Nonperturbative Fingerprints of the Many-Electron Physics ... and their Surprising Implications

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TU WIEN

- *PRL **125** 196403 **(2020)***
- *PRL **126** 056403 **(2021)***

Joint Theory seminar of **Condensed Matter departments**

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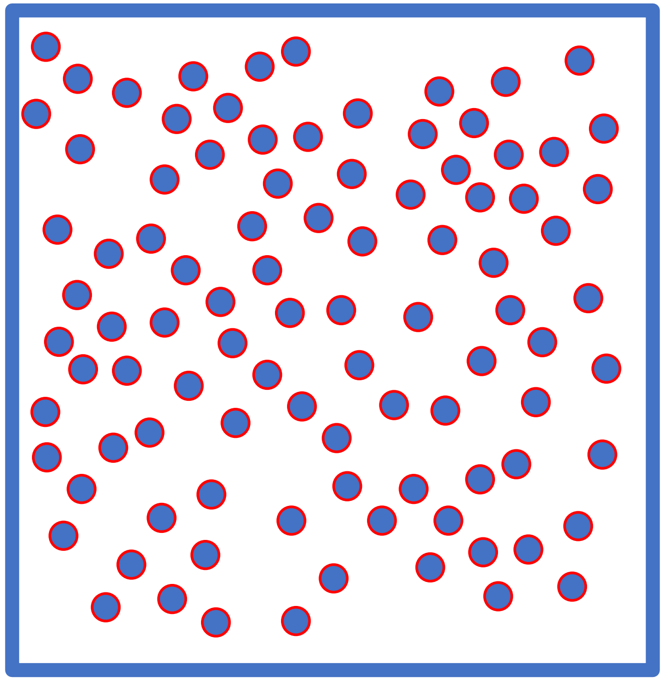
and to the Austrian Science Fund (**FWF**) for financial support through the project I 2794-N35

The two-fold challenge …

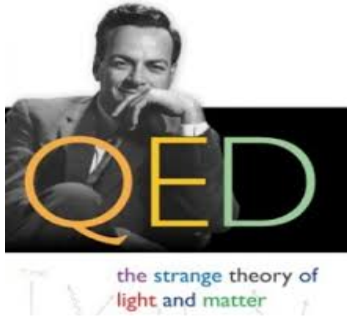
*… of the **many-electron** problem:*



~ **10^{23}** interacting fermions !

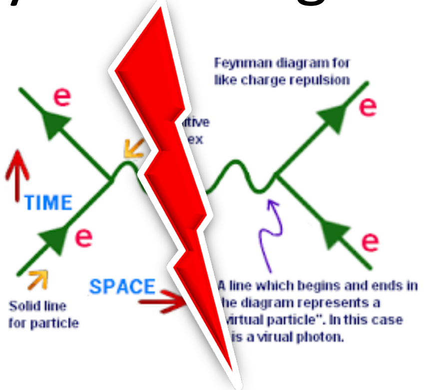
huge number of D.o.F. !

Quantum field theory as in:



NO control parameter (like **α =1/137**) for the many-body expansion !

Feynman diagrams

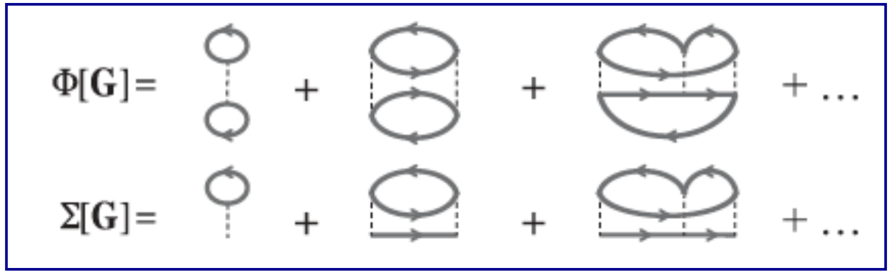


in **nonperturbative** regimes !

