TECHNISCHE UNIVERSITÄT WIEN
Vienna University of Technology

European Research Council

Divergent Precursors of the Mott Transition

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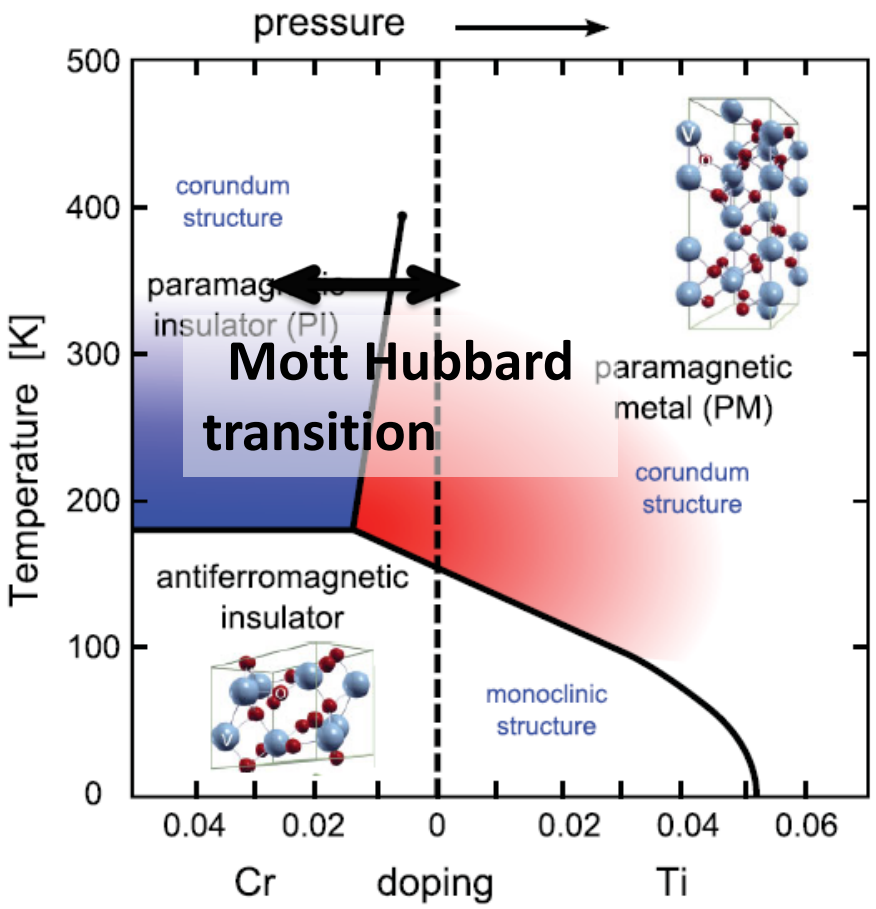
ERC Workshop, Ab-initio-DΓA

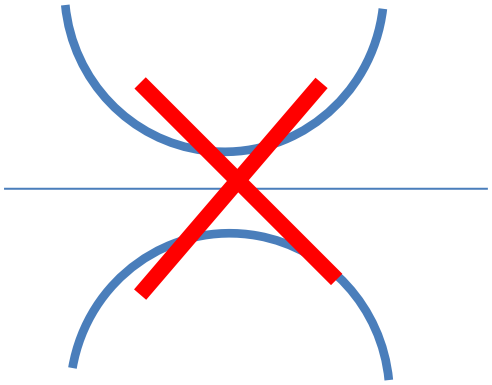
3rd September 2013

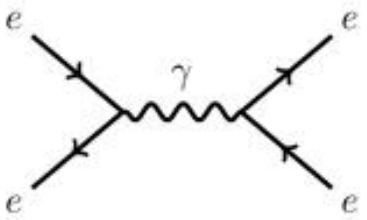
From Metallic to Insulating: the Mott transition (**MIT**)

- V_2O_3 - Mott insulator

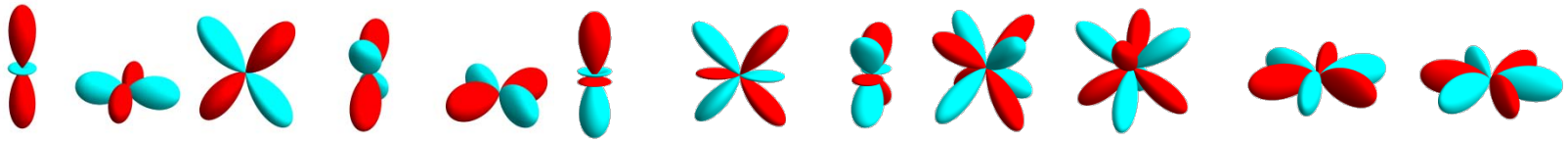


- Band insulator





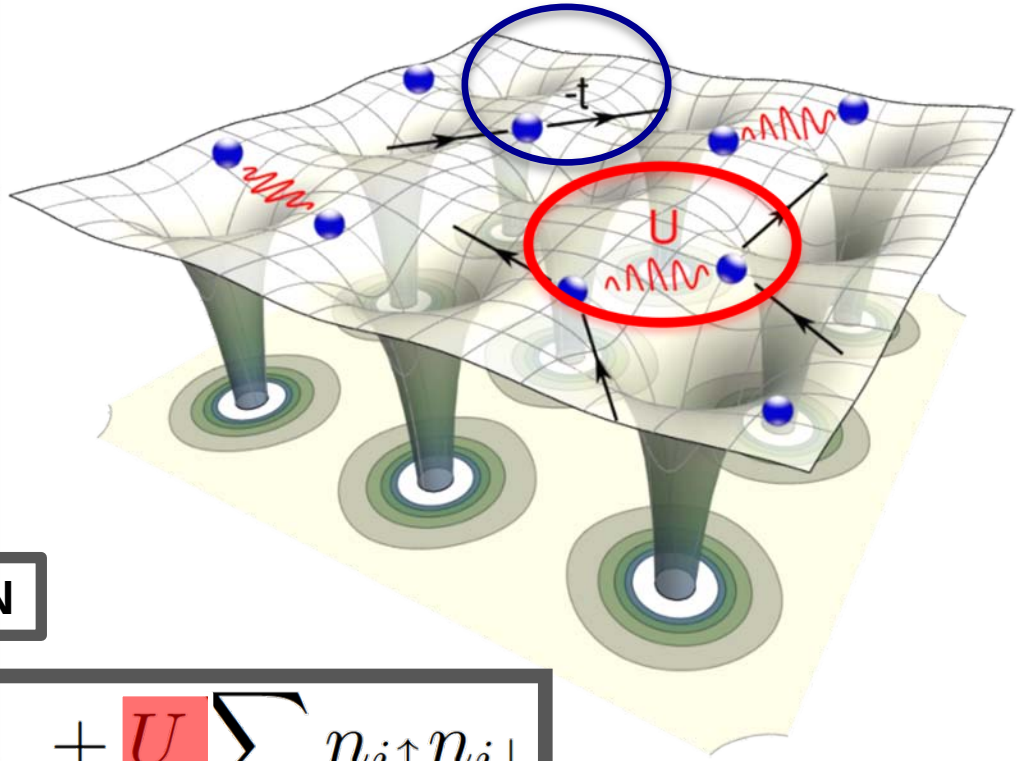
The Hubbard model



localized **d**- and **f**- orbitals

-t : electron hopping

U: local Coulomb interaction



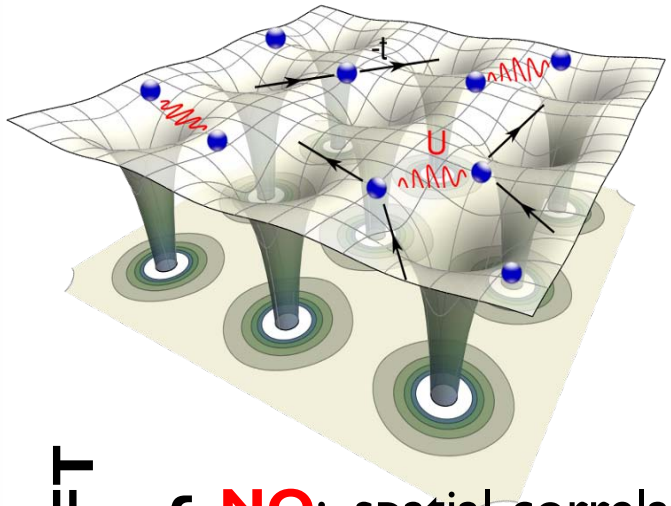
HUBBARD HAMILTONIAN

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

The Dynamical Mean Field Theory (DMFT)

