Monte-Carlo studies of metals near the onset of antiferromagnetism

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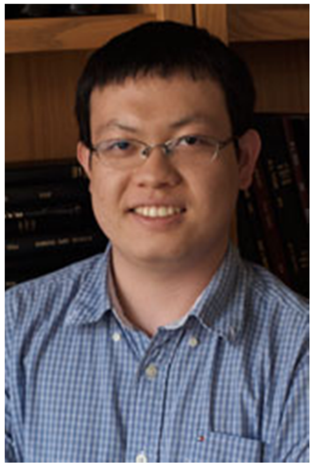
Max Gerlach
(Cologne)

Simon Trebst
(Cologne)

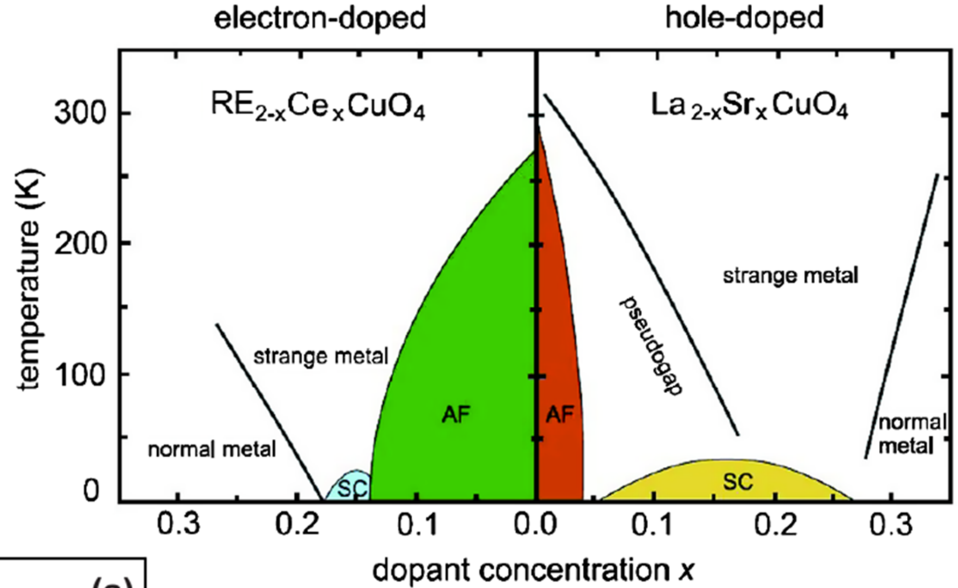


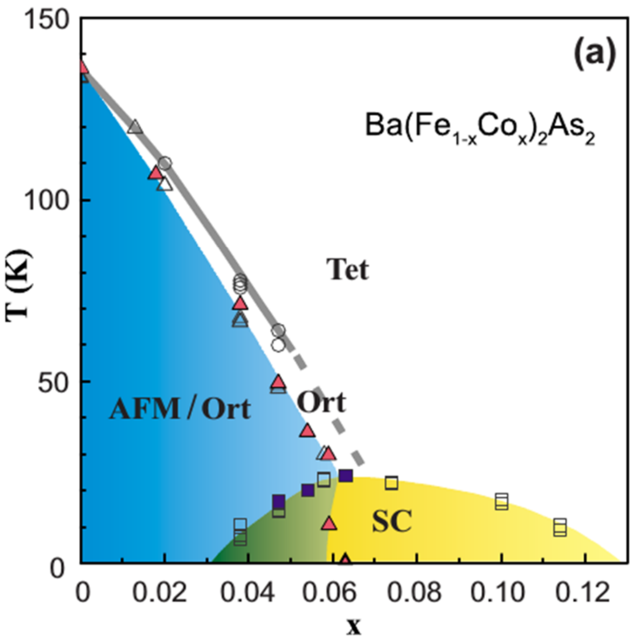
Xiaoyu Wang
(Minnesota)

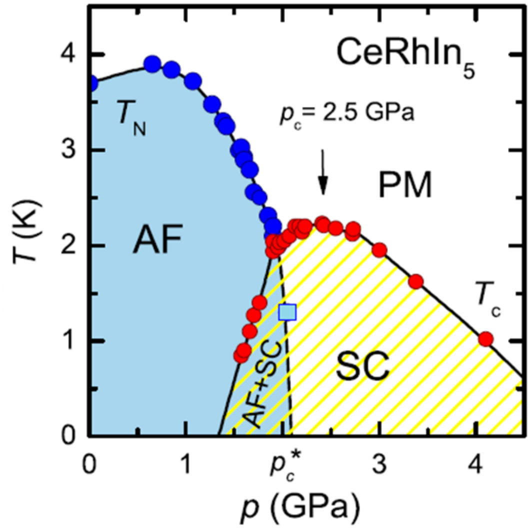
Rafael Fernandes
(Minnesota)

Erez Berg
(Chicago)

Antiferromagnetism – A common thread for unconventional superconductors

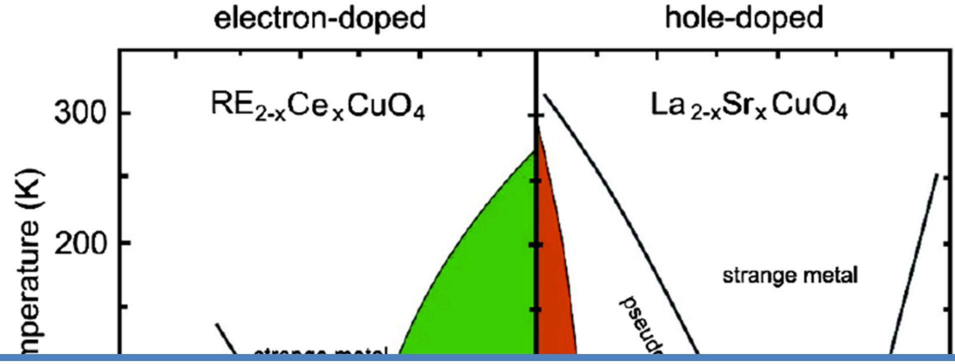




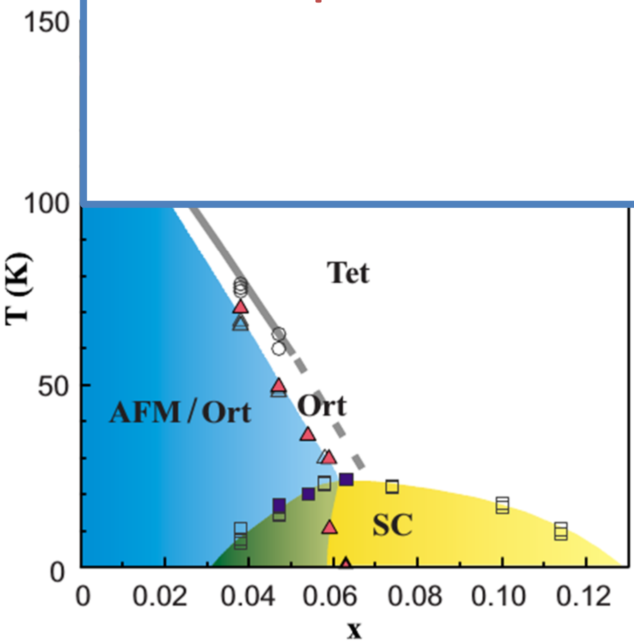


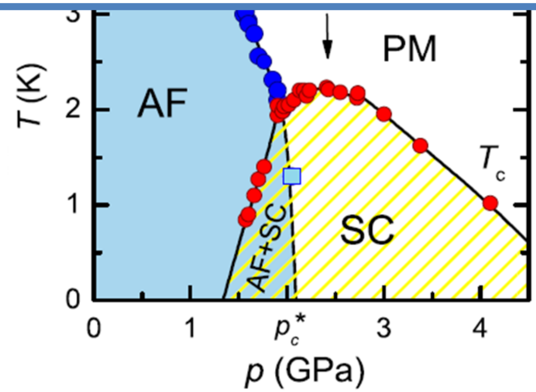
Armitage (2010), Fernandes (2010), Knebel (2009)

Antiferromagnetism – A common thread for unconventional superconductors



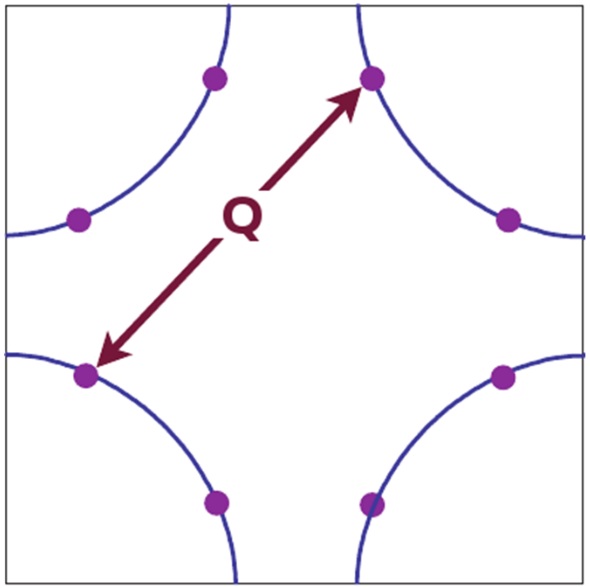
What aspects of the phenomenology of unconventional superconductors can be explained **just** by AFM fluctuations?



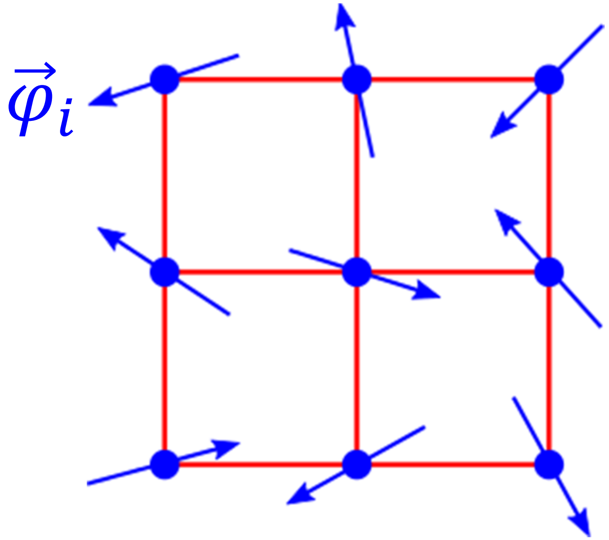


Armitage (2010), Fernandes (2010), Knebel (2009)

The model



$$S = S_{\psi} + S_{\varphi} + S_{int}$$



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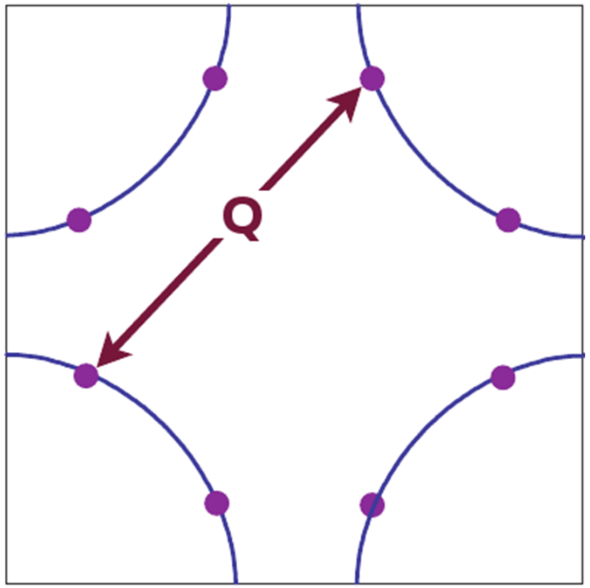

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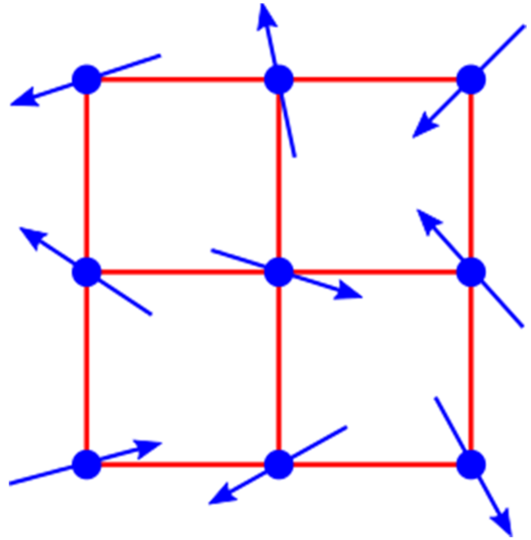
free fermions



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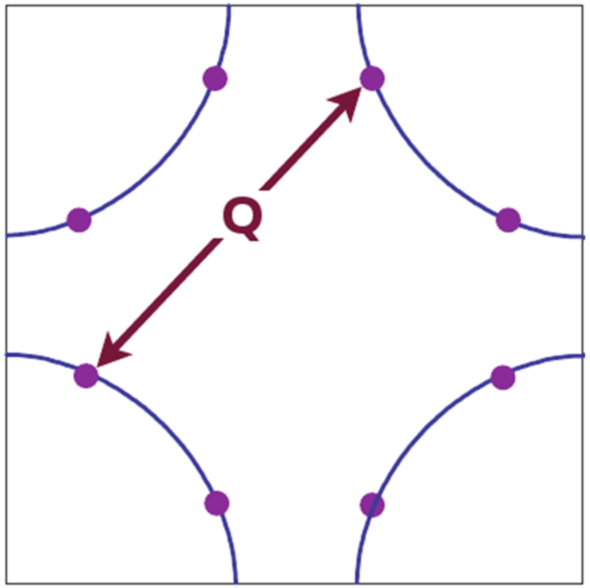

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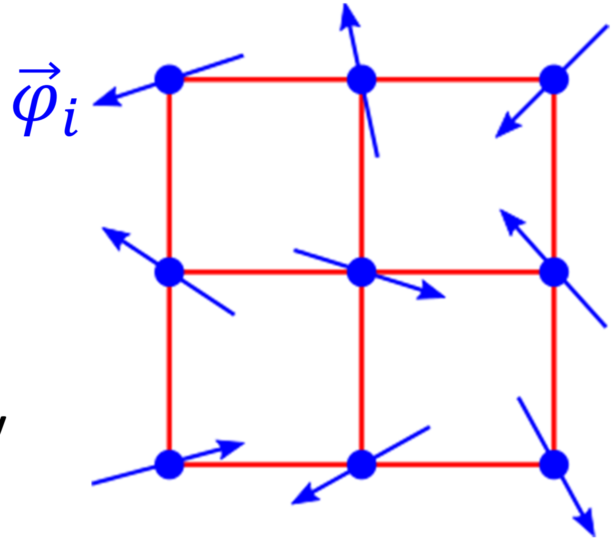
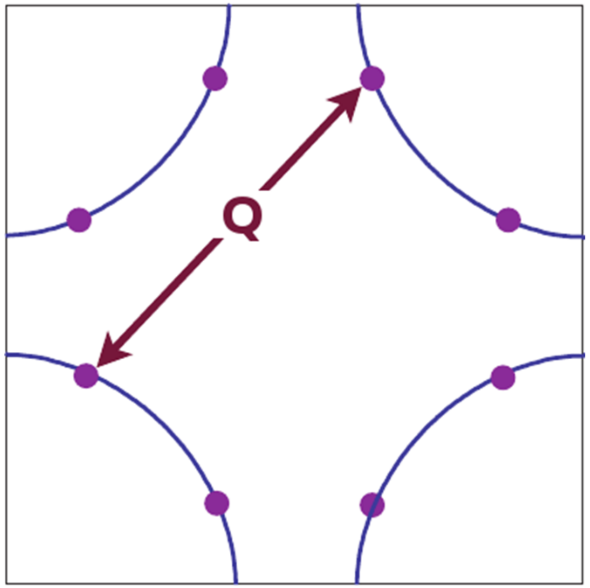
free fermions φ^4 theory



$$S_\varphi = r\vec{\varphi}^2 + \frac{1}{c^2}(\partial_\tau \vec{\varphi})^2 + \left[\nabla\left(e^{i\boldsymbol{Qx}}\vec{\varphi}\right)\right]^2 + \frac{1}{2}u(\vec{\varphi}^2)^2$$

The model



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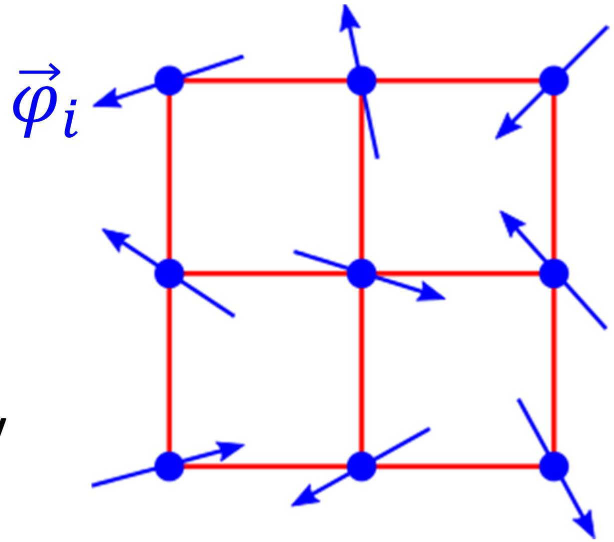
free fermions (→ S_ψ) φ^4 theory (→ S_φ)



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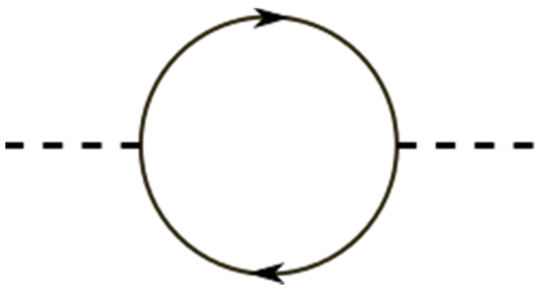
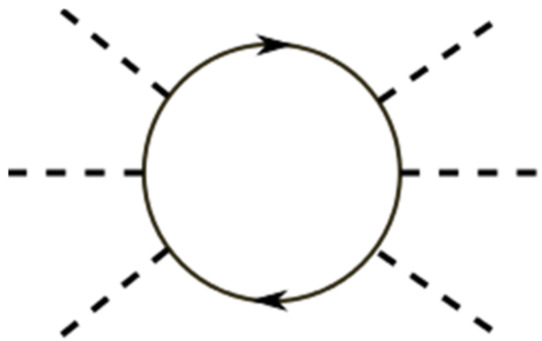
$$S_{int} = \lambda\vec{\varphi}(\psi^\dagger\vec{\sigma}\psi)$$

Hertz theory

- Integrate out the fermions
- Analyze resulting action using perturbative RG

$$S \sim |\vec{\varphi}_q|^2(r' + (\boldsymbol{q} - \boldsymbol{Q})^2 + |\omega_n|) + u_4\varphi^4 + u_6\varphi^6 \ldots.$$





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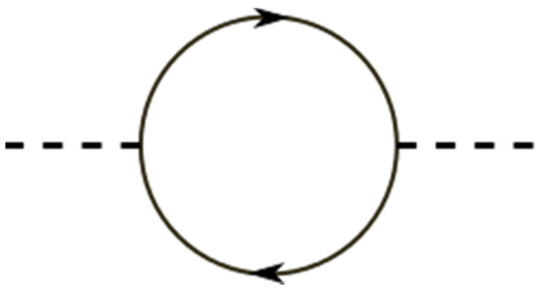
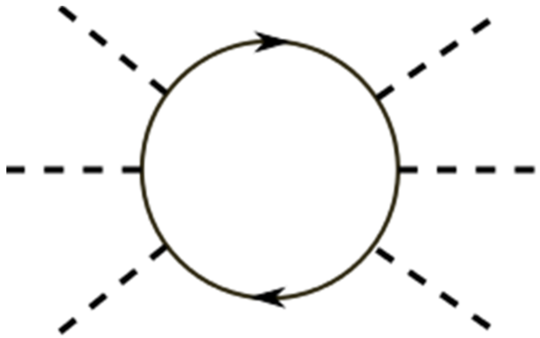
Landau damping





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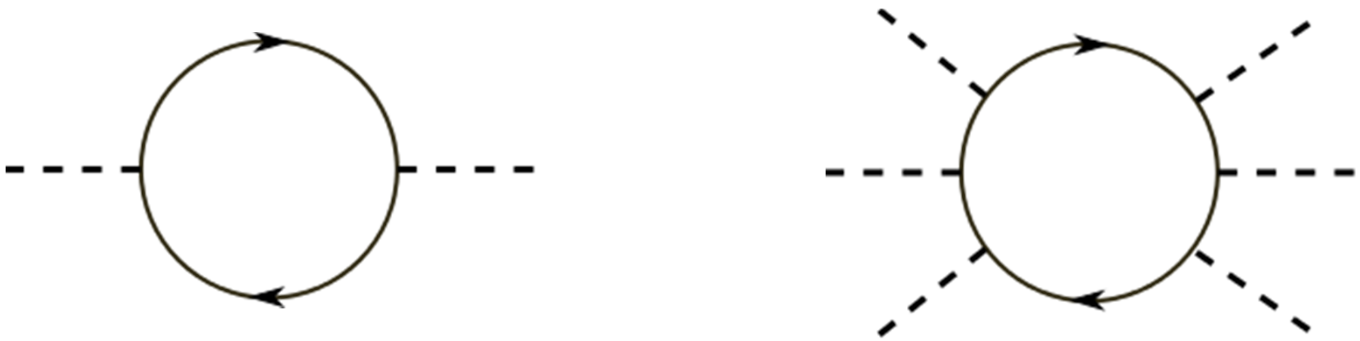

- Dynamic critical exponent z=2.
- D=2: φ^4 term is marginal: mean-field exponents + log corrections.

