Pseudogap and Fermi surface topology in doped Mott insulators

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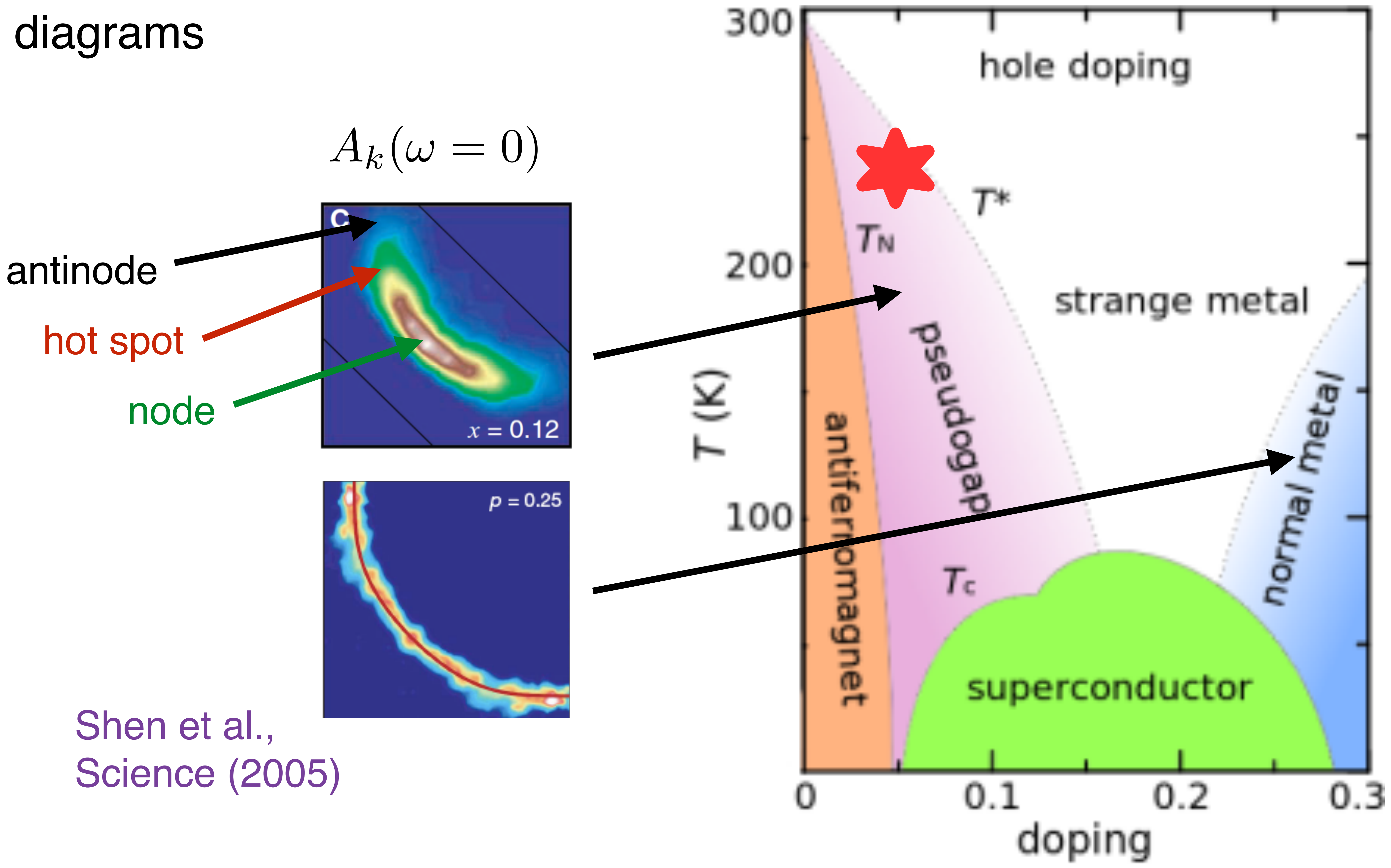
Aspen Center for Physics - March 9, 2020

Strongly-correlated materials and pseudogap physics

- Strongly-correlated systems have rich phase diagrams
- Example: cuprate superconductors
- The pseudogap region:
    - Nodal / antinodal differentiation
    - Loss of spectral weight at the antinode
- Open questions:
    - Mechanism of the pseudogap?
    - Role of Mott insulator?
    - How generic is the pseudogap?
    - Good or bad for superconductivity?
- Minimal model: 2D Hubbard model



Shen et al., Science (2005)

$$\mathcal{H} = \sum_{ij\sigma} t_{ij}\, c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

Collaborators

Ecole Polytechnique
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King's College

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Harvard University

Mathias Scheurer
Shubhayu Chatterjee
Subir Sachdev

Many discussions with

L. Taillefer,
N. Doiron-Leyraud,
O. Cyr-Choinière,
I. Paul, A. Sacuto, ...

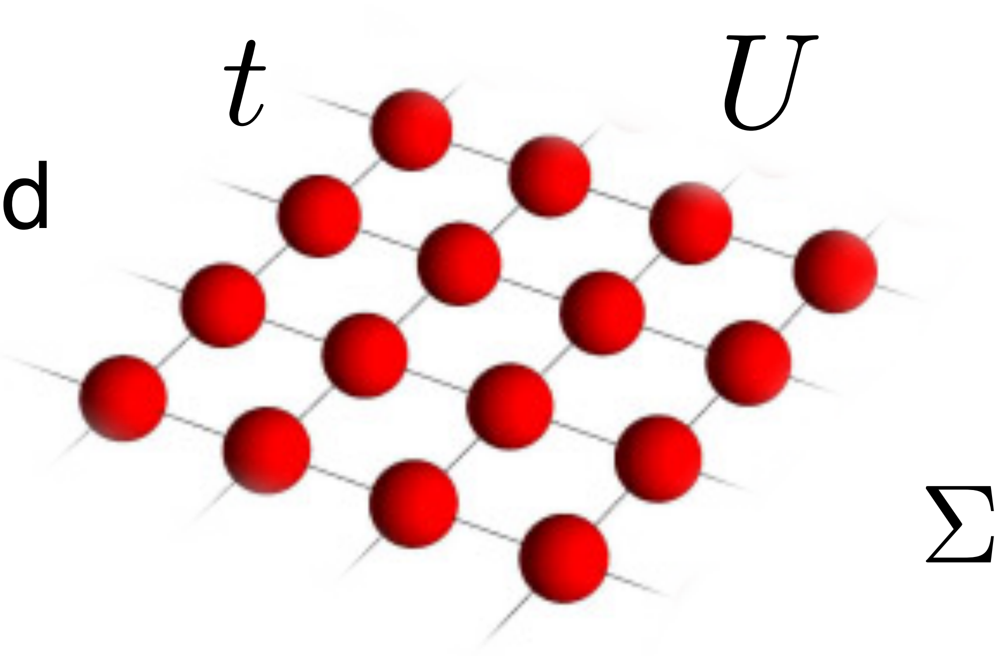
SIMONS FOUNDATION

Numerical investigation of Hubbard model:
Dynamical cluster approximation
Diagrammatic Monte Carlo

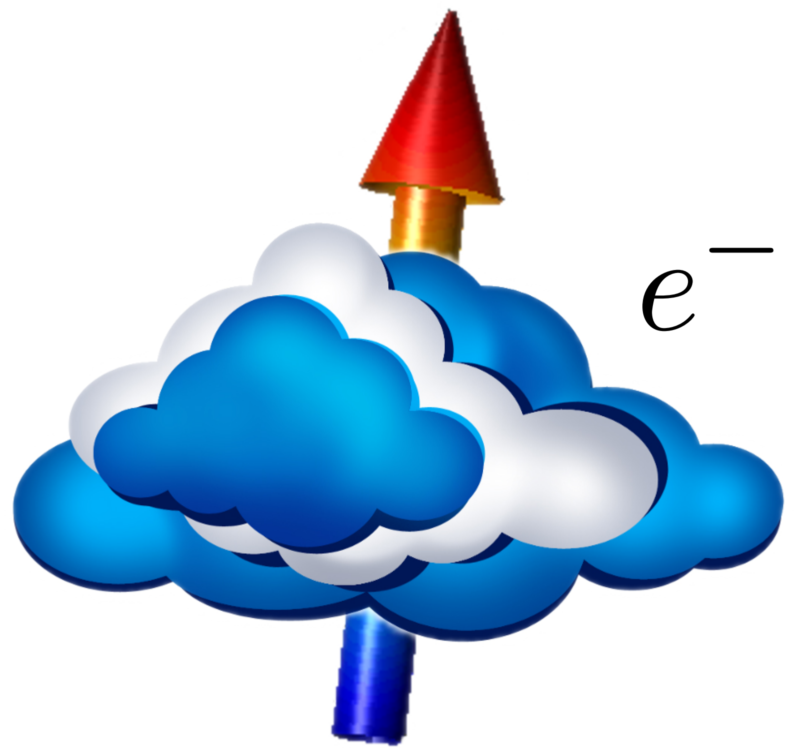
Dynamical cluster approximation

- Dynamical mean-field theory

Lattice Hubbard model

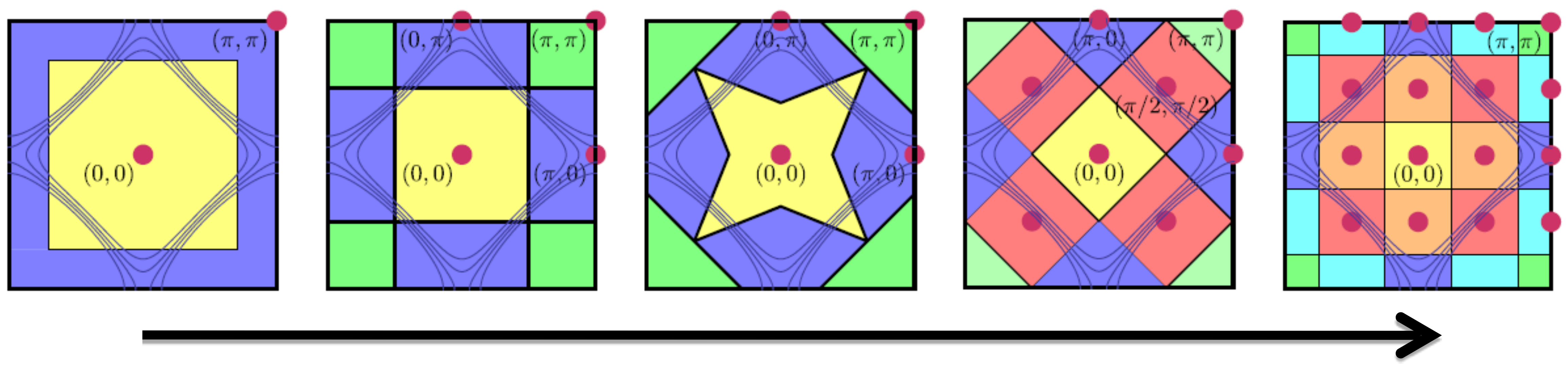


$$\Sigma(k, i\omega_n) \simeq \Sigma(i\omega_n)$$



Anderson impurity model

- Dynamical cluster approximation (DCA)



$$\Sigma(k, i\omega_n) \simeq \Sigma_K(i\omega_n)$$

In DCA, self-energy is patchwise constant
Control parameter: size of cluster

Civelli, MF, Georges, Gull, Haule, Jarrell, Katsnelson, Kotliar, Lichtenstein, Maier, Millis, Parcollet, Sordi, Tremblay, ...

Diagrammatic Monte Carlo

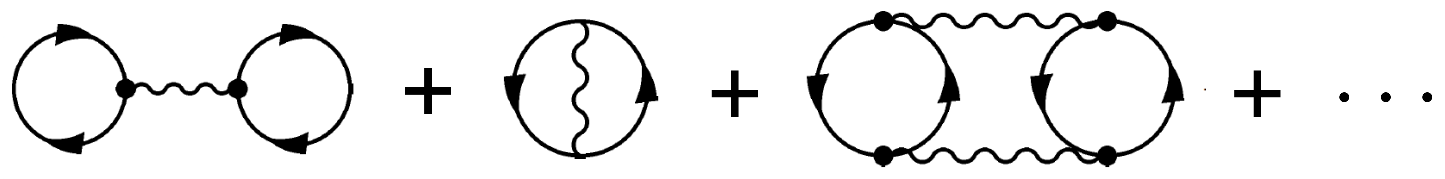
- Consider the Hubbard model on an infinite lattice at equilibrium (imaginary time)
- Write a perturbation series in U for the physical quantity of interest

$$\mathcal{A} = \sum_{n=0}^{\infty} a_n \, U^n$$

e.g. density, double occupation, Green's function, …

- From a diagrammatic point of view, e.g.

$\mathcal{A} = \ln Z =$

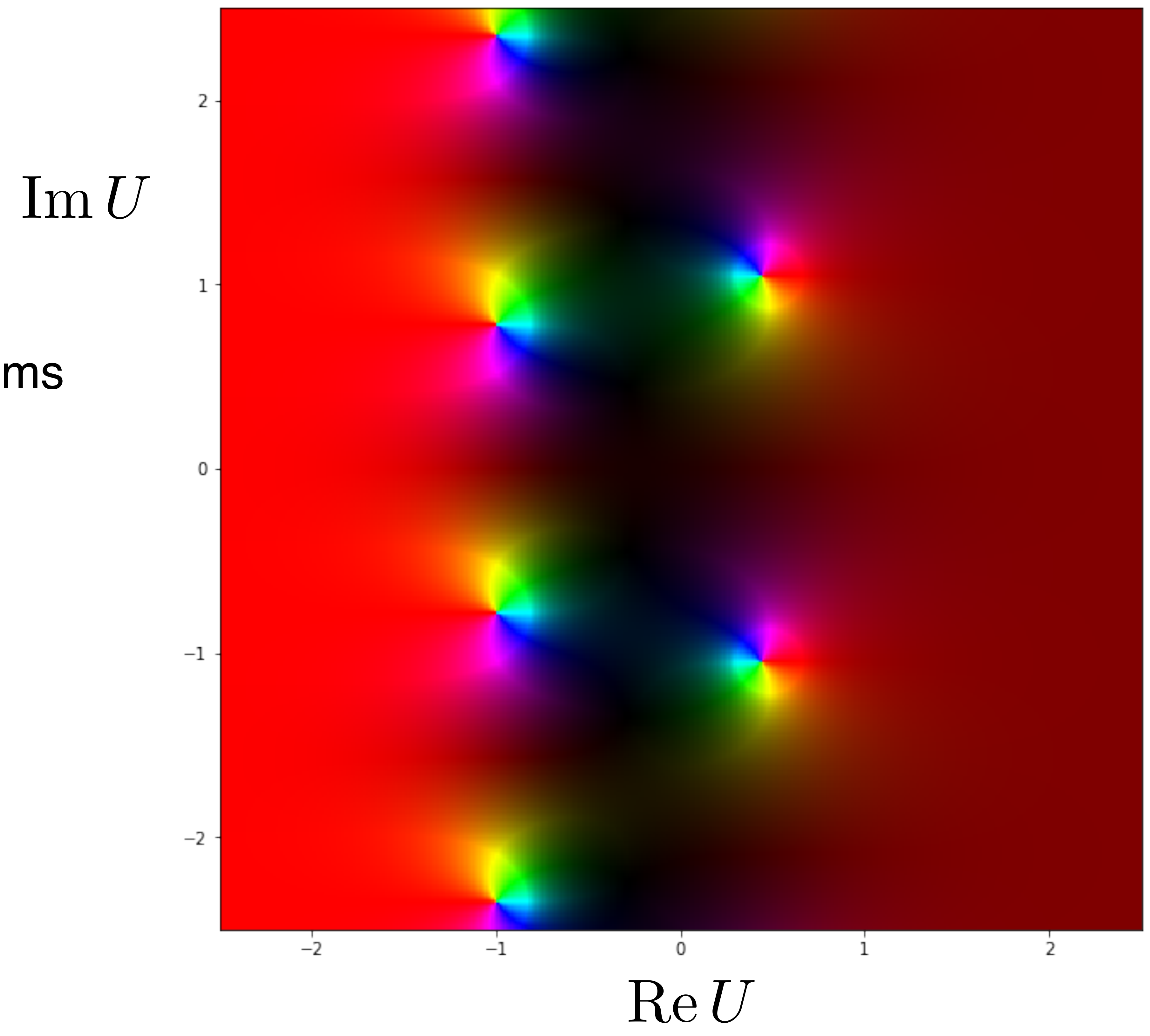


Only connected diagrams contribute to physical intensive quantities

- The series for $\mathcal{A}$ can have a finite convergence radius (poles in complex plane)
- Stochastic approach: compute a_n by Monte Carlo
- Two challenges

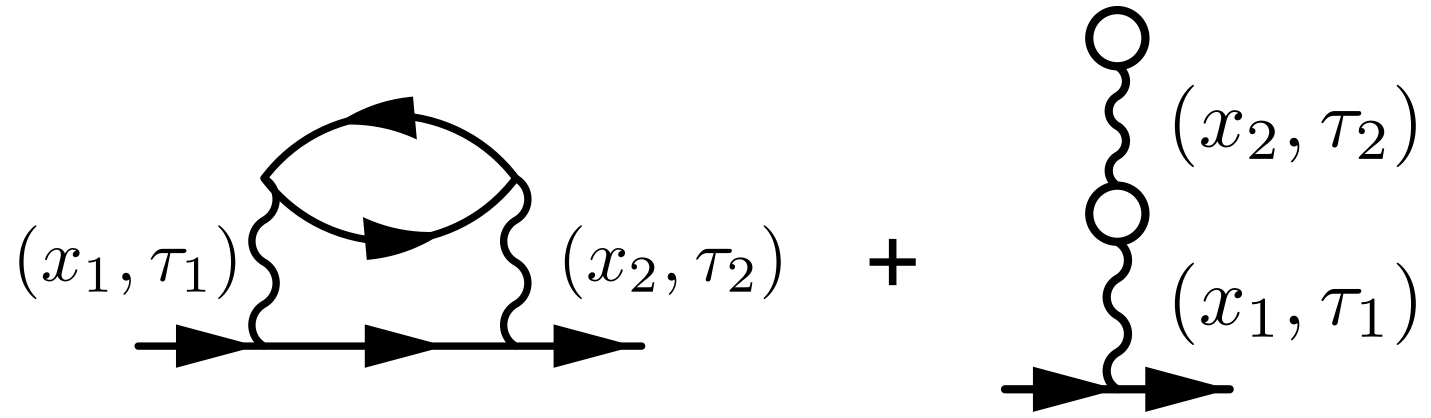
1. Fermionic sign problem → difficult to get many coefficients
2. Resumming the series → analytical structure in complex U plane?

$n(U)$ in the Hubbard atom



Challenge 1: Compute series coefficients

- Series have natural representation (e.g. connected diagrams)
- Original algorithm (DiagMC): stochastically sample topologies (≊ 6-7 orders)
- Sign problem has two origins:
  - Integration over internal variables
  - Alternating sign between different topologies
- Reduce sign problem: Sum topologies with the same set of internal vertices V
- Direct approach: huge computational effort (factorial number of diagrams)!
- CDet: Can be done in exponential time, 3^n or $n^2 2^n$, using determinants (disconnected diagrams removed recursively)



N.V. Prokofiev and B.V. Svistunov, PRL (2007)

Other approaches:

A. Taheridehkordi et al., arXiv (2019)
K. Chen and K. Haule, Nat. Comm. (2019)
M. Maček et al., arXiv (2020)

R. Rossi, PRL (2016)
A. Moutenet et al., PRB (2018); Šimkovic and Kozik, PRB (2019)

Challenge 2: Resummation of the series

- Series convergence controlled by structure in complex plane
- How do we evaluate the series beyond its convergence radius?
- Approach 1: Conformal maps, Padé approximants, …
- Approach 2: Generate new series with freedom in the starting point of the perturbation theory. Simplest idea:

$$G_0 = \frac{1}{i\omega_n + \mu - \epsilon_k} \quad \rightarrow \quad \tilde{G}_0 = \frac{1}{i\omega_n + \mu - \epsilon_k - \alpha}$$

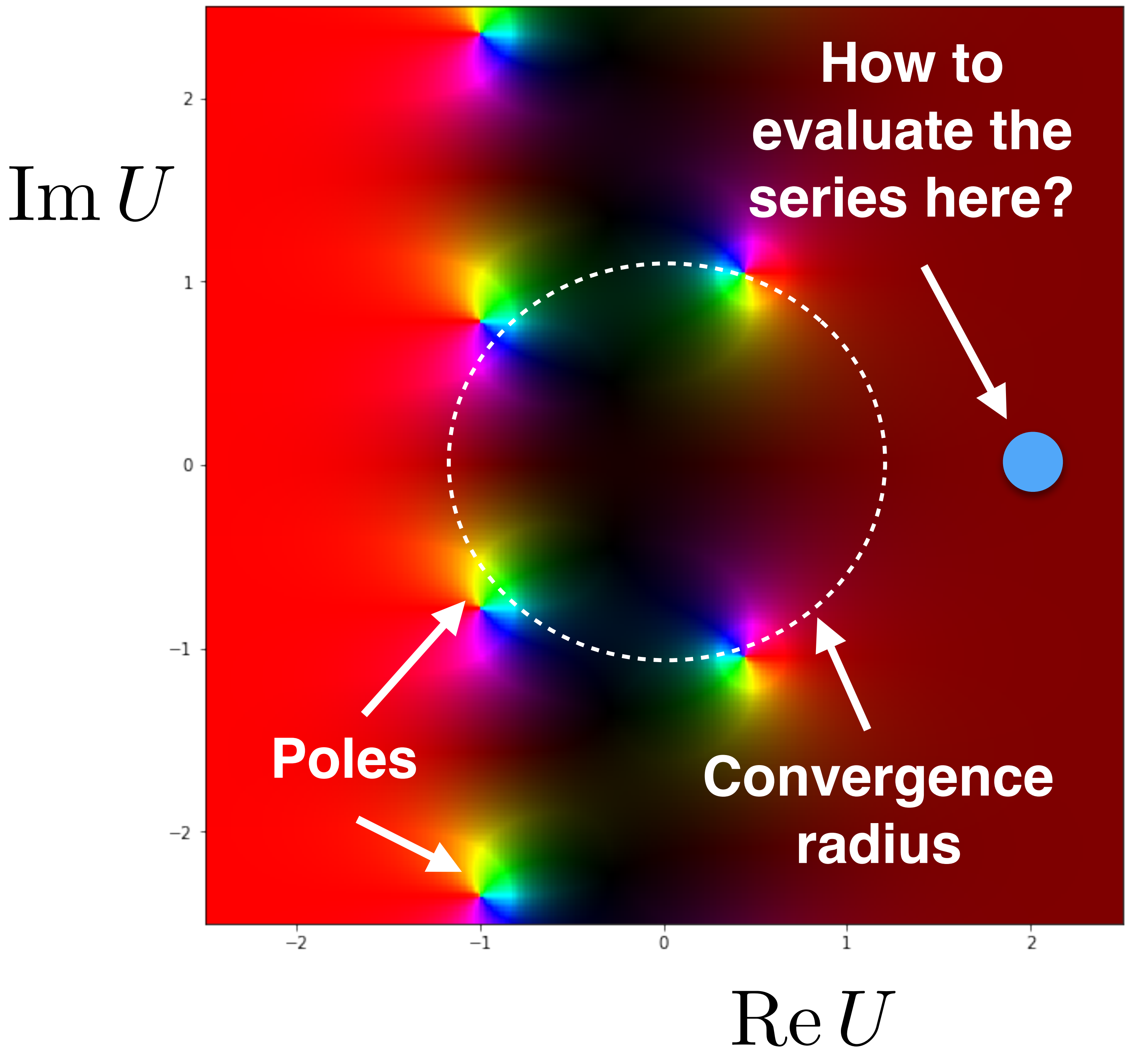
- Can be generalized to start from a renormalized propagator

$$G_0 = \frac{1}{i\omega_n + \mu - \epsilon_k} \quad \rightarrow \quad \tilde{G}_0[U] = \frac{1}{i\omega_n + \mu - \epsilon_k - \Delta_k(i\omega_n)[U]}$$