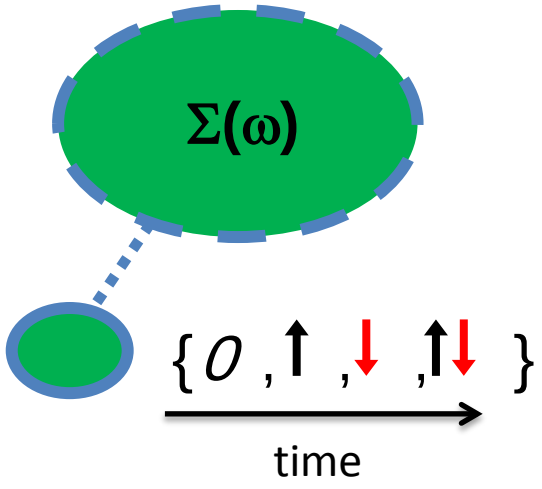
$$H = -t \sum_{\langle ij \rangle \sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

Dynamical **M**ean **F**ield **T**heory (**DMFT**)



MF in space
fluctuations in time

(d→∞)



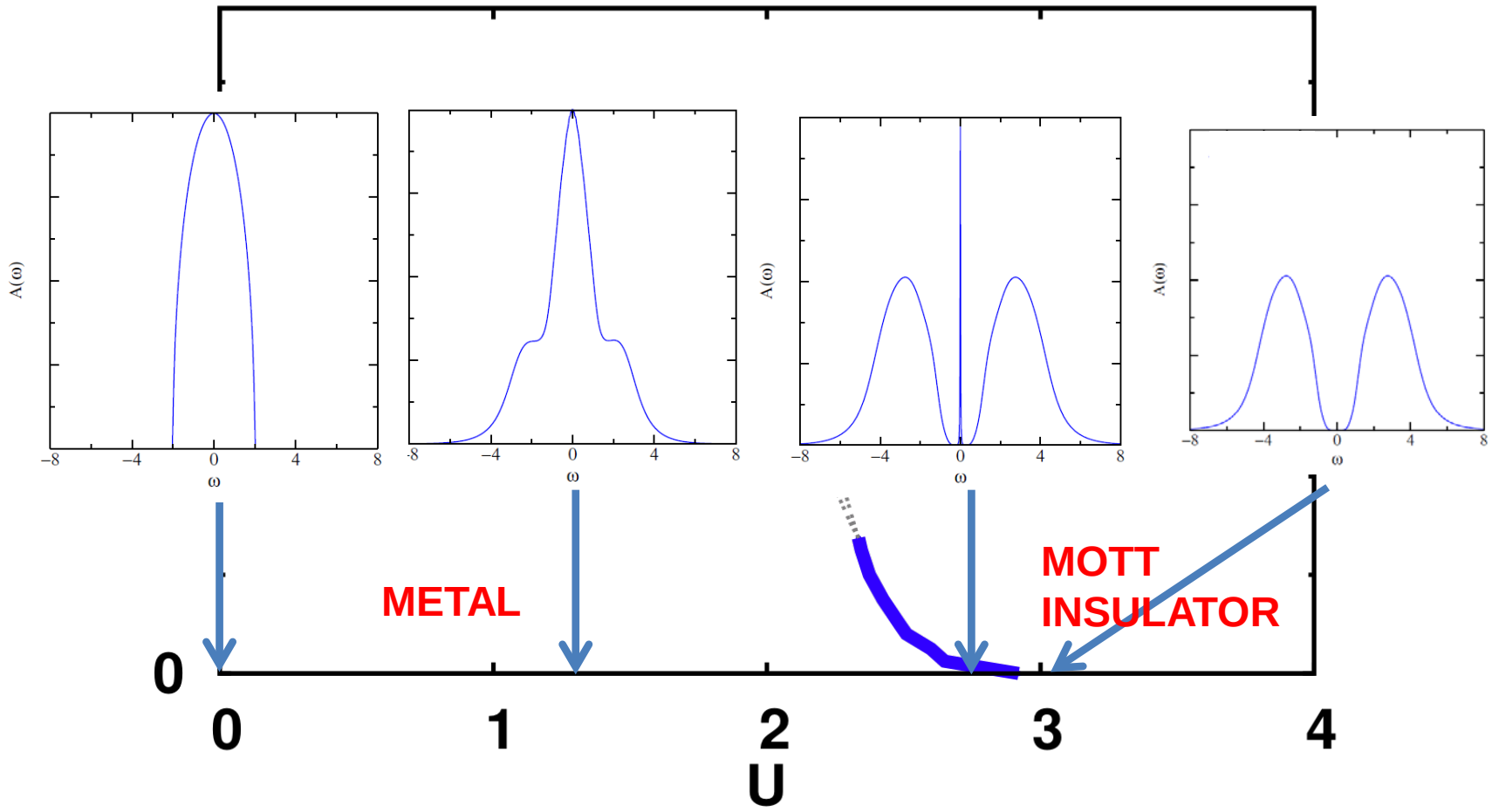
DMFT

{ **NO**: spatial correlations
YES: local **temporal** correlations

W. Metzner, D. Vollhardt, PRL 62 (`89),
A. Georges, G. Kotliar, PRB 45 (`92)

The MIT at the one-particle Level

The **phase diagram** of the Hubbard model (half-filled)



MIT data: *N. Bluemer, PhD Thesis* spectral data: *R. Zitzler, PhD Thesis*

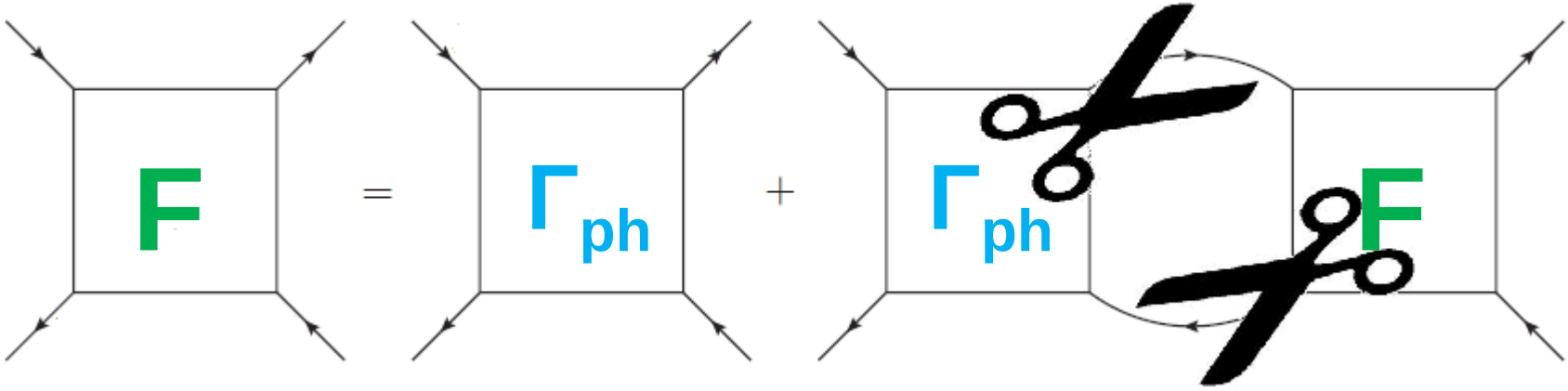
Reminder: two-particle Quantities

Parquet equation

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

Bethe-Salpeter equations

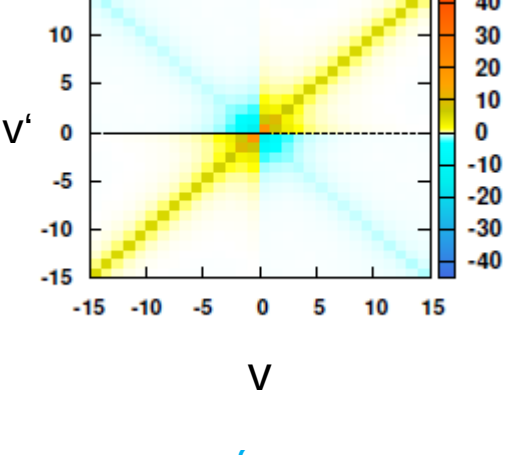
$$F = \Gamma_{ph} + \Phi_{ph} \Rightarrow \boxed{\Gamma_c = \chi_c^{-1} - \chi_0^{-1}}$$



