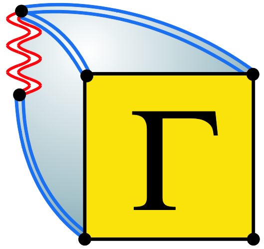
Dynamical vertex approximation (DΓA)

Karsten Held (TU Wien)

Jülich, September 18st , 2014

- **Reducibility & parquet equation**
- **Methods: DΓA, DF, 1PI, DMF²RG**
- **Critical exponents 3D Hubbard model**
- **Fate of false Mott transition in 2D Hubbard model**



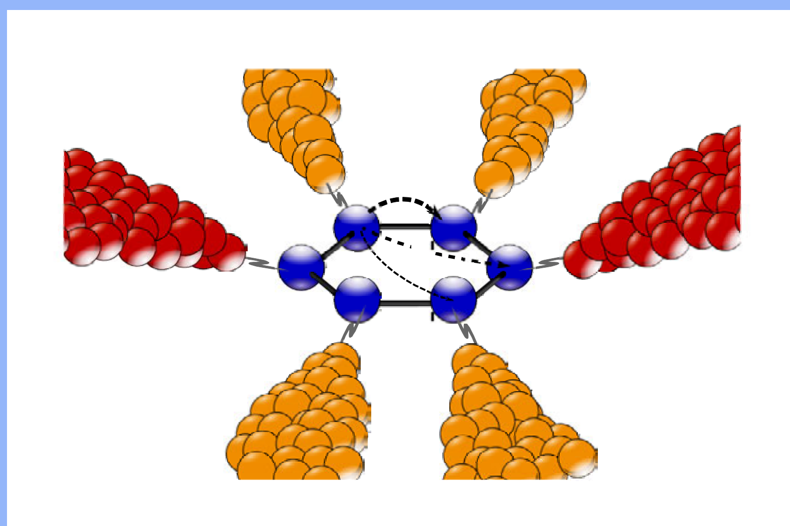
Motivation: why correlations beyond DMFT

(a) quantum criticality

(b) high temperature superconductivity

(c) heterostructures

(d) nanostructures and molecules

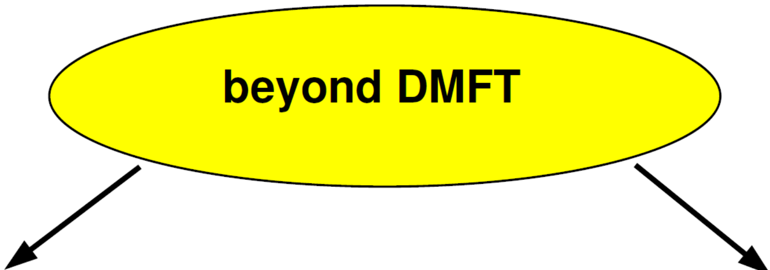


DΓA: weak localization in nanostructures
quantum chemistry

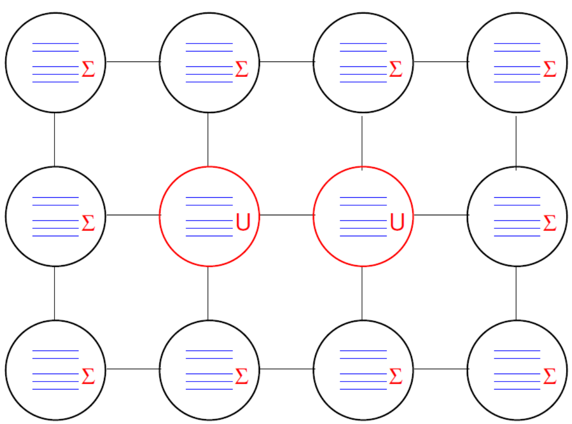
Two routes beyond DMFT:

Correlations beyond DMFT:

d-, p-wave superconductivity, pseudogaps, (para-)magnons, quantum criticality

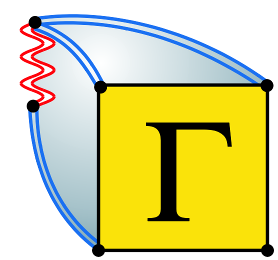


Cluster extensions



Hettler et al.'98, Lichtenstein, Katsnelson'00
Kotliar et al.'01, Potthoff et al.'03

diagrammatic extensions



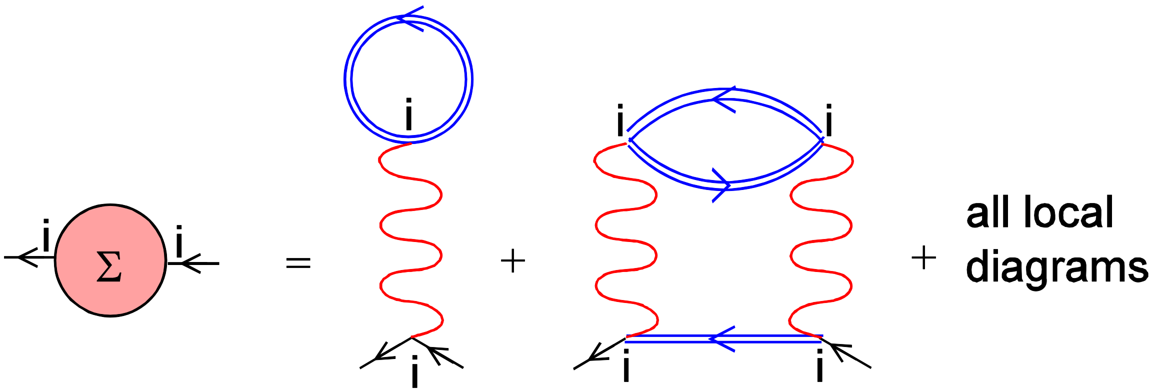
DΓA: Toschi, Katanin, KH'07
DF: Rubtsov et al.'08
… 1PI, DMF^{2}RG

Dynamical vertex approximation (DΓA)

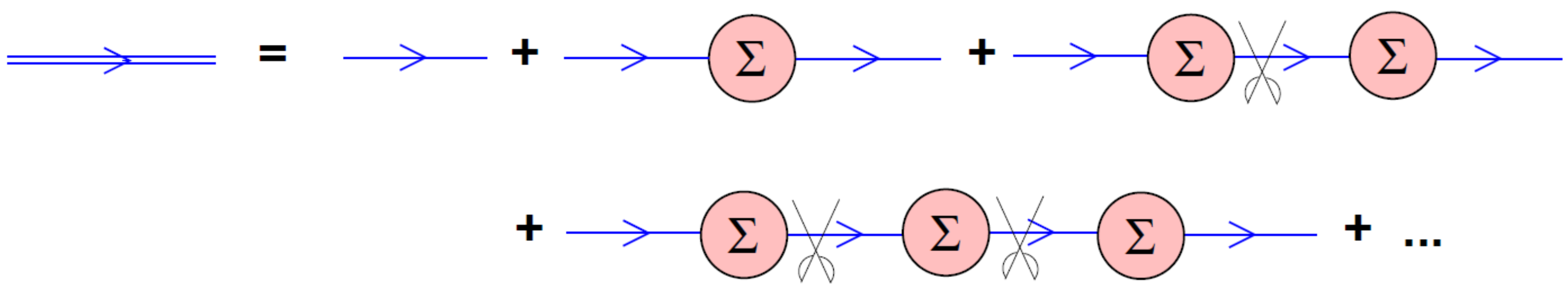
Resummation of Feynman diagrams in terms of locality

***local* n-particle fully irreducible vertex**

n=1: DMFT - local 1-particle fully irreducible vertex Σ



Σ: one-particle irreducible one-particle vertex



Dynamical vertex approximation (DΓA)

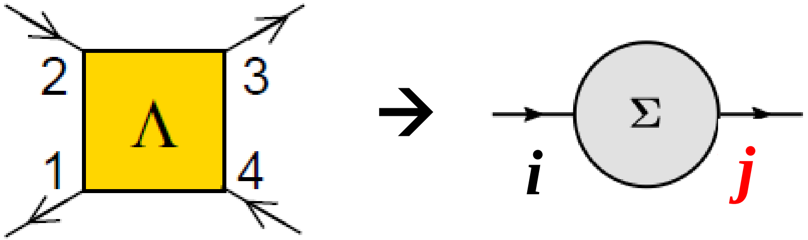
Resummation of Feynman diagrams in terms of locality

***local* n-particle fully irreducible vertex**

n=1: DMFT - local 1-particle fully irreducible vertex Σ

n=2: DΓA - local 2-particle fully irreducible vertex Λ

→ non-local correlations

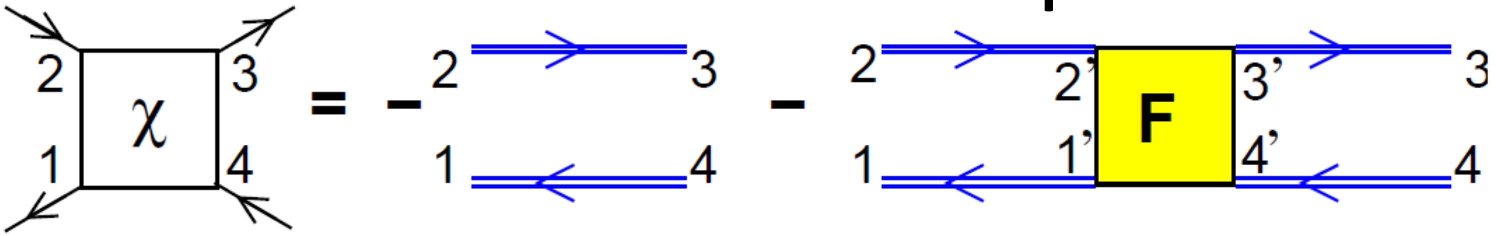


...