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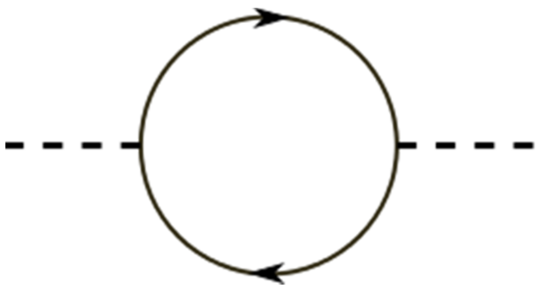
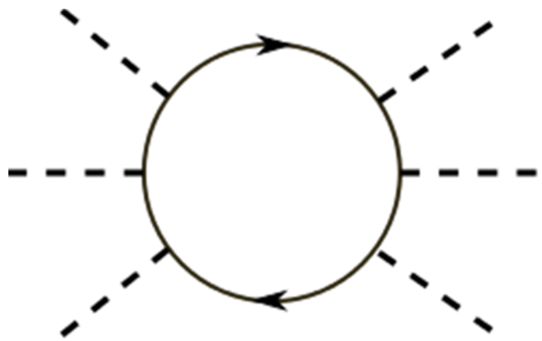


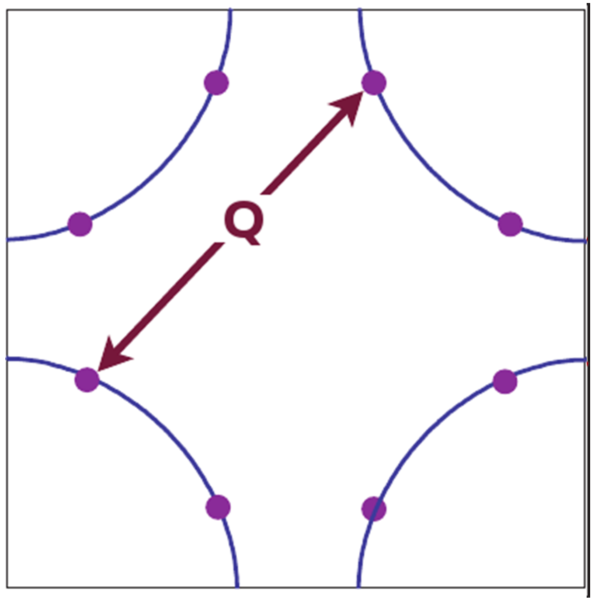


- Dynamic critical exponent z=2.
- D=2: φ^4 term is marginal: mean-field exponents + log corrections.
- Dangerous procedure - integrating out gapless DOF.

Determinant Quantum Monte Carlo

$$S_{\mathrm{eff}} = S_{\varphi} + \log(\det(G))$$

The sign problem: $\det(G)$ is complex

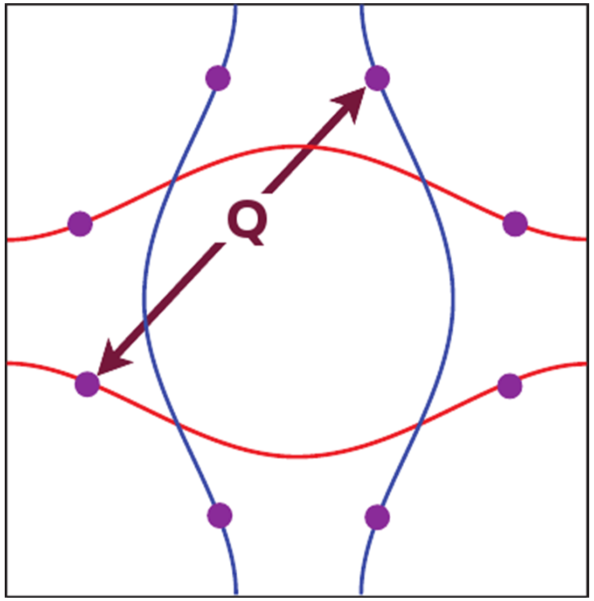


Determinant Quantum Monte Carlo

$$S_{eff} = S_{\varphi} + \log(\det(G))$$

The sign problem: $\det(G)$ is complex

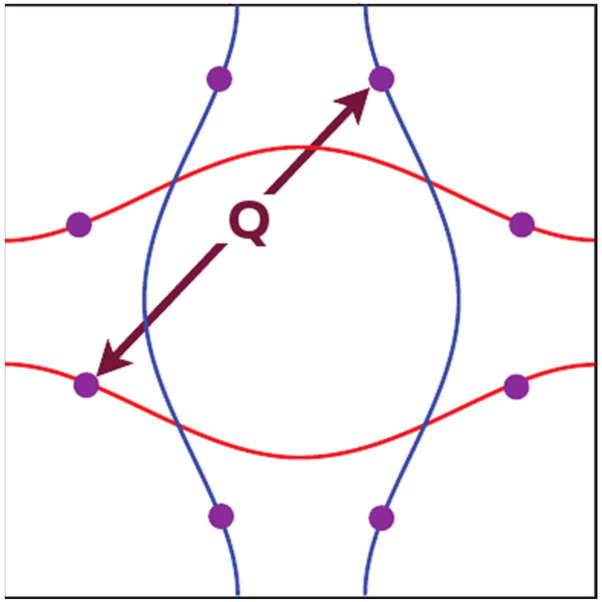
Solution: deform the FS away from the hot spots



Effective "time reversal symmetry" of the action: no sign problem

Berg, Metlitski, Sachdev, Science (2012)

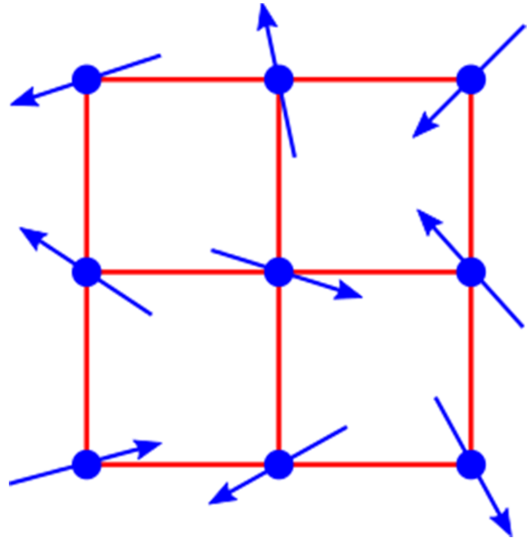
The model



$$S = S_{\psi} + S_{\varphi} + S_{in}{}^{t}$$

free fermions φ^4 theory

$\vec{\varphi}_i$



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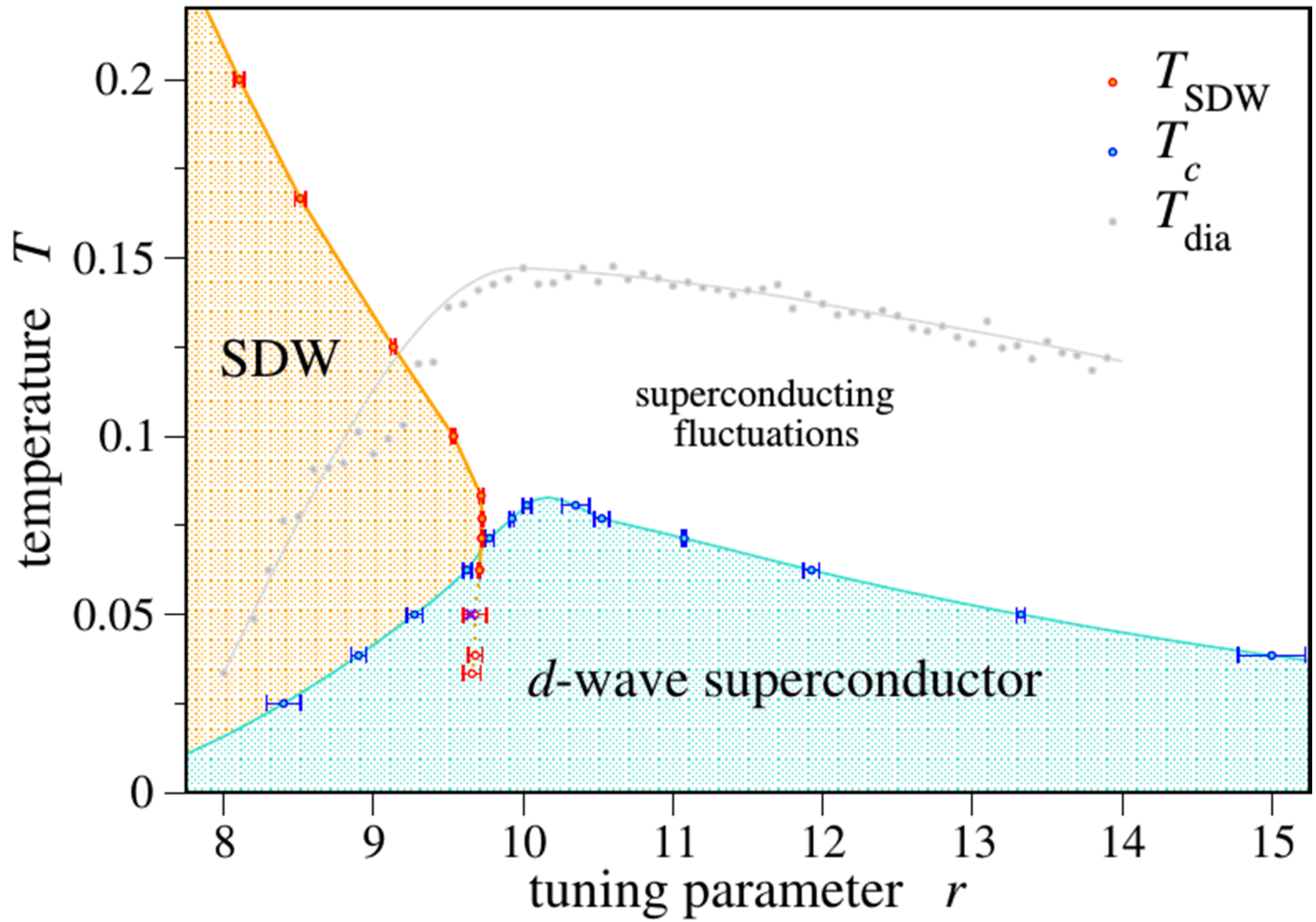
$$S_{in}{}^{t} = \lambda\vec{\varphi}(\psi_1^{\dagger}\vec{\sigma}\psi_2 + \psi_2^{\dagger}\vec{\sigma}\psi_1)$$

Easy plane AFM order $\vec{\varphi} = \left(\varphi_x, \varphi_y\right)$

Part I

Phase diagram

YS, Gerlach, Trebst, and Berg, PRL (2016)

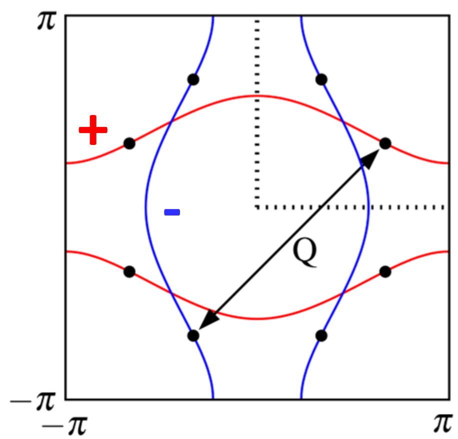


T_{SDW}
T_c
T_{dia}
SDW
superconducting fluctuations
d-wave superconductor
temperature T
tuning parameter r
0.2
0.15
0.1
0.05
0
8
9
10
11
12
13
14
15

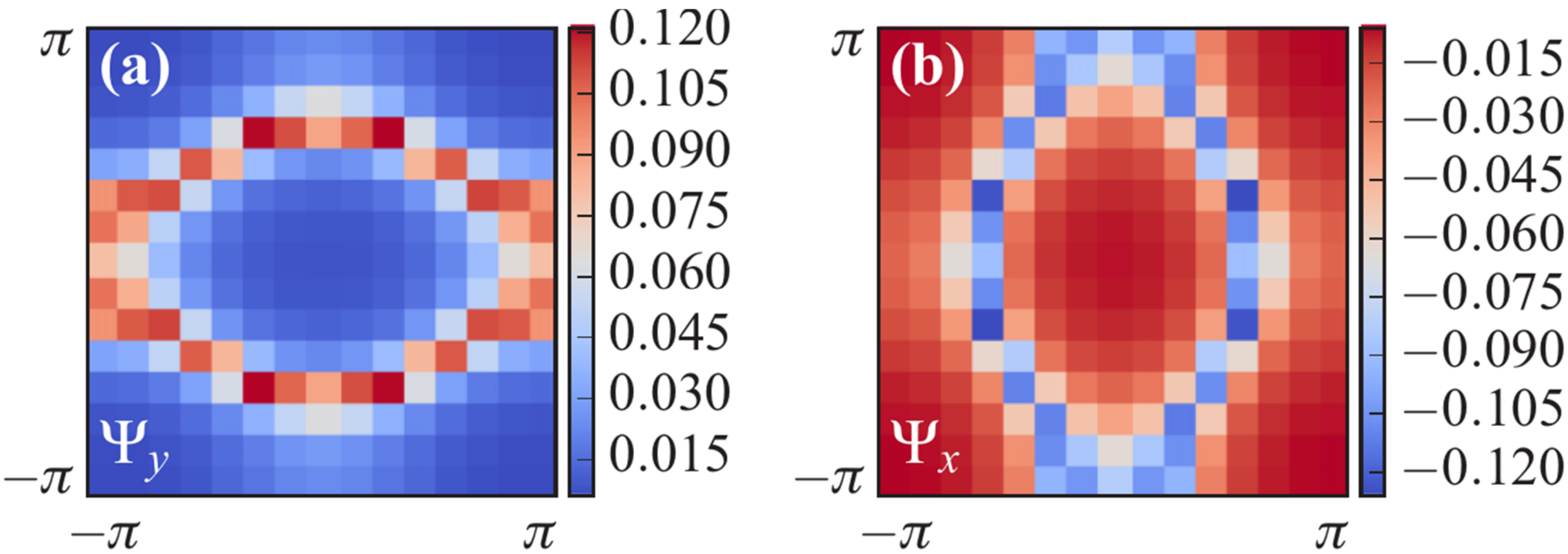
Superconductivity

Nodeless d-wave

$\Psi = \psi_{1\uparrow}\psi_{1\downarrow} - \psi_{2\uparrow}\psi_{2\downarrow}$



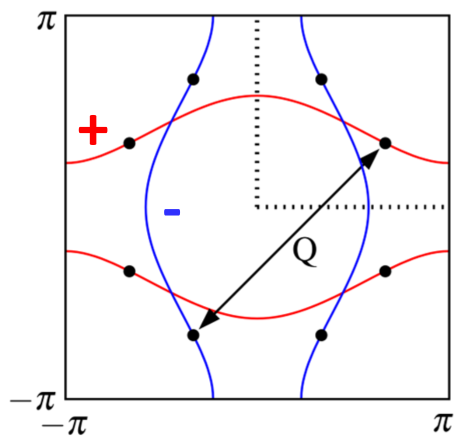
Superconductivity



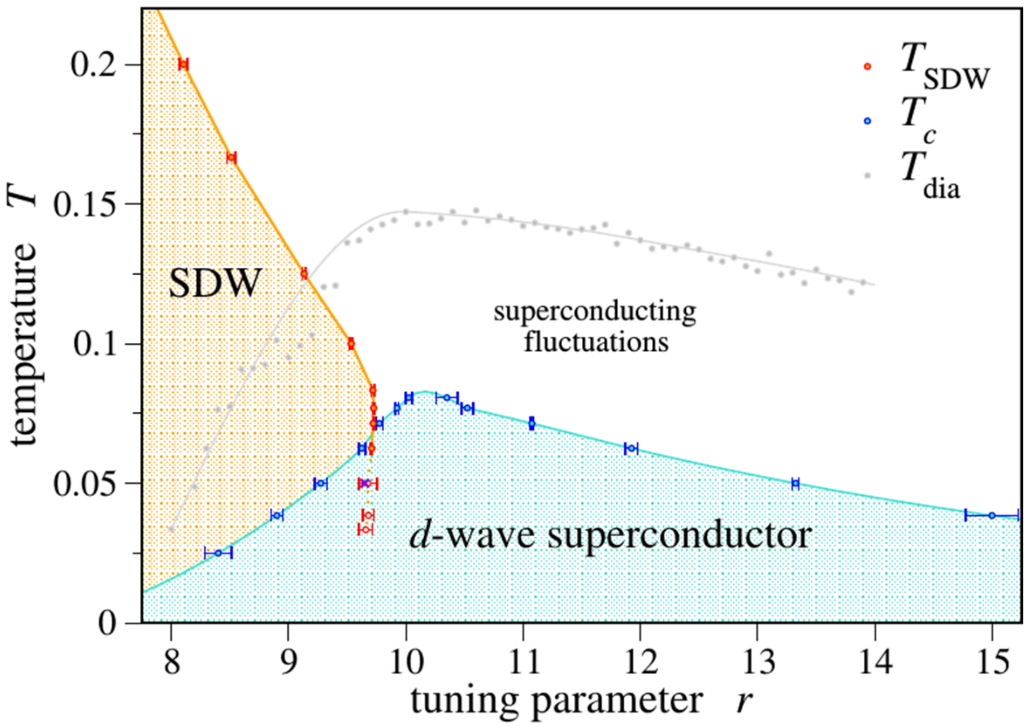
Nodeless d-wave

$$\Psi \ = \psi_{1\uparrow}\psi_{1\downarrow} - \psi_{2\uparrow}\psi_{2\downarrow}$$

