A functional RG perspective on the 2d Hubbard model

Sabine Andergassen

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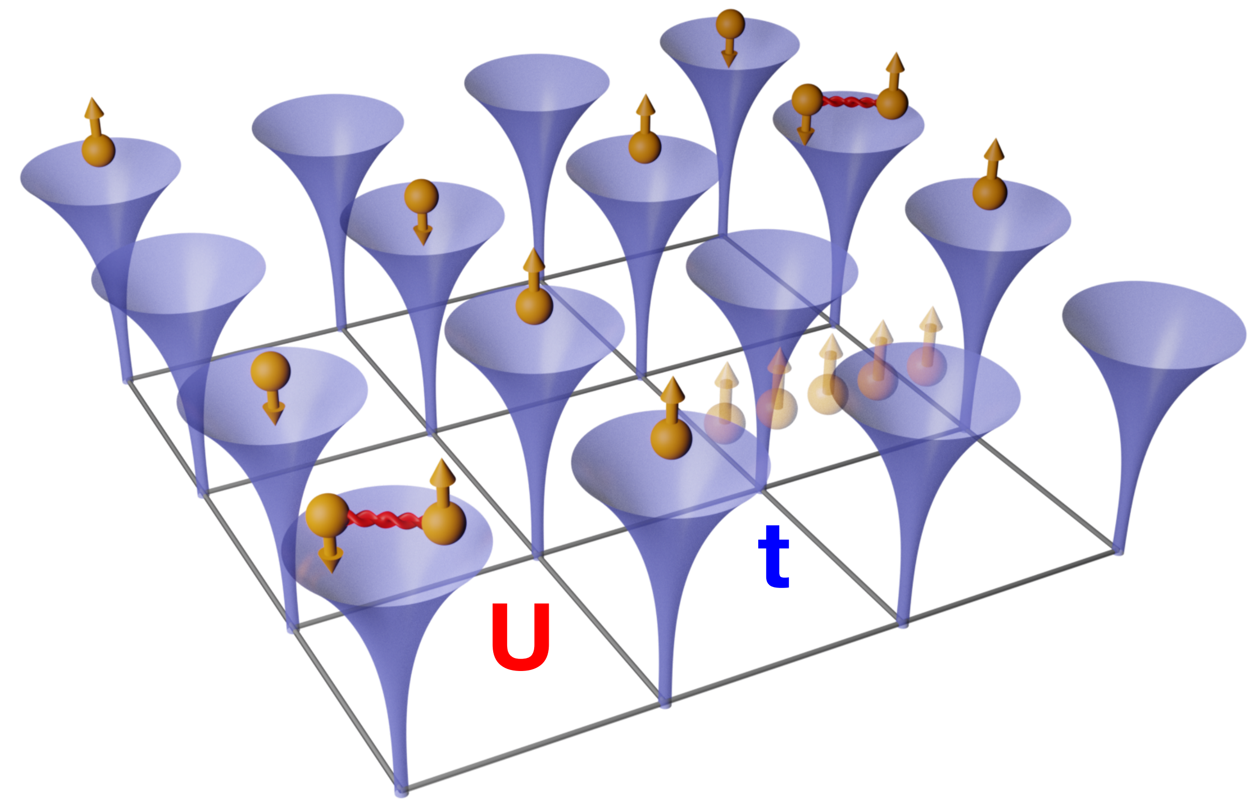
DFG Deutsche Forschungsgemeinschaft

EBERHARD KARLS UNIVERSITÄT TÜBINGEN

The Hubbard model as paradigm model

represents the fundamental model for interacting quantum systems and electronic correlations

$$H = -t \sum_{\langle ij \rangle \sigma} \left(\hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + h.c. \right) + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$



Generalizations and extensions:

- other lattice geometries (in particular honeycomb, triangular, Kagome)
- attractive Hubbard model → Poster by A. Al-Eryani
- multi-orbital models
- models with non-local interactions

Reviews appeared in ARCMP: Arovas *et al.* (2021), and from a computational perspective: Qin *et al.* (2021)

Recent reviews on numerical results (I)

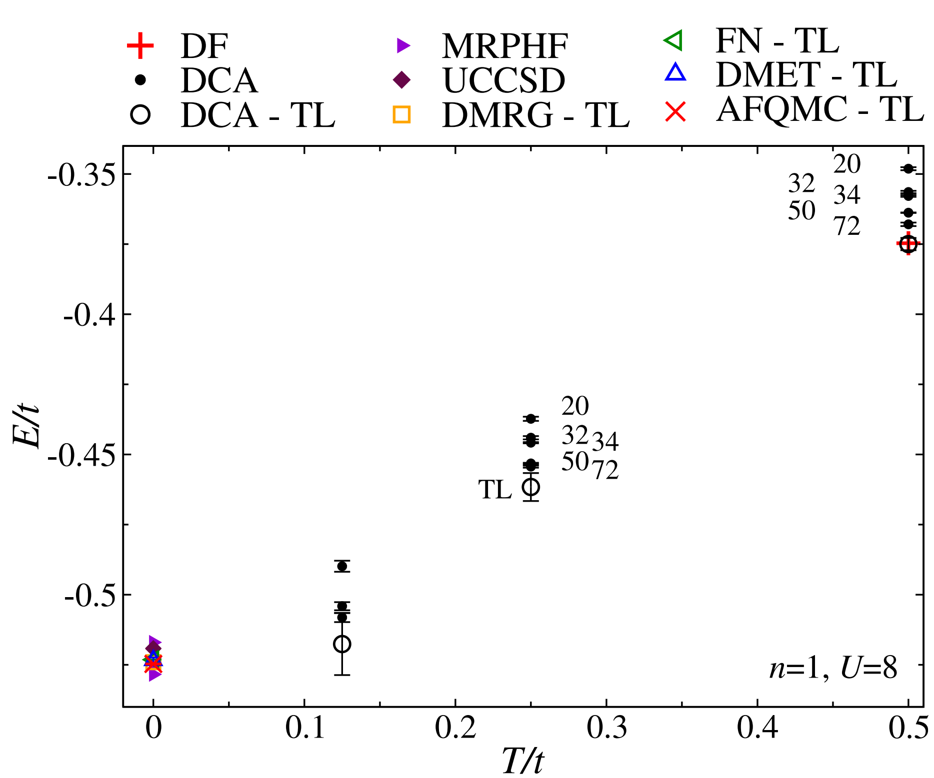
PHYSICAL REVIEW X **5,** 041041 (2015)

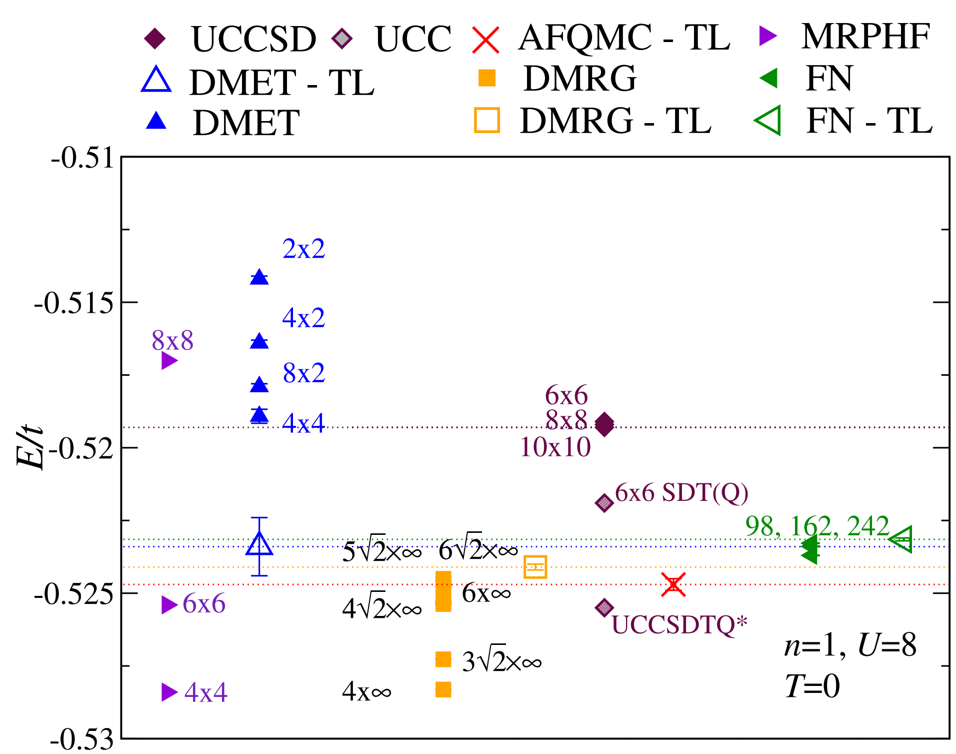
Solutions of the Two-Dimensional Hubbard Model: Benchmarks and Results from a Wide Range of Numerical Algorithms

J. P. F. LeBlanc,[1] Andrey E. Antipov,[1] Federico Becca,[2] Ireneusz W. Bulik,[3] Garnet Kin-Lic Chan,[4] Chia-Min Chung,[5] Youjin Deng,[6] Michel Ferrero,[7] Thomas M. Henderson,[3,8] Carlos A. Jiménez-Hoyos,[3] E. Kozik,[9] Xuan-Wen Liu,[6] Andrew J. Millis,[10] N. V. Prokof'ev,[11,12] Mingpu Qin,[13] Gustavo E. Scuseria,[3,8] Hao Shi,[13] B. V. Svistunov,[11,12] Luca F. Tocchio,[2] I. S. Tupitsyn,[11] Steven R. White,[5] Shiwei Zhang,[13] Bo-Xiao Zheng,[4] Zhenyue Zhu,[5] and Emanuel Gull[1,*]

ground-state and excited-state properties

(energies, double occupancies, and Matsubara self-energies) in various regimes





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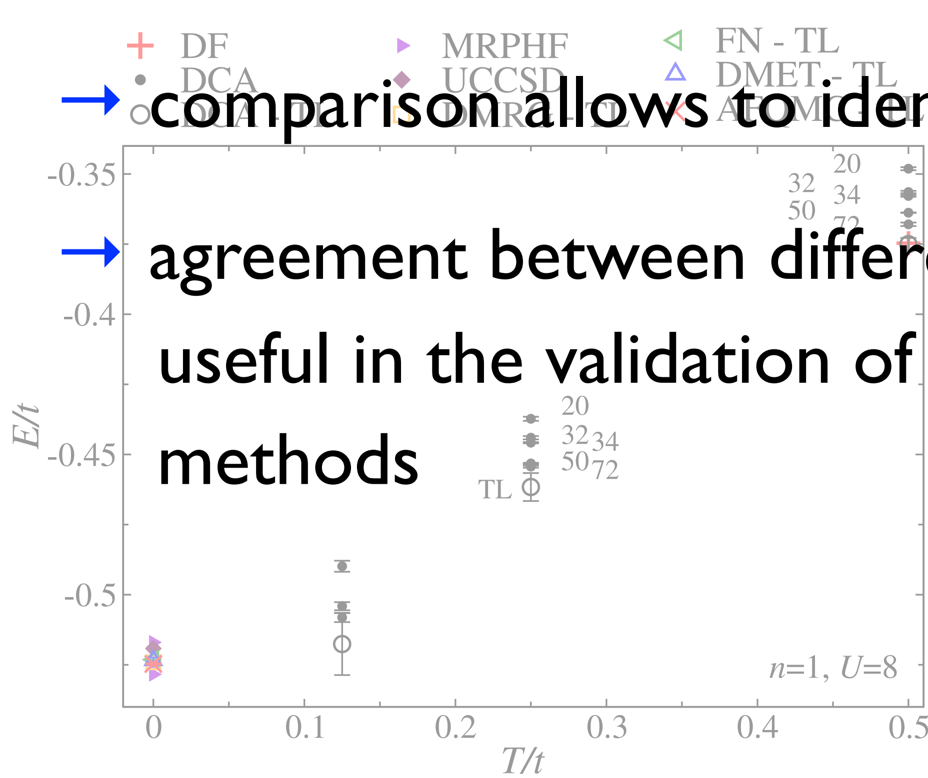
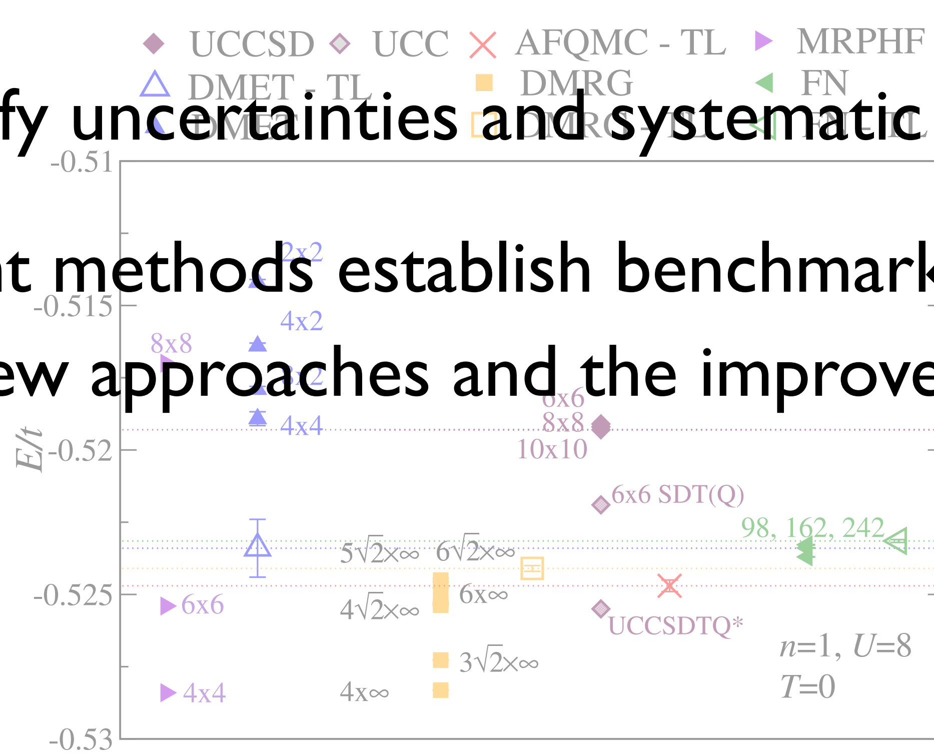
ground-state and excited-state properties
(energies, double occupancies, and Matsubara self-energies) in various regimes

→ comparison allows to identify uncertainties and systematic errors

→ agreement between different methods establish benchmark results, useful in the validation of new approaches and the improvement of existing methods





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Conclusion:

- all methods have difficulty in physically interesting intermediate coupling regime, close to half-filling

- understanding of dynamical correlation functions much less advanced than of ground-state properties

"Development of new methods, or improvement of existing methods to deal with this regime, is urgently needed."

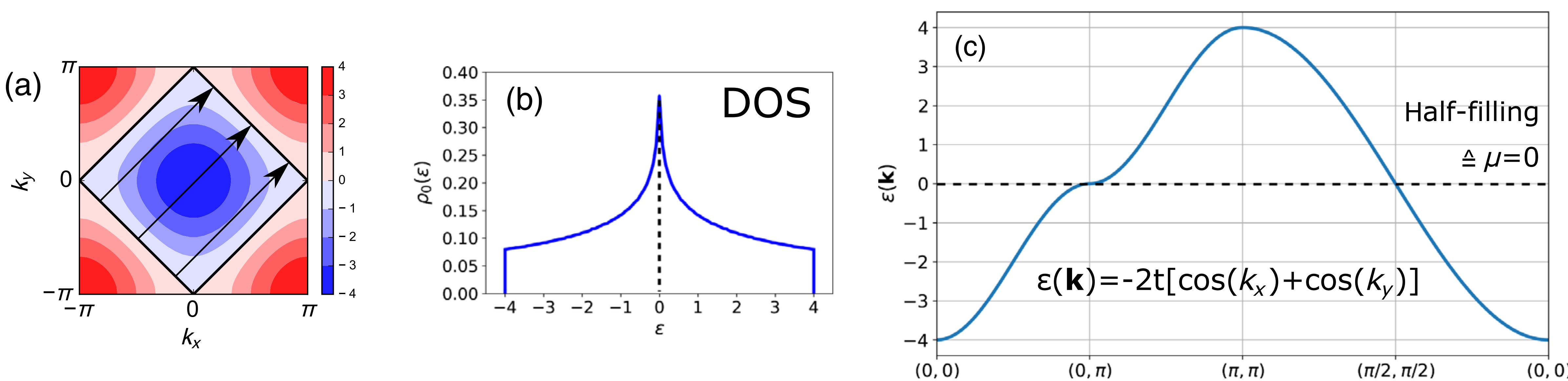
Recent reviews on numerical results (II)

PHYSICAL REVIEW X **11,** 011058 (2021)

Tracking the Footprints of Spin Fluctuations: A MultiMethod, MultiMessenger Study of the Two-Dimensional Hubbard Model

Thomas Schäfer[1,2,3,*] Nils Wentzell[4] Fedor Šimkovic IV,[1,2] Yuan-Yao He,[4,5] Cornelia Hille[6] Marcel Klett,[6,3] Christian J. Eckhardt[7,8] Behnam Arzhang,[9] Viktor Harkov[10,11] François-Marie Le Régent[2] Alfred Kirsch,[2] Yan Wang,[12] Aaram J. Kim[13] Evgeny Kozik[13] Evgeny A. Stepanov[10] Anna Kauch[7] Sabine Andergassen[6] Philipp Hansmann[14,15] Daniel Rohe[16] Yuri M. Vilk,[12] James P. F. LeBlanc[9] Shiwei Zhang[4,5] A.-M. S. Tremblay[12] Michel Ferrero[1,2] Olivier Parcollet[4,17] and Antoine Georges[1,2,4,18]

half-filled Hubbard model at ***weak coupling*** as testing ground



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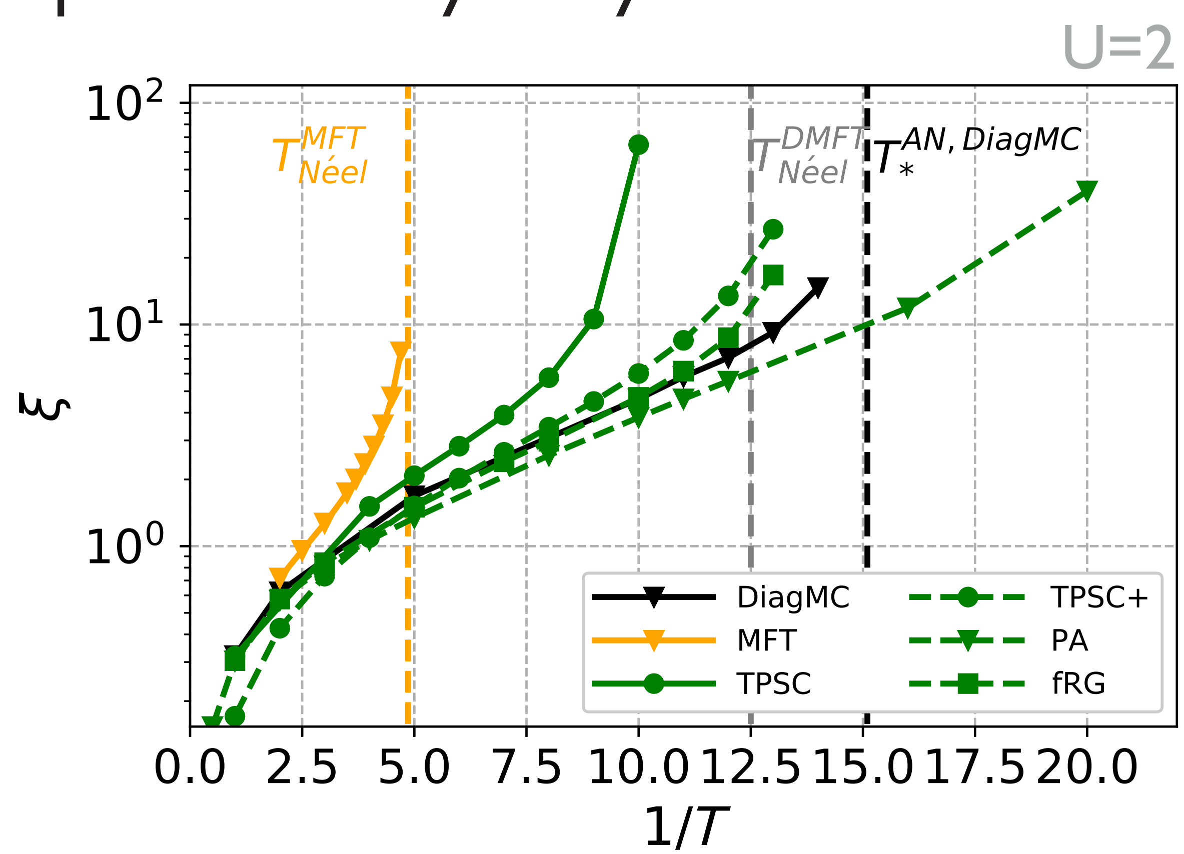
half-filled Hubbard model at ***weak coupling*** as testing ground

