Quantum criticality and superconductivity in diagrammatic extensions of DMFT

Karsten Held (TU Wien)

Jülich, Sept. 21st 2018

- **Motivation**
- **Synopsis: Dynamical vertex approximation (DΓA)**
- **Quantum criticality in 3D Hubbard model**
- **Quantum criticality in 2D periodic Anderson model**
- **Superconductivity in 2D Hubbard model**

Rev. Mod. Phys. 90, 025003 (2018)

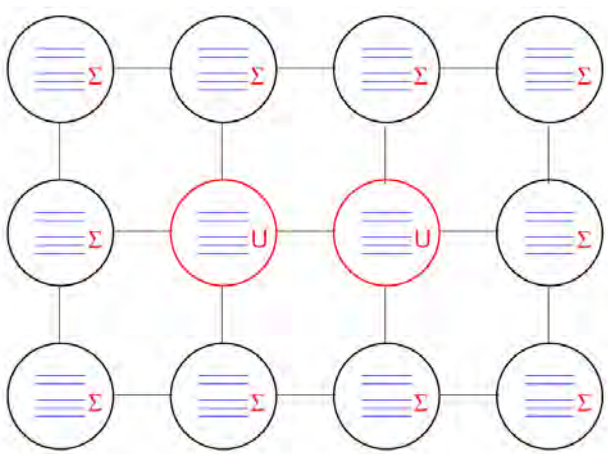
Please ask questions

Motivation I: 2 routes beyond DMFT:

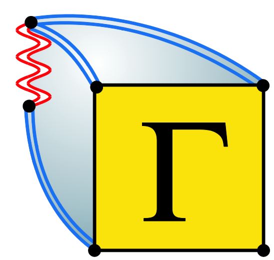
Correlations beyond DMFT:

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

Cluster extensions | **diagrammatic extensions**



Hettler et al.'98, Lichtenstein, Katsnelson'00
Kotliar et al.'01, Potthoff et al.'03, Maier et al.'05



DΓA: Toschi, Katanin, KH'07
DF: Rubtsov et al.'08
1PI, TRILEX …

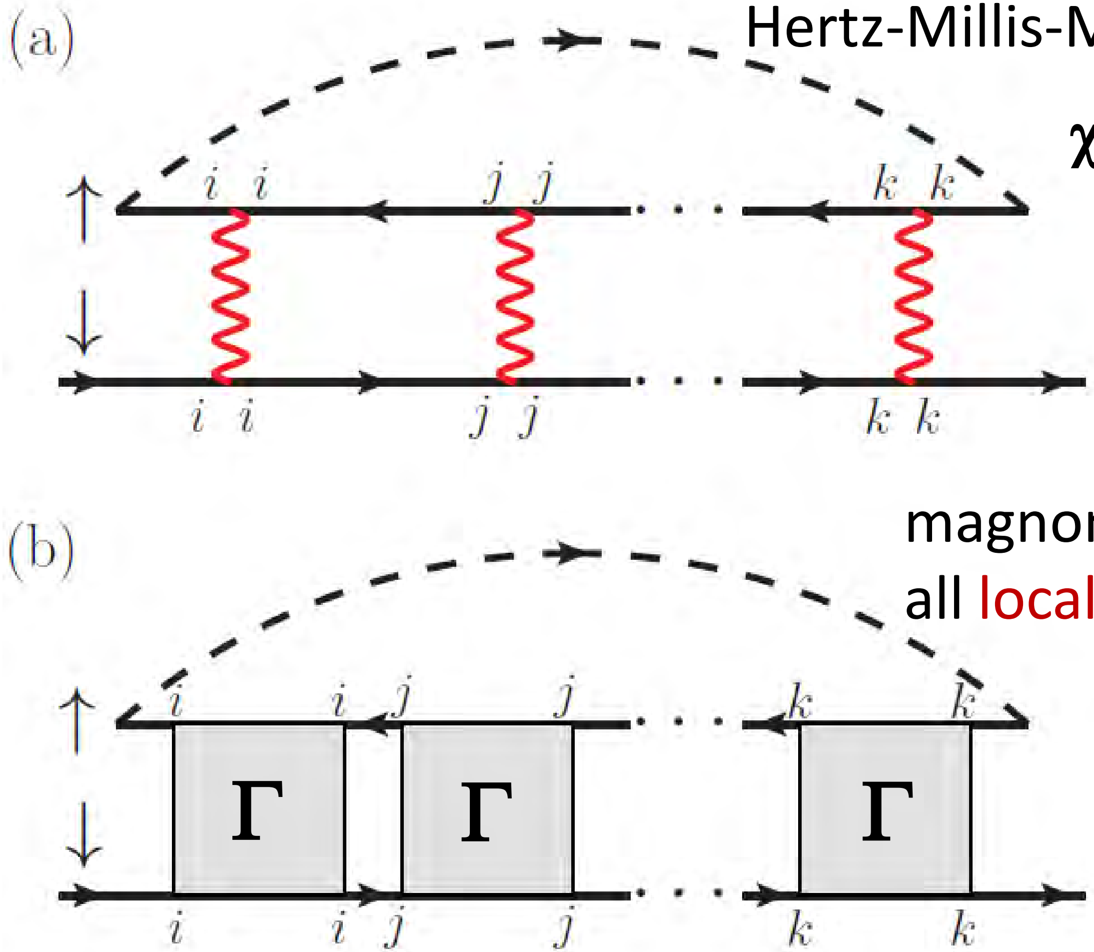
RMP'18

Motivation II

Take spin fluctuations

magnon self-energy Edwards-Hertz
Hertz-Millis-Moriya theory for QCP

$$\chi^{q,\omega} = \chi_0^{q,\omega}/(1-U\chi_0^{q,\omega})$$



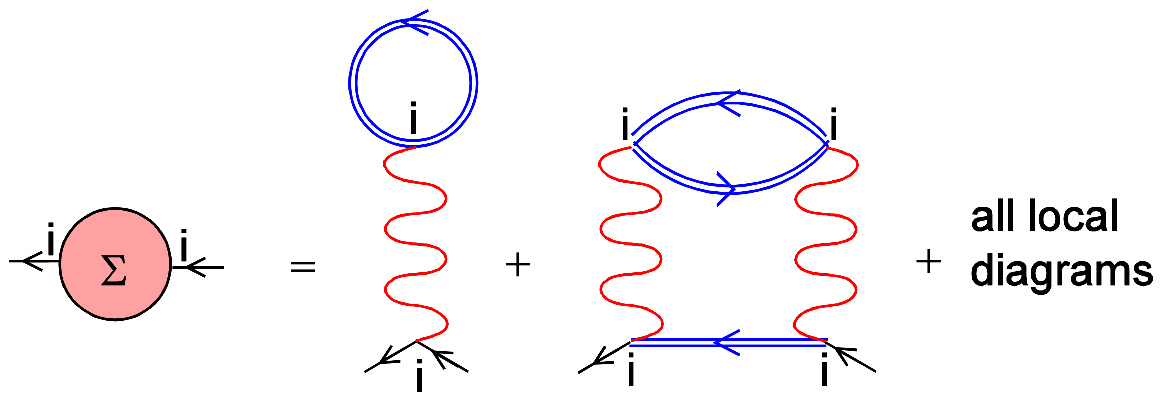
magnons but now including all local DMFT physics

Dynamical vertex approximation (DΓA)

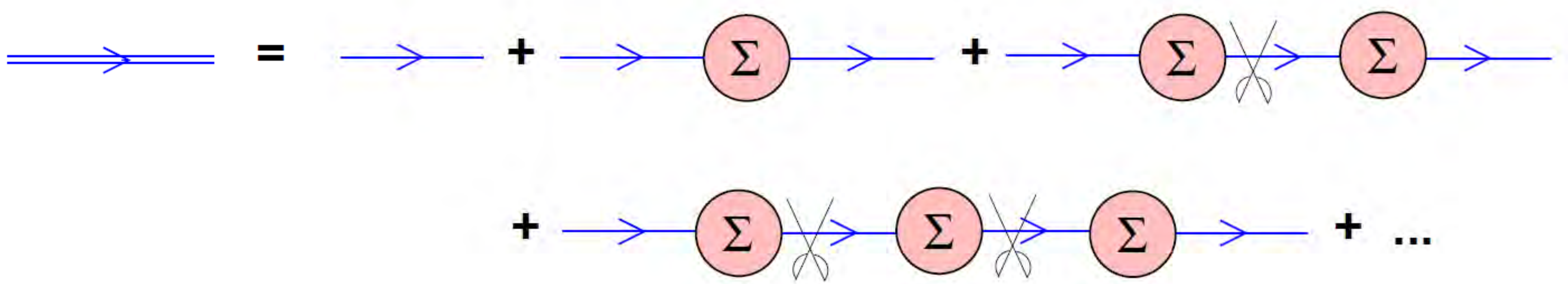
Resummation of Feynman diagrams in terms of locality

n-particle fully irreducible vertex *approximated as local*

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

n-particle fully irreducible vertex *approximated as local*

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

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

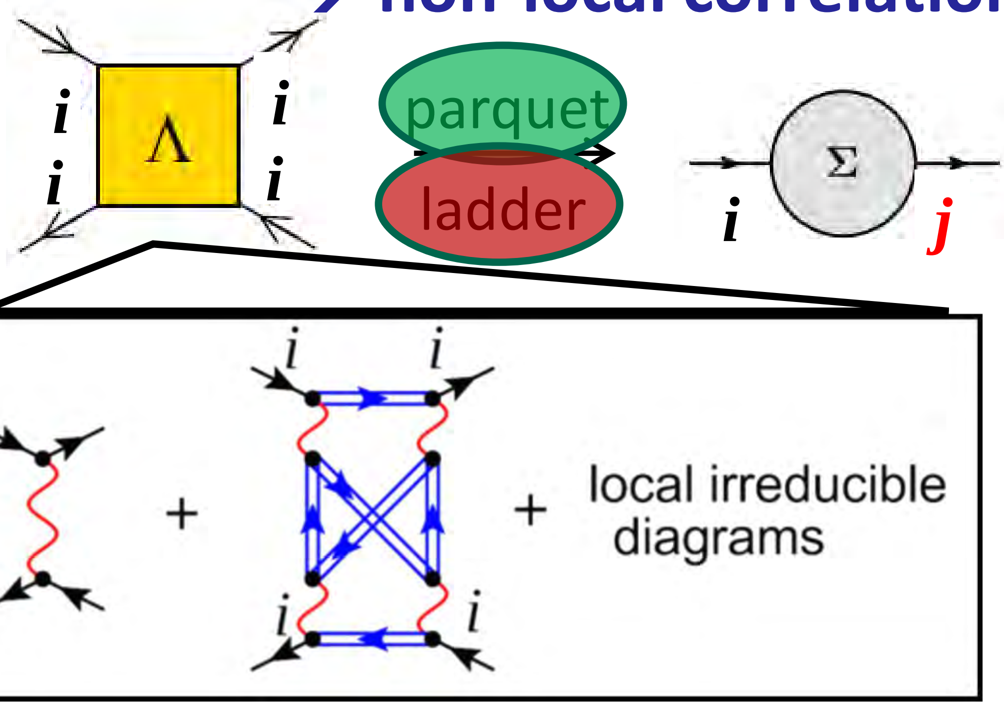
→ **non-local correlations**

n=3: error estimate

Ribic et al. PRB'17, 18

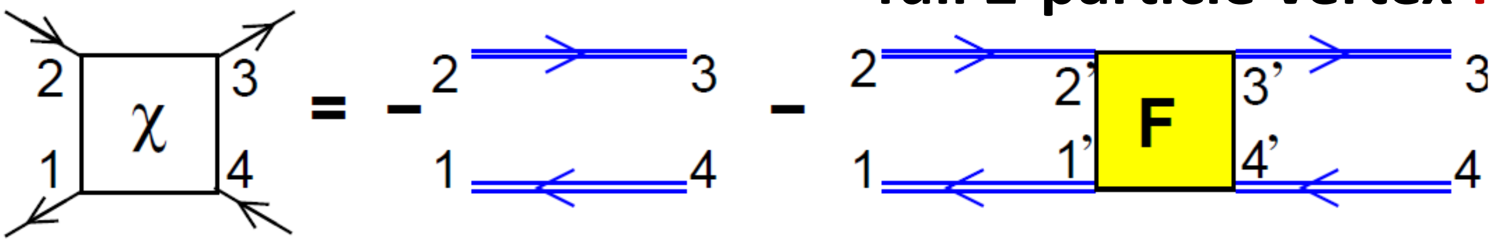
...