No sharp feature at the hotspots

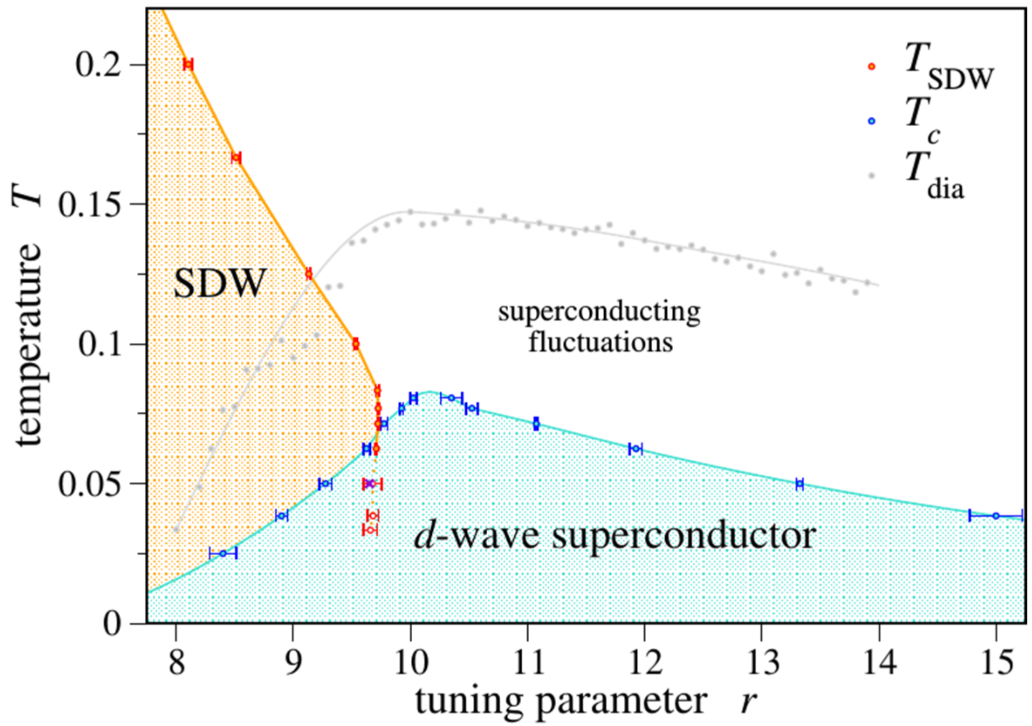


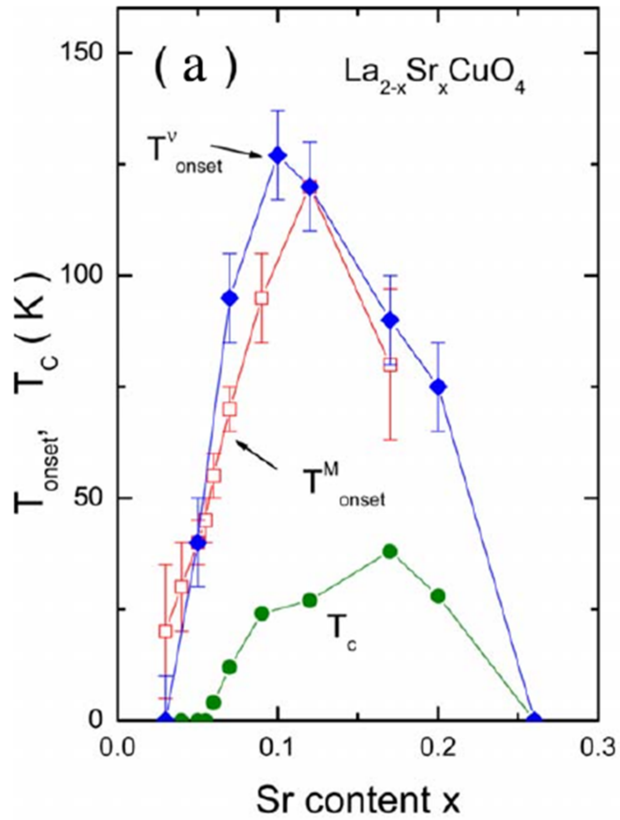
Superconducting fluctuations



Diamagnetism onsets at
T$\sim 2T_c$

Superconducting fluctuations

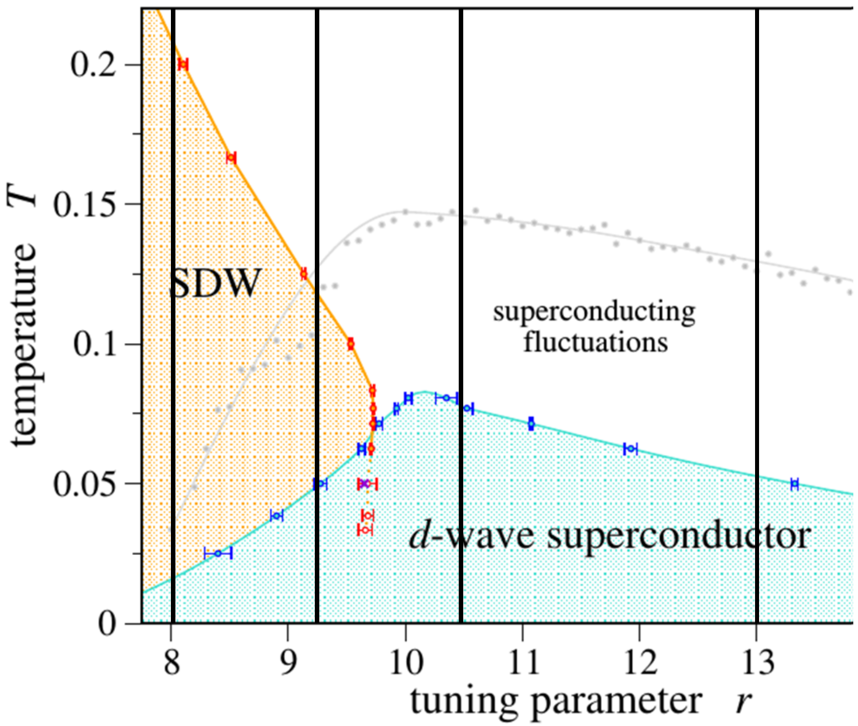


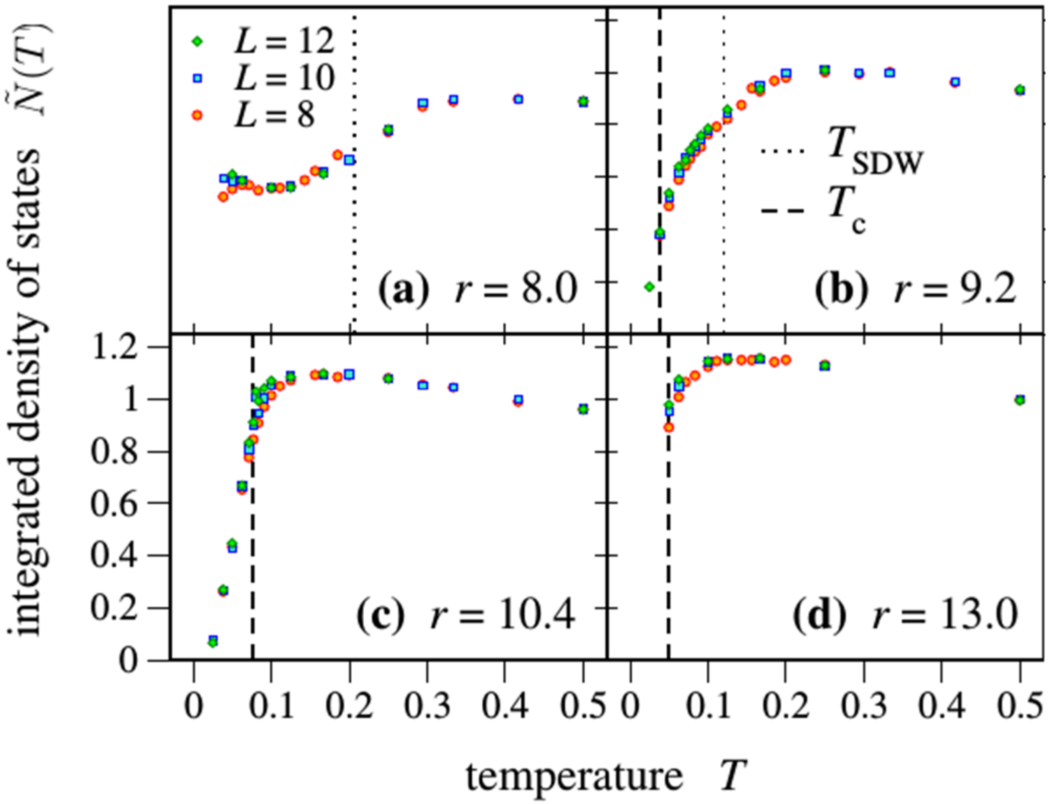


Diamagnetism onsets at
$T\sim 2T_c$

Similar to hole-doped cuprates
Li et al. PRB (2010)

“Pseudogap”

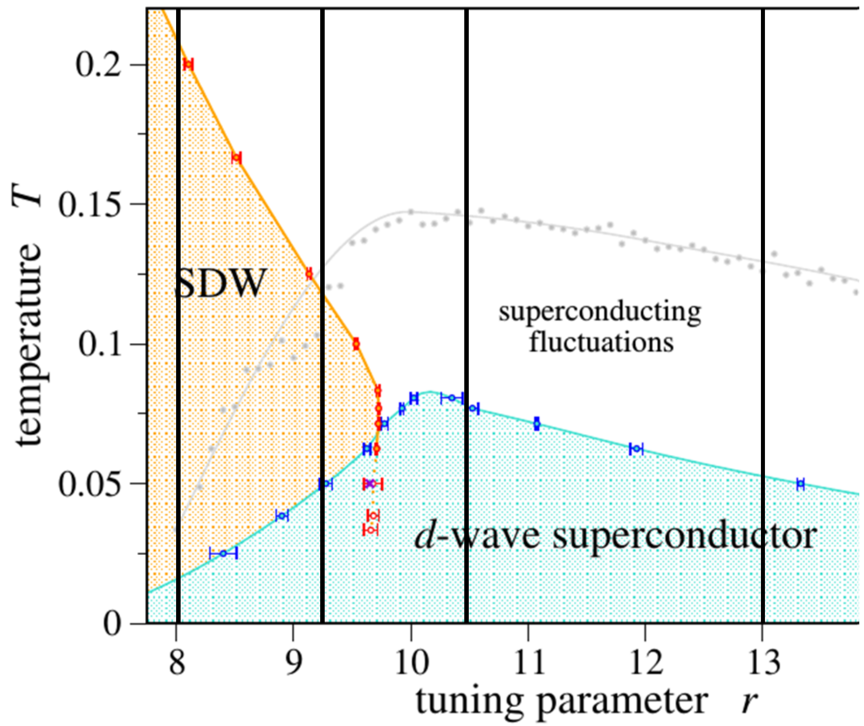


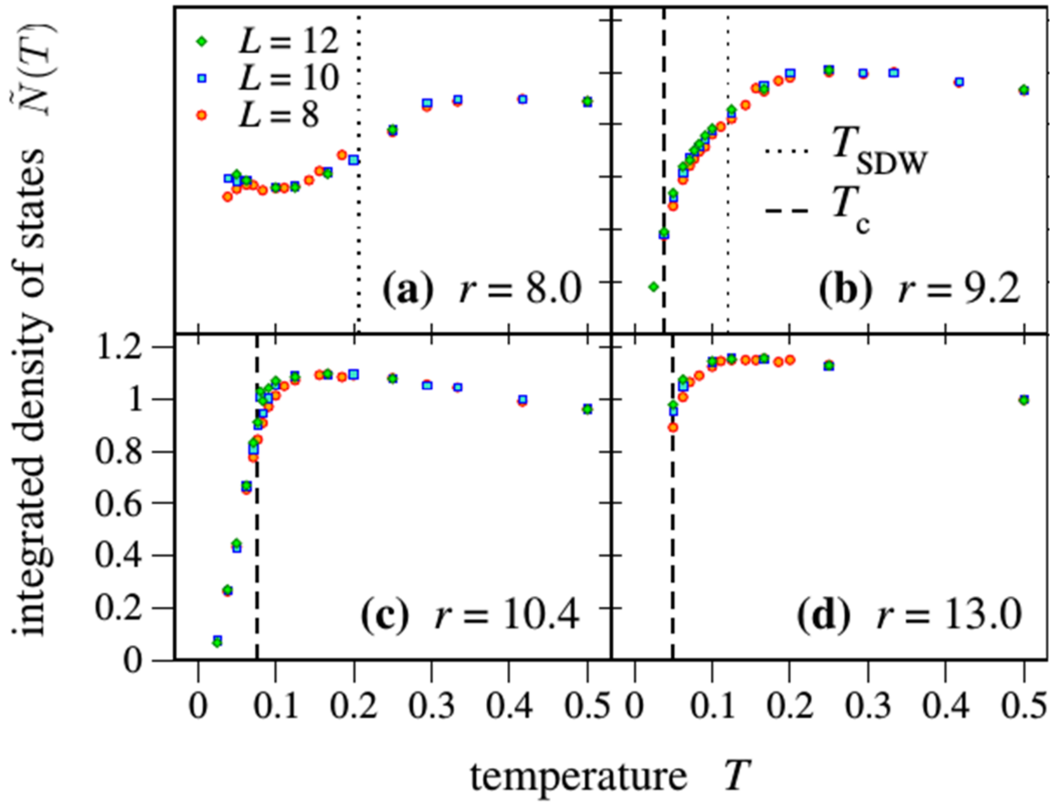


Reduction in the tunneling density of states onsets at $T \sim 1.5\max(T_c, T_{SDW})$

$$\widetilde{N}(T) = \frac{1}{T}\int d\,\omega \frac{N(\omega)}{2\cosh(\frac{\beta\omega}{2})}$$

“Pseudogap”





Reduction in the tunneling density of states onsets at $T \sim 1.5\mathrm{ma}^{\mathrm{X}}(T_c, T_{SD}{}^{W})$

Unlike hole-doped cuprates

$$\widetilde{N}(T) = \frac{1}{T}\int d\,\omega\,\frac{N(\omega)}{2\cosh(\frac{\beta\omega}{2})}$$

Charge-density waves

$$n_{-}(\vec{x}) = e^{i\,\vec{q}\vec{x}}(n_1(\vec{x}) - n_2(\vec{x}))$$

Weak enhancement of short-range CDW fluctuations with a d-wave form factor.

The optimal CDW wavevector is **not** an inter-hotspot wavevector, but is determined by band structure.

Always much weaker than SC correlations

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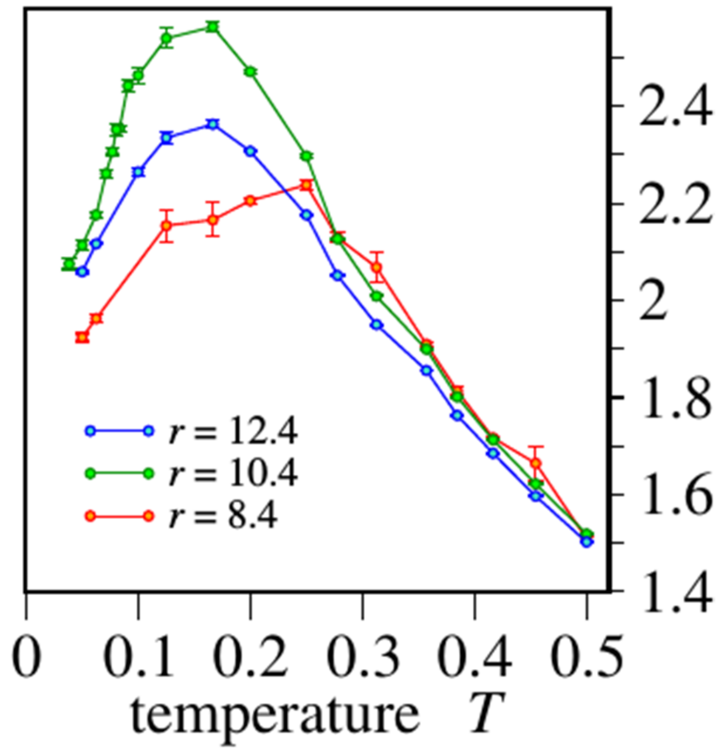


Summary of part I

- High Tc, d-wave SC phase peaked close to AFM QCP.
- Loss of tunneling density of states and diamagnetism above Tc, track Tc.
- No tendency towards charge order.

Part II

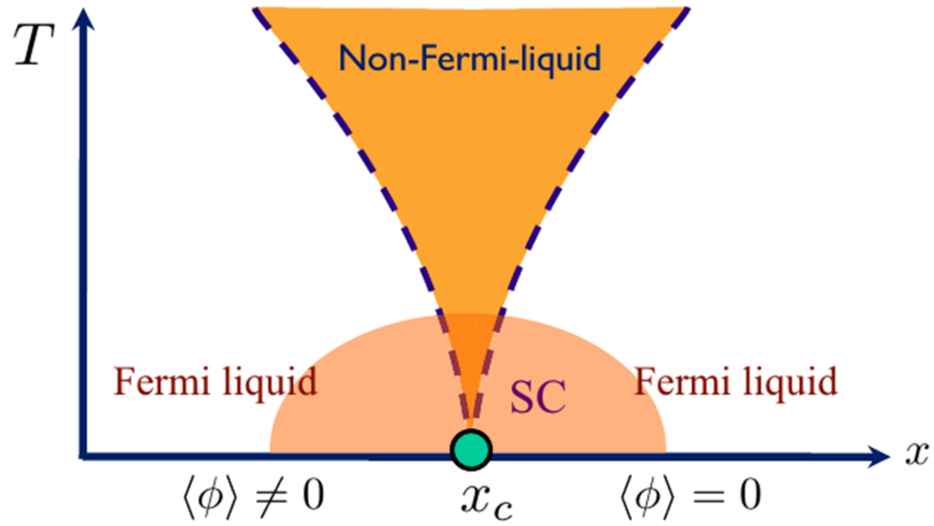
Quantum critical properties

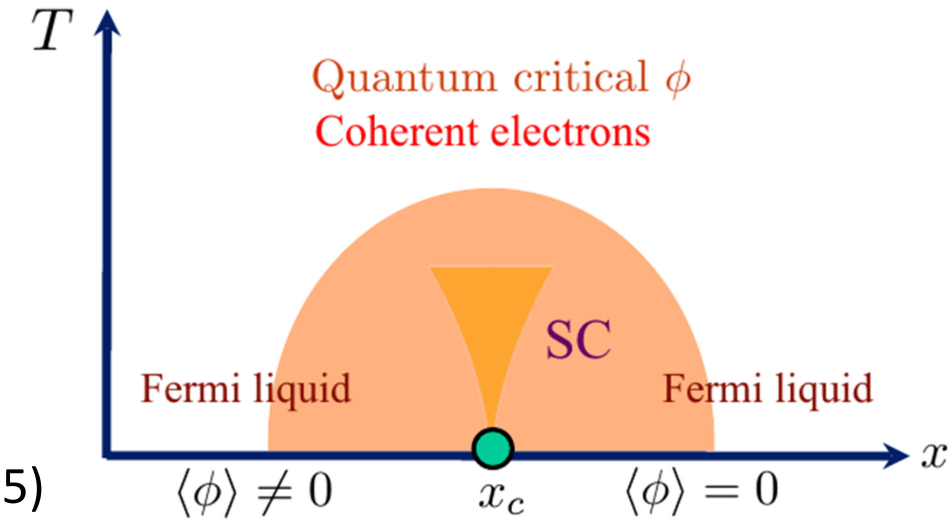
Gerlach, YS, Berg, and Trebst, PRB (2017)

Much like in experiment, superconductivity always hides the QCP

We can't get rid of SC – sign problem.

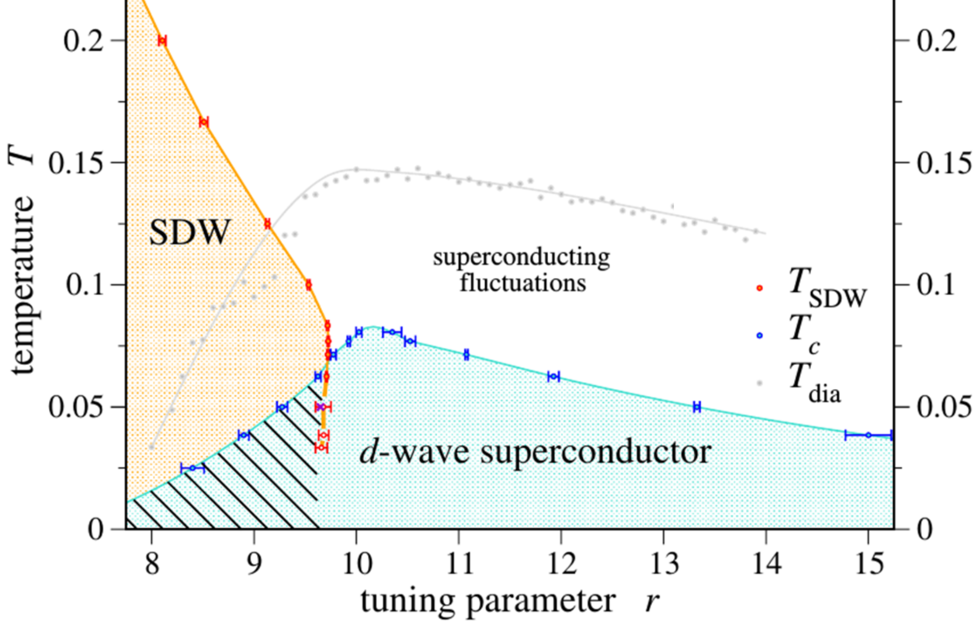
Is there a temperature window where physics of the 'metallic' QCP is seen?