Two-particle Quantities in DMFT : Γ_c – from Weak to Strong Coupling

$\Gamma_c(\nu,\nu',\omega=0)-U$

U=1.20



- Fixed temperature evolution with U, T=0.10
- Reproducible by common perturbation theory

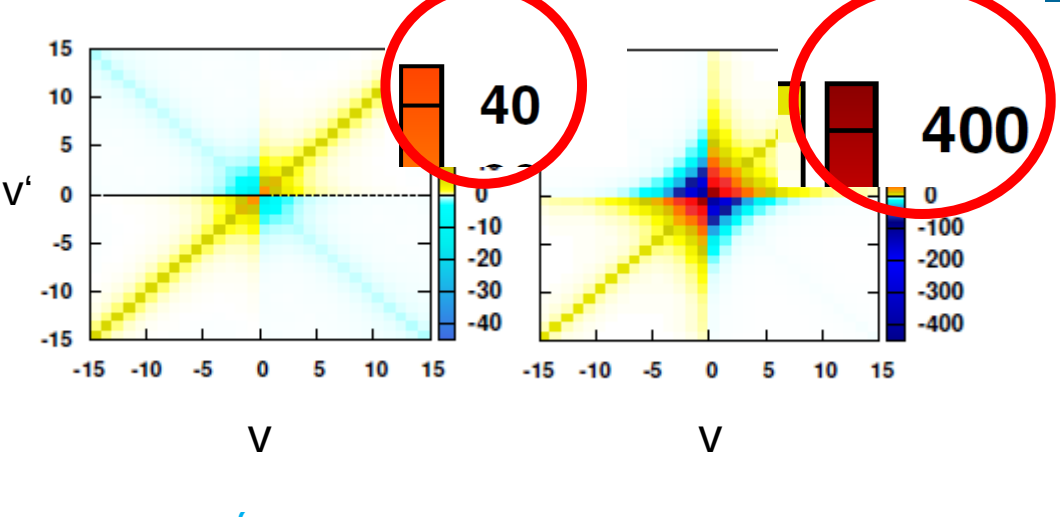
$$\Gamma_c^{\nu,\nu',\omega} = [(\chi_c^{\nu,\nu'})^{-1}]^{\omega} - [(\chi_0^{\nu,\nu'})^{-1}]^{\omega}$$

β=10.0(4t)$^{-1}$
half-filling, 2D
DMFT(QMC)

T. Schäfer , G. Rohringer, O. Gunnarsson, S. Ciuchi, G. Sangiovanni and A. Toschi, PRL 110, 246405 (2013)

Two-particle Quantities in DMFT : Γ_c – from Weak to Strong Coupling

$\Gamma_c(\nu,\nu',\omega=0)-U$ U=1.20 $\Gamma_c(\nu,\nu',\omega=0)-U$ U=1.27



- Strong enhancement at low frequencies
- Becomes predominant over the diagonals

$$\Gamma_c^{\nu,\nu',\omega} = [(\chi_c^{\nu,\nu'})^{-1}]^{\omega} - [(\chi_0^{\nu,\nu'})^{-1}]^{\omega}$$

$\beta=10.0(4t)^{-1}$
half-filling, 2D
DMFT(QMC)

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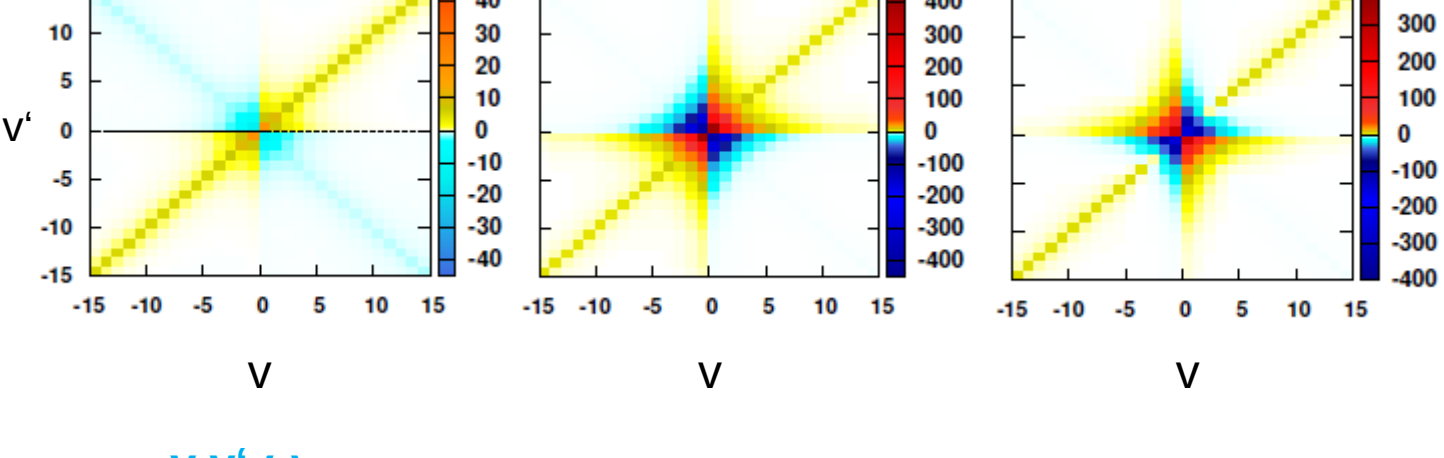
Two-particle Quantities in DMFT : Γ_c – from Weak to Strong Coupling

$\Gamma_c(\nu,\nu',\omega=0)-U$ U=1.20

$\Gamma_c(\nu,\nu',\omega=0)-U$ U=1.27

$\Gamma_c(\nu,\nu',\omega=0)-U$ U=1.28



- Inverted signs
- PT cannot reproduce this inverted sign

$$\Gamma_c^{\nu,\nu',\omega} = [(\chi_c^{\nu,\nu'})^{-1}]^{\omega} - [(\chi_0^{\nu,\nu'})^{-1}]^{\omega}$$