- The counter terms can still be computed with determinants: Renormalized determinant approach (RDet)
- Allows to reach much lower temperatures in Hubbard model

R. Rossi, F. Šimkovic, M. Ferrero, arXiv (2020)

$n(U)$ in the Hubbard atom

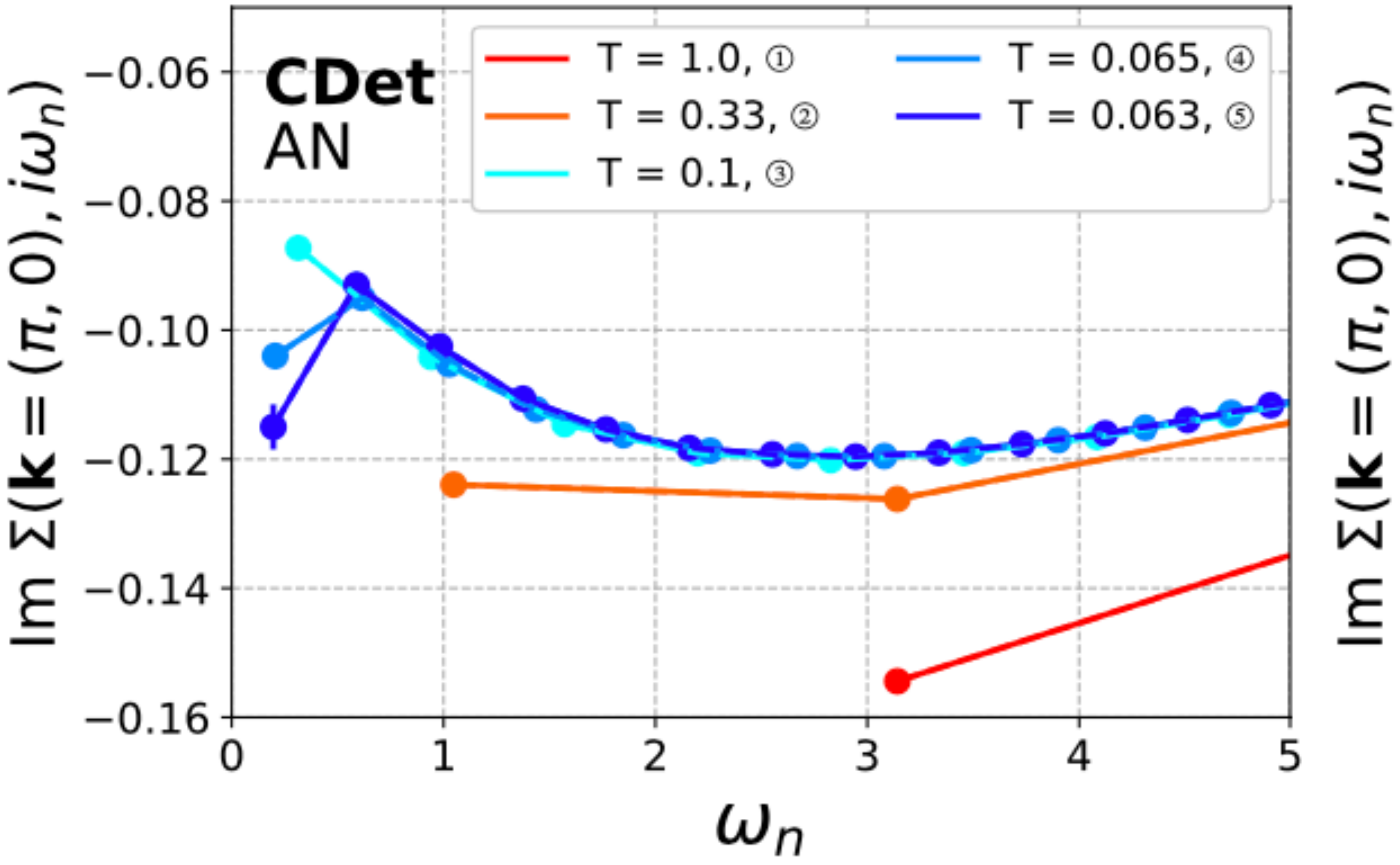


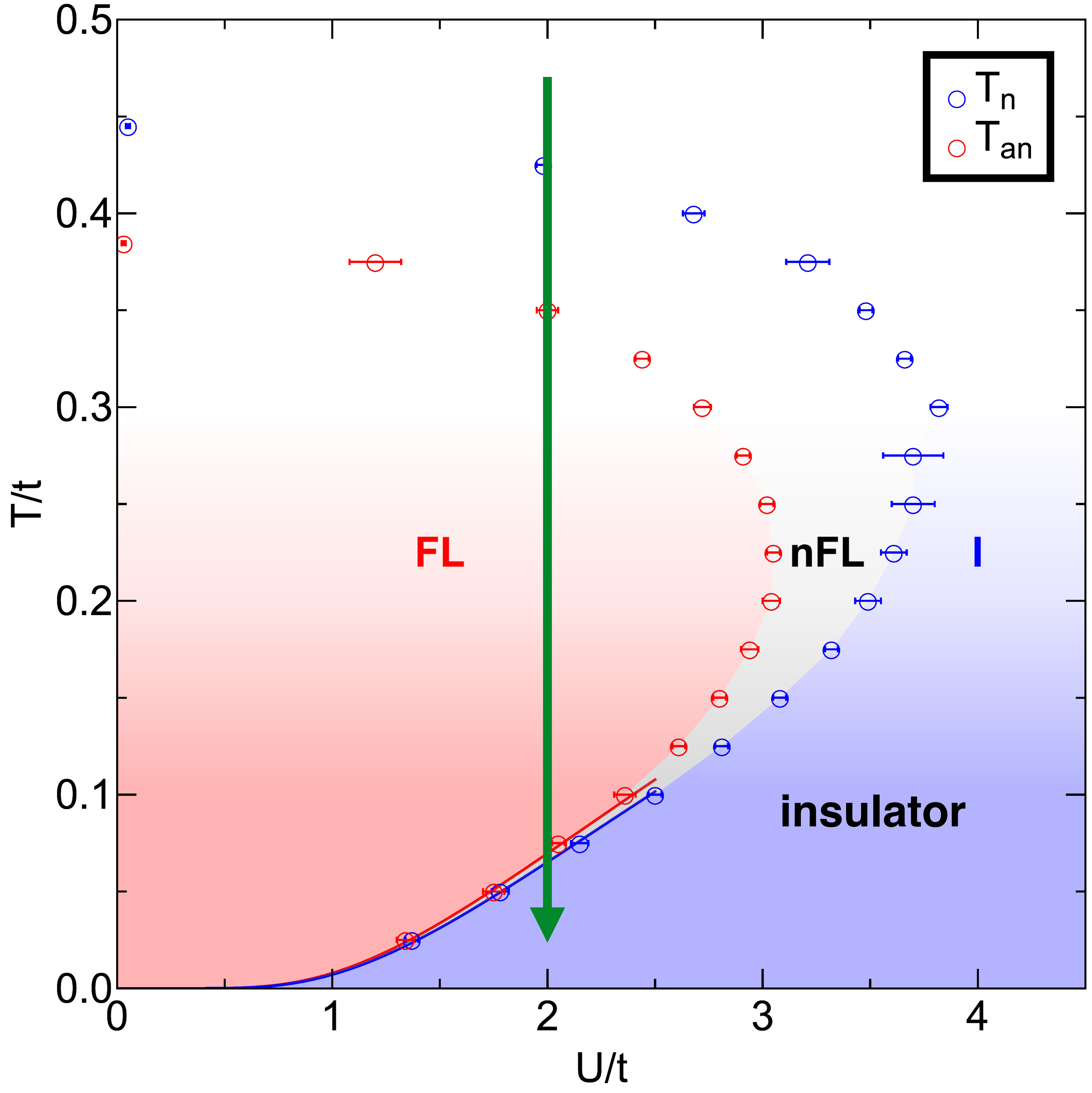
R. Profumo et al., PRB (2015)
W. Wu et al., PRB (2017)
F. Šimkovic et al., PRB (2019)
C. Bertrand et al., PRX (2019)

Existence of pseudogaps in the Hubbard model

Half-filled Hubbard model

- Exact solutions in the weak- to intermediate-coupling regime
- Two crossovers:
  - High-temperature incoherent → Fermi liquid
  - Fermi liquid → pseudogap (long-range AF correlation)
- Limitation: Resummation becomes very difficult in pseudogap regime despite absence of a true phase transition





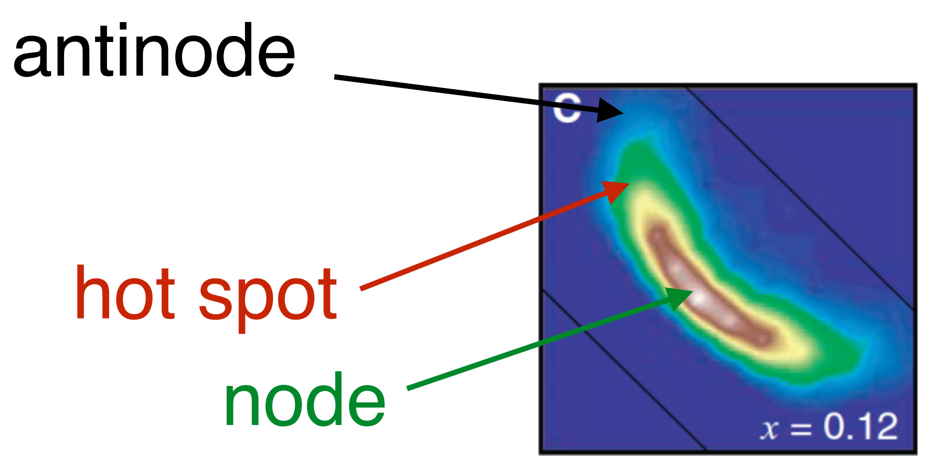
F. Šimkovic et al., PRL (2020)
A. Kim et al., PRL (2020)
T. Schäfer et al., in preparation (2020)

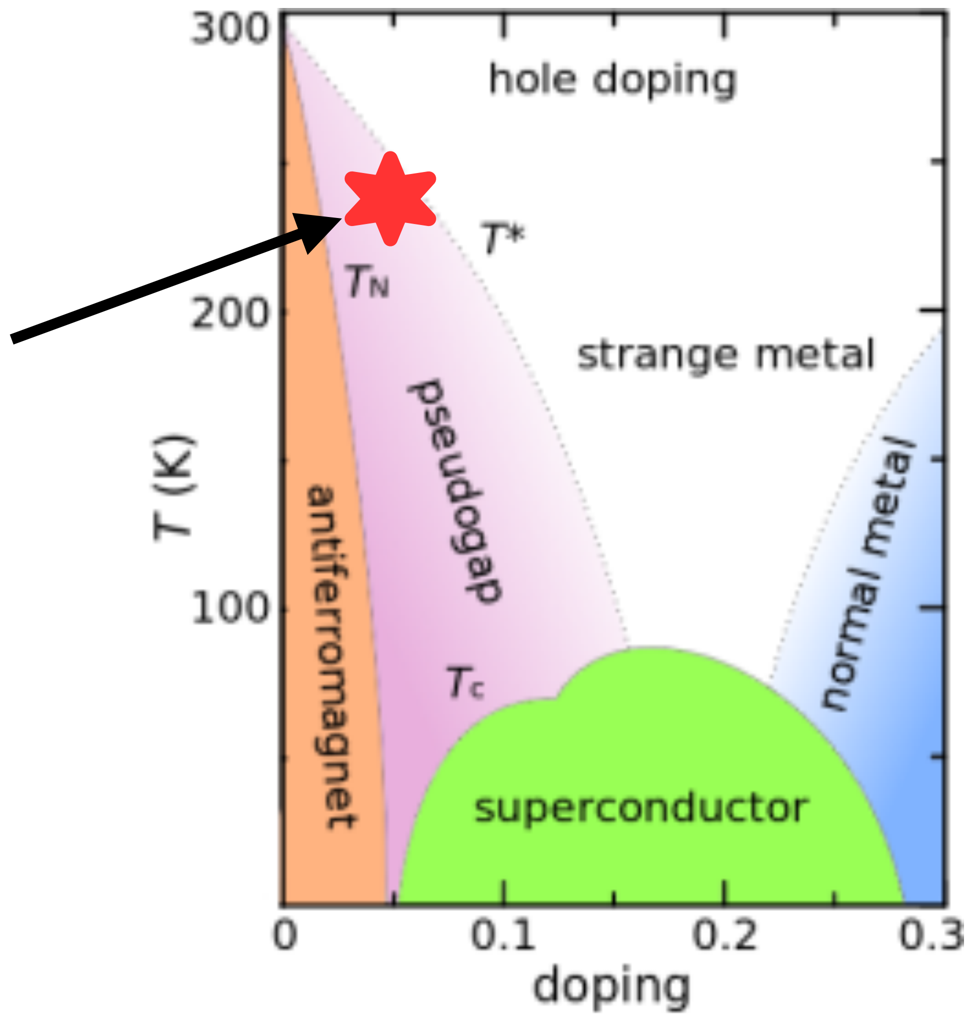
Pseudogap in hole-doped Hubbard model

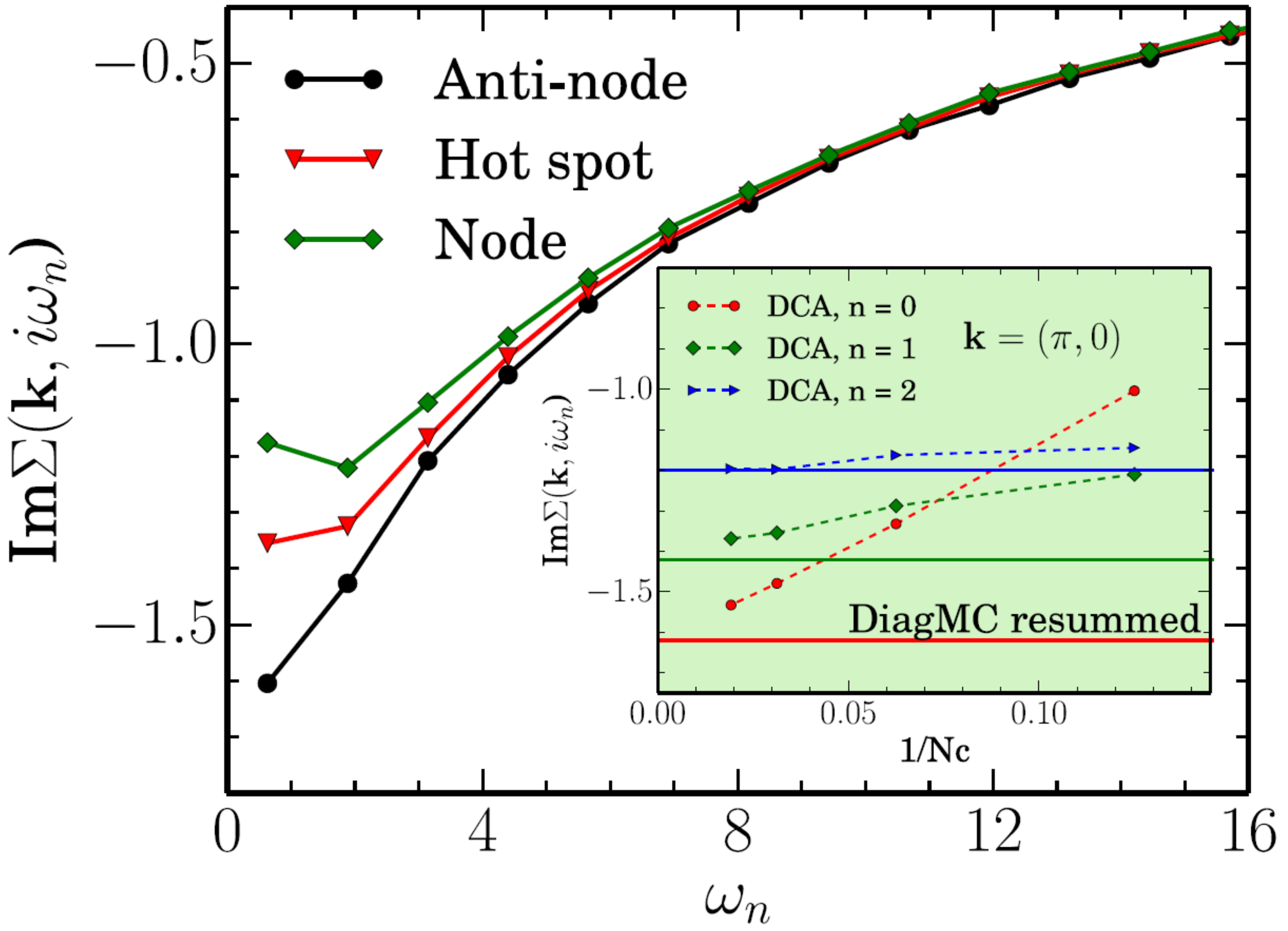
- With the diagMC algorithm, converged results for

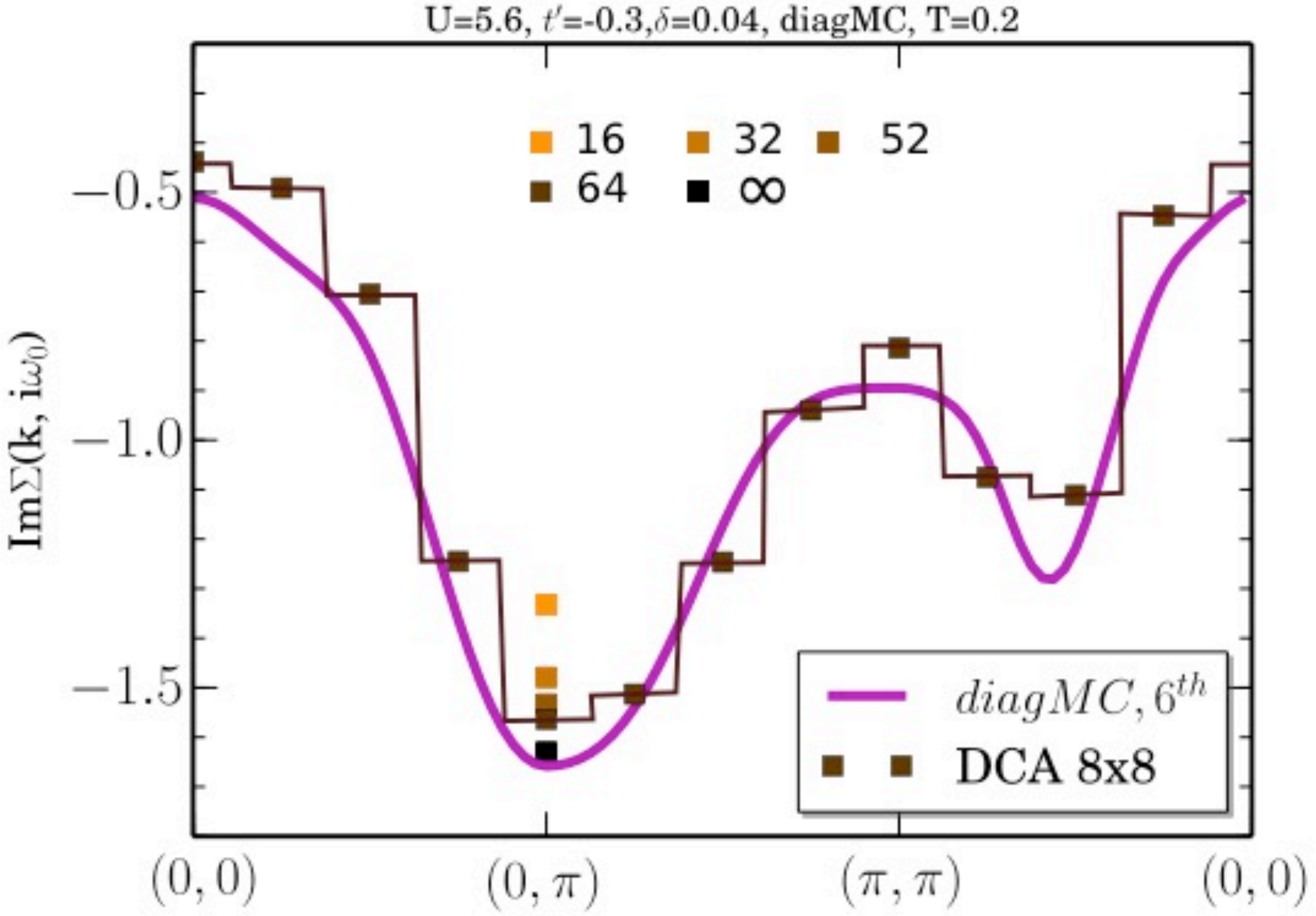
$$U = 5.6t \quad t' = -0.3t \quad T = 0.2t \quad \delta \simeq 4\%$$