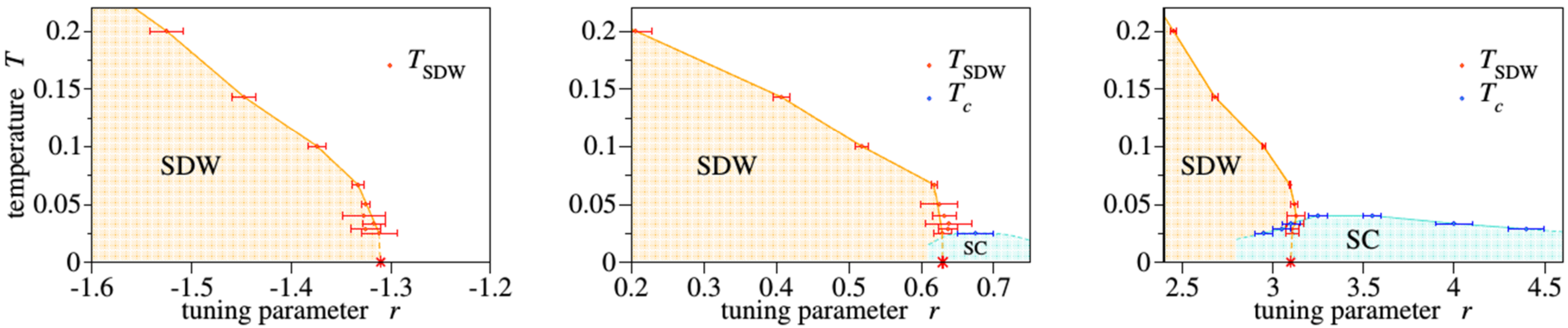


Metlitski et al. PRB (2015)

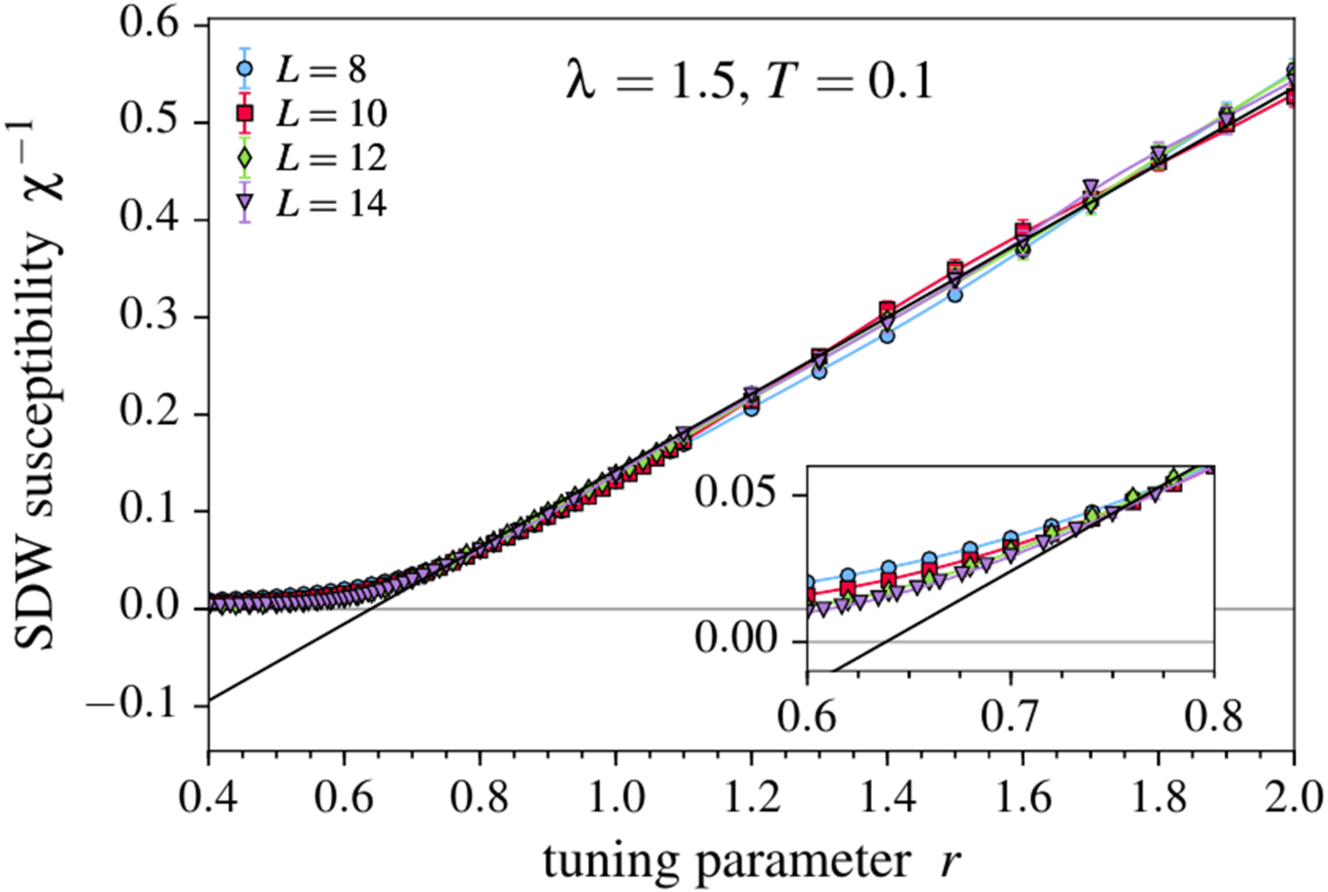
$\lambda = 3$



(a) $\lambda = 1$ **(b)** $\lambda = 1.5$ **(c)** $\lambda = 2$

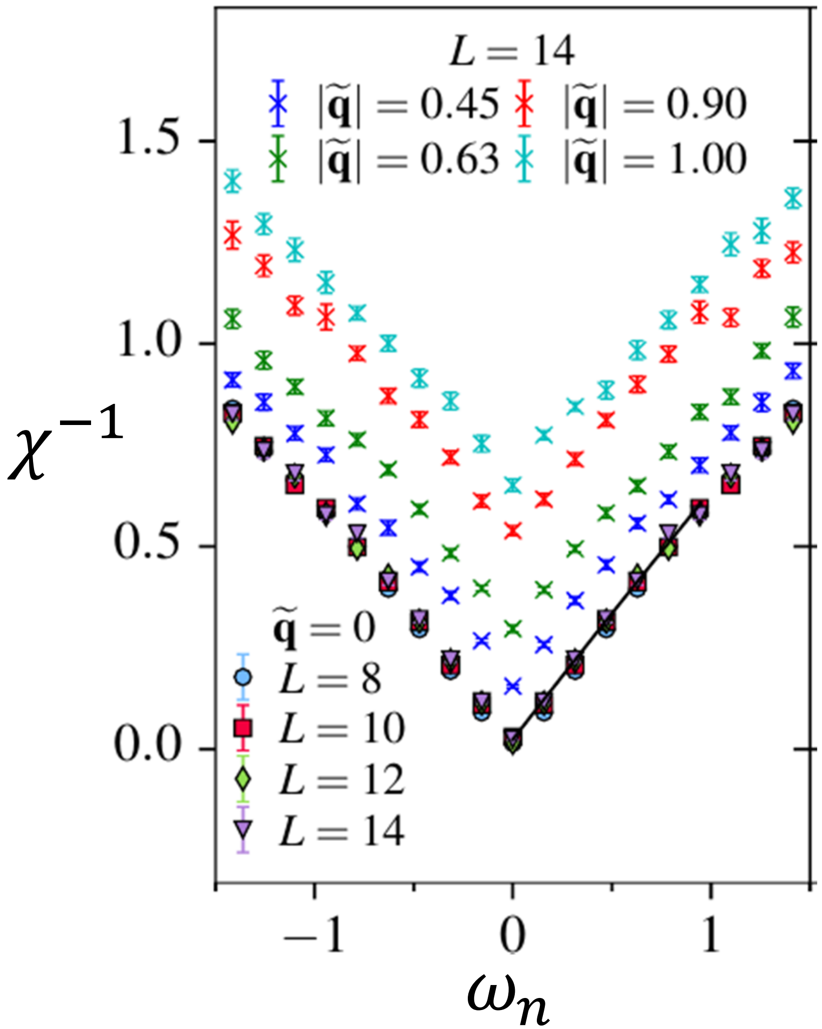


Magnetic fluctuations



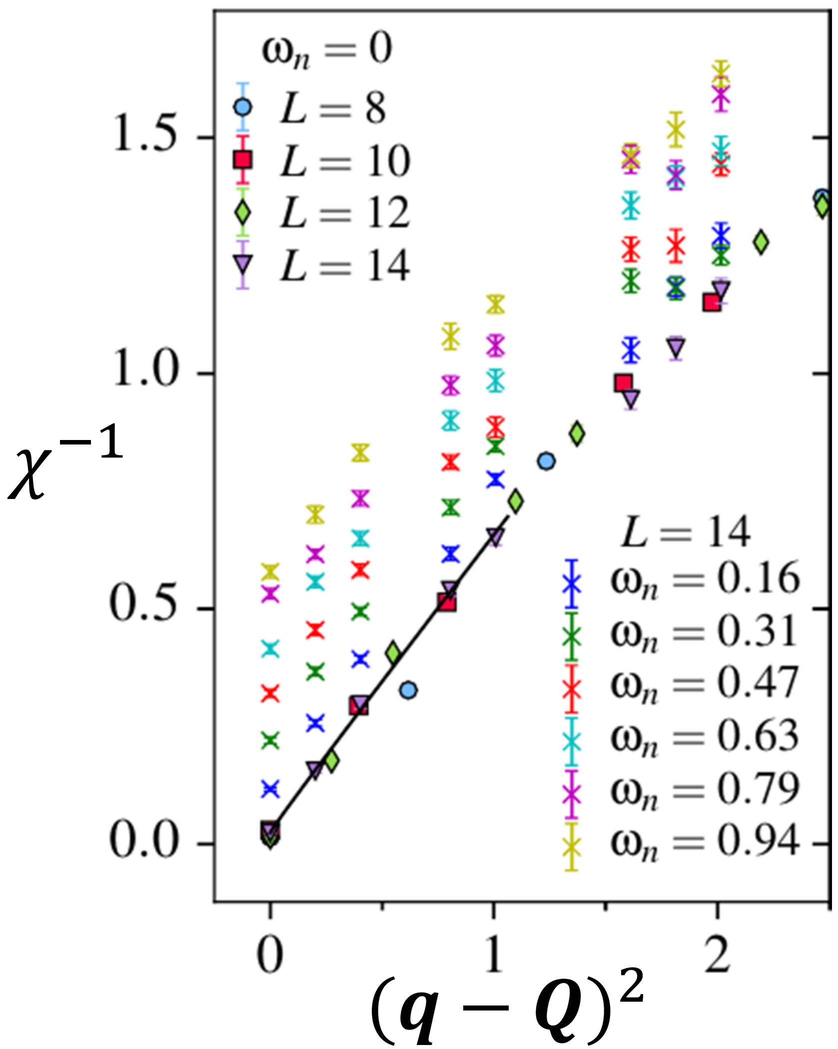
$$\chi^{-1} = a_r(r - r_{c0})$$

Magnetic fluctuations



$$\chi^{-1} = a_r(r - r_{c0}) + a_\omega|\omega_n|$$

Magnetic fluctuations



$$\chi^{-1} = a_r(r - r_{c0}) + a_\omega|\omega_n| + a_q(\boldsymbol{q} - \boldsymbol{Q})^2$$

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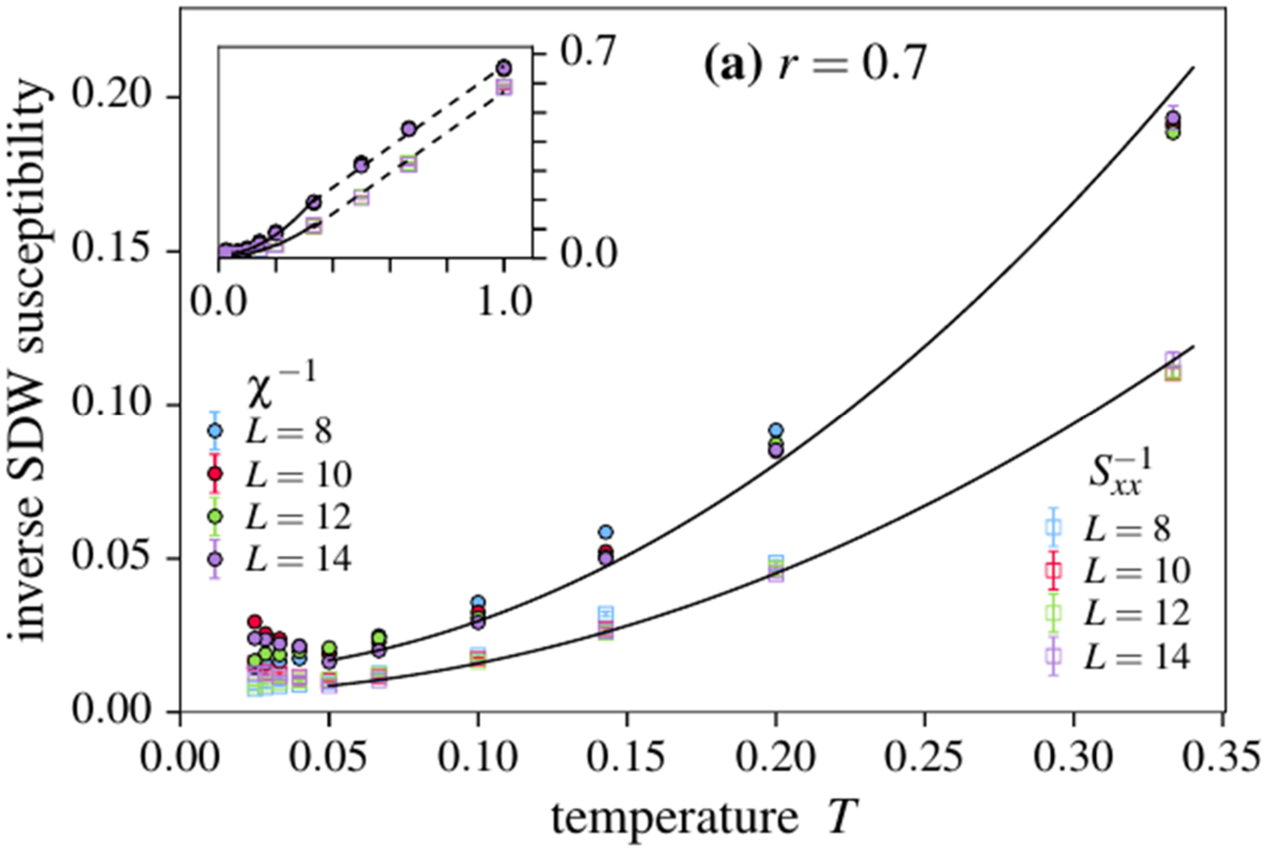
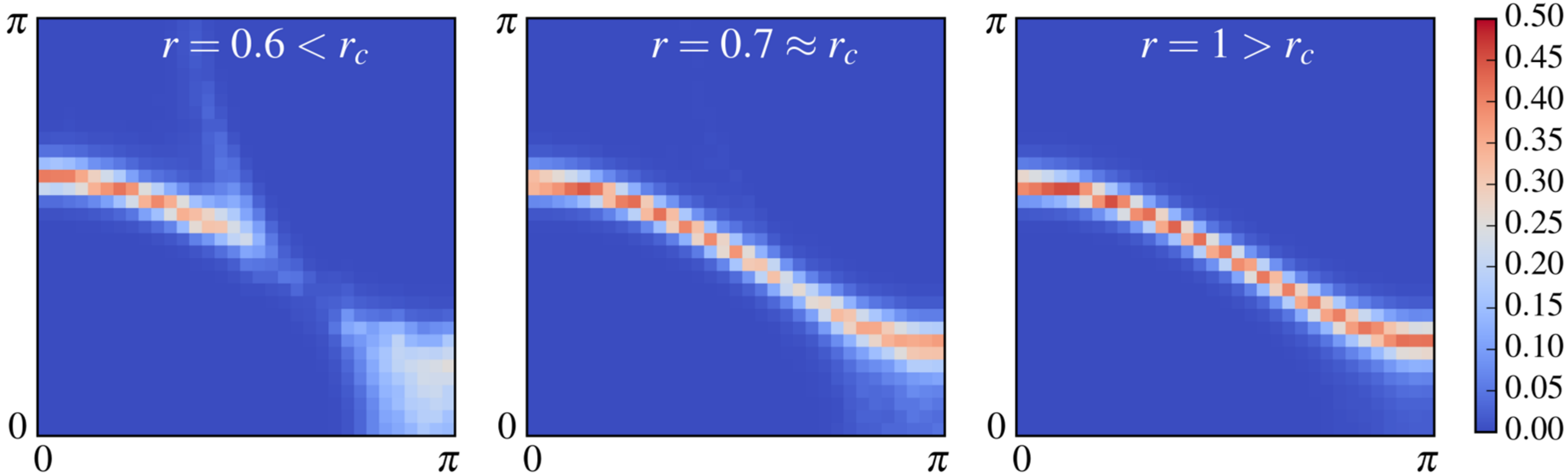
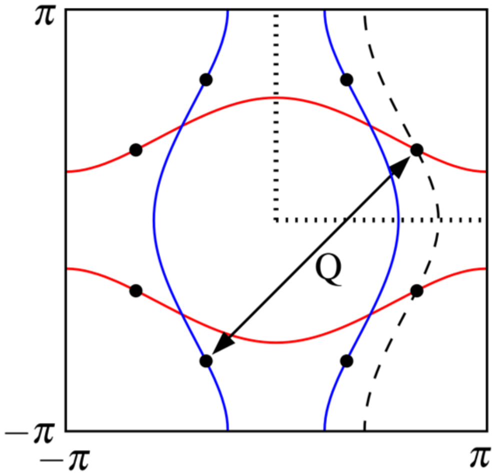


$$\chi^{-1} = a_r(r - r_{c0}) + a_\omega|\omega_n| + a_q(\boldsymbol{q} - \boldsymbol{Q})^2 + f(r, T)$$

Single-fermion properties

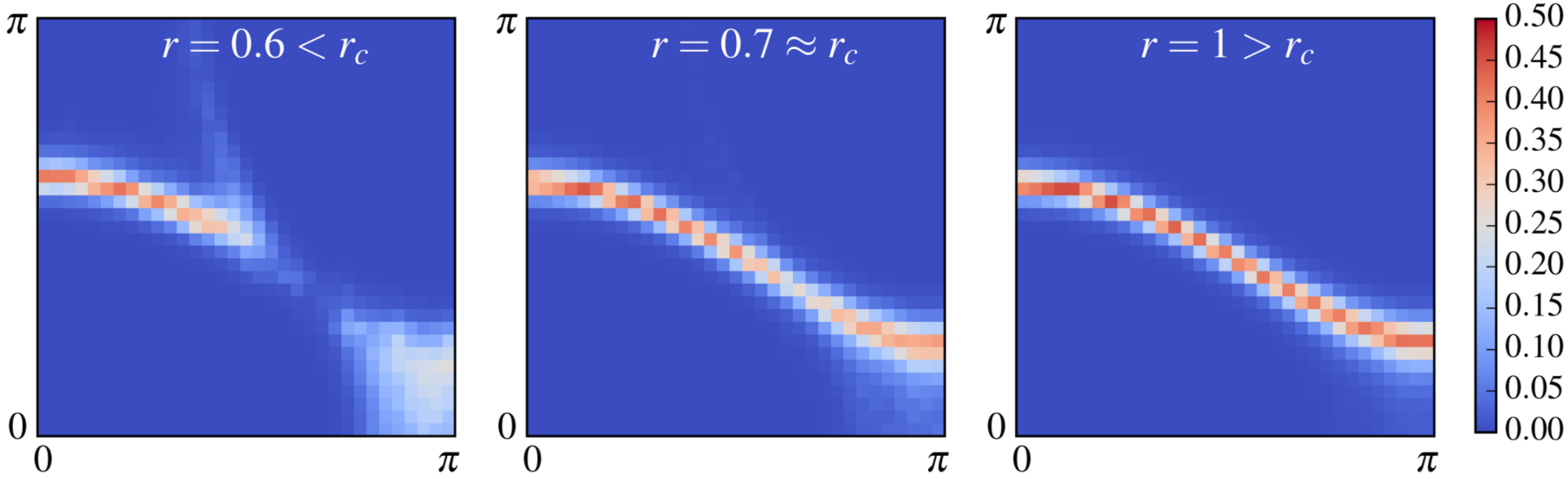


$$G_k\left(\tau = \frac{\beta}{2}\right) = \int d\omega \frac{A_k(\omega)}{2\cosh\left(\frac{\beta\omega}{2}\right)}$$

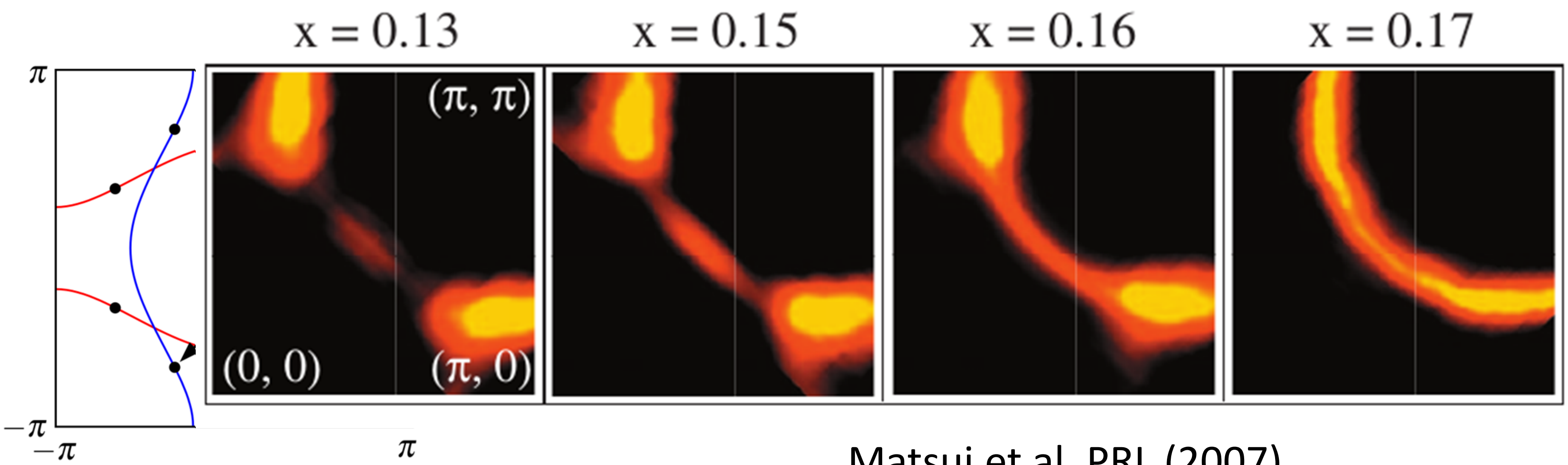


A lot like ARPES MDC: *A* integrated over a window of size ~*T*

Single-fermion properties



$Nd_{2-x}Ce_xCuO_4$



Matsui et al. PRL (2007)