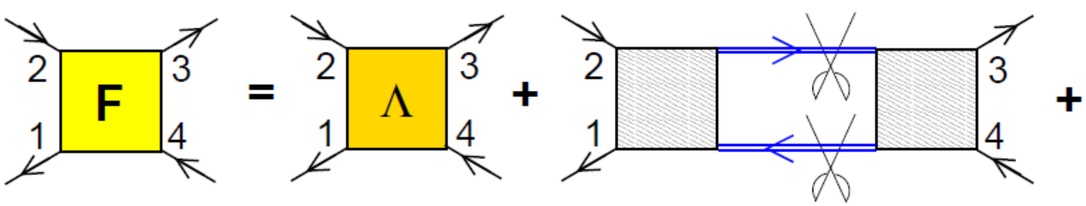
n→∞: exact

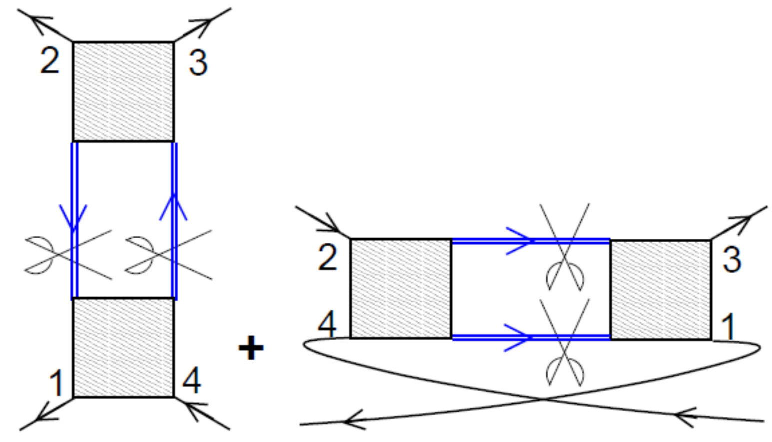
Two-particle irreducibility

full 2-particle vertex F



3 ways (channels) to cut two lines





$F = \Lambda + \Phi_{ph} + \Phi_{\overline{ph}} + \Phi_{pp}$

full vertex

parquet equation

Two-particle irreducibility

Parquet equation:

$$F = \Lambda + \Phi_{ph} + \Phi_{\overline{ph}} + \Phi_{pp}$$

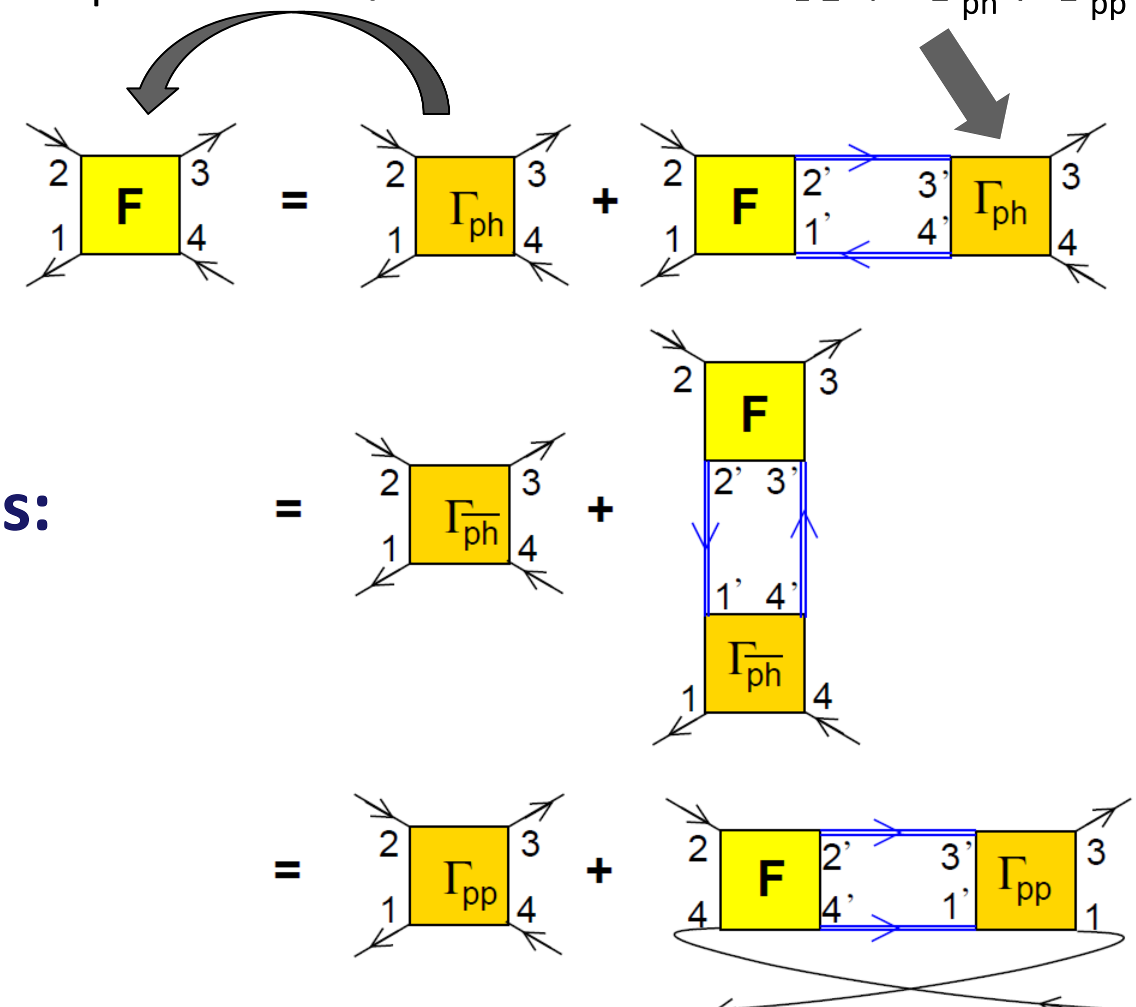
$$F = \Phi_r + \Gamma_r$$

$$r \in \{ph, \overline{ph}, pp\}$$

defines Γ_r

$$\Phi_{ph} = F - \Gamma_r$$

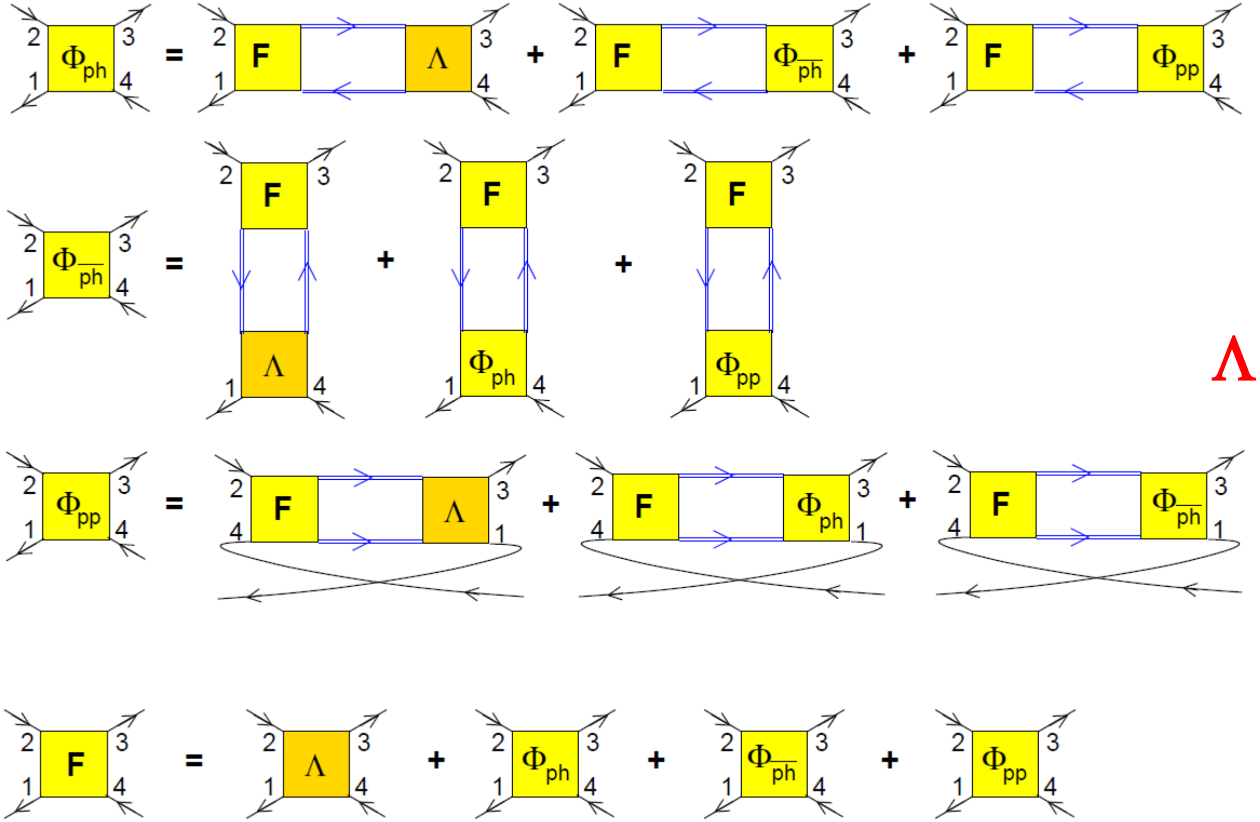
$$F - \Phi_{ph} = \Lambda + \Phi_{\overline{ph}} + \Phi_{pp}$$



Bethe Salpeter equations:

$$F = \Gamma_r + \int F\,GG\,\Gamma_r$$

Parquet equations



Λ given

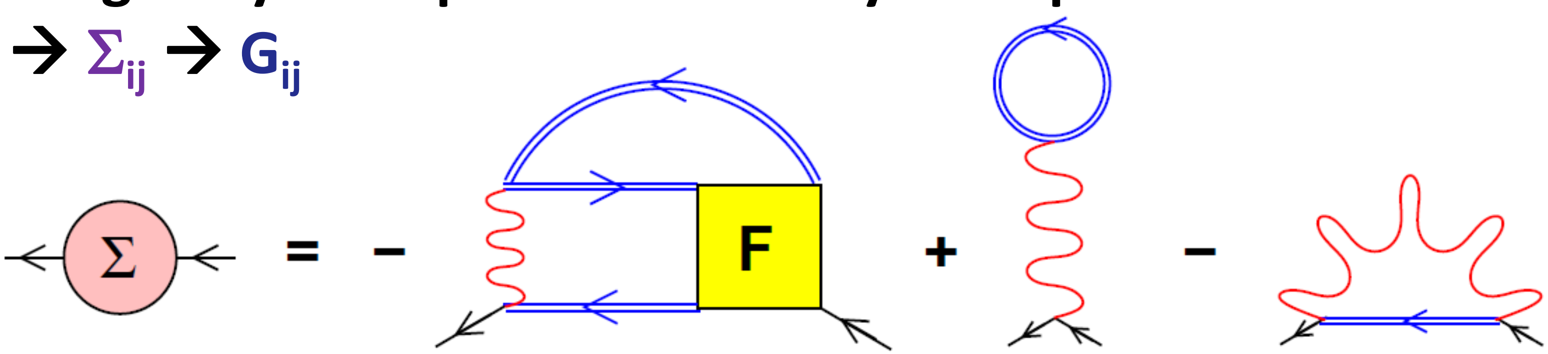
→ F, Φ_{ph}, $\Phi_{\overline{ph}}$, Φ_{pp}, Σ, G

Λ = U (parquet approx.)

Λ = Λ_{loc} (DΓA)

Schwinger-Dyson eq. of motion & Dyson equation

$F_{ijkl} \rightarrow \Sigma_{ij} \rightarrow G_{ij}$



Why DΓA?