- Top of pseudogap region
- Clear nodal / antinodal differentiation
- Antinode hotter than hotspot ≠ weak-coupling





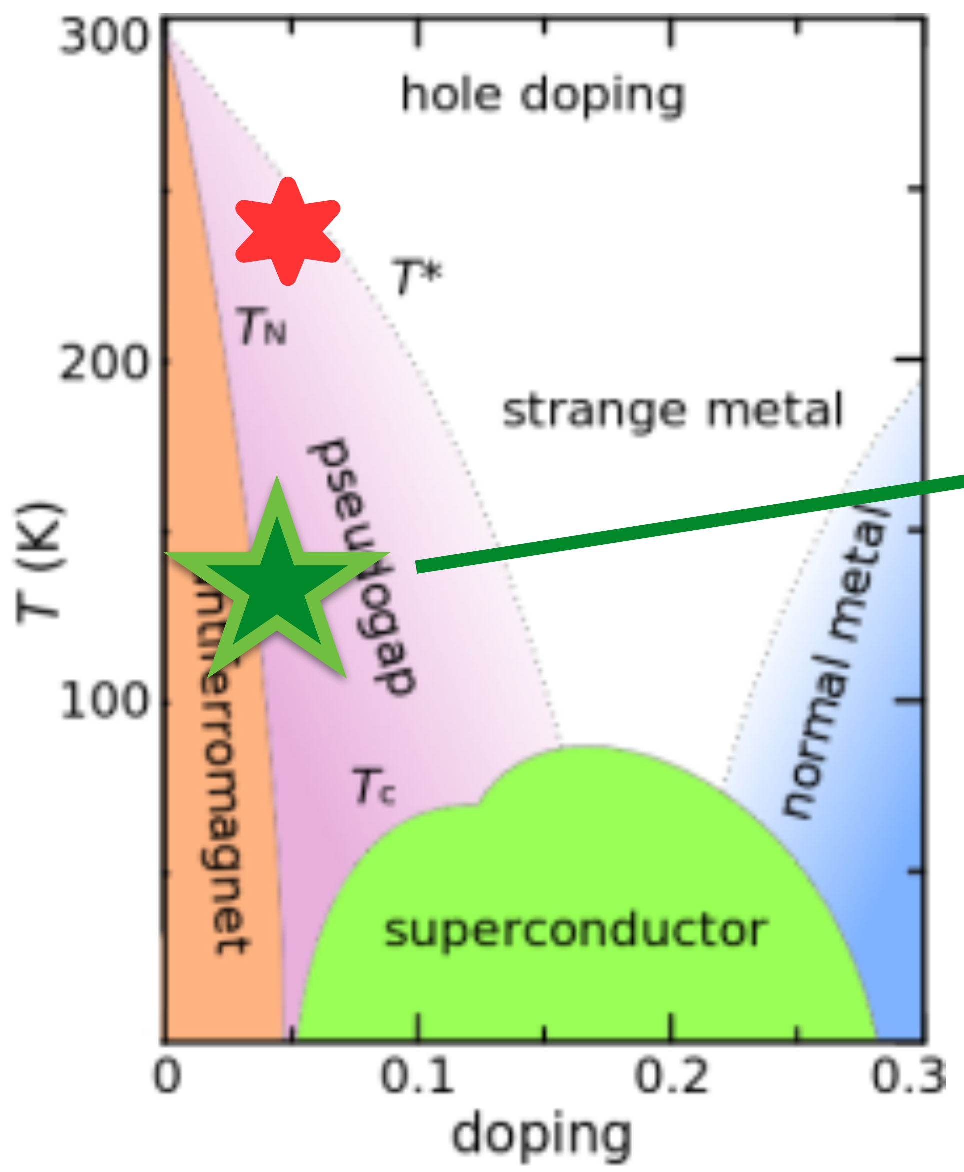


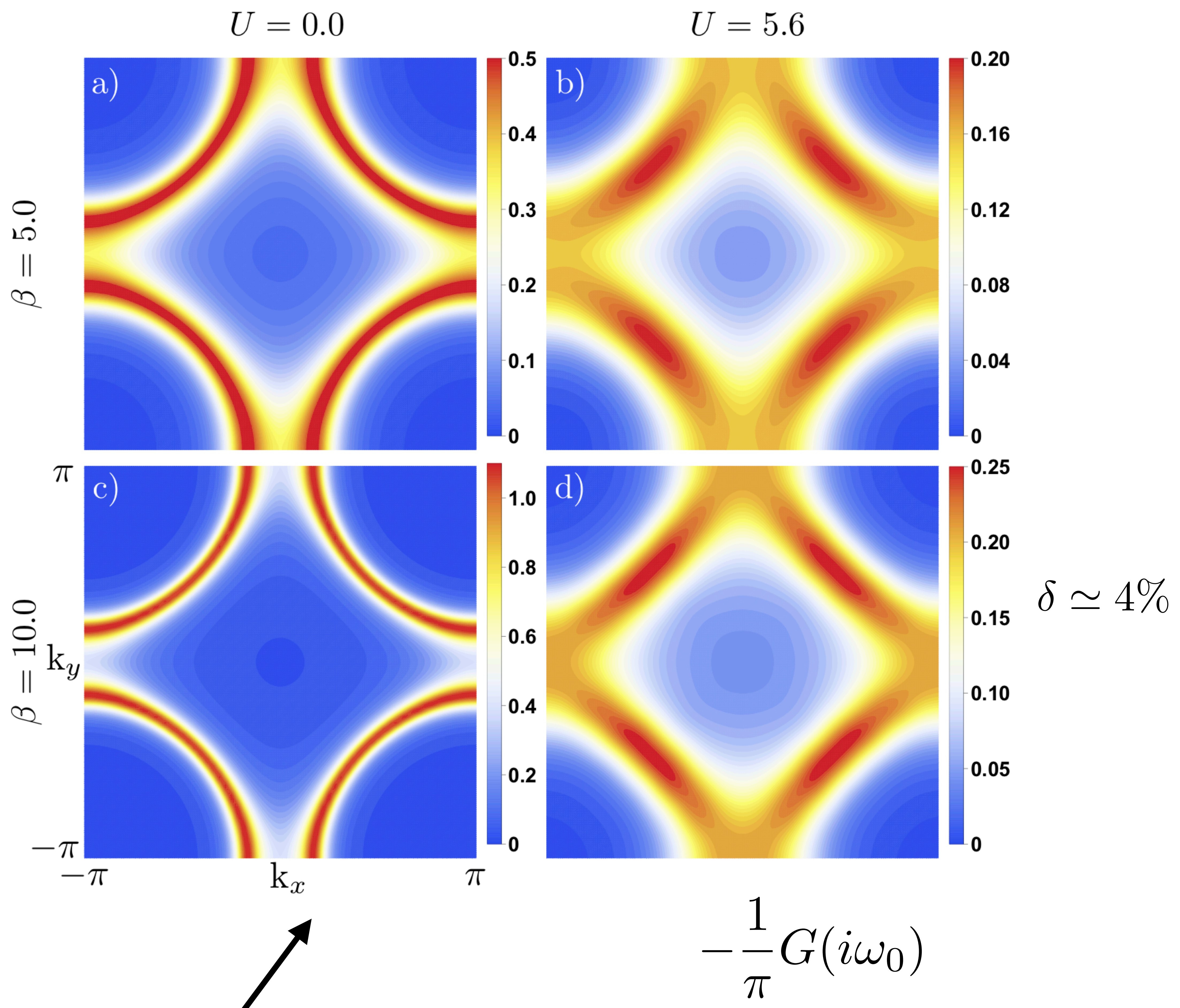


W. Wu et al., PRB (2017)

Pseudogap in hole-doped Hubbard model

- We can now reach temperatures that are twice as low





obtained from RDet

- However, there is only a weak reinforcement of the nodal / antinodal differentiation
- Larger value of the interaction U?

R. Rossi, F. Simkovic and M. Ferrero, arXiv (2020)

Origin of the pseudogap

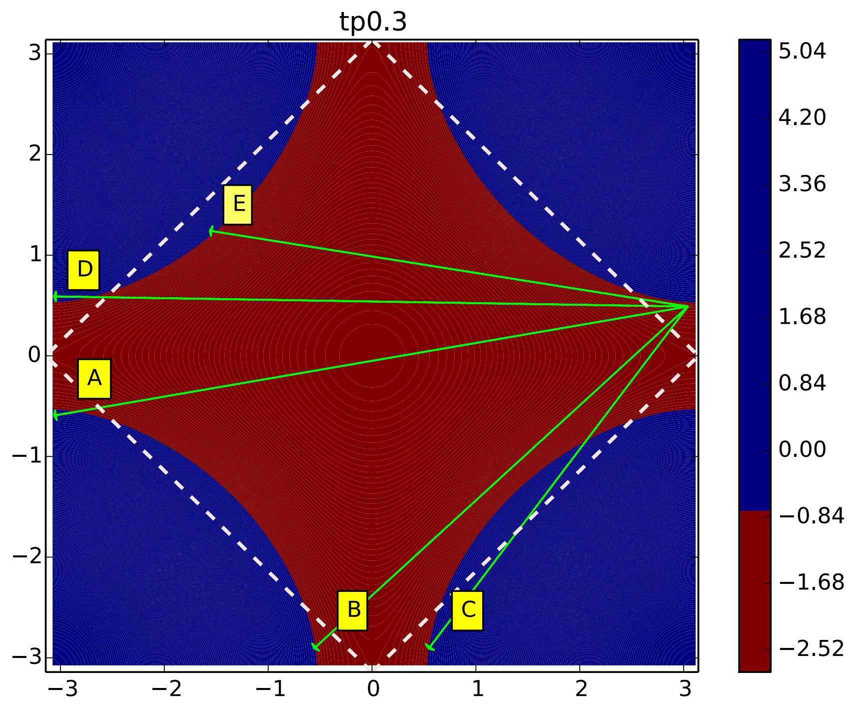
Origin of the pseudogap: fluctuation diagnostics

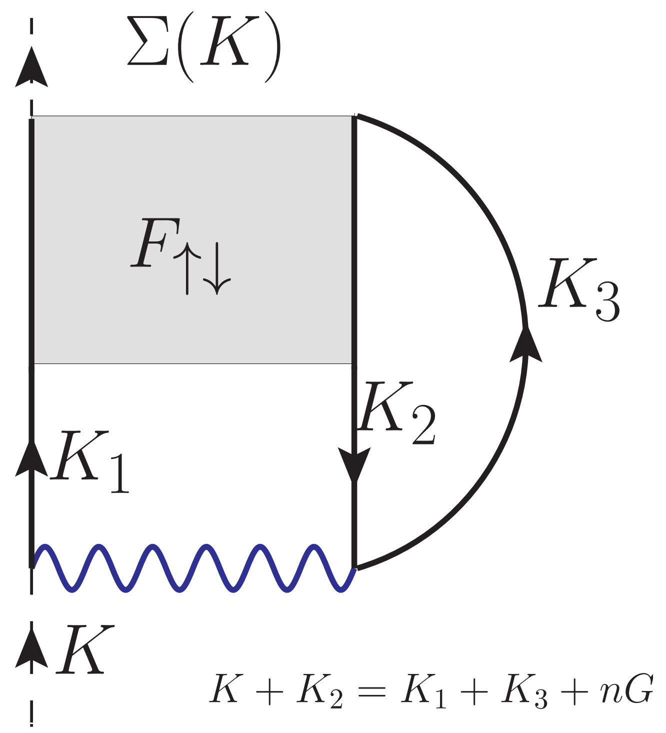
- Fluctuation analysis

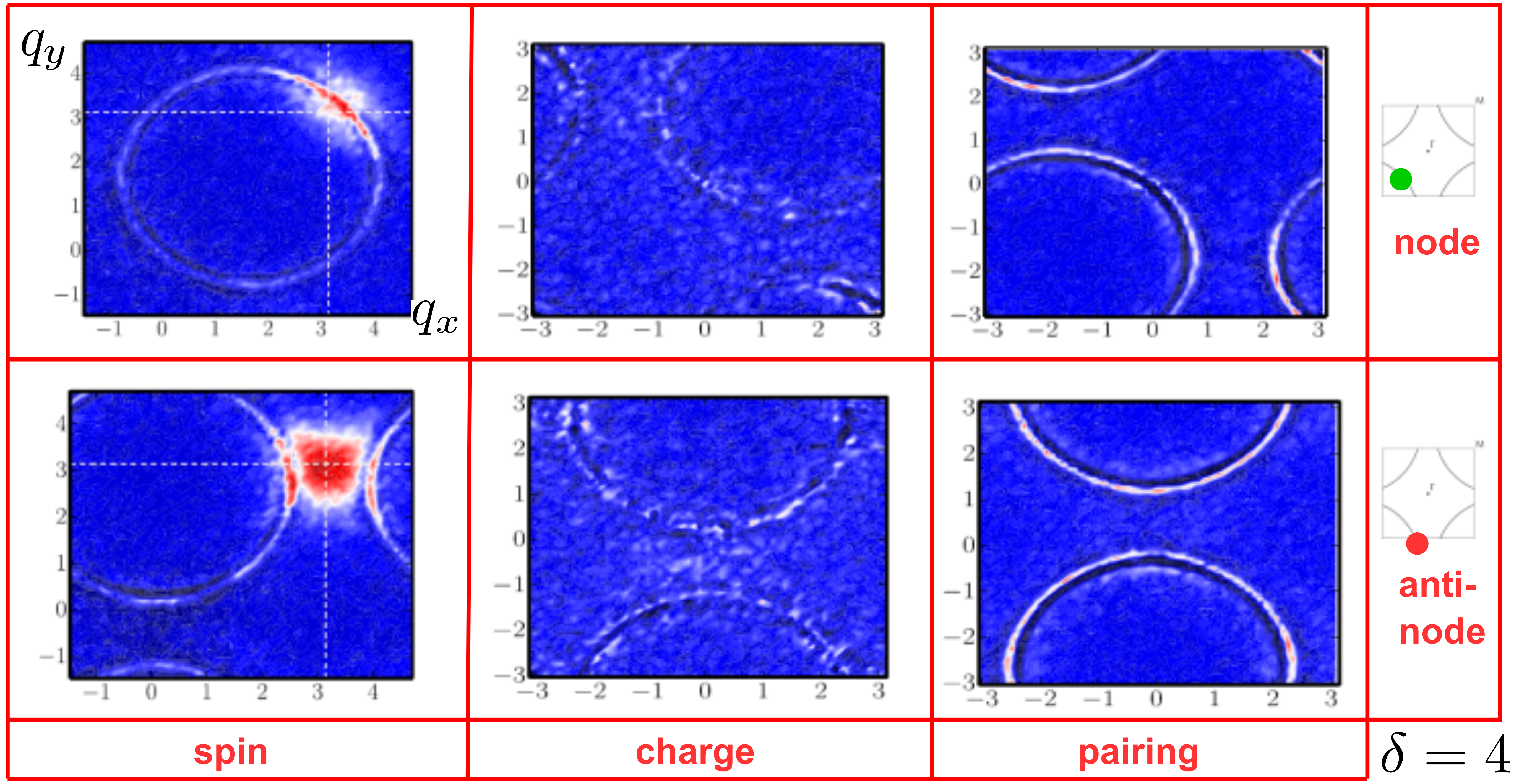
  O. Gunnarson, T. Schäfer, et al., PRL (2015)

$$\Sigma(K) = \sum_q \Sigma_X^q(K) + \frac{Un}{2}$$

- Distribution of momenta gives info about nature of scattering
- Spin, charge and pairing representations
- Charge and pairing featureless
- Spin: Fermi surface scattering at node, commensurate at antinode
- From spin susceptibility: $\boxed{\xi \simeq 1.5}$
- Pseudogap due to short-range, antiferromagnetic correlations







$\delta = 4\%$

$U = 5.6t, T = 0.2t$

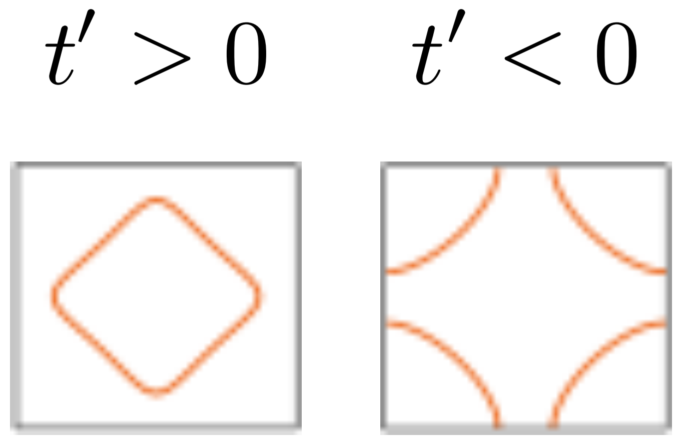
W.Wu, M. Ferrero, A. Georges and E. Kozik, PRB (2017)

Origin of the pseudogap: pole in self-energy

W. Wu, A. Georges, MF, PRX (2018)
M.S. Scheurer et al., PNAS (2018)

- Systematic 8-site DCA calculations

$$\mathcal{H} = \sum_{ij\sigma} t_{ij}\, c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

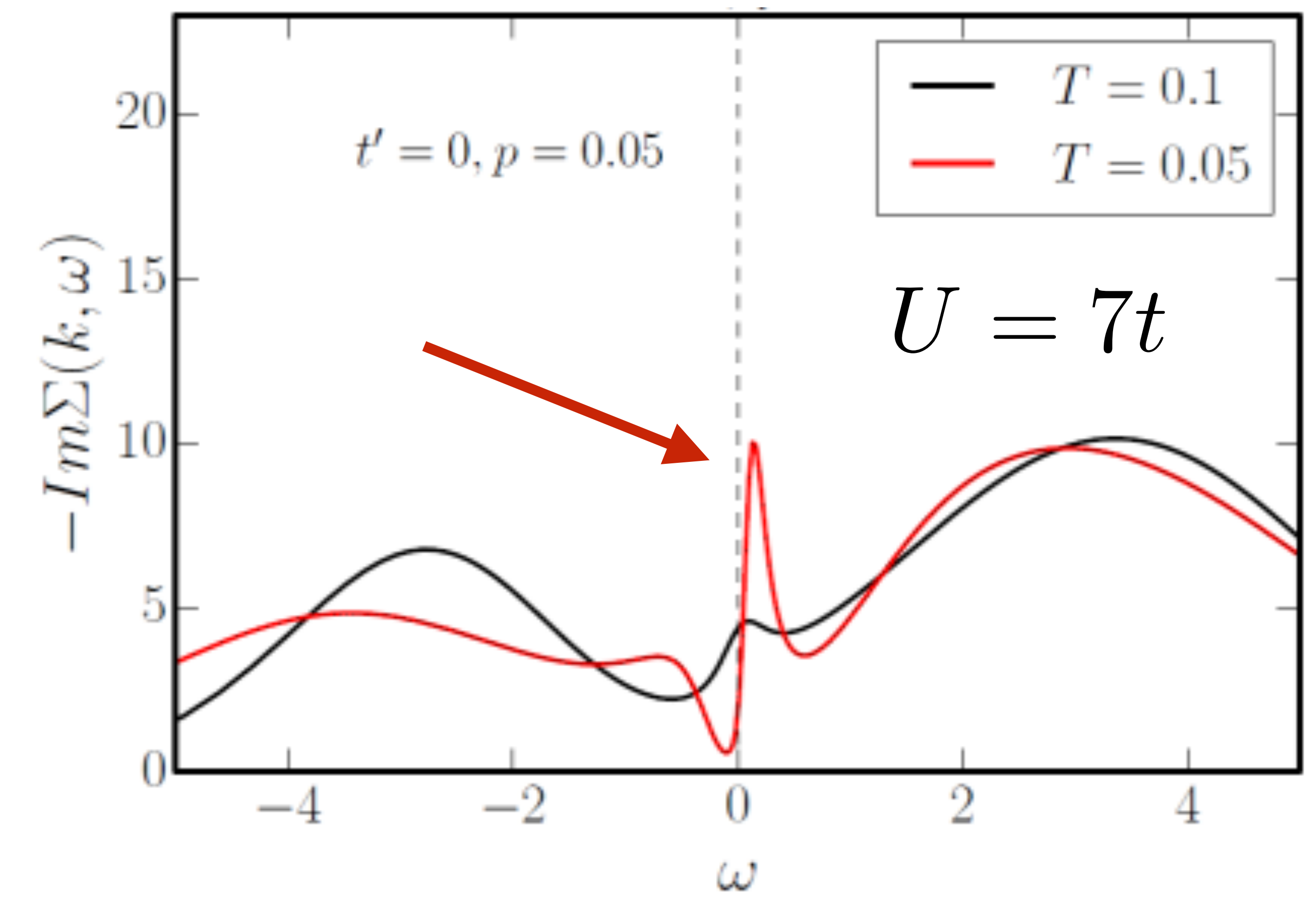


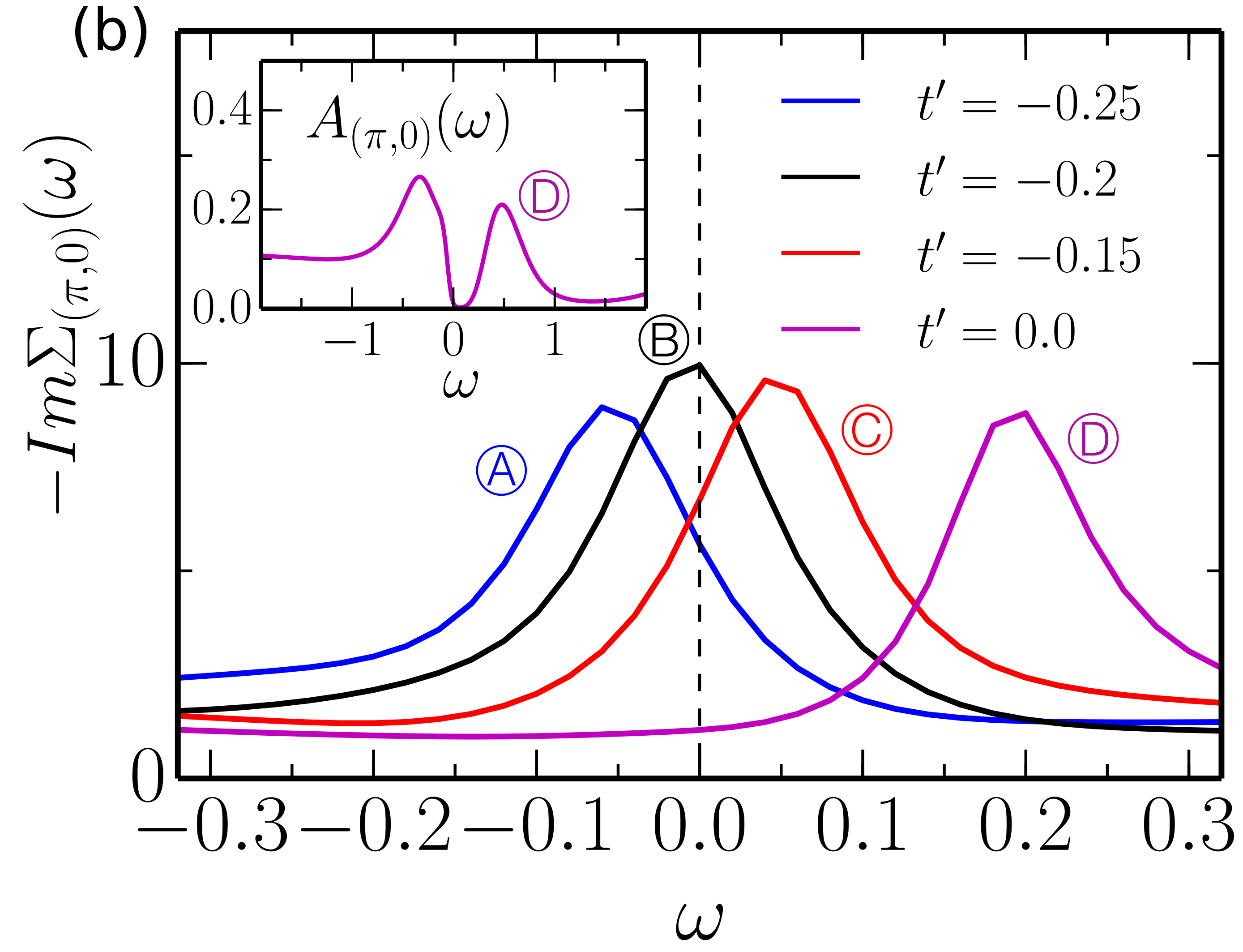
- As shown in previous works: pseudogap stems from pole-like feature in antinodal self-energy
- Pole is asymmetric and moves with nearest-neighbor hopping t’
- Asymmetry of pole changes Fermi surface topology