Quasiparticle weight

$$G_{\boldsymbol{k}}\left(\tau\sim\frac{\beta}{2}\right)=Z_{\boldsymbol{k}}(T)\,\frac{e^{-\epsilon_{\boldsymbol{k}}\left(\tau-\frac{\beta}{2}\right)}}{2\cosh\left(\frac{\beta\epsilon_{\boldsymbol{k}}}{2}\right)}$$

$$Z_{\boldsymbol{k}}(T\to 0)=Z_{\boldsymbol{k}}$$

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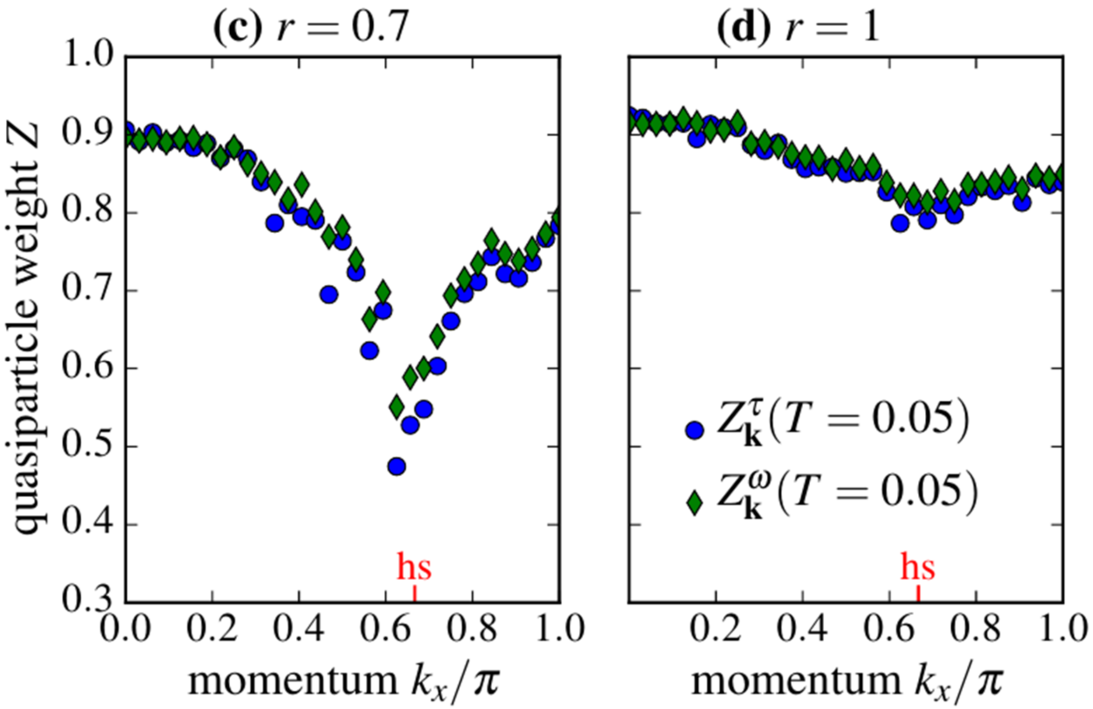

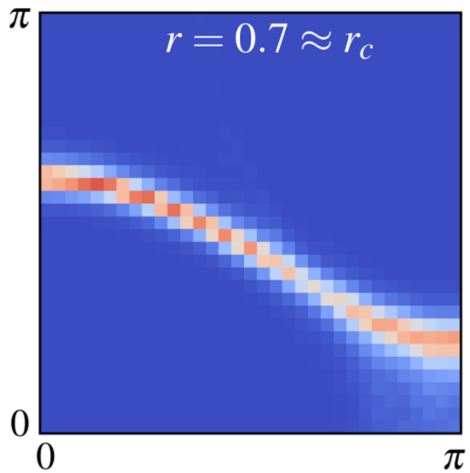

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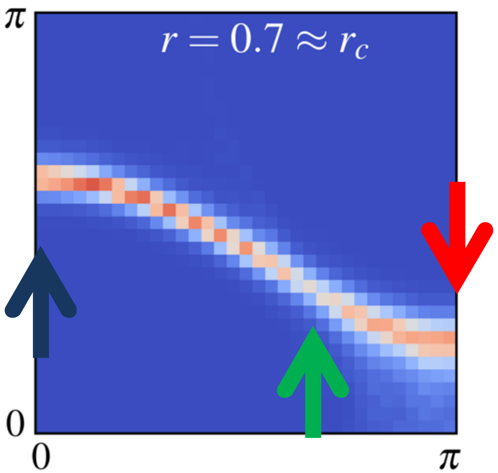
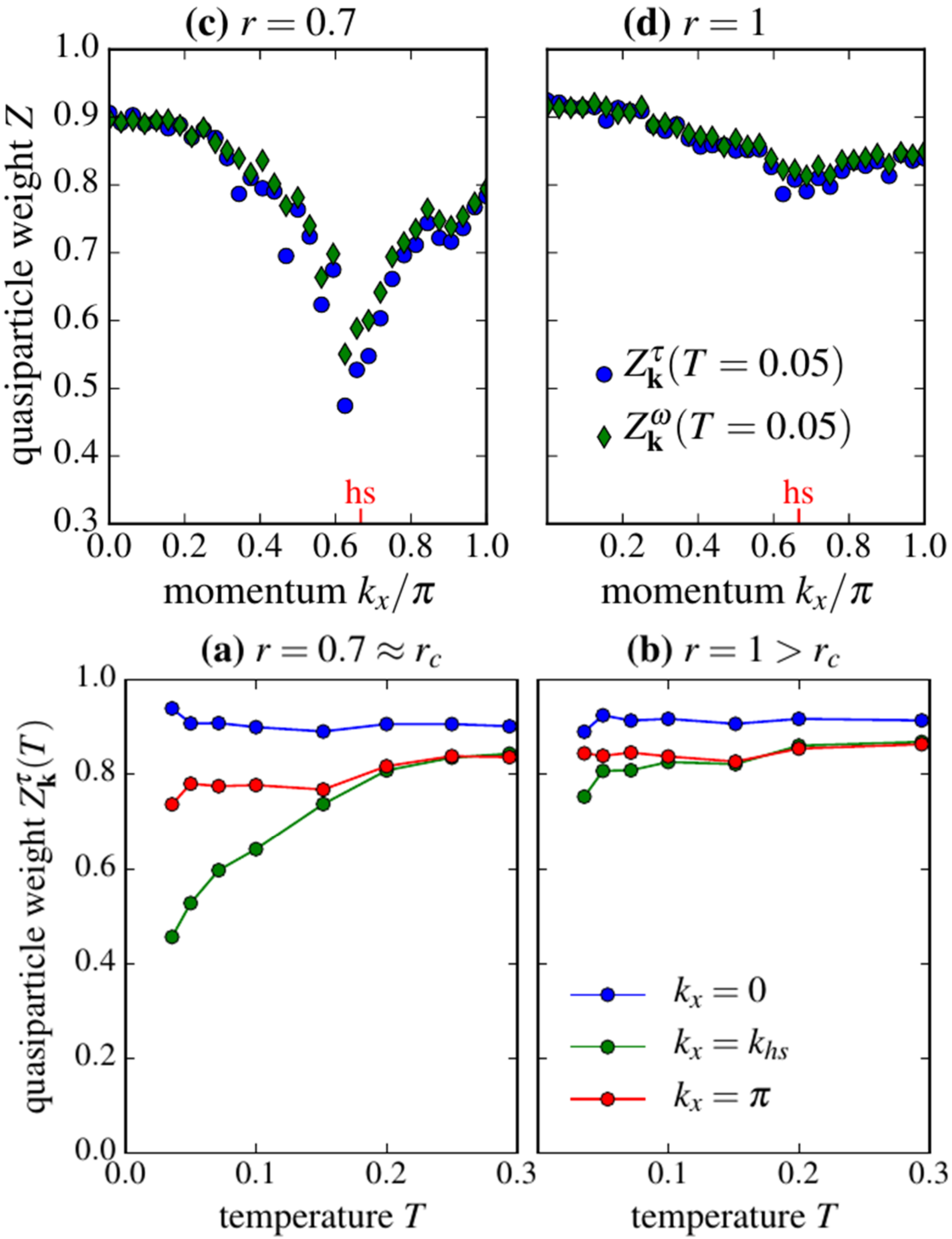
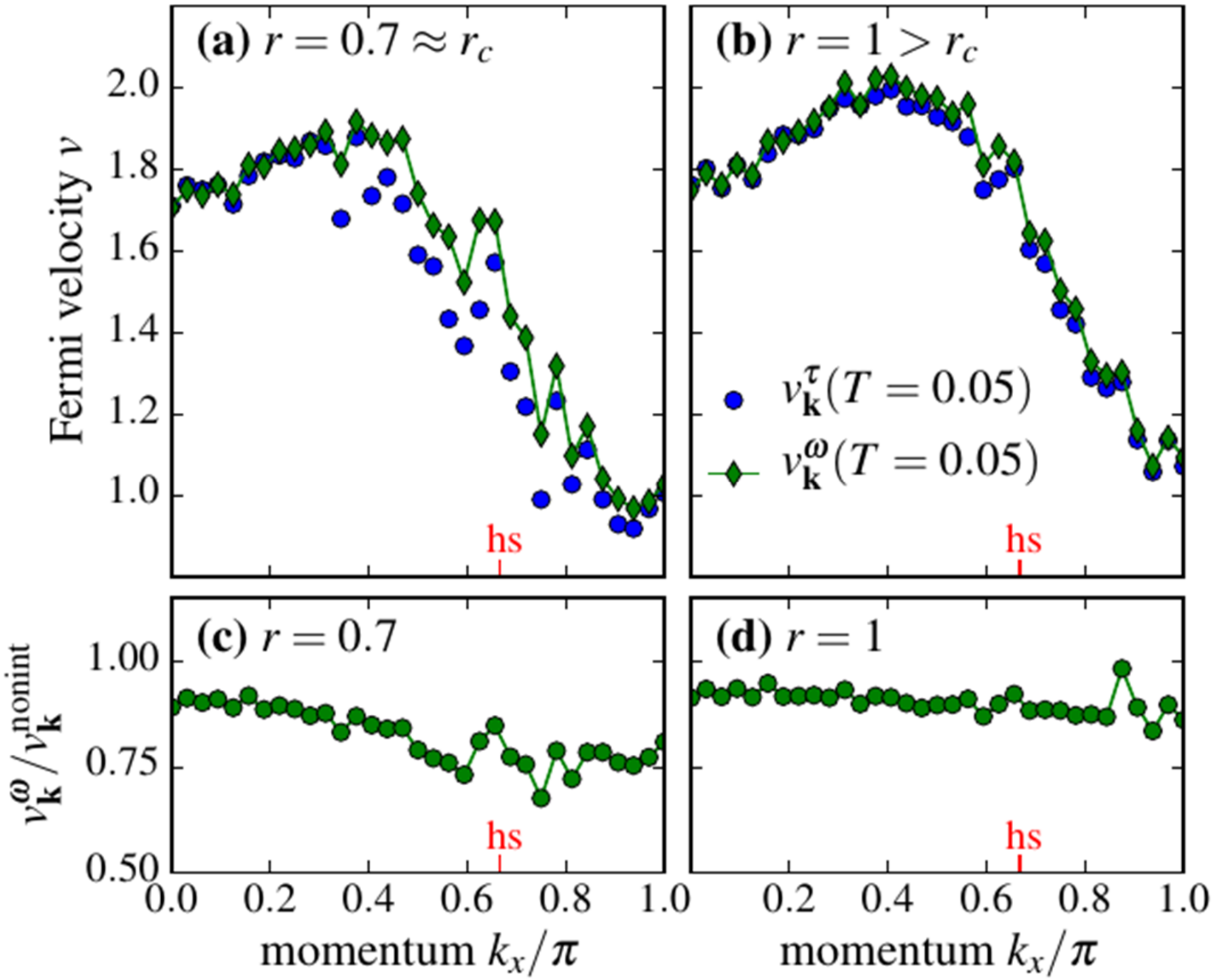
$$G_{\boldsymbol{k}}\left(\tau\sim\frac{\beta}{2}\right)=Z_{\boldsymbol{k}}(T)\frac{e^{-\epsilon_{\boldsymbol{k}}(\tau-\frac{\beta}{2})}}{2\cosh\left(\frac{\beta\epsilon_{\boldsymbol{k}}}{2}\right)}$$

$$Z_{\boldsymbol{k}}(T\rightarrow 0)=Z_{\boldsymbol{k}}$$



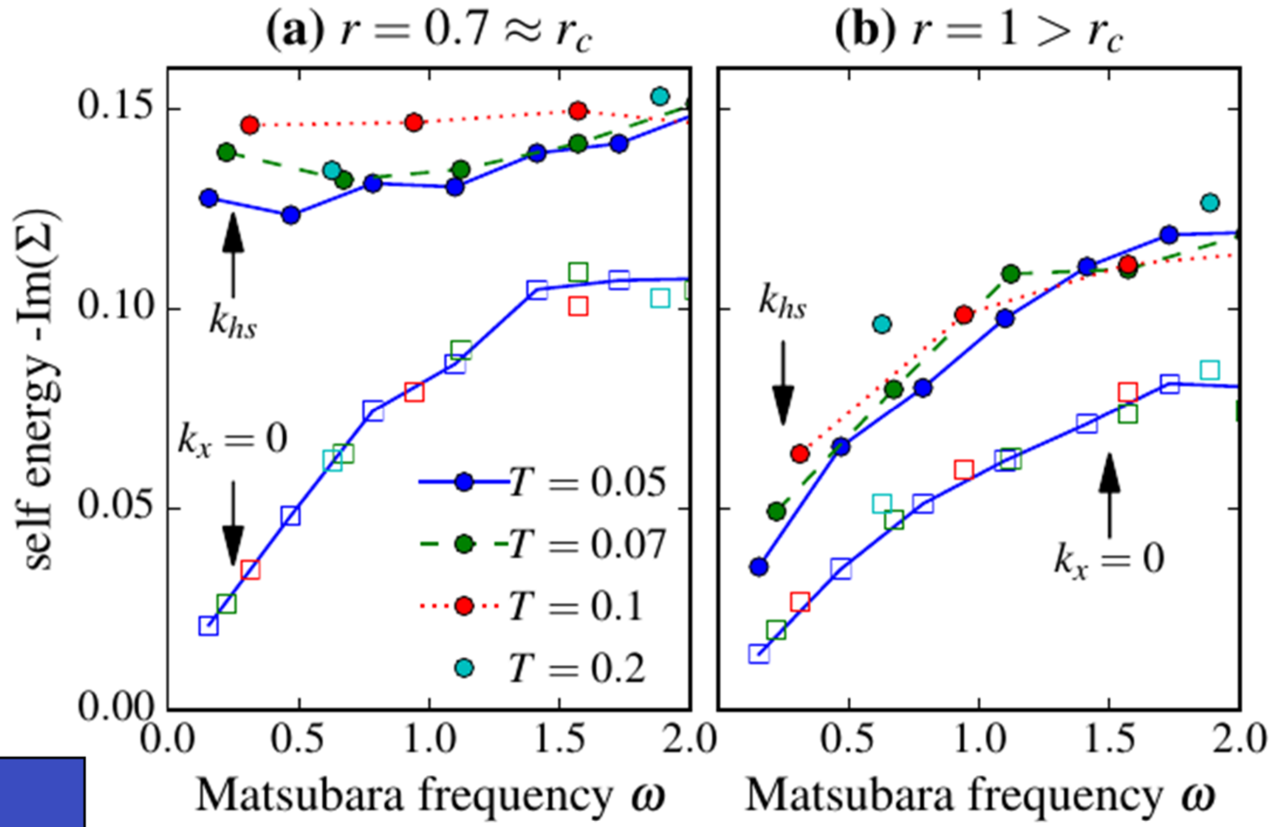


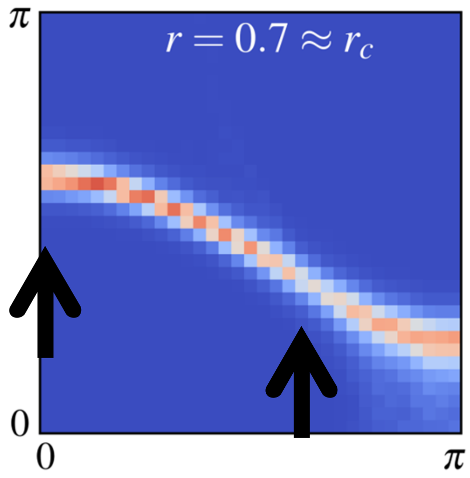
Velocity renormalization



v_f is renormalized, minor feature at hotspots.

Self energy

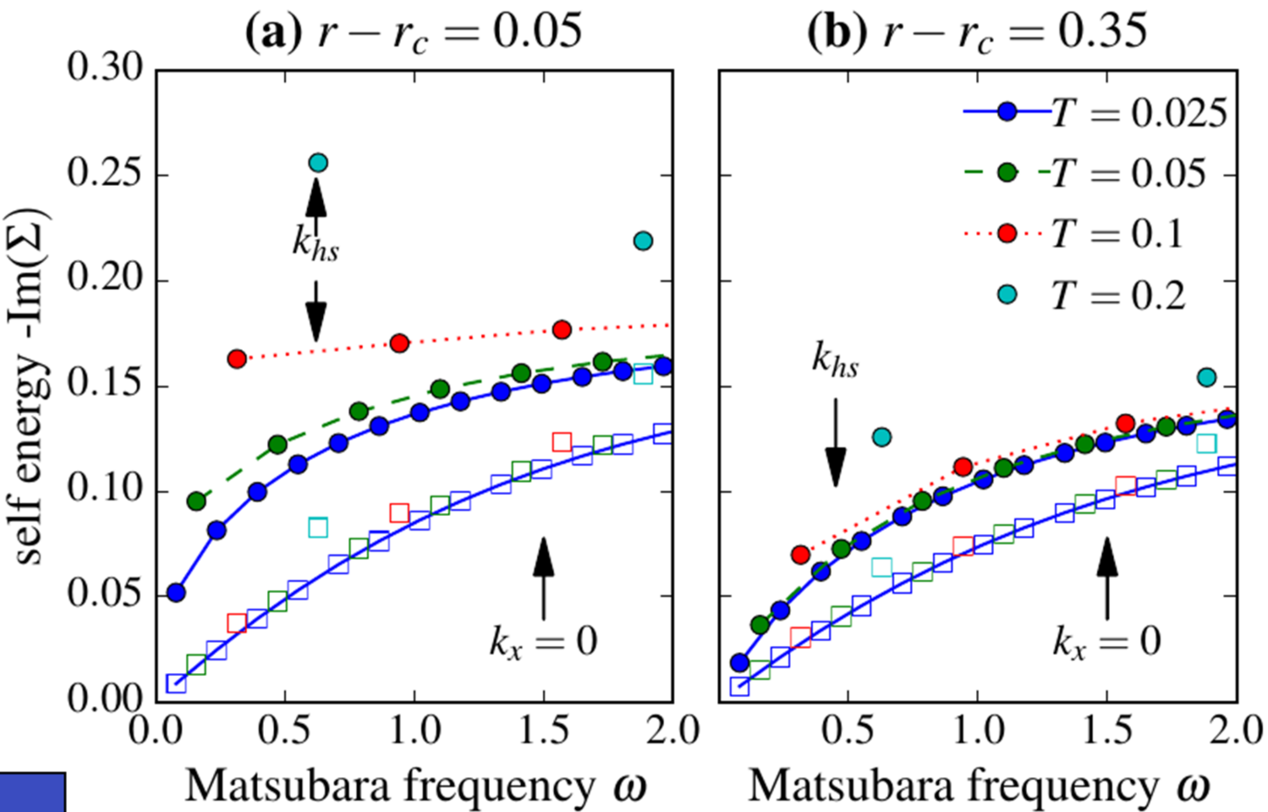


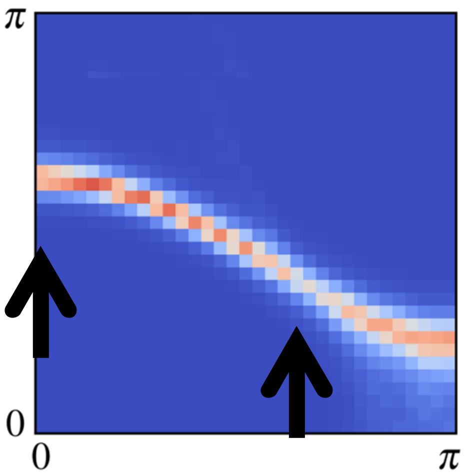


$\mathrm{Im}\Sigma_{\boldsymbol{k}_{hs}} \sim \mathrm{con}^{\mathrm{S}}$! (but small)

No singularity on FS ?!?