n→∞: exact

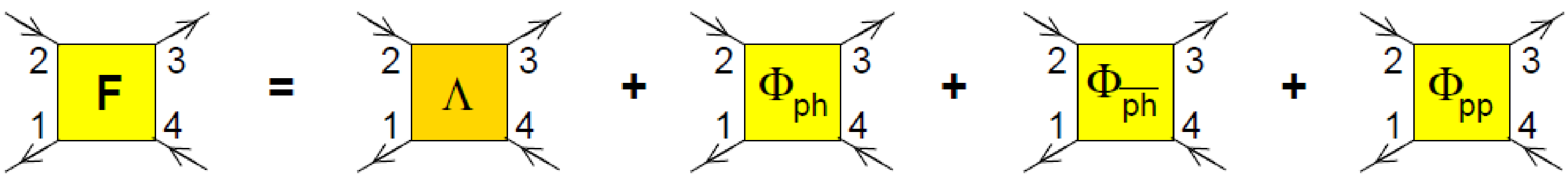


Two-particle irreducibility

full 2-particle vertex F



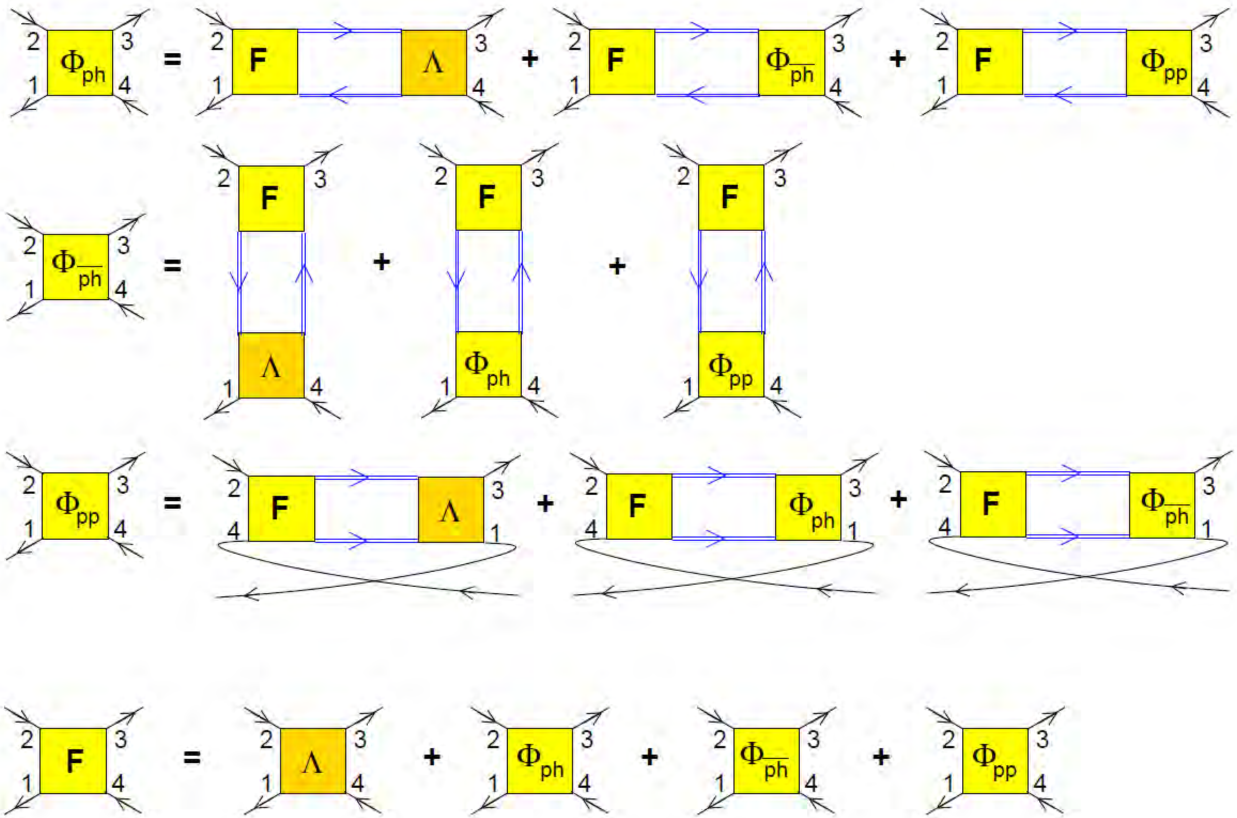
3 ways (channels) to cut two lines



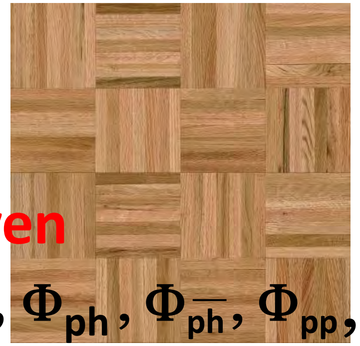
full vertex Λ Φ_{ph} $\Phi_{\overline{ph}}$ Φ_{pp}

parquet equation

Parquet equations



3 Bethe-Salpeter eq.



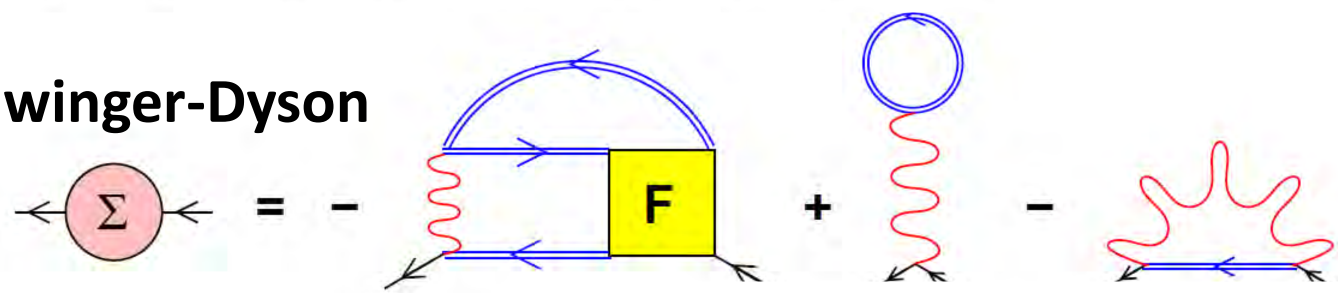
Λ **given**

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

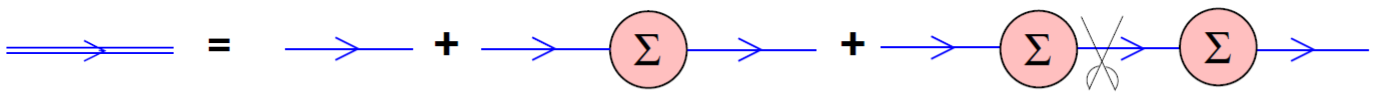
Λ = U (parquet approx.)

$\Lambda = \Lambda_{loc}$ (DΓA)

Schwinger-Dyson

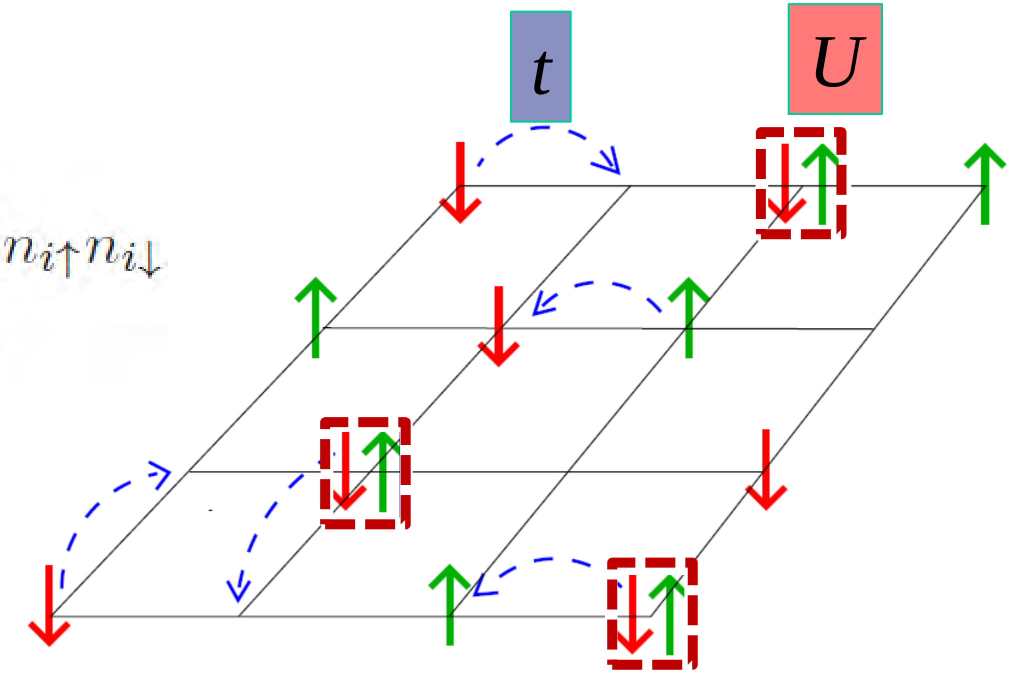


Dyson equation



ladder DΓA results: 3D Hubbard model

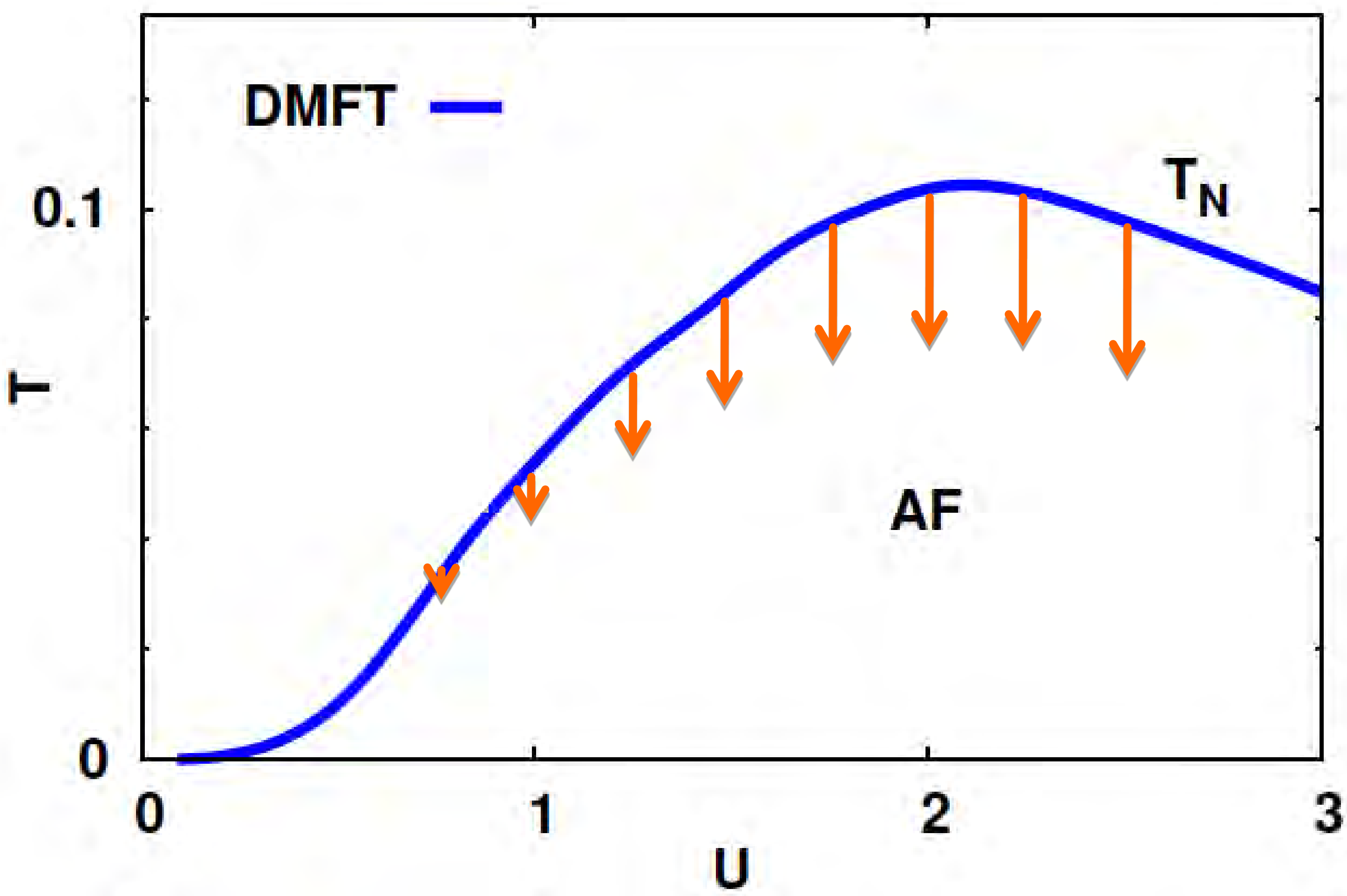
$$H = -t \sum_{\langle ij \rangle \sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$