$$\mathrm{Re}\Sigma_K(\omega = 0) = \frac{1}{\pi}\int_{0+}^{\infty} \frac{\mathrm{Im}\Sigma_K(\omega') - \mathrm{Im}\Sigma(-\omega')}{\omega'} d\omega'$$

$$\tilde{\epsilon}_{(\pi,0)} = \epsilon_{(\pi,0)} - \mu + \mathrm{Re}\Sigma_{(\pi,0)}(\omega = 0)$$

renormalized dispersion

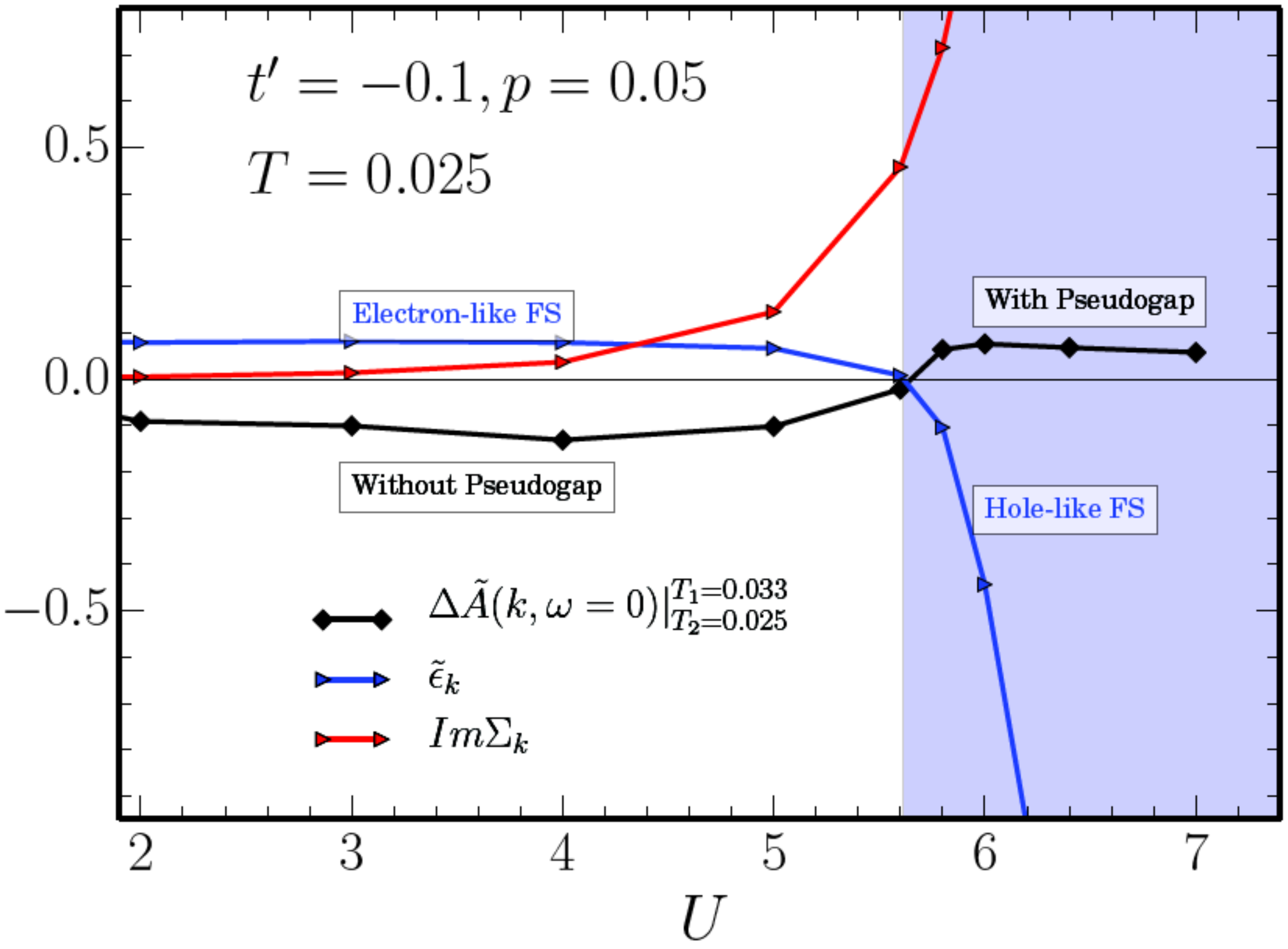




Rapid crossover between weak and strong coupling

Entering the strong-coupling regime

- The renormalized dispersion changes very abruptly at $U \simeq 5.5$

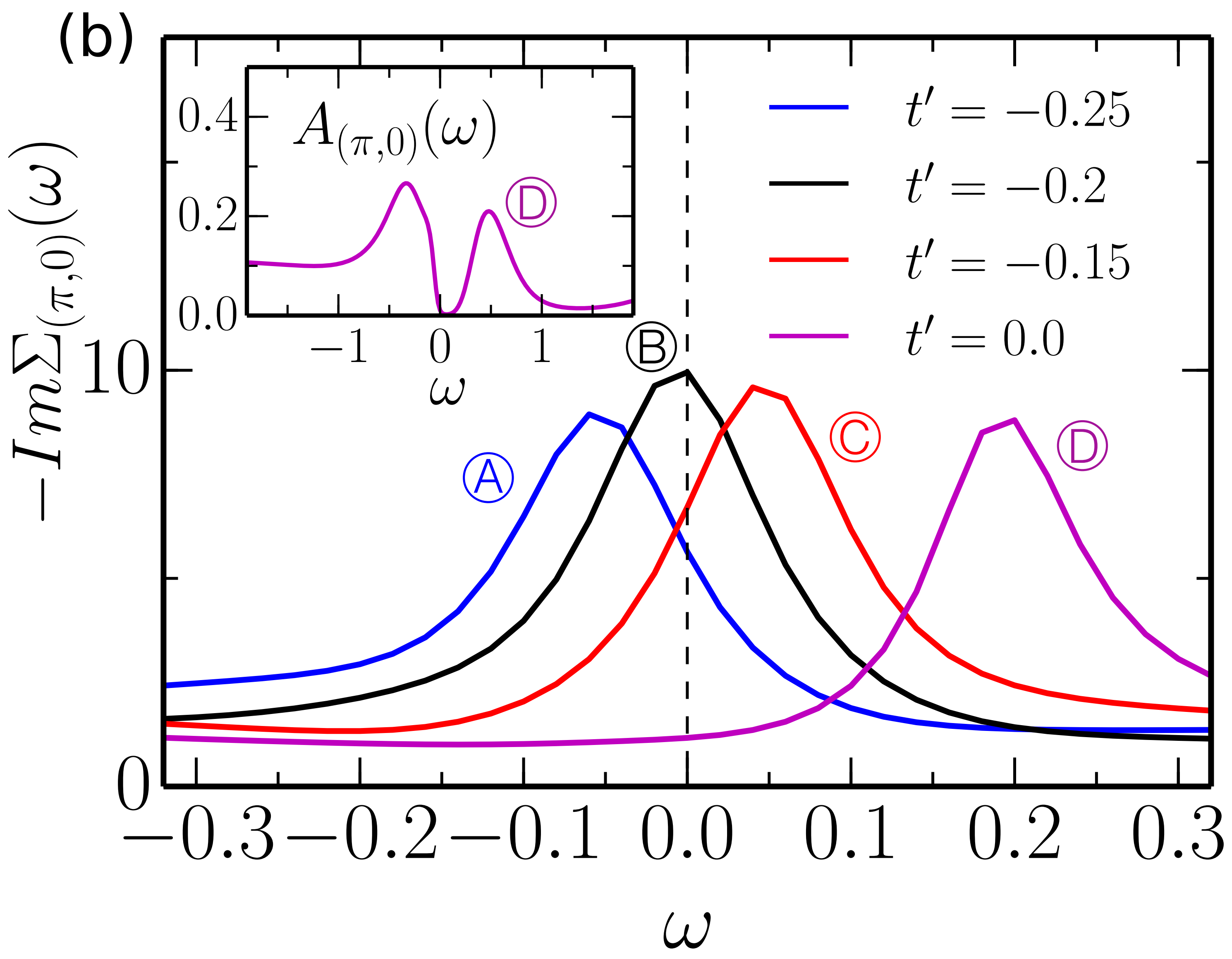


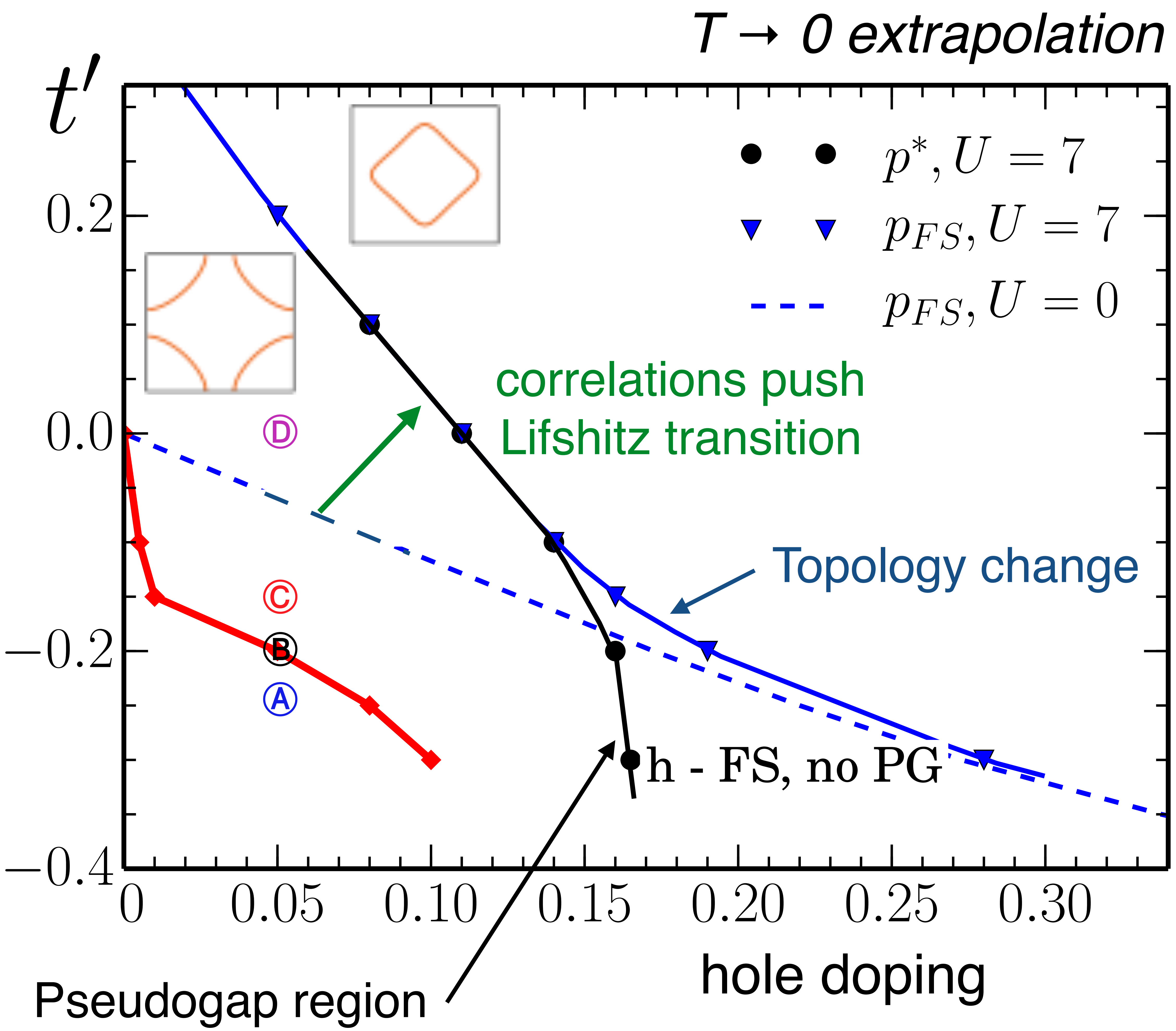
Fermi surface topology and pseudogap

Fermi surface topology and pseudogap

- Pole in self-energy → Fermi surface strongly modified by interactions
- The pseudogap only exists on hole-like Fermi surfaces!
- Compatible with experimental body on cuprates

S. Benhabib et al, PRL (2015); A. Kaminski et al., PRL (2015)
C.E. Matt et al., PRB (2015); T. Yoshida et al., PRB (2006)
S. Badoux et al., Nature (2016)

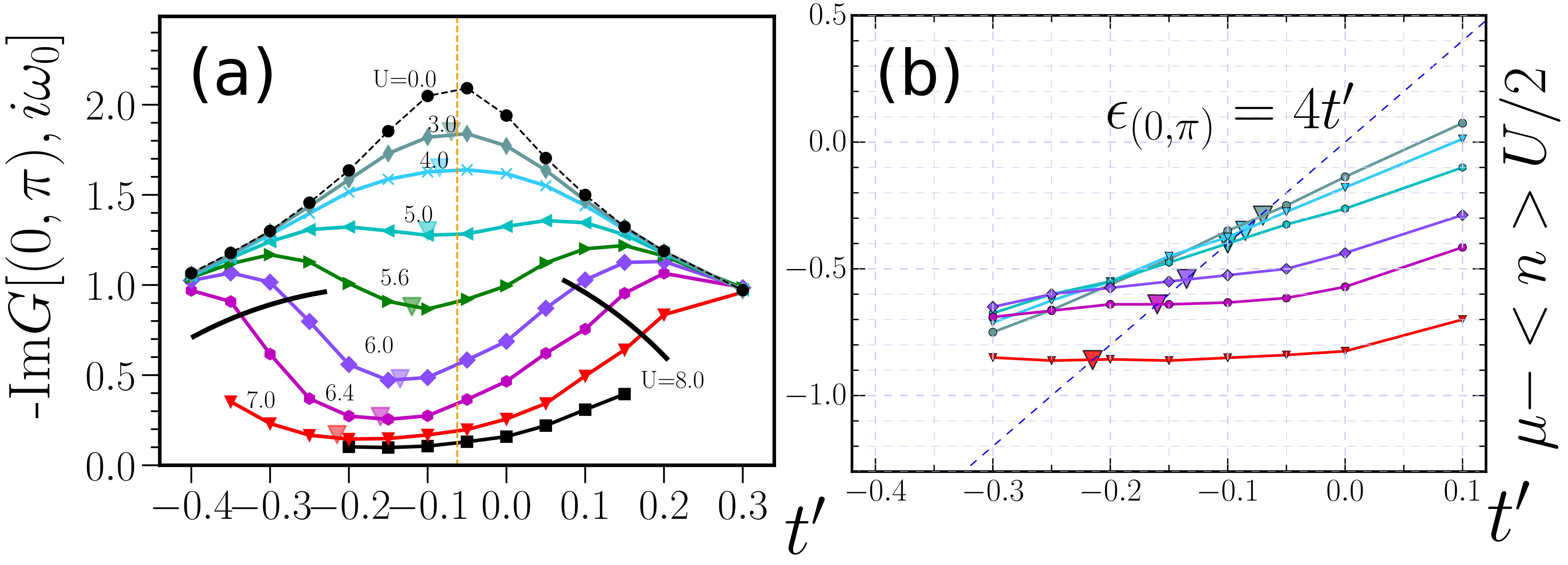


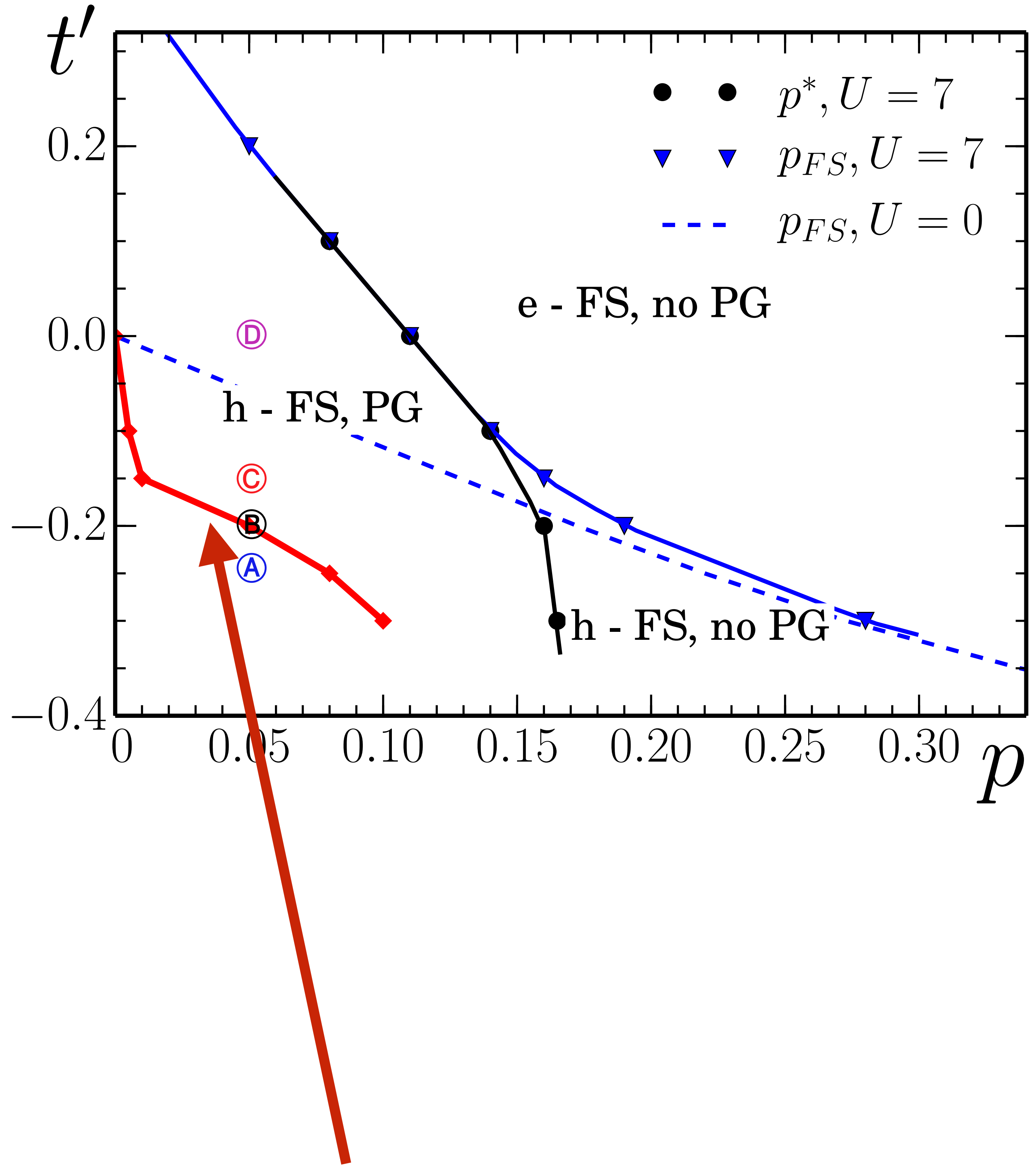


W. Wu, A. Georges, MF, PRX (2018)

Self-energy pole and the van Hove singularity

- Red line: pole at zero energy in the antinodal self-energy
- Can we characterize the red line?