Two main
routes
to approximations

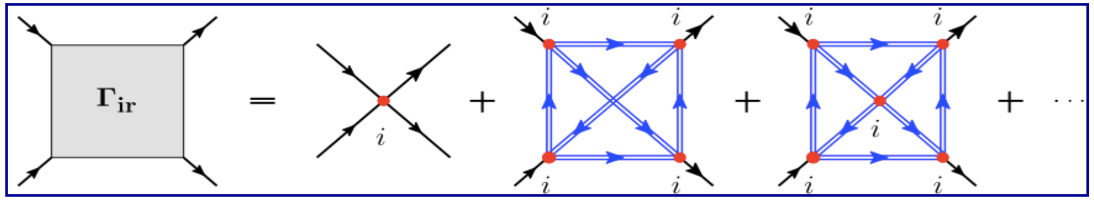
1. Luttinger-Ward formalism ➔ *“conserving theories„*

$$\Omega[G] = \tilde{\Omega}[G_0, G] + \Phi[G] \;\Rightarrow\; \Sigma = \frac{\delta\Phi}{\delta G};\; \Gamma_{ch}^{IRR} = \frac{\delta^2\Phi}{\delta G^2}$$



2. Crossing symmetries ➔ *“Pauli principle„*

$$\Sigma = \int \Gamma\, GGG \text{ with } \Gamma \Leftarrow \Gamma^{IRR} = \text{BSE } \textit{and / or} \text{ parquet}$$



Nonperturbative

Tw main
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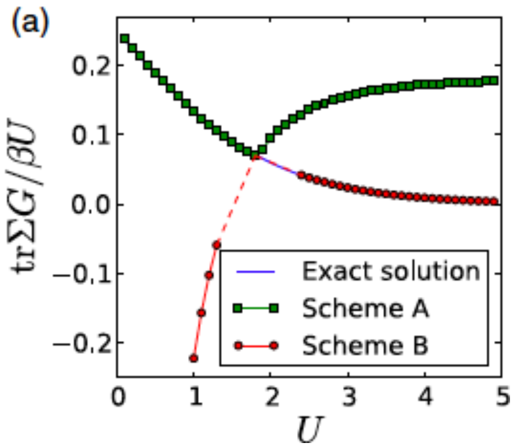
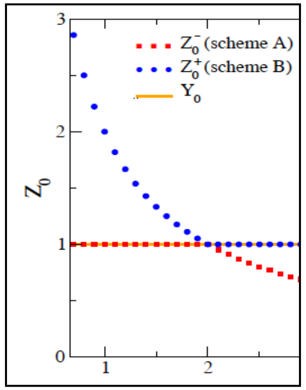
to approx nations

breakdown!

1. Luttinger-Ward functionals

I. Multivaluedness of LW functional

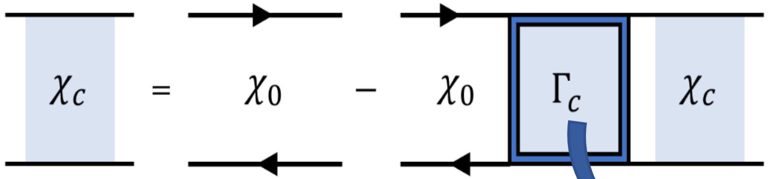


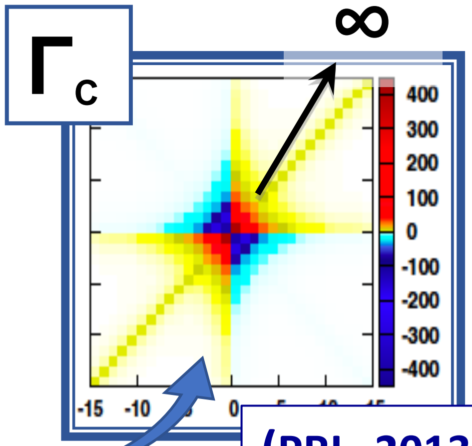


E. Kozik et al., PRL (2015)
A.Stan et al., NJP (2015)
R. Rossi et al., PRB (2015)
W.Tarantino, et al., PRB (2017)
J.Vucicevic, et al. PRB (2018)
A.J. Kim et al. arXiv:2012.06159
K.Van Houcke et al., arXiv:2102.04508