DΓA results in 3 dimensions

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

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



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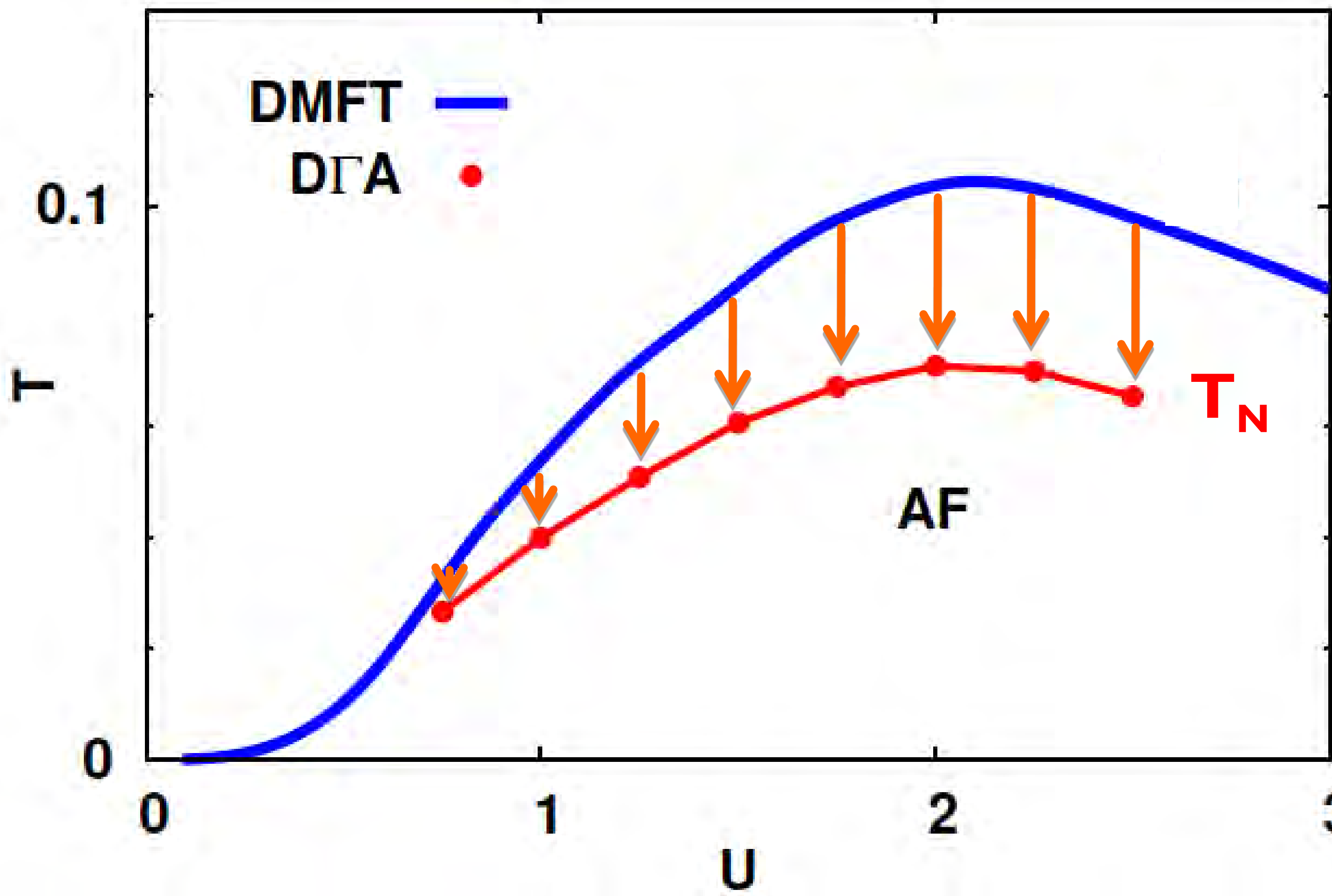
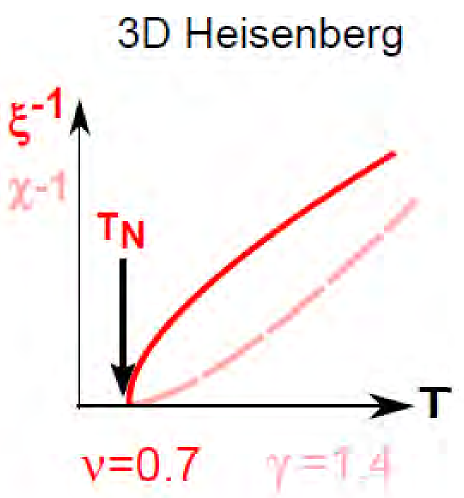
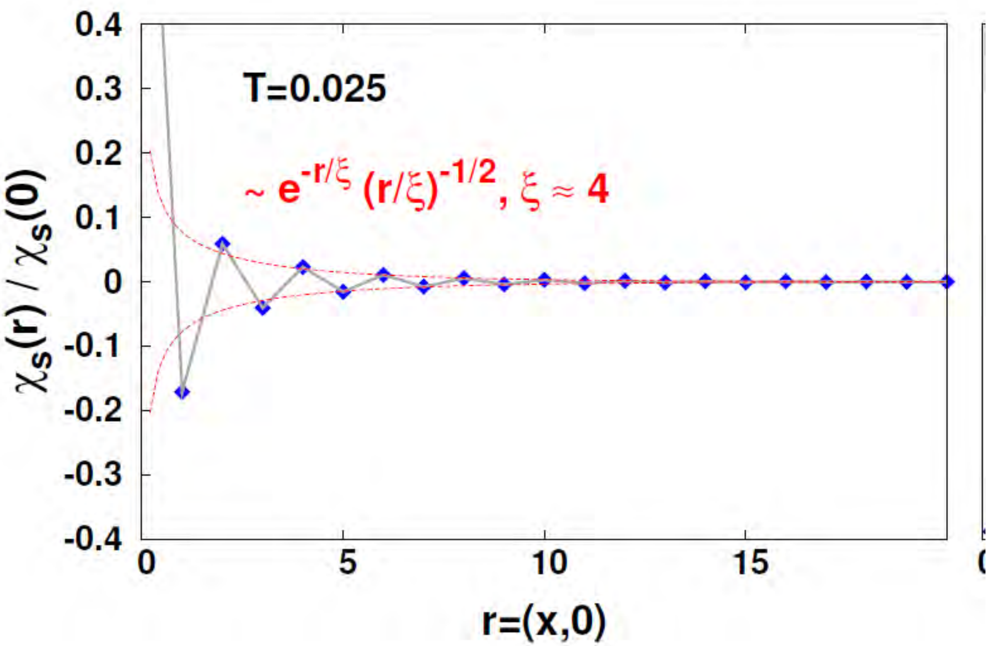


Intermezzo: critical exponents

Critical exponents





susceptibility $\chi^{-1} \sim (T - T_c)^{\gamma}$

correlation length $\xi^{-1} \sim (T - T_c)^{\nu}$

$\chi_S(r) = \langle S(r)S(0) \rangle \sim (r/\xi)^{-1/2}\, e^{-r/\xi}$

Fisher'67 relation

$\gamma/\nu = 2 - \eta \quad (\eta \sim 0)$

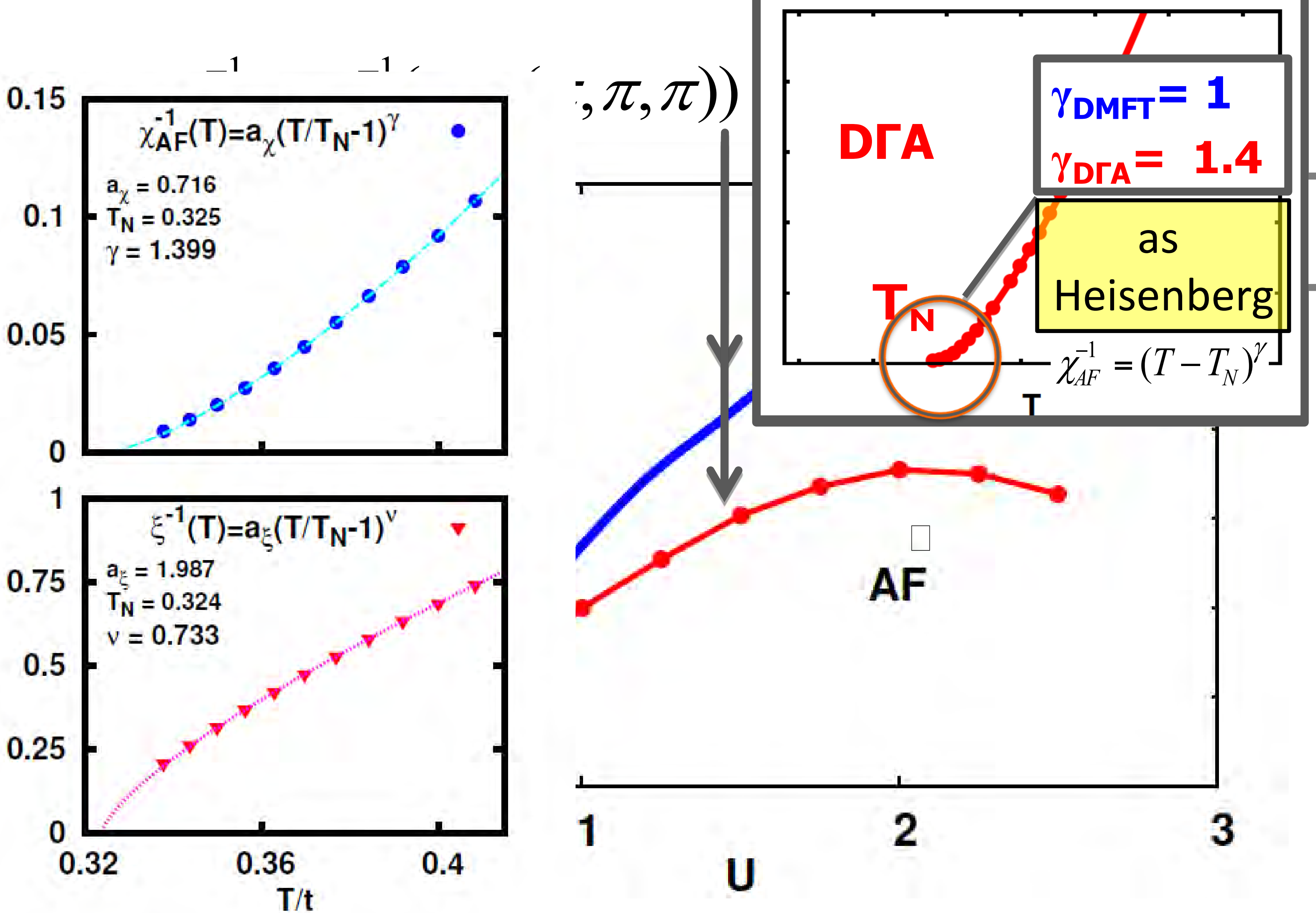
in practice: Ornstein-Zernike'16

$\chi_q^{\omega=0} \sim 1/[\,(q-Q)2 + \xi^{-2}]$

$\rightarrow \chi = \chi_Q^{\omega=0}, \xi$

universality: γ, ν only depend on d, symmetry order param.

