_\lambda = \lambda \int_{\mathbf{x},\tau} \vec{\phi}\cdot\bar{\psi}_\alpha \vec{\sigma}_{\alpha\beta}\psi_\beta$$

$$S_B = \int_{\mathbf{q},i\Omega} \chi_0^{-1}(\mathbf{q}, i\Omega)\vec{\phi}_q \cdot \vec{\phi}_{-q}$$

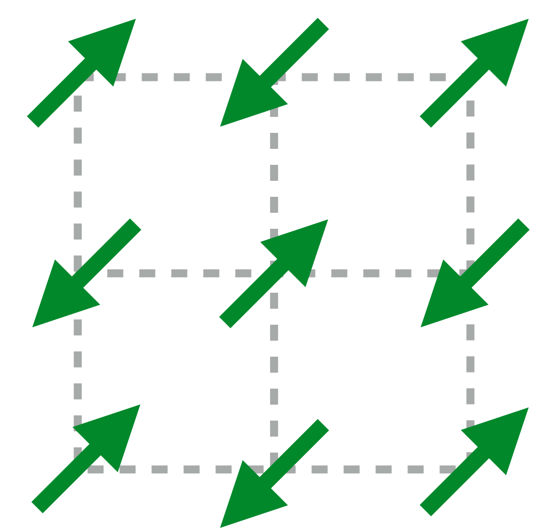
- Spin fluctuation peaked at **Q**

$$\chi_0^{-1}(\mathbf{q}, i\Omega) = r_0 + (\mathbf{q}-\mathbf{Q})^2 + \frac{\Omega^2}{v_s^2}$$

$r_0 > 0$:



$r_0 < 0$:

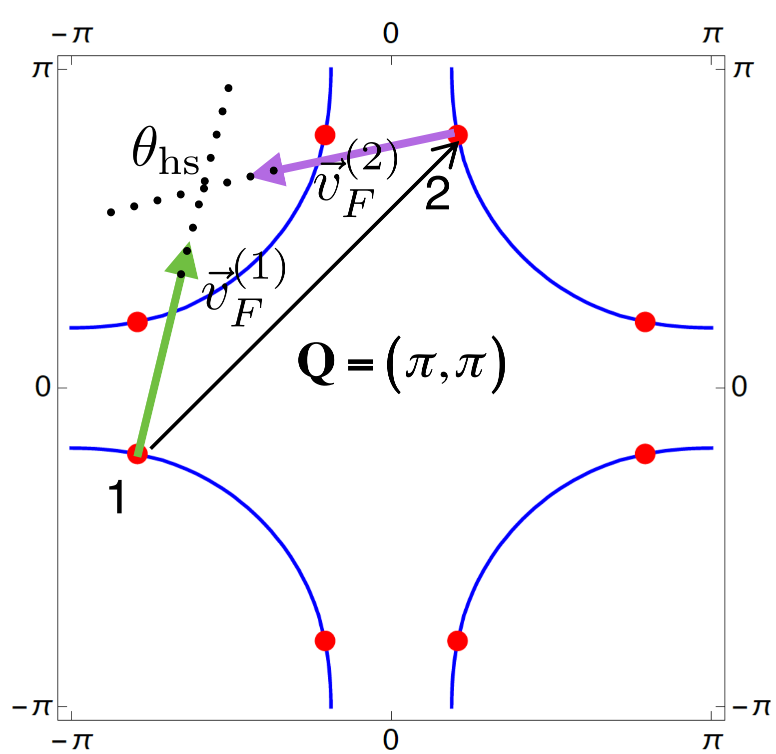


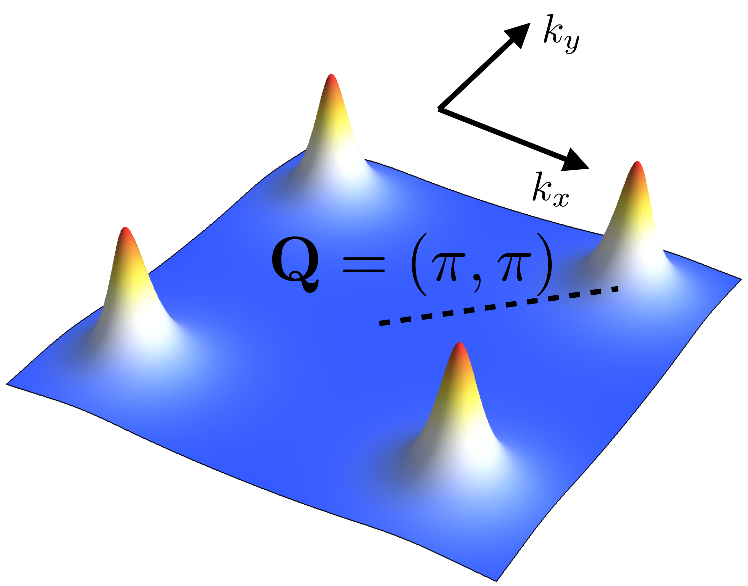
Néel order

- Hot spots: Points on the Fermi surface that couple strongly to spin fluctuations

- Low-energy physics governed by linearized hot spot approximation:

$$\varepsilon_{i,\mathbf{k}} \approx \mathbf{v}_F^{(i)} \cdot (\mathbf{k} - \mathbf{k}_{\rm hs}^{(i)});\ \ i = 1, 2$$



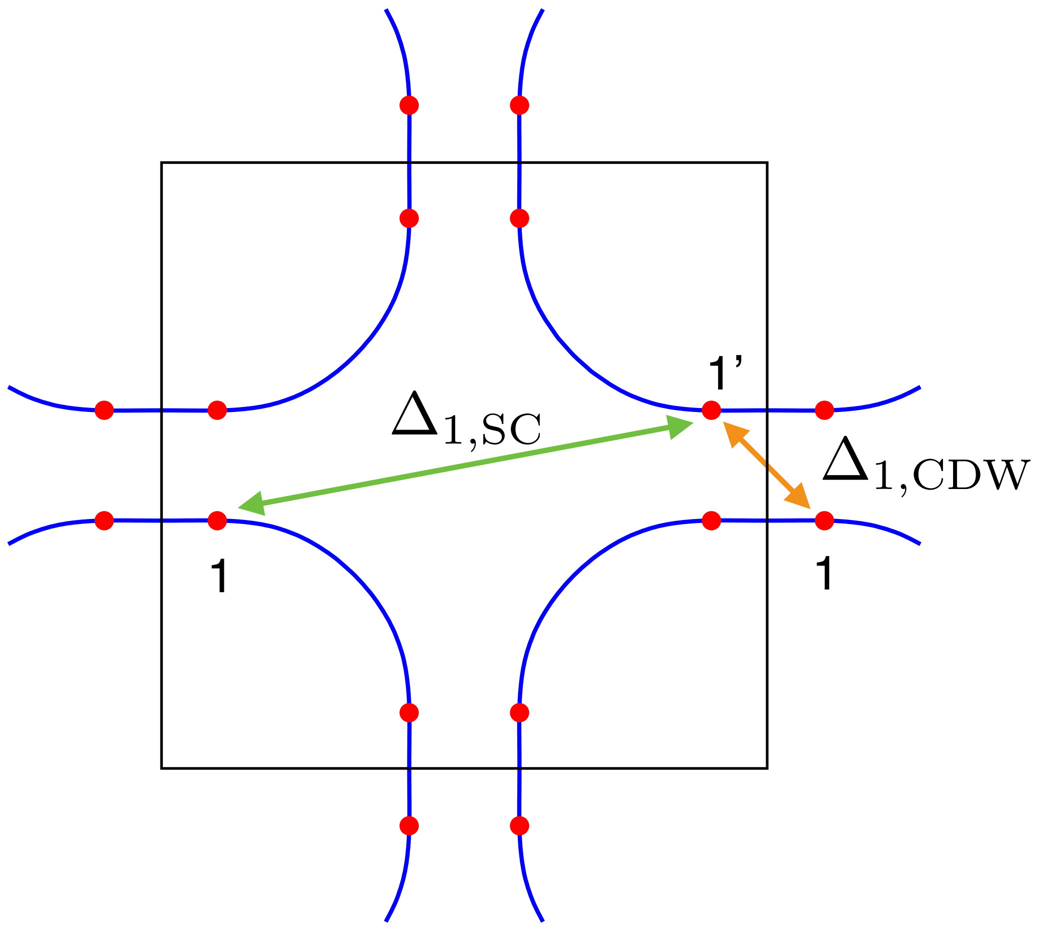


Abanov, Chubukov & Schmalian, Adv. in Phys. (2003)
Metlitski & Sachdev, PRB (2010) …

- Emergent SU(2) symmetry at each pair of hot spots

$$\begin{pmatrix} \psi_{i,\mathbf{k}\uparrow} \\ \psi_{i,\mathbf{k}\downarrow} \end{pmatrix} \to \begin{pmatrix} \psi^\dagger_{i,-\mathbf{k}\downarrow} \\ -\psi^\dagger_{i,-\mathbf{k}\uparrow} \end{pmatrix} \; ; \; i = 1, 2$$

- Enlarged order parameter O(4): complex SC and CDW
  - Relevant to hole-doped cuprates?



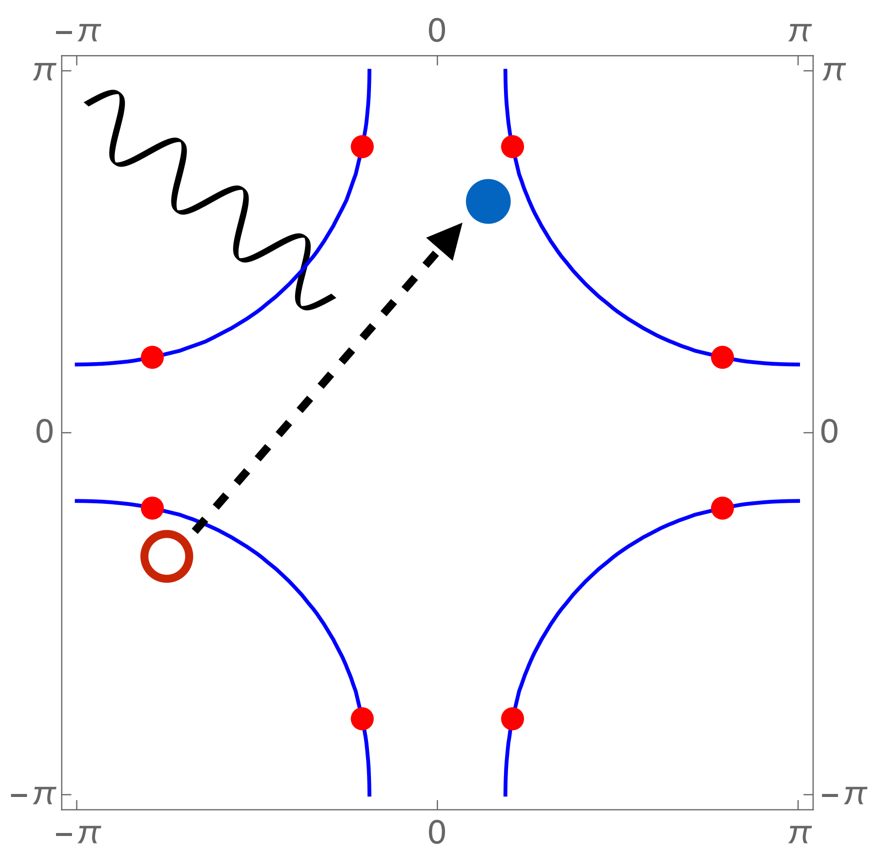
$$\Delta_{1,\text{SC}} = \langle \psi_{1,\uparrow}\psi_{1',\downarrow} - \psi_{1,\downarrow}\psi_{1',\uparrow} \rangle$$

$$\Delta_{1,\text{CDW}} = \langle \psi_{1,\uparrow}\psi^\dagger_{1',\uparrow} + \psi_{1,\downarrow}\psi^\dagger_{1',\downarrow} \rangle$$