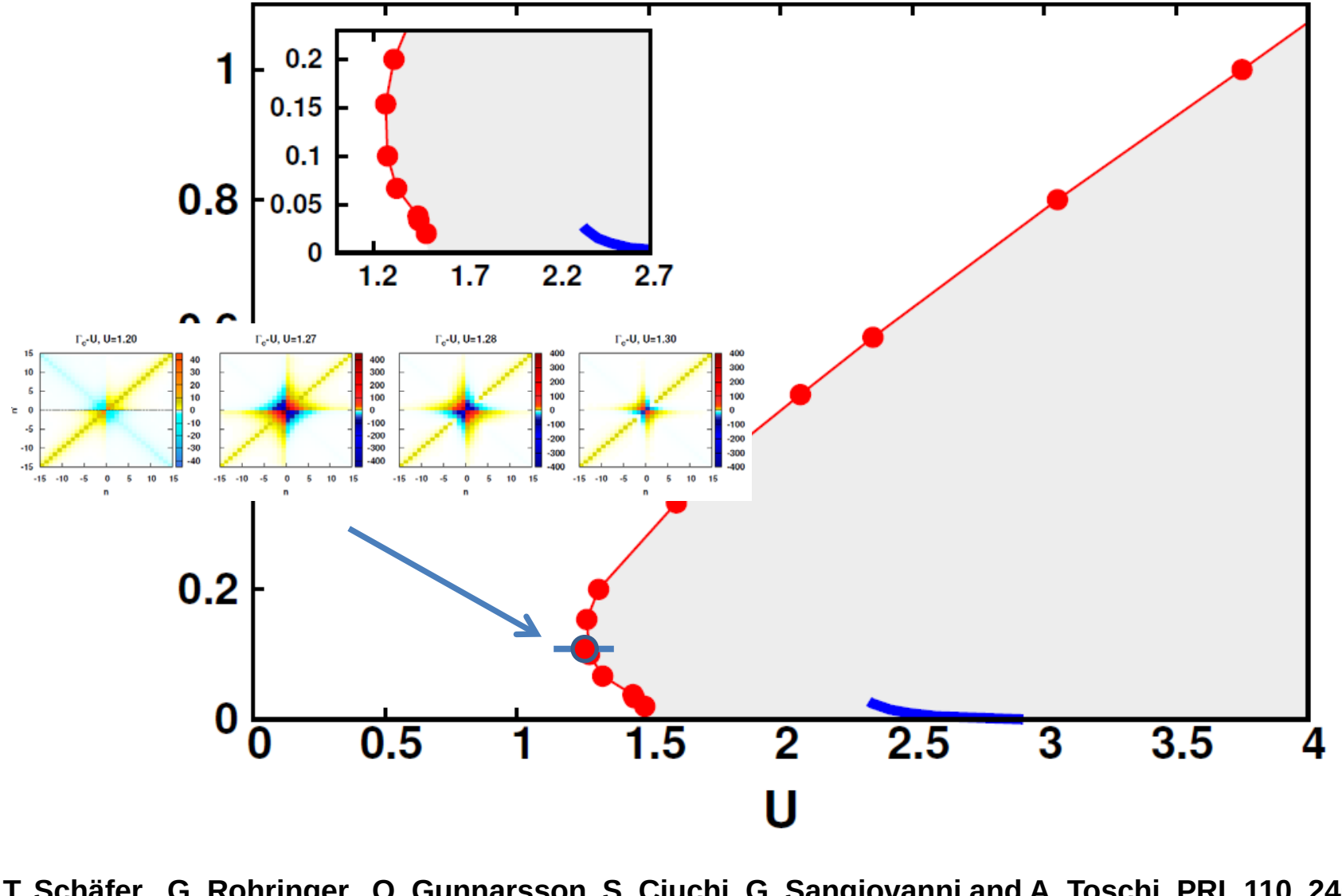
Γ_c → ∞

$[(\chi_c^{\nu,\nu'})^{-1}]^{\omega} - [(\chi_0^{\nu,\nu'})^{-1}]^{\omega}$ → " 0" (→eigenvalue)

β=10.0(4t)$^{-1}$
half-filling, 2D
DMFT(QMC)

T. Schäfer , G. Rohringer, O. Gunnarsson, S. Ciuchi, G. Sangiovanni and A. Toschi, PRL 110, 246405 (2013)

Divergency Line of Γ_c: Possible Interpretations



T. Schäfer , G. Rohringer, O. Gunnarsson, S. Ciuchi, G. Sangiovanni and A. Toschi, PRL 110, 246405 (2013)

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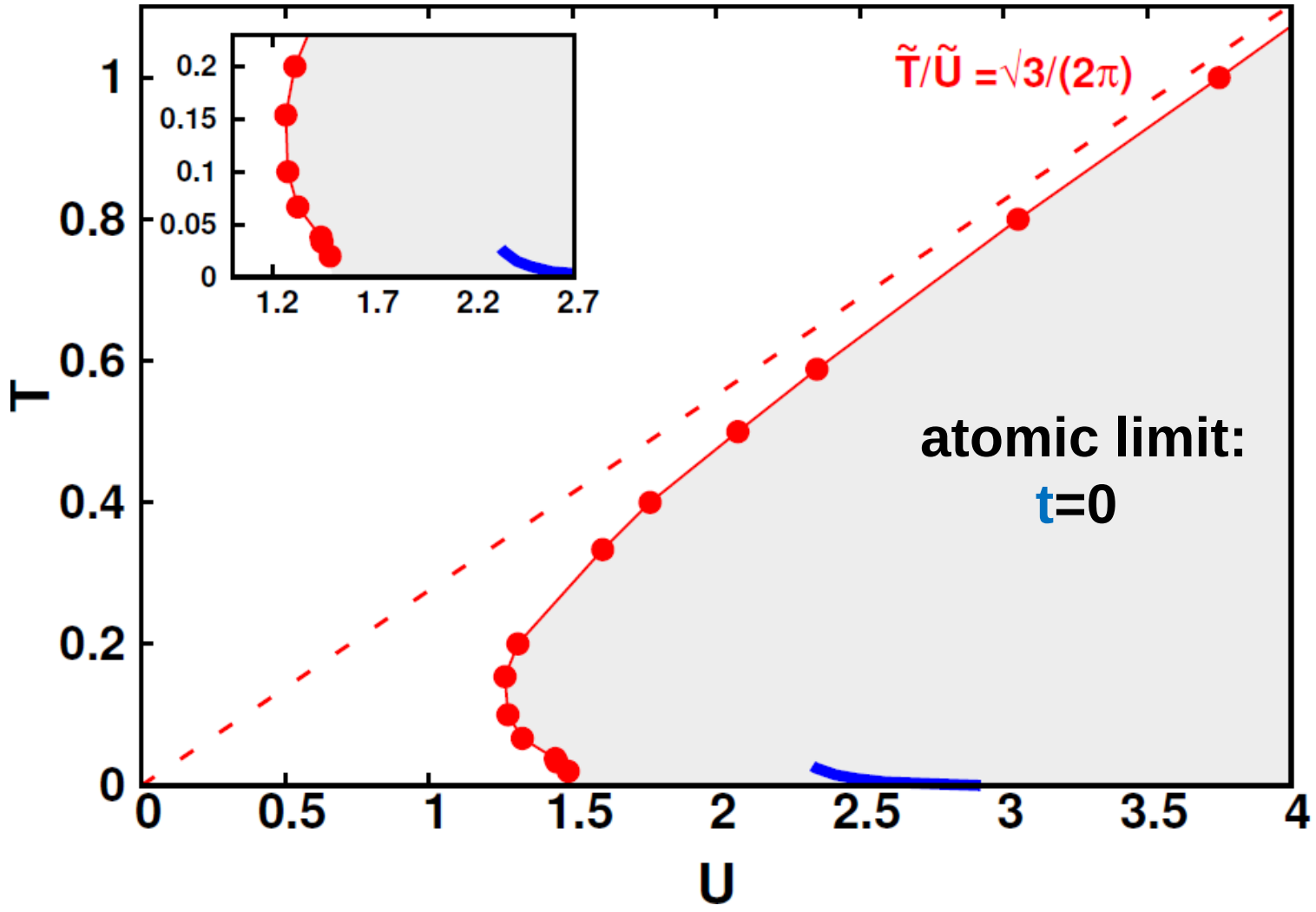
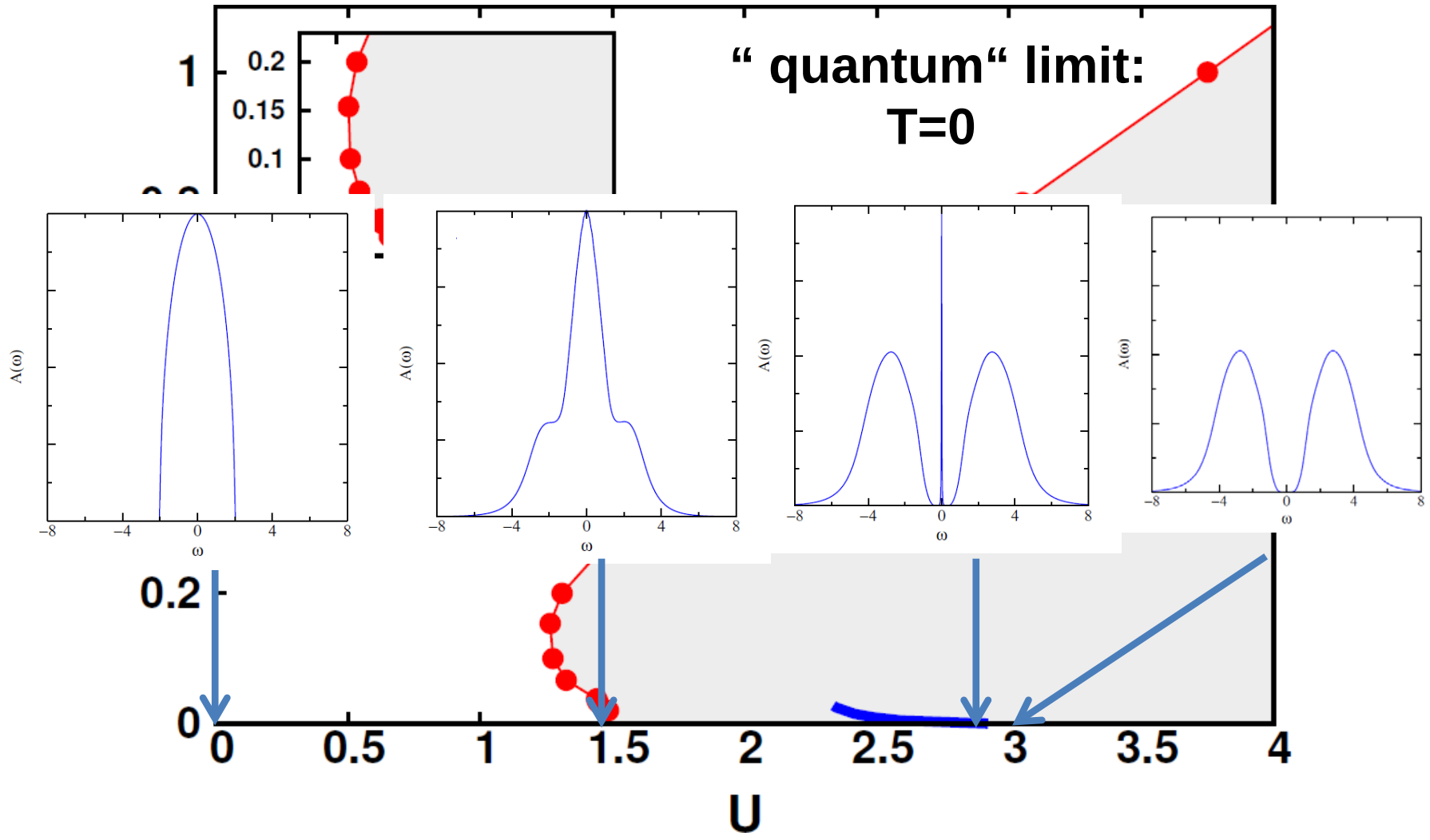