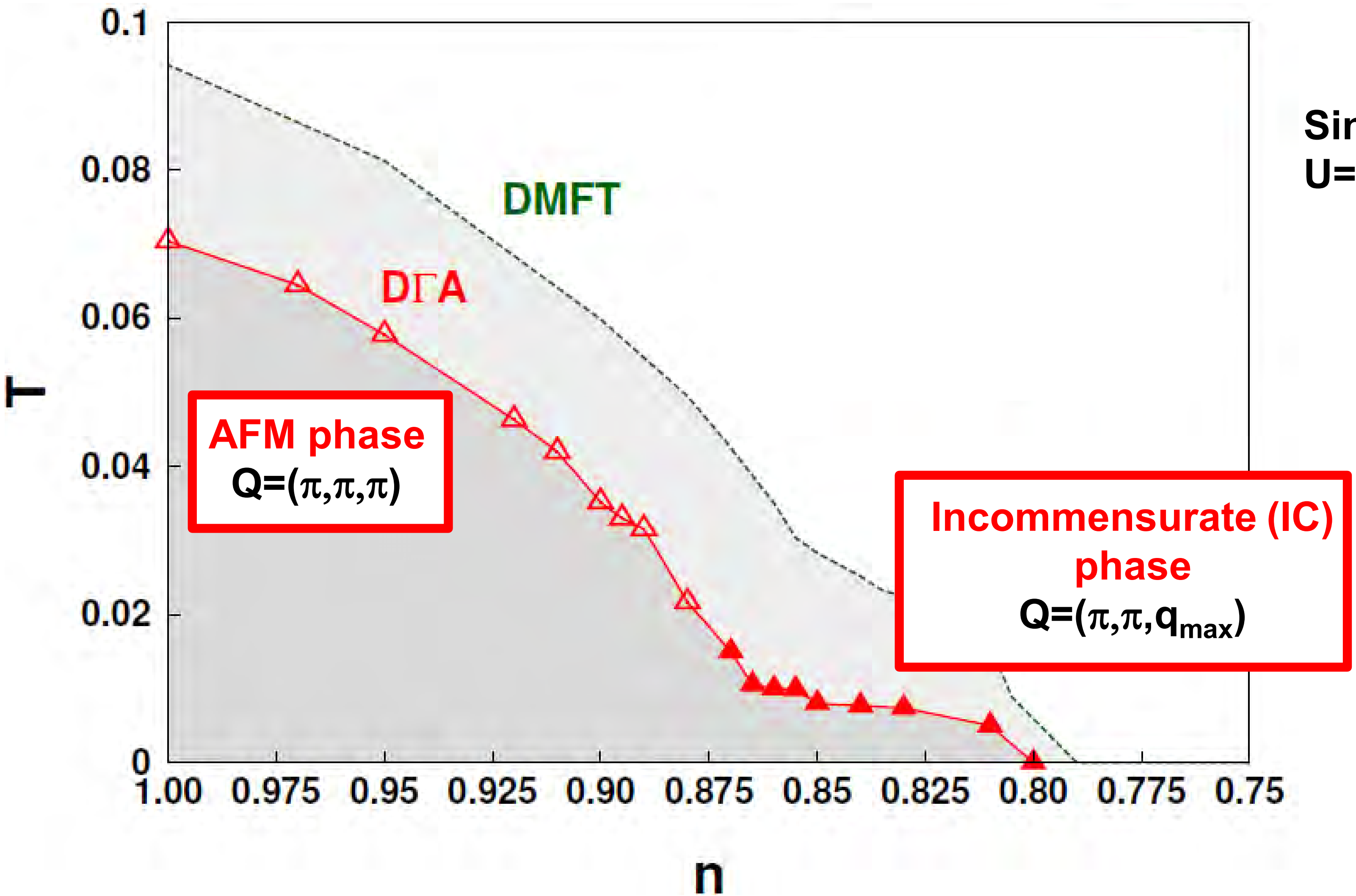
DΓA results in 3 dimensions



c
H
H
F
A

c
H
U
D

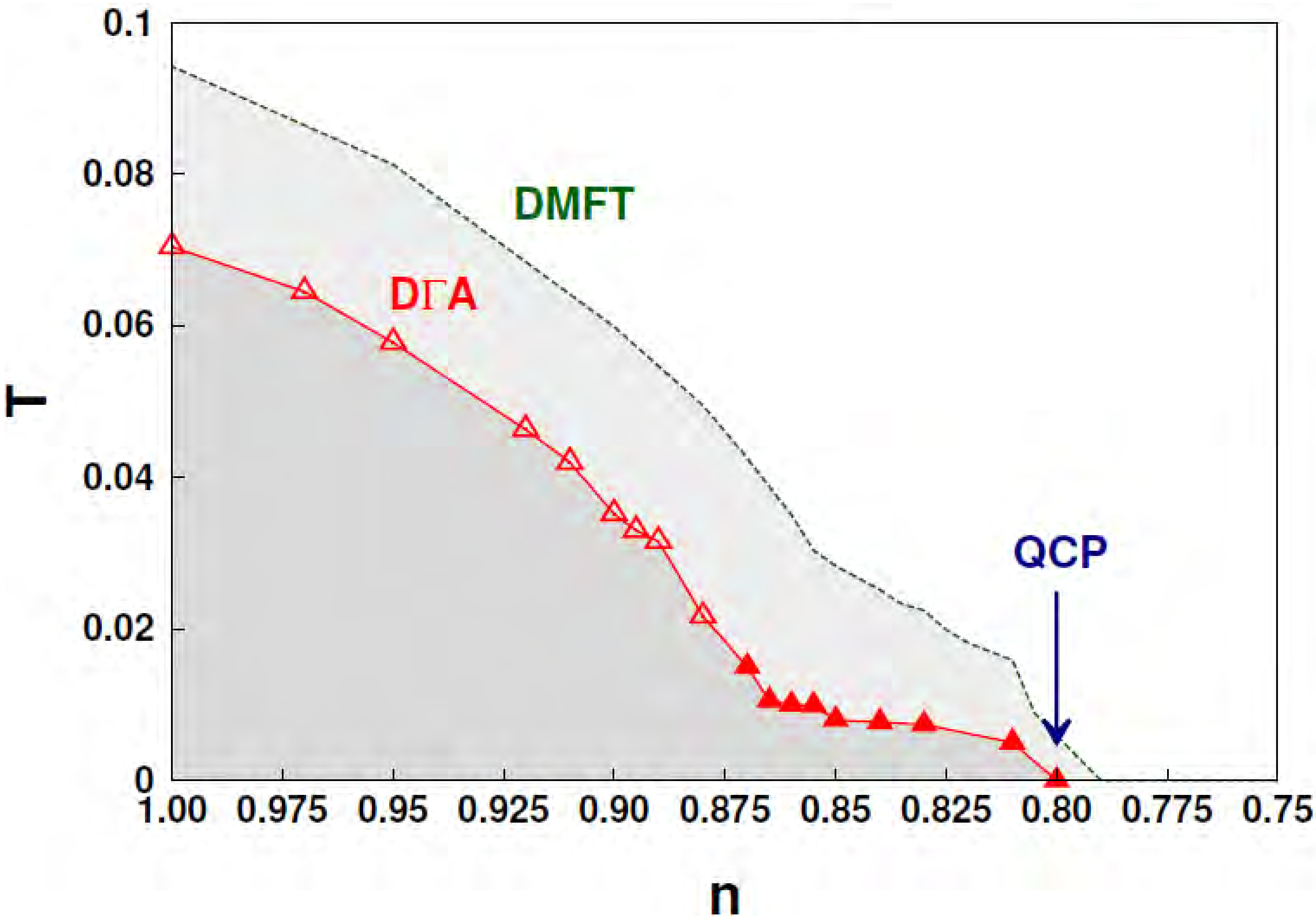
Quantum phase transition in $\color{red}{3}$ dimensions



Single band
U=2 [2√6t]

T. Schäfer et al. PRL 119 0946402 (2017)

Quantum phase transition in 3 dimensions



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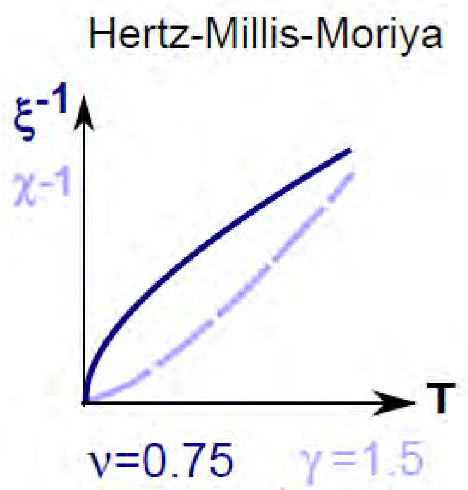
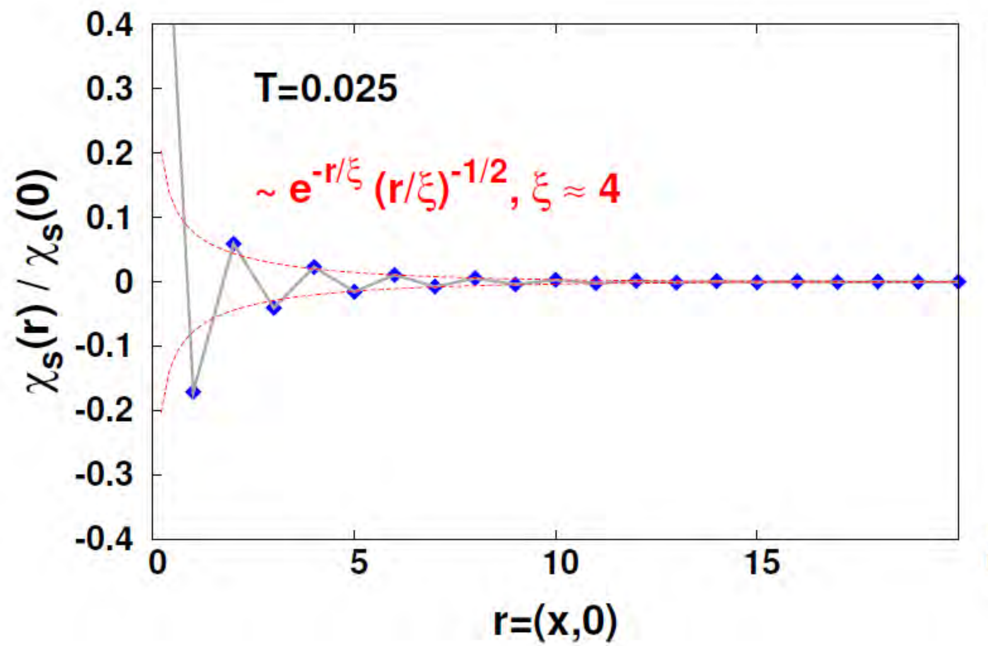
Intermezzo: quantum critical exponents

Critical exponents





susceptibility $\chi^{-1} \sim (T-T_c)^{\gamma}$

correlation length $\xi^{-1} \sim (T-T_c)^{\nu}$

$d_{eff}=z+d$

$z=2$, AF metal

$z=1$, AF insualtor

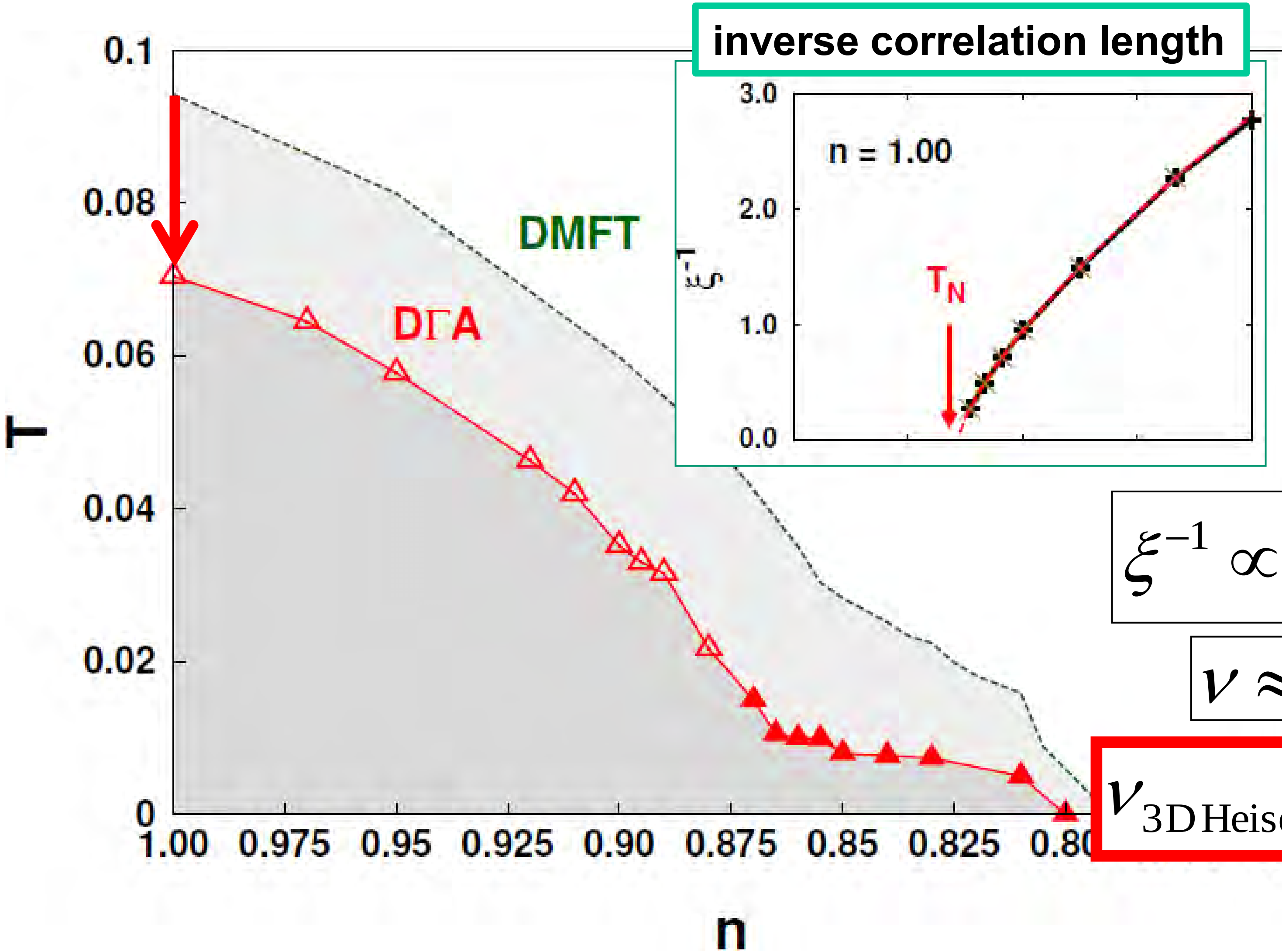
QCP quantum fluctuations in $\tau \in [0, 1/T]$

correlation length in time $\xi_\tau^{-1} \sim T^{z\nu}$

Chubukov, Sachdev, Ye'94

Troyer, Imada, Ueda'97

Quantum phase transition in 3 dimensions



Single band
U=2 [2√6t]