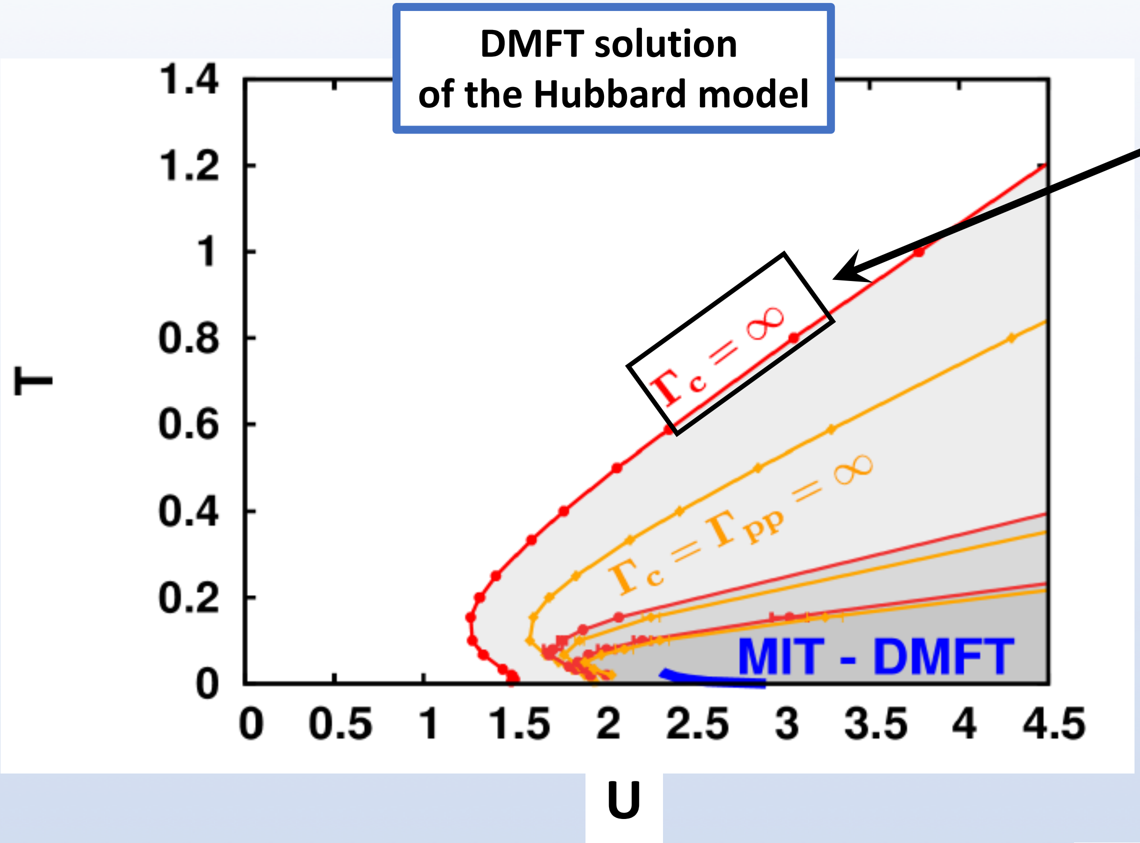
2. Crossing symmetries

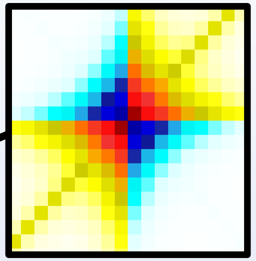
II. Divergences of irreducible vertices





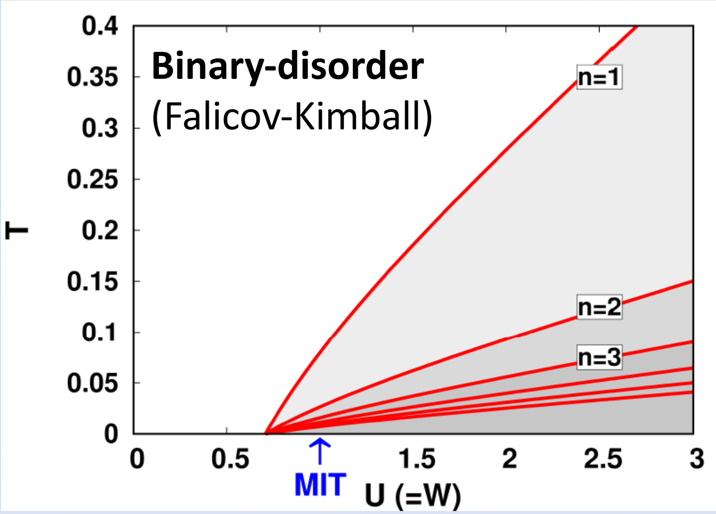
(PRL, 2013)