T. Schäfer et al., PRL 110, 246405 (`13), G. Rohringer et al., PRB 86 125114 (`12),
H. Hafermann et al., EPL 85 27707 (`09), S. Pairault et al., Eur. Phys. J. B 16 85-105 (2000)

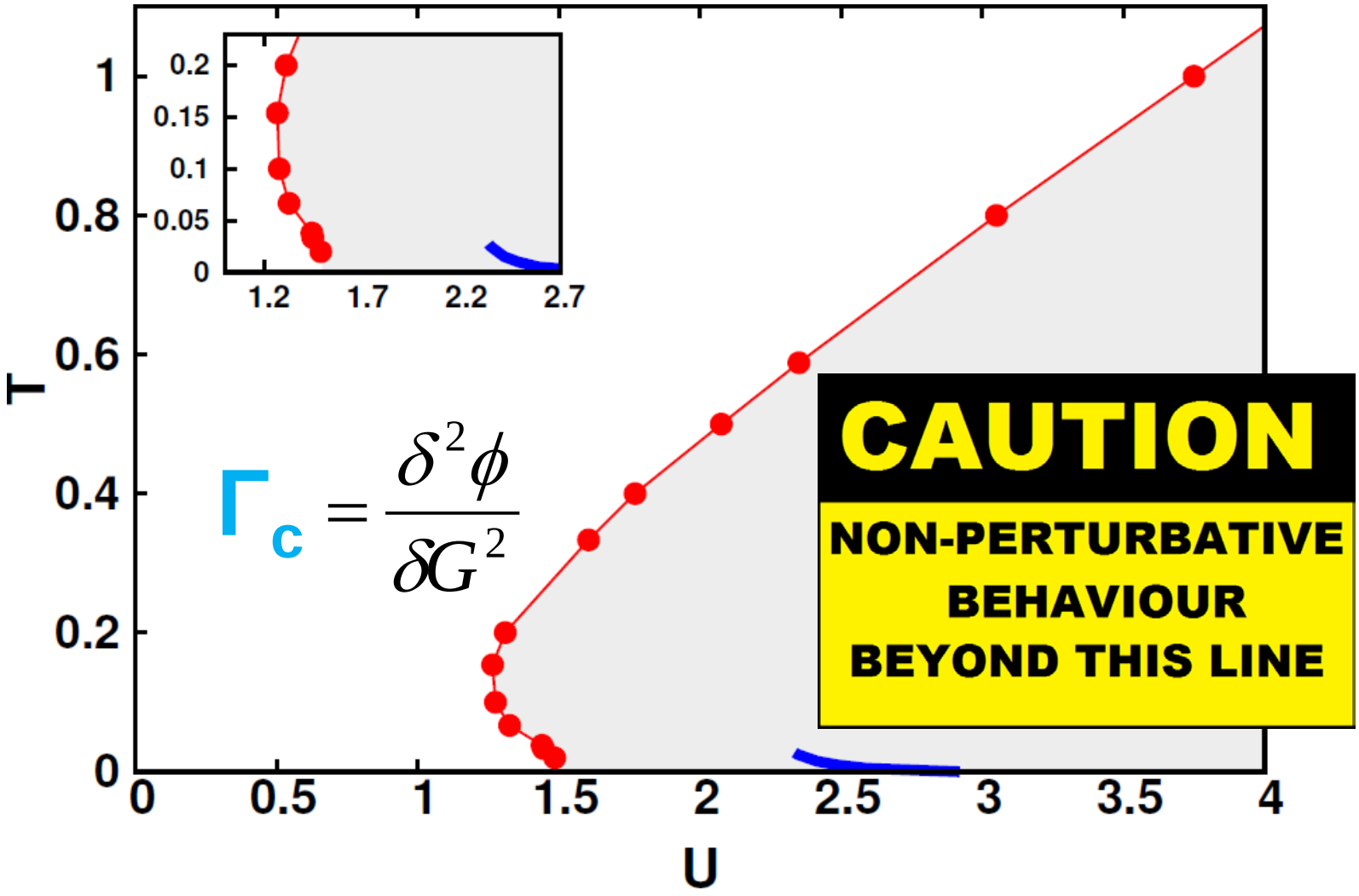
Divergency Line of Γ_c: Possible Interpretations