Here the self-energy has a pole at zero energy

- We observe that maximum scattering when the Hartree-shifted Fermi surface goes through the van Hove singularity

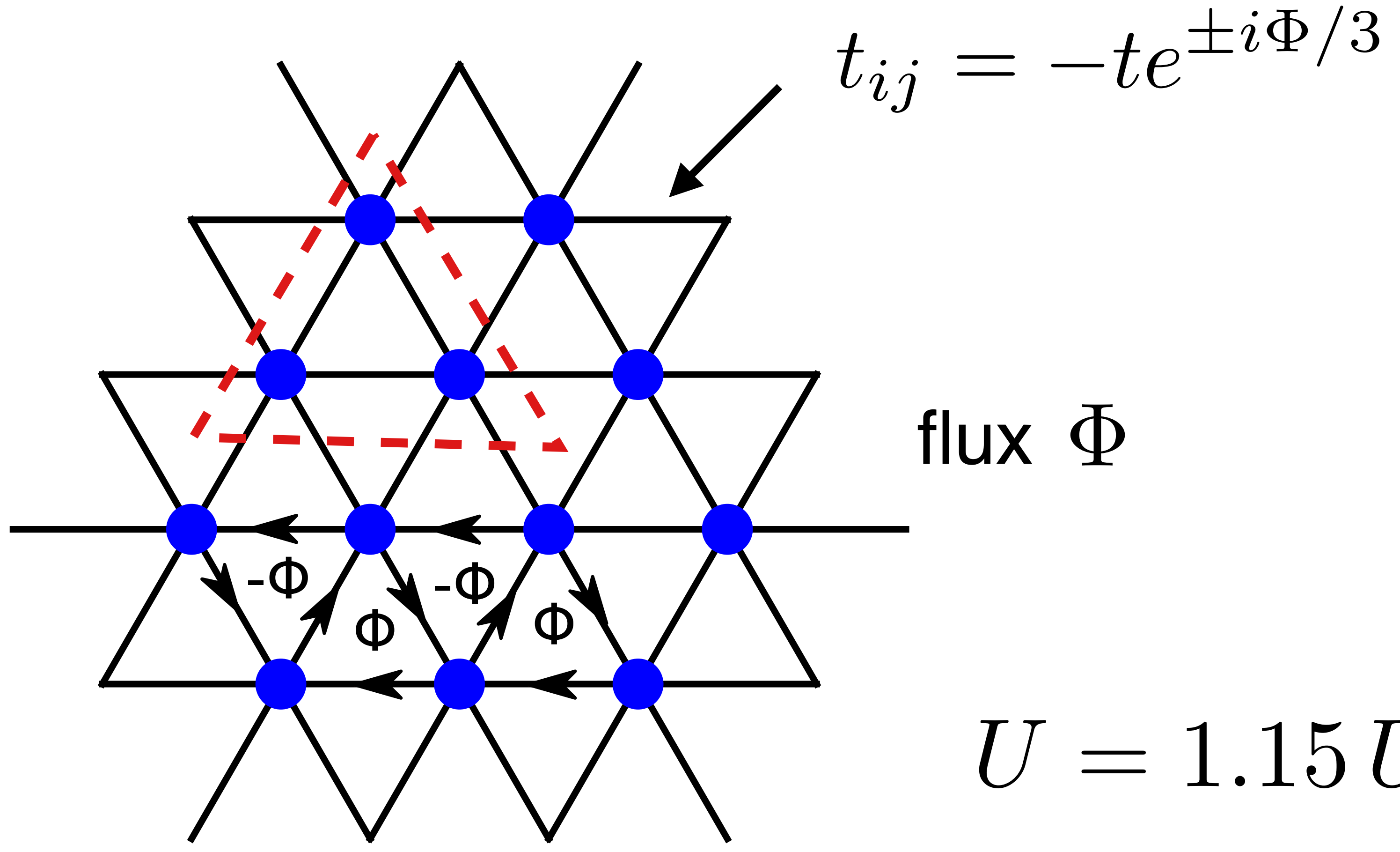
$$\boxed{\epsilon(K_{\mathrm{vH}}) - \mu + \frac{\langle n \rangle}{2} U = 0} \qquad K_{\mathrm{vH}} = (0, \pi)$$

- How generic is this result? What role does the van Hove singularity play?

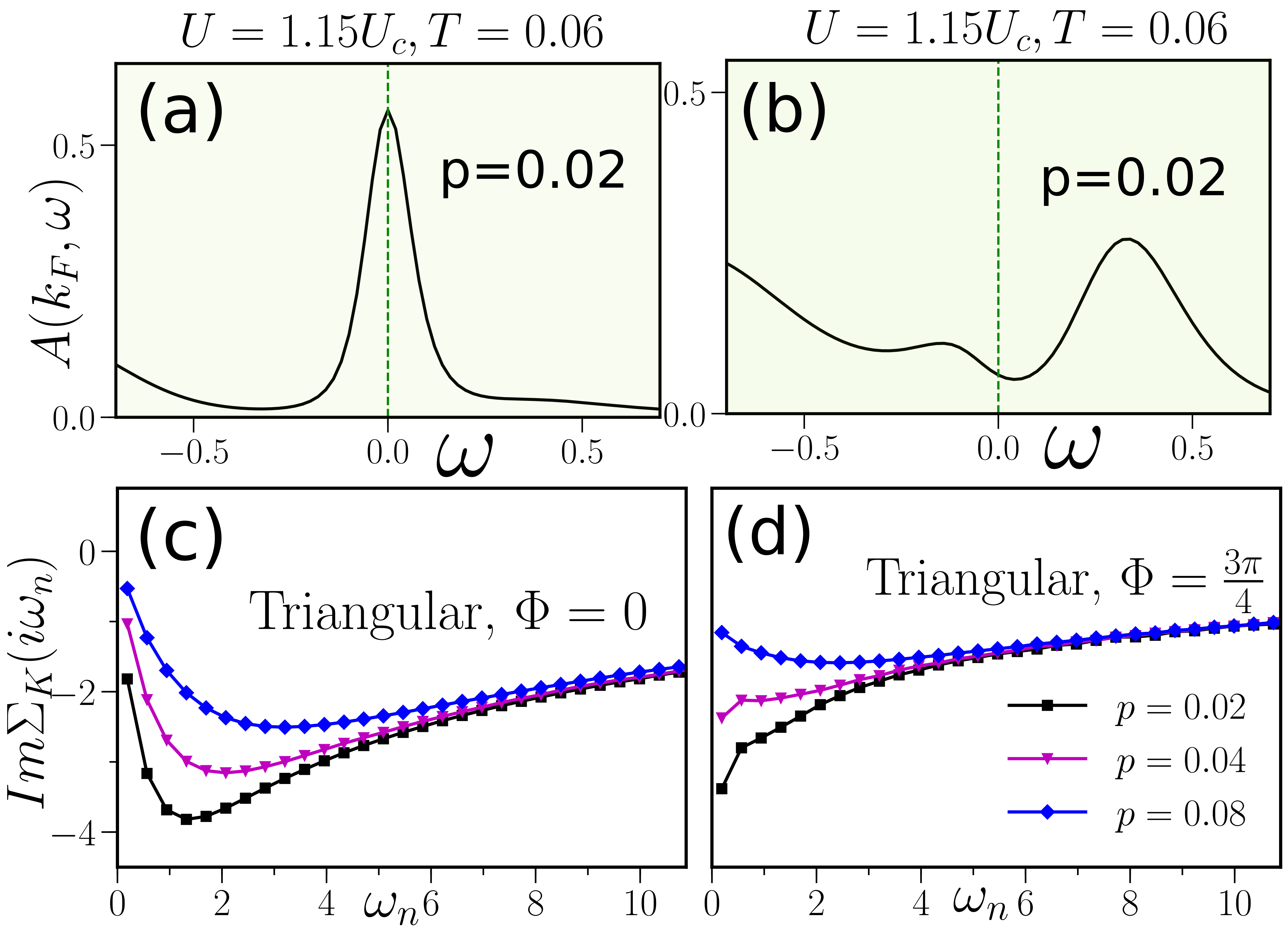
Fermi surface topology and pseudogap in other models

- Non-intuitive relationship between pseudogap and Fermi surface topology
- We systematically investigate several models with different fermiologies
- Here we show results for triangular lattice with flux
- At low doping, pseudogap only for some fluxes
- The absence of a pseudogap at $\Phi = 0$ is not related to frustration (same Heisenberg limit)
- Flux changes → van Hove singularity changes

W. Wu et al. arXiv (2020)



$U = 1.15\, U_c^{\mathrm{Mott}}$



$\Phi = 0$

$\Phi = \frac{3\pi}{4}$

Role of the van Hove singularity?

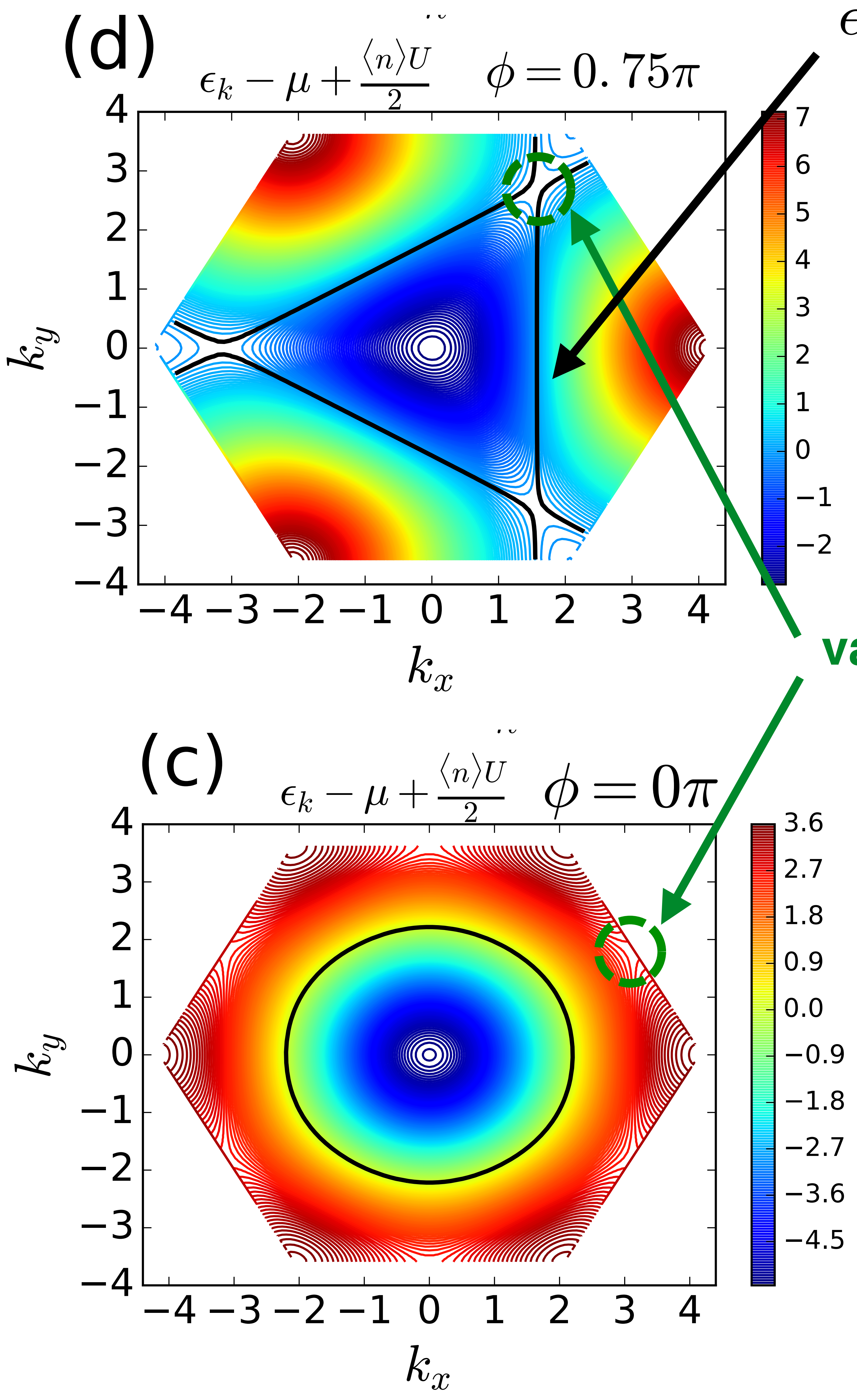
- On the square two-dimensional Hubbard model we found that the pseudogap is maximum when

$$\epsilon(K_{\mathrm{vH}}) - \mu + \frac{\langle n\rangle}{2}U = 0$$

- The same relation holds for the triangular lattice →
- Also true for square lattice with asymmetric hopping

$$\epsilon_k = -2t\Big(\cos(k_x) + \cos(k_y)\Big) - 4t''' \cos(2k_x)\cos(k_y)$$

- Change in fermiology → shift the vHs away → turn off the pseudogap
- Even though we are clearly in the strong-coupling regime, the van Hove singularity is a key player in the construction of the pseudogap



$$\epsilon(k) - \mu + \frac{\langle n\rangle}{2}U = 0$$

$$\boxed{\Phi = \frac{3\pi}{4}}$$

van Hove singularity

$$\boxed{\Phi = 0}$$

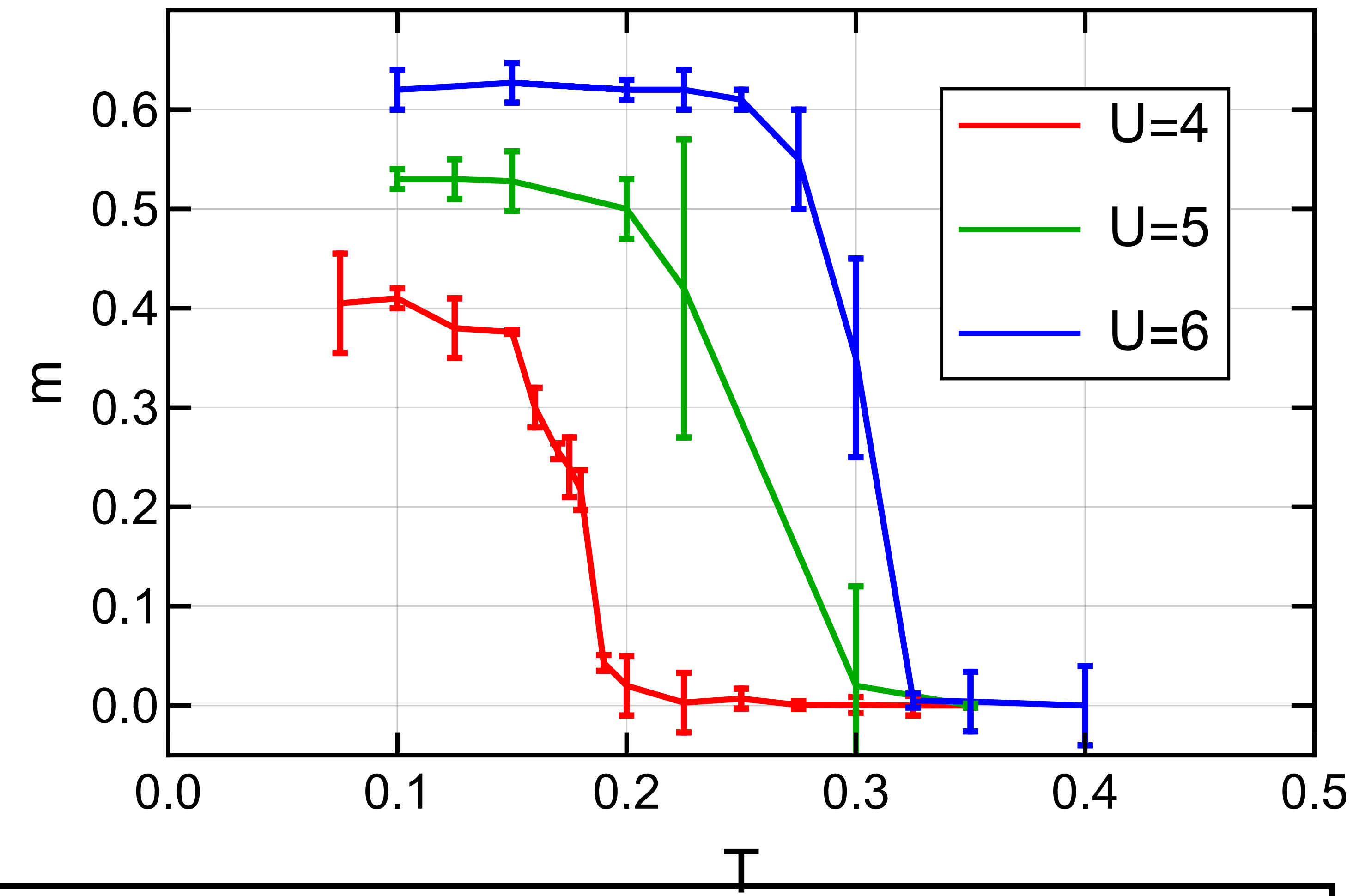
Conclusions and perspective

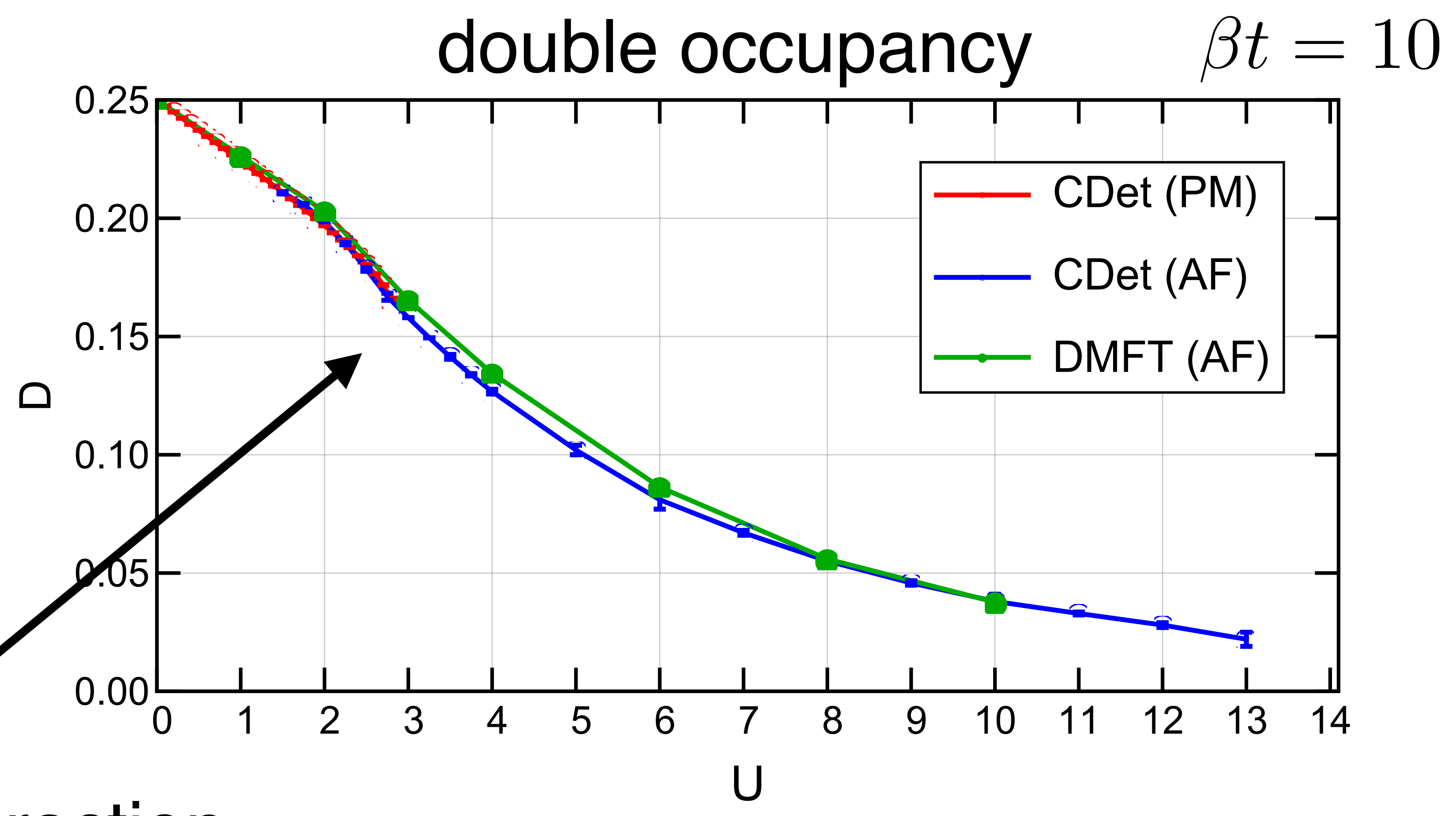
A recipe for the pseudogap

- The pseudogap is sensitive to the fermiology of the non-interacting system
- The sum of 3 ingredients seems to be necessary for the onset of a pseudogap:
  - (Short-range) antiferromagnetic correlations
  - A van Hove singularity
  - The Fermi surface defined by $\epsilon(k) - \mu + \frac{\langle n \rangle}{2} U = 0$ must be close to the vHs
- Not weak-coupling physics!
  - Short correlation length
  - No pseudogap if no van Hove singularity
- Having fine k-resolution is essential to make further progress