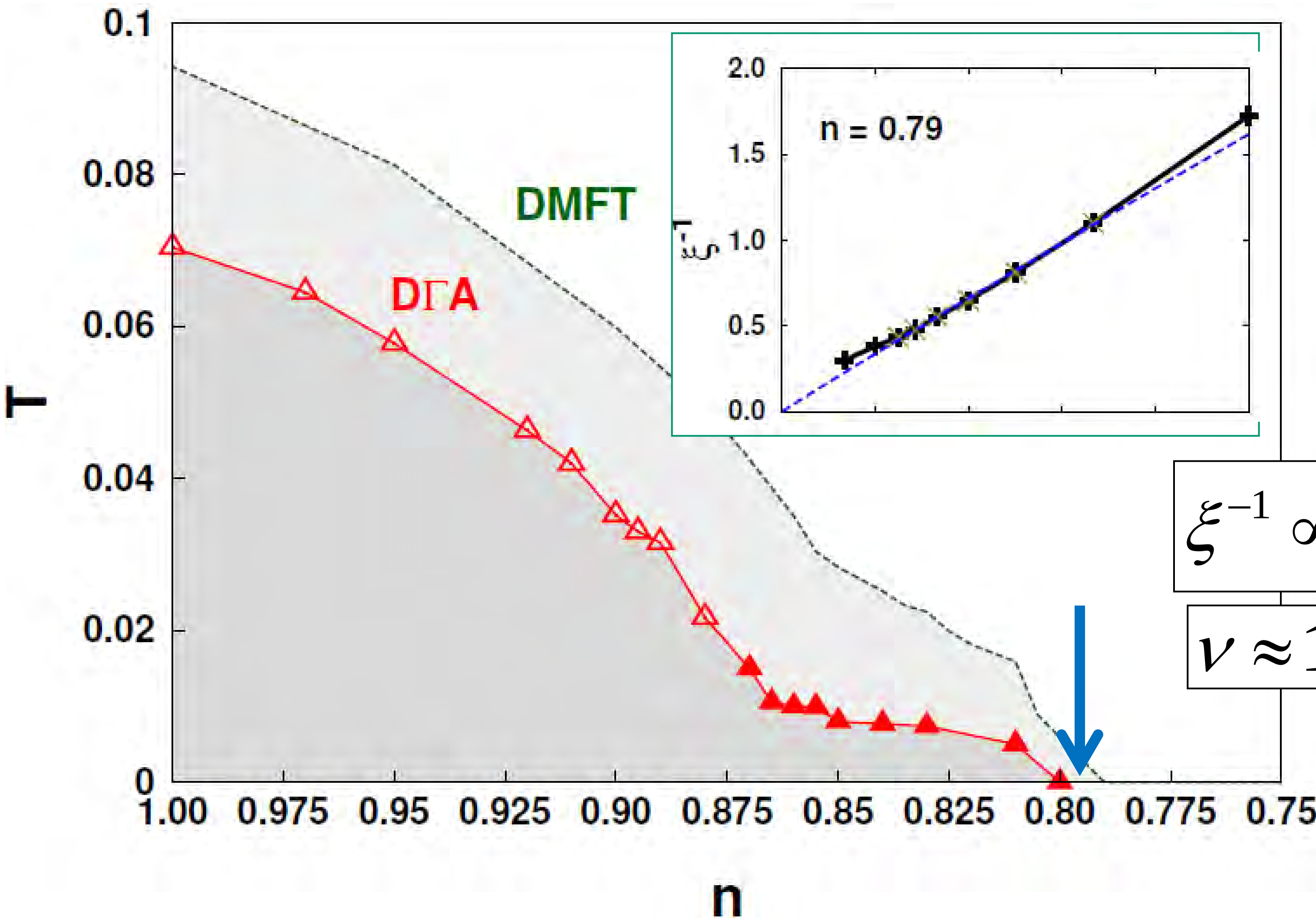
$$\xi^{-1} \propto |T - T_N|^{\nu}$$

$$\nu \approx 0.72$$

$$\nu_{3D\,\mathrm{Heisenberg}} \approx 0.7$$

T. Schäfer et al. PRL 119 0946402 (2017)

Quantum phase transition in 3 dimensions



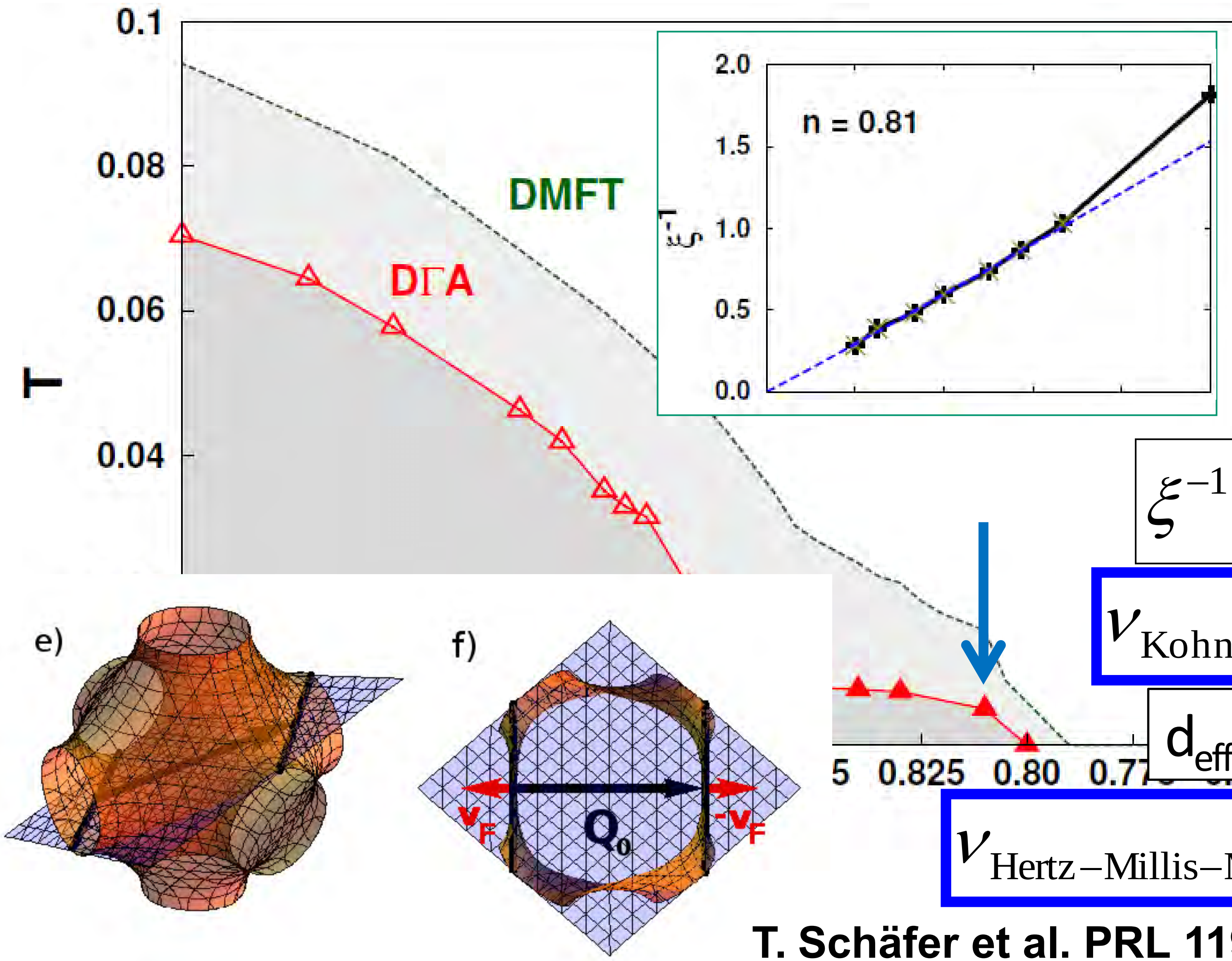
Single band
U=2 [2√6t]

$$\xi^{-1} \propto |T|^{\nu}$$

$$\nu \approx 1.00$$

T. Schäfer et al. PRL 119 0946402 (2017)

Quantum phase transition in 3 dimensions



Single band
U=2 [2√6t]

$$\xi^{-1} \propto |T|^{\nu}$$

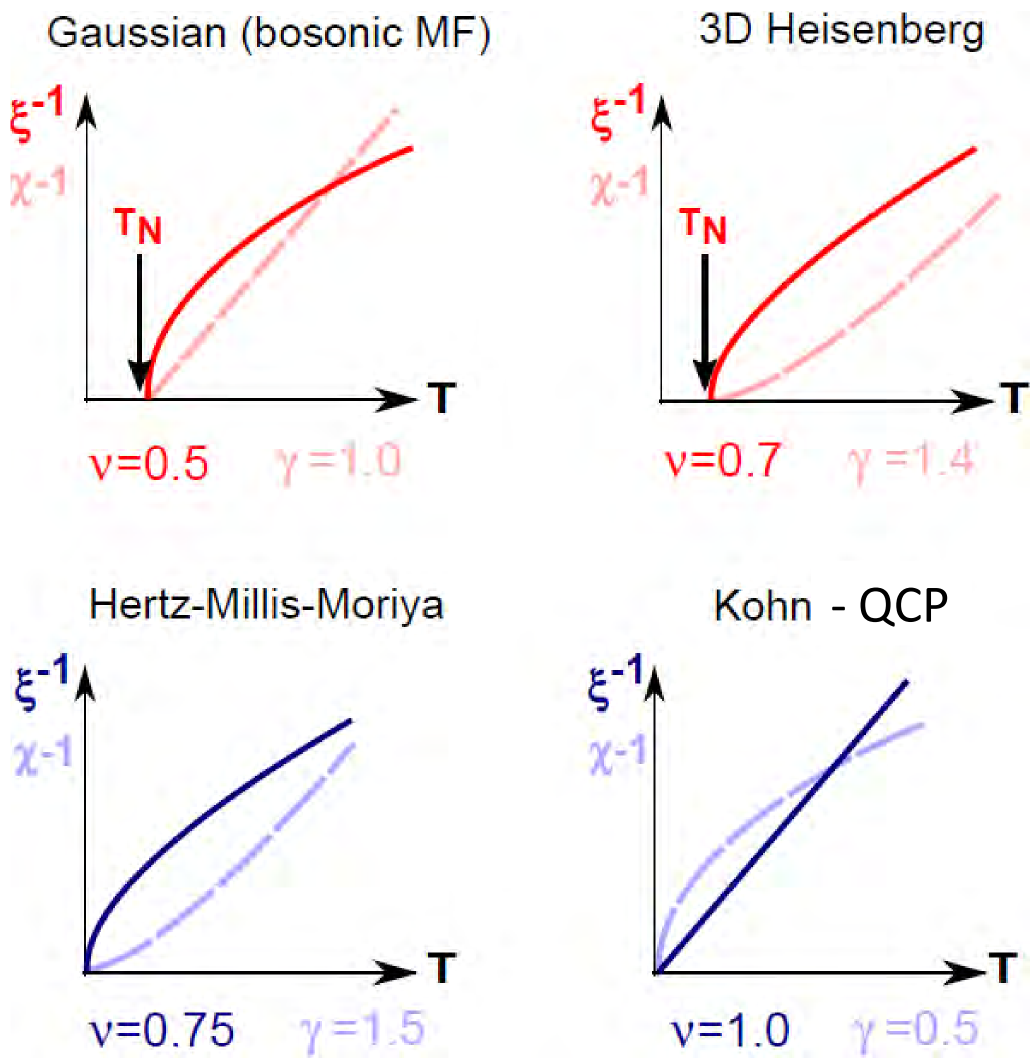
$$\nu_{\text{Kohn/QCP}} = 1.0$$

$d_{eff}=z+d=2+3>4$

$$\nu_{\text{Hertz-Millis-Moriya}} = 0.75$$

T. Schäfer et al. PRL 119 0946402 (2017)

(Quantum) critical exponents



correlation length

$\xi^{-1} \sim T^{\nu}$

susceptibility

$\chi^{-1} \sim T^{\gamma}$

Kohn-QCP:
strong deviation from
$\gamma = 2\nu$ $(\eta \sim 0)$

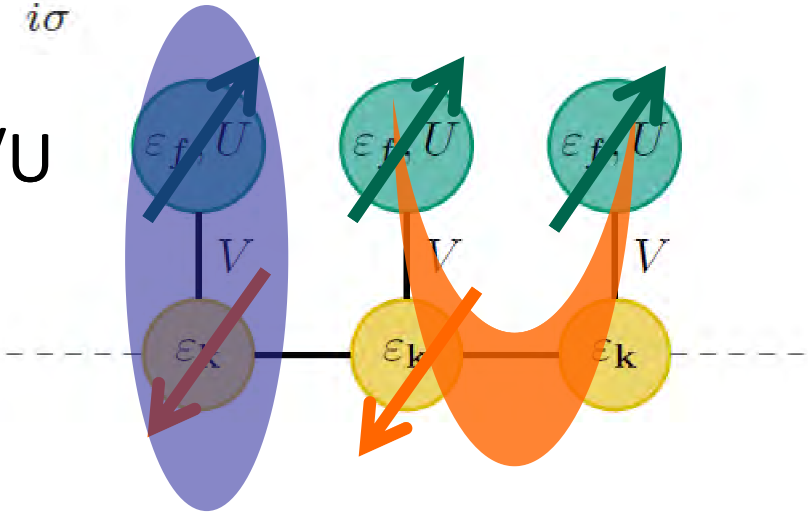
Quantum criticality 2D periodic Anderson model