→ comparative study of state-of-the-art quantum many-body methods:

- benchmark methods (dQMC)
- (dynamical) mean-field methods
- cluster extensions of DMFT
- vertex-based extensions of DMFT
- other approaches (TPSC, fRG, PA)



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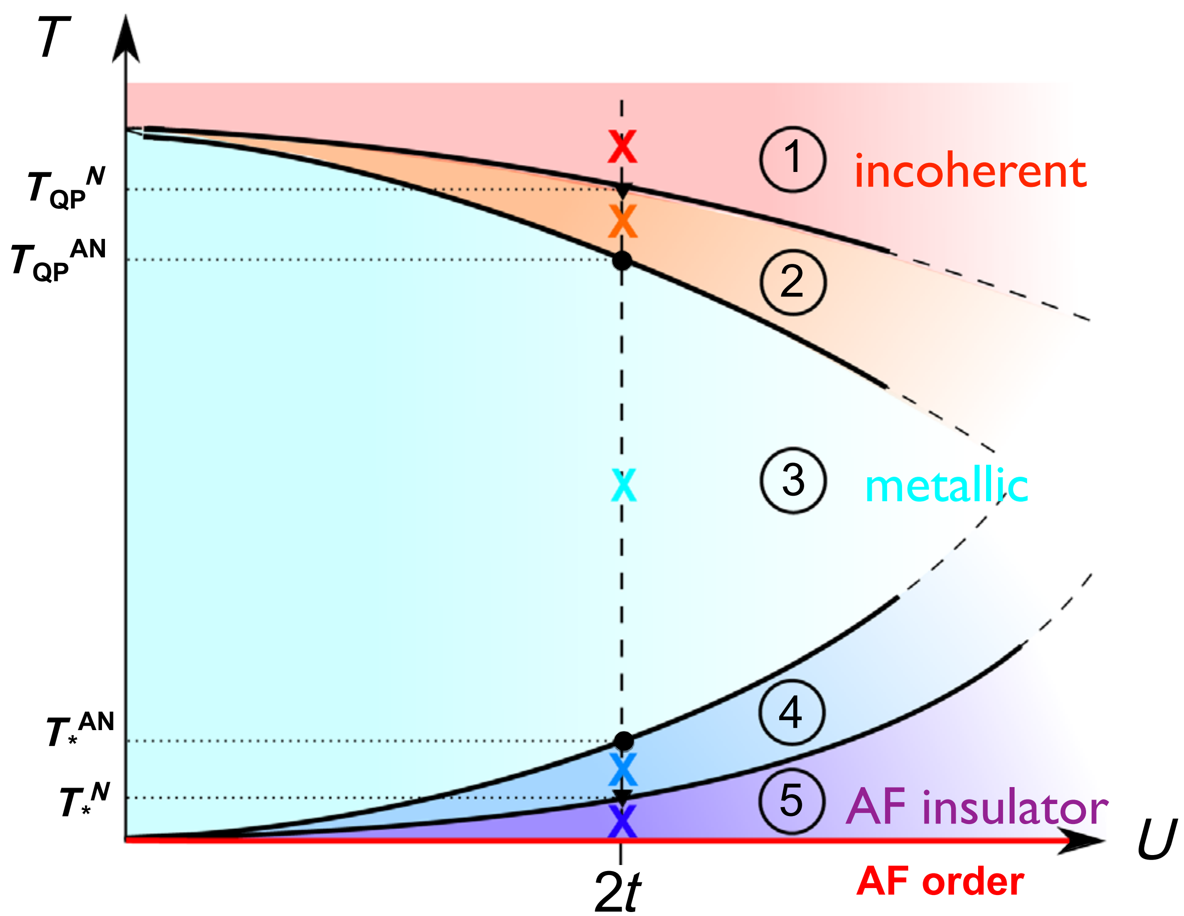

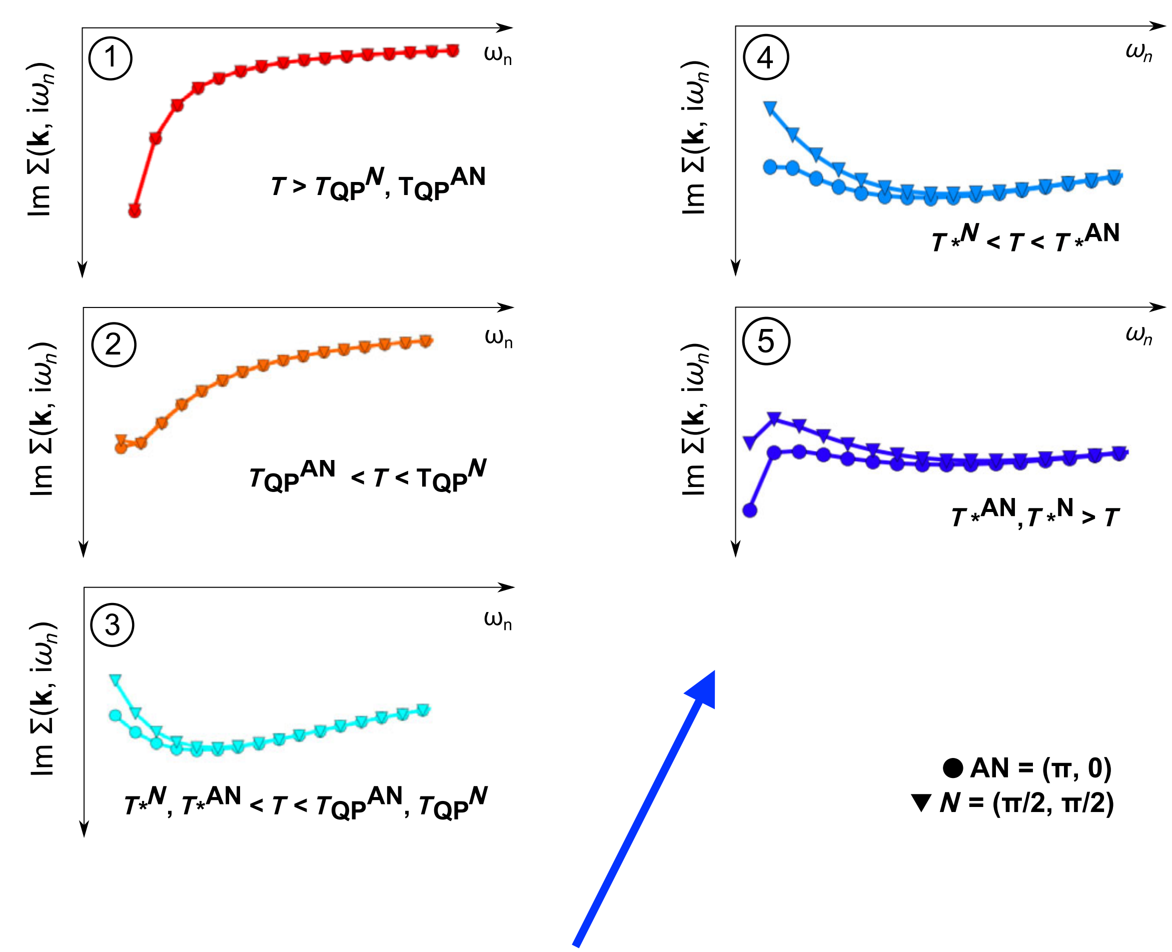

pseudogap opening due to AF fluctuations

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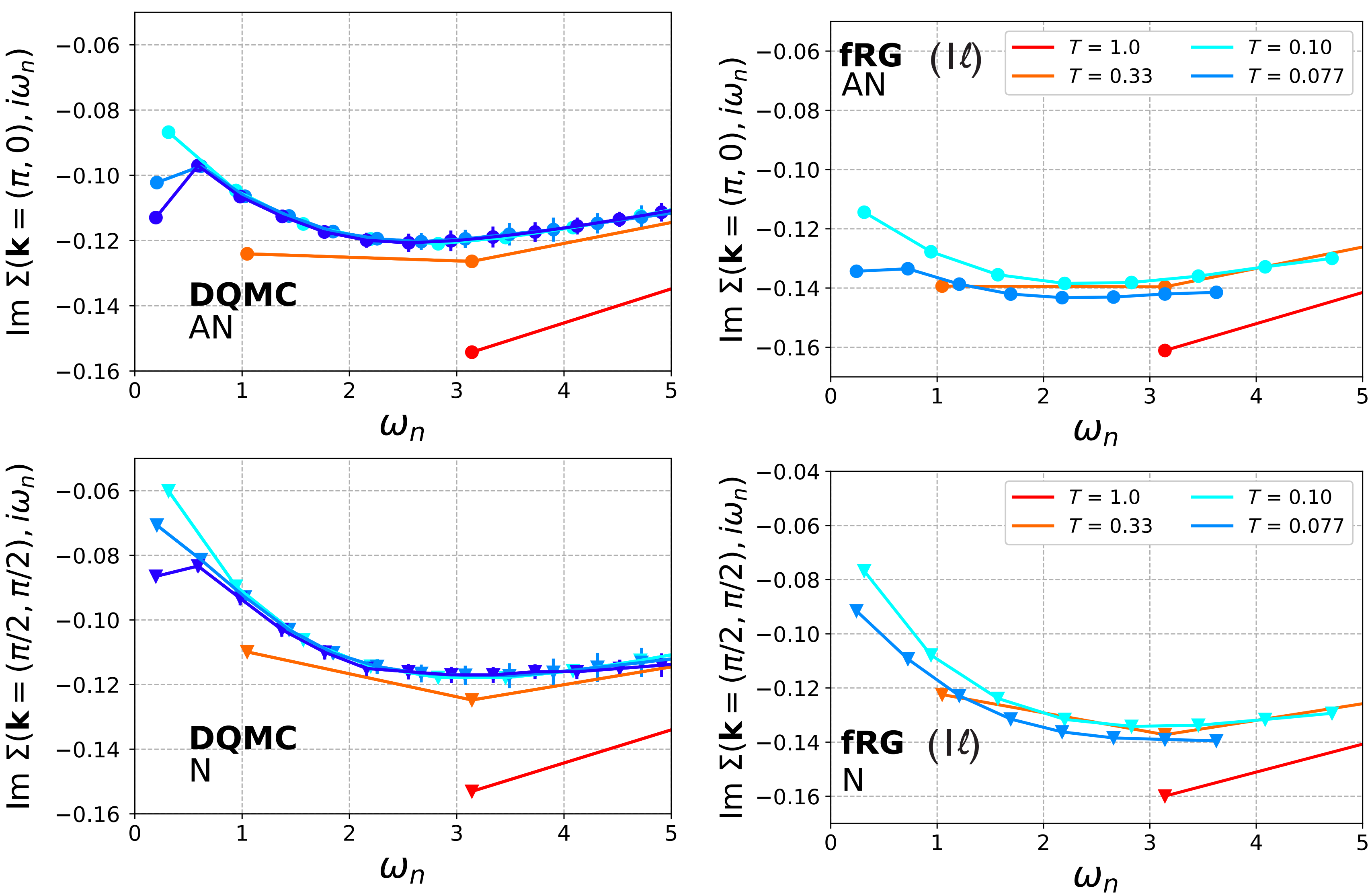

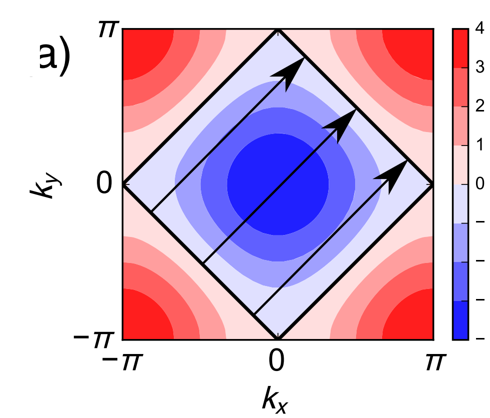

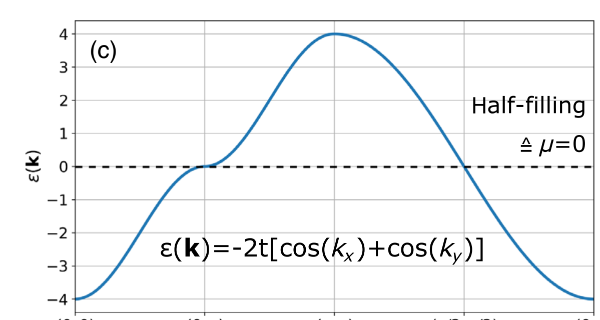

Recent reviews

Functional RG (fRG)

Physics Reports
Volume 910, 10 May 2021, Pages 1-114

The nonperturbative functional renormalization group and its applications

N. Dupuis [a], L. Canet [b], A. Eichhorn [c, d], W. Metzner [e], J.M. Pawlowski [d, f], M. Tissier [a], N. Wschebor [g]

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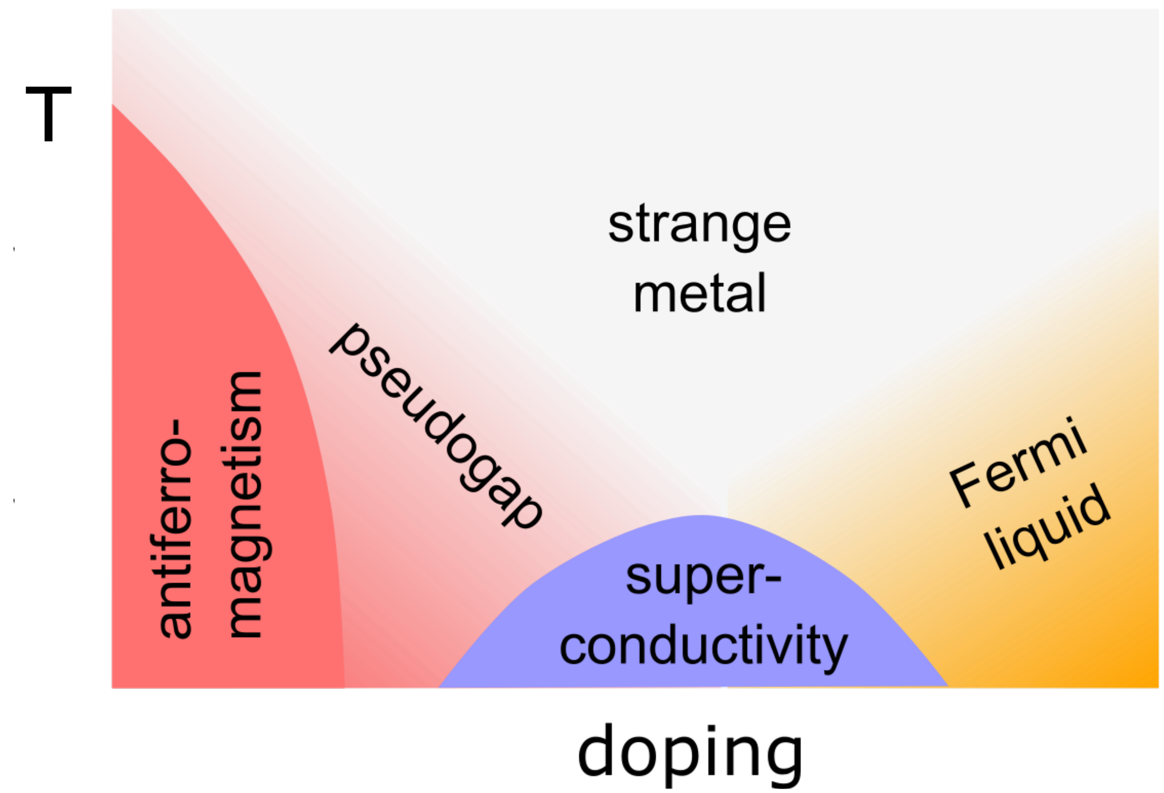
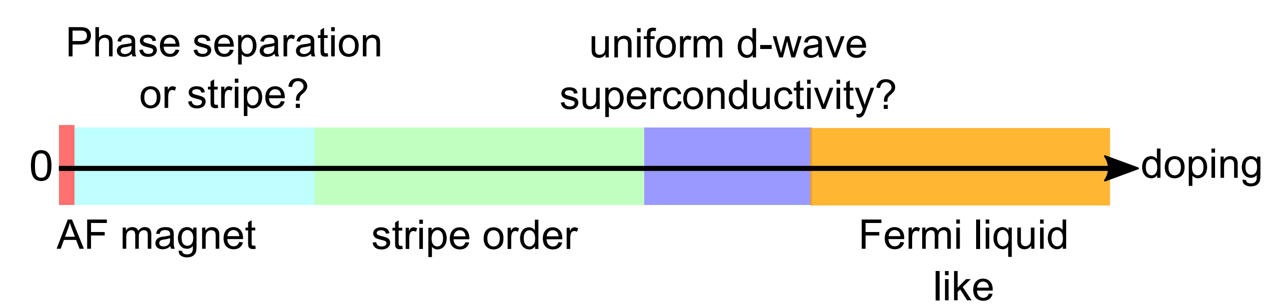
Renormalization in condensed matter: Fermionic systems – from mathematics to materials

Manfred Salmhofer

Salmhofer (1999); Berges *et al.*, PR (2002); Kopietz *et al.*, (2010); Metzner *et al.*, RMP (2012)

Phase diagram



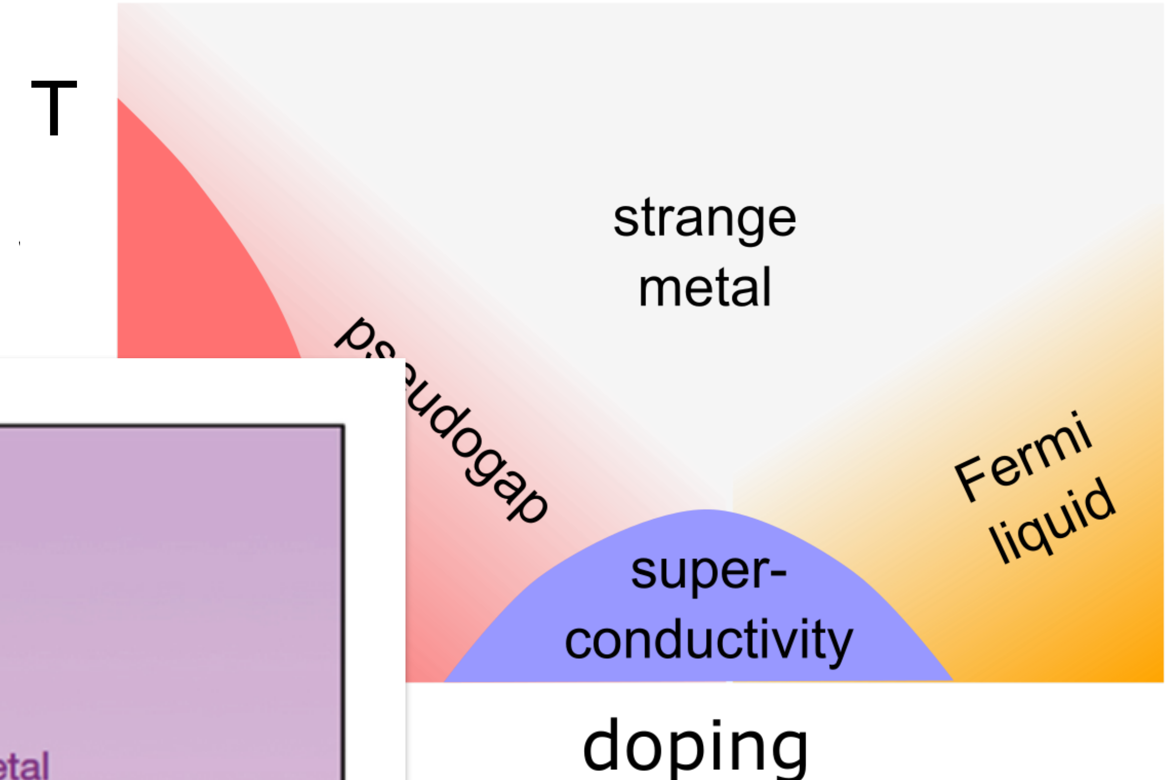


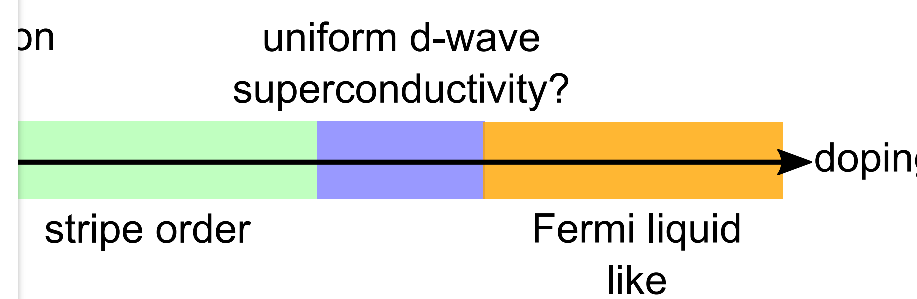
precise phase boundaries hard to determine - especially in the intermediate-to-strong interaction limit - due to:

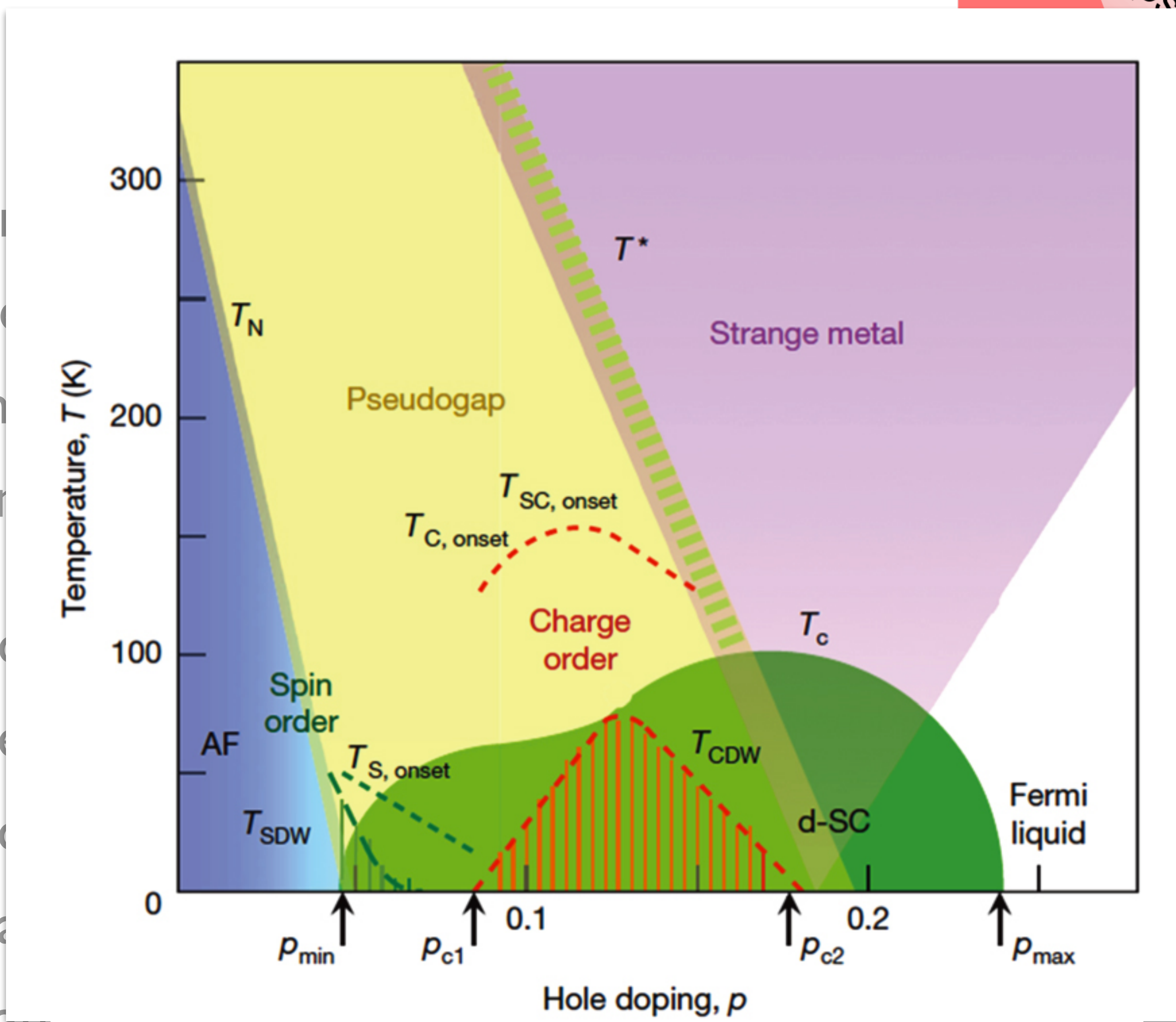
- divergent correl. length at continuous phase transitions hinders finite-size scaling
- energetic differences of competing phases often very small
- crossover regions with different physical properties
- approximate methods tend to break symmetries and overemphasize ordered phases

Qin *et al.*, ARCMP (2021)

Phase diagram







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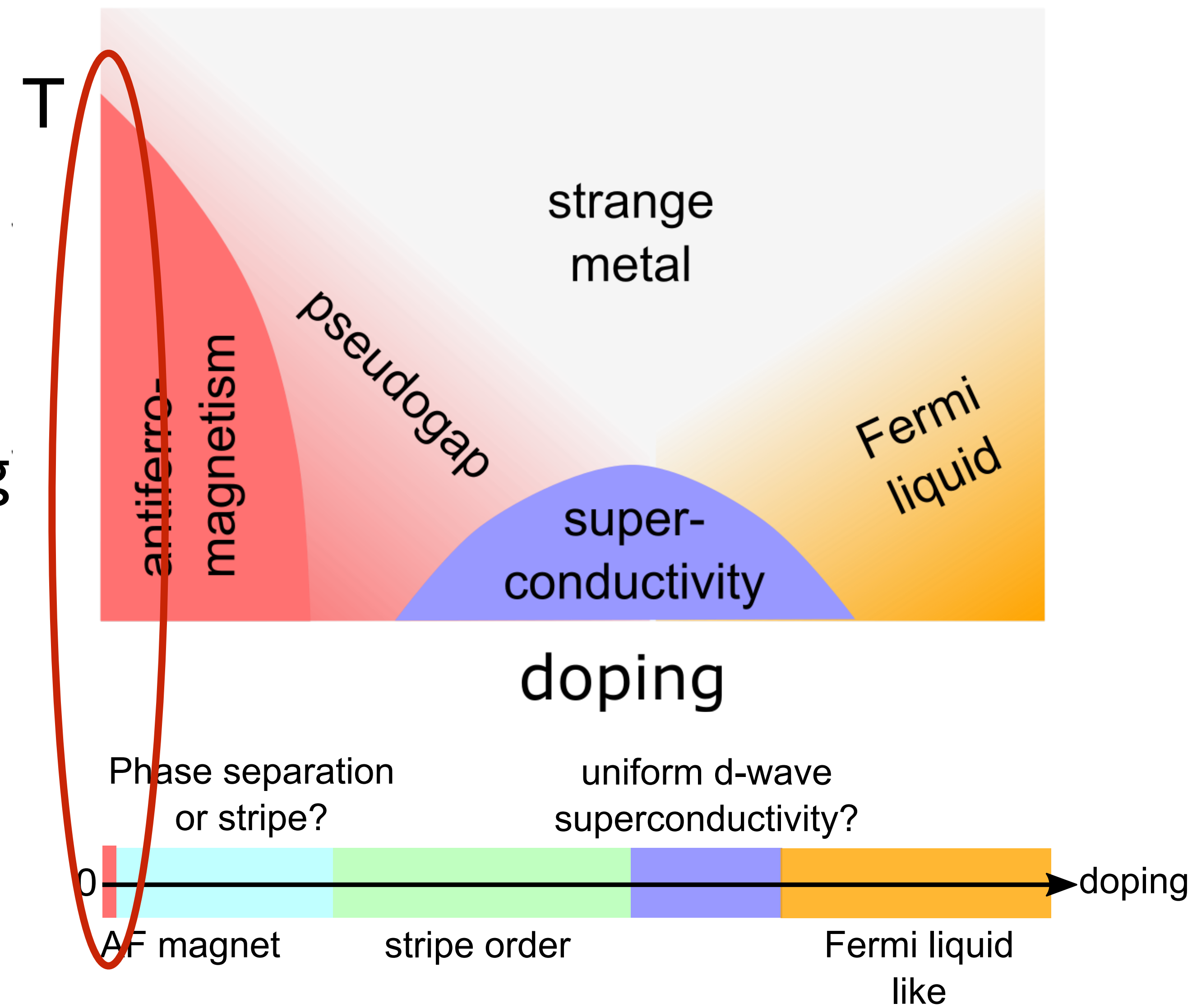
- c … itions hinders finite-size scaling
- e … ery small
- c … es
- a

and overemphasize ordered phases

Keimer *et al.*, Nature (2015)

The Hubbard model at half filling

ξ grows exponentially when reducing T → long-range fluctuations lead to weak-coupling pseudogap and eventually suppress magnetic ordering (Mermin-Wagner)



weak coupling

ground state is insulating (charge gap for any interaction strength U) with AF Neel order

strong coupling

Mott gap

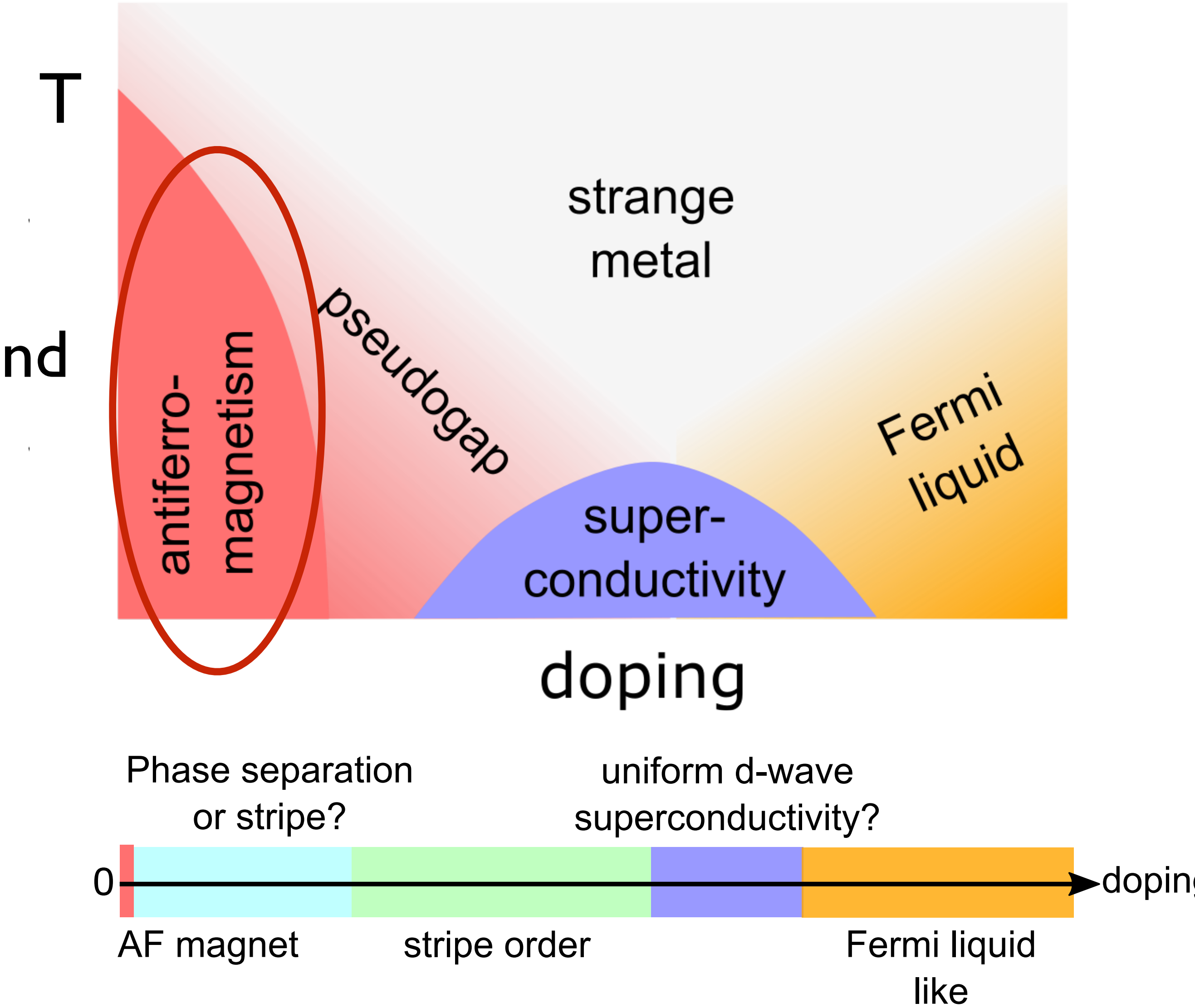
→ crossover at U~4t

The doped 2D Hubbard model at weak coupling

Antiferromagnetic order

AF order with generally incomm. wave vectors away from half-filling found already in mean-field theory

→ also indicated by diverging interactions and susceptibilities in fRG flows



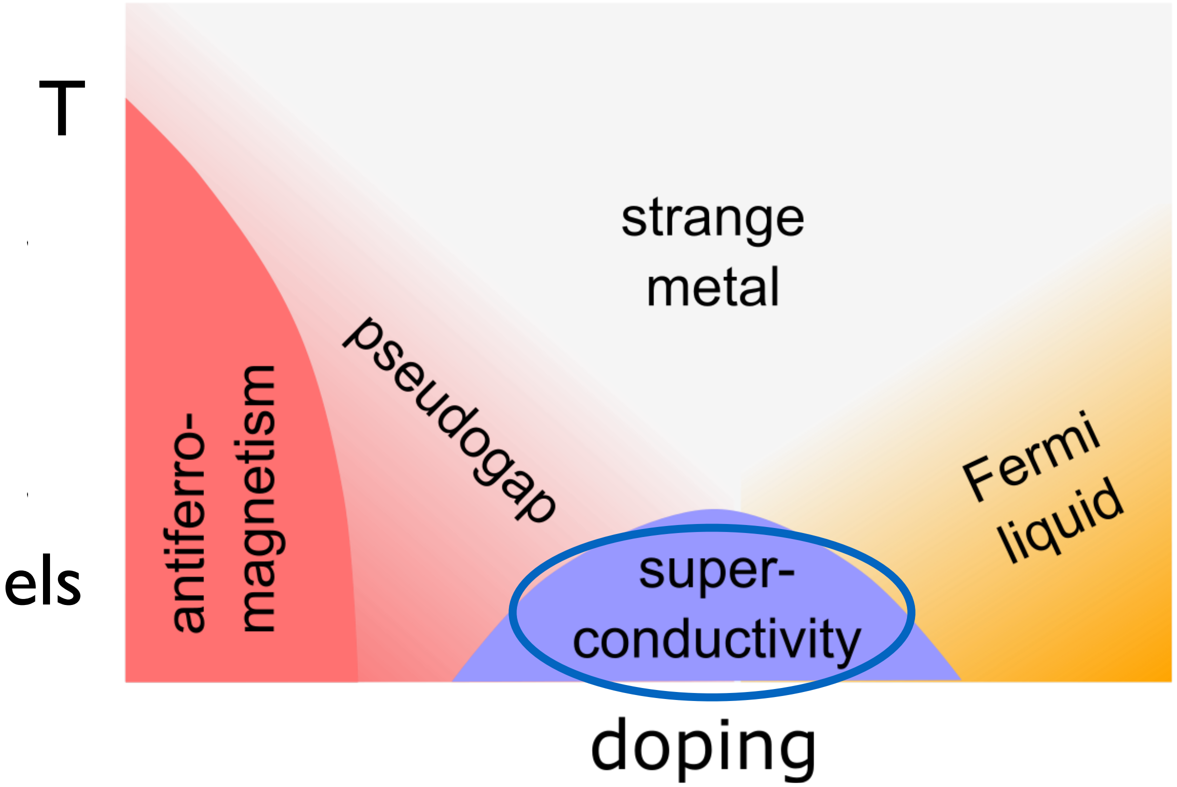
Halboth and Metzner, PRL (2000); Huseman and Salmhofer, PRB (2009); Eichhorn *et al.*, PRE (2013); Lauscher *et al.*, PRD (2000)

The doped 2D Hubbard model at weak coupling

Superconductivity

suggested by perturbative expansions

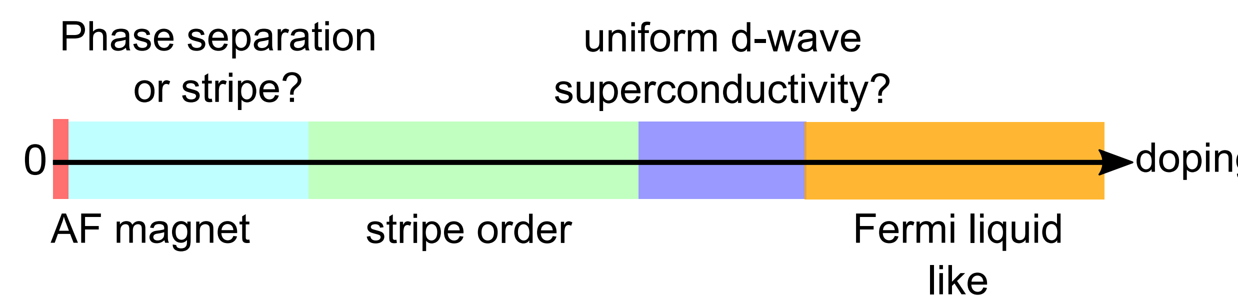
Scalapino, PR (1995)



fRG treatment of *all* fluctuation channels

on equal footing extends summation

in selected channels



→ only unbiased stability analysis

provided conclusive evidence

for existence of *d*-wave superconductivity with a sizable energy gap

at moderate interaction strength !

Zanchi and Schulz, PRB (2000); Halboth and Metzner, PRL&PRB (2000);
Honerkamp and Salmhofer, PRL (2001); Honerkamp *et al.*, PRB (2001)

The doped 2D Hubbard model at weak coupling

Superconductivity

suggested by perturbative expansions

Scalapino, PR (1995)

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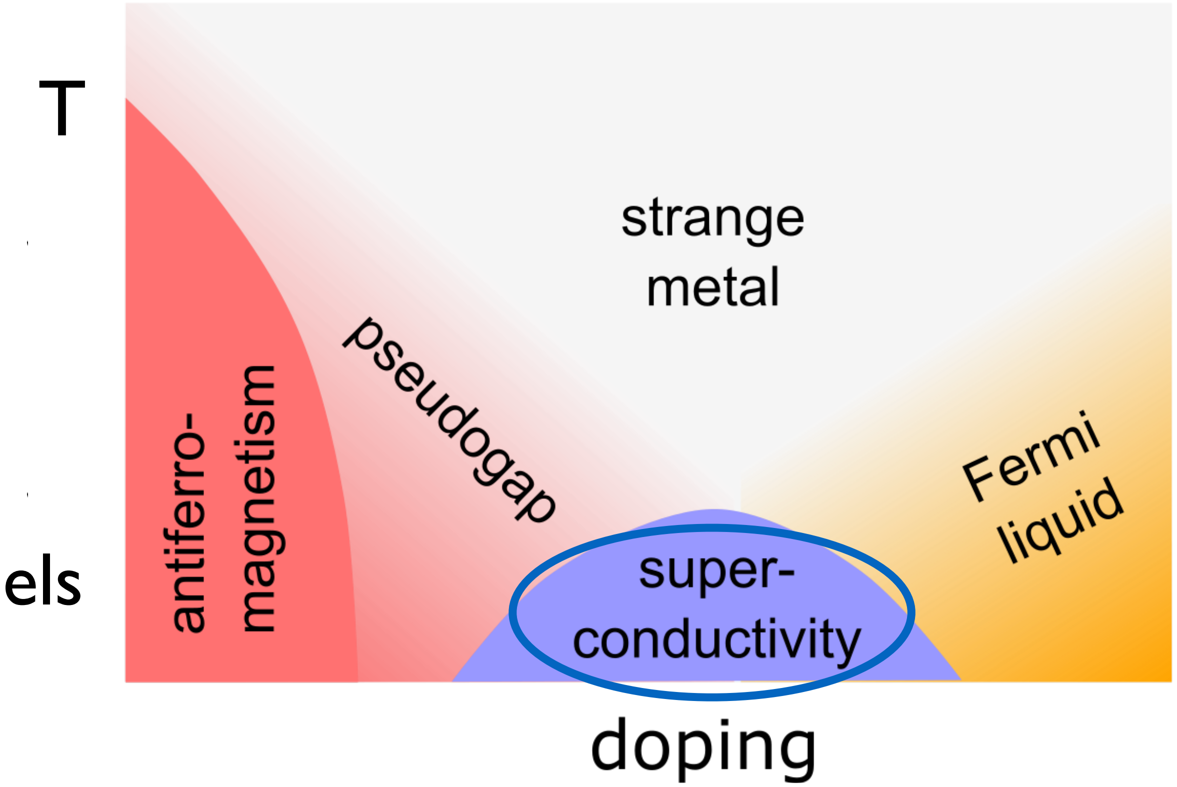
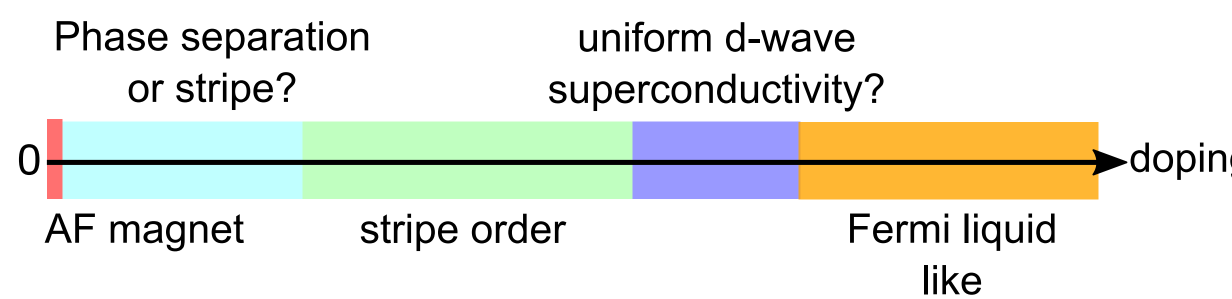




convincing evidence established also by other methods

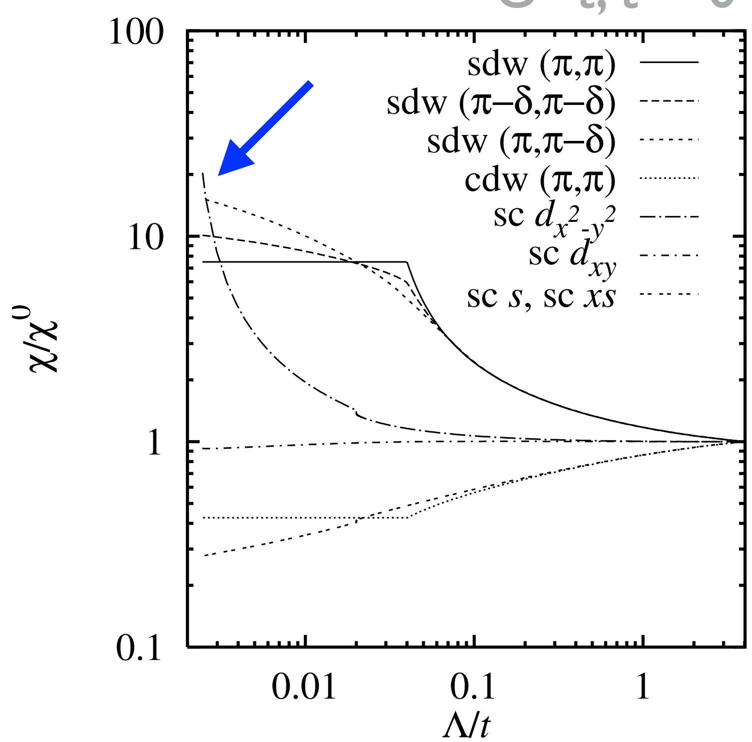
Kyung et al., PRB (2003); Raghu *et al.*, PRB (2010); Deng *et al.*, EPL (2015); Simkovic *et al.*, PRB (2021)