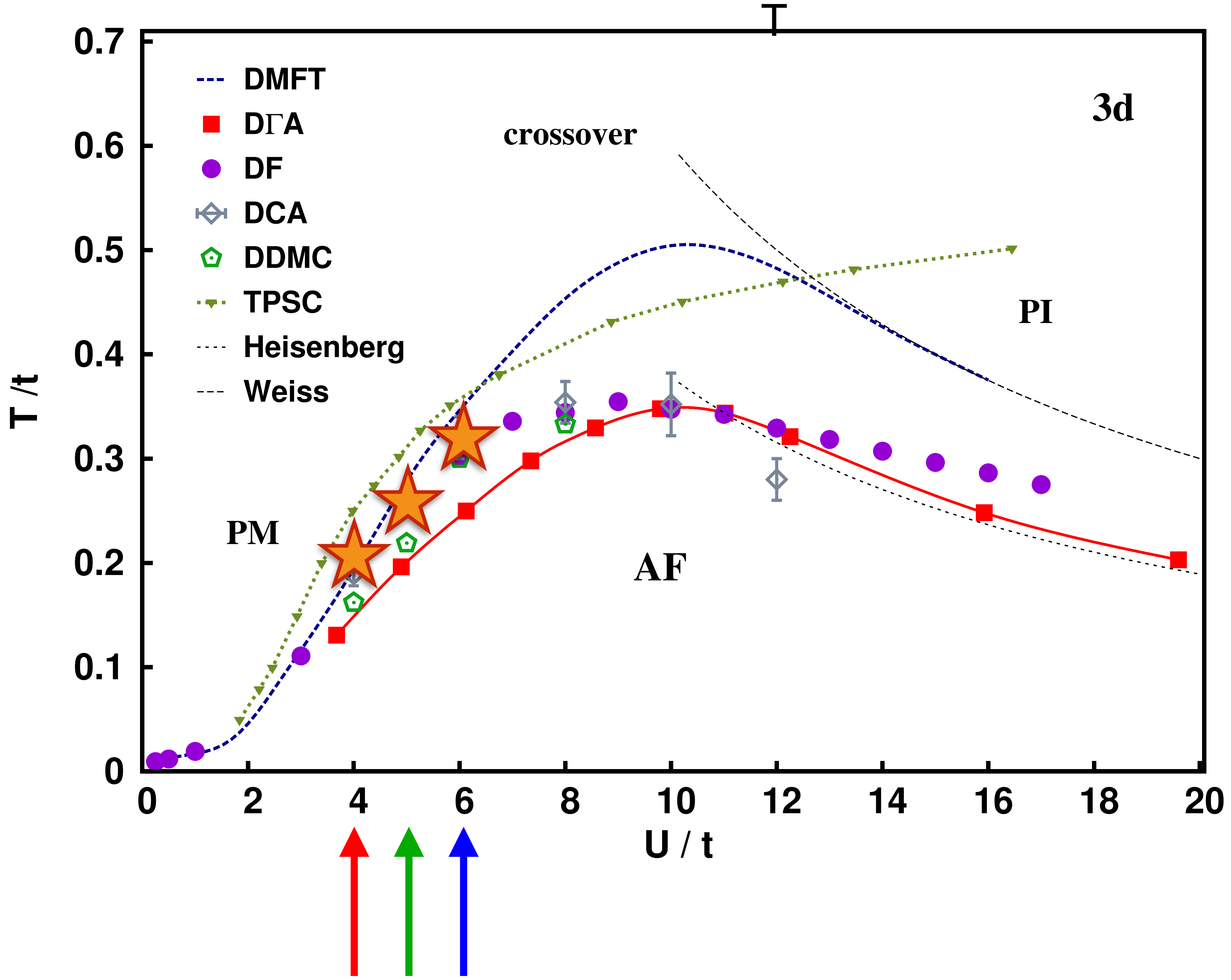
Diagrammatic Monte Carlo: future developments

- Recent efforts:
  - Broken-symmetry phases:
    e.g. AF order in 3D half-filled Hubbard model
  - Better starting points for perturbation series:
    e.g. AF-ordered starting point in 2D half-filled Hubbard model



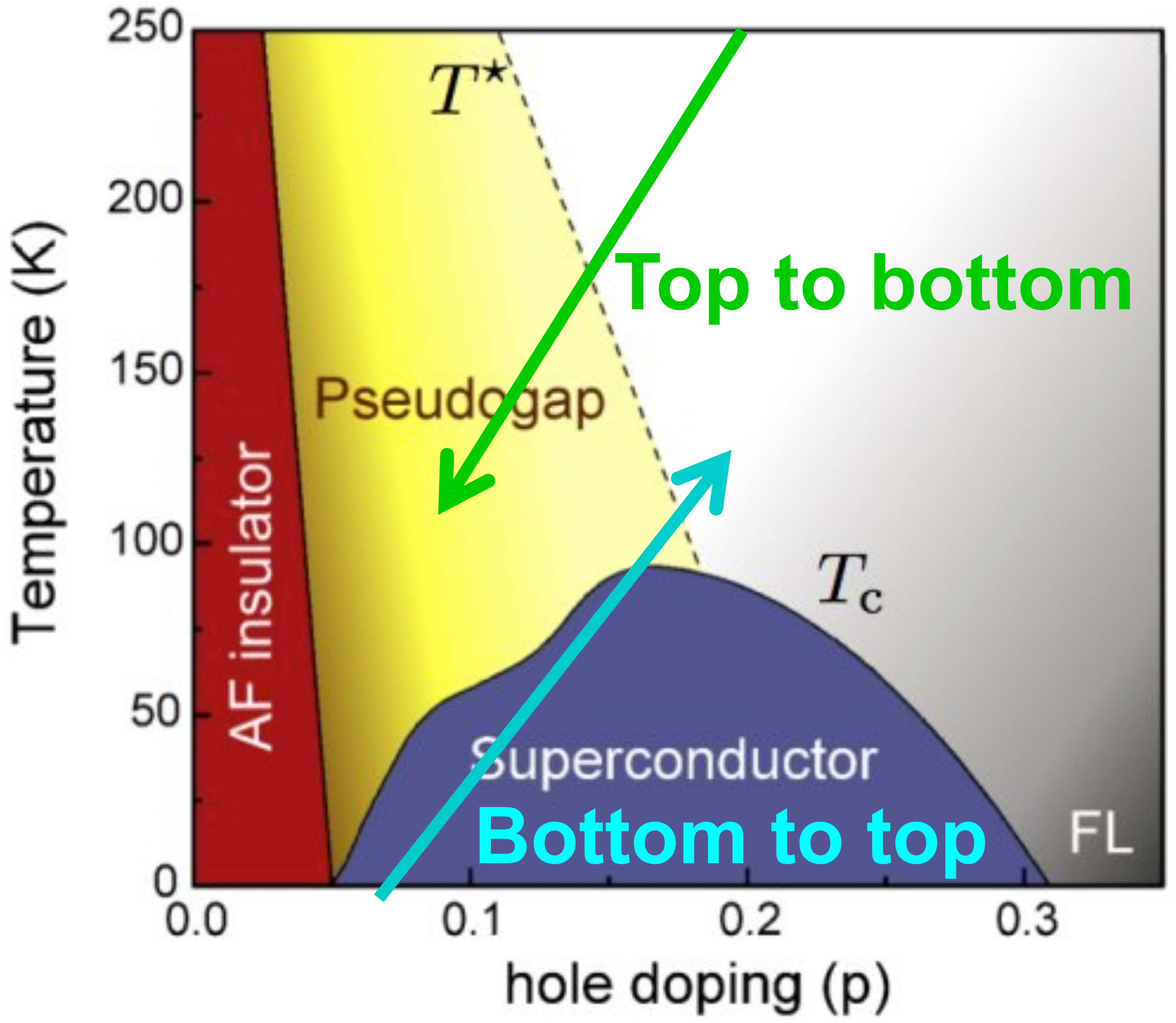


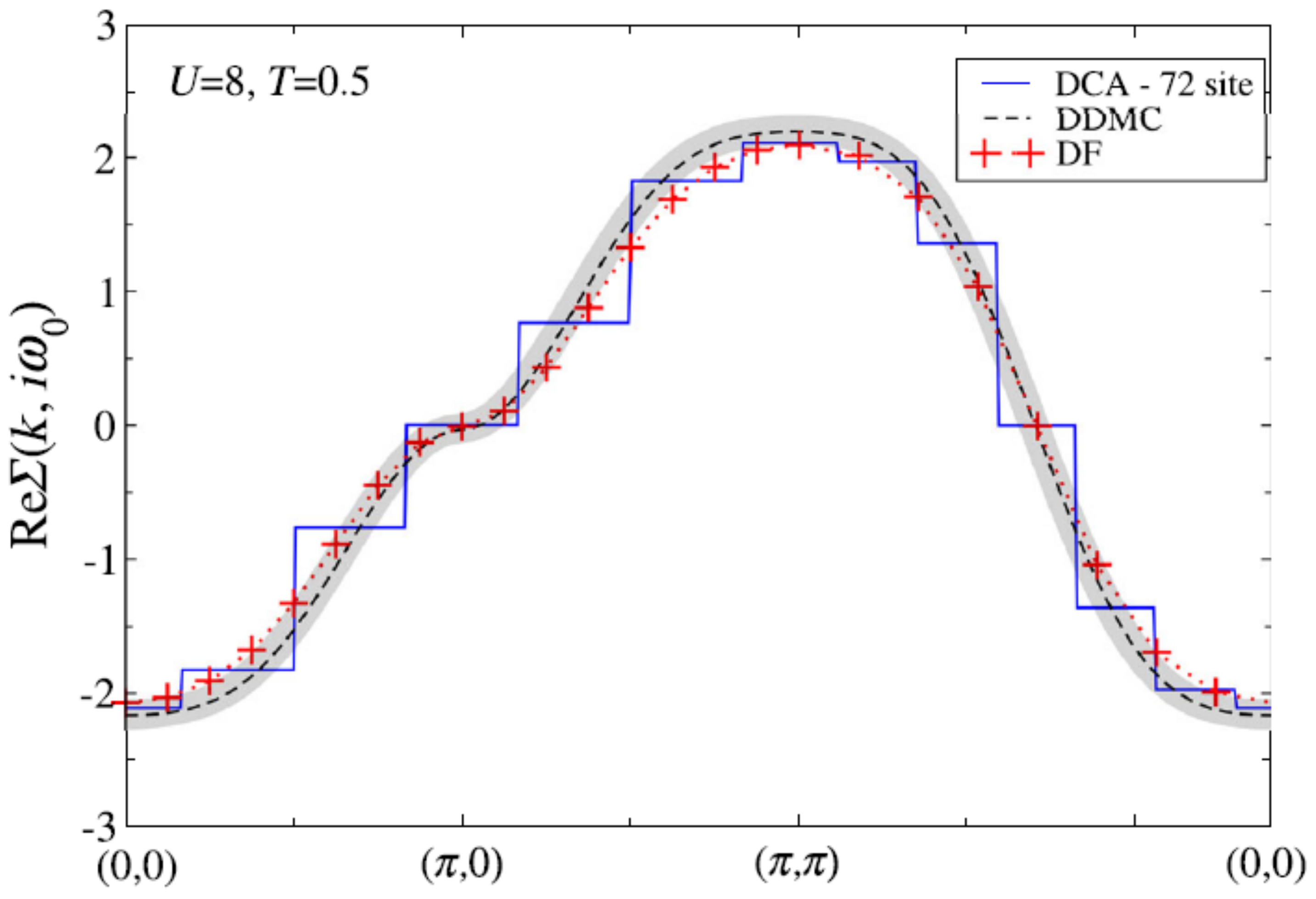
largest interaction
value with standard CDet



Many other approaches to the Hubbard model

- Important progress in computational approaches
- Bottom-to-top: DMRG, PEPS, MERA, METTS, …
  S.R. White, PRL (1992); U. Schollwöck, RMP (2005); F. Verstraete and J. I. Cirac (2004); E.M. Stoudenmire and S.R. White, NJP (2010), …
- Top-to-bottom: DMFT and extensions (cluster DMFT, DΓA, dual fermions, bosons, TRILEX), quantum Monte Carlo (diagMC, CDet, DQMC), …
  A. Georges et al., RMP (1996); T. Maier et al., RMP (2005); N. V. Prokof'ev and B. V. Svistunov, PRL (2007); R. Blankelbacer, D. Scalapino and R.L. Sugar, PRD (1981); A. Toschi et al., PRB (2007); A.N. Rubtsov, PRB (2008); T. Ayral, O. Parcollet, PRB (2015, 2016); R. Rossi, PRL (2017), …
- Agreement in non-trivial regimes
- There are efforts to compare approaches / make them complementary!
  - Benchmarks (e.g. J.P.F. LeBlanc et al., PRX (2015); T. Schäfer et al., in preparation)
  - Shake hands between methods





J.P.F. LeBlanc et. al, PRX (2015)

Putting Modern Many-Body Computations to the Test: a Multi-Messenger, Multi-Method Study of the Half-Filled Two-Dimensional Hubbard Model at Weak Coupling

T. Schäfer[a,b,*], N. Wentzell[c], F. Šimkovic IV[a,b], Y.-Y. He[c,d],
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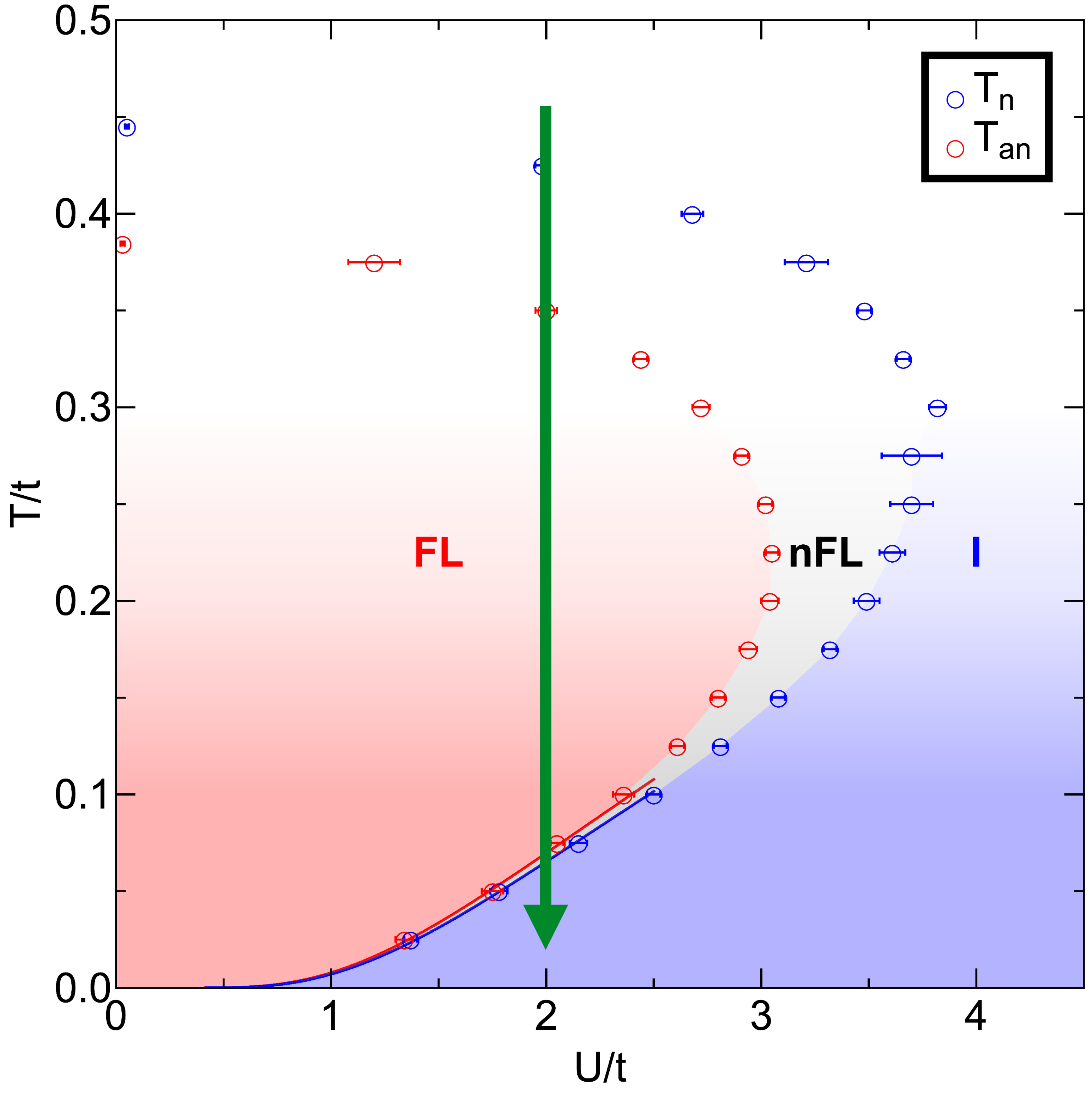
F.-M. Le Régent[b], A. Kirsch[b], Y. Wang[j], A. Kim[k], E. Kozik[k], E. A. Stepanov[i],
A. Kauch[f], S. Andergassen[e], P. Hansmann[l], Y. M. Vilk[j], J. LeBlanc[h],
S. Zhang[c,d], A.-M. Tremblay[j], M. Ferrero[a,b], O. Parcollet[c], and A. Georges[a,b,c,m]



Test parameters

- 2D unfrustrated square lattice
- Half-filled
- U = 2t

Observables (as function of T)

- Coherence temperature T_{QP}
- ”Pseudogap” temperature T_*
- Magnetic susceptibility χ
- Magnetic correlation length ξ
- Double occupancy D

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→ MPI Stuttgart

T. Schäfer et al., in preparation (2020)

Putting many-body methods to the test

Numerically exact techniques

- Diagrammatic Monte Carlo (CDet)
- Lattice quantum Monte Carlo (DQMC)

(Dynamical) mean field theory

- Mean field theory (MFT)
- Dynamical mean field theory (DMFT)

$$\mathcal{H} = -t \sum_{\langle ij \rangle \sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

Extensions of DMFT

Cluster extensions

- Dynamical cluster approximation (DCA)
- cellular DMFT (cDMFT)

Diagrammatic extensions

- Dynamical vertex approximation (DΓA)
- Dual fermion (DF)
- Dual boson (DB)
- Triply irreducible local expansion (TRILEX)

Other common many-body techniques

- Two-particle self-consistent approach (TPSC)
- Functional renormalization group (fRG)
- Parquet approximation (PA)

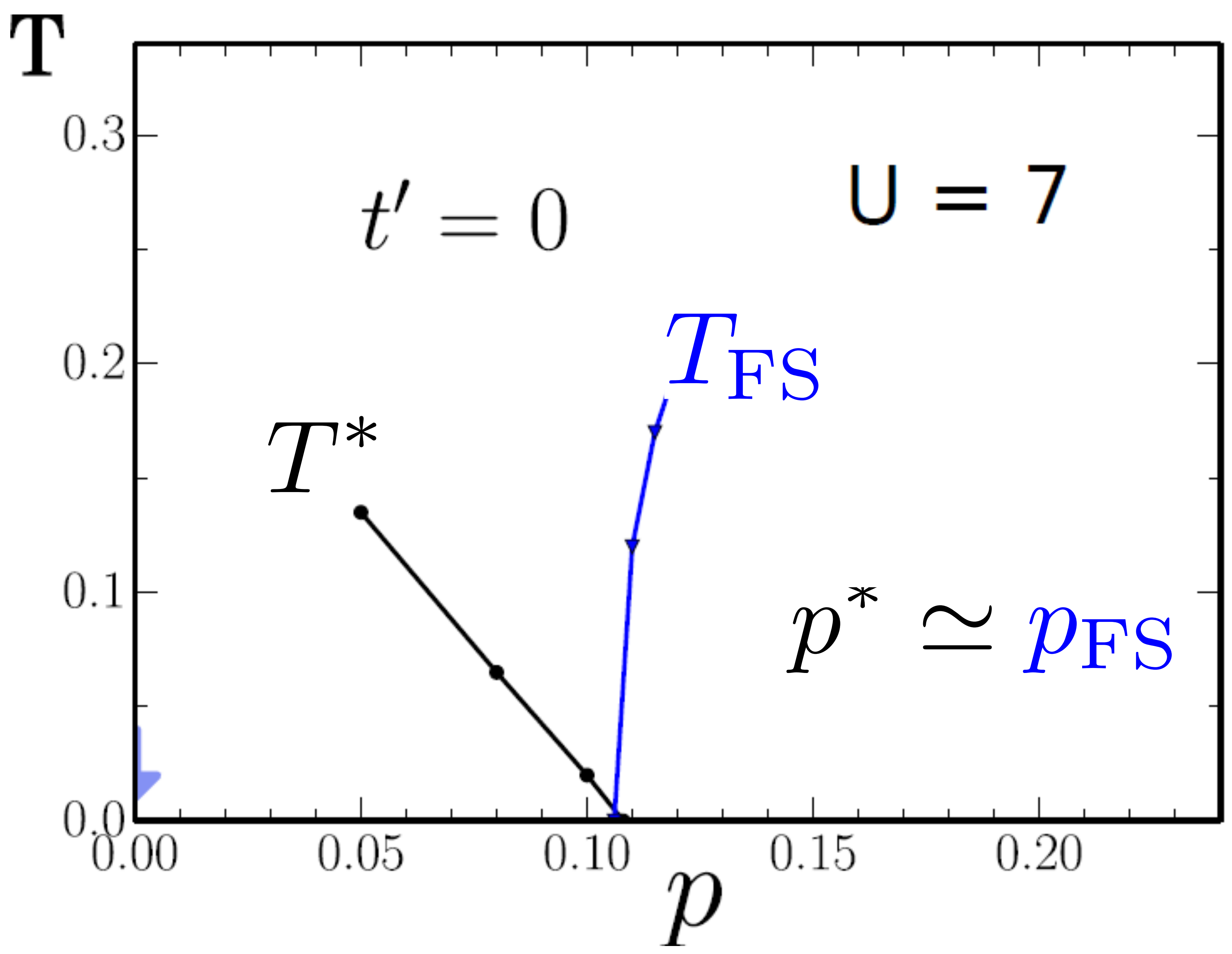
T. Schäfer et al., in preparation (2020)

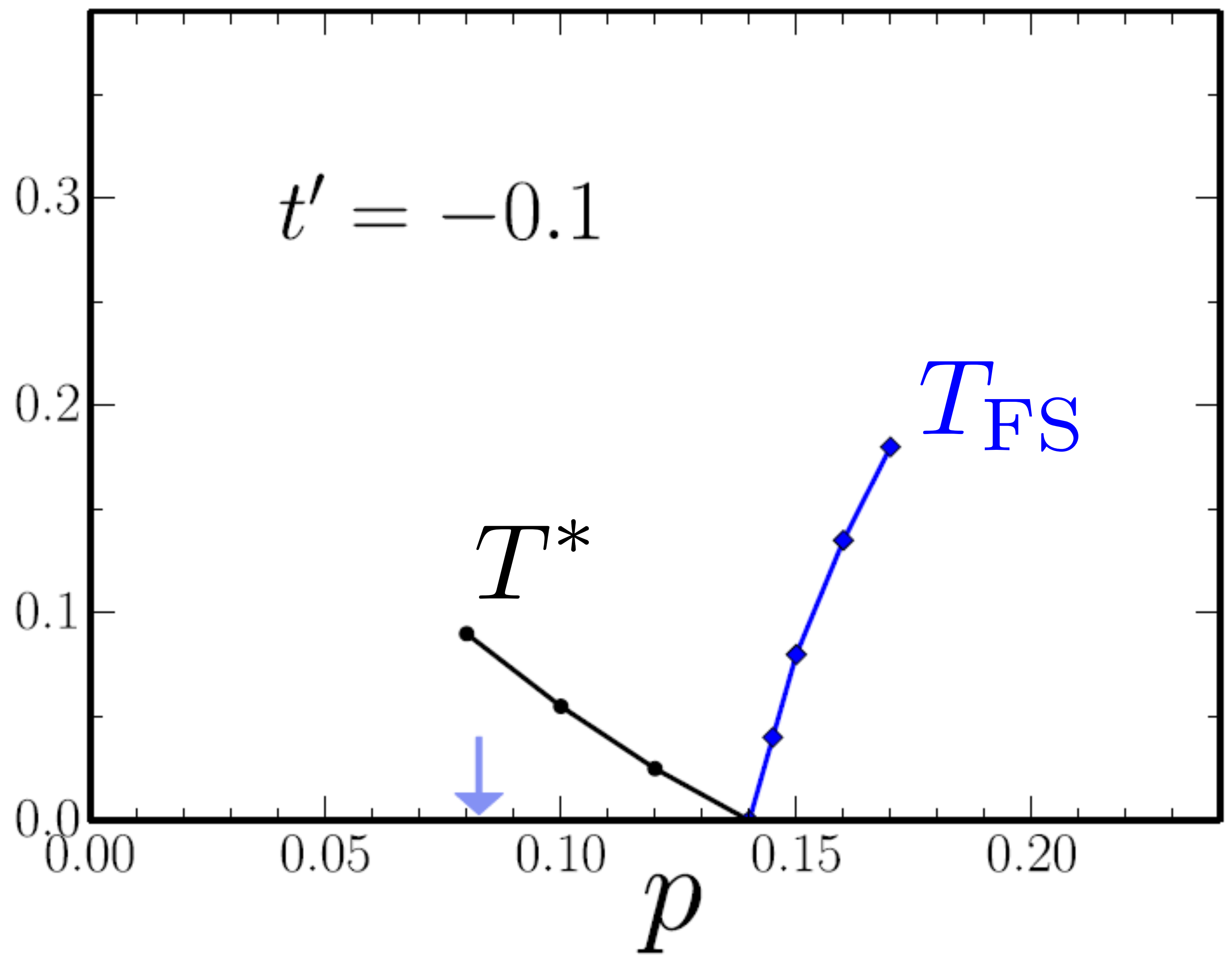
Thank you for your attention!