- **Quantum criticality in 3D Hubbard model** $d_{eff}=z+d=2+3$
- **Quantum criticality in 2D periodic Anderson model** $d_{eff}=1+2$

Quantum criticality 2D periodic Anderson model

$$H_{PAM} = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} a^{+}_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma} + \varepsilon_f \sum_{i\sigma} f^{+}_{i\sigma} f_{i\sigma} + \sum_{\mathbf{k}\sigma} V_{\mathbf{k}} \left(a^{+}_{\mathbf{k}\sigma} f_{\mathbf{k}\sigma} + f^{+}_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma} \right) + U \sum_i f^{+}_{i\sigma} f_{i\sigma} f^{+}_{i\bar{\sigma}} f_{i\bar{\sigma}} - \mu \sum_{i\sigma} \left(f^{+}_{i\sigma} f_{i\sigma} + a^{+}_{i\sigma} a_{i\sigma} \right). \quad (4)$$

Effective spin interaction $J = 4V^2/U$



Competition between

1) **Kondo $T_K \sim e^{-1/(\rho_0 J)}$**
2) **RKKY $T_c \sim \chi_0 J^2$**

in the following: half-filling (Kondo insulator)

Quantum criticality 2D periodic Anderson model

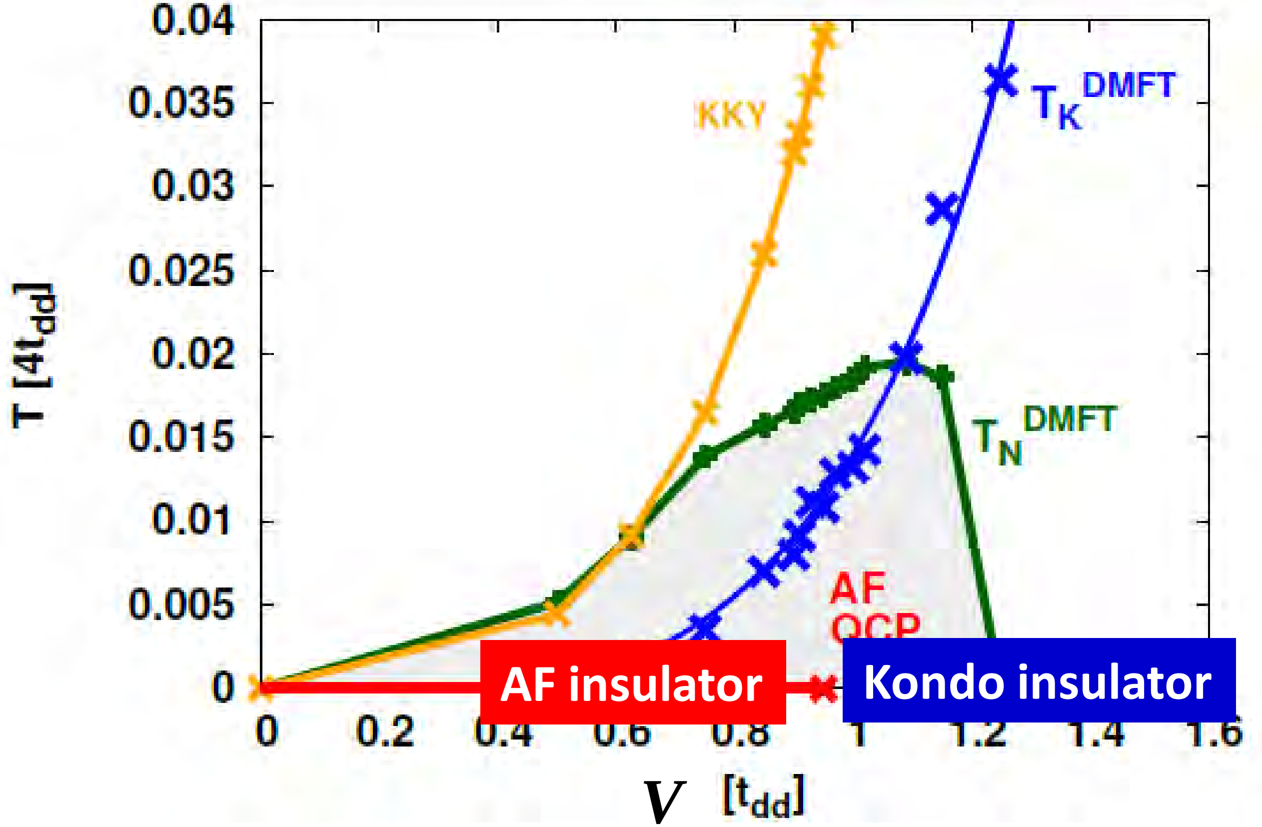
Doniach phase diagram in DMFT and DΓA

(competition between Kondo and RKKY)