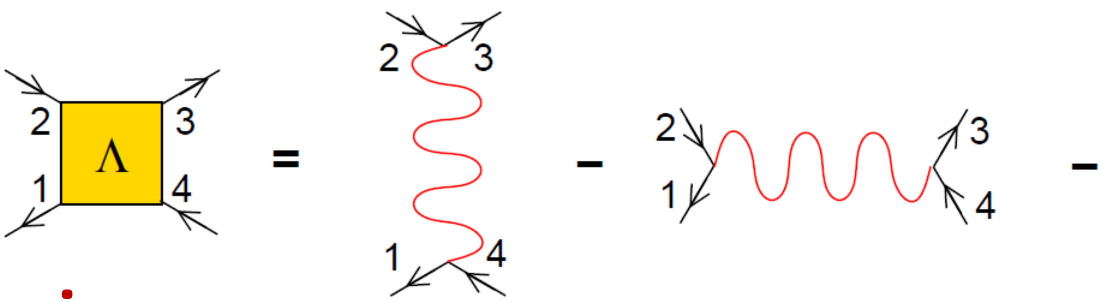
1) Physics: our understanding either based on

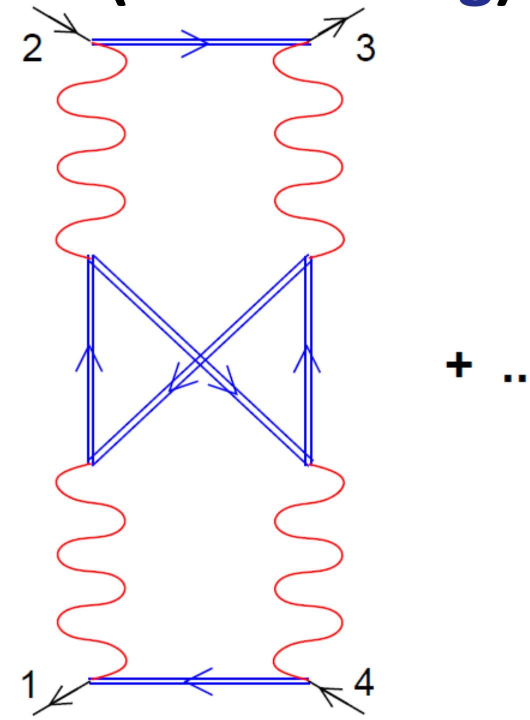
1-particle [qp renormalization, Mott transition etc…] or

2-particle level [(para)magnons, (quantum)criticality]

2) Diagrammatics:

includes DMFT, plus non-local contributions (few missing)



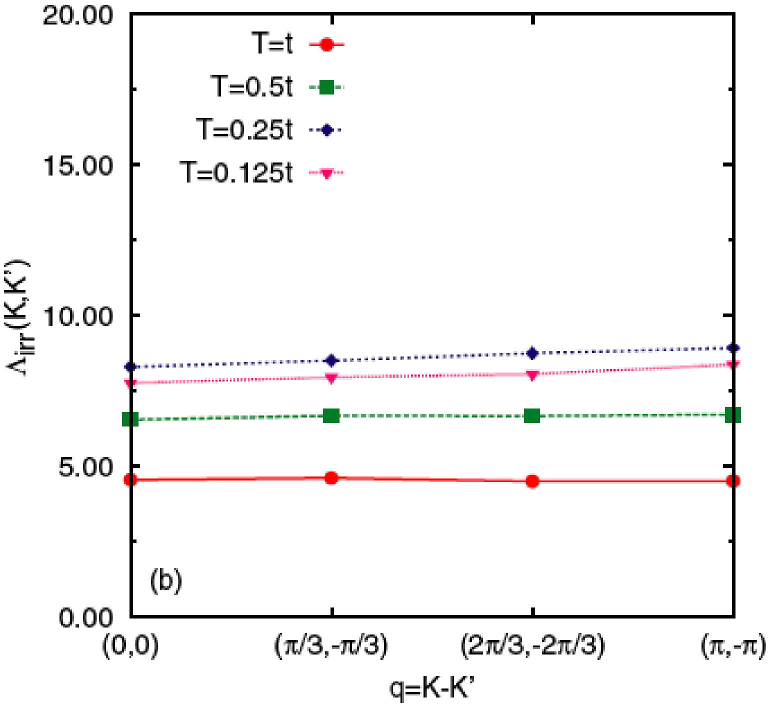


3) Numerics:

fully irreducible vertex is local.

3) Fully irreducible vertex is local!

The fully irreducible vertex Λ_{irr} is local (*k*-independent) !

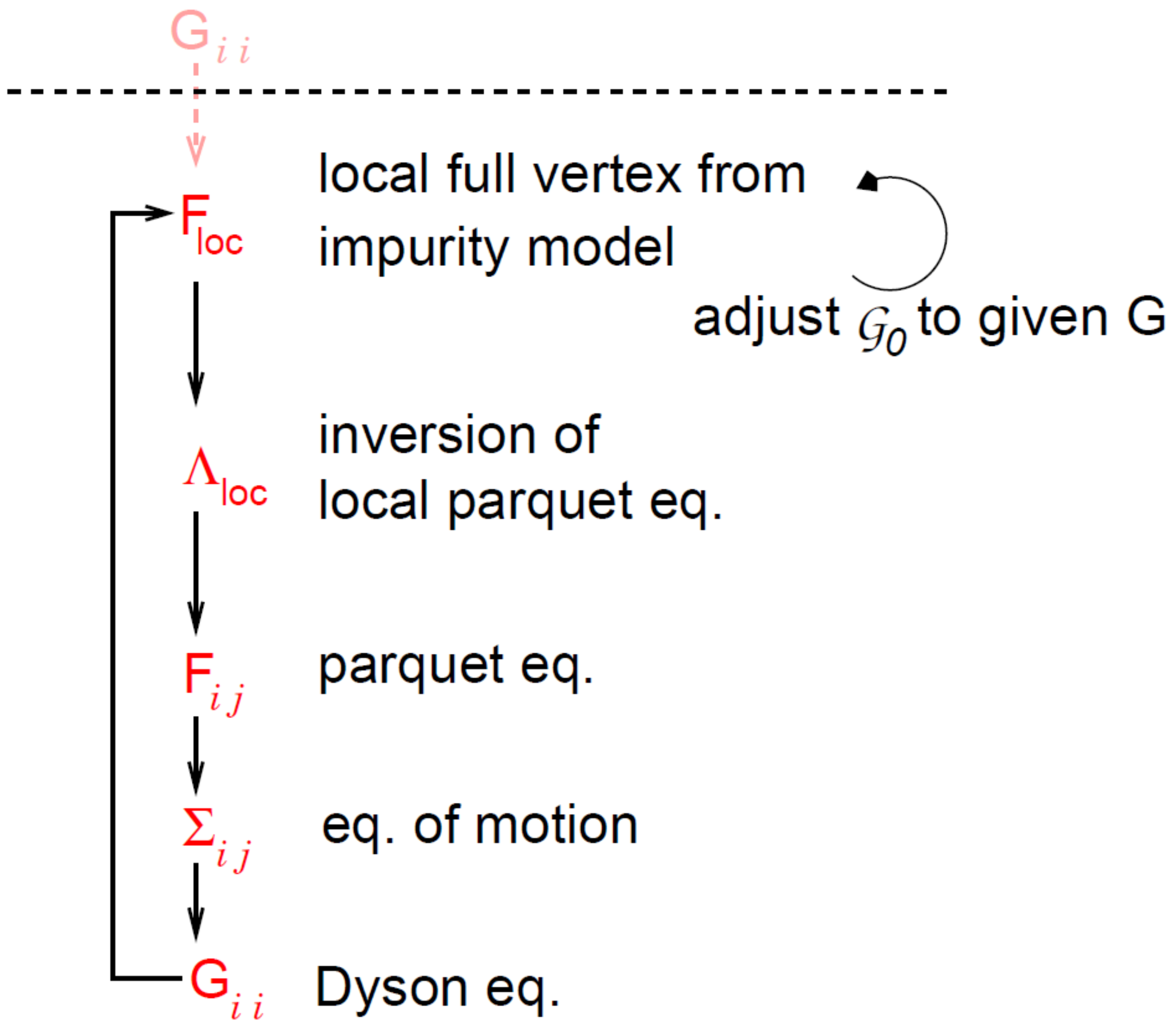


DCA, 2D-Hubbard model, U=4t, n=0.85,

$\nu=\nu'=\pi/\beta$, $\omega=0$

Maier et al. PRL 96 (2006)

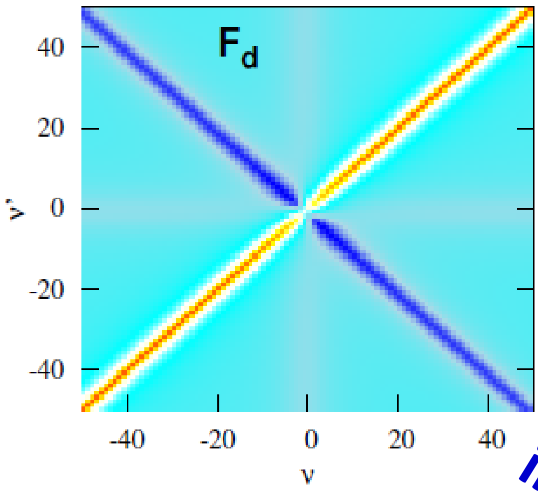
DΓA algorithm



Calculation of local irreducible vertex

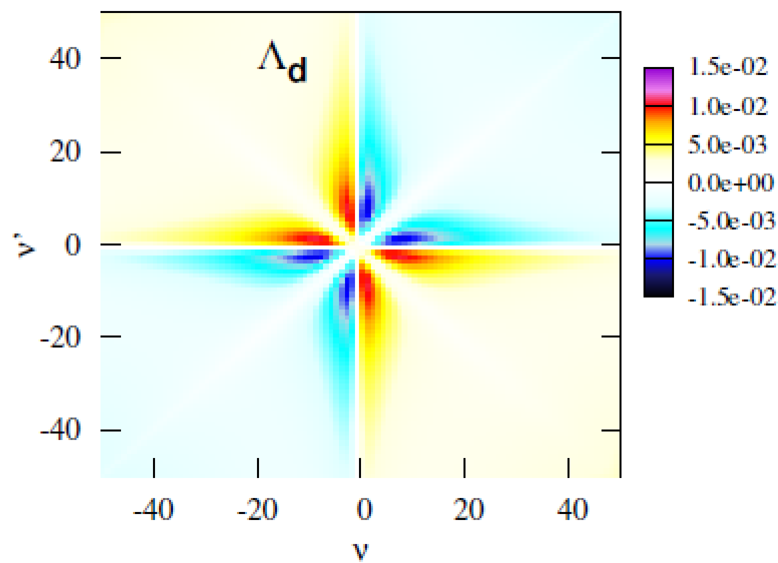
full vertex F (from SIAM, QMC or ED)

Rohringer, Valli, Toschi '12



inversion of parquet eq.