R. Bulla et al. PRL 83 136 (1999) and R. Zitzler PhD Thesis (Augsburg, 2004)

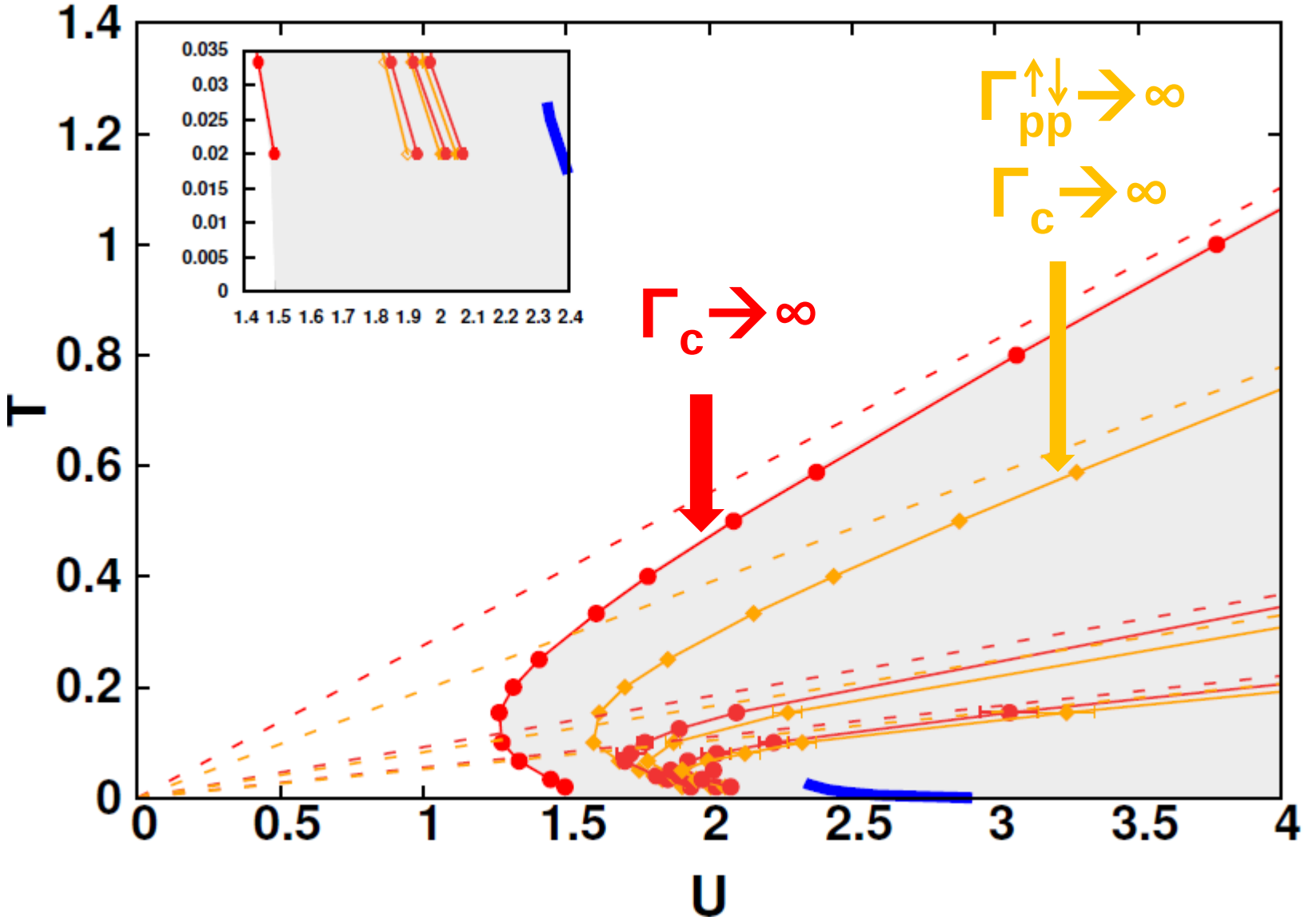
K. Byczuk et al., Nat Phys 3, 168 (‘07), K. Held, R. Peters and A. Toschi, PRL 110, 246402 (‘13)