Kondo $T_K \sim e^{-1/(\rho_0 J)}$

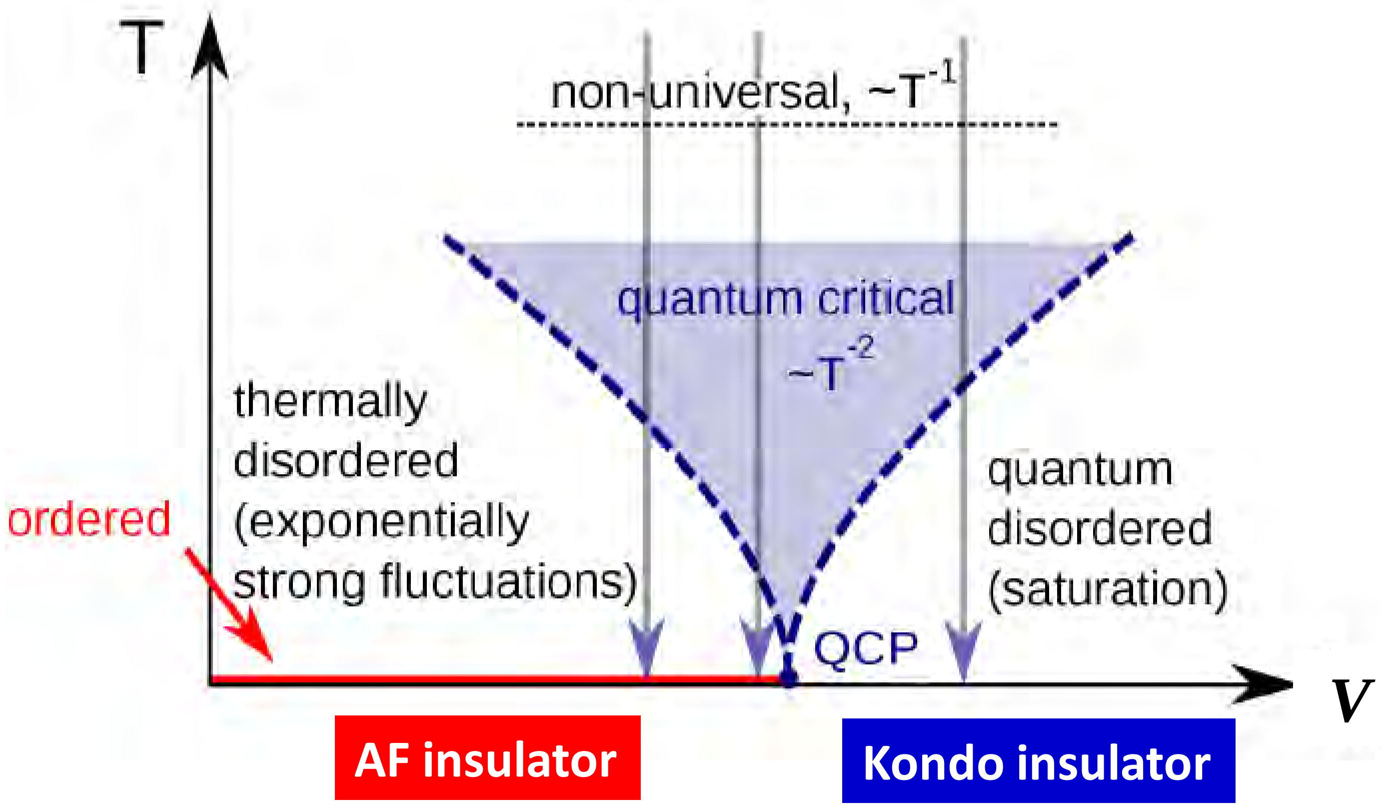
RKKY $T_c \sim \chi_0 J^2$

$J = 4V^2/U$ $\quad U=4t_{dd}$

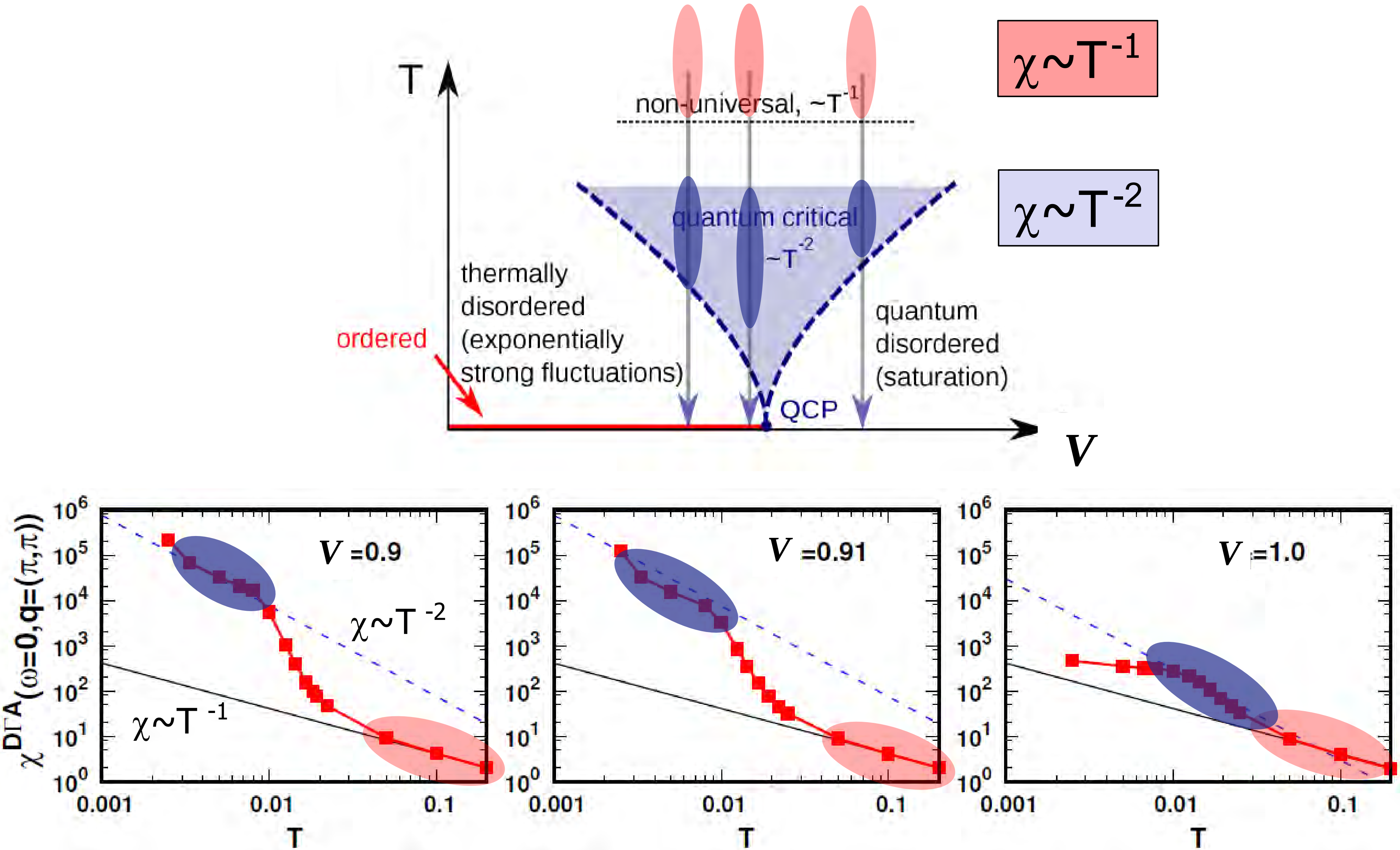


Schäfer et al. '18

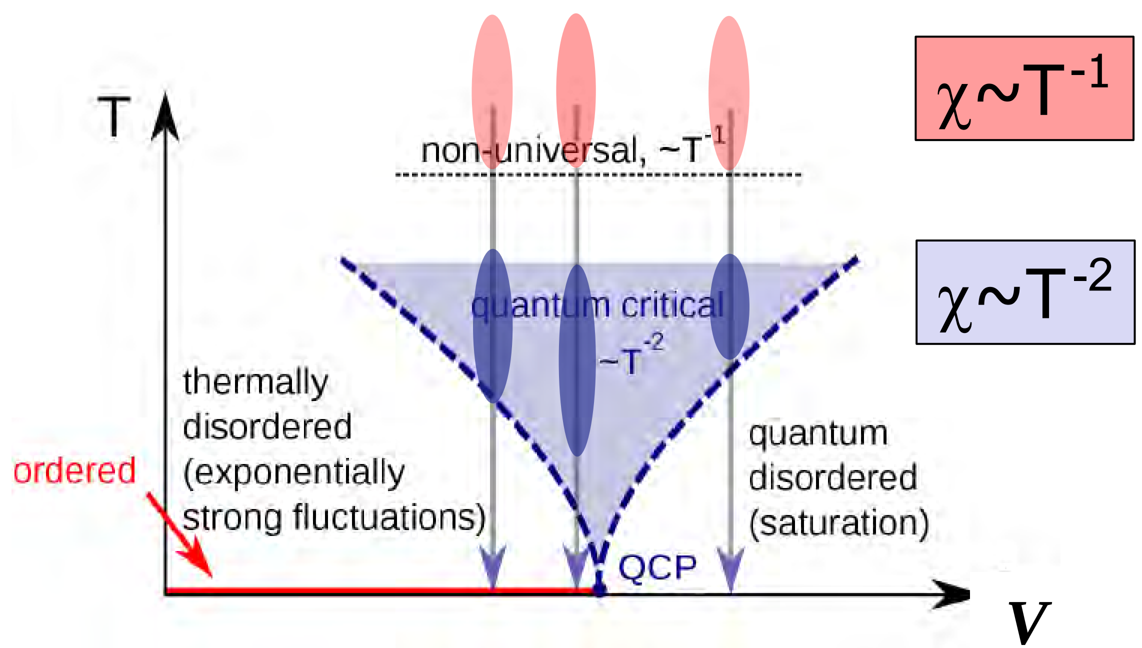
Quantum criticality 2D periodic Anderson model



Quantum criticality 2D periodic Anderson model



Quantum criticality 2D periodic Anderson model



correlation length in time $\xi_\tau^{-1} \sim T^{z\nu}$, $z=1$, correlation length $\xi^{-1} \sim T^{\nu}$

finite T → cut-off $\xi_\tau \sim 1/T$ → $\xi \sim \xi_\tau \sim 1/T$ i.e. $\nu=1$

Fisher'67 relation $\gamma/\nu = 2 - \eta$ $(\eta \sim 0)$ → $\gamma = 2$ i.e. $\chi \sim T^{-2}$

same as for Heisenber model Chakravarty et al.'88

Superconductivity in 2D

2D Hubbard model (square lattice)

Kitatani et al.'2018

Non-local spin fluctuations in ladder DΓA (ph, $\overline{\text{ph}}$ channel)

→ remove local pp contribution → Γ_{pp}

→ Eliashberg equation (pp channel)

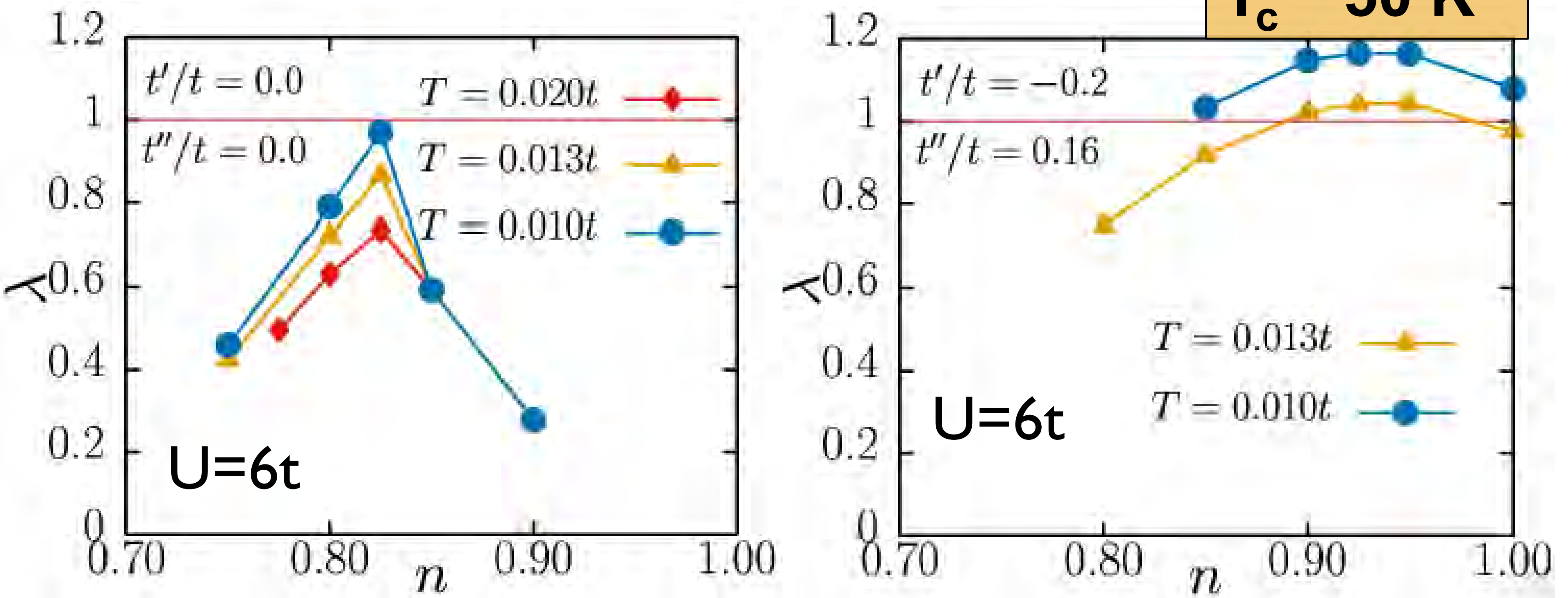
$\chi = \chi_0/(1+\Gamma_{pp}\,\chi_0)$

eigenvalue $-\lambda$

SC dome

$T_c \sim 50$ K

Leading d-wave eigenvalue λ



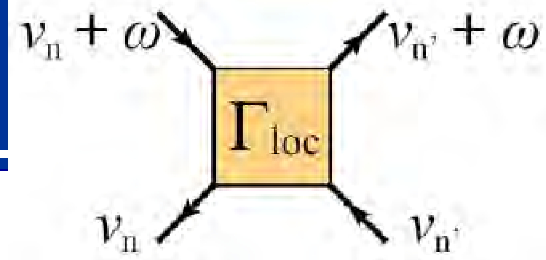
Superconductivity in 2D

Importance of vertex dynamics!

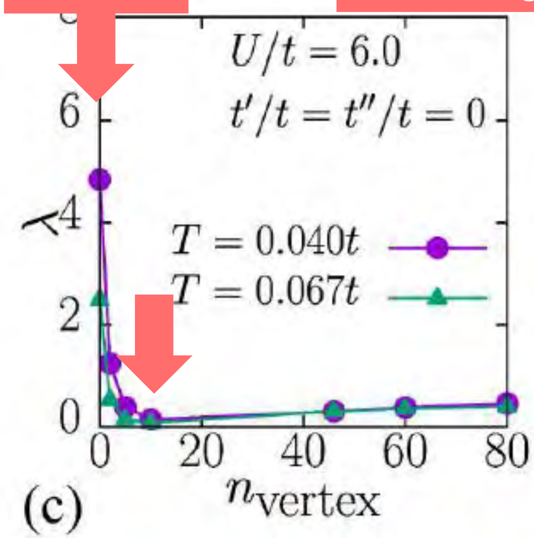
Γ=-U

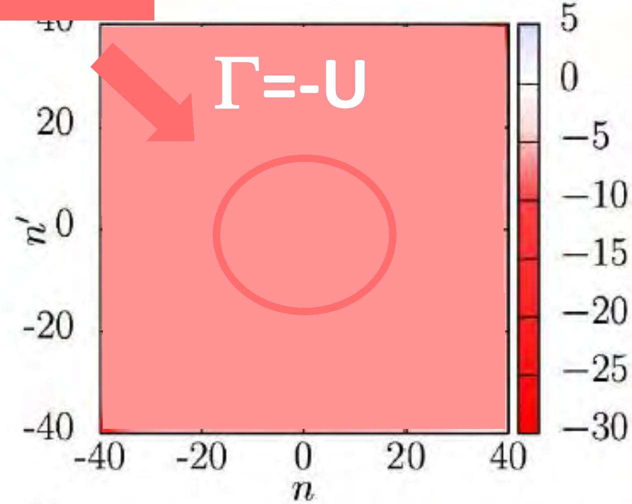
w/o $T_c \sim 400K$

local $\Gamma_m(\nu_n, \nu_{n'}, \omega)$



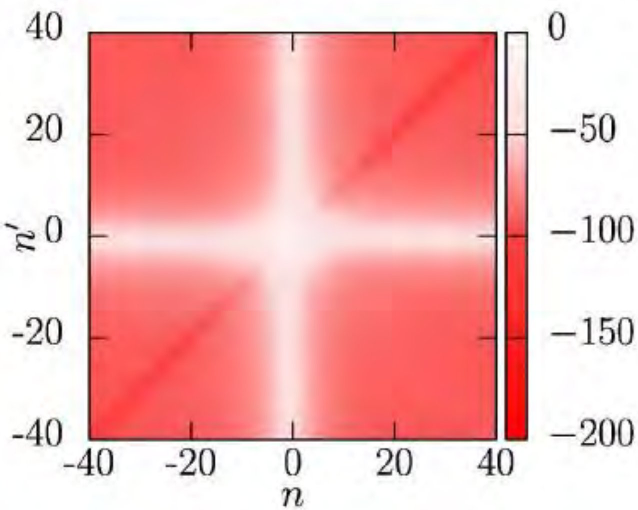
U=6t

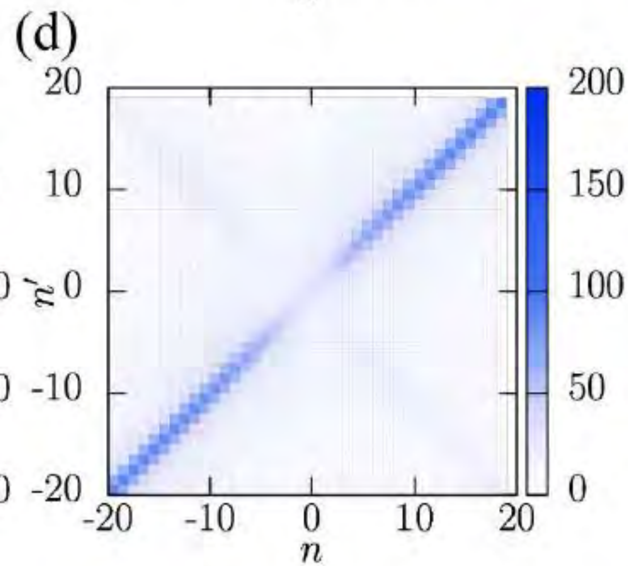




ω=0

nonlocal
F
q=(π,π)