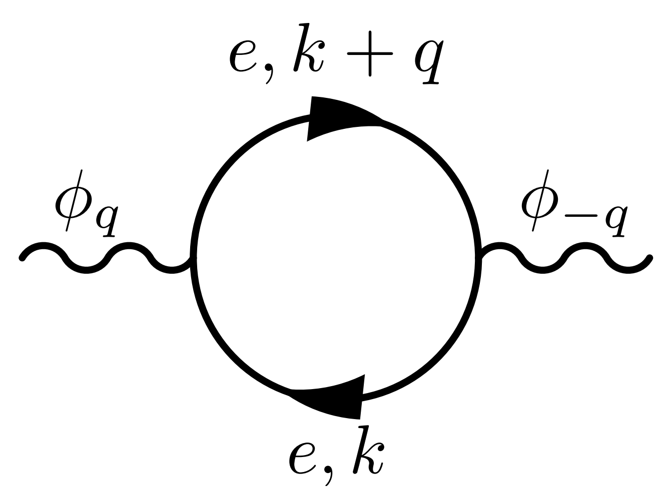
Metlitski & Sachdev, PRB (2010)
Wang, Agterberg & Chubukov, PRB (2015)

- Low frequency spin fluctuations are strongly renormalized due to the hot spots — Landau damping

$$\chi(\mathbf{q}, i\Omega_n) = \frac{1}{r_0 + (\mathbf{q} - \mathbf{Q})^2 + \Omega_n^2/v_s^2 + |\Omega_n|/\gamma} \qquad \frac{1}{\gamma} \propto \frac{\lambda^2}{v_f^2 \sin(\theta_{\text{hs}})}$$



Polarization bubble:

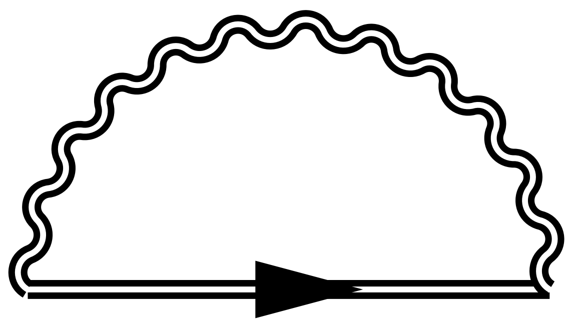


Abanov, Chubukov & Schmalian, Adv. in Phys. (2003)
Metlitski & Sachdev, PRB (2010)
Mross et al, PRB (2010) …

- How to study SC and non-FL due to quantum critical spin fluctuations?

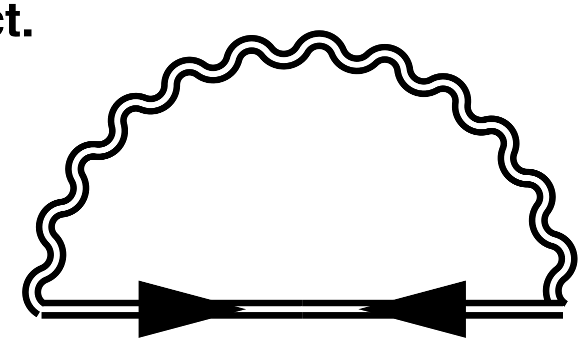
  —Hot-spot Eliashberg approximation

damped spin fluct.



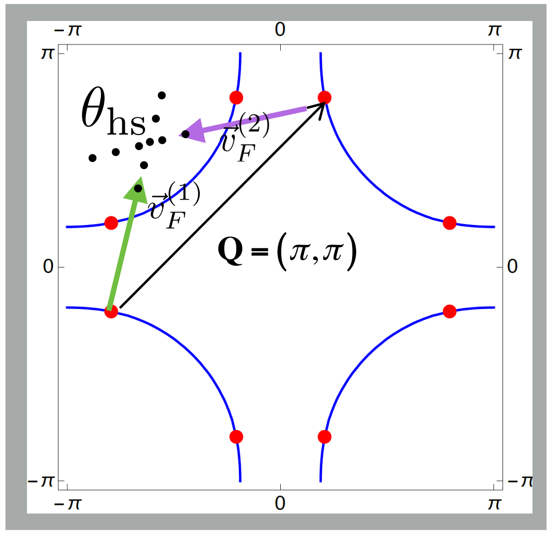
Regular part of the self-energy

$$\Sigma(\omega) \sim \sqrt{\omega}$$



Anomalous part of the self-energy

$$T_c \propto \left(\frac{\lambda^2}{v_F}\right)^2 \gamma \sim \lambda^2 \sin(\theta_{\rm hs})$$



- How to understand the angle dependence of T_c?
  - $\theta_{\rm hs} \to 0$: Spin fluct. strongly damped; insufficient to mediate pairing

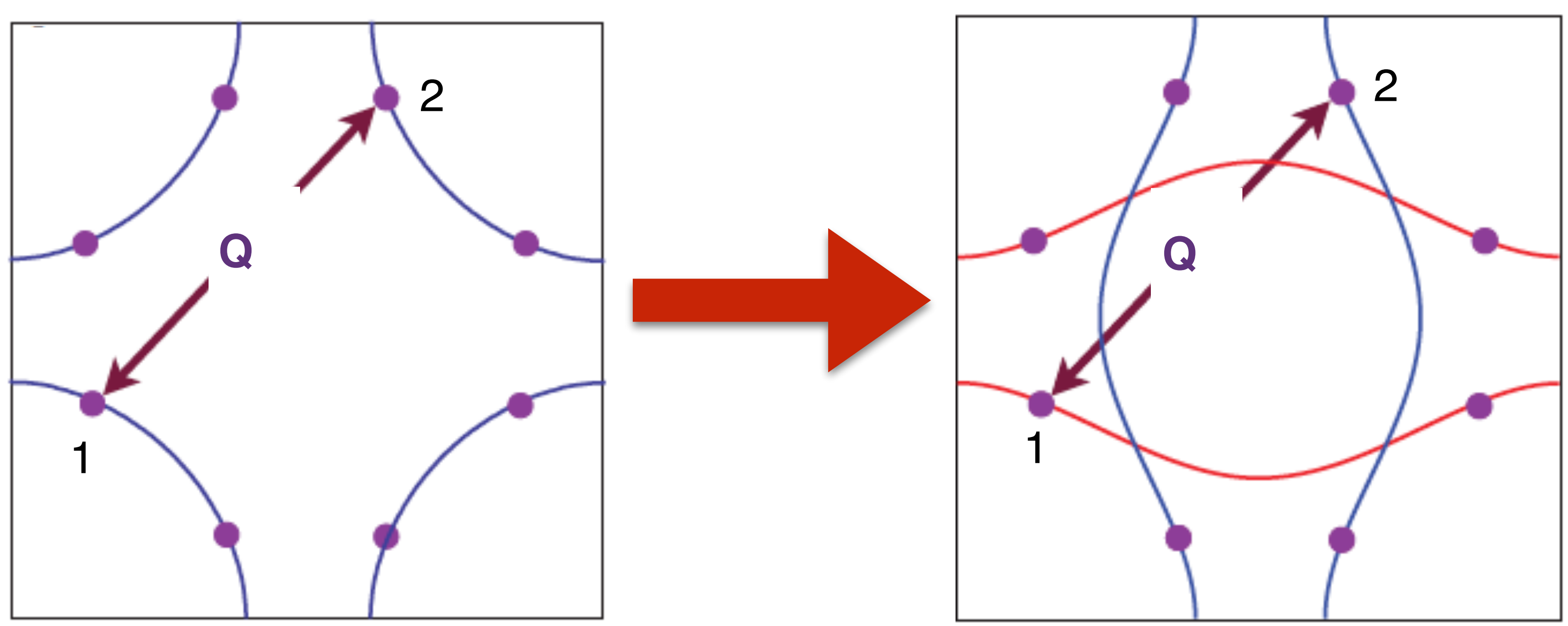
Abanov, Chubukov & Schmalian, Adv. in Phys. (2003)
Metlitski & Sachdev, PRB (2010) …

How to achieve sign-free QMC?

- How to avoid the fermion sign problem?
  - Two electron bands
  - Spin fluct. couple inter-band
- Kramer's symmetry:

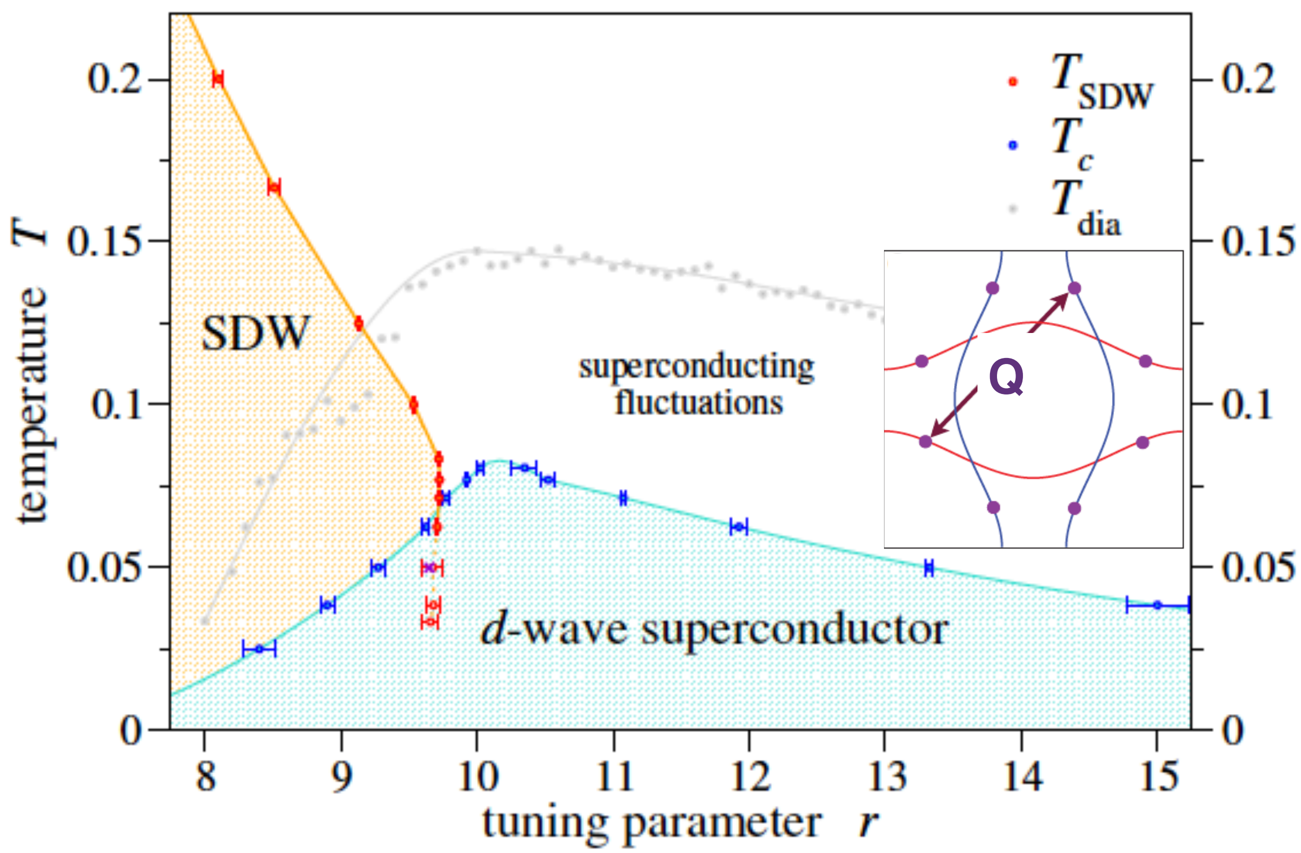
$$\tilde{U} = i\sigma_2 \otimes \tau_3 \mathcal{C}$$