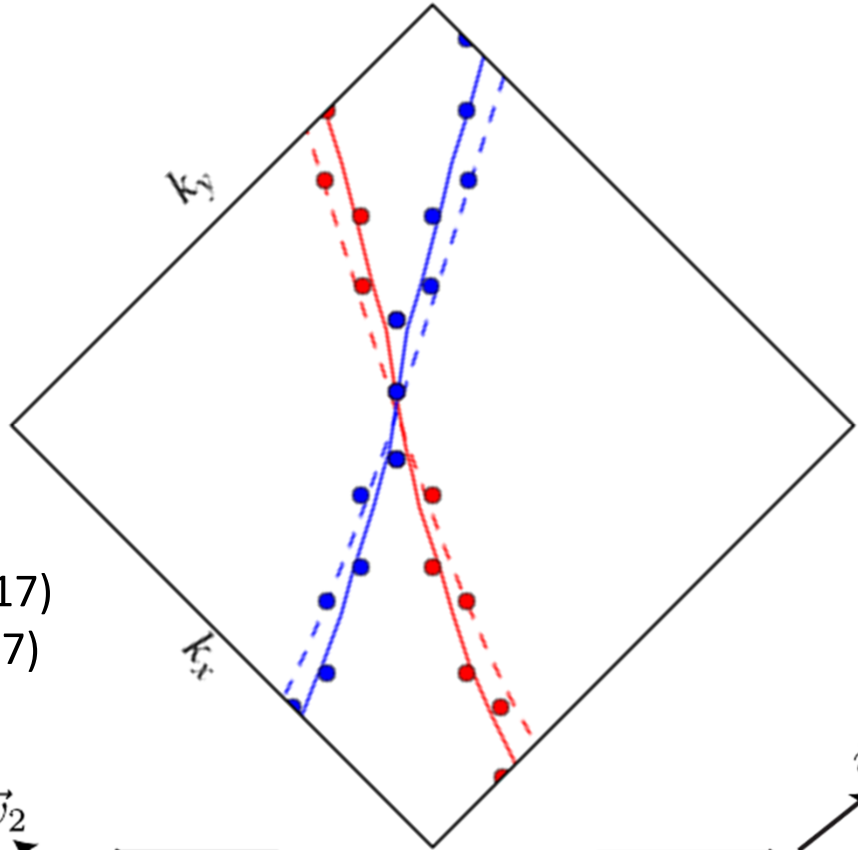
Perturbation theory



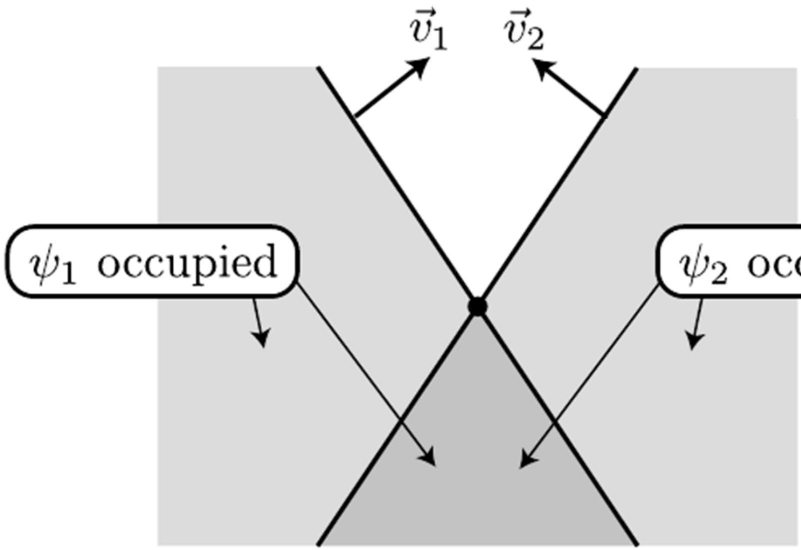


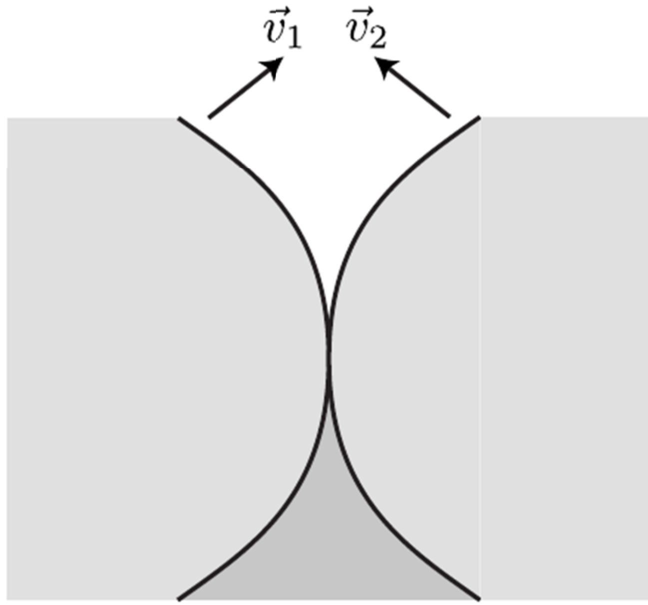
$$\Sigma_{1k}(\omega_n) = \frac{\lambda^2}{\beta L^2} \sum_{q,m} \chi_q(\Omega_m) G^0_{2,k+q}(\omega_n + \Omega_m)$$

Fermi surface



Abanov, Chubukov, PRL (2000)
Metlitski, Sachdev, PRB (2010)
Schlief , Lunz, S.S Lee, PRX (2017)
Lunz, Schlief, S.S Lee, PRB (2017)





Summary of part II

- Above Tc, the magnetic fluctuations mostly agree with Hertz-Millis theory:

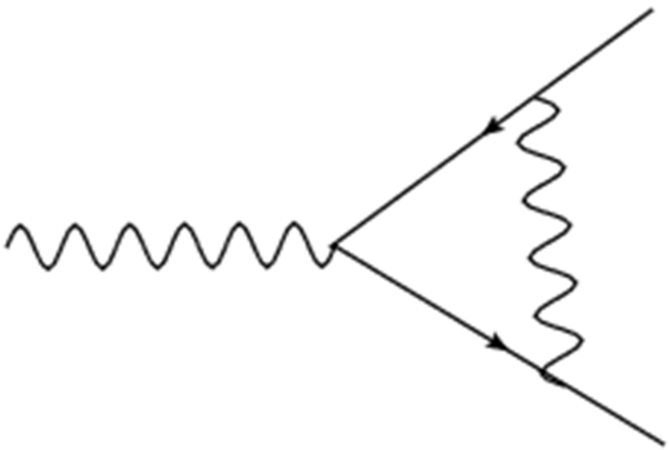
$$\chi^{-1} = A(r - r_{c0}) + Bq^2 + C|\omega_n| + f(r,T).$$

- The temperature dependence is less clear, $\chi^{-1} \sim T^2$.

- Loss of single-fermion spectral weight at the hotspots.
- Non Fermi liquid behavior: finite quasiparticle lifetime, nearly independent of T, ω.

The number of spin components

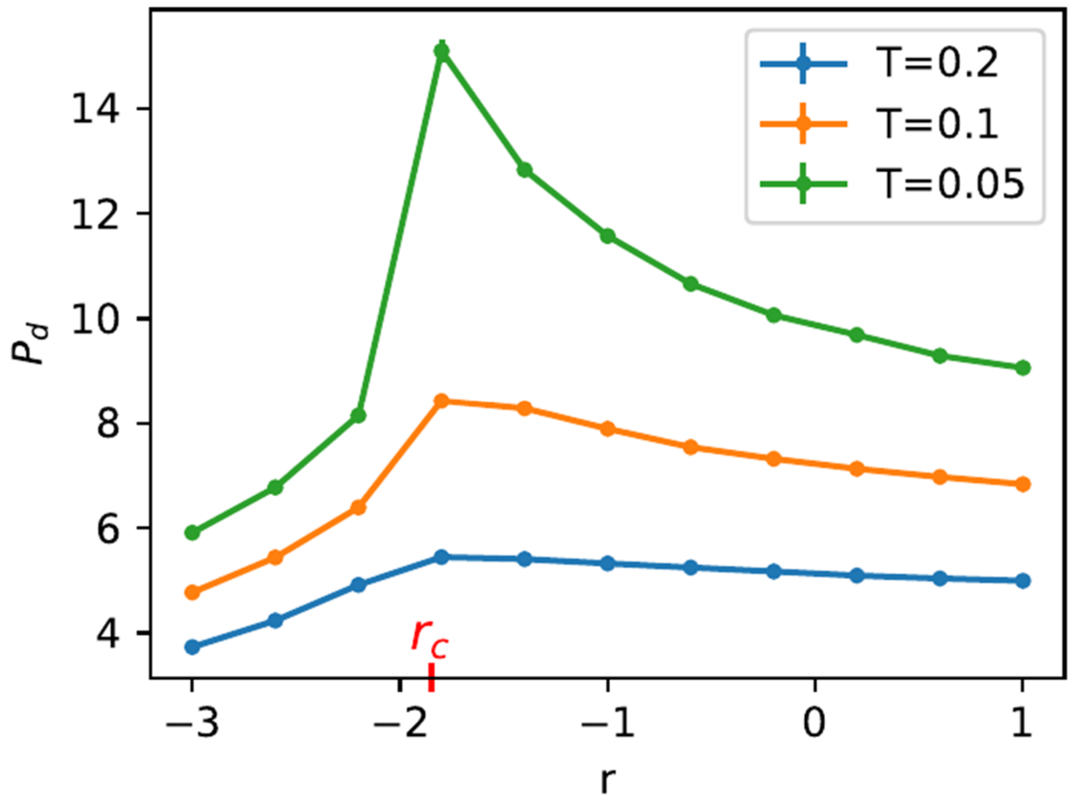
- So far we considered easy-plane magnetism, $N_B = 2$.
- In Eliashberg theory, the number of spin components doesn't matter.
- But vertex corrections are very different:



$$\propto (2 - N_B)$$

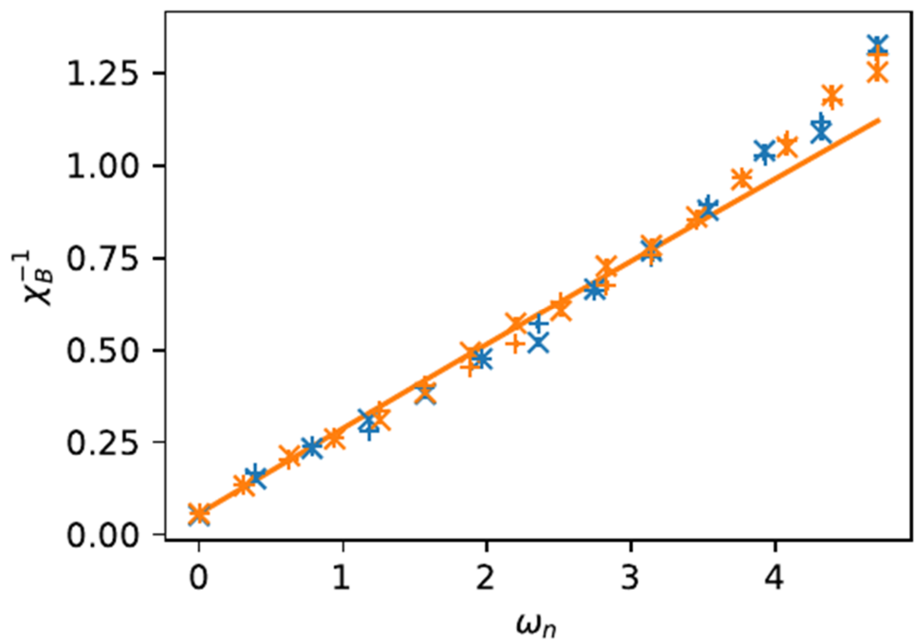
Heisenberg spins

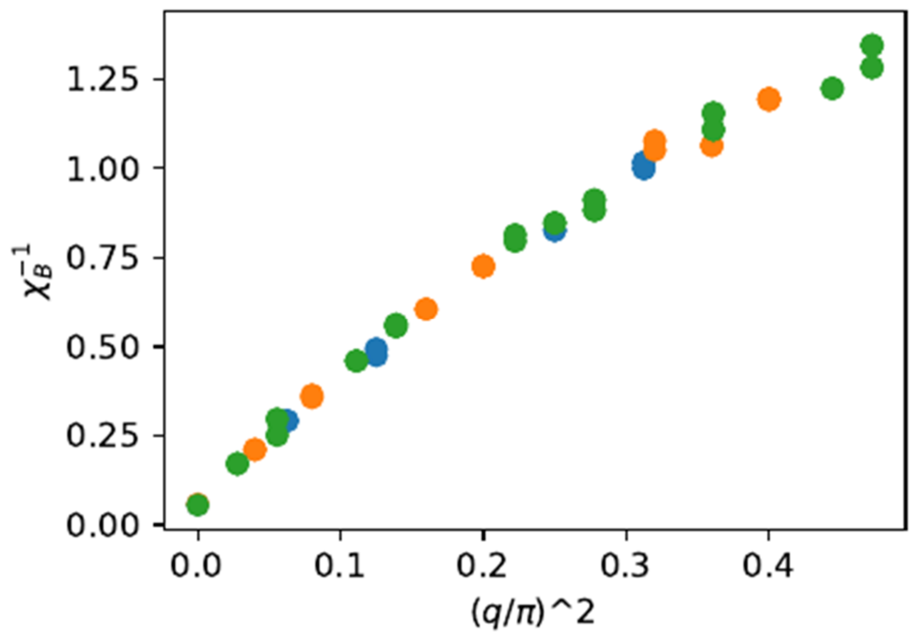
- We find very similar results. High T_c, peaked close to the AFM QCP.
- We now focus on a moderate value $\lambda = 1$ so that T_c is low.



Heisenberg spins

$\lambda = 1, T_c < 0.05 \quad r = -1.6 \approx r_c$





$$\chi^{-1} = a_r(r - r_{c0}) + a_\omega|\omega_n| + a_q(\boldsymbol{q} - \boldsymbol{Q})^2 + f(r, T)$$

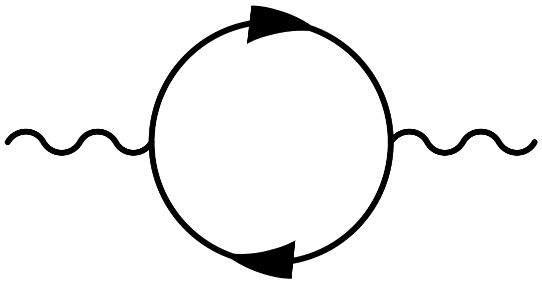
Part III

Comparison with Eliashberg theory

Wang, Schattner, Berg, and Fernandes, arXiv (2016)

Hot-spots Eliashberg approximation

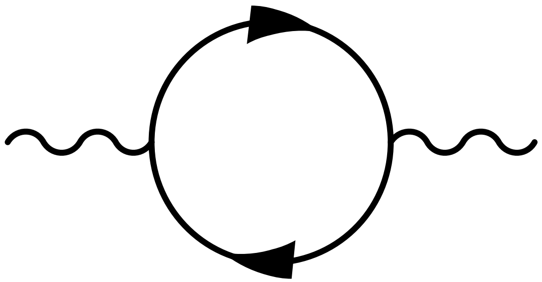
- Bosonic propagator is computed within one-loop using the bare Green's functions (no self-consistency).



$$\chi^{-1} = (r' + (\boldsymbol{q} - \boldsymbol{Q})^2 + |\omega_n|)$$

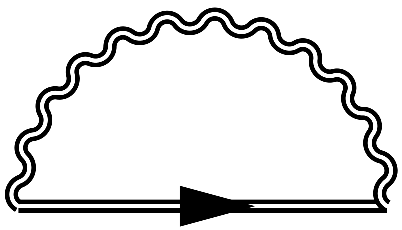
Hot-spots Eliashberg approximation

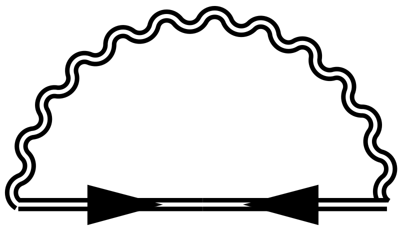
- Bosonic propagator is computed within one-loop using the bare Green's functions (no self-consistency).



$$\chi^{-1} = (r' + (\boldsymbol{q} - \boldsymbol{Q})^2 + |\omega_n|)$$

- Fermionic self-energies (normal and anomalous) are then computed self-consistently. No vertex corrections.





Hot-spots Eliashberg approximation

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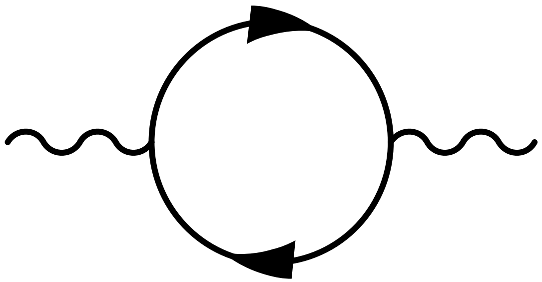

$$\chi^{-1} = (r' + (\boldsymbol{q} - \boldsymbol{Q})^2 + |\omega_n|)$$

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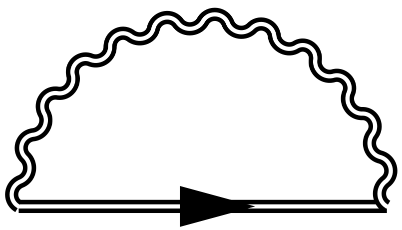
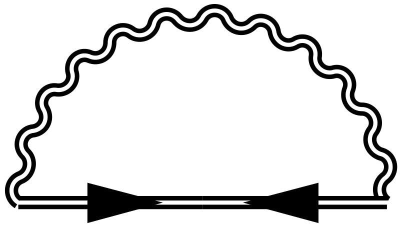
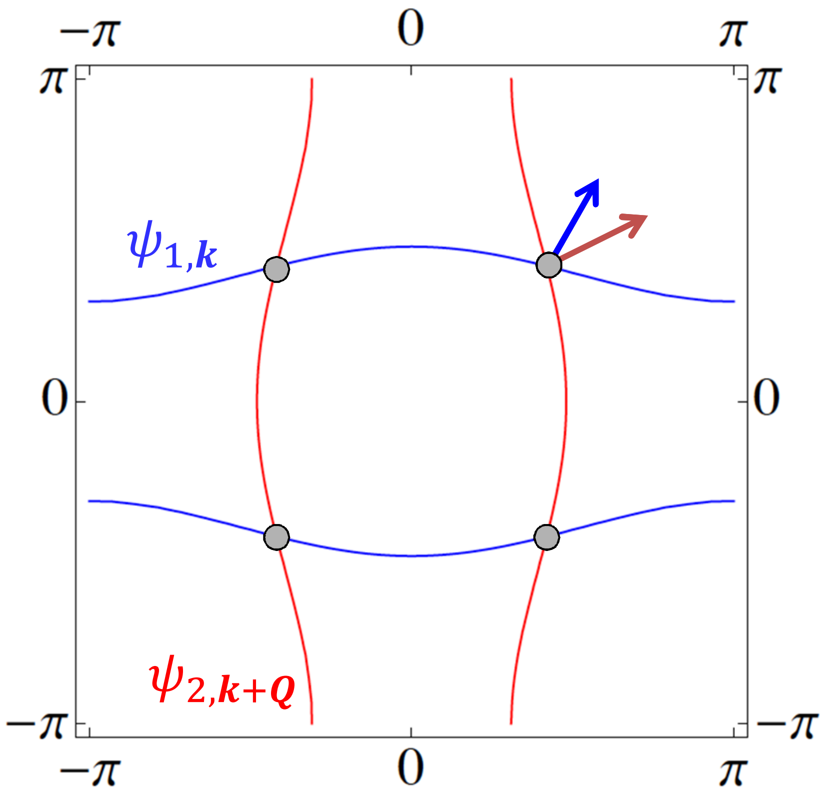
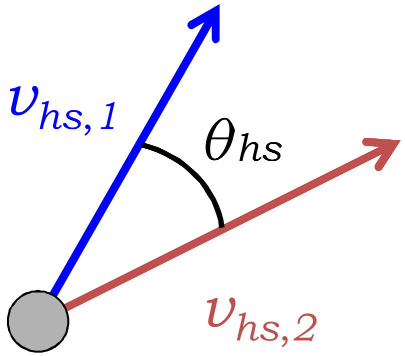




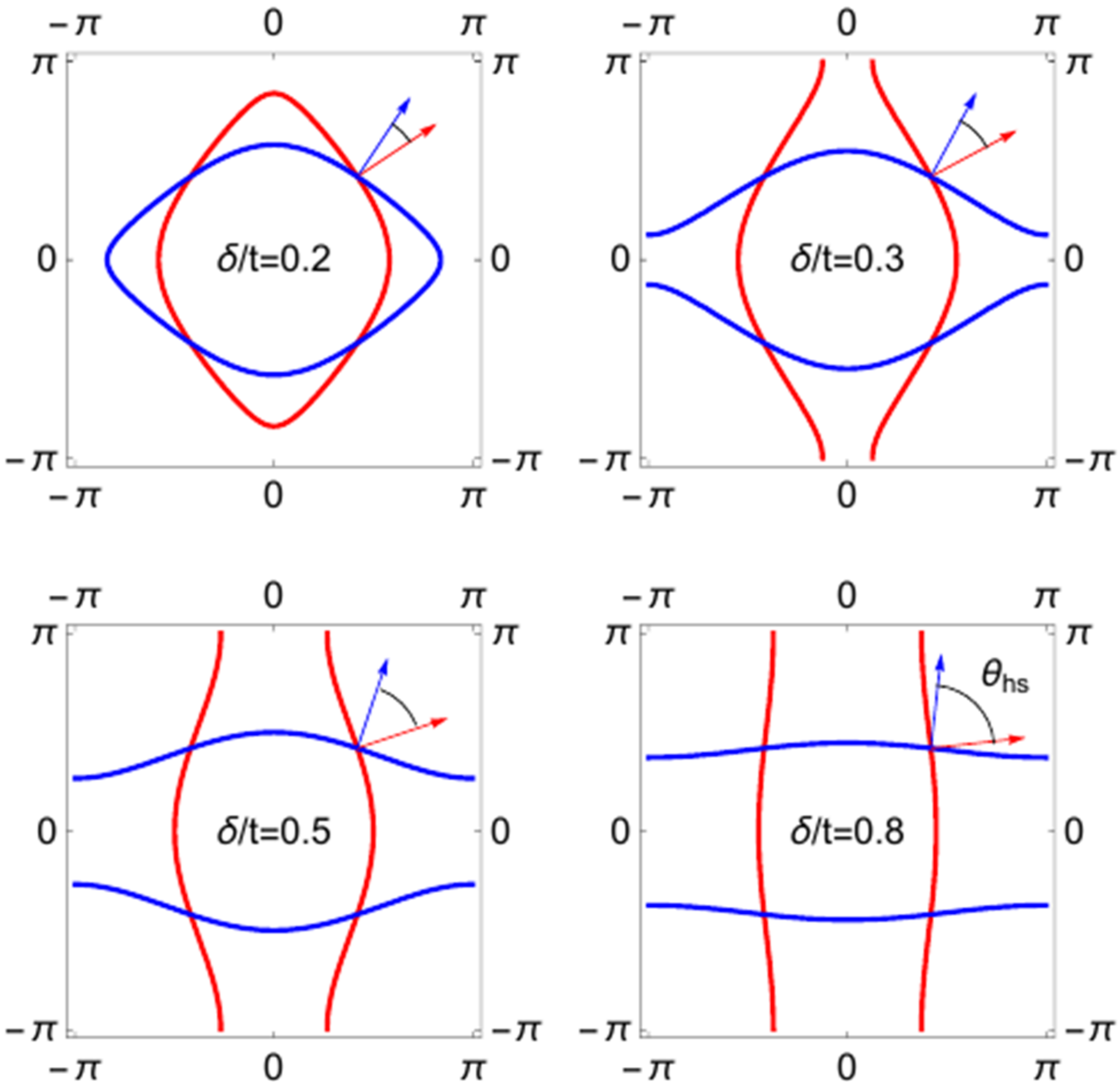
- Linearized dispersion. Self energy evaluated at the hotspots only.