Supplementary slides:

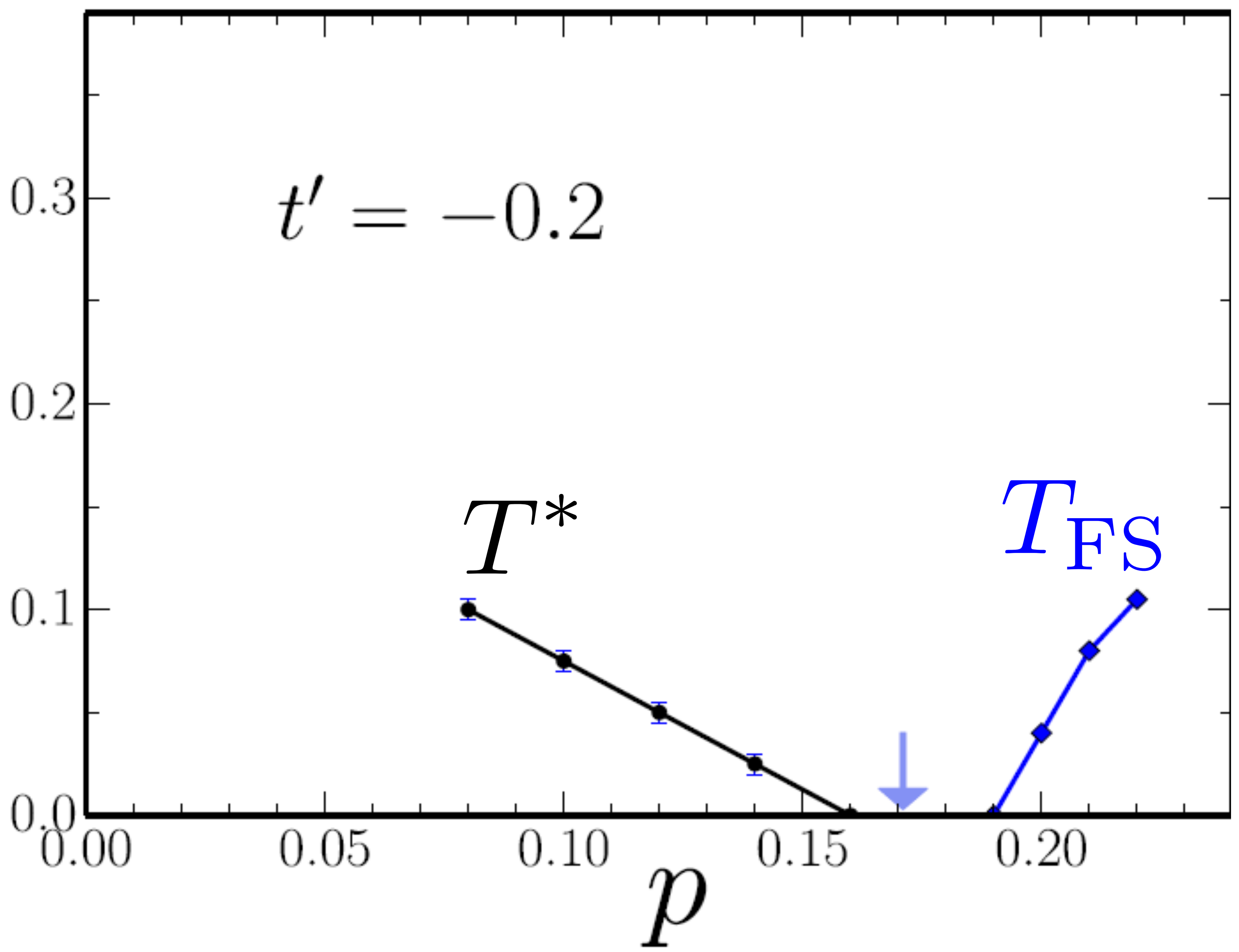
Pseudogap and Fermi surface topology

Pseudogap and Fermi surface topology





$p^* \simeq p_{\rm FS}$



$p^* < p_{\rm FS}$

Blue arrow: location of the Lifshitz transition in non-interacting system

DCA 8 sites calculations

Insights from low-energy effective theory

Sachdev, Metlitski, Qi, Xu, PRB (2009)
M.S. Scheurer et al., PNAS (2017)
W. Wu, A. Georges, MF, PRX (2017)

- We compare results with effective SU(2) gauge field theory
- Describes electrons in environment with fluctuating AF order
- Decomposition of electron fields:

Bosonic spinon

Fermionic chargon

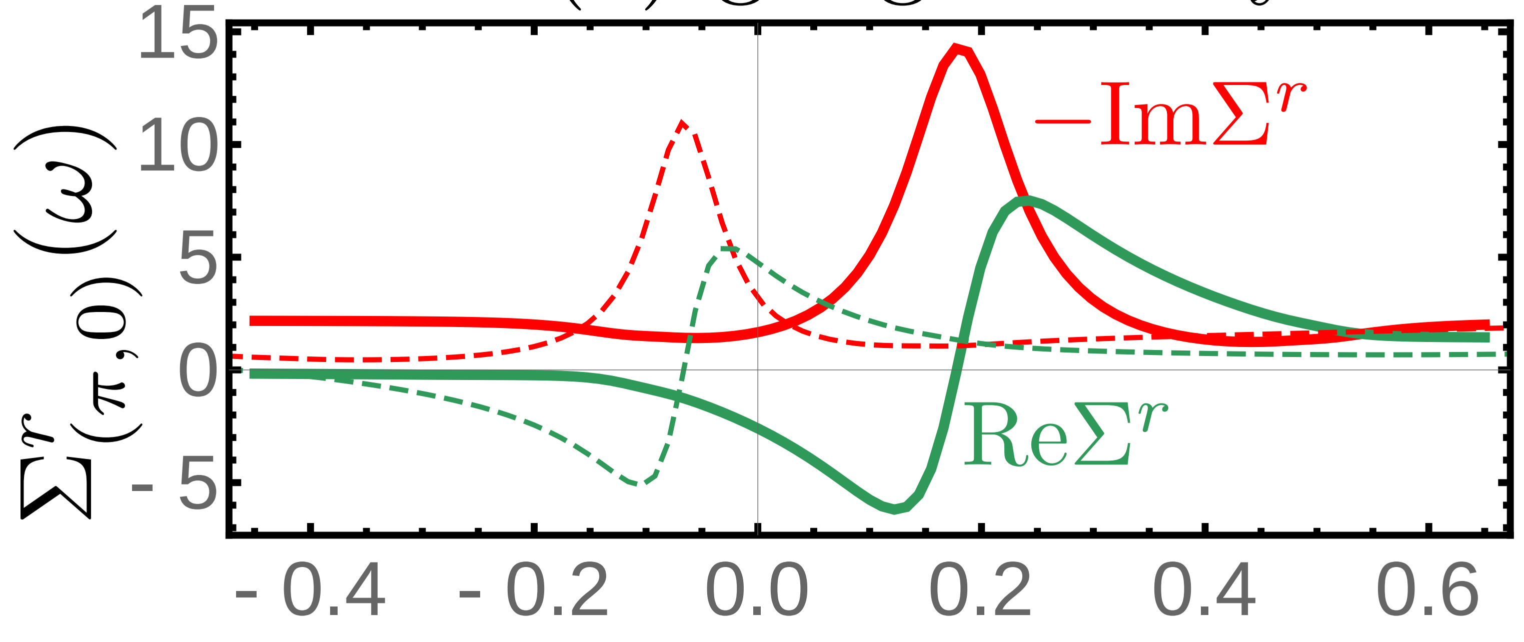
Physical electron

$$\begin{pmatrix} c_\uparrow \\ c_\downarrow \end{pmatrix} = \hat{R} \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix}$$

Introduces local SU(2) gauge invariance

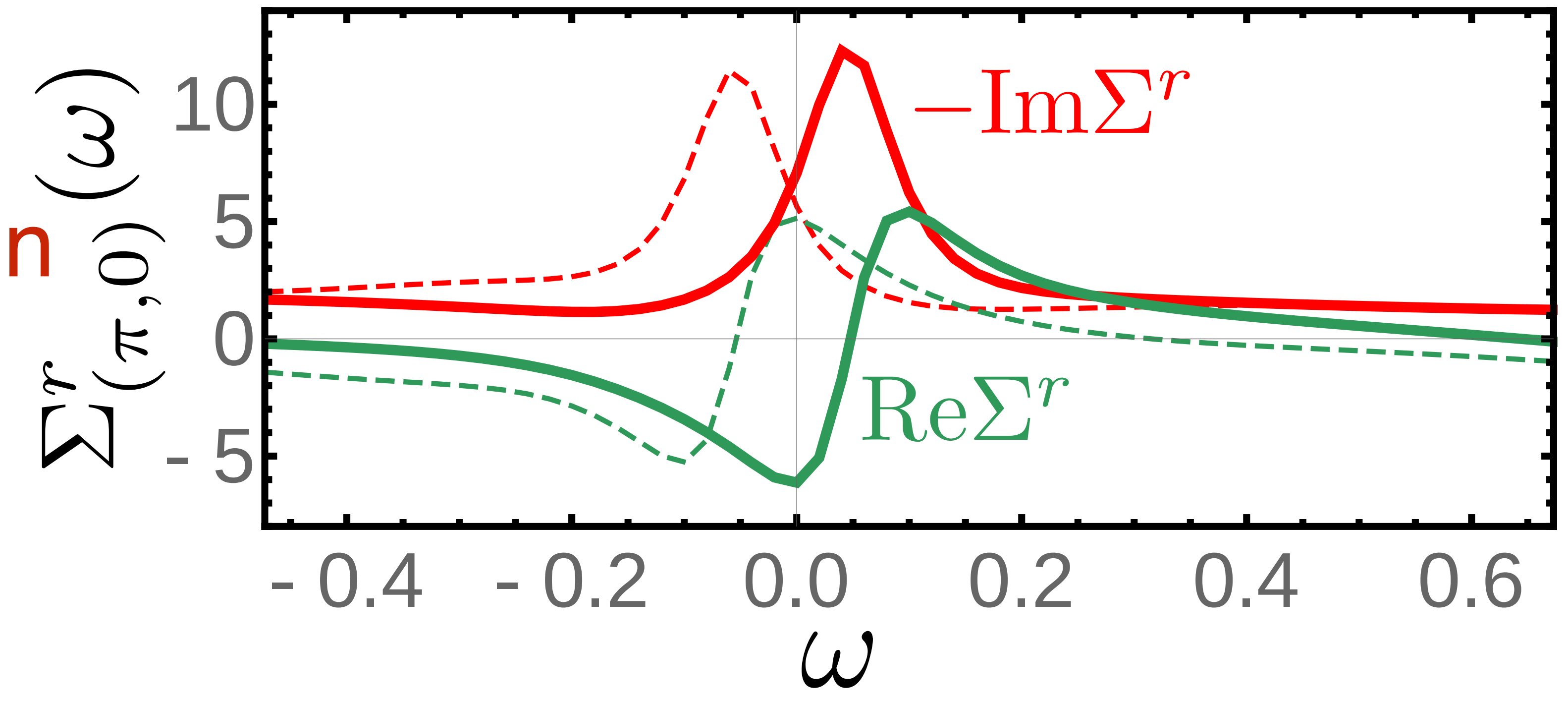
- Treated at mean-field level
- SU(2) symmetry broken while other symmetries are preserved
  → Topological order
- Good agreement with DCA
- Self-energy pole consequence of short-range AF correlations in PG region

SU(2) gauge theory



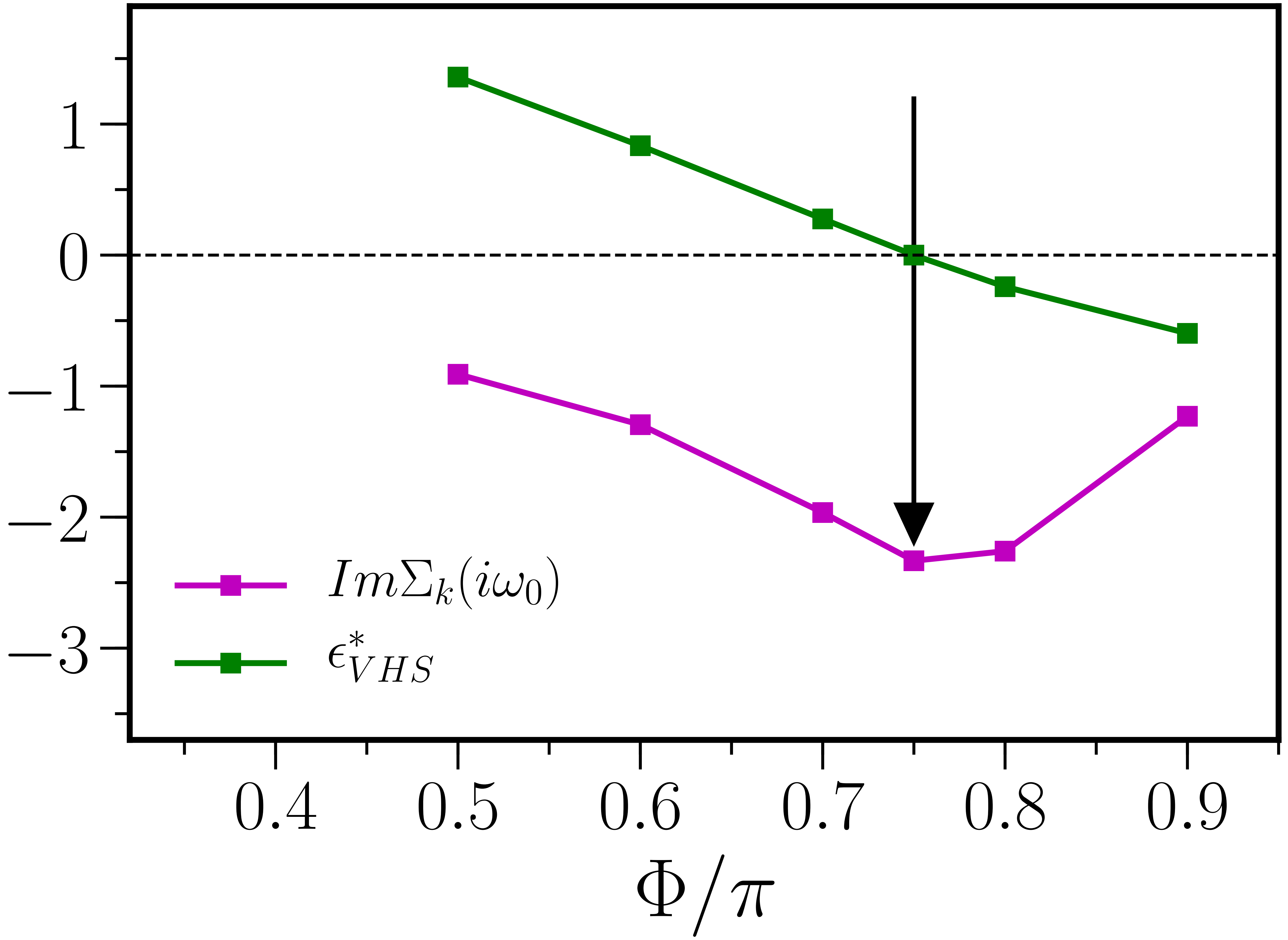
$U = 7, p = 0.05, T = 1/30$

DCA



solid/dashed: different values of t'

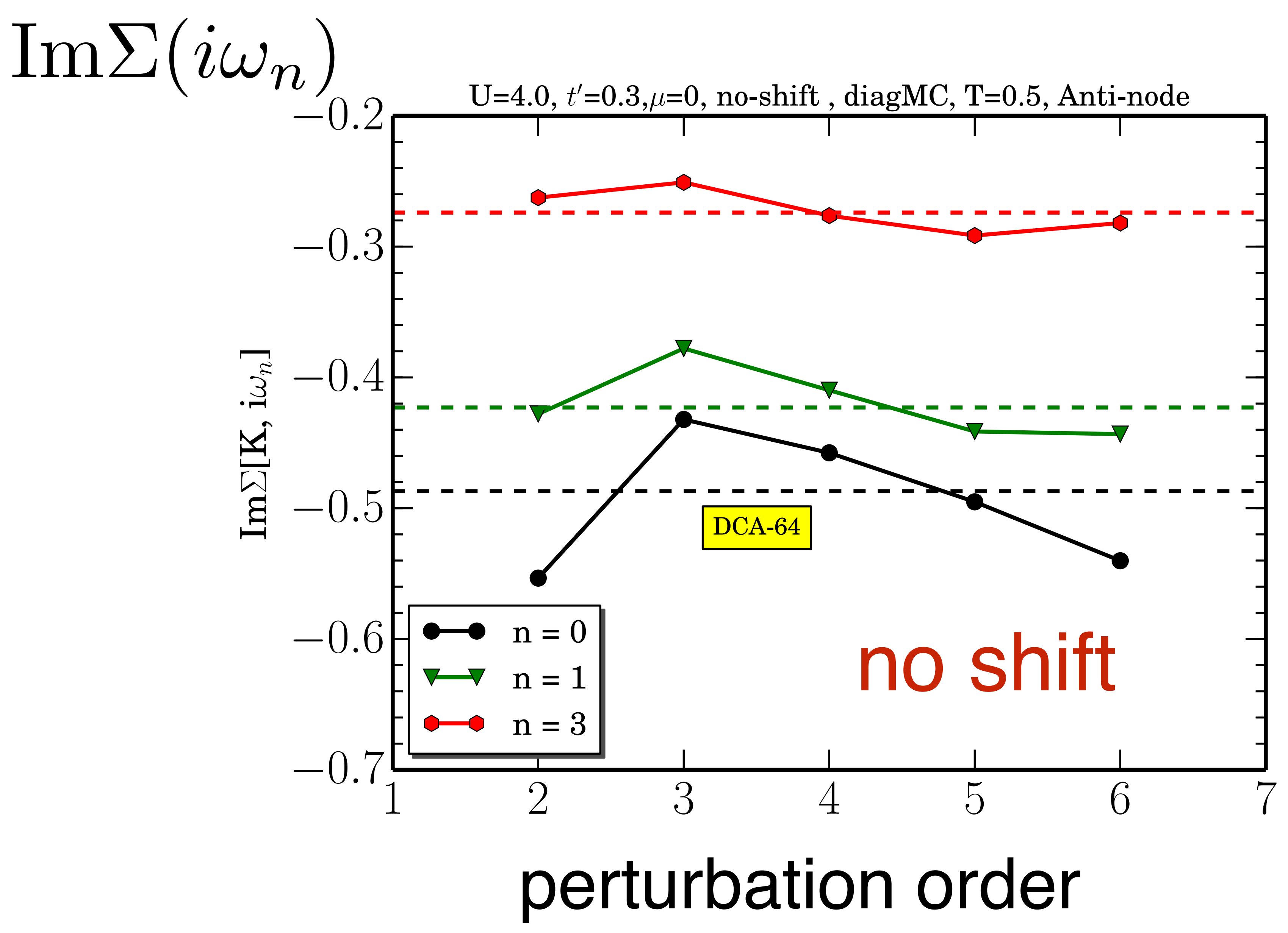
Self-energy versus flux in the triangular lattice