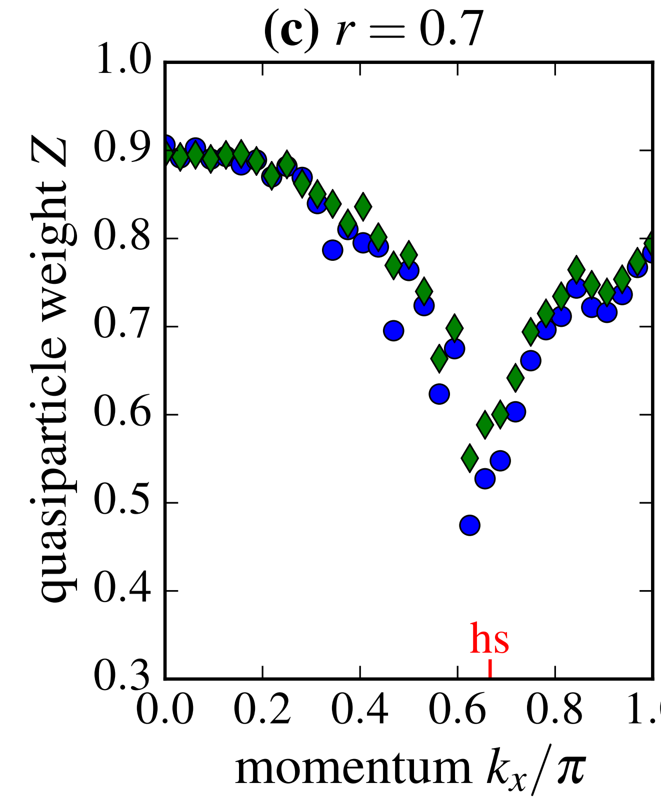
- Hot spots dominate low-energy physics



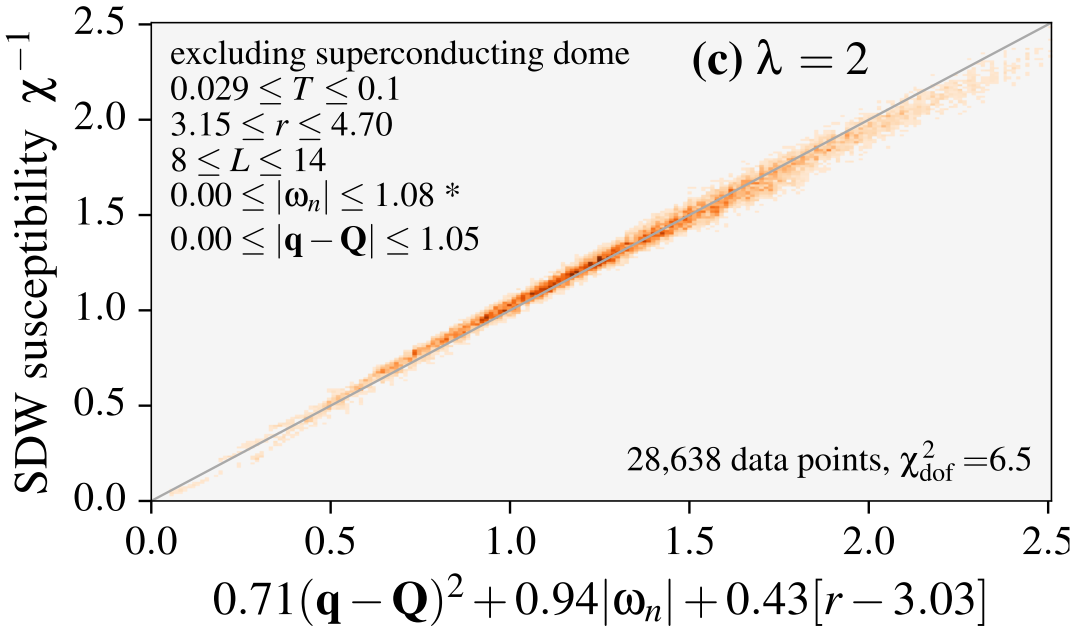
Berg, Metlitski & Sachdev, Science (2012)

Numerical characterization of low-energy properties

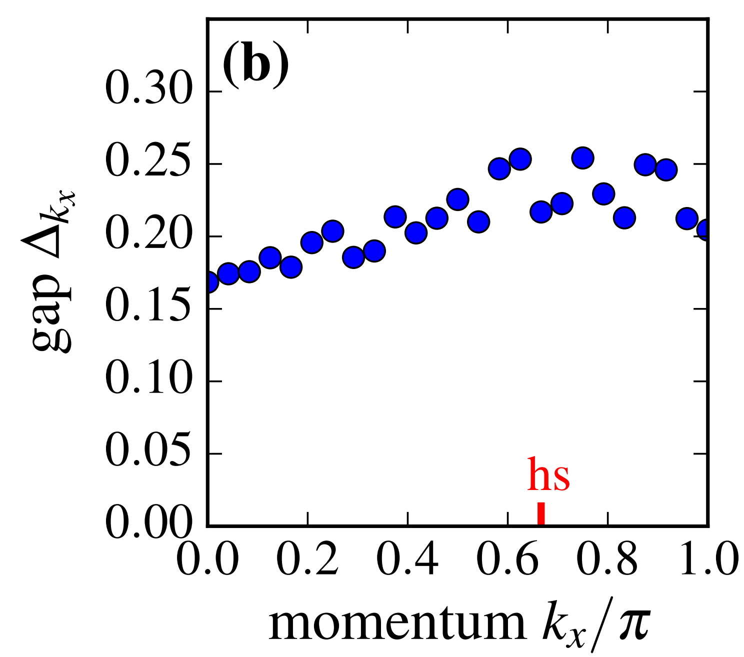




Electrons lose coherence near hot spots



Damping dynamics of spin fluct.



SC gap function **k**-independent

Schattner et al, PRL (2016); Gerlach et al, PRB (2017)

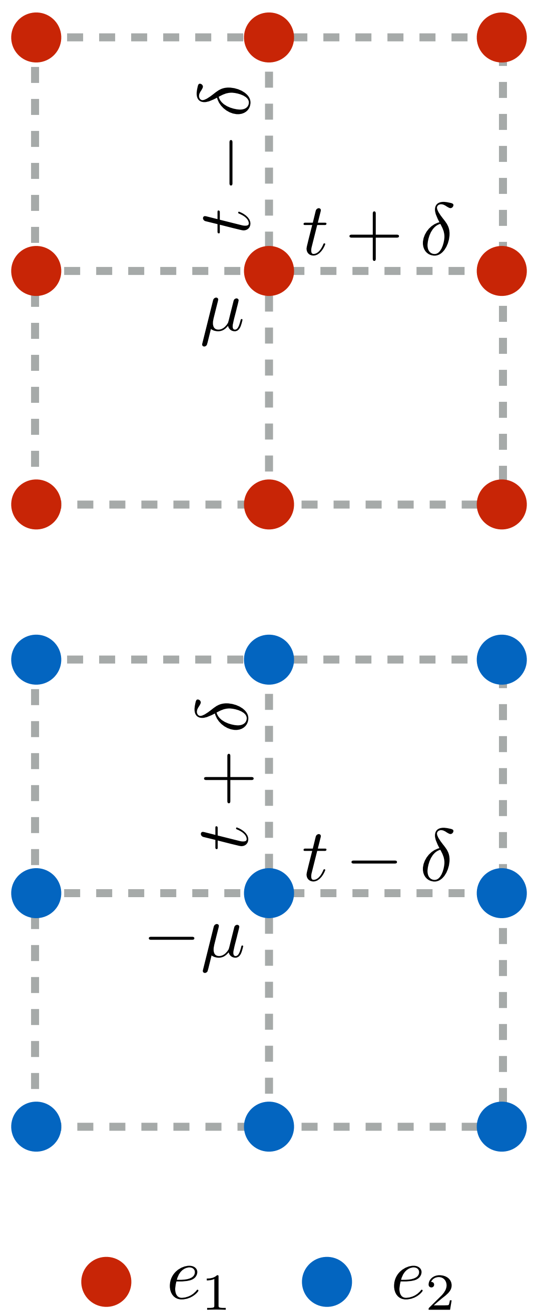
Superconductivity near QCP

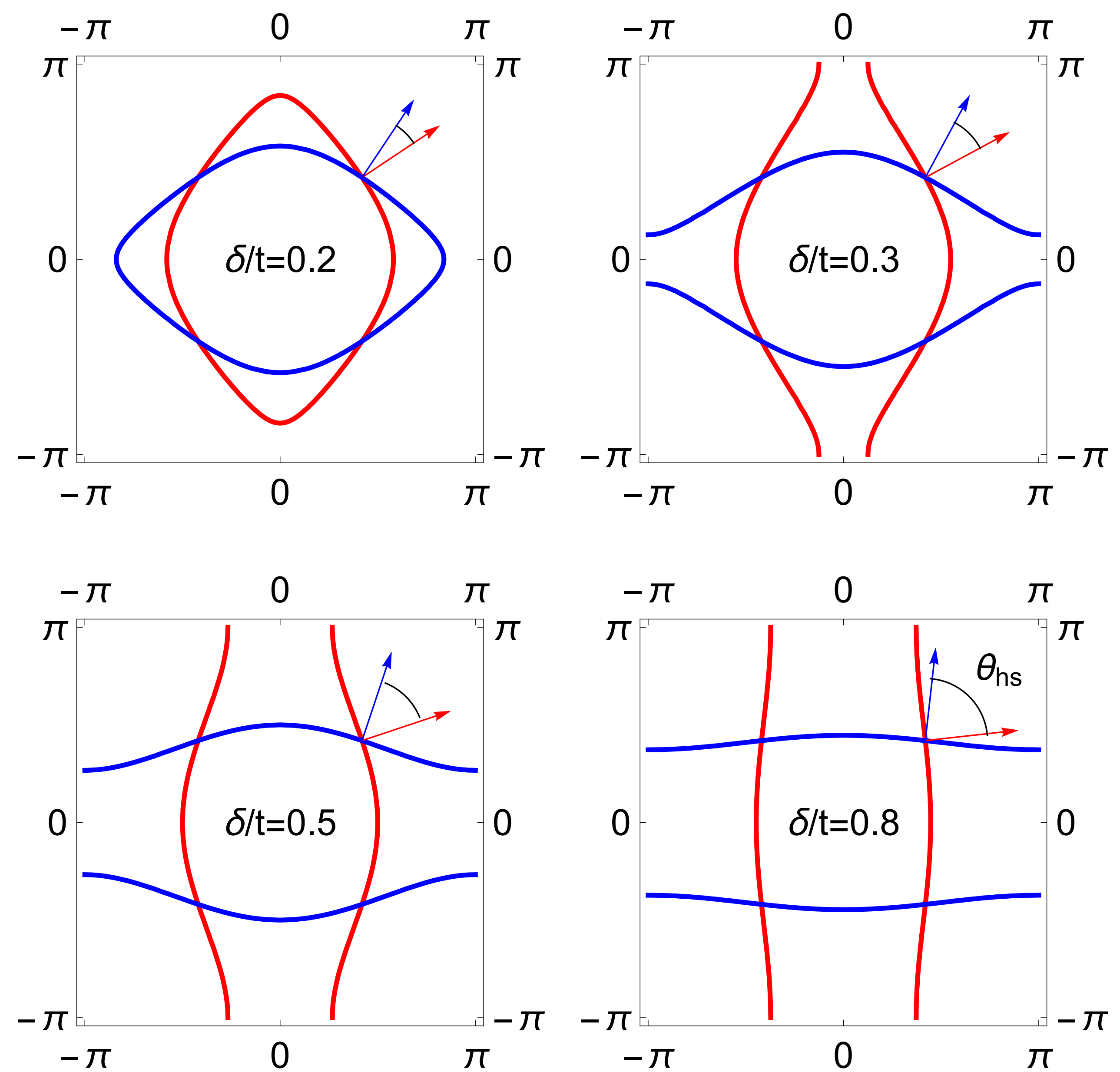
- Are the SC properties governed by the hot spots?
- Is Eliashberg approximation valid?