pairing interaction
Γ_{pp}

Superconductivity in 2D

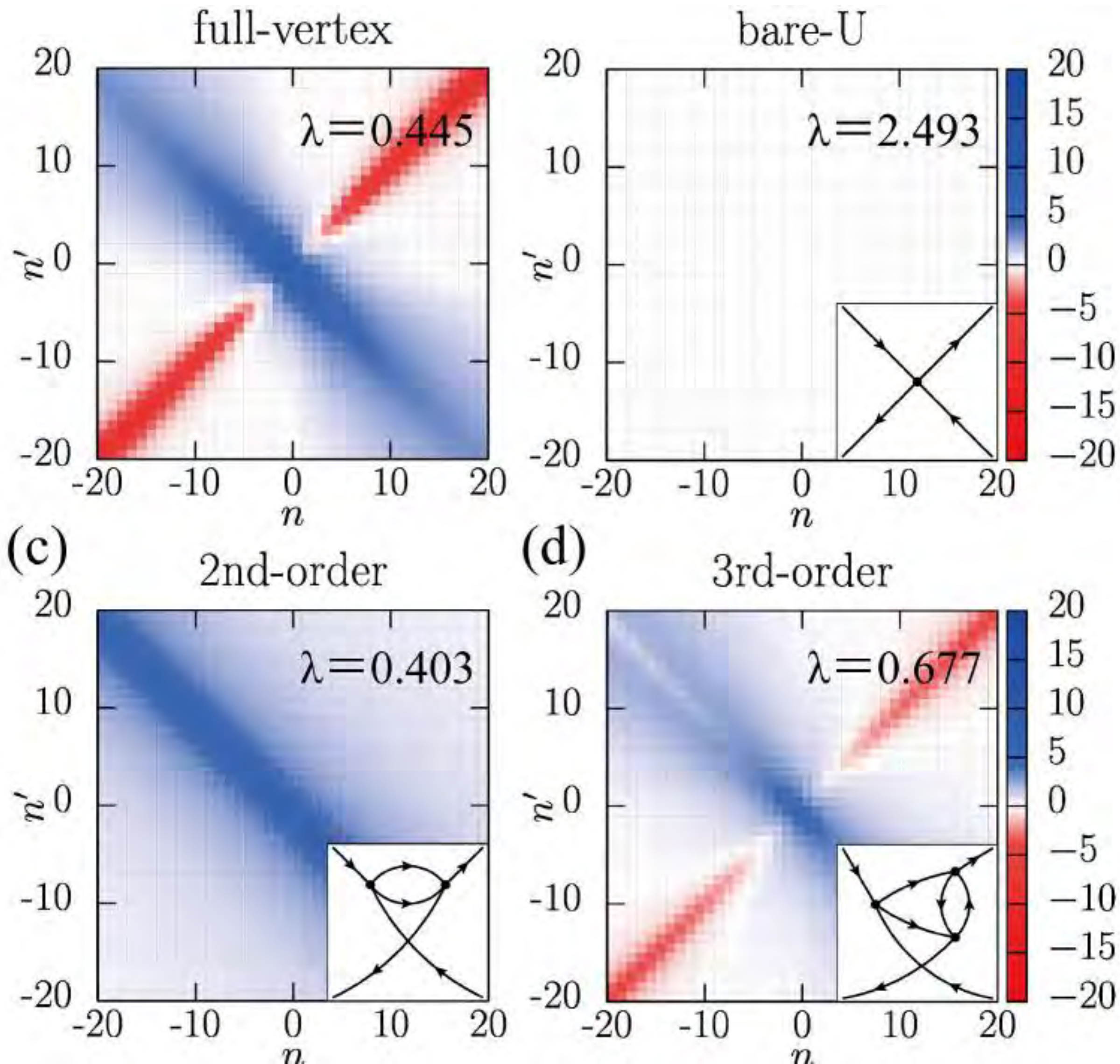
Importance of vertex dynamics!

local
Γ_m-(-U)

bare U

2nd order

3rd order



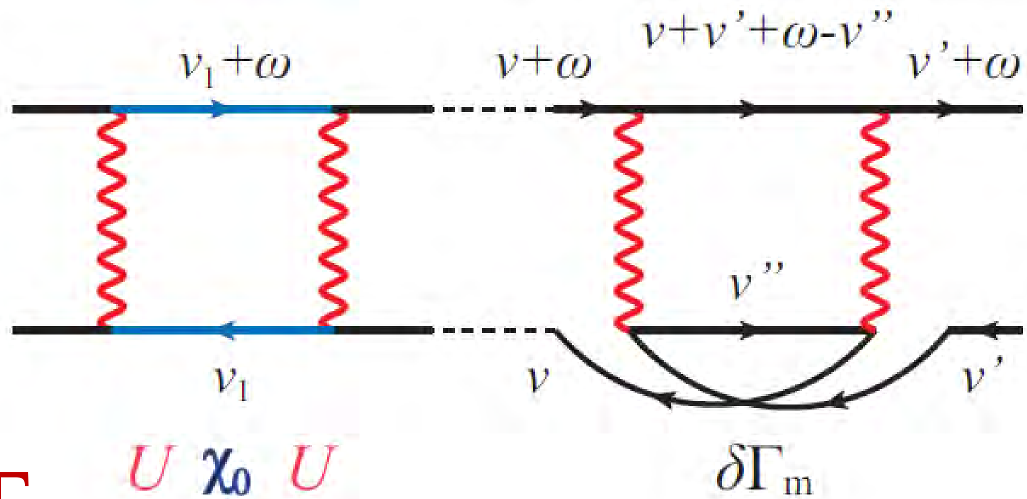
Superconductivity in 2D

Importance of vertex dynamics!

spin fluctuations

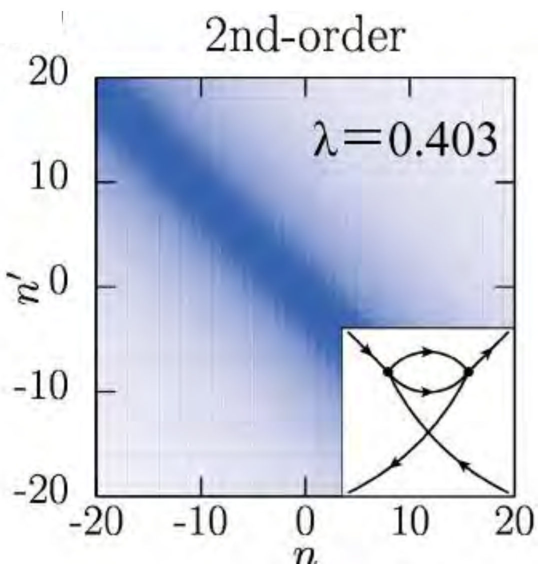
$\chi=\chi_0+\chi_0 U\chi_0+\chi_0 U\chi_0 U\chi_0+\ldots$

$= \chi_0/(1-\chi_0 U)$



suppressed by pp channel $\delta\Gamma_m$

2^{nd} order

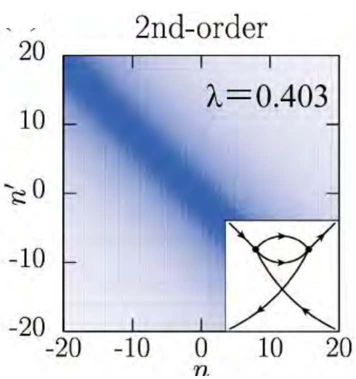


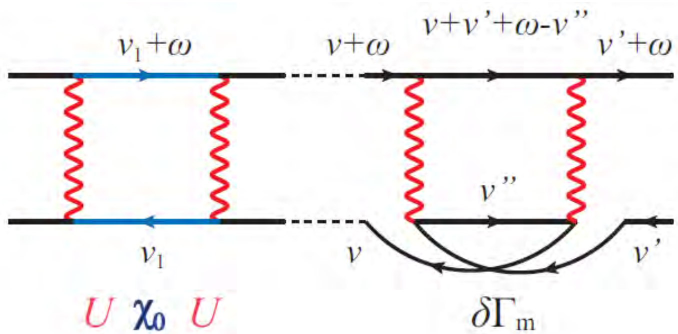
Conclusion

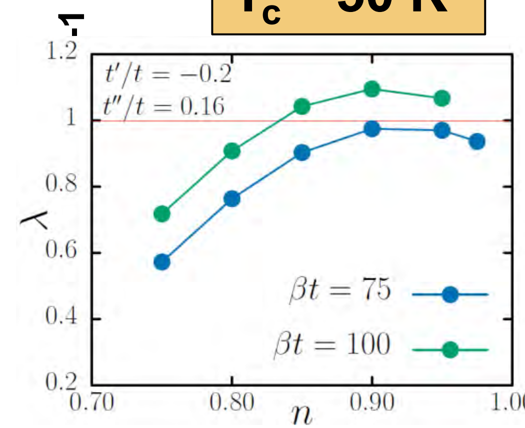
➢ **DΓA for high T_c superconductors**

SC dome
$T_c \sim 50$ K

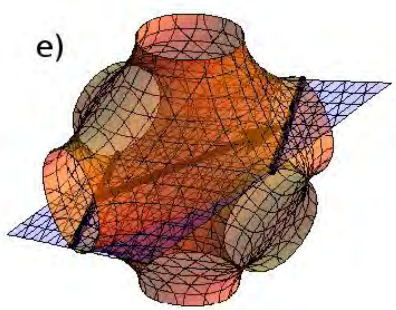
vertex dynamics suppresses T_c



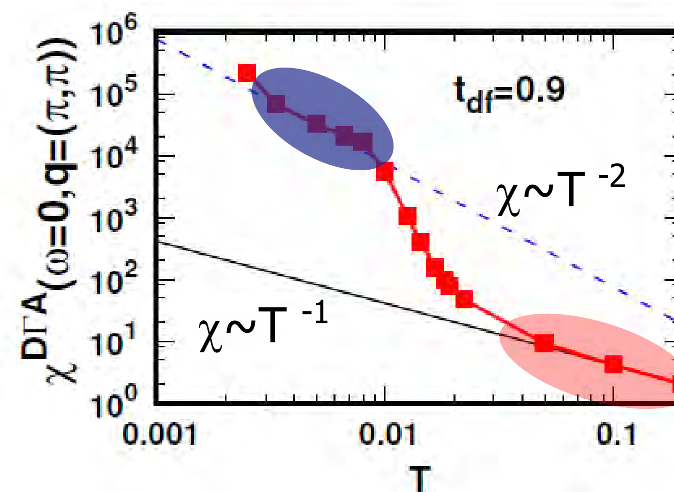




➢ **quantum criticality**
3D Hubbard model



2D periodic Anderson model



Thanks to ....

- **M. Kitatani, T. Schäfer, A. Toschi** **(TU Wien)**
- **A. Katanin (Ekaterinburg)**
- **G. Rohringer (Moskva)**

Further reading:

QCP Hubbard:	PRL 119 0946402 (2017)
SC Hubbard:	arXiv: 1801.05991
	RMP 90, 025003 (2018)

Vienna Computational Materials Laboratory ViCoM

DFG FOR1346

FWF

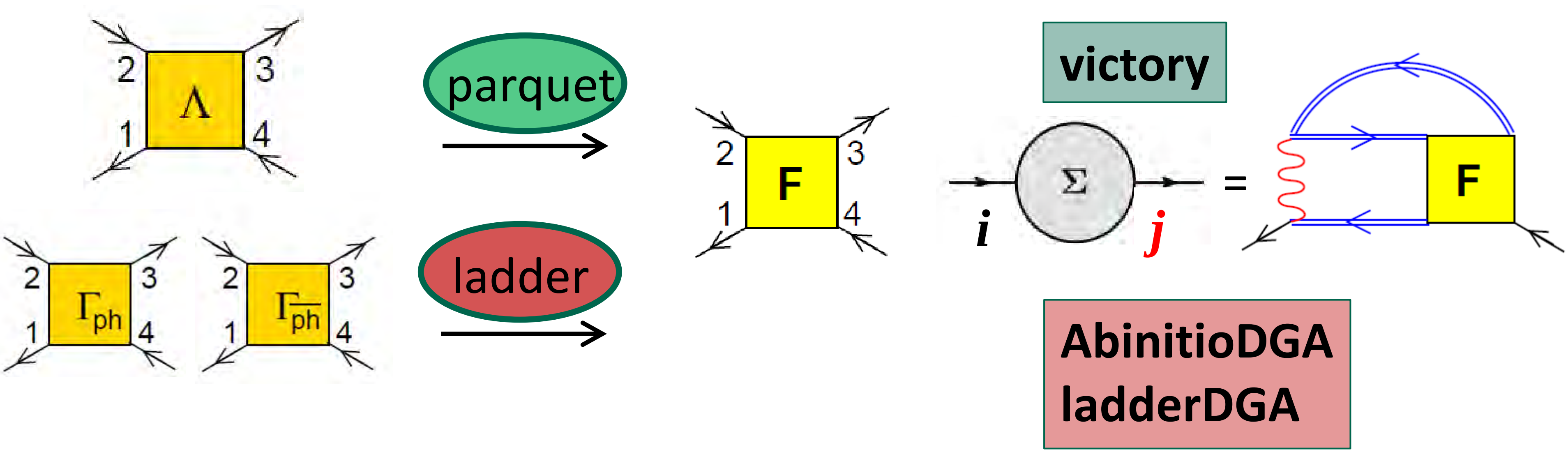
erc European Research Council

Conclusion: method

DΓA: Resummation of Feynman diagrams in terms of locality

n-particle fully irreducible vertex *approximated as local*

local ⟶ **non-local**



includes local **DMFT** correlations

and non-local correlations

(e.g. spin fluctuations)