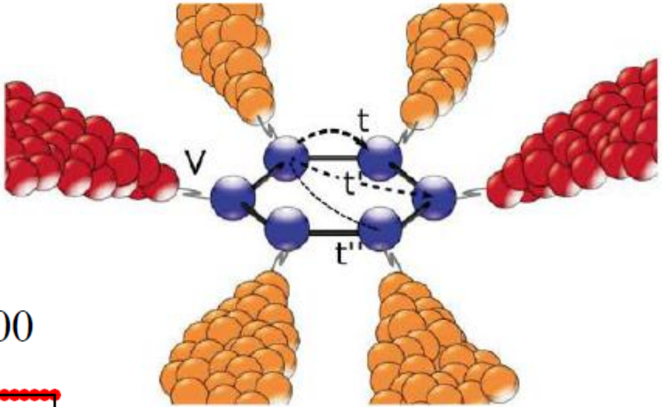
fully irreducible vertex Λ

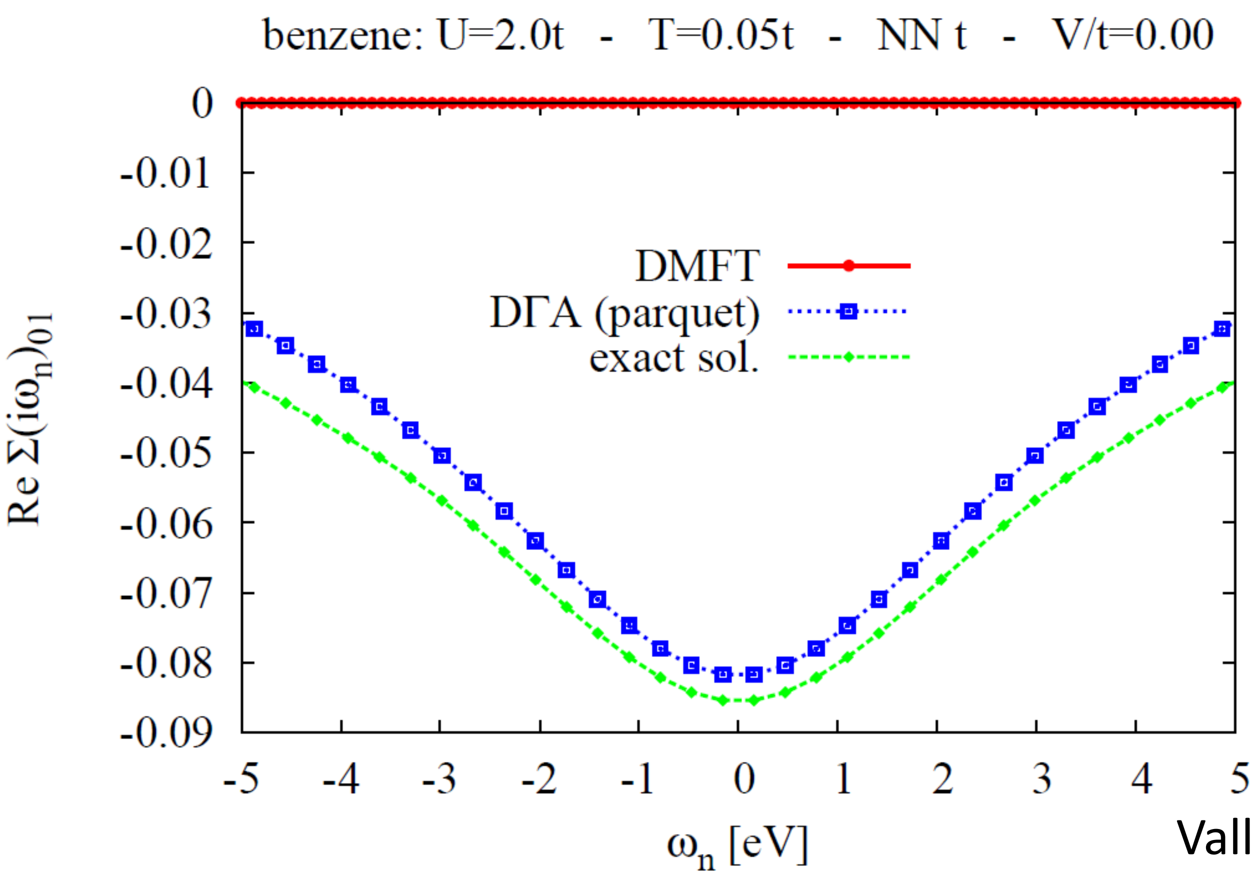


Λ ω-dep. but *k*-indep.!

DΓA with parquet equation

Benzene Hubbard ring:
comparison non-local Σ
to exact solution





Valli, Rohringer, Toschi, KH'13

Other 2-particle vertex approaches:

Dual Fermions (DF):

Rubtsov, Lichtenstein, Katsnelson ’08

functional integral with action of dual Fermions

$$S[f,f^*] = \sum_{\omega k \sigma} g_\omega^{-2} \left((\Delta_\omega - \epsilon_k)^{-1} + g_\omega \right) f^*_{\omega k \sigma} f_{\omega k \sigma} + \sum_i V_i$$

$$V[f_i,f_i^*] = -\gamma^{(4)}_{1234} f_1^* f_2 f_3^* f_4 + \gamma^{(6)}_{123456} f_1^* f_2 f_3^* f_4 f_5^* f_6 + \dots$$

1-particle reducible vertex γ

Rohringer et al. PRB ‘13

1PI: functional integral using 1-particle irreducible vertex

$$Z[\eta,\eta^+] = \int d[\widetilde{c},\widetilde{c}^+] \exp\left\{ \widetilde{c}^+_{k\sigma} \left[\zeta_\nu^{-1} - G_{0k}^{-1} \right]^{-1} \widetilde{c}_{k\sigma} + (\eta^+_{k\sigma} + \widetilde{c}^+_{k\sigma}) \phi_{k\sigma} + \phi^+_{k,\sigma} (\eta_{k\sigma} + \widetilde{c}_{k\sigma}) - \Gamma_{\mathrm{DMFT}}[\phi,\phi^+] \right\}$$

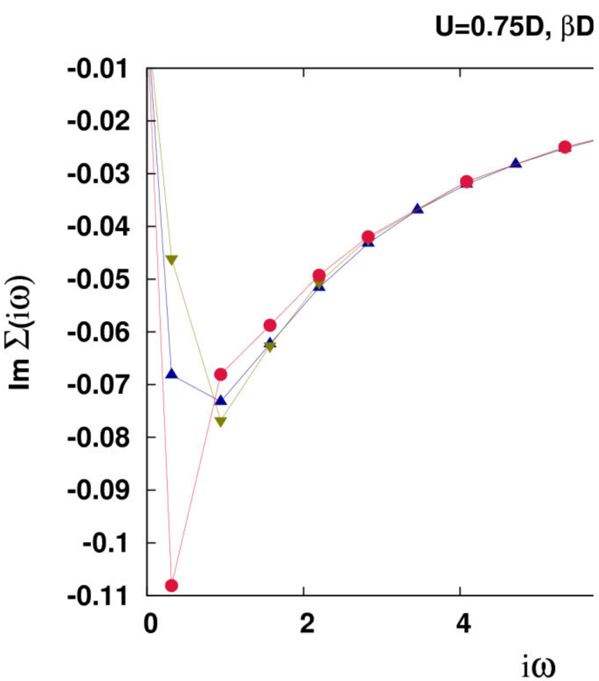
1PI unifies positive features of DF and DΓA

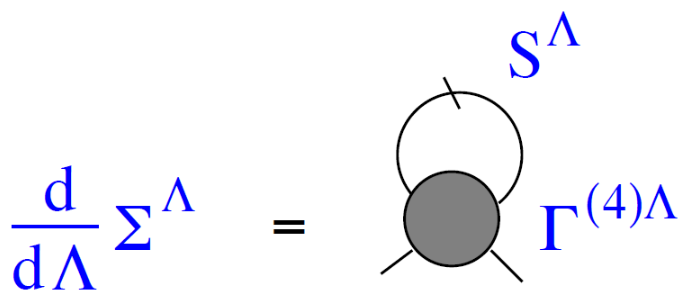
Other 2-particle approaches: DMF^{2}RG

Taranto et al.PRL'04

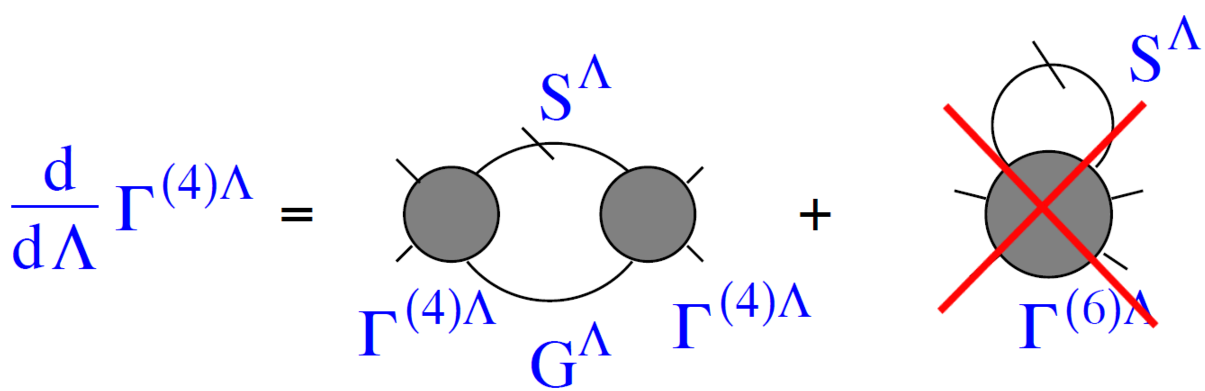
DMFT 1PI verte^2 Γ → fRG

2d Hubbard model





taken from Metzner et al.'12



Overview 2-particle vertex approaches:

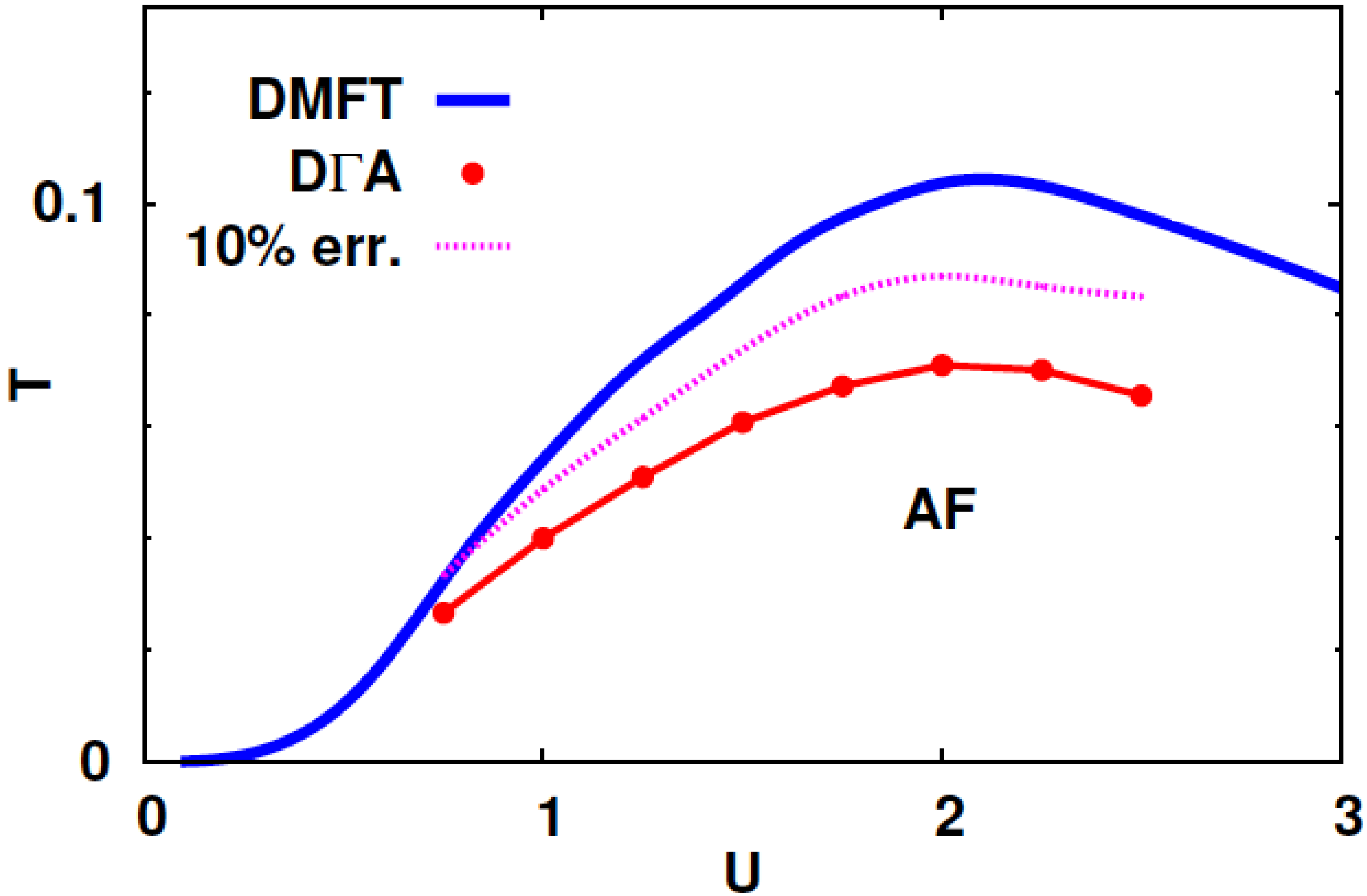
Method	local 2-particle vertex	Feynman diags
DF	1-particle reducible vertex, here F_{loc}	2nd order, ladder, parquet
1PI	1-particle irreducible vertex F_{loc}	ladder
DMF^{2}RG	1-particle irreducible vertex F_{loc}	RG flow
ladder DΓA	2-particle irreducible vertex in r Γ_r	ladder
full DΓA	2-particle fully irreducible vertex Λ	parquet