- Phys. Rev. B 95, 174520 (2017)

Band structure

- Study a series of band structures with different δ/t
- Different low-energy properties, while maintaining same bandwidth 8t





Blue band shifted by **Q**; pair of hot spots overlap

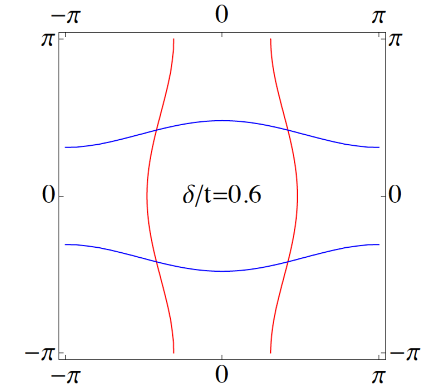
- For each band parameter δ/t :

Spin-fermion interaction: $\lambda^2 = 8t$

System sizes: $L = 8, 10, 12, 14$

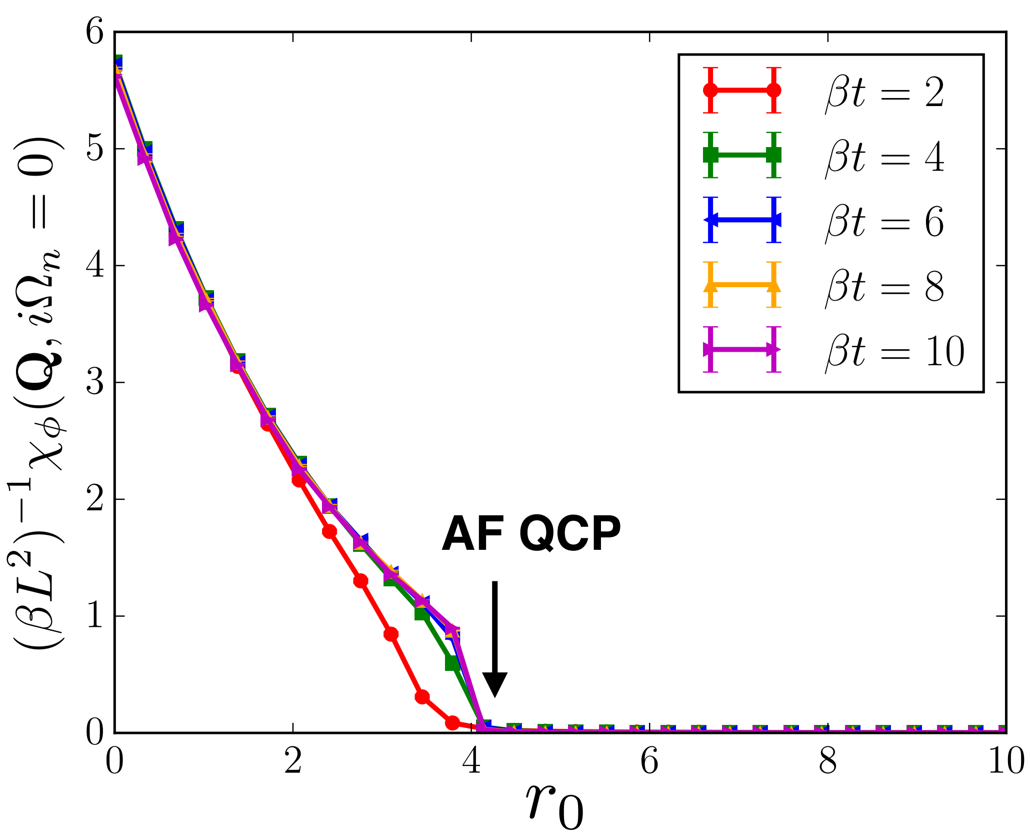
Temperatures: $T \geq 0.04t$

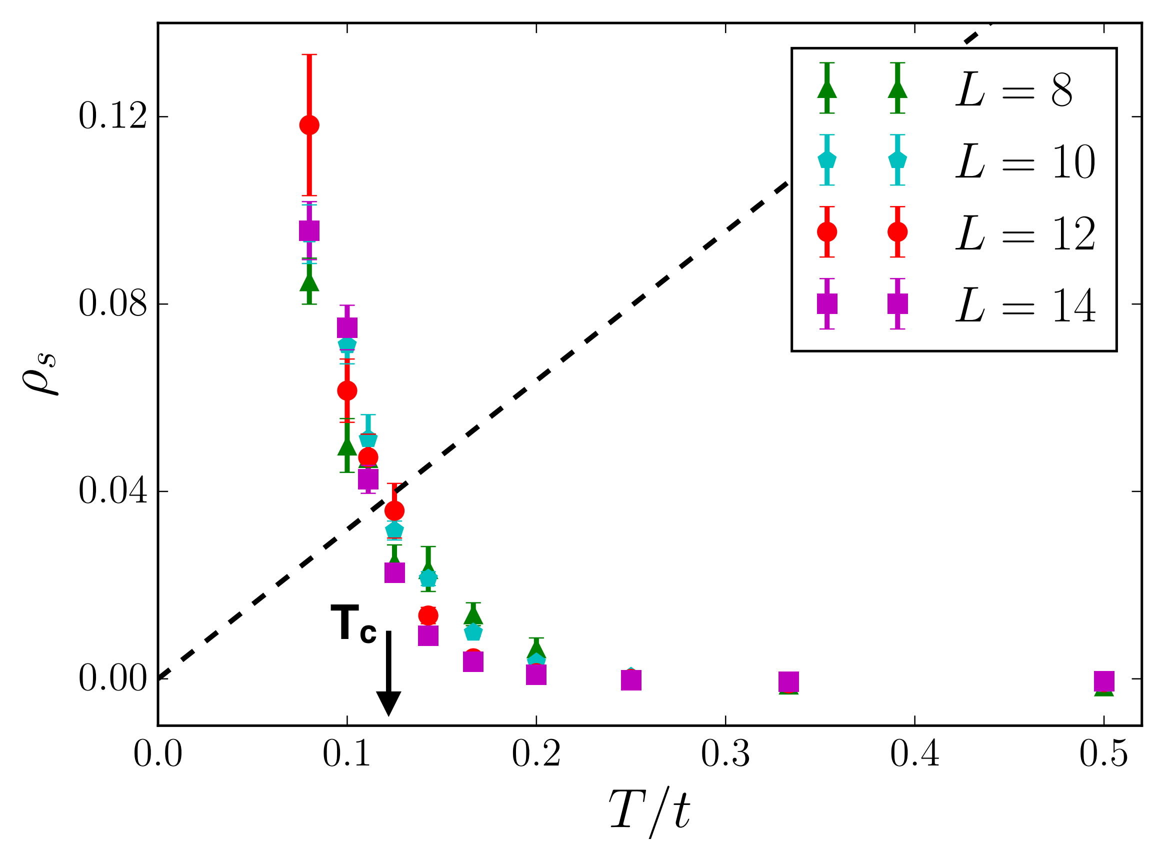
$$t \sim 100meV \Rightarrow T \sim 40K$$

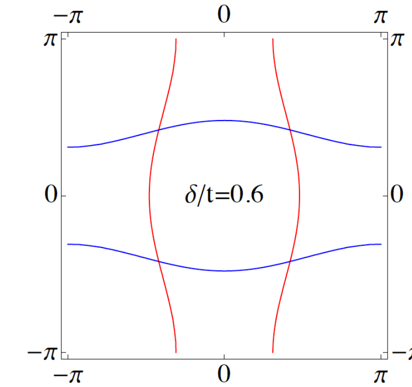


- QMC procedure:
  - Locate AF QCP by varying bare mass r_0 of spin fluct.
  - Obtain T_c via BKT criterion

$$\rho_s(T_c) = \frac{2T_c}{\pi}$$







- For each band parameter δ/t :