Hot-spots Eliashberg approximation

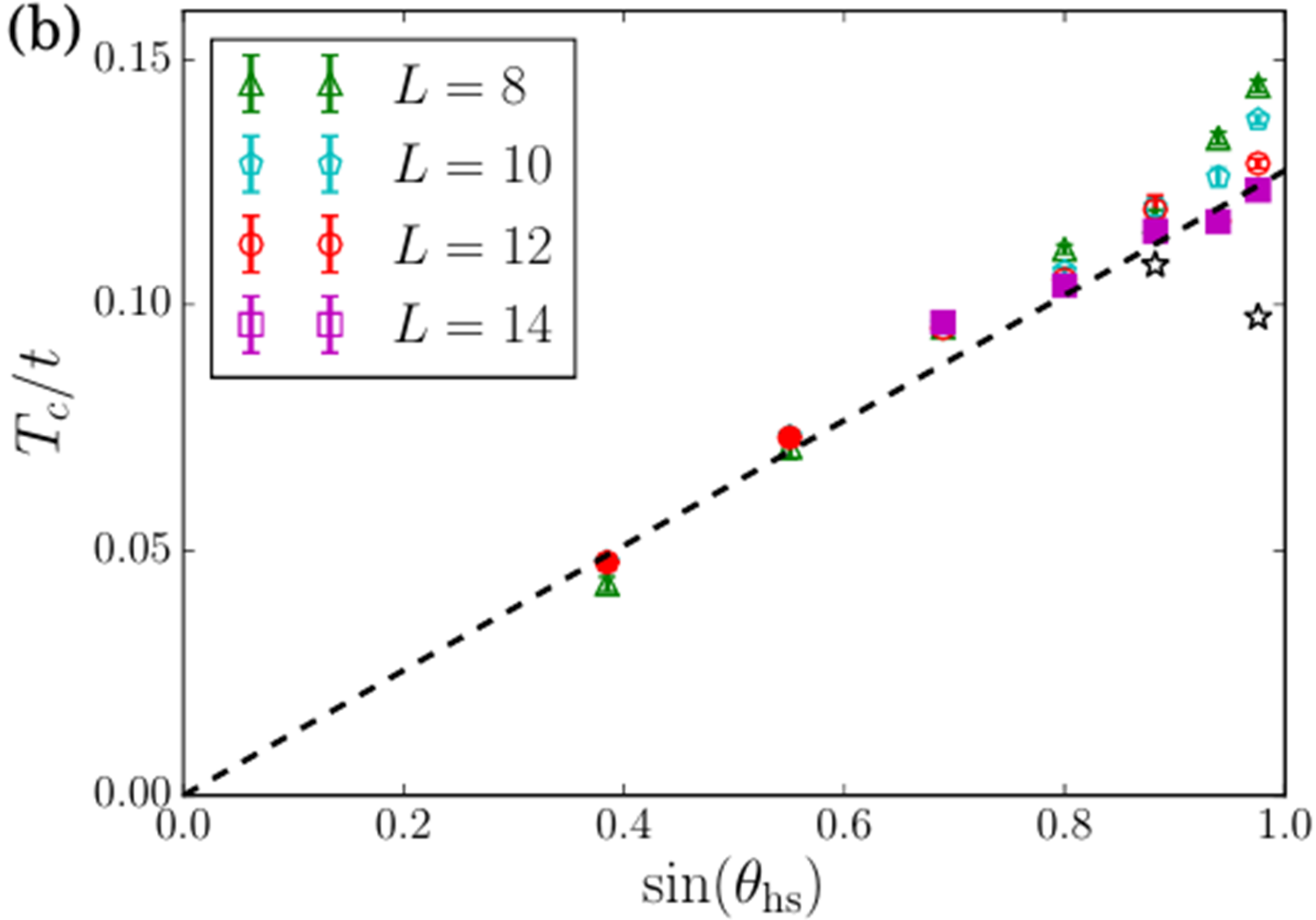




$$T_c \propto \lambda^2 \sin(\theta_{hs})$$



δ/t=0.2
δ/t=0.3
δ/t=0.5
δ/t=0.8
θhs
−π
0
π



(b)
$L = 8$
$L = 10$
$L = 12$
$L = 14$
0.15
0.10
0.05
0.00
T_c/t
0.0
0.2
0.4
0.6
0.8
1.0
$\sin(\theta_{\rm hs})$

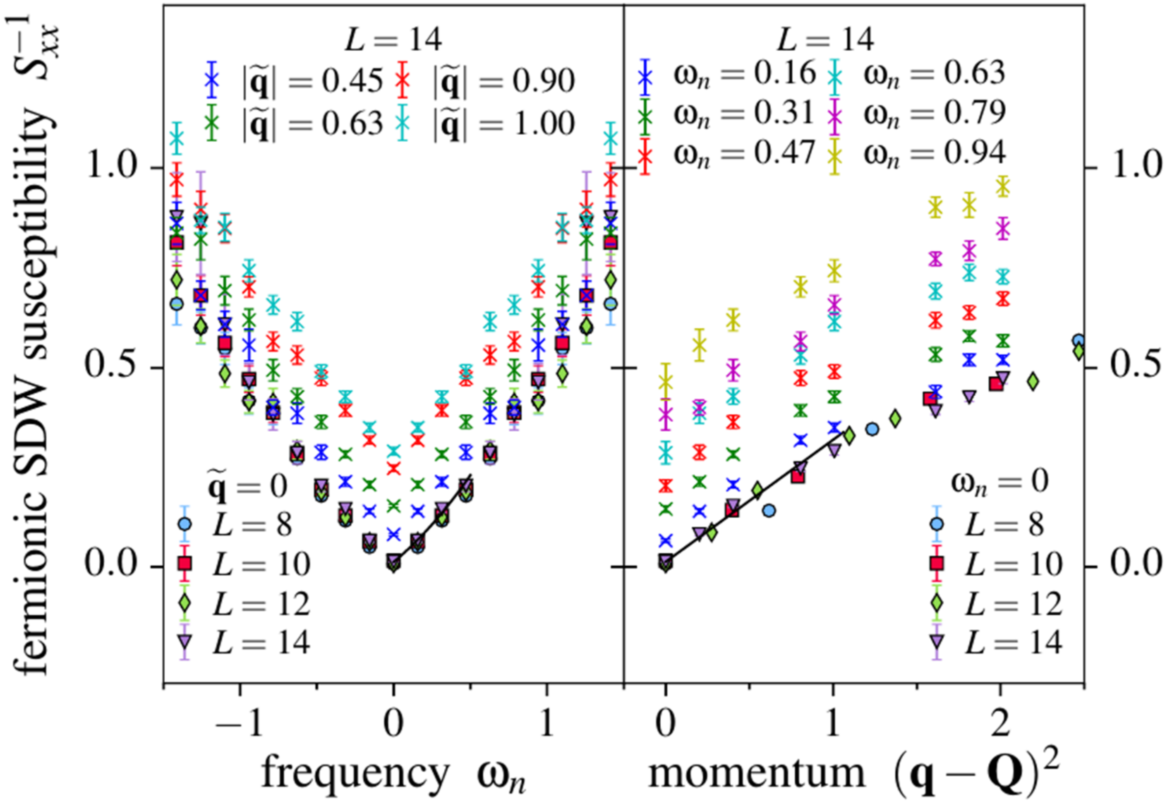
Conclusions

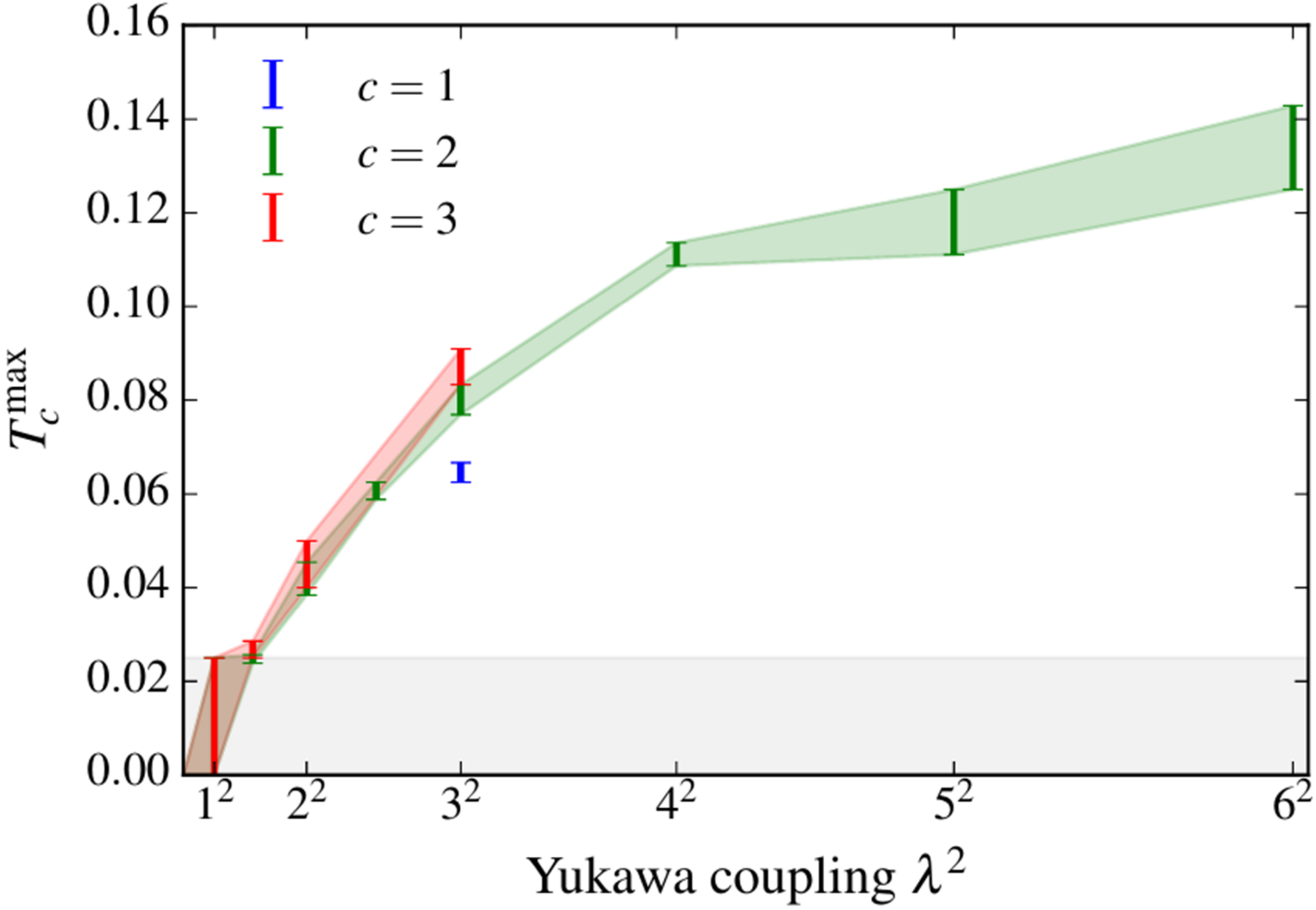
- DQMC can be used to study this type of problems!
- The phase diagram is a lot like many high-Tc superconductors.
- Unlike hole-doped cuprates
  - No pseudogap
  - No charge order
- Non-Fermi liquid above Tc
  - constant lifetime at the hotspots. Not a power law.
- Unjustified 1-loop works for most things

Magnetic fluctuations

Consistency check

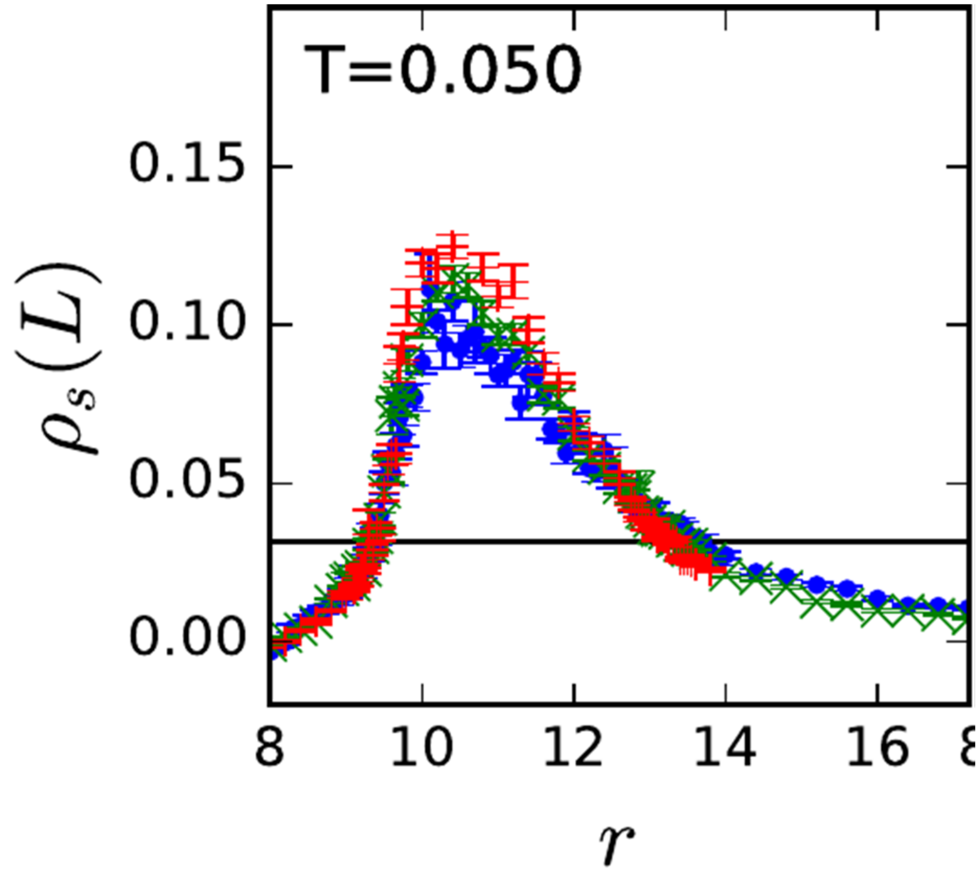
compare with a susceptibility of fermion bilinear of the same symmetry, $S_x = \psi_1^{+}\sigma_x\psi_2 + H.c.$

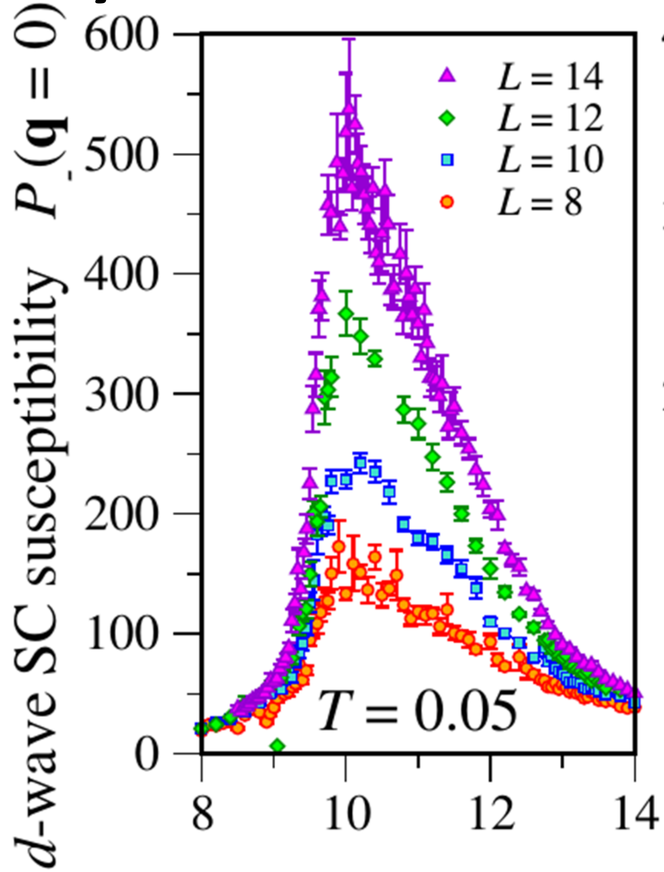




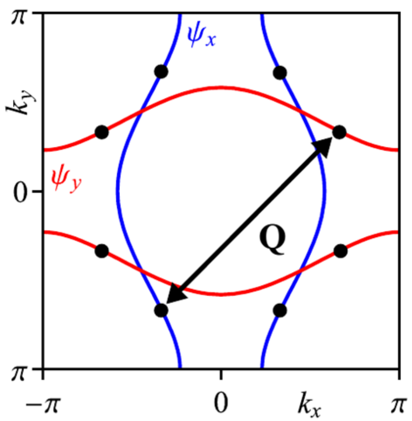
0.16
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
$c = 1$
$c = 2$
$c = 3$
$T_c^{\max}$
1^2
2^2
3^2
4^2
5^2
6^2
Yukawa coupling λ^2