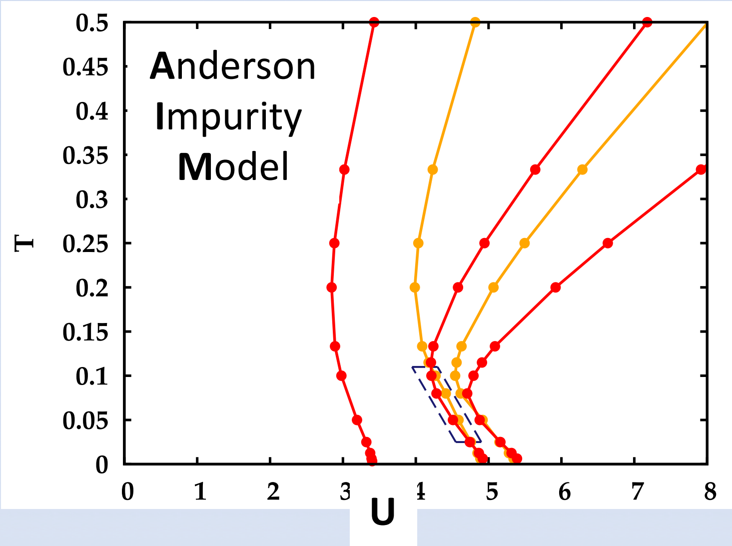


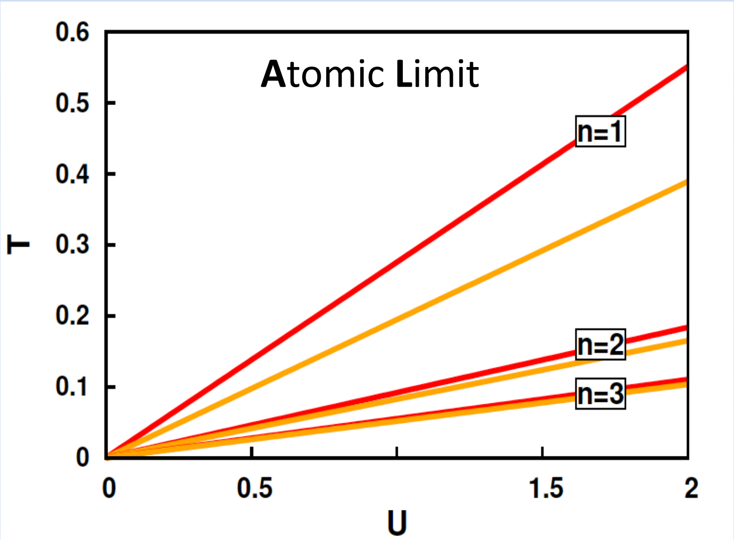


- T. Schäfer, ... and A.T., PRL **110** 246105 (2013)
- T. Schäfer, ... and A.T., PRB **94** 235108 (2016)