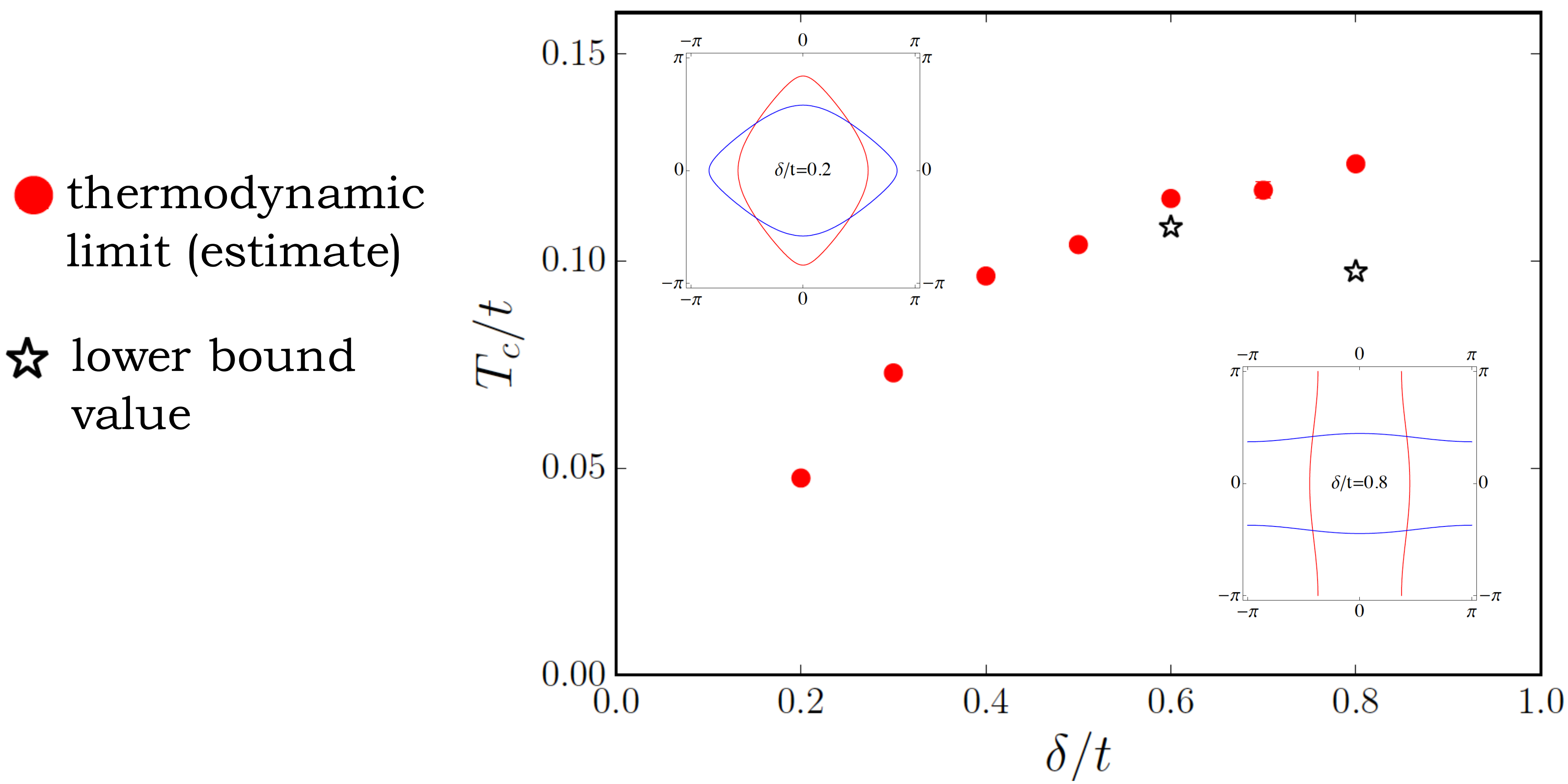
Spin-fermion interaction: $\lambda^2 = 8t$

System sizes: $L = 8, 10, 12, 14$

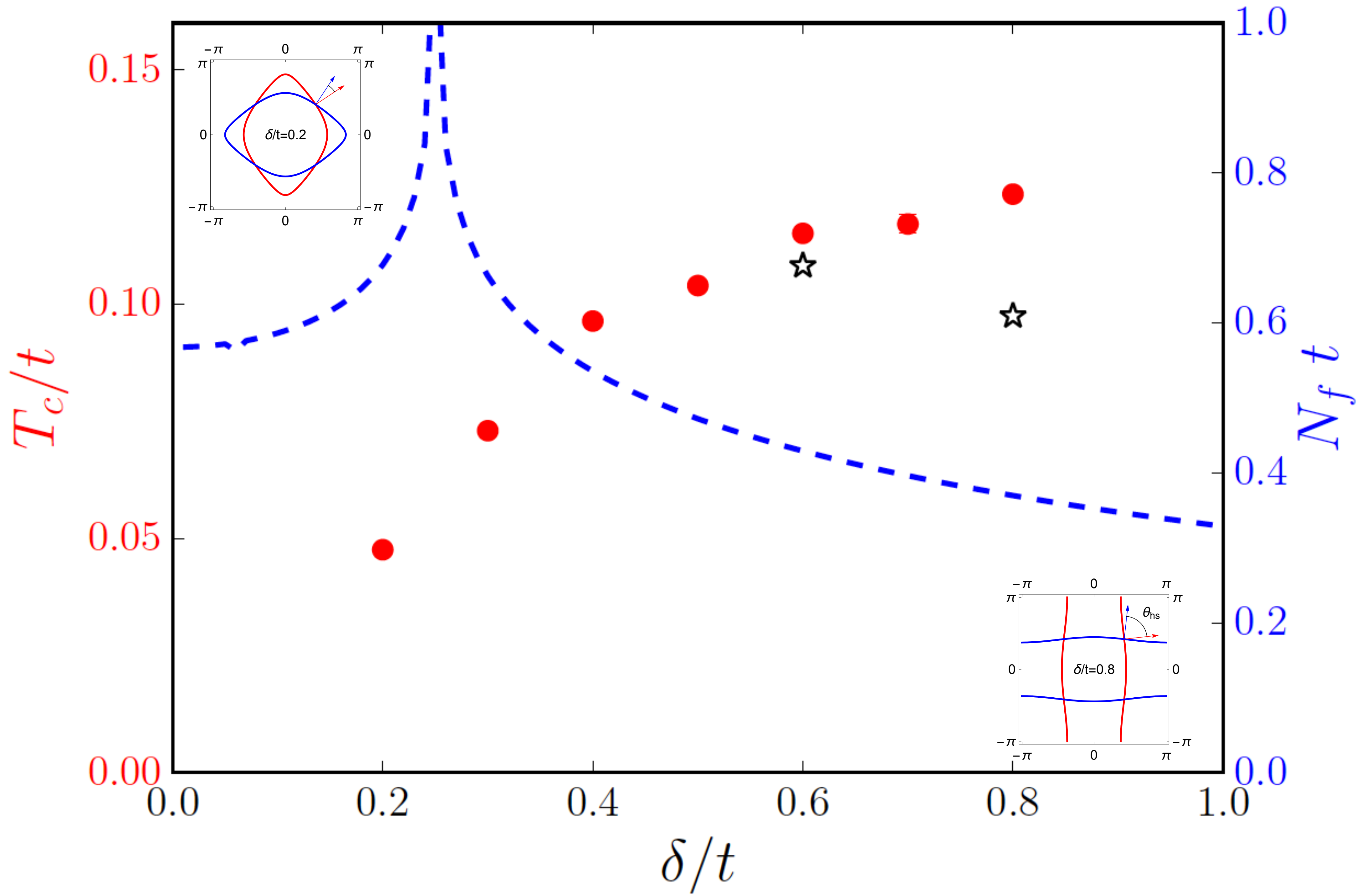
Temperatures: $T \geq 0.04t$

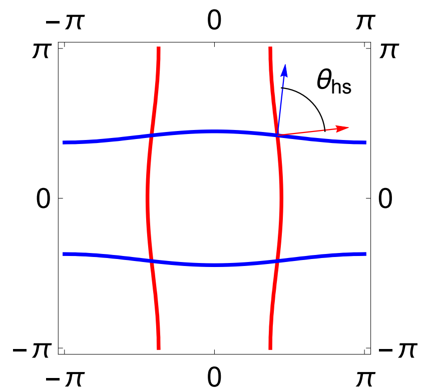
- QMC procedure:
  - Locate AF QCP by varying bare mass r_0 of spin fluct.
  - Obtain T_c via BKT criterion