Divergency Line of Γ_c: Possible Interpretations

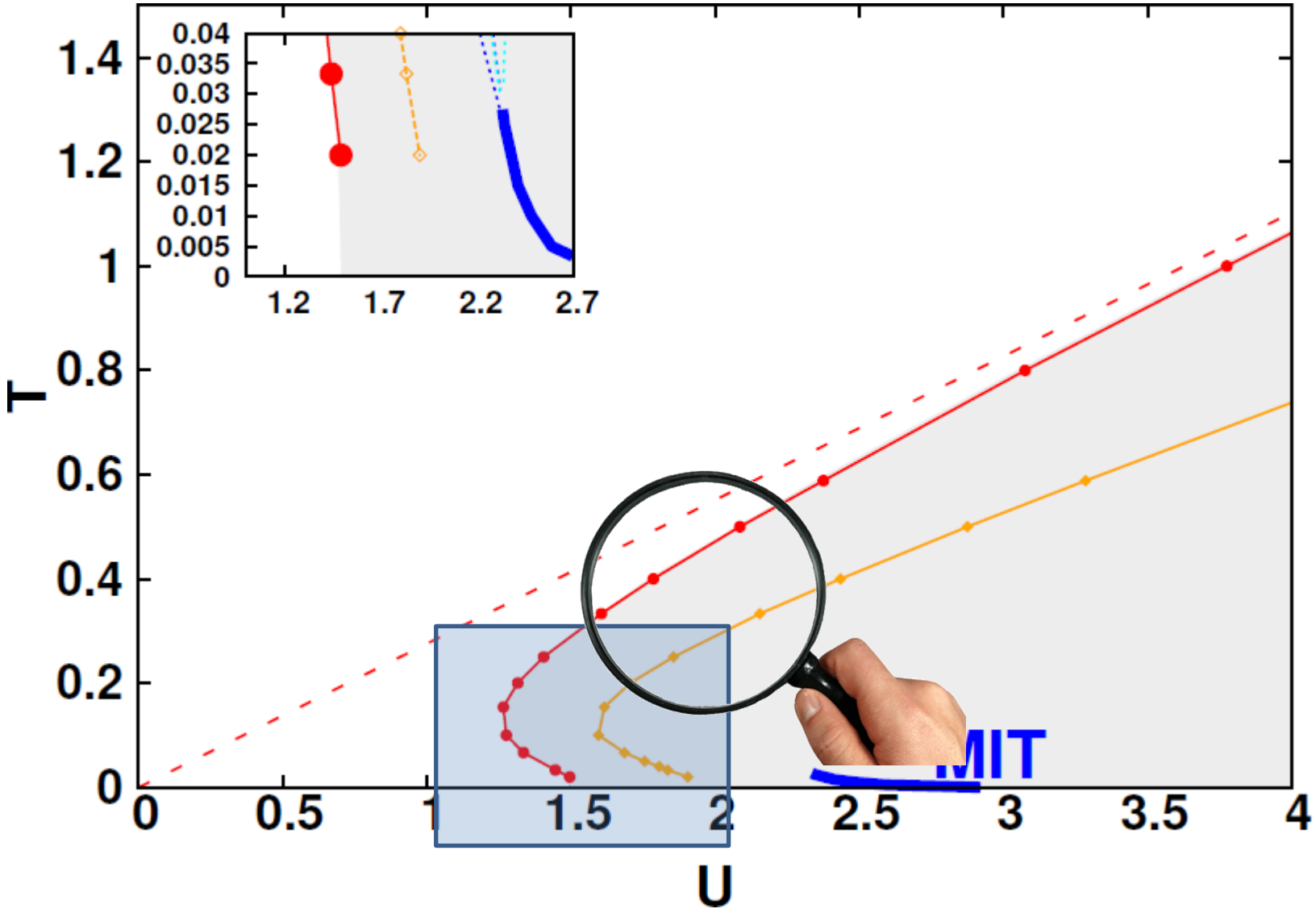


T. Schäfer et al., PRL 246405 (2013), G. Baym and L. Kadanoff PR 124 287 (`61)

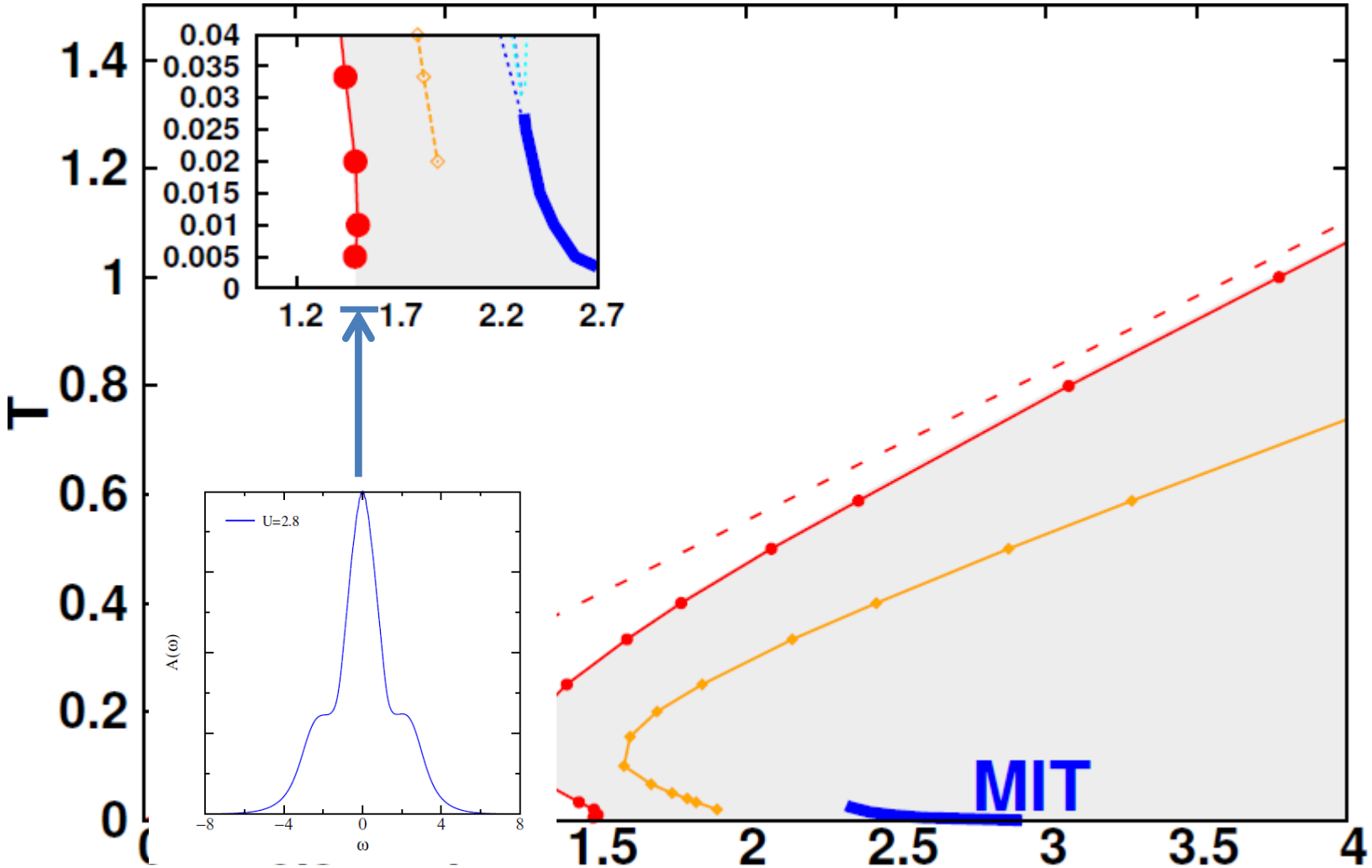
Ongoing work: Deeper Understanding of **DMFT** results



Ongoing work: Deeper Understanding of **DMFT** results



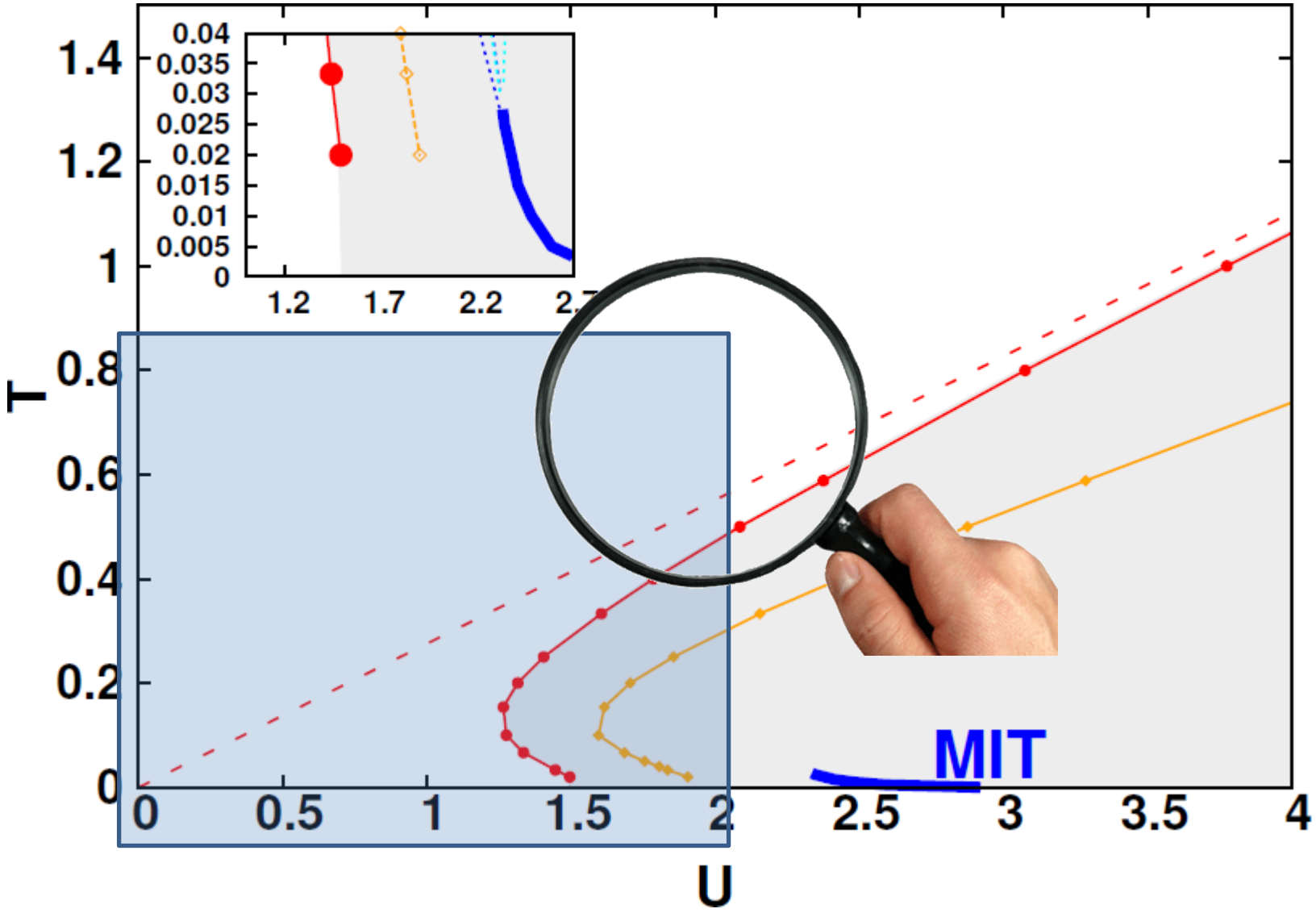
Ongoing work: Deeper Understanding of **DMFT** results