- P. Chalupa, ..., & A.T., PRB **97** 245136 (2018)
- P. Thunström, ..., & G. Rohringer, PRB **98** 235107 (2018)
- D. Springer, ..., & AT, PRB **101** 155148 (2020)

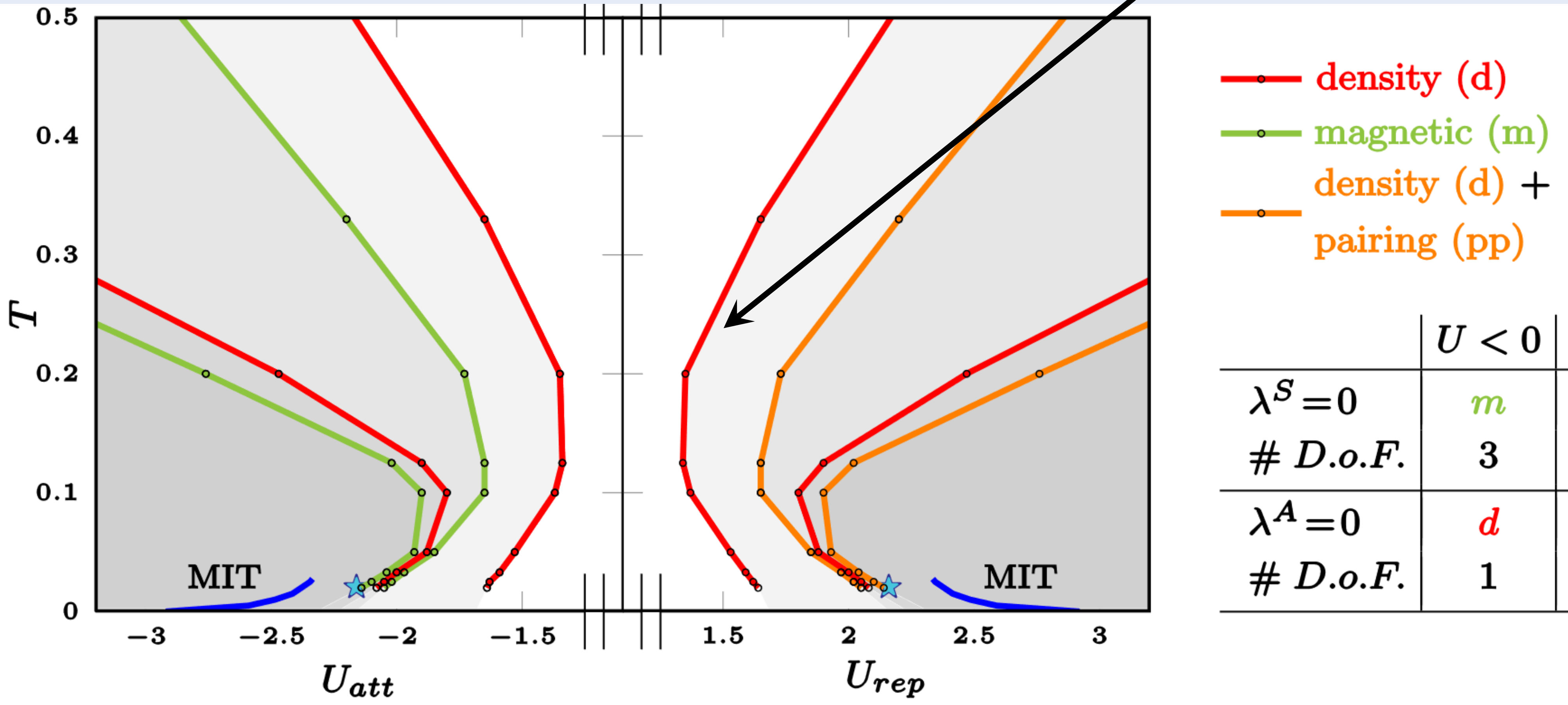


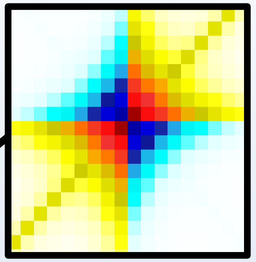




DMFT solution of the **attractive** Hubbard model

DMFT solution of the **repulsive** Hubbard model





	$U<0$	$U>0$
$\lambda^S=0$	m	d, pp
$\#$ D.o.F.	3	$1+2$
$\lambda^A=0$	d	d
$\#$ D.o.F.	1	1

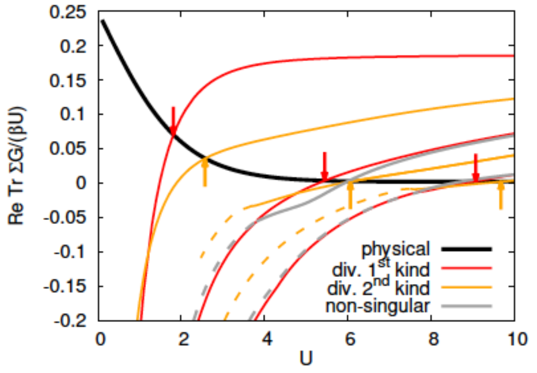