$$\rho_s(T_c) = \frac{2T_c}{\pi}$$

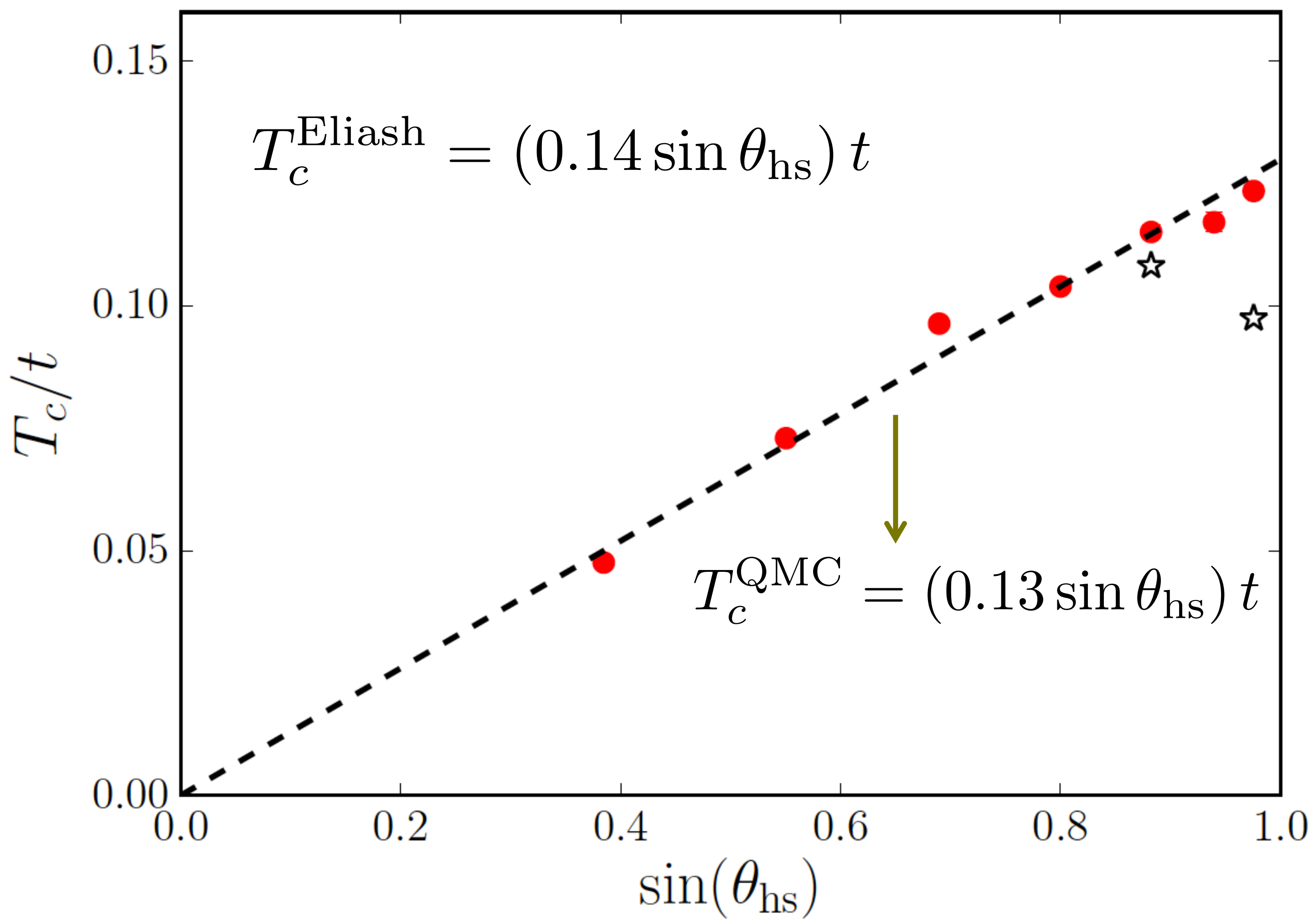


- T_c is not correlated with density of states at the Fermi energy



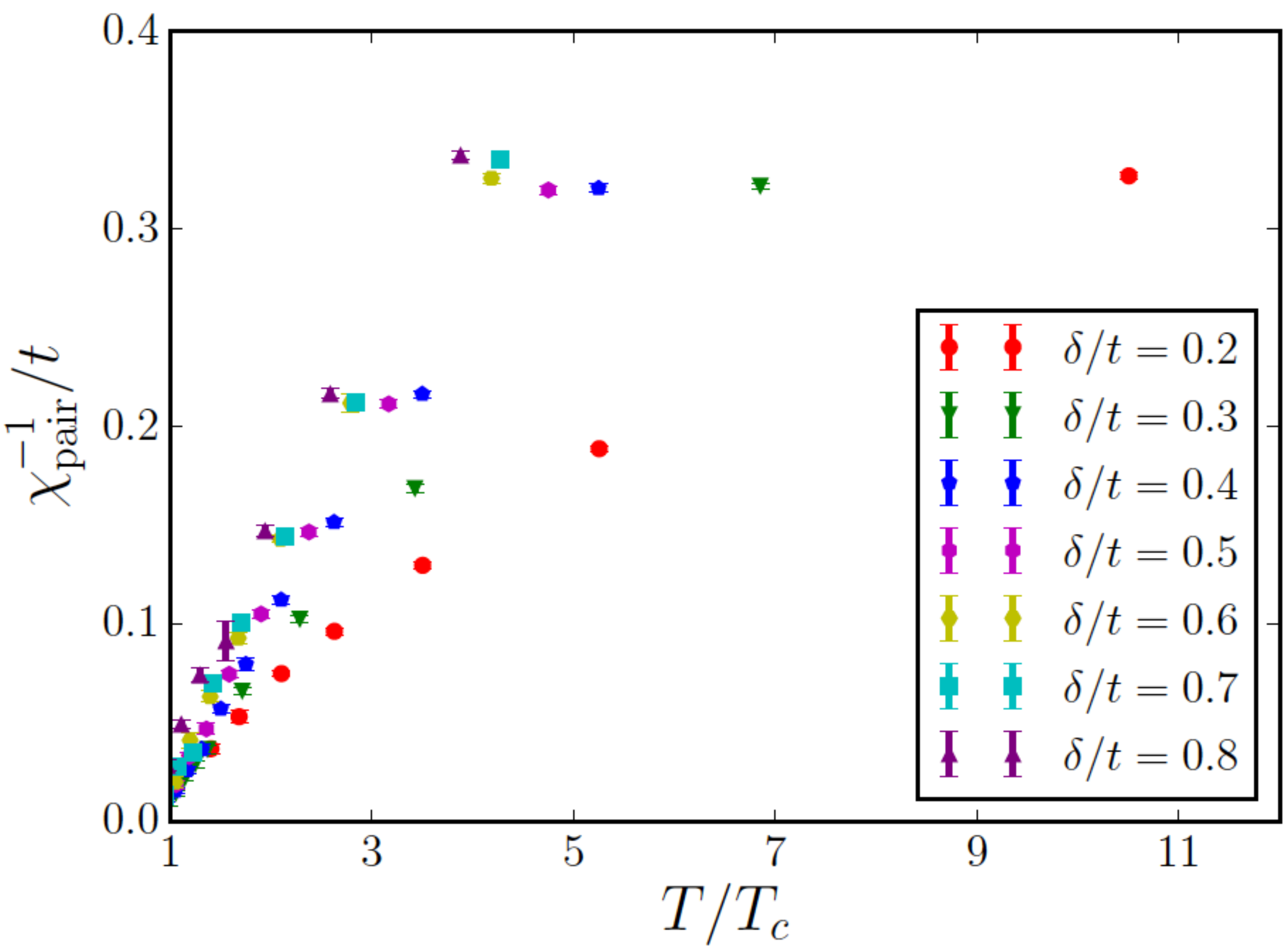


- T_c is strongly correlated with the relative angle between Fermi velocities at a pair of hot spots



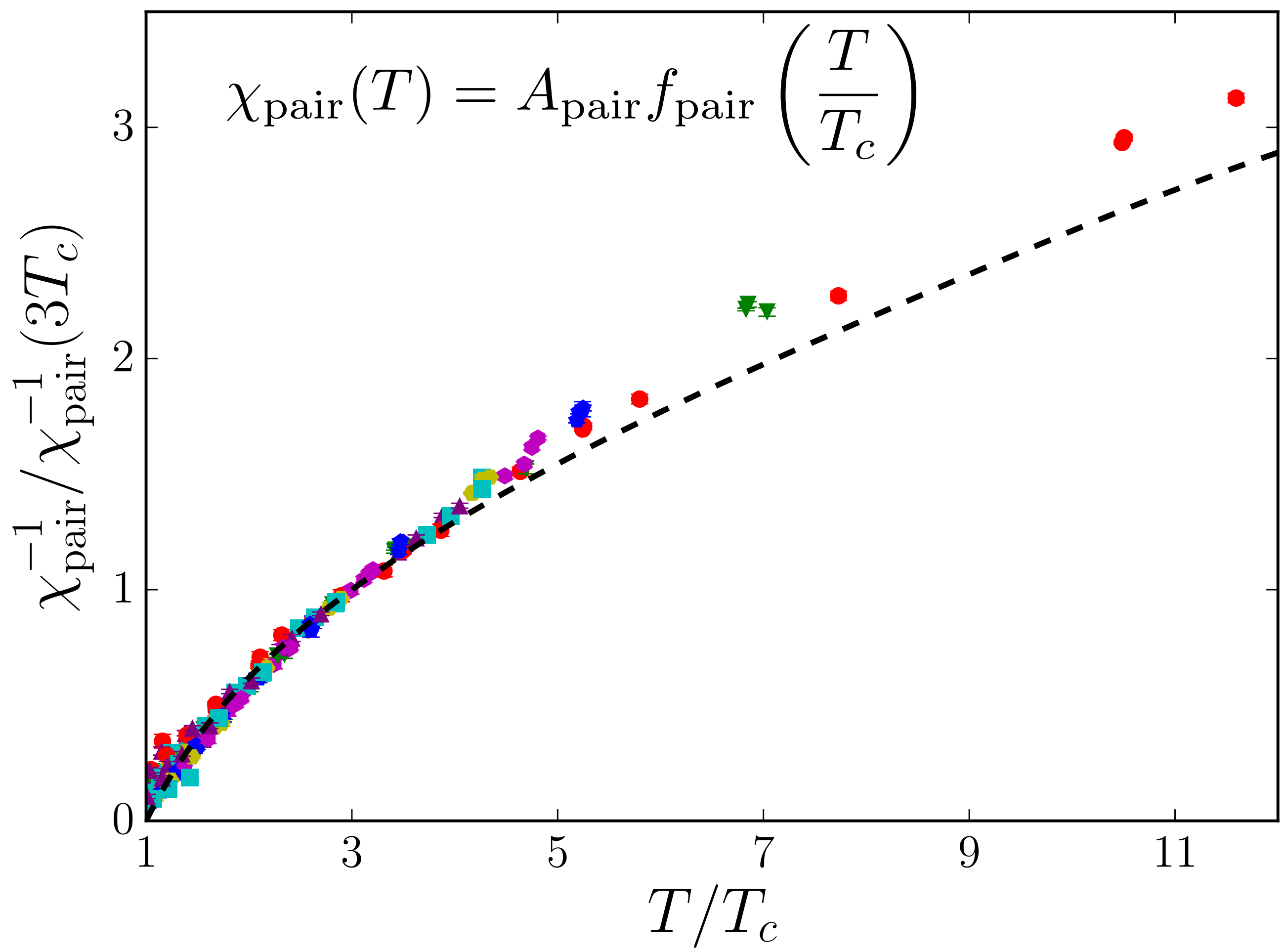
- Static pair susceptibility:

$$\chi_{\text{pair}} = \int_{\mathbf{r},\tau} \langle \hat{\Gamma}(\mathbf{r},\tau)\hat{\Gamma}^\dagger(0,0)\rangle \qquad \hat{\Gamma}(\mathbf{r},\tau) \sim \psi_\uparrow(\mathbf{r},\tau)\psi_\downarrow(\mathbf{r},\tau)$$



- Static pair susceptibility:

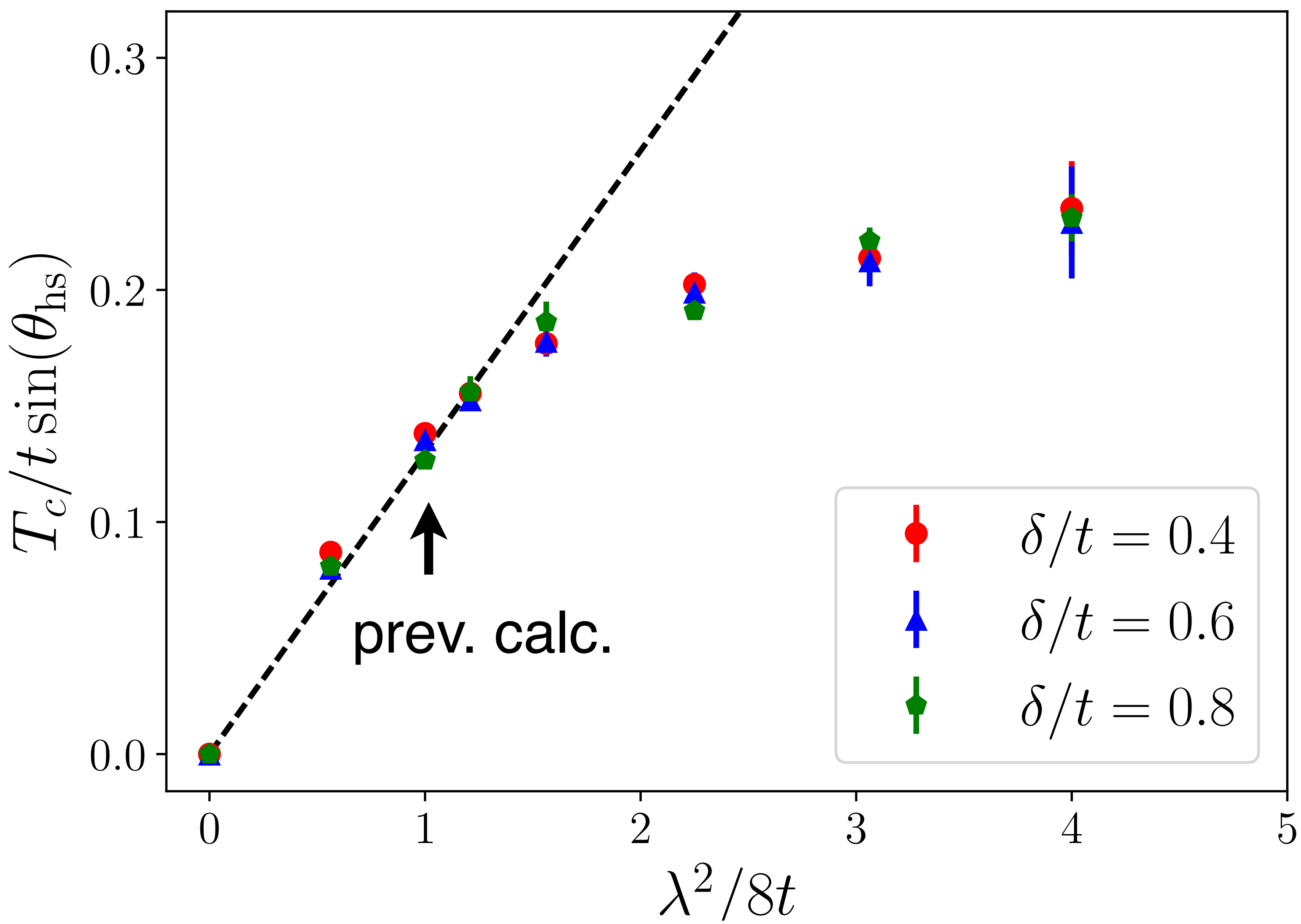
$$\chi_{\text{pair}} = \int_{\mathbf{r},\tau} \langle \hat{\Gamma}(\mathbf{r},\tau)\hat{\Gamma}^{\dagger}(0,0)\rangle \qquad \hat{\Gamma}(\mathbf{r},\tau) \sim \psi_{\uparrow}(\mathbf{r},\tau)\psi_{\downarrow}(\mathbf{r},\tau)$$