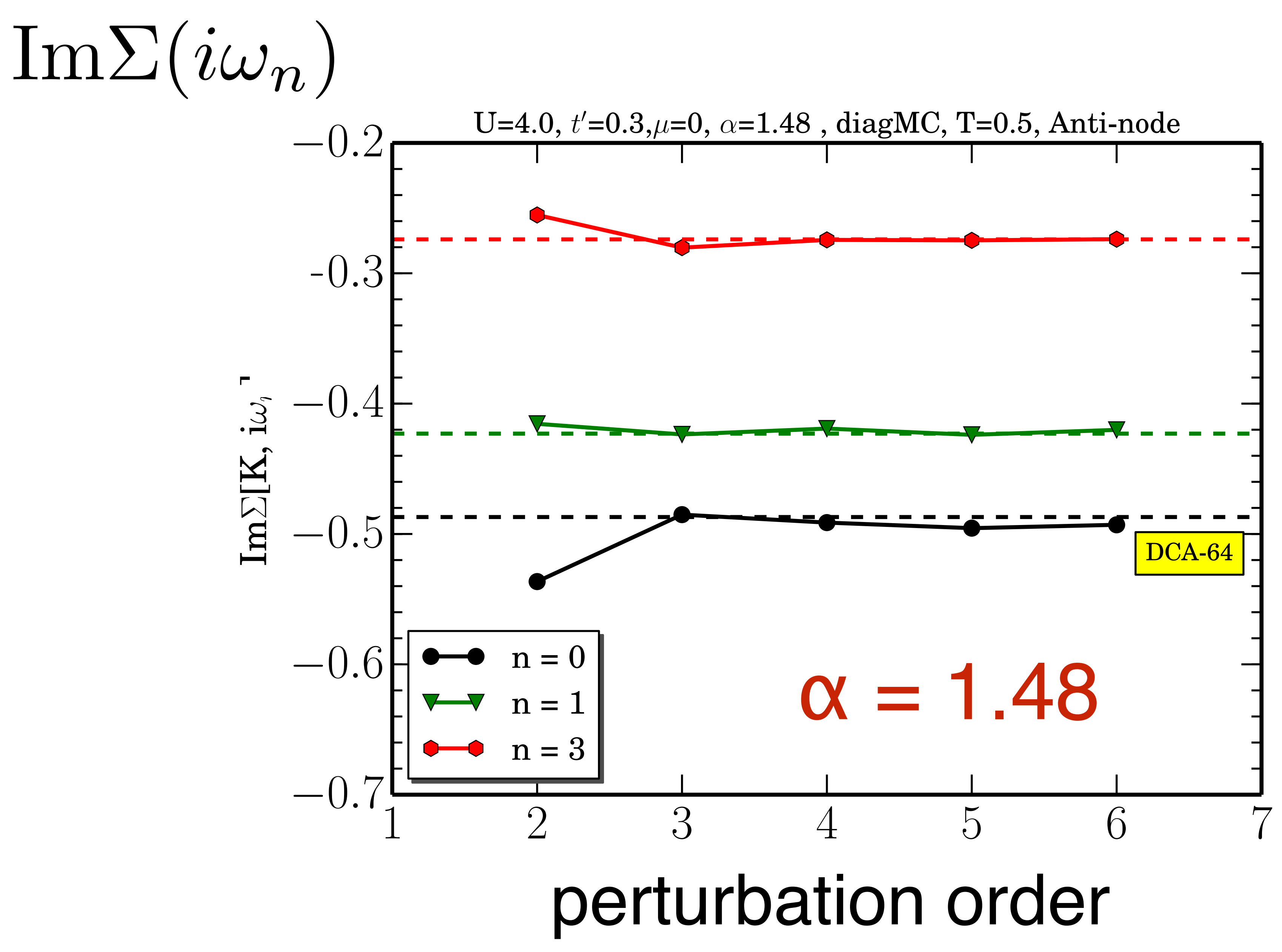


Supplementary slides:
Diagrammatic Monte Carlo

The “chemical potential” shift

- Tuning the shift can lead to much better series





- This static shift is easily implemented within CDet
- Often, a good choice for α is to take a value such that $\tilde{G}_0$ is the static mean-field solution of the problem

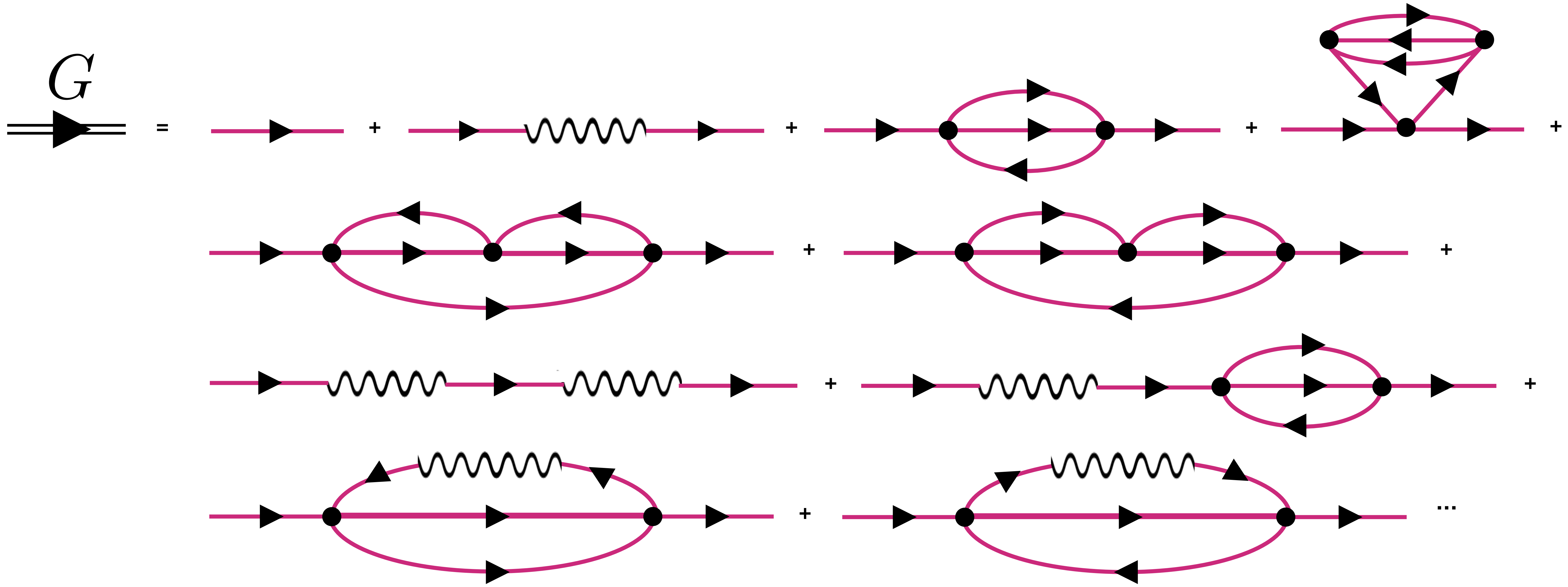
Profumo et al., PRB (2015)
W.Wu et al., PRB (2017)

Renormalized determinant approach (RDet)

- Can the idea be generalized?

$$\hat{G}_0 = \frac{1}{i\omega_n + \mu - \epsilon_k - \alpha - \Delta_k(i\omega)}$$

- Counter terms:



R. Rossi, F. Šimkovic,
M. Ferrero, arXiv (2020)

Renormalized determinant approach (RDet)

- Can the counter terms still be computed with determinants? Yes!

R. Rossi, F. Šimkovic,
M. Ferrero, arXiv (2020)

- What should one put for $\Delta_k(i\omega_n)$?

$$\hat{G}_0 = \frac{1}{i\omega_n + \mu - \epsilon_k - \alpha - \Delta_k(i\omega)}$$

  - A hybridization function with a gap

$$\Delta(U^2) \leftarrow \frac{\tilde{\Delta} U^2}{i\omega_n}$$

We explored several values for $\tilde{\Delta}$

  - Local DMFT self-energy

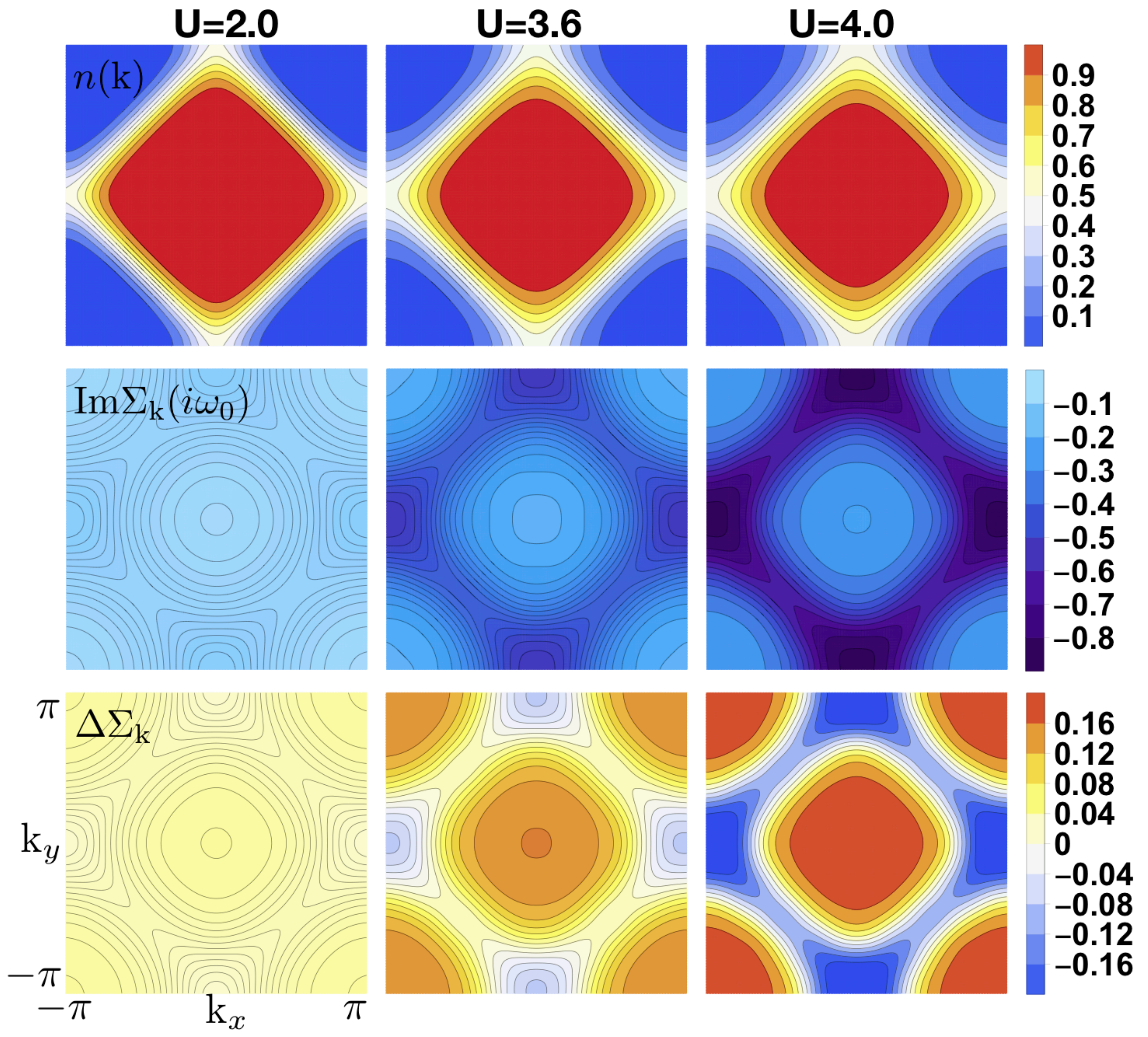
$$\Delta(U^2) \leftarrow \Sigma_{\mathrm{loc}}^{\mathrm{DMFT}}$$

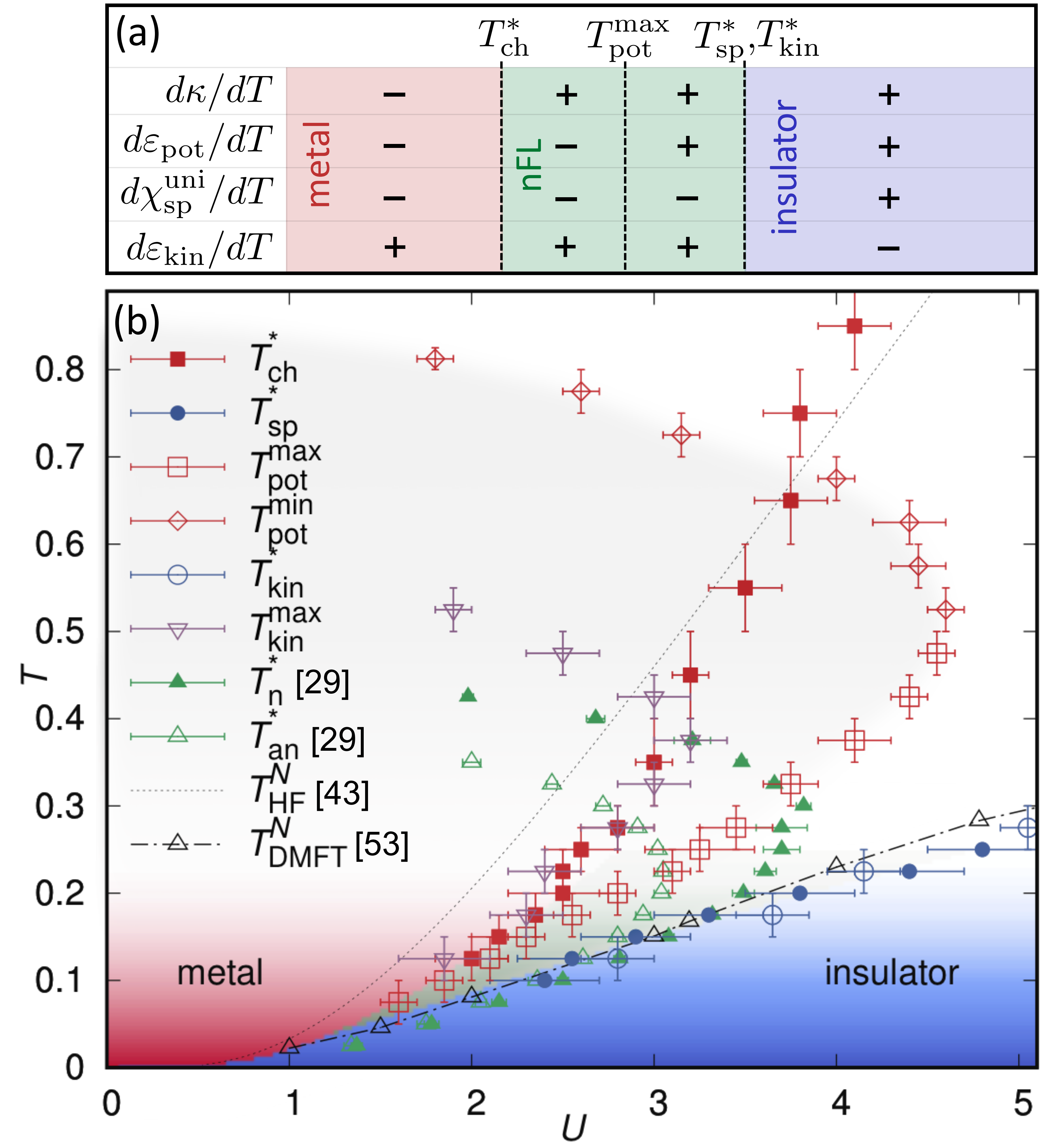
- Observables: density, double occupancy, Green functions, self-energies, etc.

Half-filled Hubbard model

- Crossover documented by many observables

$\beta t = 5$





(a)	metal	nFL		insulator
$d\kappa/dT$	−	+	+	+
$d\varepsilon_{\mathrm{pot}}/dT$	−	−	+	+
$d\chi^{\mathrm{uni}}_{\mathrm{sp}}/dT$	−	−	−	+
$d\varepsilon_{\mathrm{kin}}/dT$	+	+	+	−

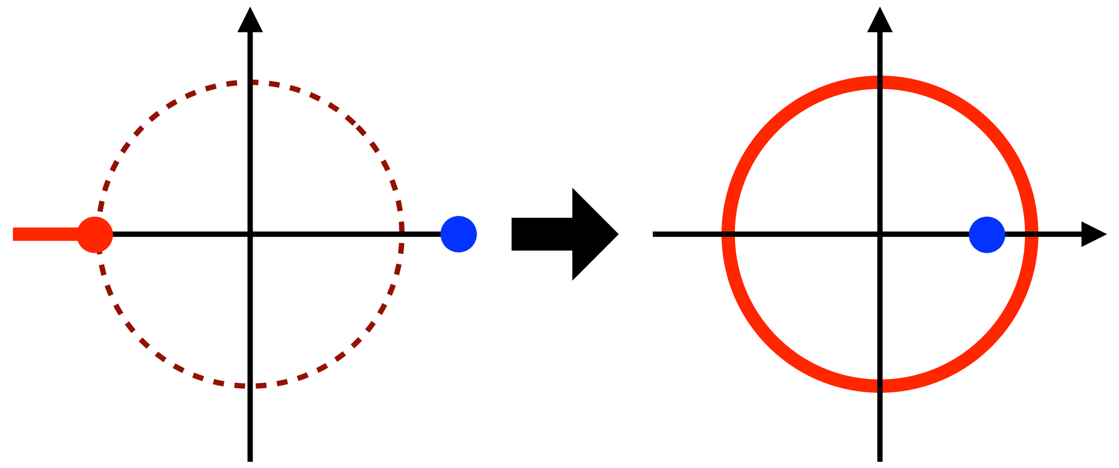
- <u>Limitation</u>: Resummation becomes very hard in incoherent regime despite absence of a true phase transition

F. Šimkovic et al., PRL (2020)
A. Kim et al., PRL (2020)

Freedom of non-interacting propagator

- Series convergence controlled by structure in complex plane
- How do we evaluate the series beyond its convergence radius?

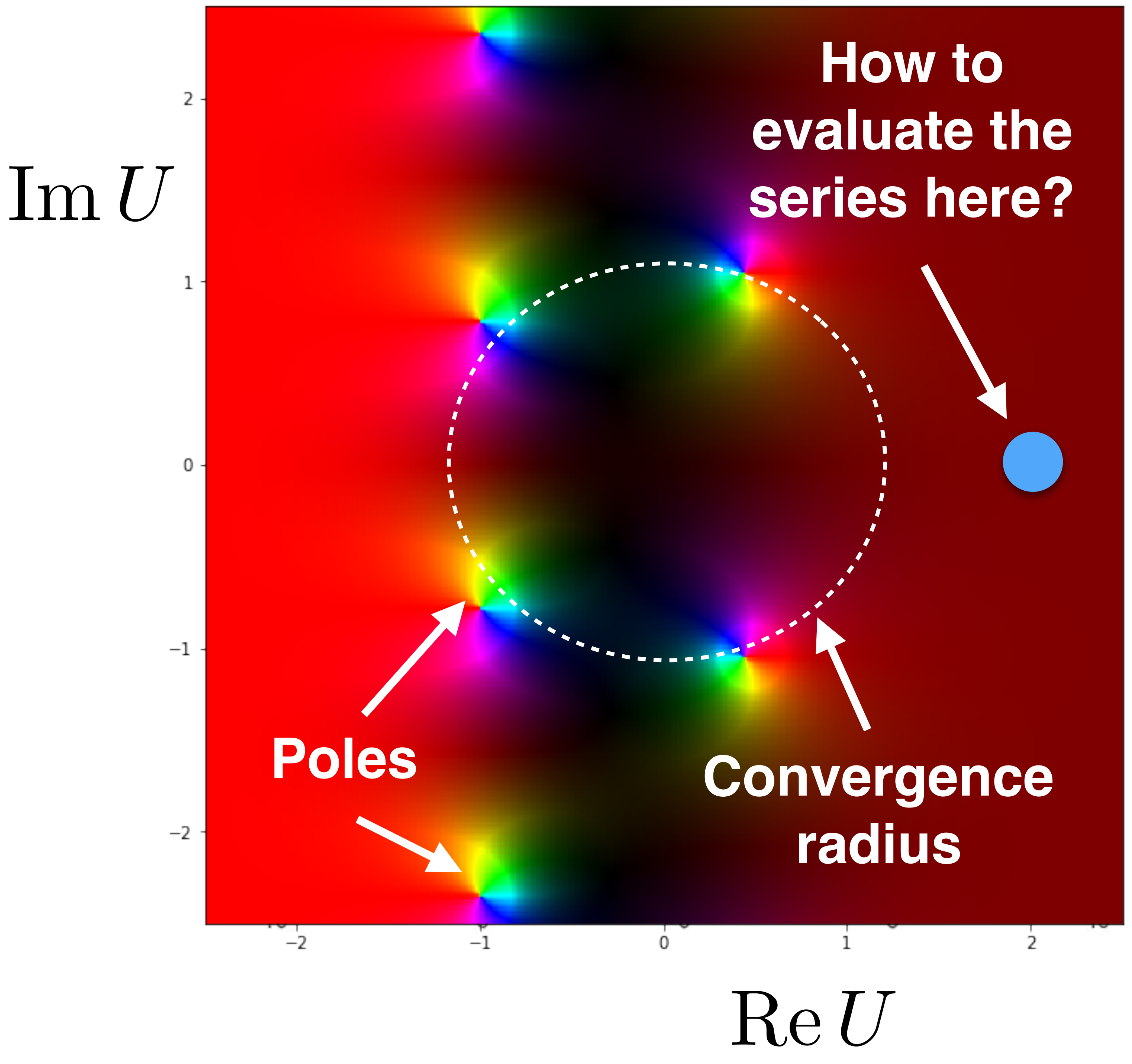
- Approach 1: Conformal maps, Padé approximants, Integral approximants, …



- Approach 2: Generate new series with freedom in the starting point of the perturbation theory

$$G_0 = \frac{1}{i\omega_n + \mu - \epsilon_k} \to \tilde{G}_0 = \frac{1}{i\omega_n + \mu - \epsilon_k - \alpha}$$

$n(U)$ in the Hubbard atom



How to evaluate the series here?

Poles

Convergence radius

R. Profumo et al., PRB (2015)
W. Wu et al., PRB (2017)
F. Šimkovic et al., PRB (2019)
C. Bertrand et al., PRX (2019)