DΓA results: 3D and 2D Hubbard model

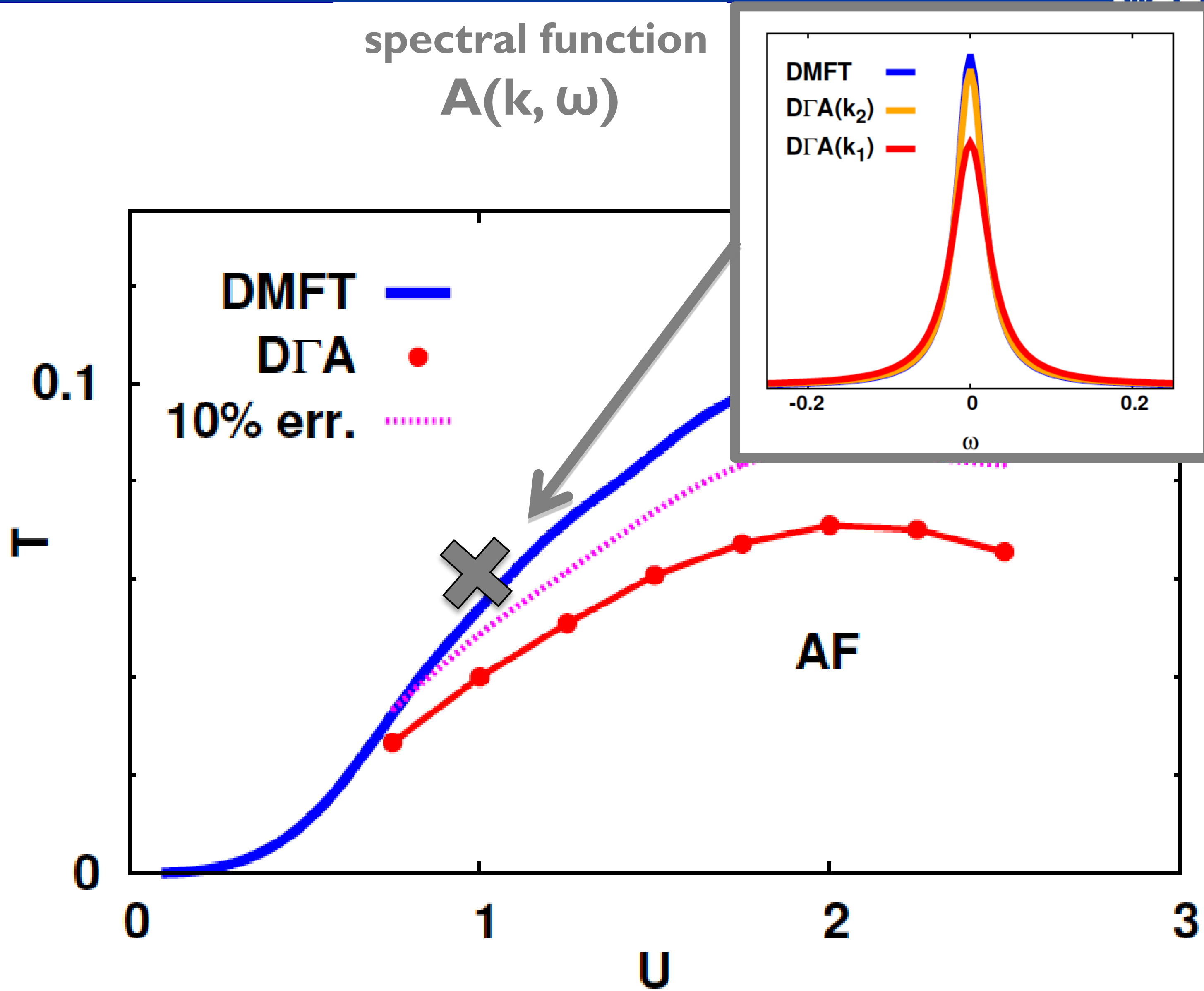
DΓA results in 3 dimensions

Phase diagram: Hubbard model in **d=3** (cubic lattice D=1, half-filling)

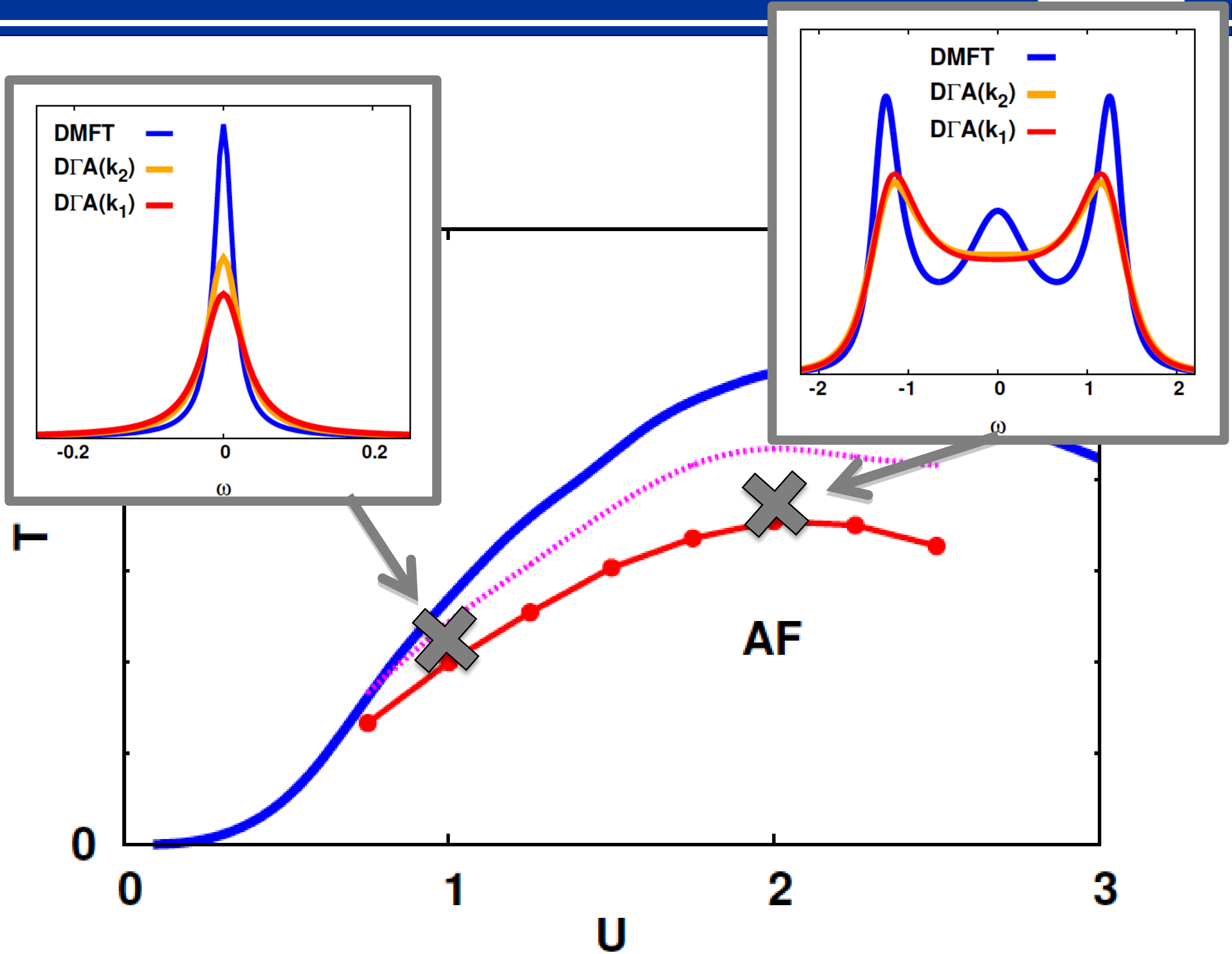
G. Rohringer *et al.*, PRL (2011)