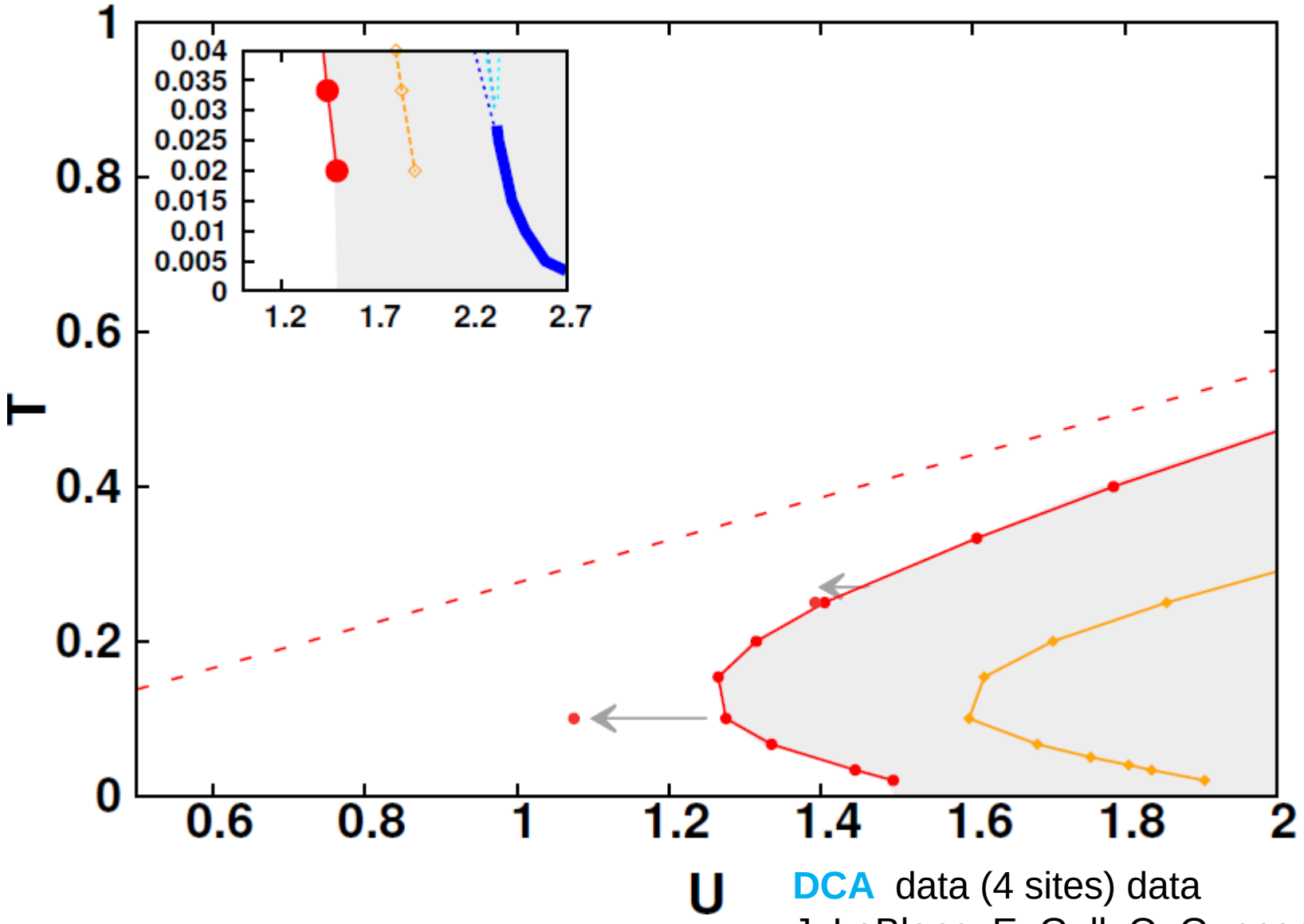
R. Zitzler PhD Thesis (Augsburg, 2004)

DMFT (CT-QMC) data
M. Wallerberger

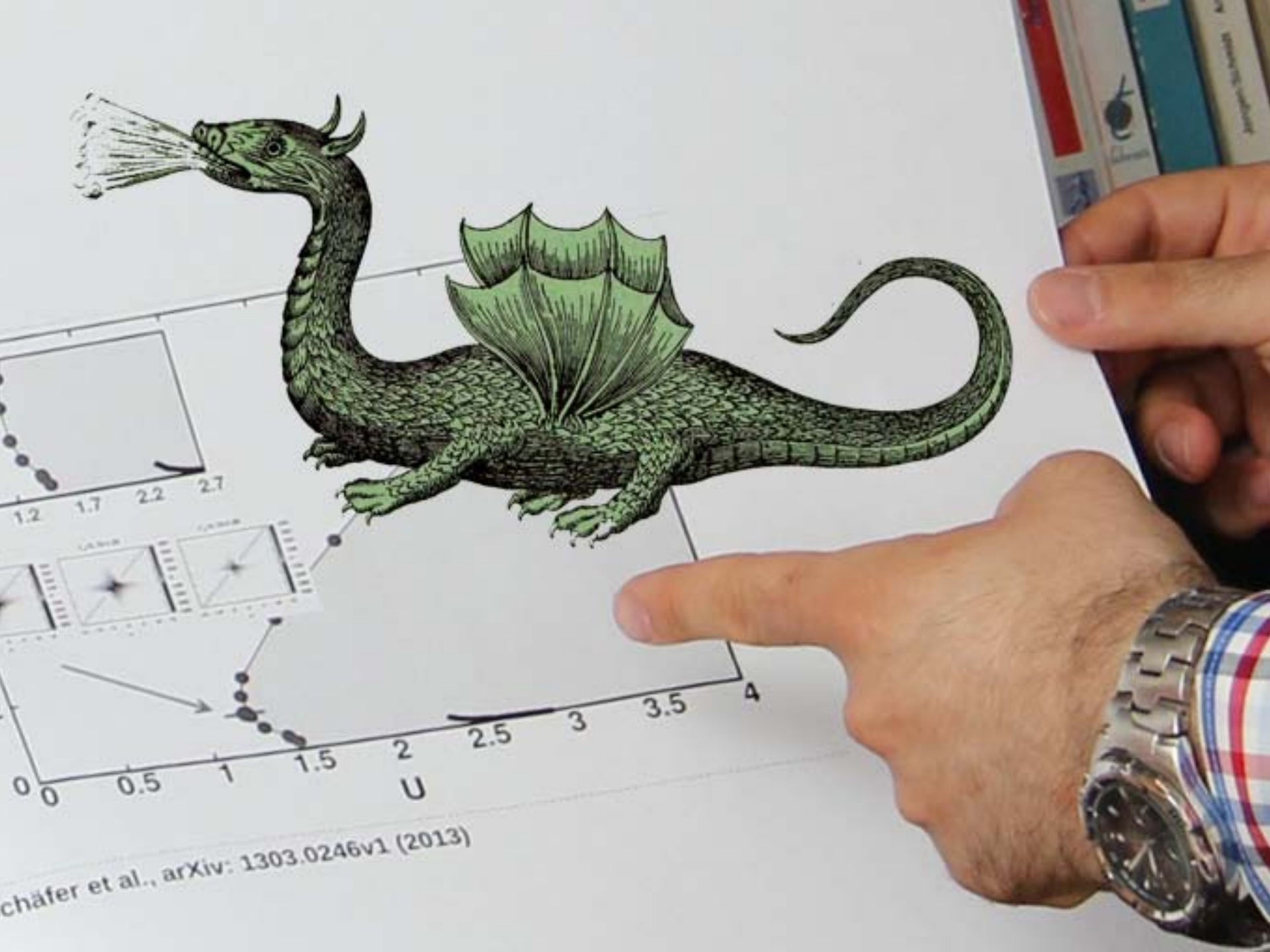
Ongoing work: Including short-ranged Correlations (**DCA**)



Ongoing work: Including short-ranged Correlations (**DCA**)

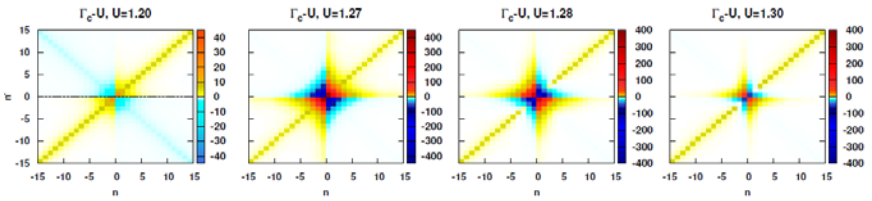


DCA data (4 sites) data
J. LeBlanc, E. Gull, O. Gunnarsson


1.2
1.7
2.2
2.7
0
0.5
1
1.5
2
2.5
3
3.5
4
U
chäfer et al., arXiv: 1303.0246v1 (2013)

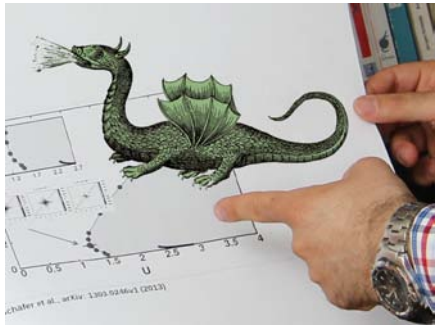
Conclusions and Outlook

First **precursors** of MIT **in metallic phase:**
divergence of Γ_c



New region in **phase diagram**:

Mathematically clear separation of
weakly and **strongly** correlated regions



Outlook/Ongoing: multiple divergency lines, low temperatures.
inclusion of spatial correlations (**DCA**),
doping

Special thanks to A. Toschi, G. Rohringer and Florian Aigner (PR)
(http://www.tuwien.ac.at/aktuelles/news_detail/article/8264/)