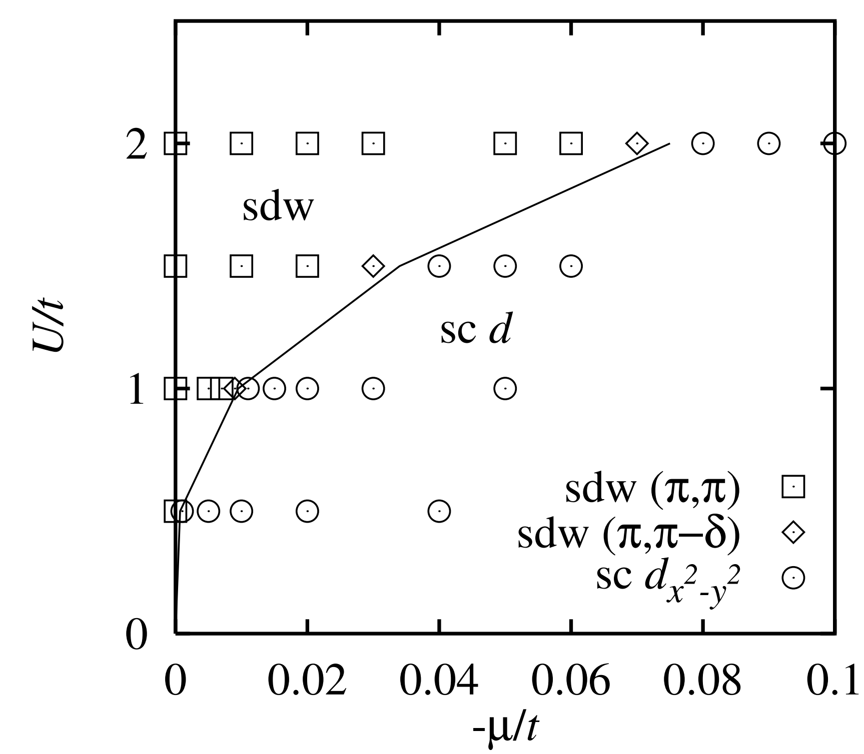
d-wave superconductivity

T=0

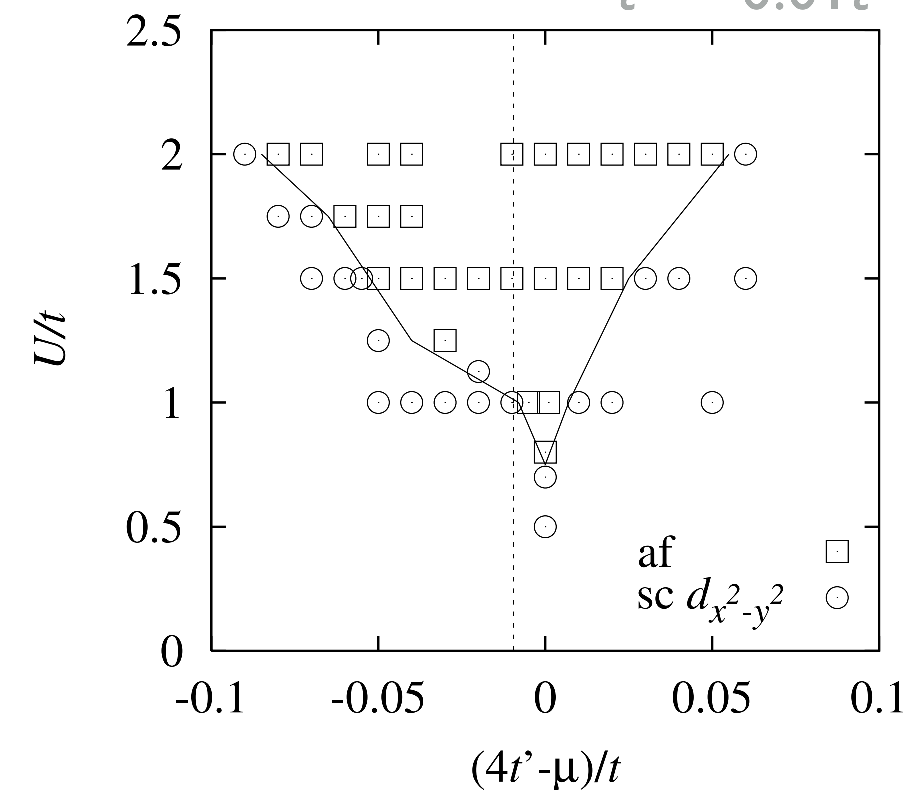
ground state identified from divergences of two-particle vertex and susceptibilities at some critical cutoff

U=t, t'= 0





t'= −0.01t

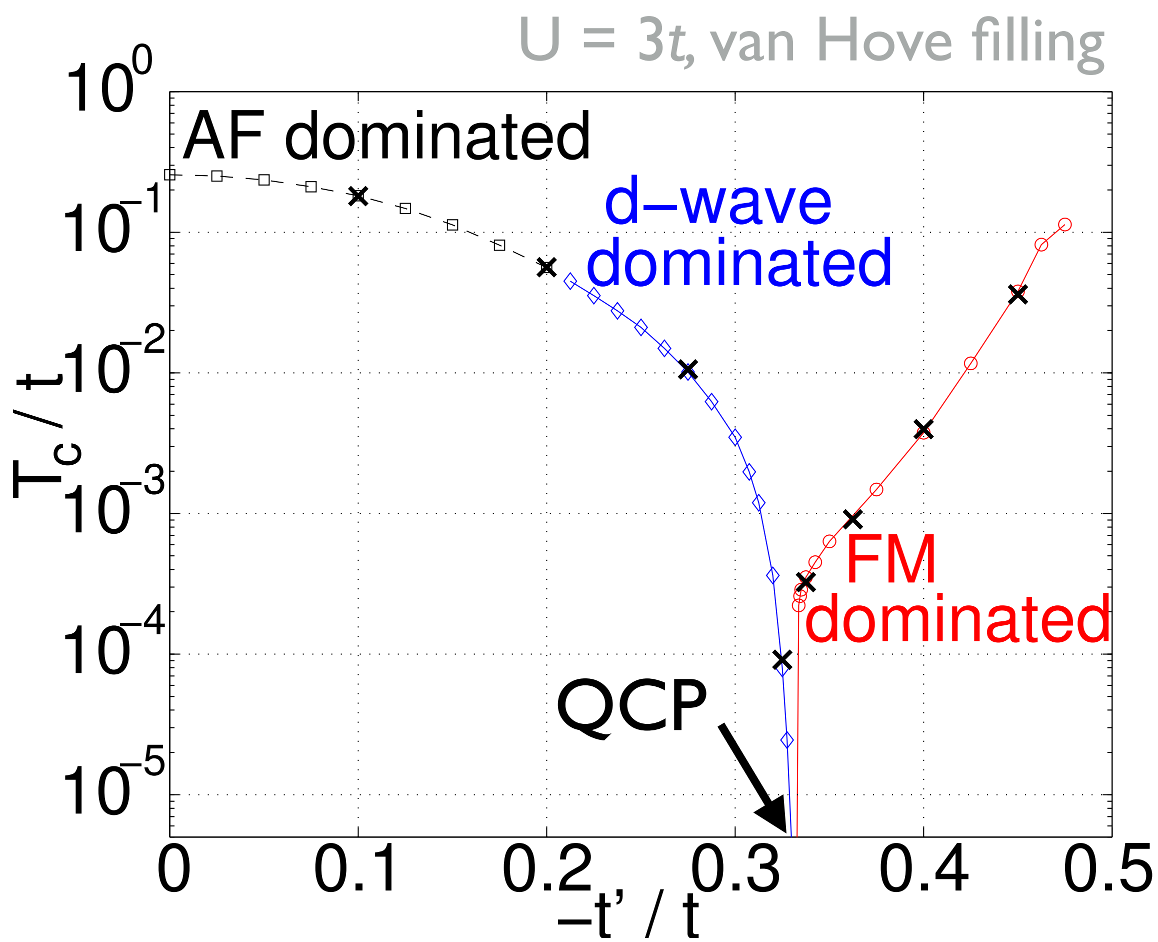


(static approxim.)

Halboth and Metzner, PRL&PRB (2000)

d-wave superconductivity

T>0



pseudo-critical T in a temperature flow

(≠ true critical T)

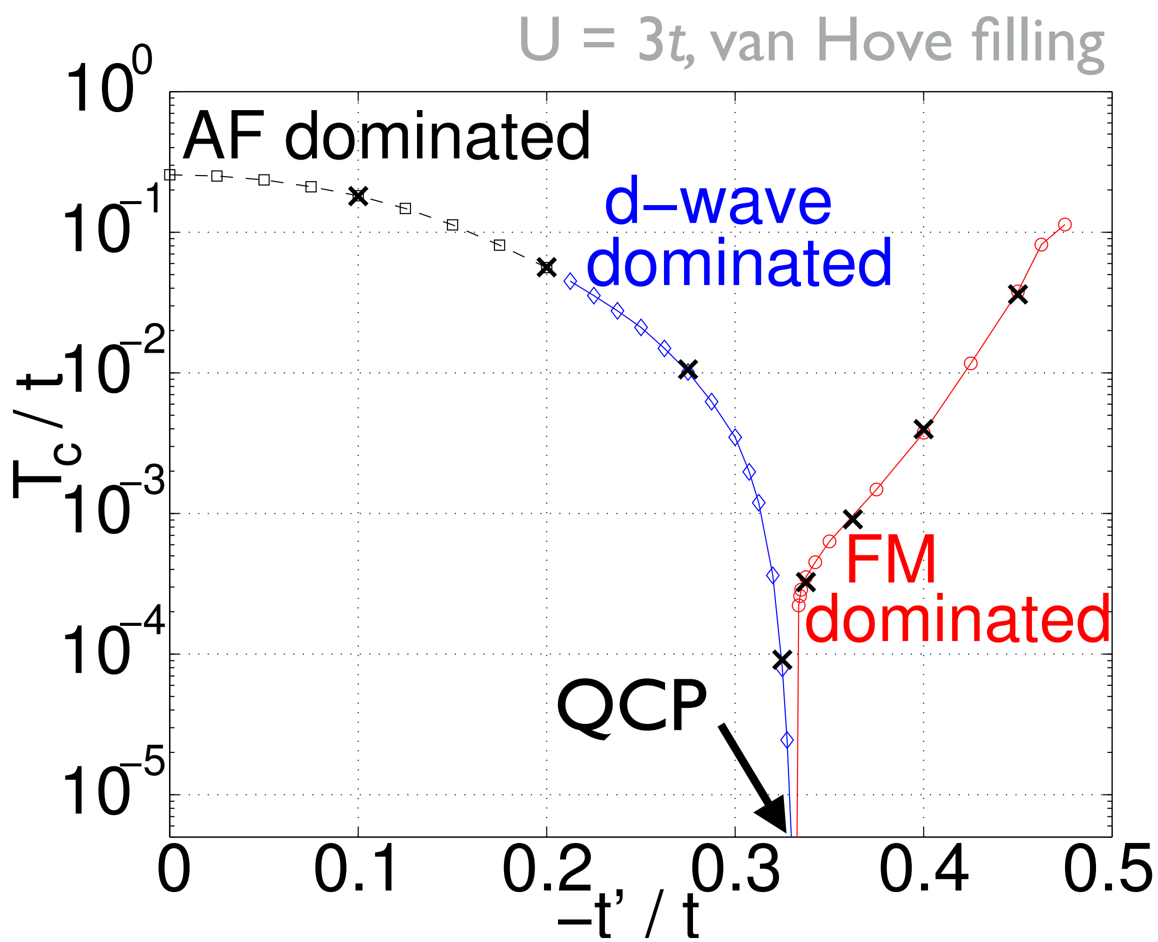
Note:

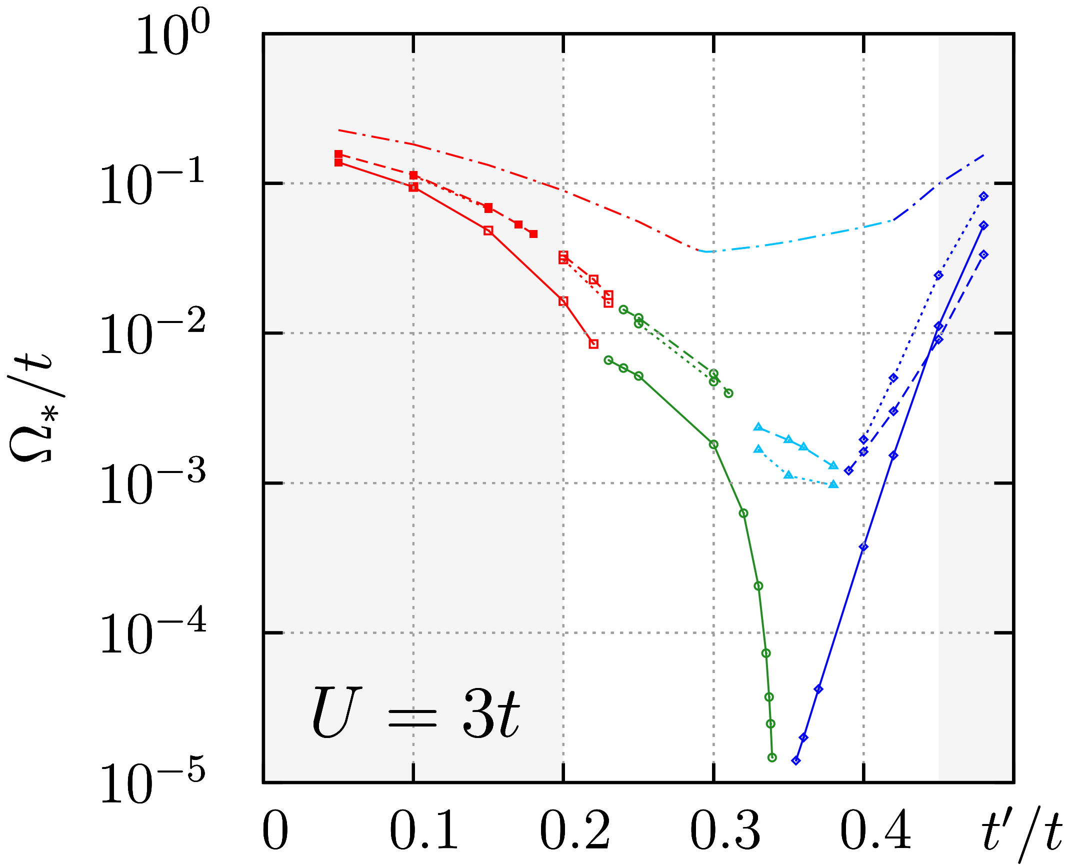
- that order parameter fluctuations suppressing actual transition T in 2d not captured by 2. order truncation
- also static approximation insufficient beyond weak coupling regime

Honerkamp and Salmhofer, PRL (2001)

d-wave superconductivity

T>0





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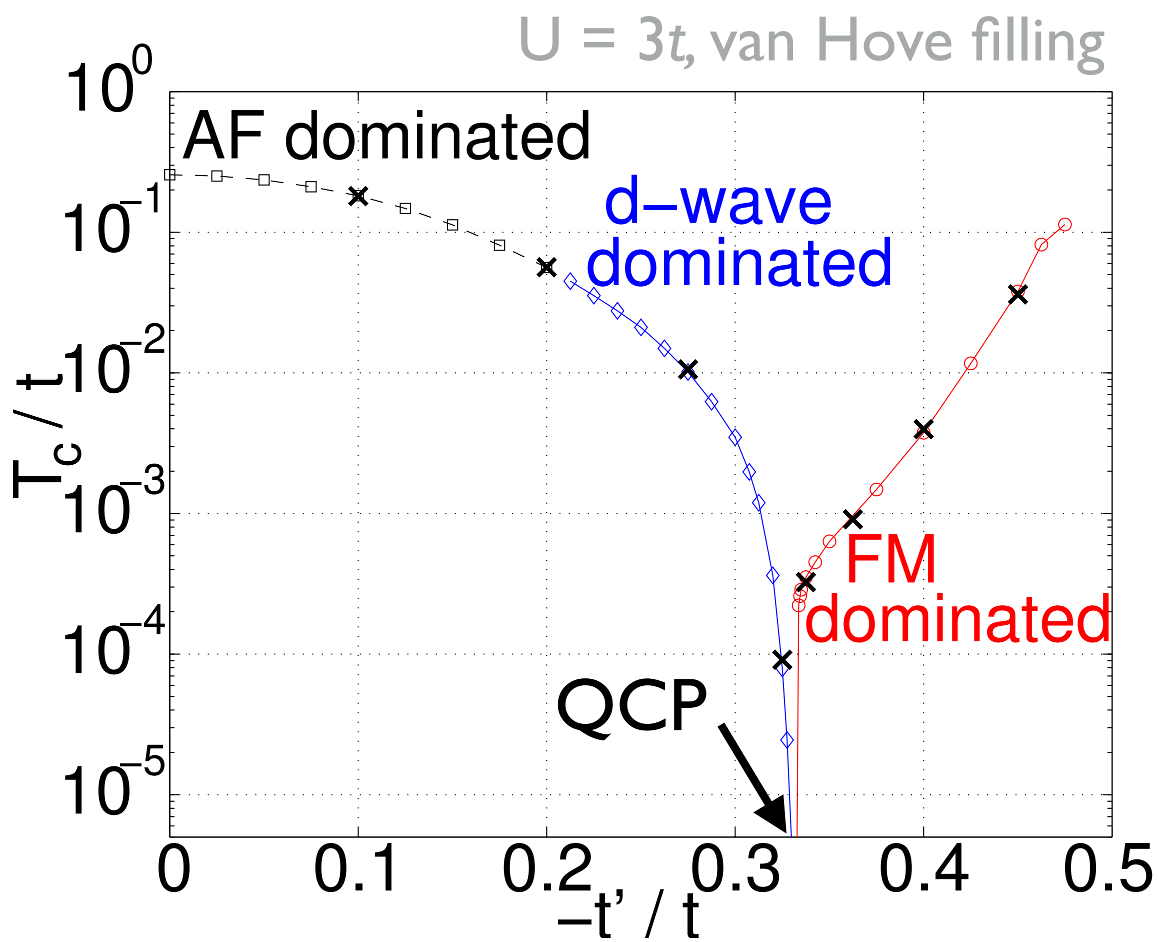
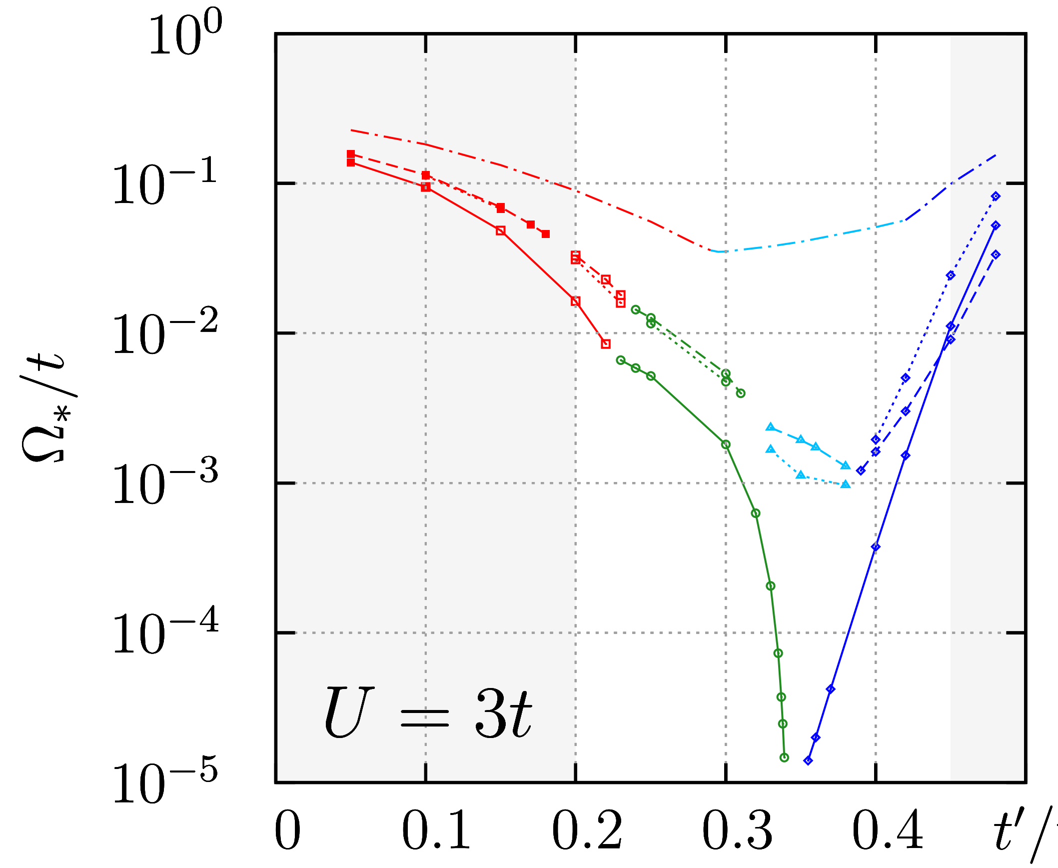
Giering and Salmhofer, PRB (2012); Honerkamp and Salmhofer, PRL (2001)

d-wave superconductivity

T>0





Note:

- that order parameter fluctuations suppressing actual transition T in 2d not captured by 2. order truncation
- also static approximation insufficient beyond weak coupling regime

→ development of improved vertex parametrizations

Order parameters and critical temperatures

symmetry breaking such as magnetic order or superconductivity associated with divergence at pseudo-critical scale

→ to continue flow, order parameter needs to be implemented:

Fermionic flows

including tiny symmetry breaking field that develops into a finite order parameter below critical scale

Eberlein and Metzner, PRB (2014)

Flows with order-parameter fields

flow of collective bosonic order parameter fields obtained by Hubbard-Stratonovich decoupling

Baier *et al.*, PRB (2004); Krahl *et al.*, PRB (2009); Friederich *et al.*, PRB (2010&11)

Renormalized mean-field theory

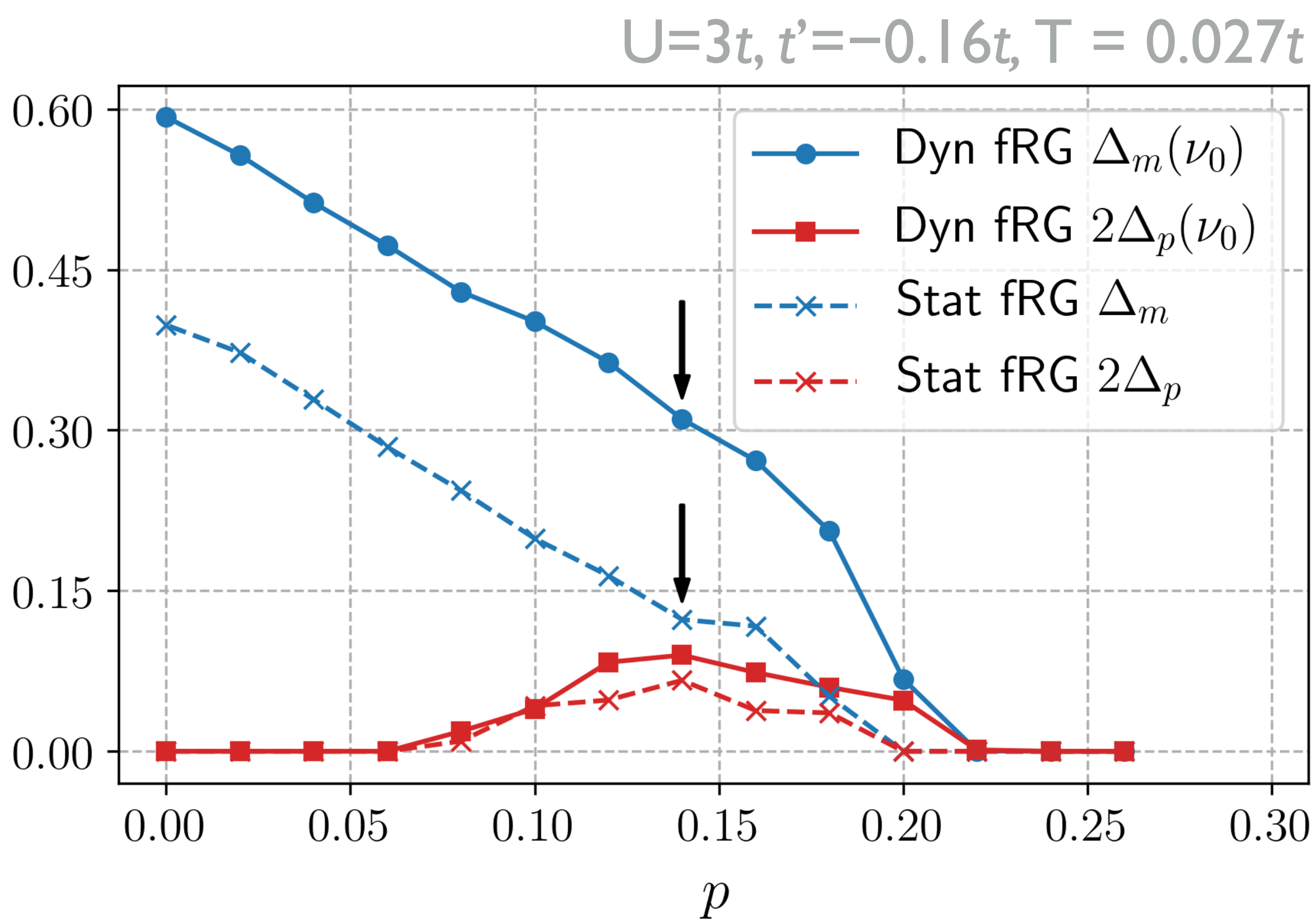
combination of flow equations at high scales with mean-field approximation at low scales (fRG+MF)

Reiss *et al.*, PRB (2007); Wang *et al.*, PRB (2014); Yamase *et al.*, PRL (2016)

Order parameters and critical temperatures

Amplitudes of magnetic and pairing gap

mean-field theory treatment of gap formation below energy scale of spontaneous symmetry breaking

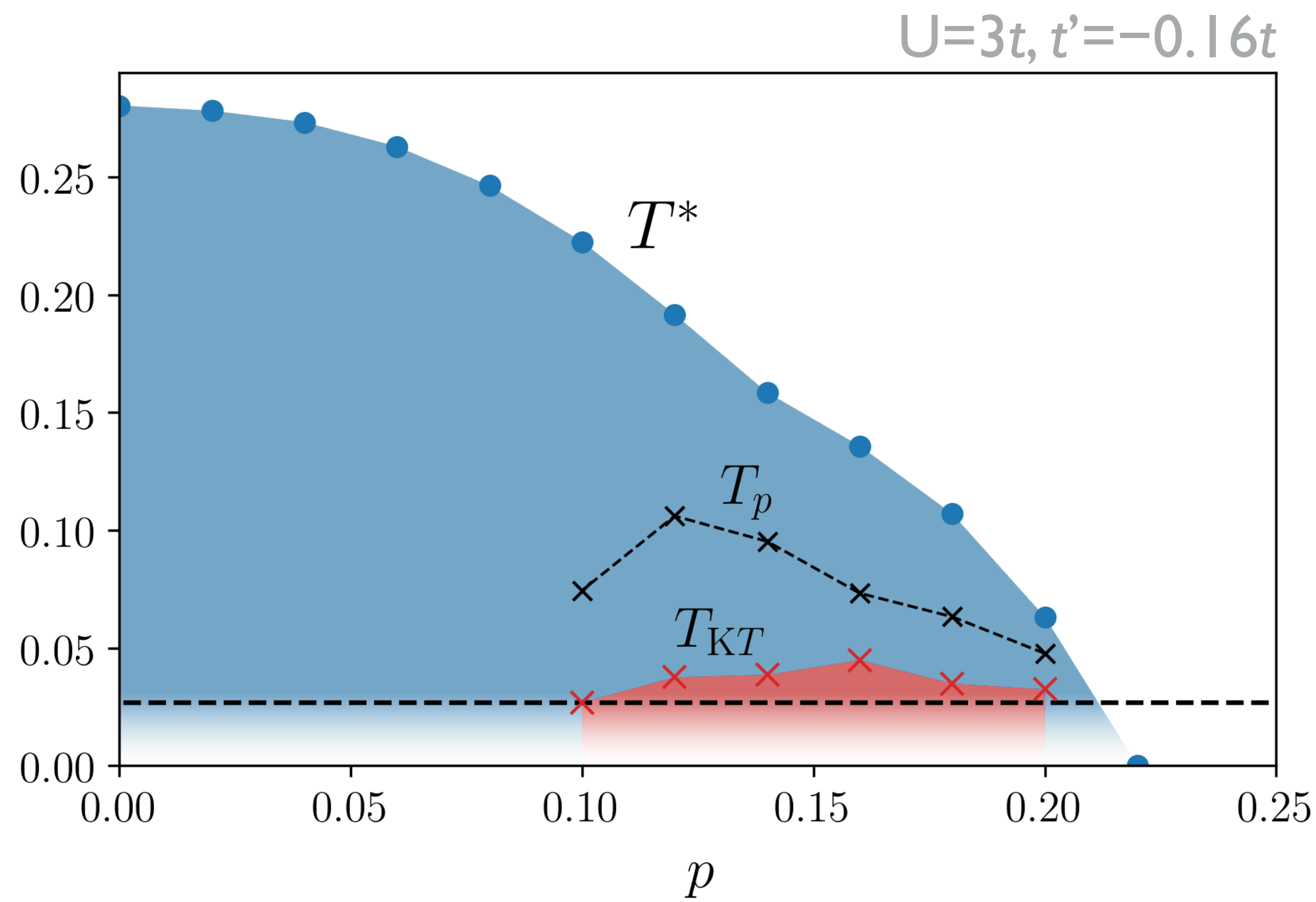


full frequency dependence of interaction vertices and gap functions confirms important previous results in static approximation !

Vilardi *et al.*, PRB (2020)

Order parameters and critical temperatures

Phase diagram



- sizable doping regime with robust pairing coexisting with Neel or incomm. AF
- Kosterlitz-Thouless determined from superfluid phase stiffness

→ superconducting dome centred around 15% hole doping

Vilardi *et al.*, PRB (2020)

Establishing a new level of accuracy

fRG in first implementation provides

- possibility to scan parameter space due to reduced numerical effort
- physical picture and ***qualitative*** agreement with experiments

Algorithmic advancements

- efficient parametrization of vertex function
- multiloop extension

Application to 2D Hubbard model

→ quantitative description at weak-to-intermediate couplings

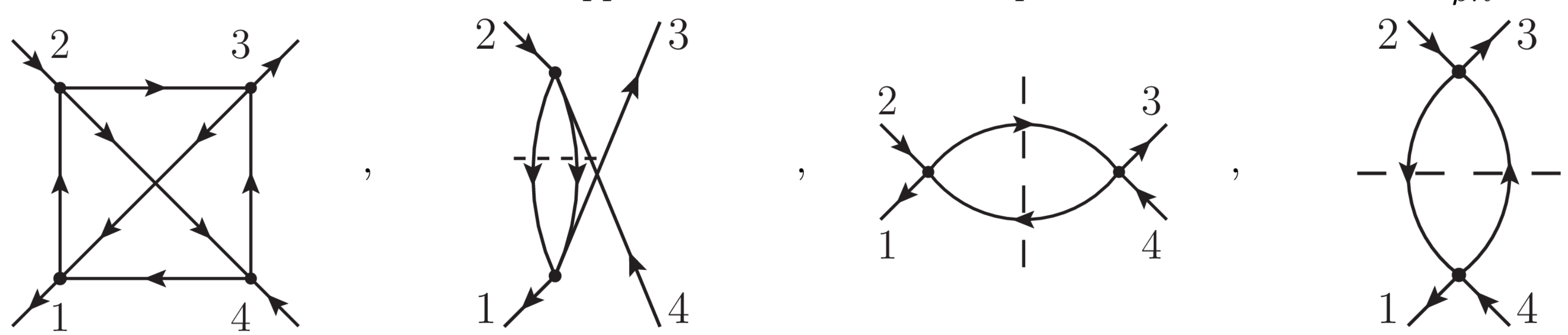
→ towards strong coupling by combination with DMFT

→ unbiased and optimized approach towards ***quantitative*** predictions

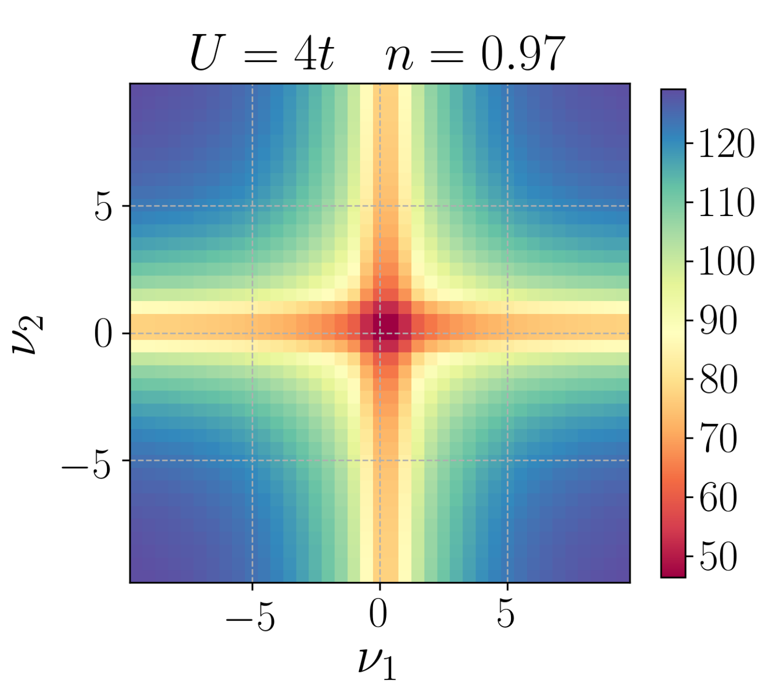
Efficient parametrization of vertex function

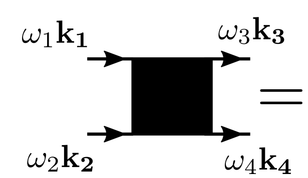
- formulation using diagrammatic parquet decomposition

$$\Lambda \approx U \quad + \quad \Phi_{pp} \quad + \quad \Phi_{ph} \quad + \quad \Phi_{\overline{ph}}$$

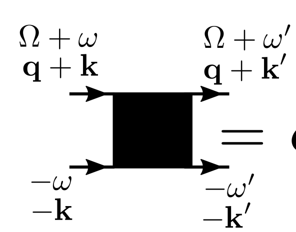


- full frequency ***and*** momentum dependence challenging:





$$= \gamma_4(\overbrace{\omega_1, \omega_2, \omega_3}^{N_\omega^3}, \overbrace{\mathbf{k_1}, \mathbf{k_2}, \mathbf{k_3}}^{(N_{k_x} \times N_{k_y})^3})$$



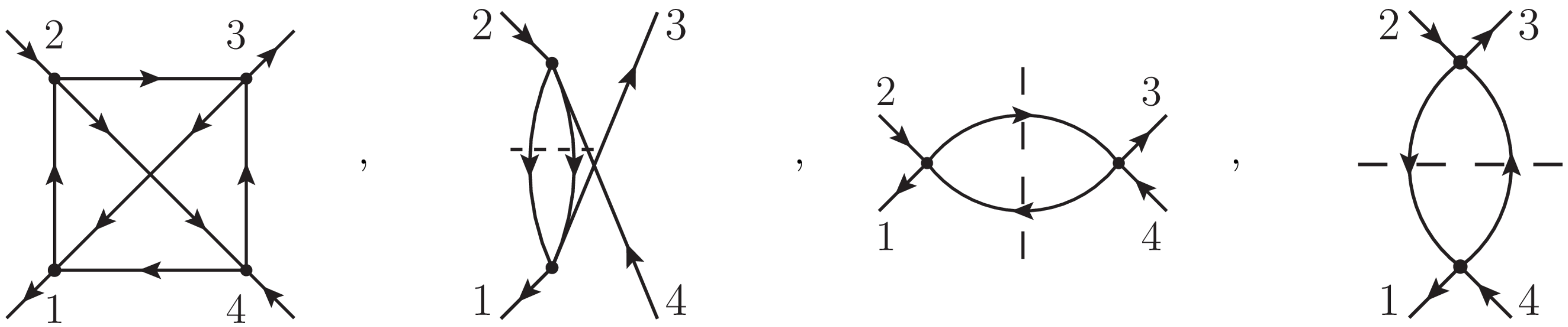
$$= \phi_{pp}(\overbrace{\Omega, \omega, \omega'}^{(N_\Omega) \times (N_\omega)^2}, \underbrace{\mathbf{q}, \mathbf{k}, \mathbf{k'}}_{(N_{q_x} \times N_{q_y}) \times (N_{k_x} \times N_{k_y})^2})$$

Husemann *et al.*, PRB (2012); Vilardi *et al.*, PRB (2018); Tagliavini *et al.*, SciPost Phys. (2019)

Efficient parametrization of vertex function

- formulation using diagrammatic parquet decomposition

$$\Lambda \approx U \quad + \quad \Phi_{pp} \quad + \quad \Phi_{ph} \quad + \quad \Phi_{\overline{ph}}$$



- **momentum dependence** with "truncated unity" fRG (TU-fRG)

  → expansion in form factors $\quad \mathbb{1} = \int d\mathbf{p}' \sum_n f_n^*(\mathbf{p}') f_n(\mathbf{p})$

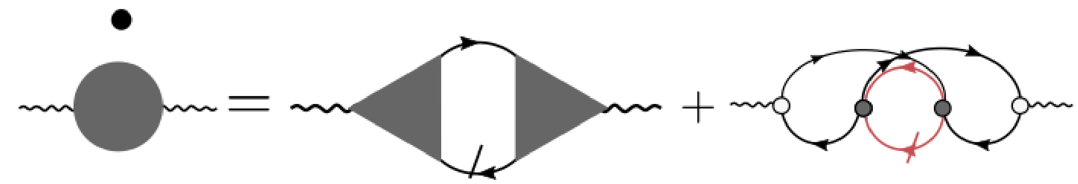
- **frequency dependence**

  → considerable reduction of numerical effort by including asymptotics

$$\phi_r(i\omega_l, i\nu_o, i\nu_{o'}, \mathbf{q}, \mathbf{k}, \mathbf{k}') = \mathcal{R}_r(i\omega_l, i\nu_o, i\nu_{o'}, \mathbf{q}, \mathbf{k}, \mathbf{k}') + \mathcal{K}_{2,r}(i\omega_l, i\nu_o, \mathbf{q}, \mathbf{k}) + \bar{\mathcal{K}}_{2,r}(i\omega, i\nu_{o'}, \mathbf{q}, \mathbf{k}') + \mathcal{K}_{1,r}(i\omega_l, \mathbf{q})$$