DΓA results in 3 dimensions

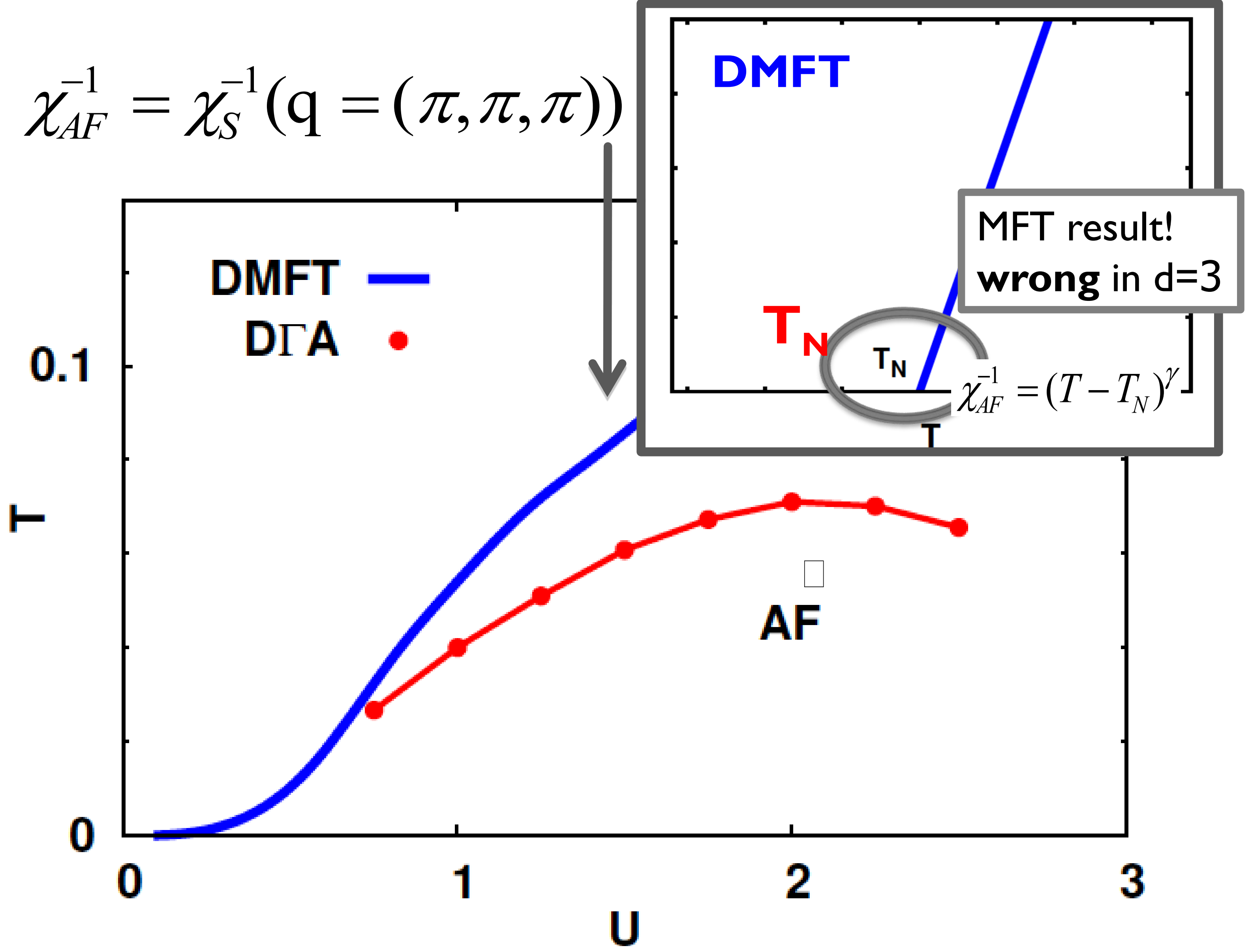


DΓA results in 3 dimensions

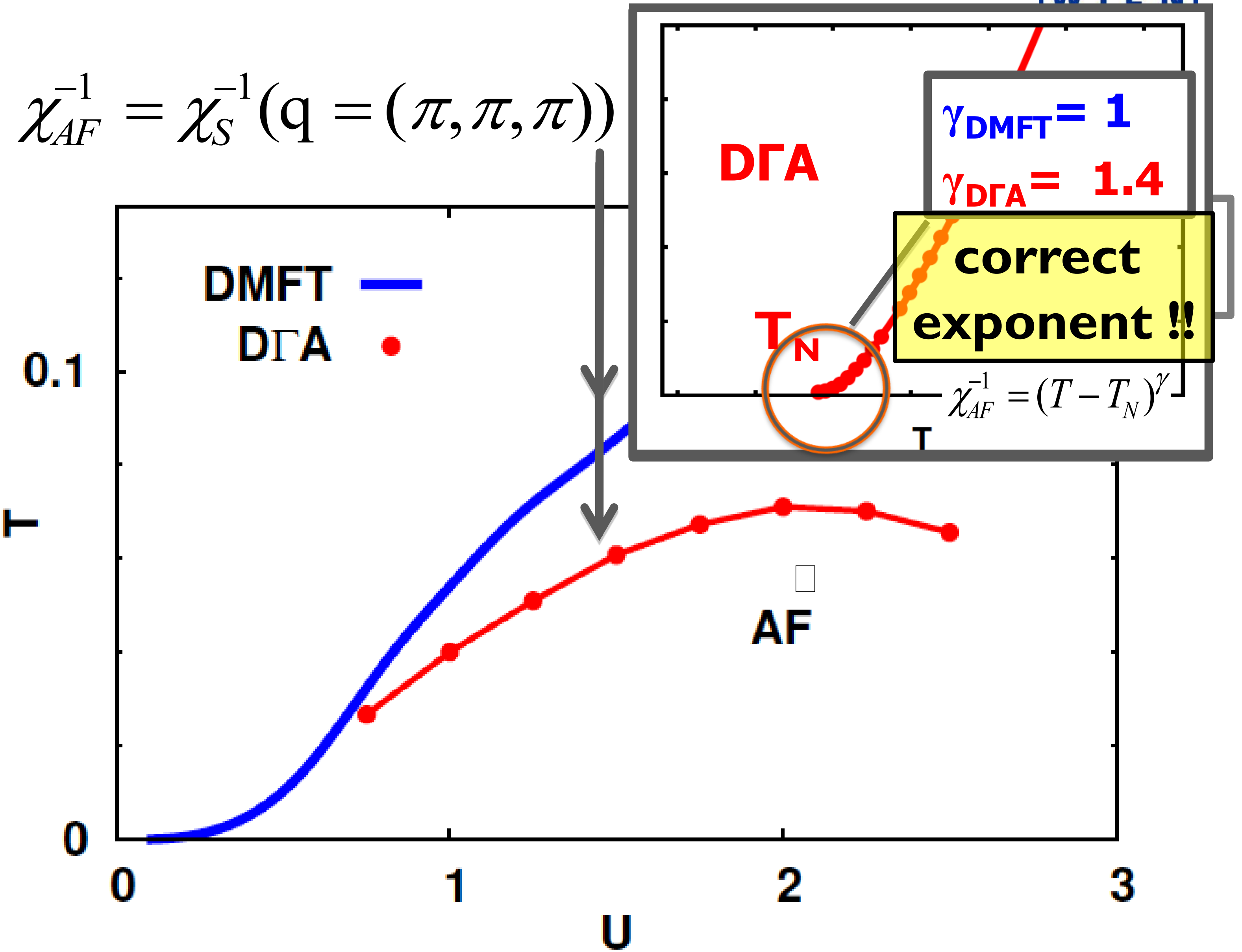


DΓA results in 3 dimensions

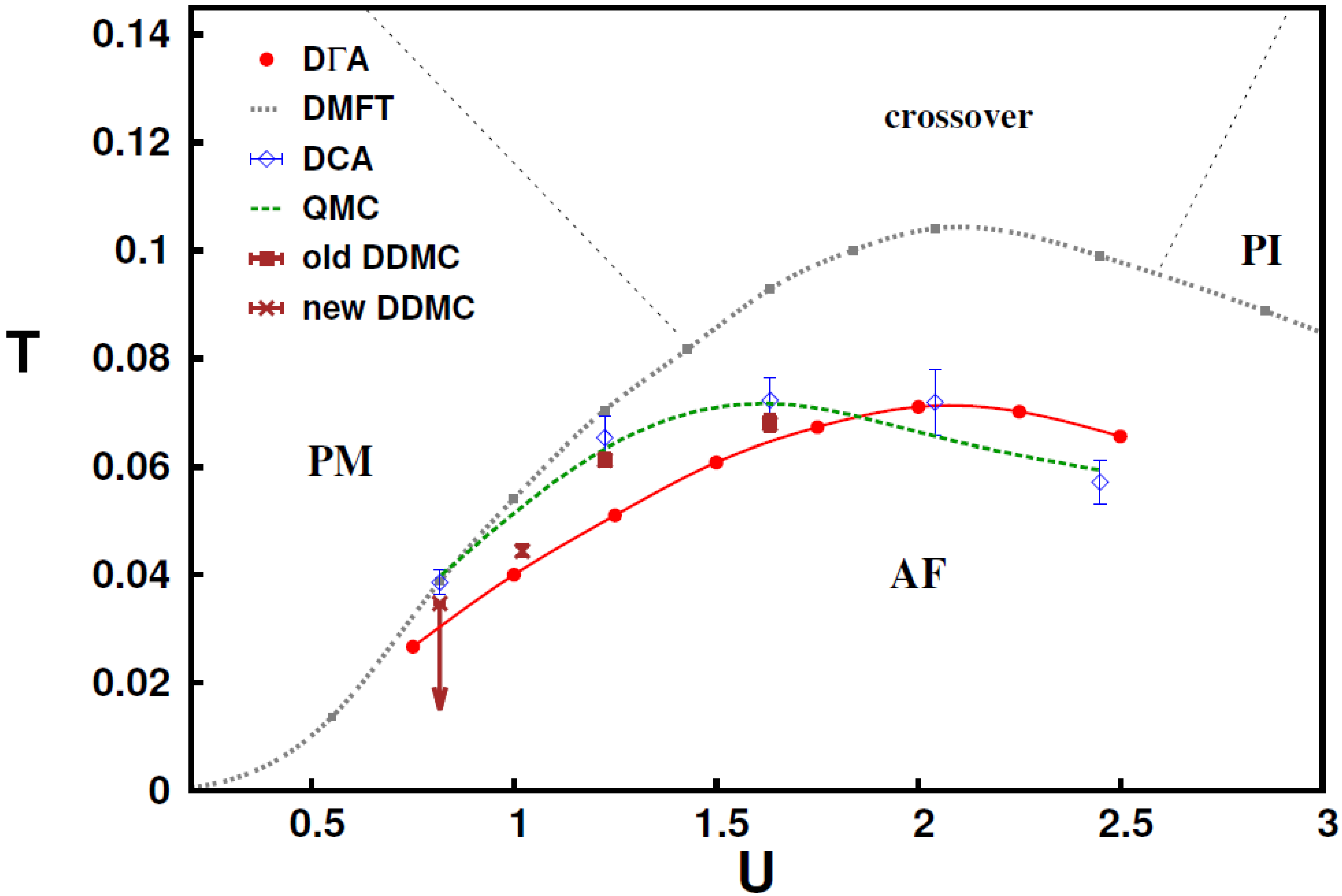
$$\chi_{AF}^{-1} = \chi_S^{-1}(\mathrm{q} = (\pi,\pi,\pi))$$



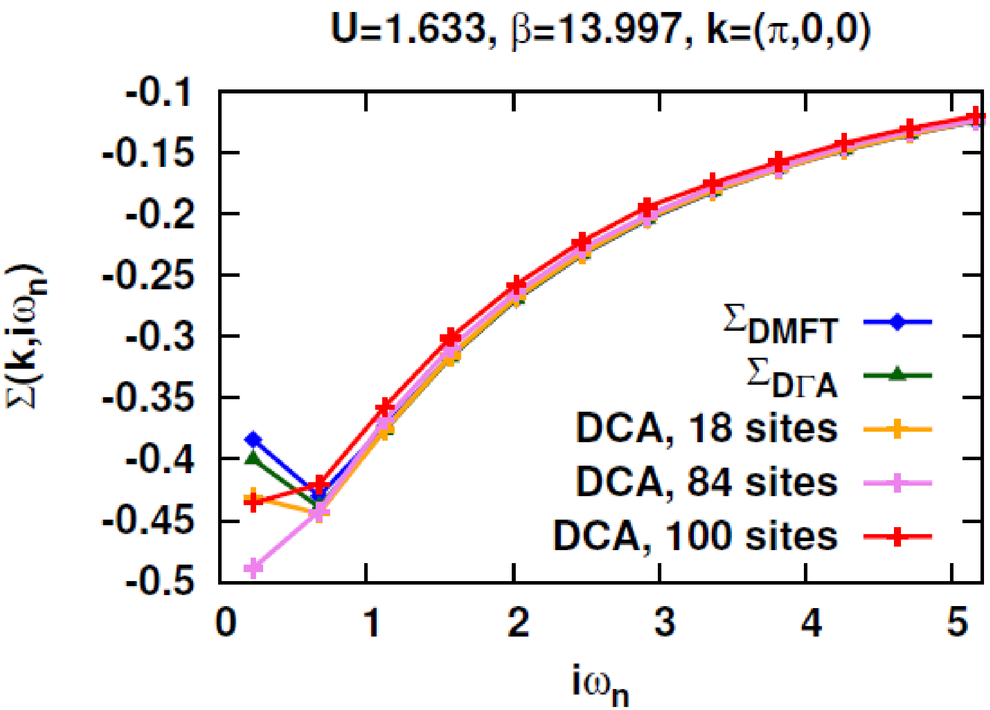
DΓA results in 3 dimensions



Comparison with DCA, QMC



Comparison of self energy



DΓA vs. DCA by Gull et al.