Superconductivity



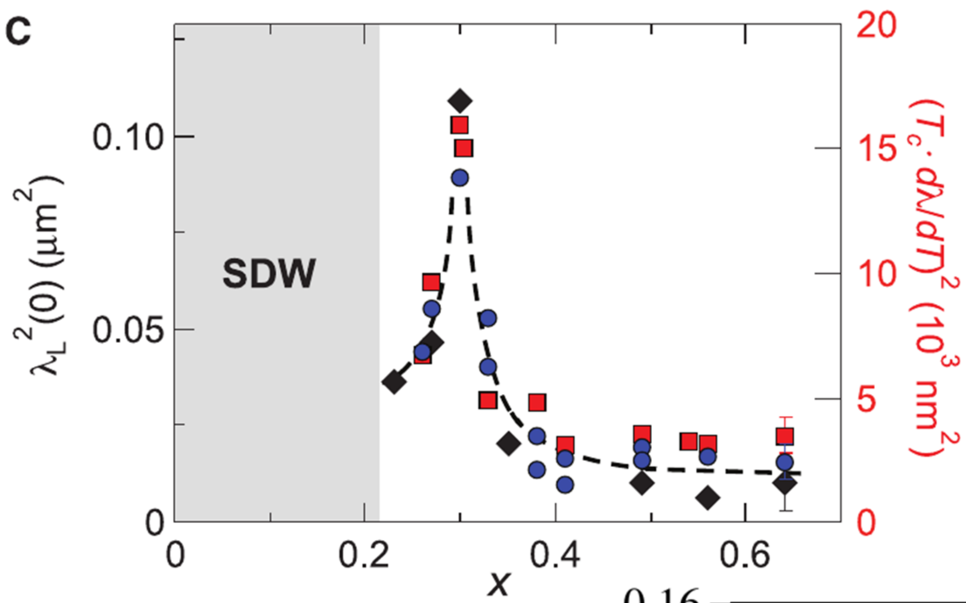


$$\rho_s(T_c) = \frac{2}{\pi} T_c$$

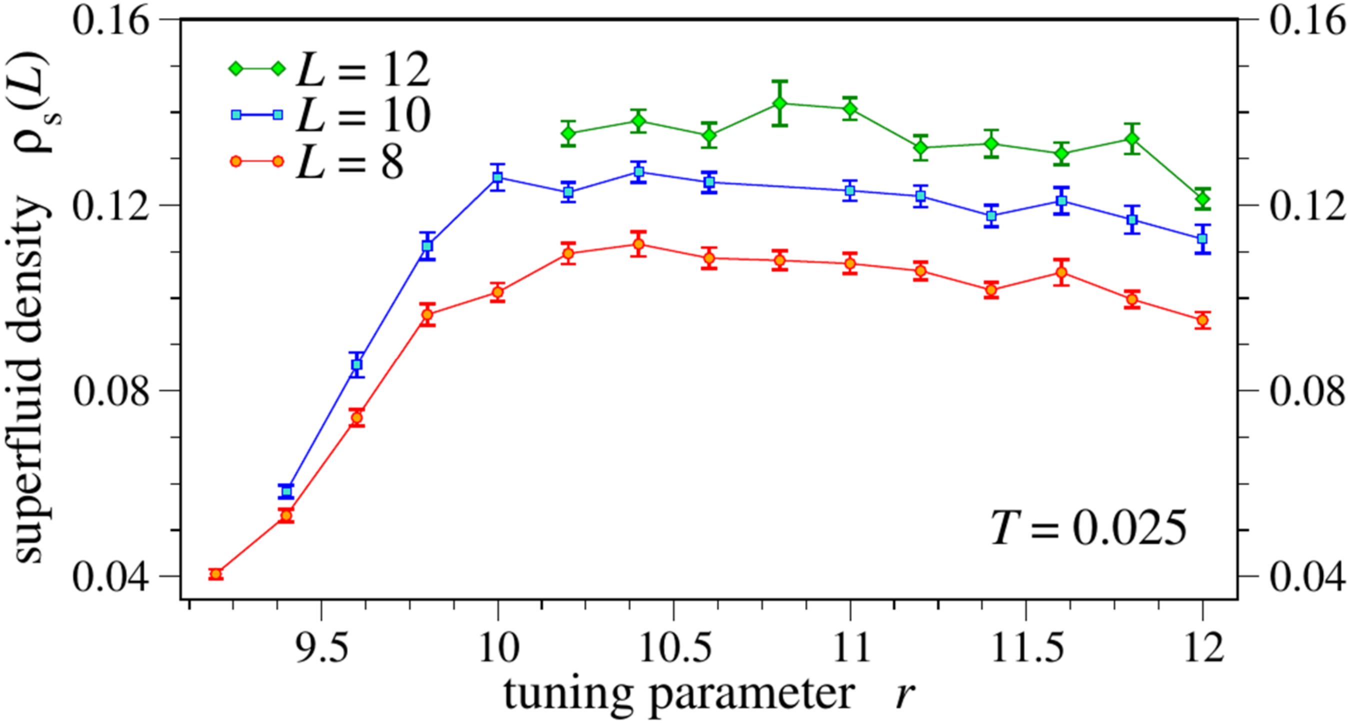


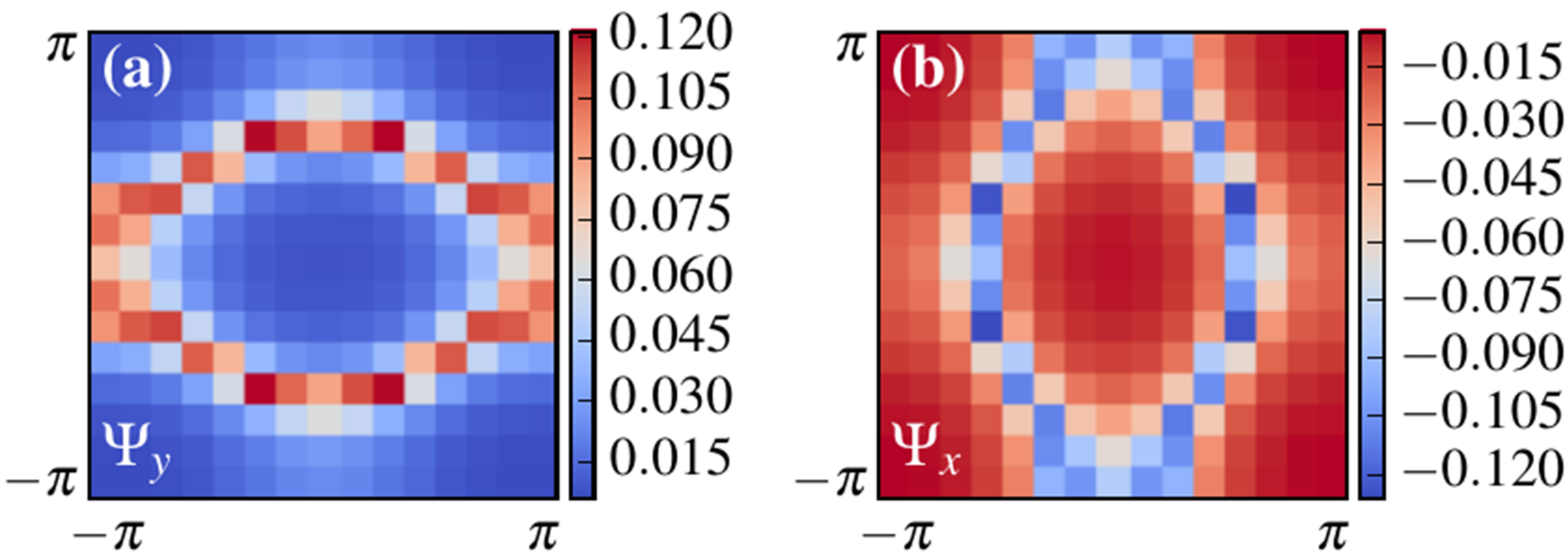
$$\Delta_- = c^\dagger_{x\uparrow} c^\dagger_{x\downarrow} - c^\dagger_{y\uparrow} c^\dagger_{y\downarrow}$$

Superfluid density



Hashimoto et al.,
Science (2012)

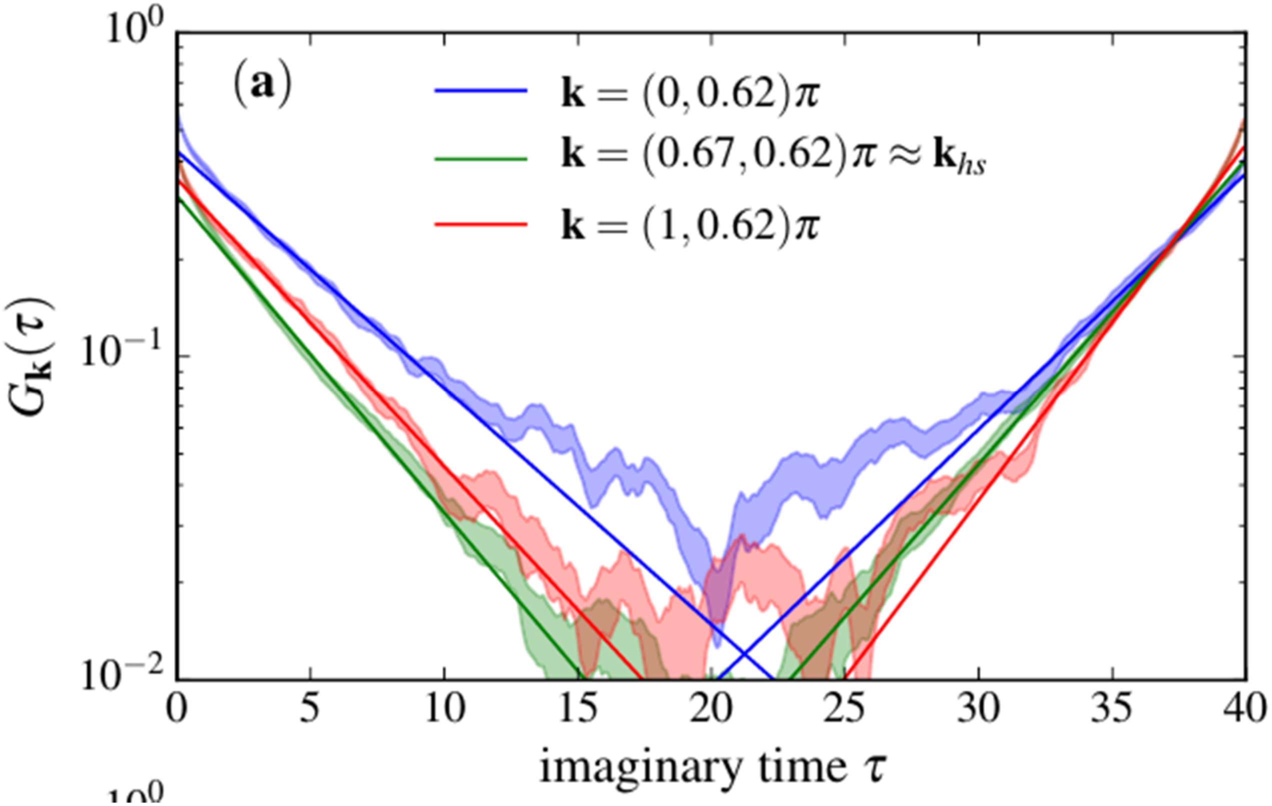




Momentum resolved pairing susceptibility close to T_c

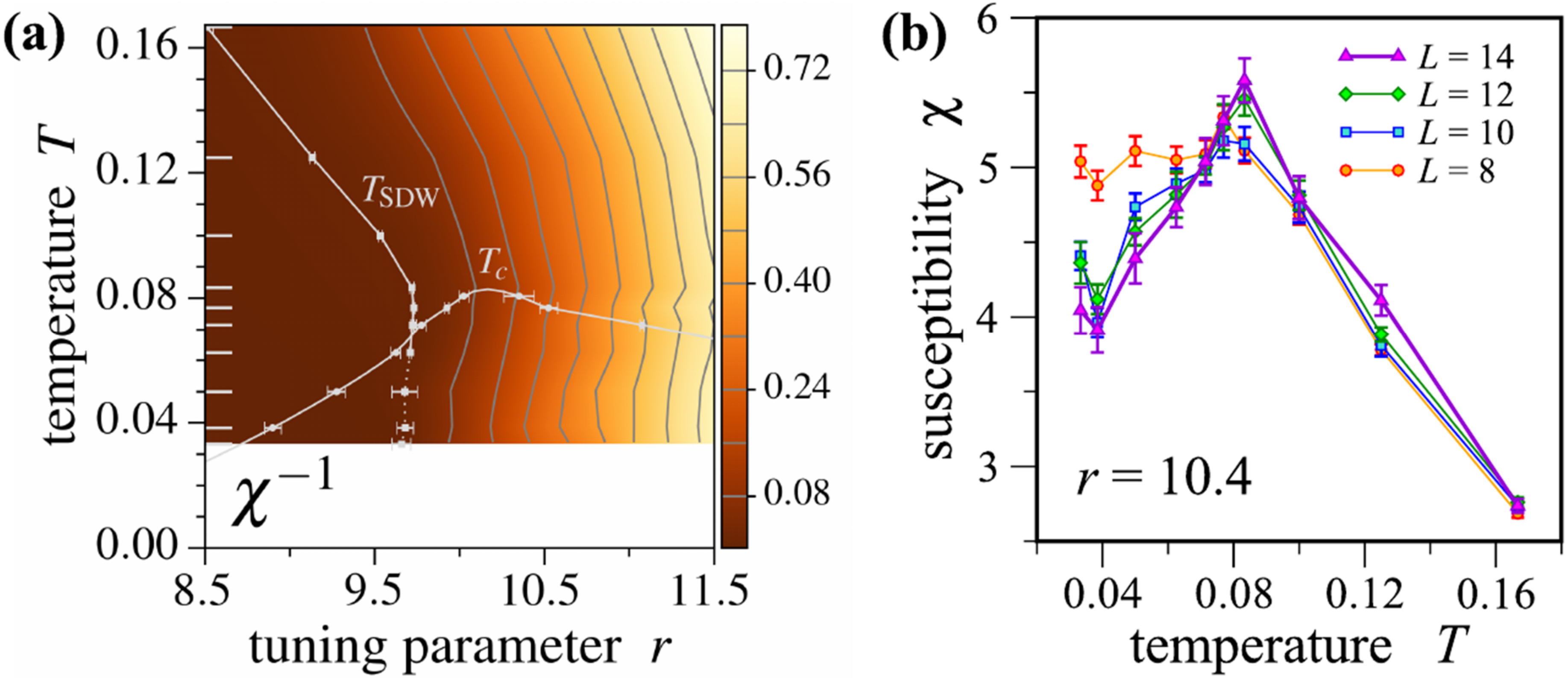
$$P_{k\alpha;k'\alpha'} = \int d\tau \langle \Psi_{k\alpha}(\tau)\, \Psi^{+}_{k'\alpha'}(0) \rangle$$

$\Psi^{opt}_{k\alpha}$ the optimal wavefunction.



$$G_{\mathbf{k}}(\tau) = \frac{1}{1 + e^{-\beta E_{\mathbf{k}}}} \left(u_{\mathbf{k}}^2 e^{-E_{\mathbf{k}}\tau} + v_{\mathbf{k}}^2 e^{-E_{\mathbf{k}}(\beta - \tau)} \right)$$

Competition of magnetism and superconductivity



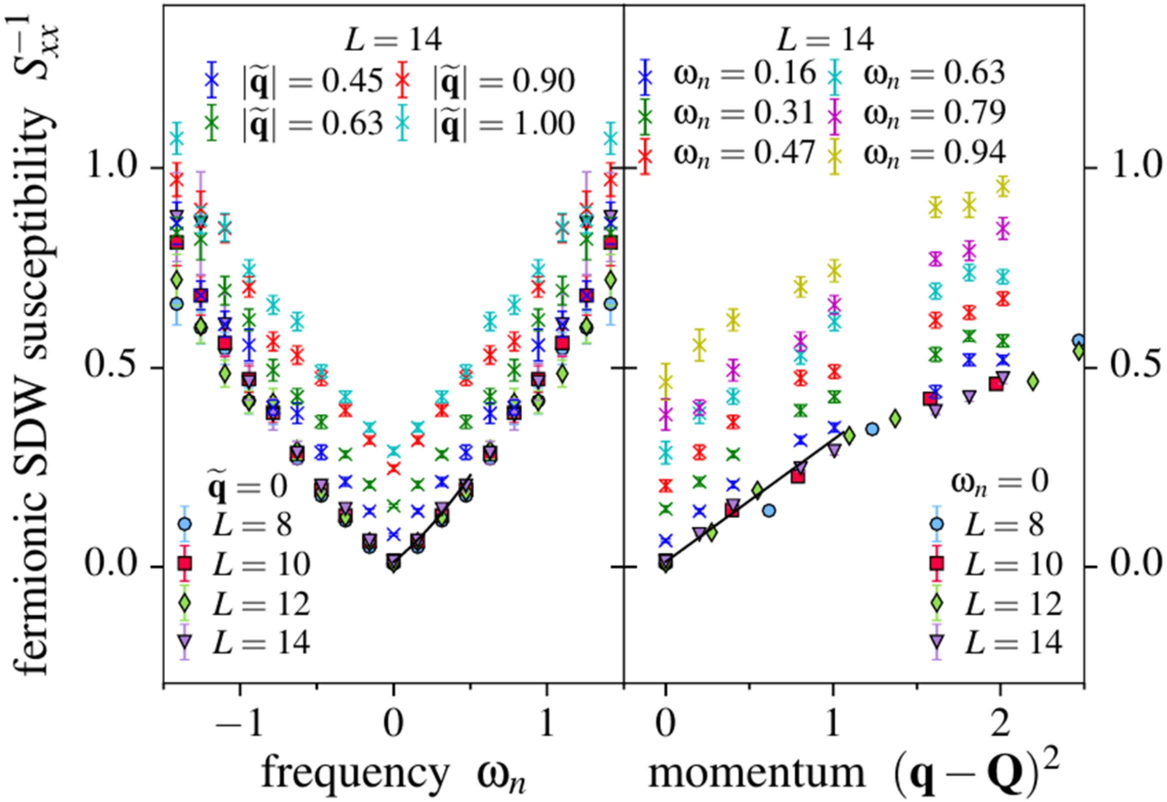
Bending of the magnetic phase boundary

Peak in susceptibility at $T \sim T_c$

Magnetic fluctuations

Consistency check

compare with a susceptibility of fermion bilinear of the same symmetry, $S_x = \psi_1^{+}\sigma_x\psi_2 + H.c.$

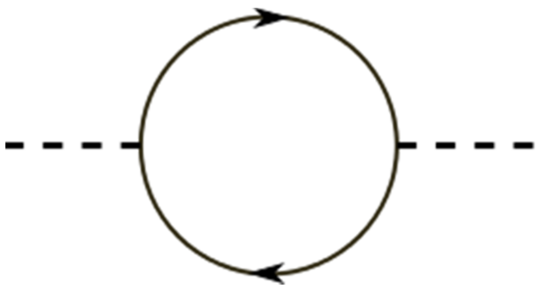


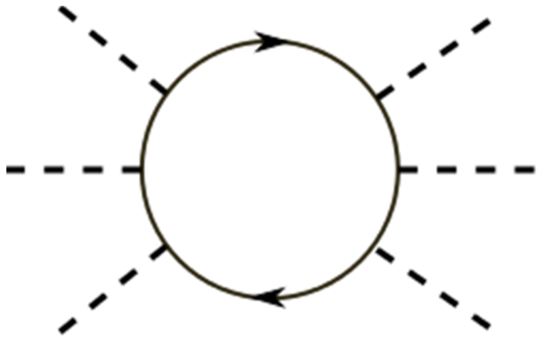
Hertz theory

$$S \sim |\vec{\varphi}_q|^2 (r' + (\boldsymbol{q} - \boldsymbol{Q})^2 + |\omega_n|) + u_4 \varphi^4 + u_6 \varphi^6 + \cdots .$$

φ^{2n} terms are non-local and marginal. Infinitely many marginal terms!

Abanov and Chubukov, PRL (2004)



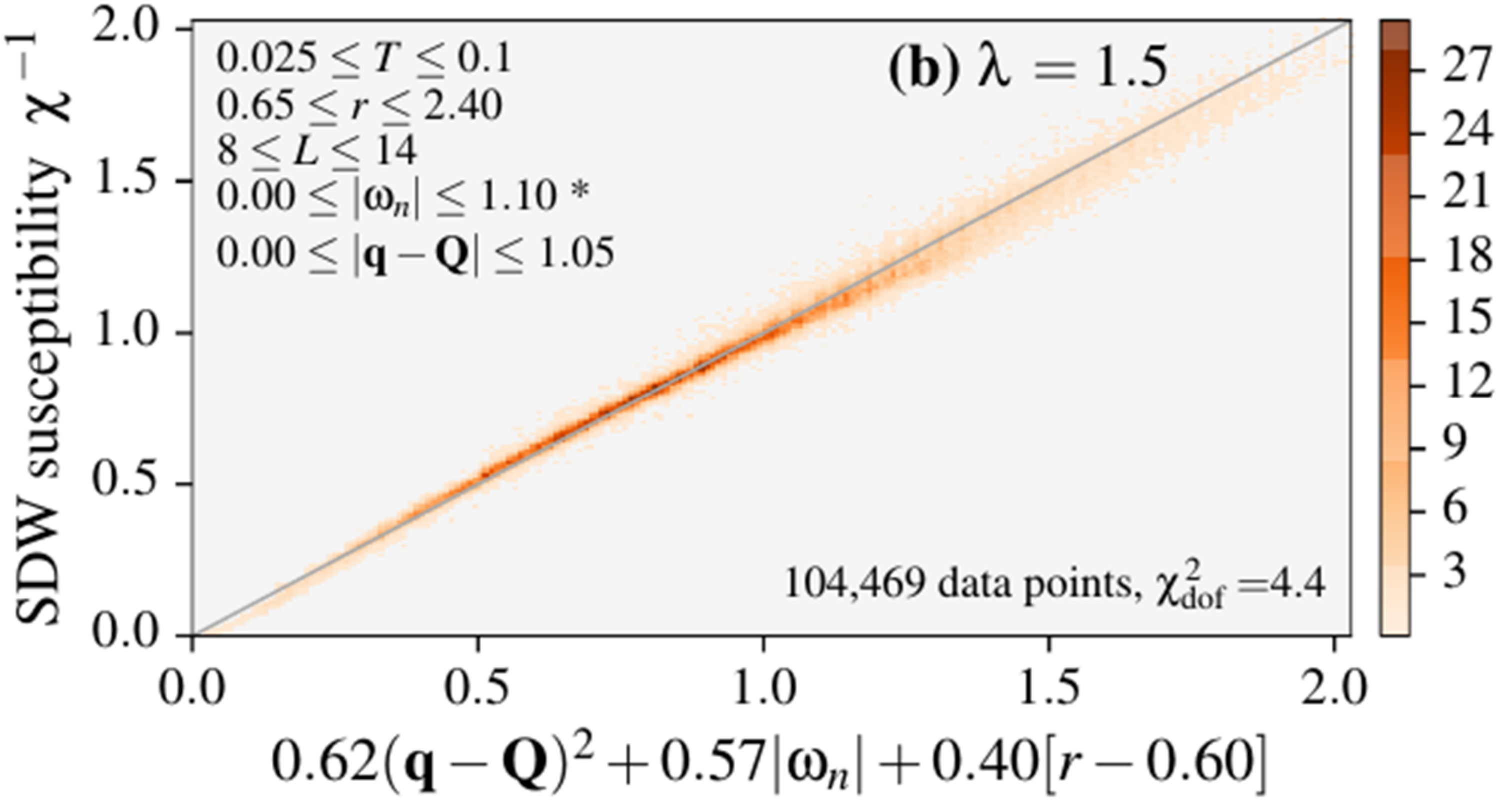


Large N (fermion flavors)?

Naïve counting in 1/N doesn't work

S.S Lee, PRB (2009)
Metlitski and Sachdev, PRB (2010)

Magnetic fluctuations



$$\chi^{-1} = a_r(r - r_{c0}) + a_\omega|\omega_n| + a_q(\boldsymbol{q} - \boldsymbol{Q})^2 + f(r, T)$$