- Scaled susceptibilities collapse onto a ***single universal curve***
- The curve is fitted well by hot spot Eliashberg approximation

- T_c dependence on the spin-fermion interaction strength: unbounded?

$$S_\lambda = \lambda \int_x \vec{\phi} \exp(i\mathbf{Q}\cdot\mathbf{x}) \cdot \sum_{\alpha\beta} \bar{\psi}_\alpha \vec{\sigma}_{\alpha\beta} \psi_\beta$$

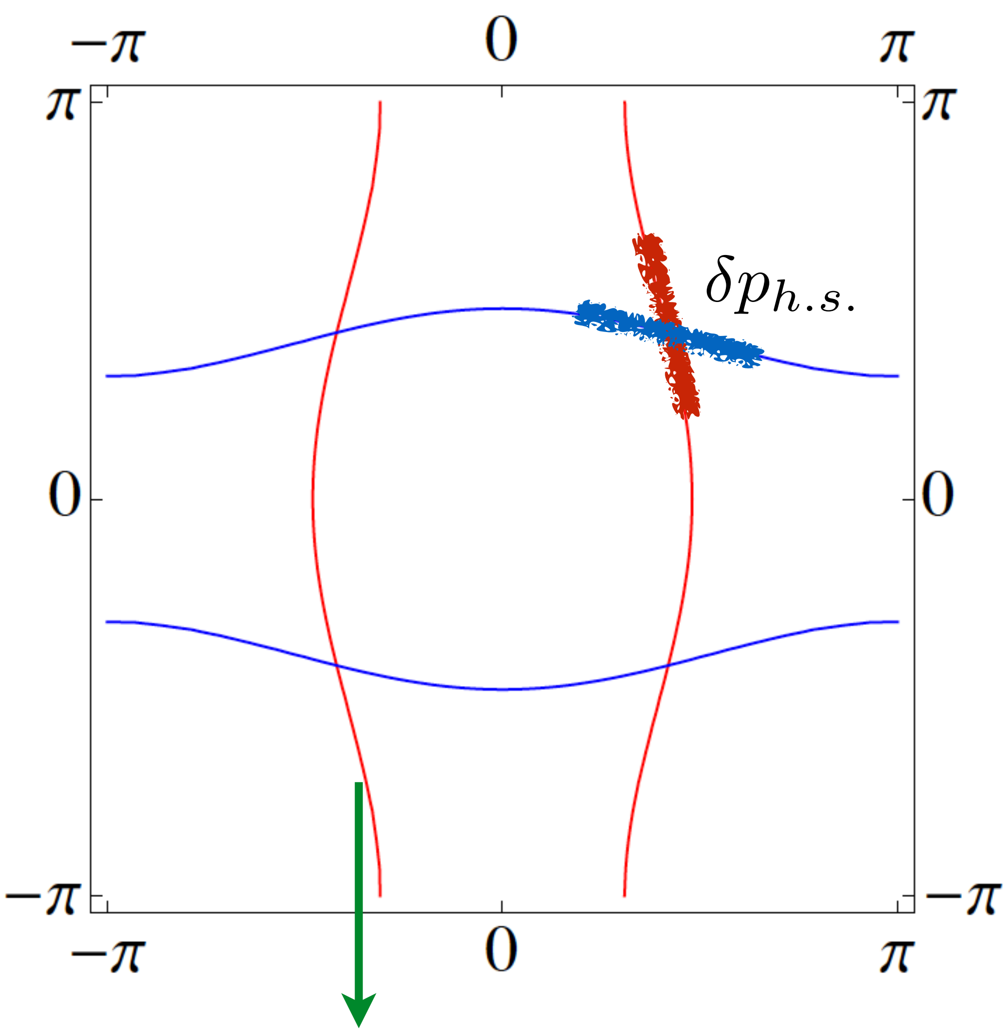


$T_c^{max} \approx 0.2t$

Saturation of Tc deviates from linearized hot spot approx. $T_c \propto \lambda^2 \sin\theta_{\rm hs}$

- Damped spin fluct. propagator:

$$\chi^{-1}(\mathbf{q}, i\Omega_n) = r_0 + (\mathbf{q} - \mathbf{Q})^2 + \boxed{\frac{|\Omega_n|}{\gamma}} \rightarrow (\delta p_{h.s.})^2$$



$|\mathbf{q} - \mathbf{Q}| \sim p_0$

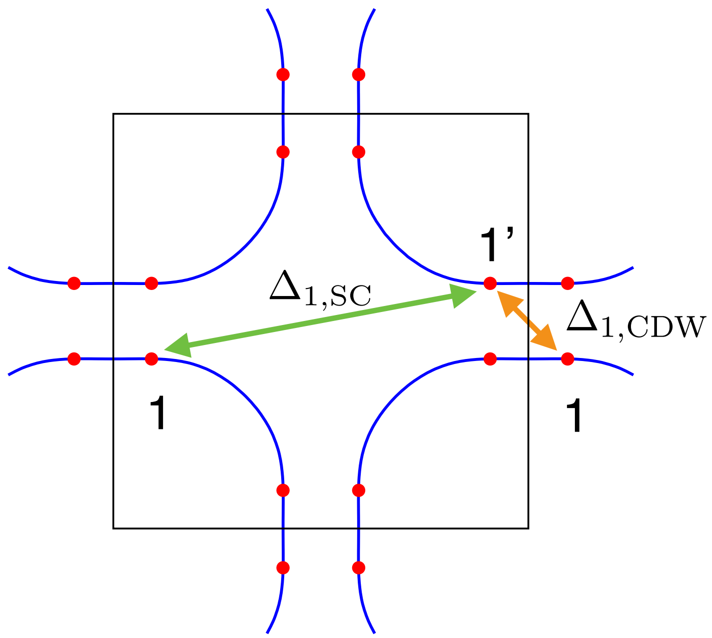
$$\frac{\delta p_{h.s.}}{p_0} \sim 1$$

- The whole Fermi surface becomes “hot”
- T_c saturates at crossover from hot-spot dominated to Fermi-surface dominated pairing.

Brief Summary

- Hot spots govern SC properties near AF QCP up to large interactions comparable with fermionic bandwidth
- T_c saturates to a few percent of the bandwidth at the crossover from hot-spot dominated to Fermi-surface dominated pairing
- Despite uncontrolled, Eliashberg approximation shows quantitative agreement with numerical results
  - Why are vertex corrections absent?

- Phys. Rev. B 95, 174520 (2017)



Emergent low-energy symmetry

- Emergent low-energy symmetry from the hot spots
  - Near-degeneracy between CDW and SC
  - Robust symmetry against perturbations?
  - Can it be responsible for CDW in cuprates?
    - Exotic charge order *not* relying on Fermi surface nesting

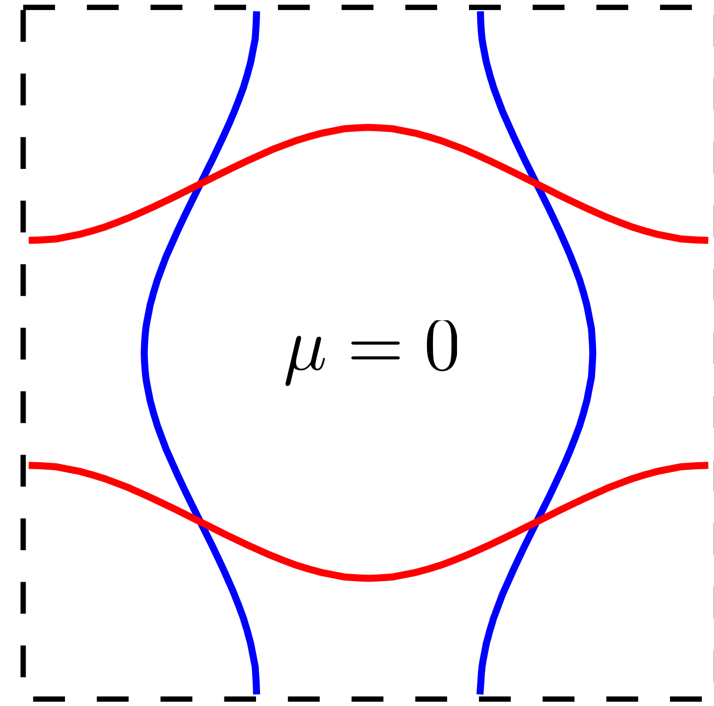
- arXiv:1710.02158

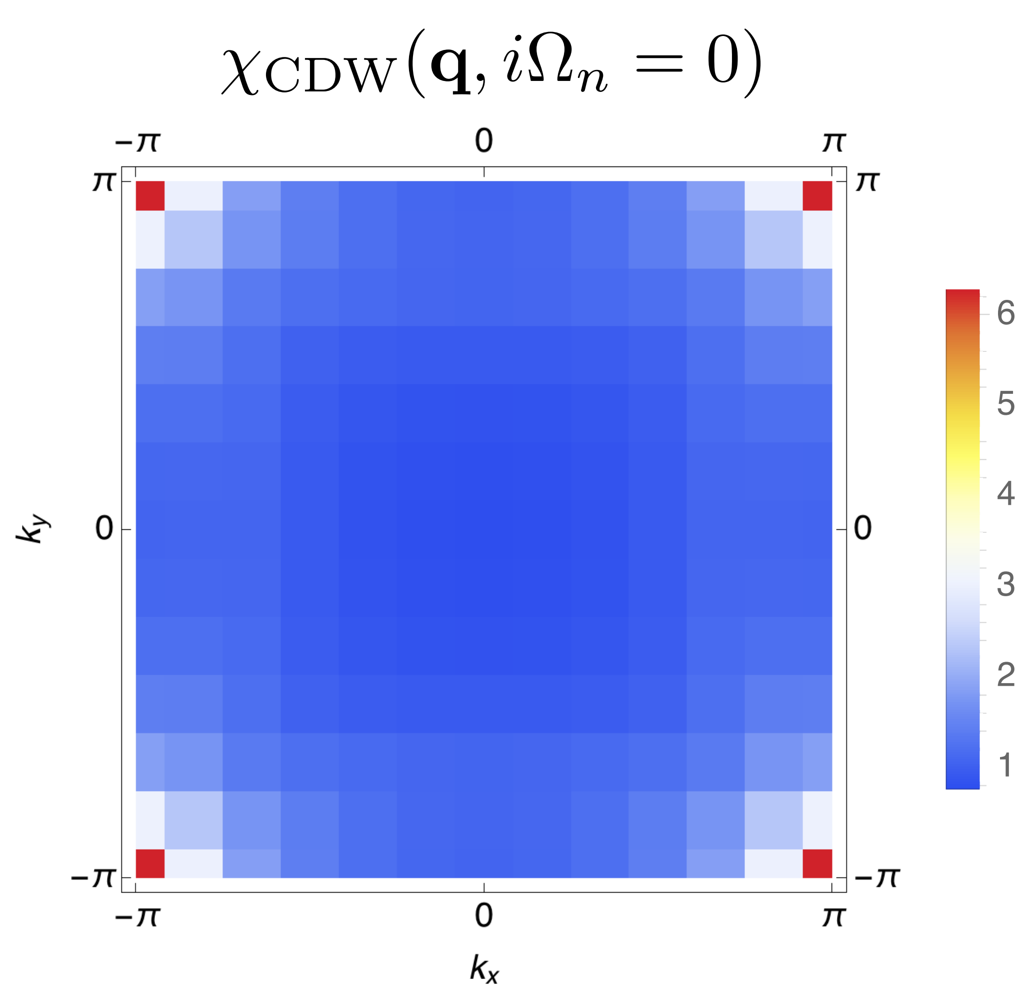
- Bipartite lattice at half-filling: exact SU(2) symmetry
  - SC and (π,π) CDW transform like a three-component order parameter
  - Similar symmetries have been studied, e.g., negative-U Hubbard model