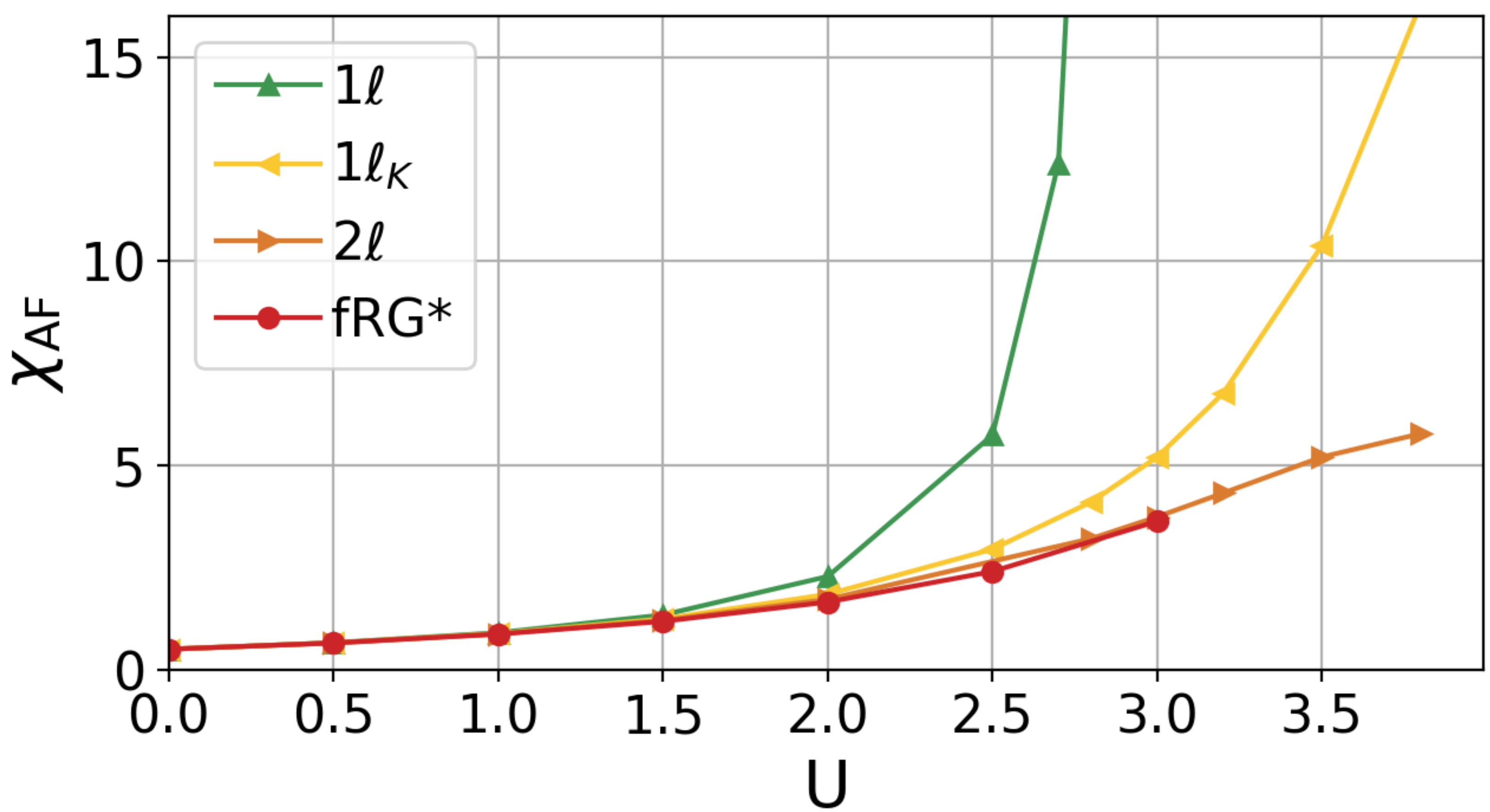
Husemann and Salmhofer, PRB (2009); Lichtenstein *et al.*, PRB (2017); Karrasch *et al.*, EJP (2008); Wentzell *et al.*, PRB (2020)

Multiloop extension



- improves truncation by partial inclusion of higher order vertex contributions
- recovers parquet approximation (PA) at infinite loop order

  → solution satisfies exact relations and is ***independent*** of cutoff !



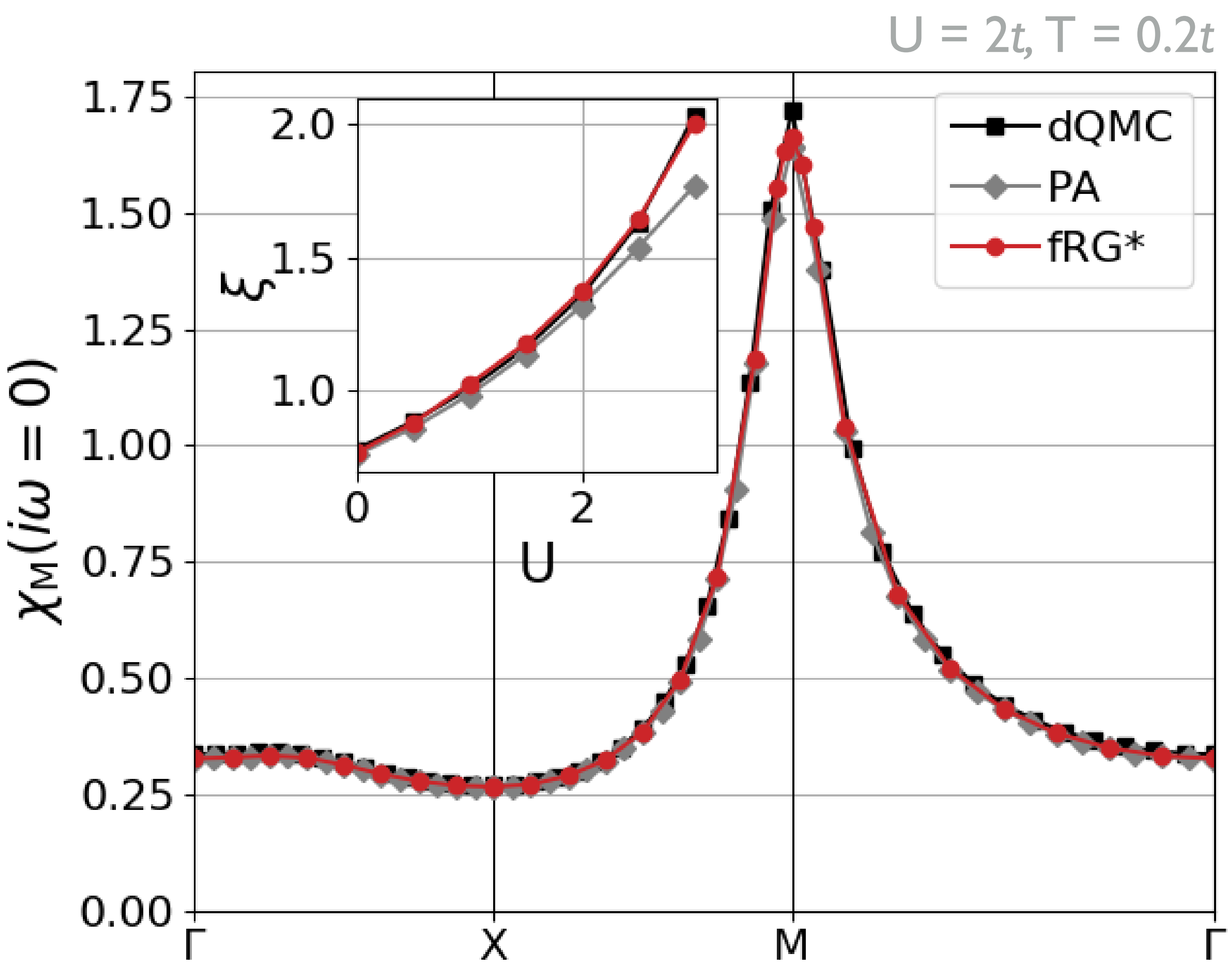
half-filling, T = $0.2t$

- strong suppression of pseudocritical temperature
- main effect already at 2ℓ, which appears to be almost at loop convergence

Kugler and von Delft, PRL (2018); Tagliavini *et al.*, SciPost Phys. (2019)

Multiloop fRG results

Magnetic susceptibility at half filling



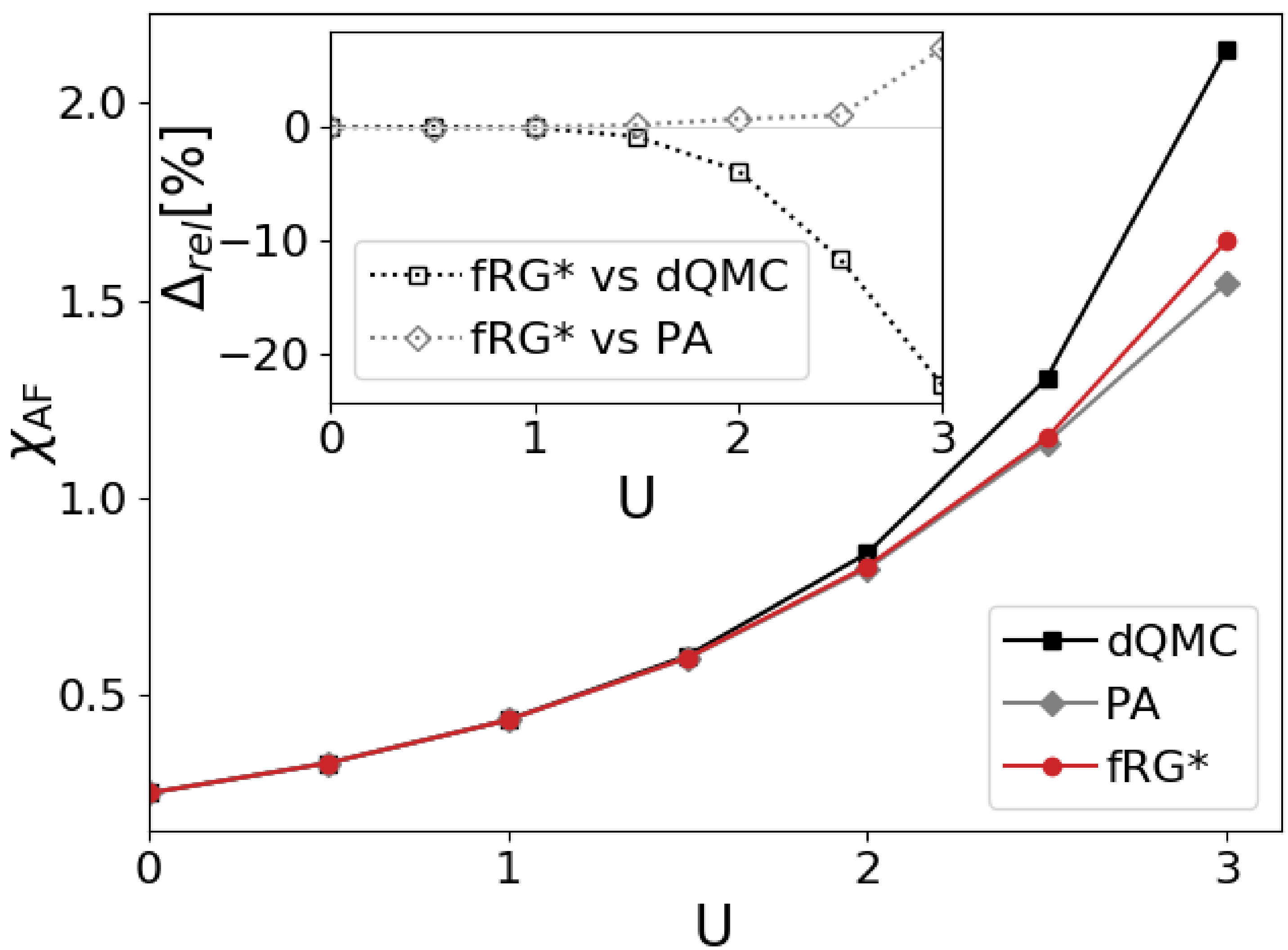
- AF peak dominant at half-filling
- **excellent agreement** with PA and determinant dQMC → ***quantitative fRG*** !

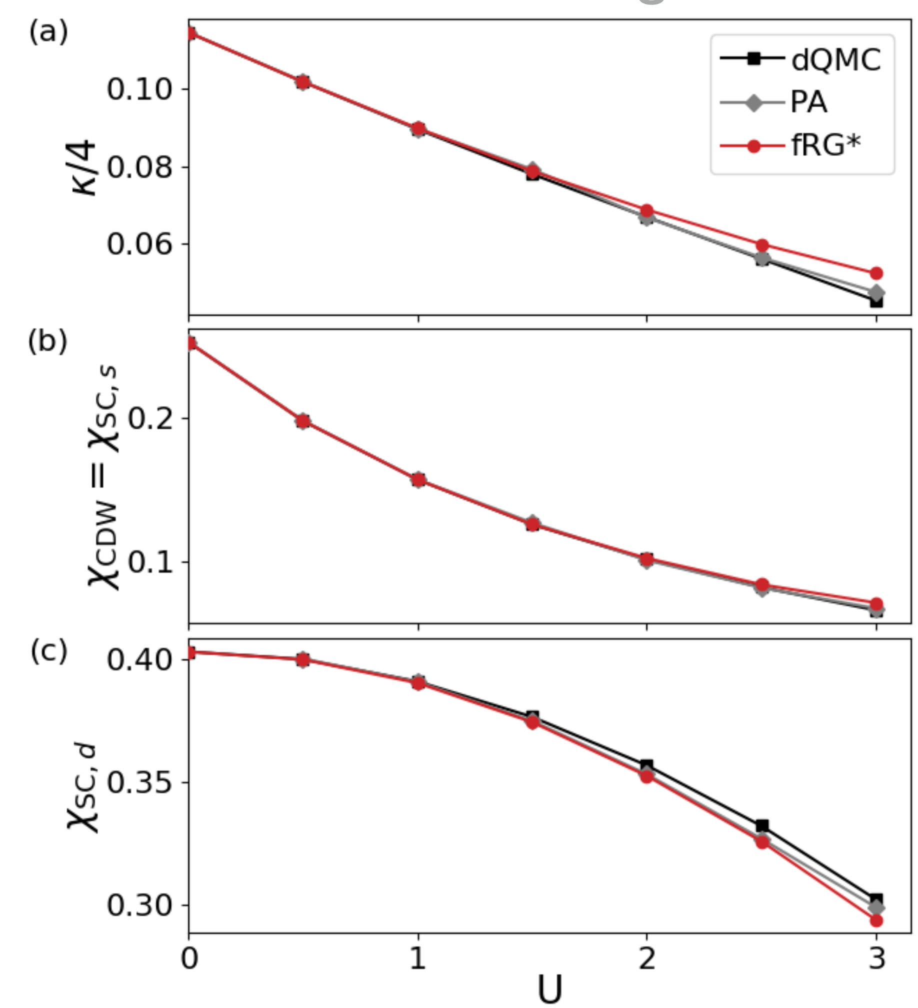
Hille *et al.*, PRReserach (2020)

Multiloop fRG results

Evolution with interaction

half filling, T = 0.2t





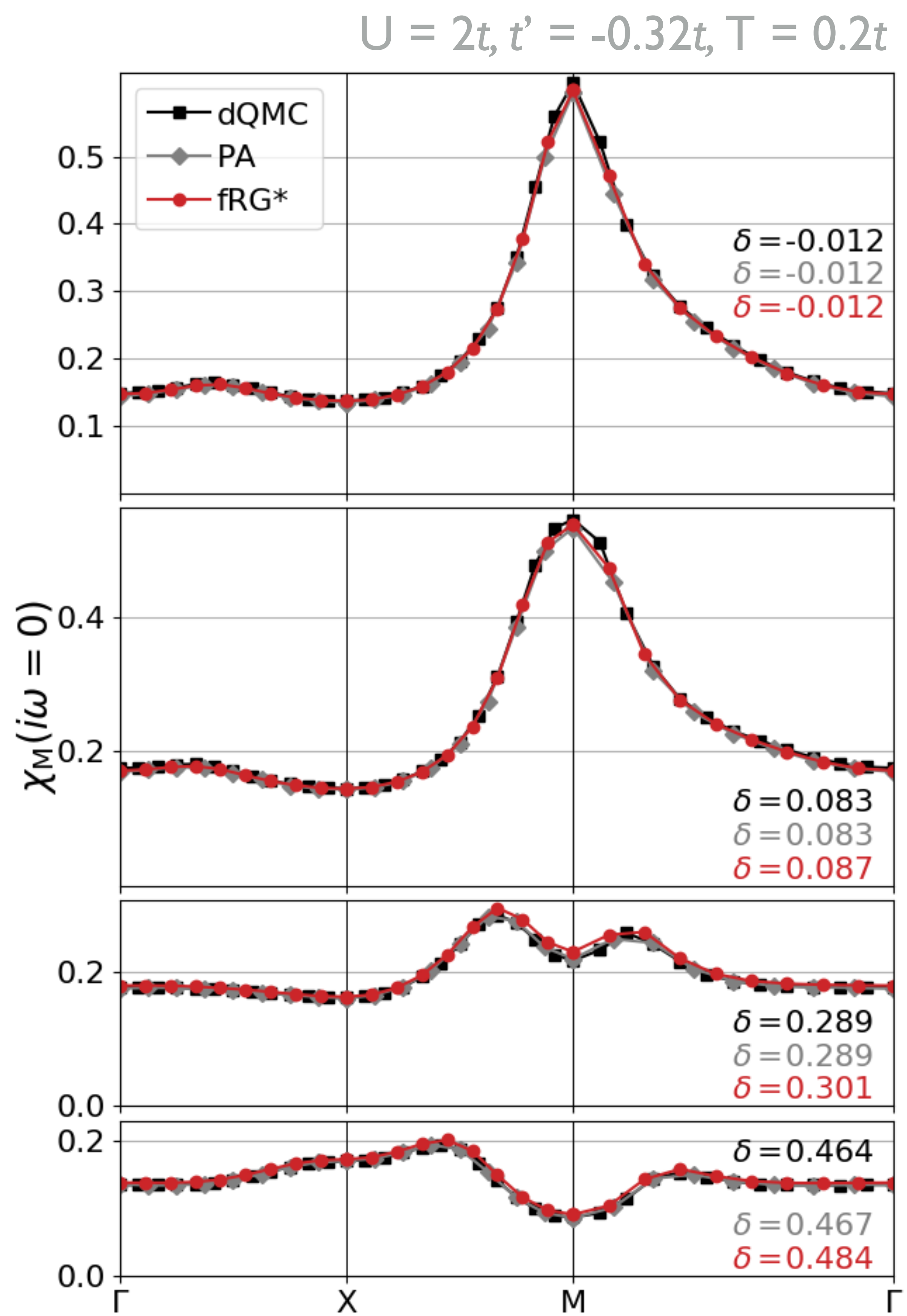
deviations with increasing interaction (corrections to dQMC of 4. order)

→ convergence becomes more challenging

Hille *et al.*, PRReserach (2020)

Multiloop fRG results

Magnetic susceptibility at finite doping



very high accuracy, despite convergence

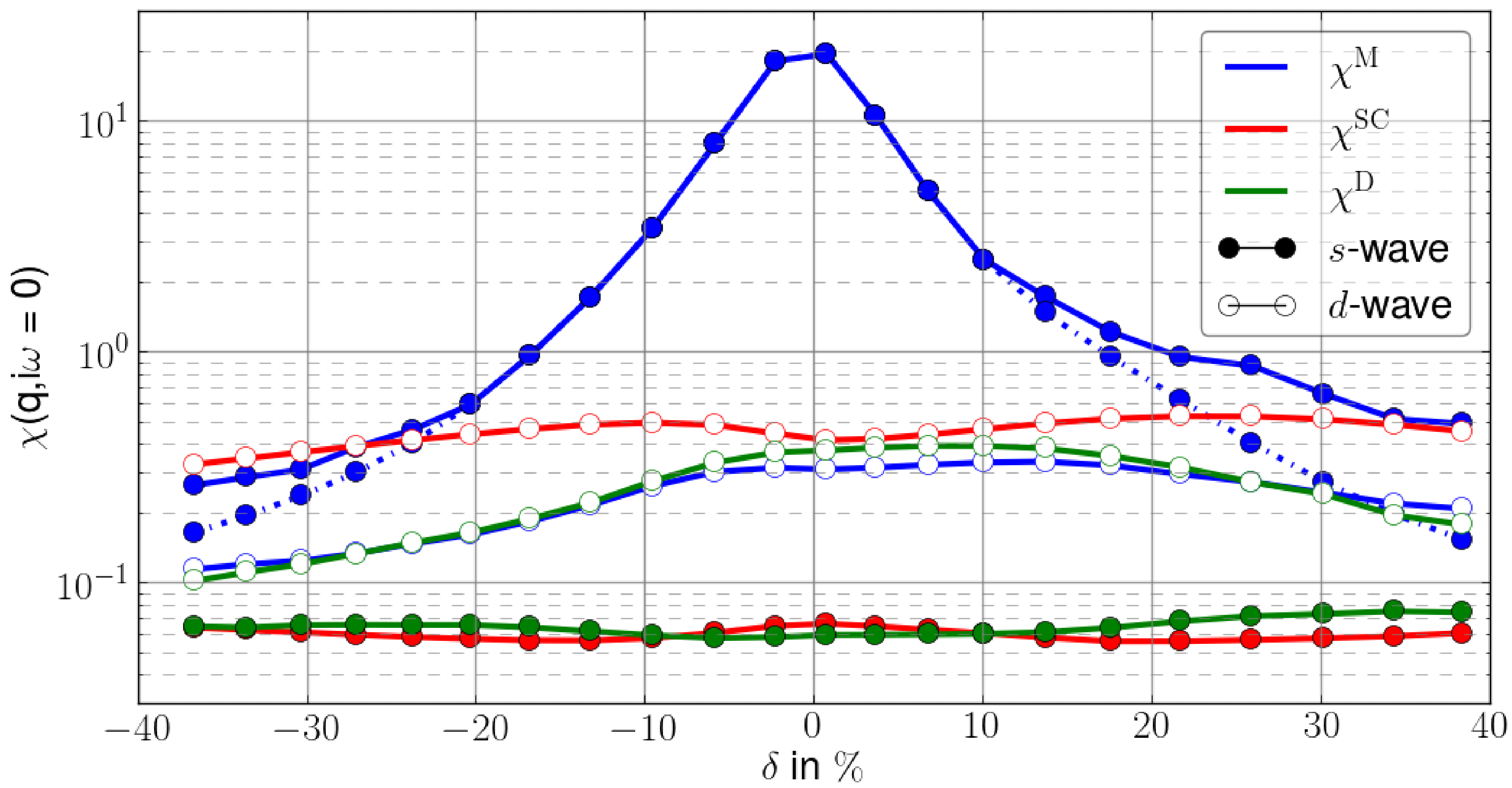
in form factors not fully achieved

Hille *et al.*, PRReserach (2020)