3d Hubbard (D=1)

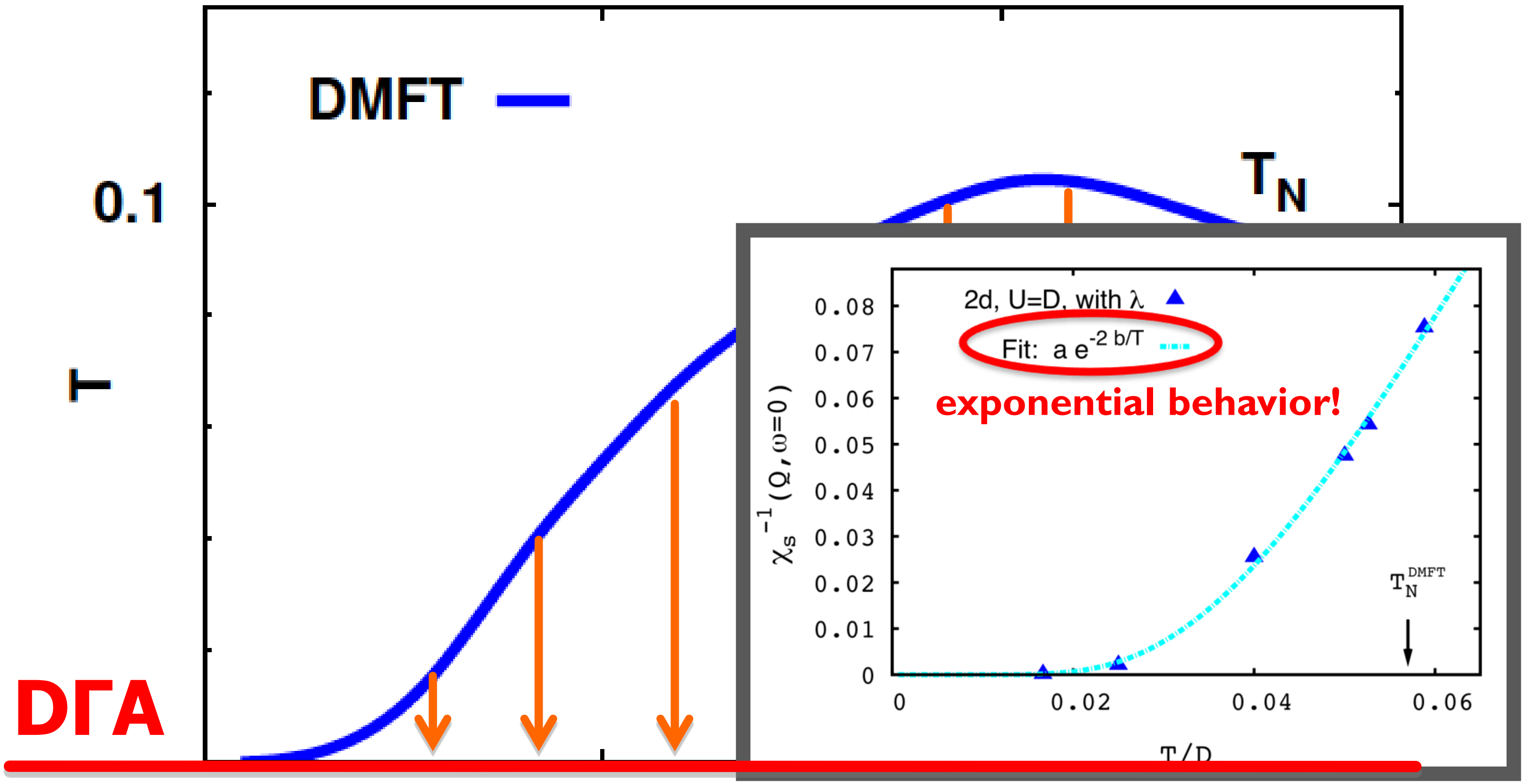
Rohringer et al'13

DΓA results in 2 dimensions

Phase diagram:

Hubbard model in **d=2**

G. Rohringer *et al.*, PRL (2011)



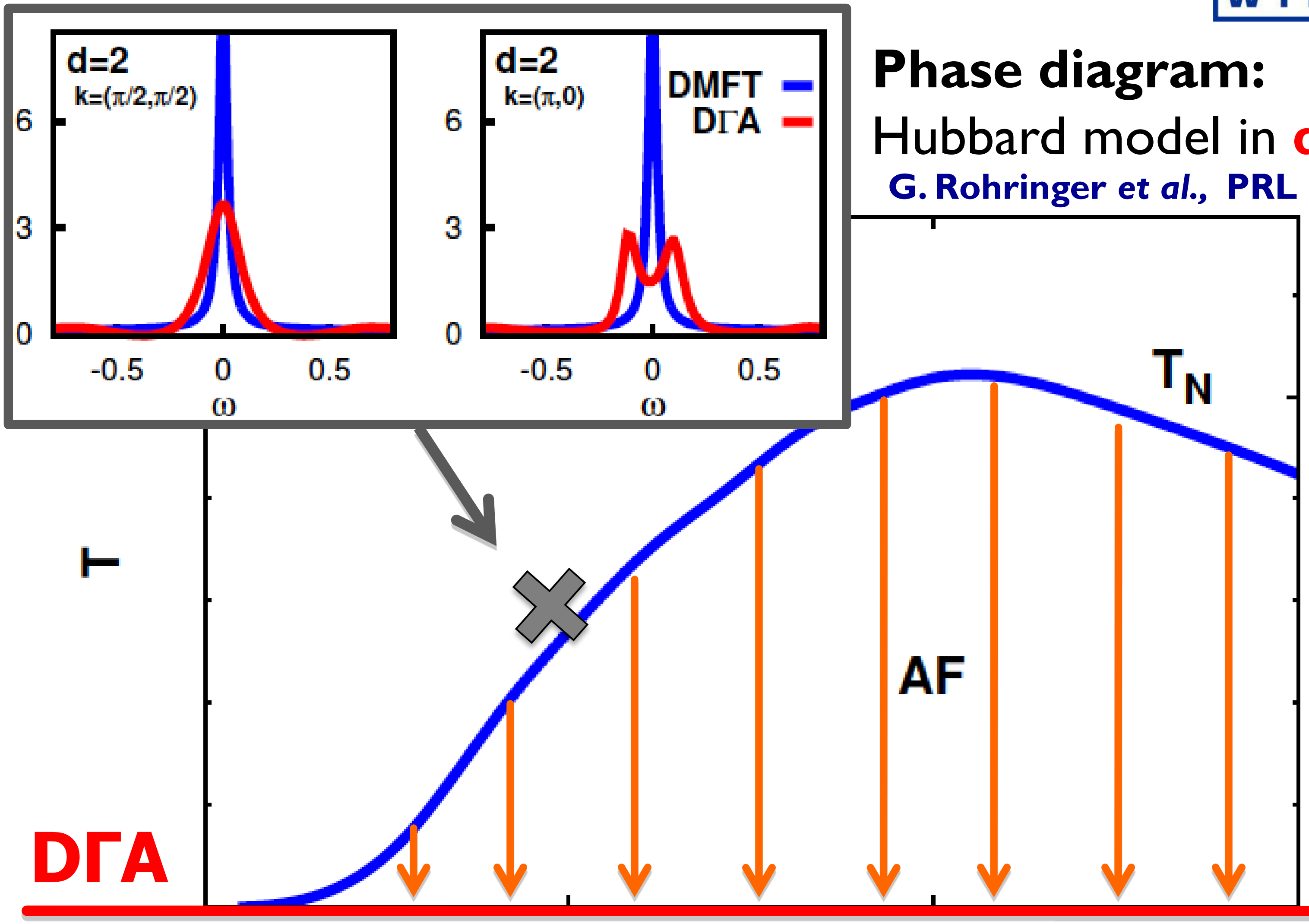
$T_N = 0$ ➔ Mermin-Wagner Theorem in d = 2!

DΓA results in 2 dimensions

Phase diagram:

Hubbard model in **d=2**

G. Rohringer *et al.*, PRL (2011)

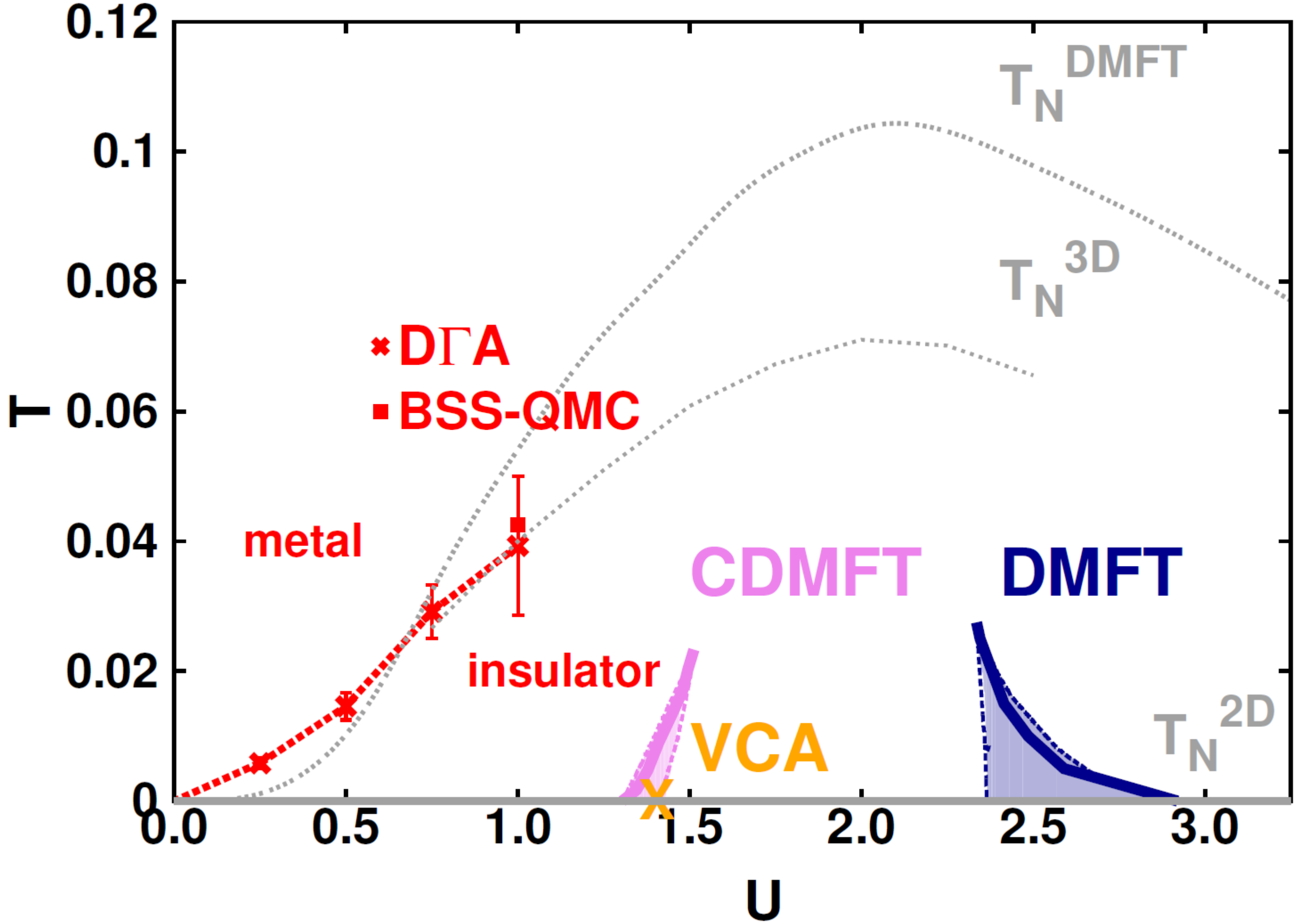


$T_N = 0$ ➔ Mermin-Wagner Theorem in d = 2!

Fade of false Mott transition in 2D

T. Schäfer et al. arXiv:1405.7250

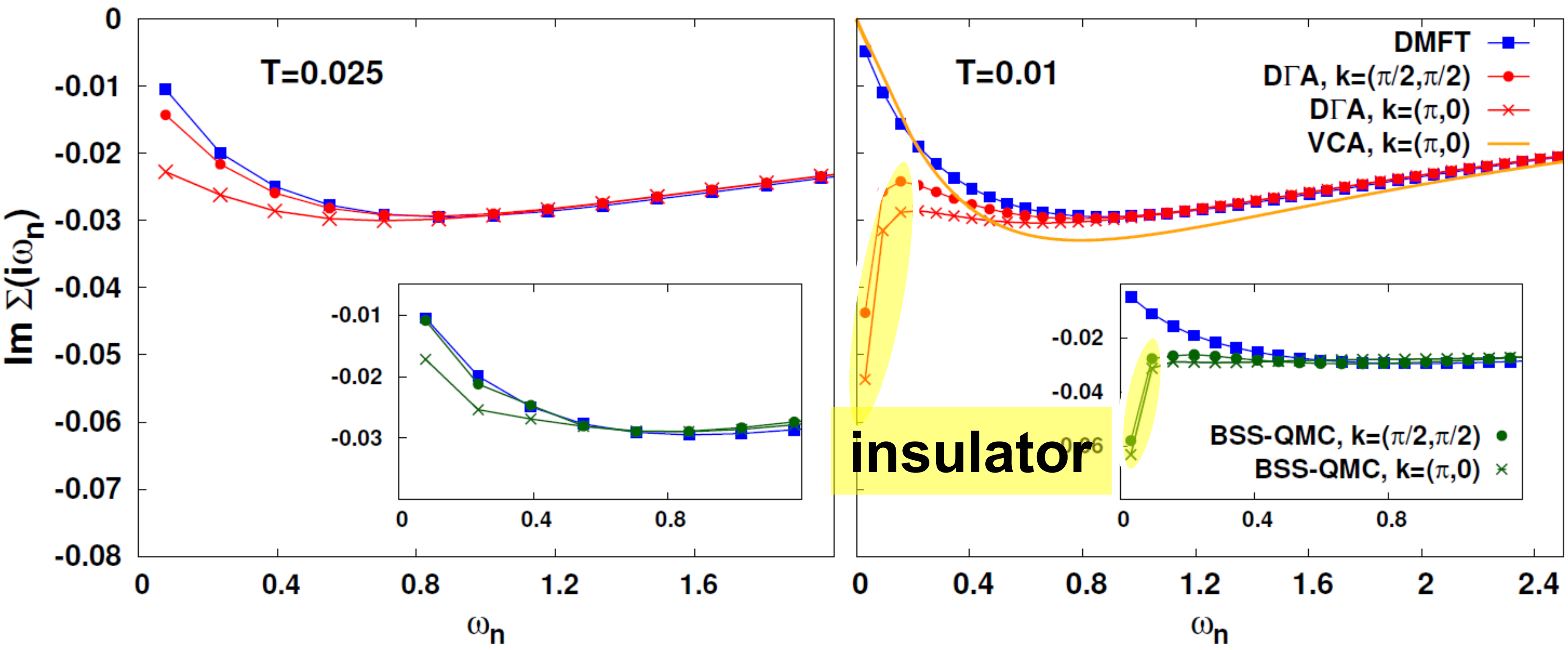
2D Hubbard model on square lattice (4t ≡ 1)



Fade of false Mott transition in 2D

T. Schäfer et al. arXiv:1405.7250

2D Hubbard model on square lattice (U=0.5 * 4t)



Fade of false Mott transition in 2D

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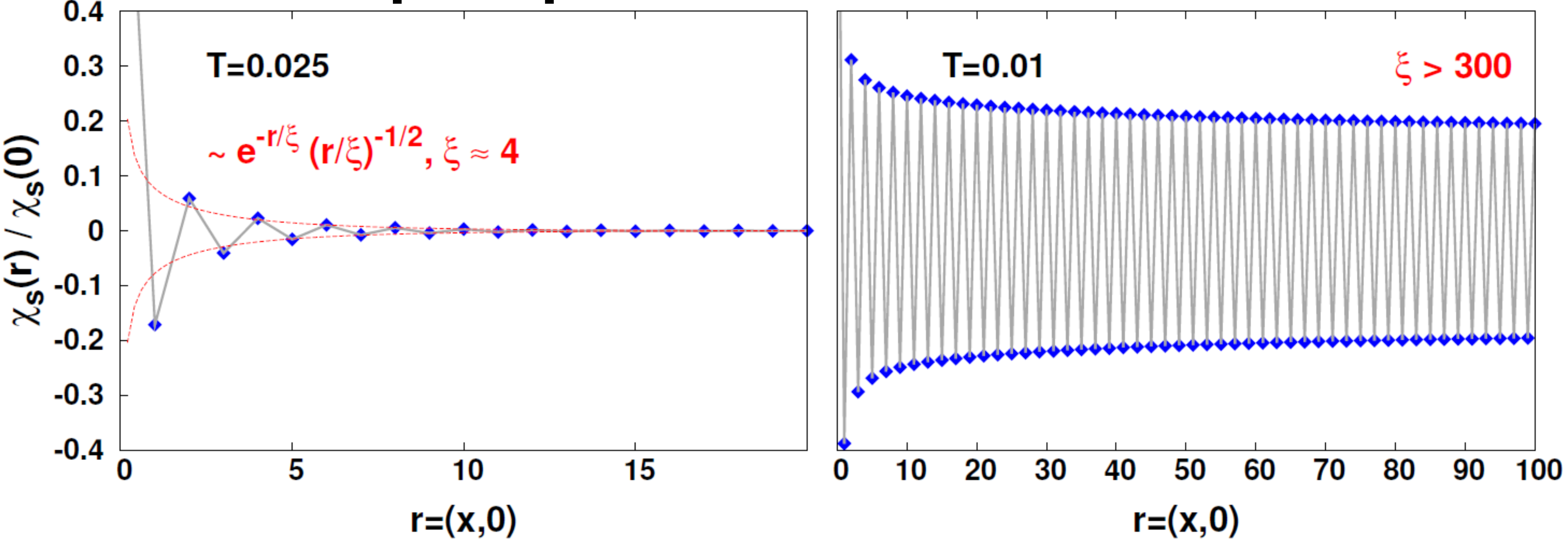
2D Hubbard model on square lattice (U=0.5 * 4t)

spin-spin correlation function



Origin of gap: long-range antiferromagnetic correlations of Slater type (H_U energy gain)

× no effective Heisenberg model (Anderson'87)

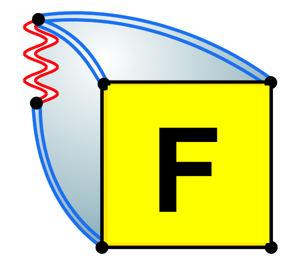
√ similar to TPSC (Tremblay et al. '07)

Conclusion

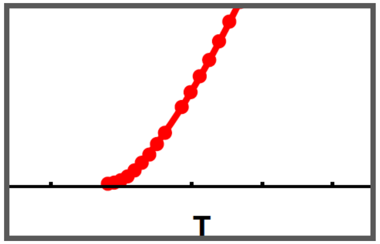
- **DF: reducible** local vertex

- **1PI & DMF^{2}RG: 1-particle irreducible** local vertex

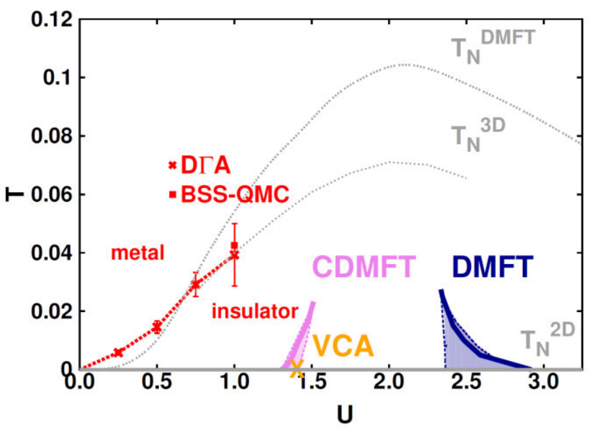
- **DΓA:** fully, **2-particle irreducible** local vertex Λ
  → full vertex **F** via parquet equations



- **DΓA: critical exponents**



- **DΓA: metal-insulator transition**
  → $U_c=0$



Thanks to ....

- A. Katanin (Ekaterinburg)
- A. Toschi, G. Rohringer, A. Valli, C. Tarato, T. Schäfer (TU Wien)
- S. Andergassen (Uni Wien), W. Metzner (Stuttgart)

Further reading:

PRB 75, 045118 (2007), PRB 80, 075104 (2009), Ann. Phys. 523, 698 (2011), PRL 107, 256402 (2011) PRB 88, 115112 (2013), arXiv:1405.7250

PhD, postdoc position available

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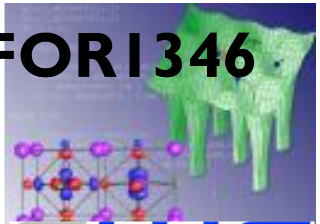

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