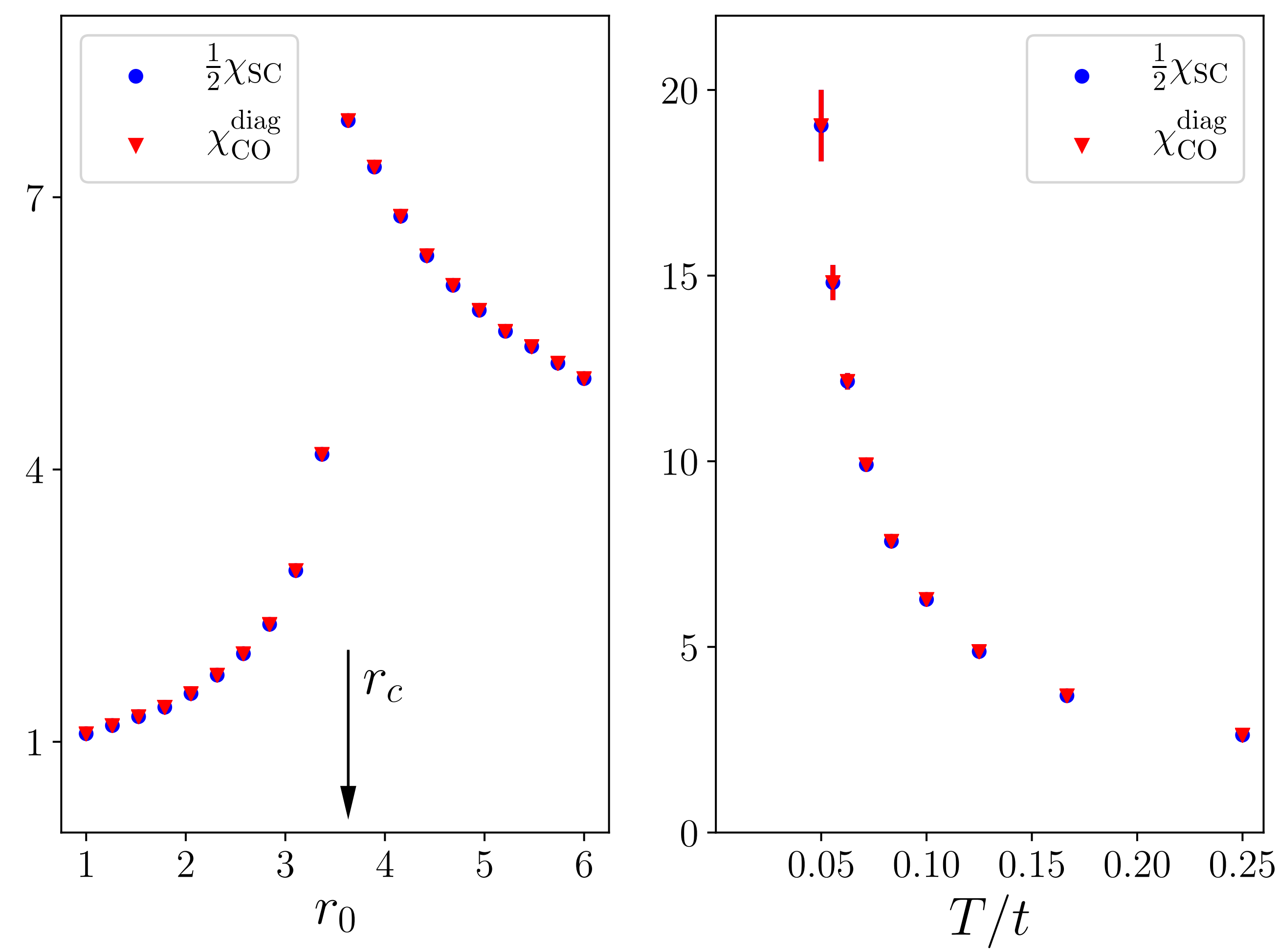
Moreo & Scalapino, PRL (1991)
Chakravarty, Laughlin, Morr & Nayak, PRB (2001)

- Away from half-filling, exact lattice symmetry is broken, however emergent hot spot symmetry is still present

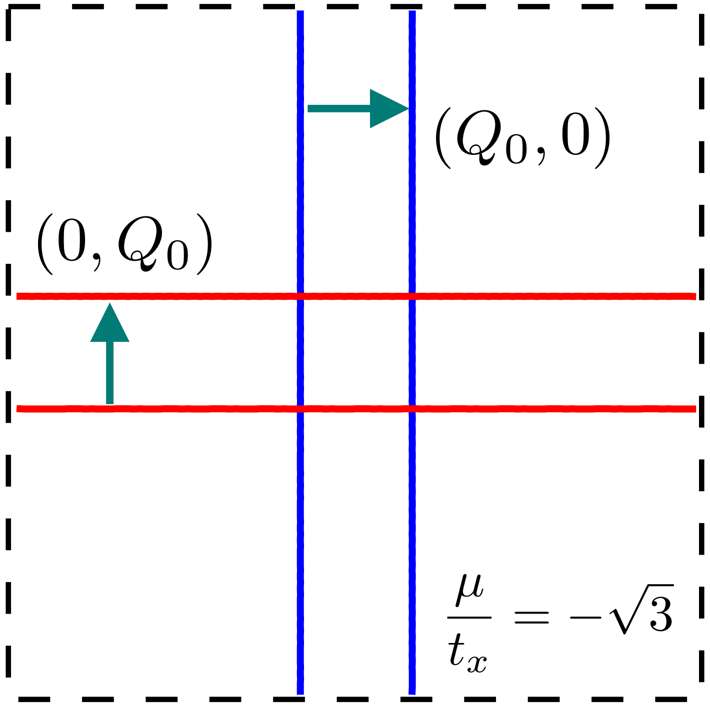
- Half-filling
- Results unchanged by band dispersion
- d-wave SC and CO enhanced by AFM QCP

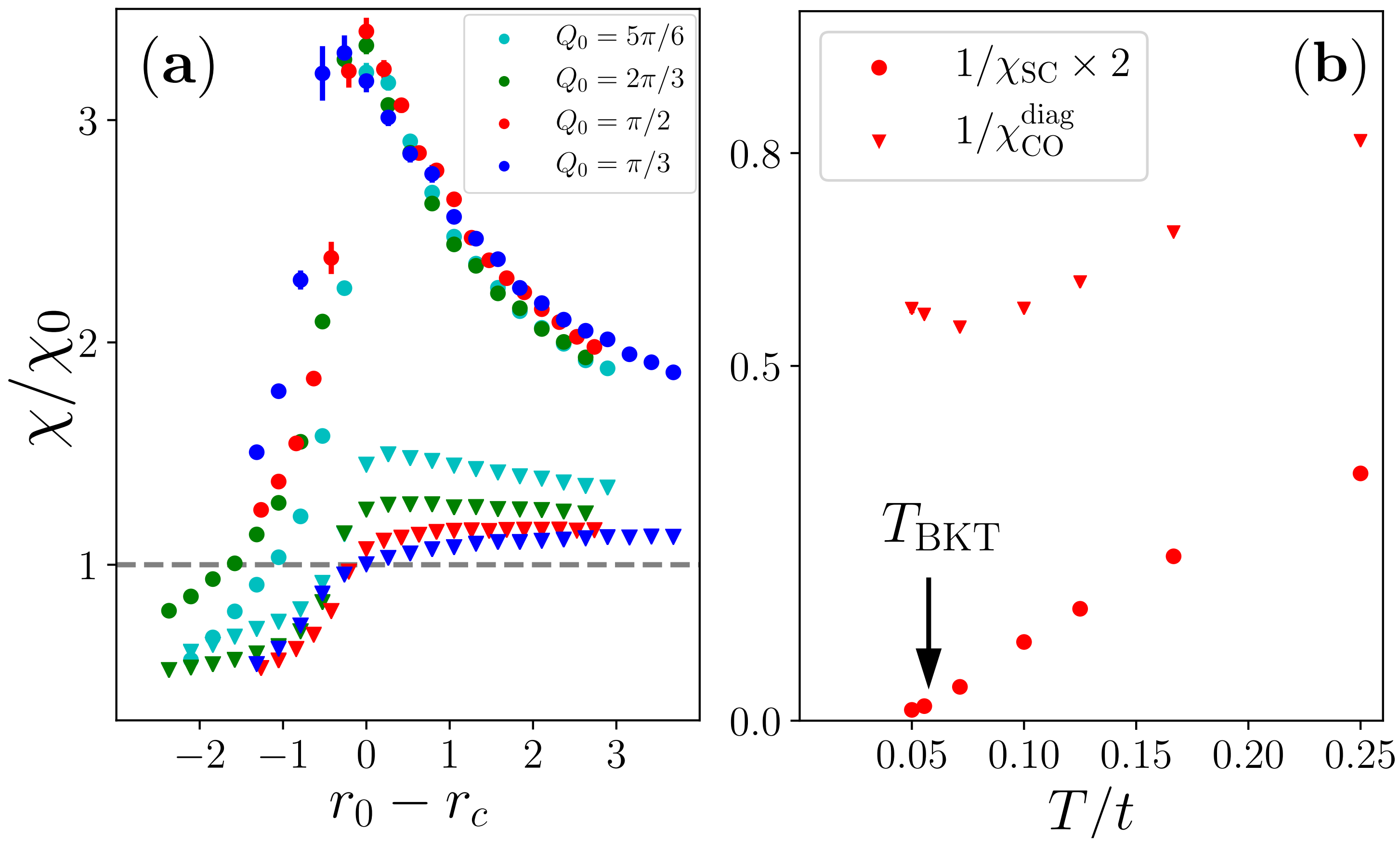






- Away from Half-filling





- Charge order always subleading to SC
- Emergent symmetry not found
    - Symmetry breaking terms at lattice level are relevant

Fradkin, Kivelson, Tranquada, RMP (2015)

Summary

- Sign-problem-free DQMC is a useful tool to study metallic QCP physics
- Hot spots govern SC properties near AF QCP up to large interactions comparable with fermionic bandwidth
- T_c saturates to a few percent of the bandwidth at the crossover from hot-spot dominated to Fermi-surface dominated pairing
- Despite uncontrolled, hot spot Eliashberg approximation works very well up to moderately strong coupling
- The emergent hot spot symmetry does not play a role in enhancing charge correlations
    - Need to look for charge order in more sophisticated models

- Phys. Rev. B 95, 174520 (2017)
- arXiv:1710.02158