2ℓ fRG study

→ Poster S. Heinzelmann

Susceptibilities as a function of doping



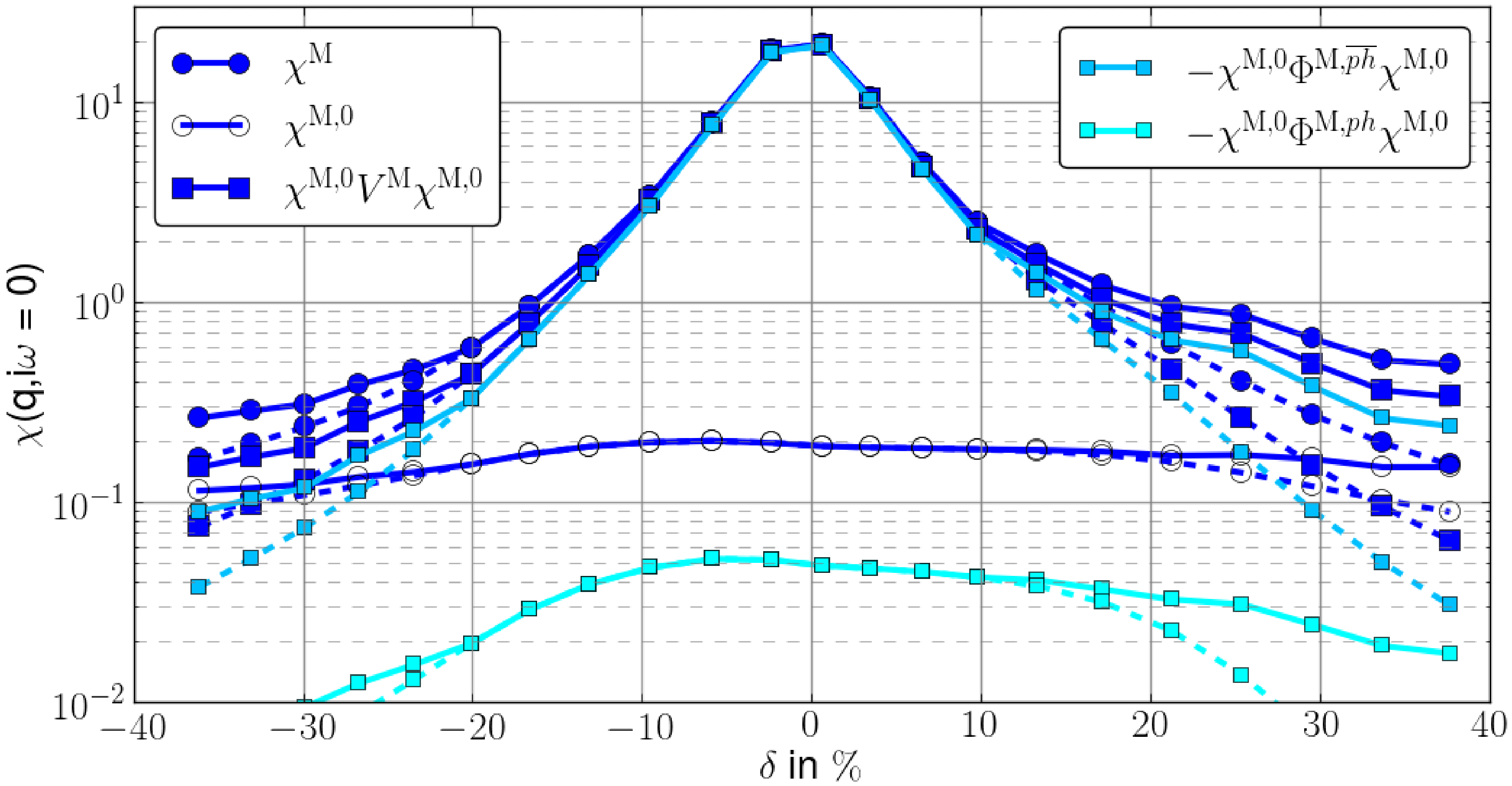
U = 3t, t' = -0.15t, T = 0.067t

- AF fluctuations dominate → become incommensurate at larger doping
- superconducting d-wave fluctuations expected to grow at lower T
- large effect of multiloop corrections included in 2ℓ, correct to $O(U^3)$

2ℓ fRG study

Fluctuation diagnostics

$$\chi^X(\mathbf{q},i\omega) = \sum_{i\nu} \mathbf{\Pi}^X(\mathbf{q},i\omega,i\nu) + \sum_{i\nu,i\nu'} \mathbf{\Pi}^X(\mathbf{q},i\omega,i\nu)\mathbf{V}^X(\mathbf{q},i\omega,i\nu,i\nu')\mathbf{\Pi}^X(\mathbf{q},i\omega,i\nu')$$
$$:= \chi^{X,0}(\mathbf{q},i\omega) + \left[\chi^{X,0}\mathbf{V}^X\chi^{X,0}\right](\mathbf{q},i\omega)$$



magnetic channel

***vertex driven*,**

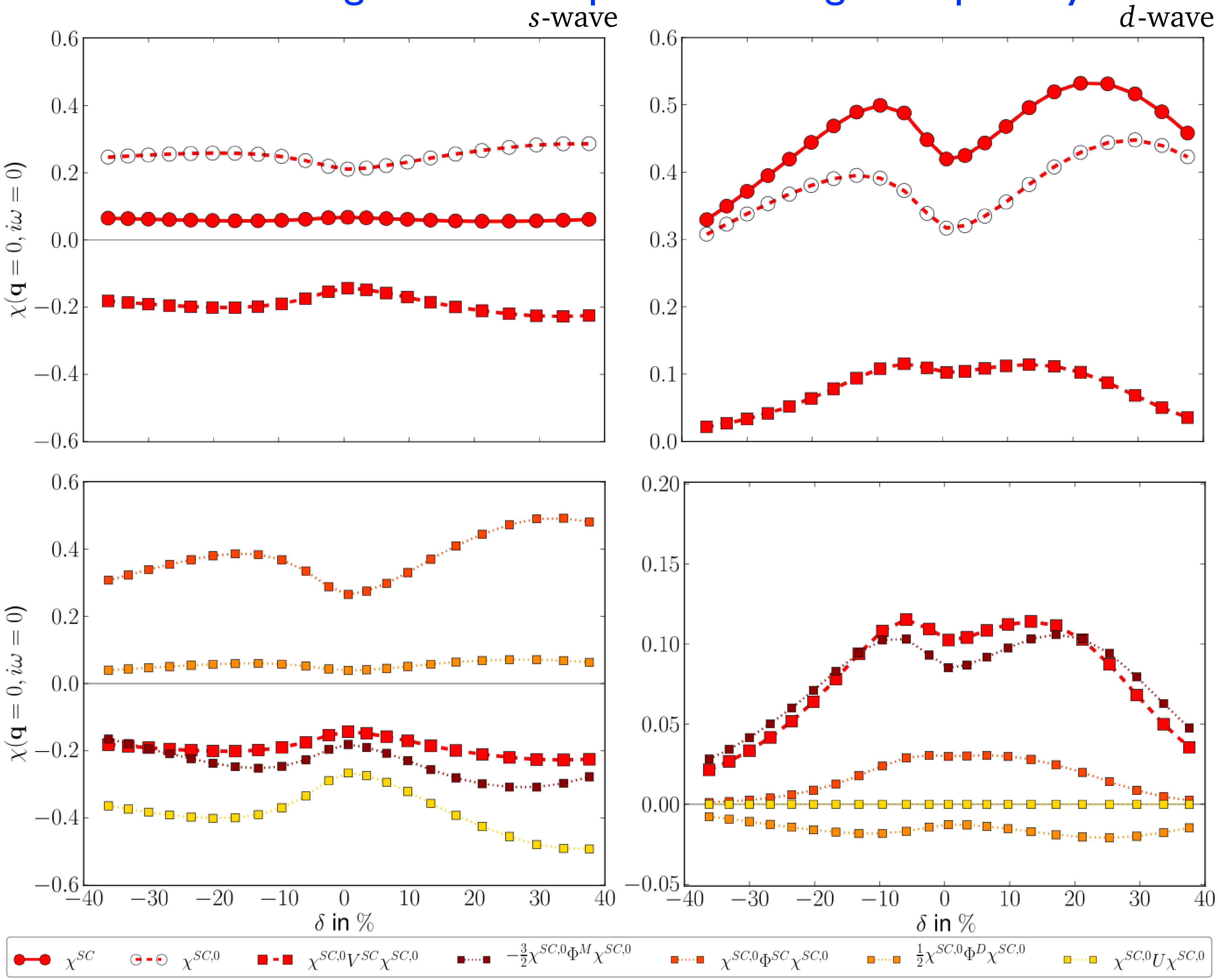
in particular by

crossed p-h channel

Gunnarsson *et al.*, PRL (2015)

2ℓ fRG study

Fluctuation diagnostics of superconducting susceptibility



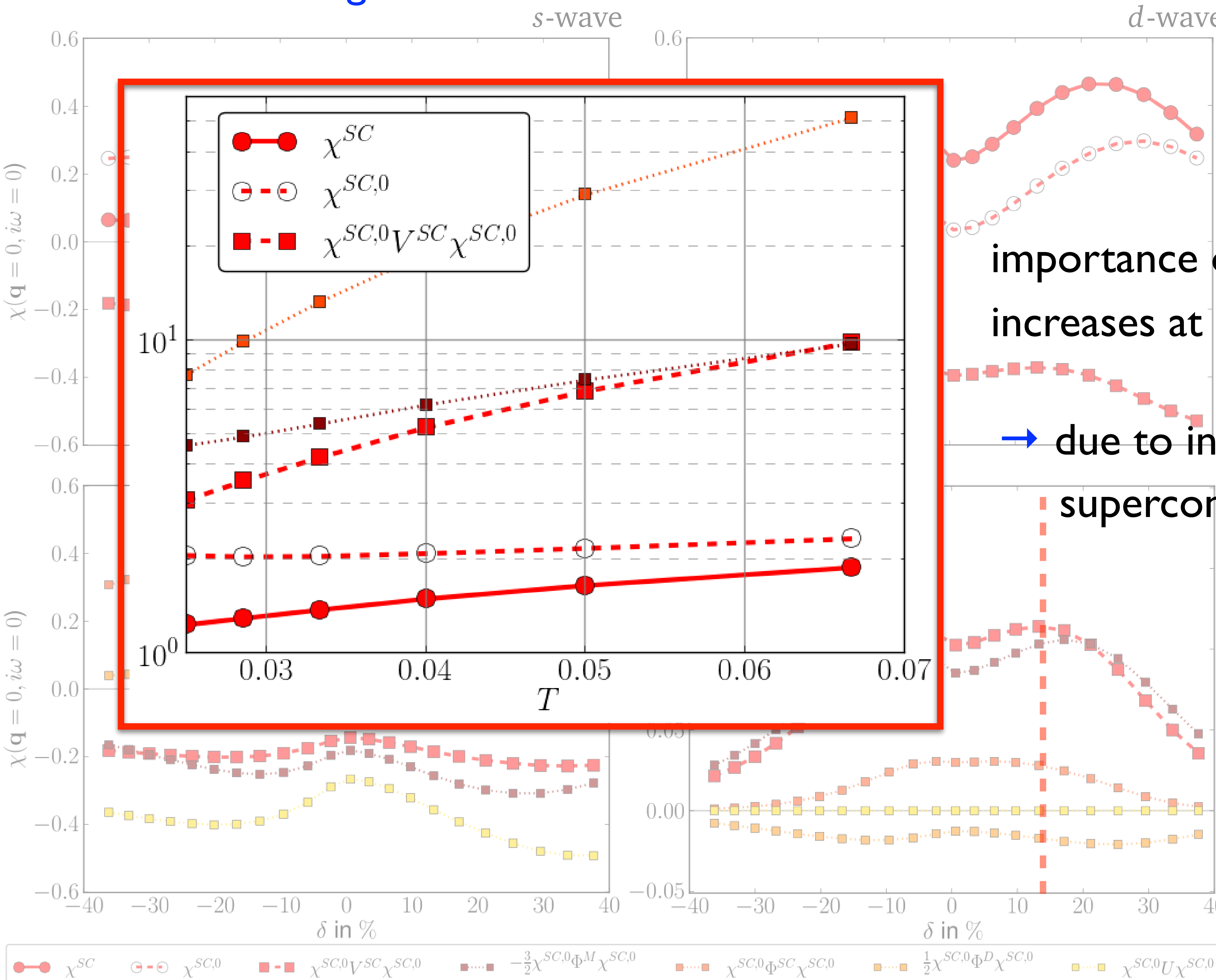
- cancellation effects in s-wave

- d-wave still bubble dominated

- leading vertex contribution due to impact of ***magnetic channel***

2ℓ fRG study

Fluctuation diagnostics



importance of vertex corrections increases at lower T

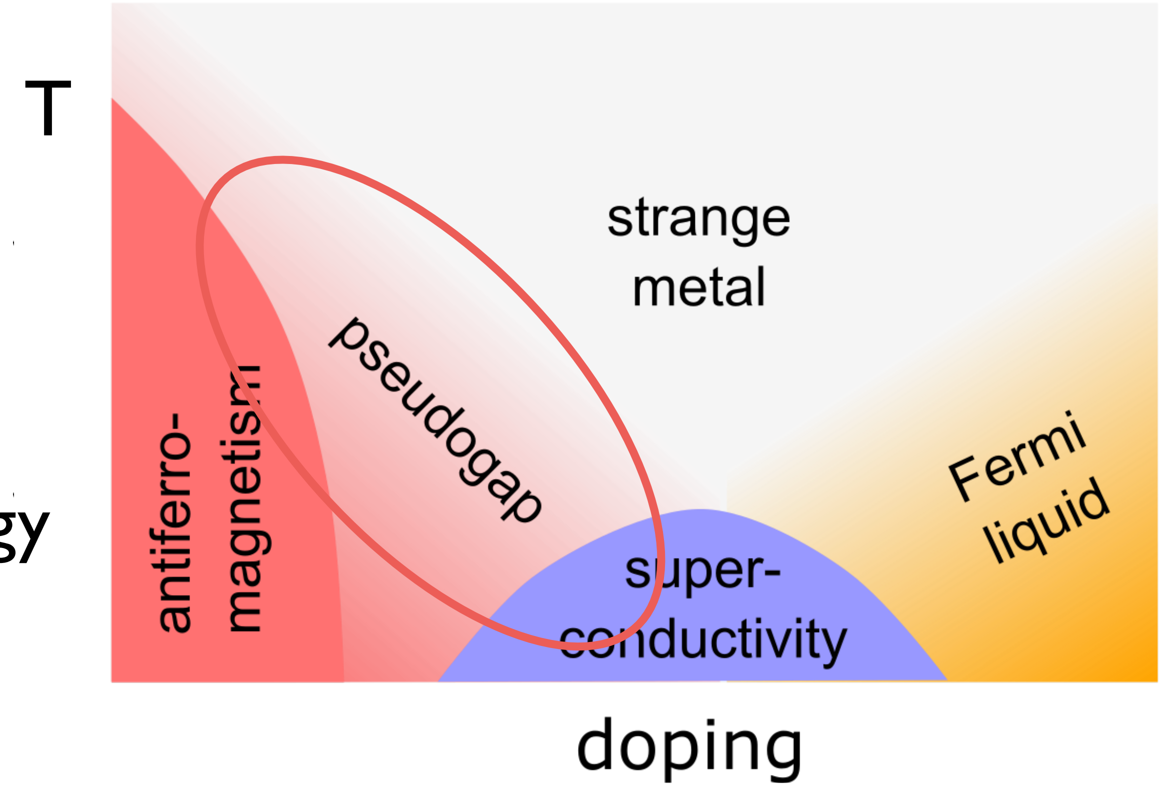
→ due to influence of superconducting channel

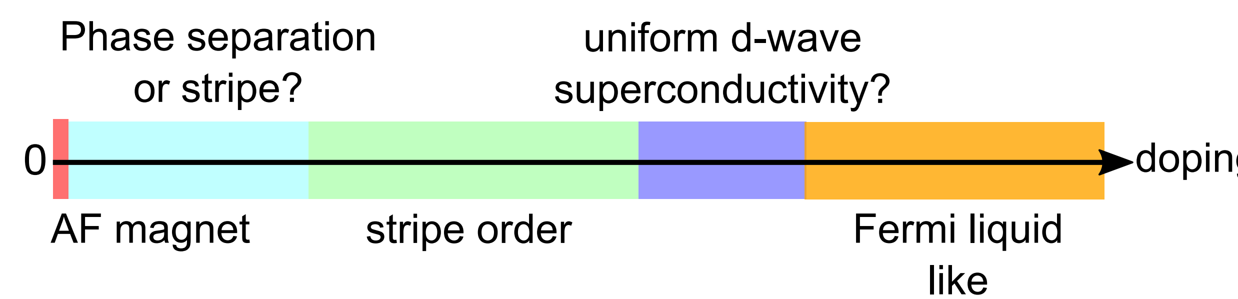
The doped 2D Hubbard model at weak coupling

Pseudogap

refers to a momentum-dependent suppression of the single-particle spectral function near the Fermi energy

→ induced by long-range AF fluct.





underlying mechanism can be understood already at 2. order of self-energy:

Ornstein-Zernike form of spin susceptibility

$$\chi_{\mathrm{sp}}(\mathbf{q}, i\Omega_n = 0) = \frac{A}{(\mathbf{q}-\mathbf{Q})^2 + \xi^{-2}}$$

predicts spectral gap for momenta close to the hot spots

Vilk et al., JdP (1997); Wu *et al.*, PRB (2017); Hille *et al.*, PRReasearch (2020)

2ℓ fRG results

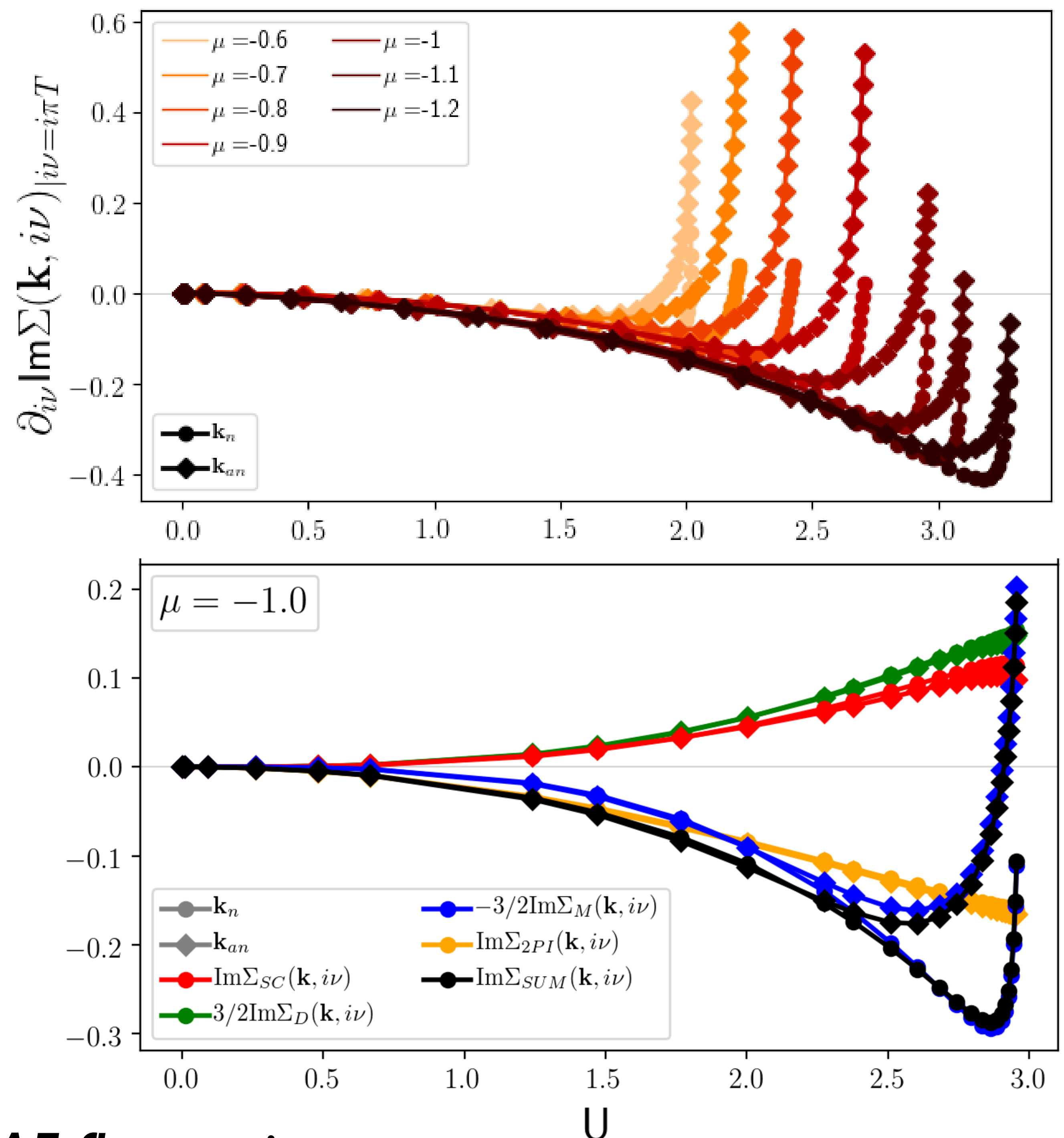
→ Poster H. Braun

Pseudogap opening

for small T quasi-particle weight determined by slope of Im Σ at lowest frequencies

- momentum-selective pseudogap opening
- fluctuation diagnostics: (incomm.) AF fluctuations responsible for pseudogap opening also at finite doping

t'=-0.15t, T=0.05t



→ pseudogap ***driven by long-ranged AF fluctuations***

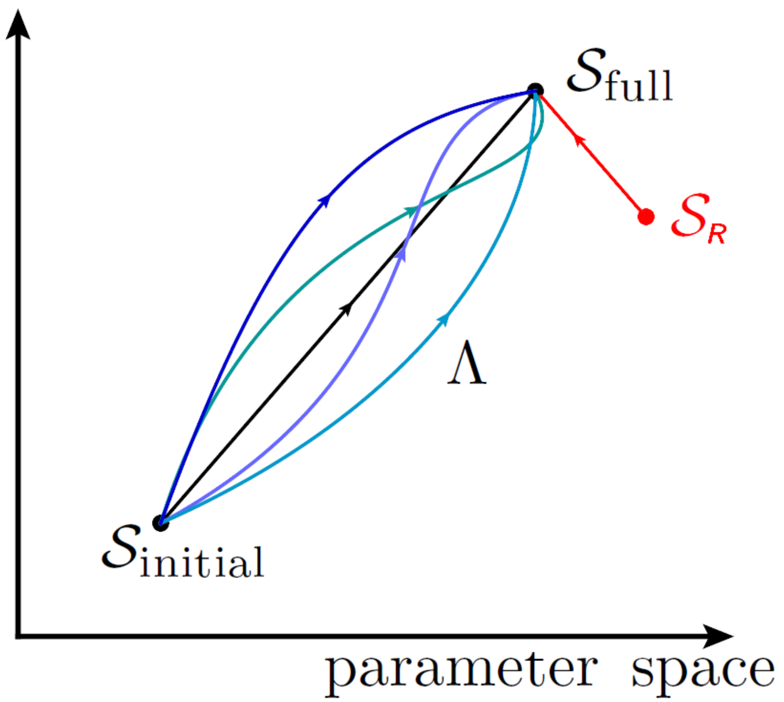
Extension to correlated starting points

exploit freedom of choice for cutoff and $\mathcal{S}_{\text{initial}}$

→ include correlation effects already in initial conditions

→ reduce truncation error by starting 'closer' to final action

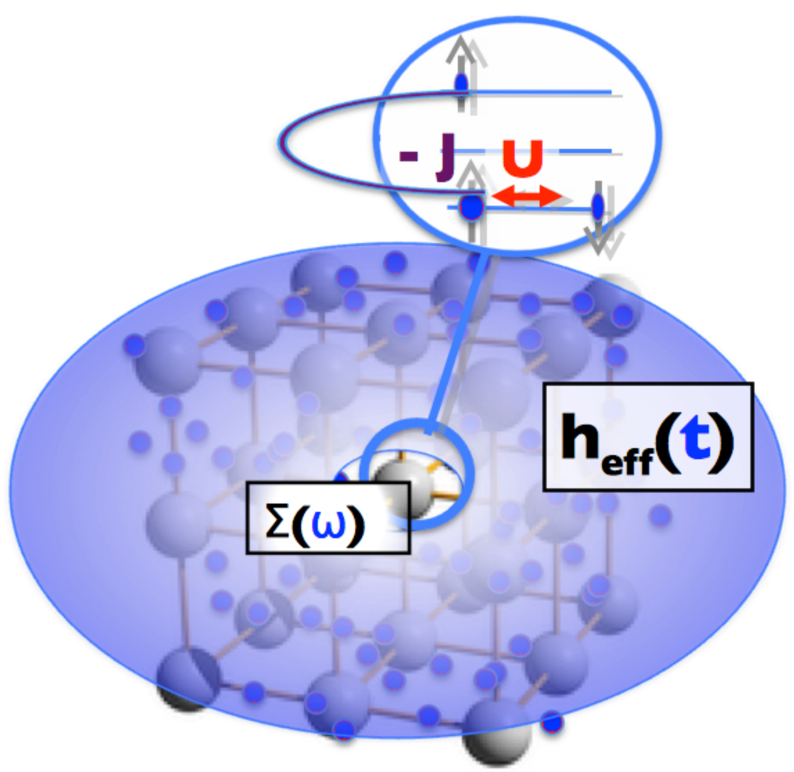
Wentzell *et al.*, PRB (2015)



Starting from Dynamical Mean Field Theory (DMFT):

non-perturbative treatment of local correlations

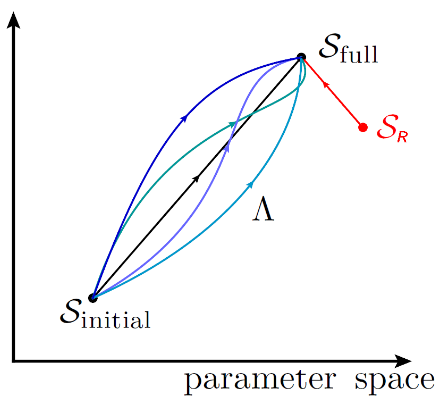
- exact solution in the limit $d \to \infty$
- strong-coupling regime accessible

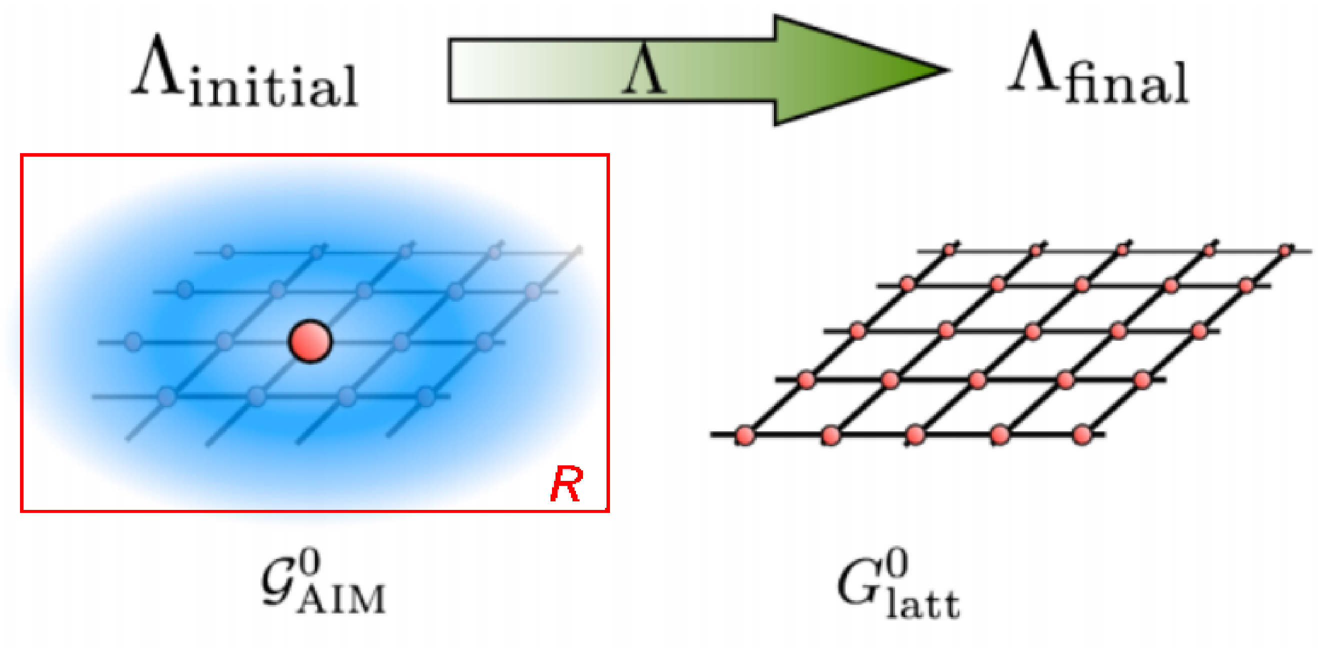


BUT lack of *non-local* spatial correlations

Metzner and Vollhardt, PRL (1989); Georges and Kotliar, PRB (1992)

Combination of DMFT and fRG: DMF^{2}RG





- **new initial condition:** local DMFT solution $\Sigma^{\Lambda_{\rm in}} = \Sigma^{\rm DMFT}(i\omega)$

$$\Gamma^{\Lambda_{\rm in}} = \Gamma^{\rm DMFT}(i\omega_1', i\omega_2', i\omega_1)$$

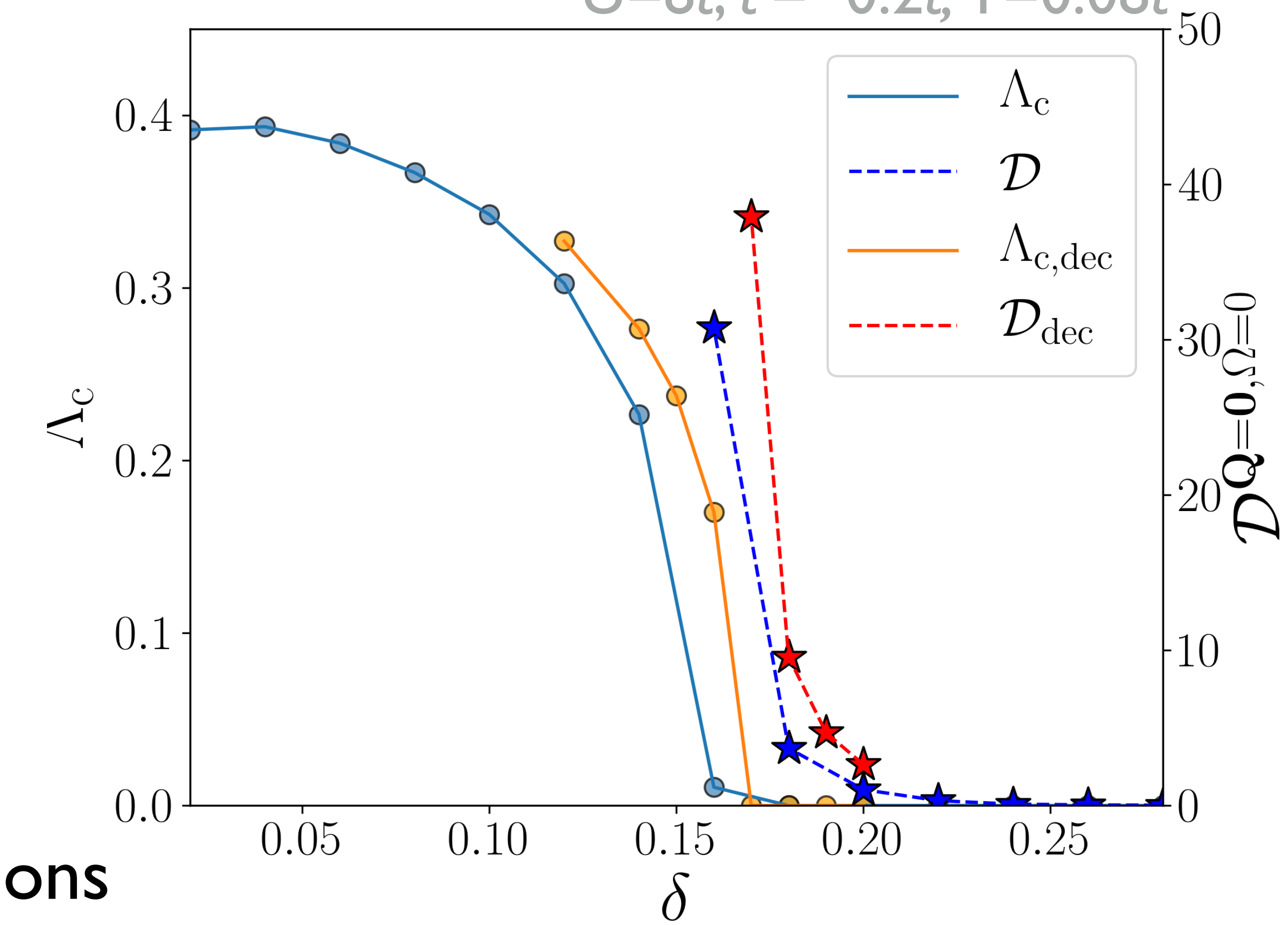
- *local* correlations fully accounted for by DMFT starting point
- *non-local* correlations generated by RG flow unbiasedly in all channels !

Taranto *et al.*, PRL (2014); Vilardi *et al.*, PRB (2019)

(1ℓ) DMF^{2}RG results

Critical flow parameter for AF instability and maximal d-wave pairing interaction

- magnetic instability for doping range where experimentally pseudogap opening is observed
- sizable d-wave pairing interaction at edge of AF regime
  (at lower dopings flow has to be stopped before it can fully develop)
  → driven by strong magnetic fluctuations
- no major impact of channel interplay



→ d-wave pairing driven by (nonlocal) magnetic fluctuations

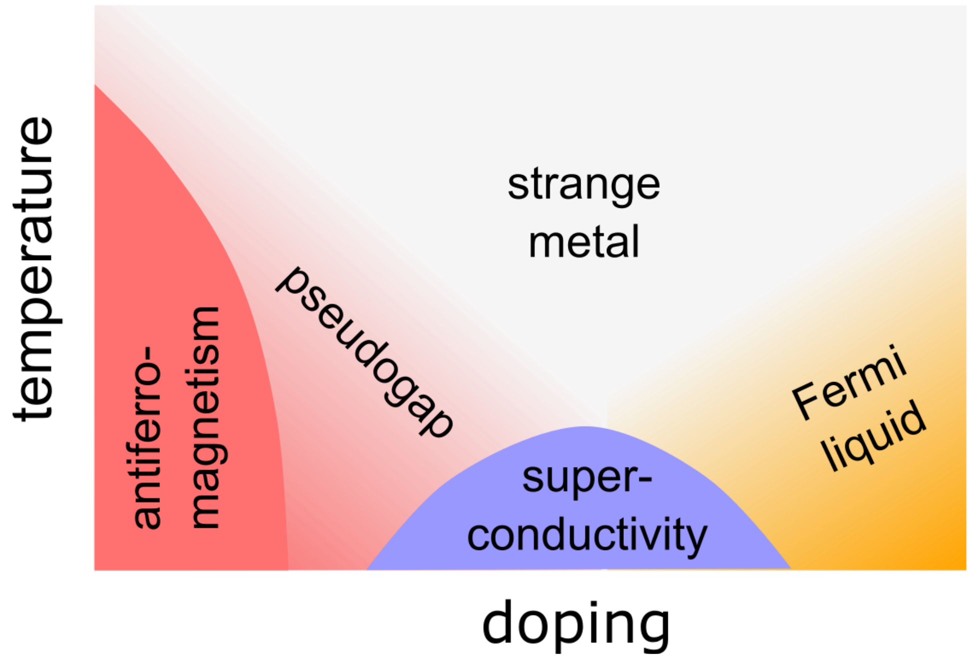
Vilardi *et al.*, PRB (2019)

Summary and outlook

→ controlled numerical solutions in various regions of the phase diagram available

→ despite all progress, many open challenges remain:

- precise locations of phase boundaries, in particular of d-wave superconductivity
- extension to more orbitals and/or longer ranged interactions
- real-time evolution and real frequency observables



Qin *et al.* (2021)

Thank you!

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Deutsche Forschungsgemeinschaft

Single-boson exchange representation

→ Poster K. Fraboulet

Decomposition in terms of *U*-reducibility

Krien *et al.*, PRB (2019)

$$\underbrace{U \pm \phi^X_{kk'}(q)}_{\text{2P-reducible}} = \underbrace{h^X_k(q)\, D^X(q)\, h^X_{k'}(q)}_{U\text{-reducible}} + \underbrace{\mathcal{R}^X_{kk'}(q)}_{U\text{-irreducible}}$$

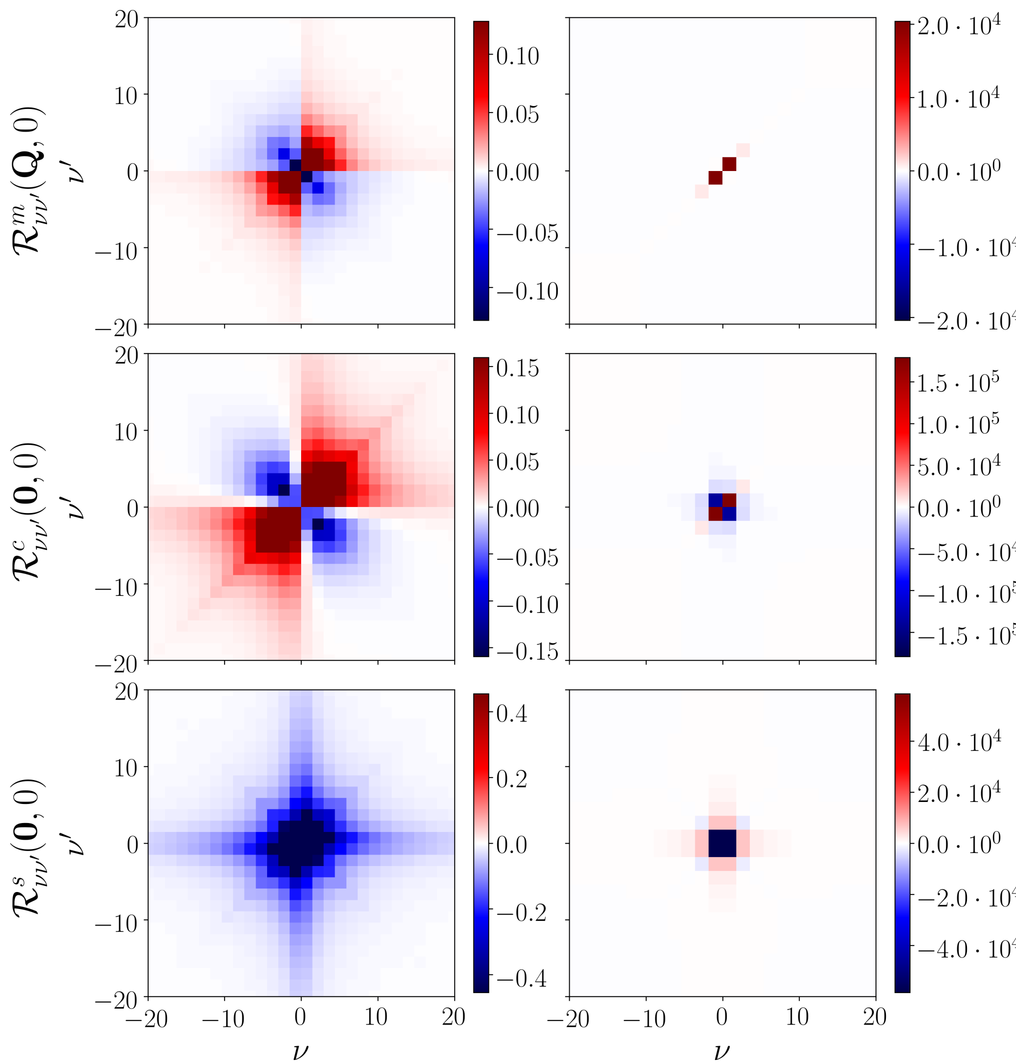
→ allows to

- simplify vertex complexity
- clearly identify collective excitations

→ extremely localised frequency structures in rest function at strong coupling

→ feasibility of multiloop DMF^{2}RG

$U = 4t$ $U = 16t$



Bonetti *et al.*, PRResearch (2021)