❖ D. Springer, …., & AT, PRB **101** 155148 (2020)

Nonperturbative

breakdown!

I. Multivaluedness of LW functional

BOTH numerically ....



EQUIVALENT ASPECTS
of the SAME „phenomenon“ !!!

[PRL ***119*** *046402 (2017)]*

II. Divergences of irreducible vertices

... AND analytically !

$$\sum_{\nu'} \chi_c^{\nu\nu'(\omega=0)} \left[1/G_0^{(2)}(\nu') - 1/G_0^{(1)}(\nu')\right] = O\left[\left(1/G_0^{(2)} - 1/G_0^{(1)}\right)^2\right].$$

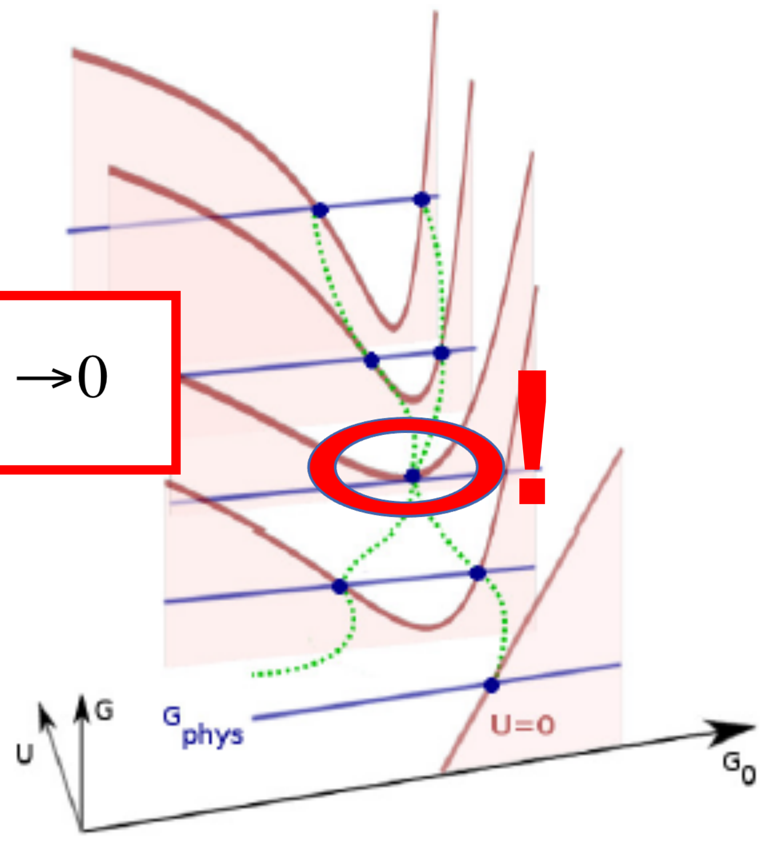
Heuristic picture:

G = G[G$_0$]

$$\frac{\delta G}{\delta \Sigma} = \frac{\delta G}{\delta G_0}\frac{\delta G_0}{\delta \Sigma} \to 0$$

(I) Multivaluedness of LW functional

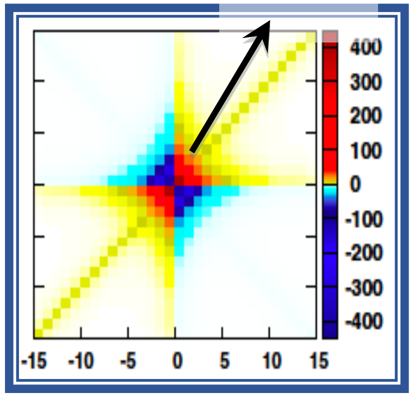
$$\frac{\delta G}{\delta G_0} \to 0$$



(II) Divergences of irreducible vertices

$$\Gamma_{ch}^{IRR}[G] = \frac{\delta^2 \Phi}{\delta G^2} = \frac{\delta \Sigma}{\delta G} \to \infty$$

∞



O. Gunnarsson, ... , & AT, PRL **119** 046402 (2017)

algorithmic challenges

I. Multivaluedness of LW functional

iterative/self-consistent (=``bold'') approaches

Diagrammatic Monte Carlo

Nested Cluster Schemes

[E. Kozik et al., PRL (2015); A.Stan et al., NJP (2015);
R. Rossi et al. , PRB (2015); J.Vucicevic, et al. PRB (2018), ….]

II. Divergences of irreducible vertices

parquet-based methods

dynamical vertex approximation (**DΓA**)

QUADRILEX

[A.Toschi et al., PRB (2007); O. Gunnarsson et al., PRB (2016)
T.Ayral et al. , PRB (2016); G. Rohringer et al. , PRB (2018); ….]

Outline

1) What is the **``origin”** of the **breakdown** in many-body perturbation theories ?

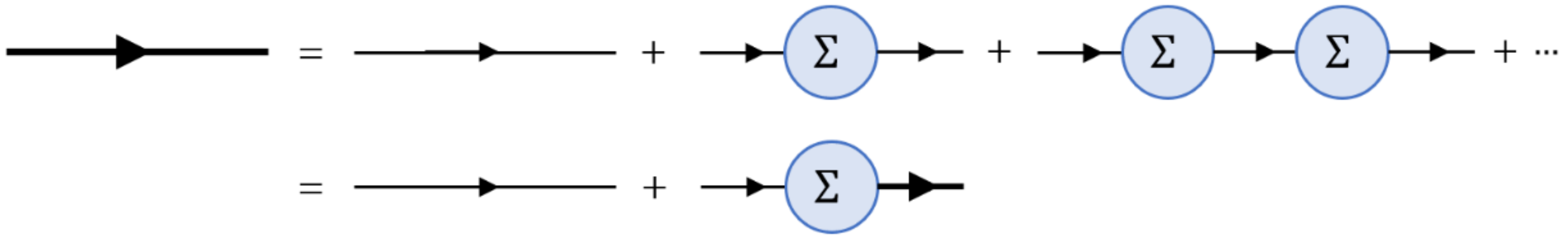
- How to ``read’’ the physics from the 2P quantities
- **FINGERPRINTS** of the local moment formation and of its Kondo screening

2) Are there relevant **physical consequences?**

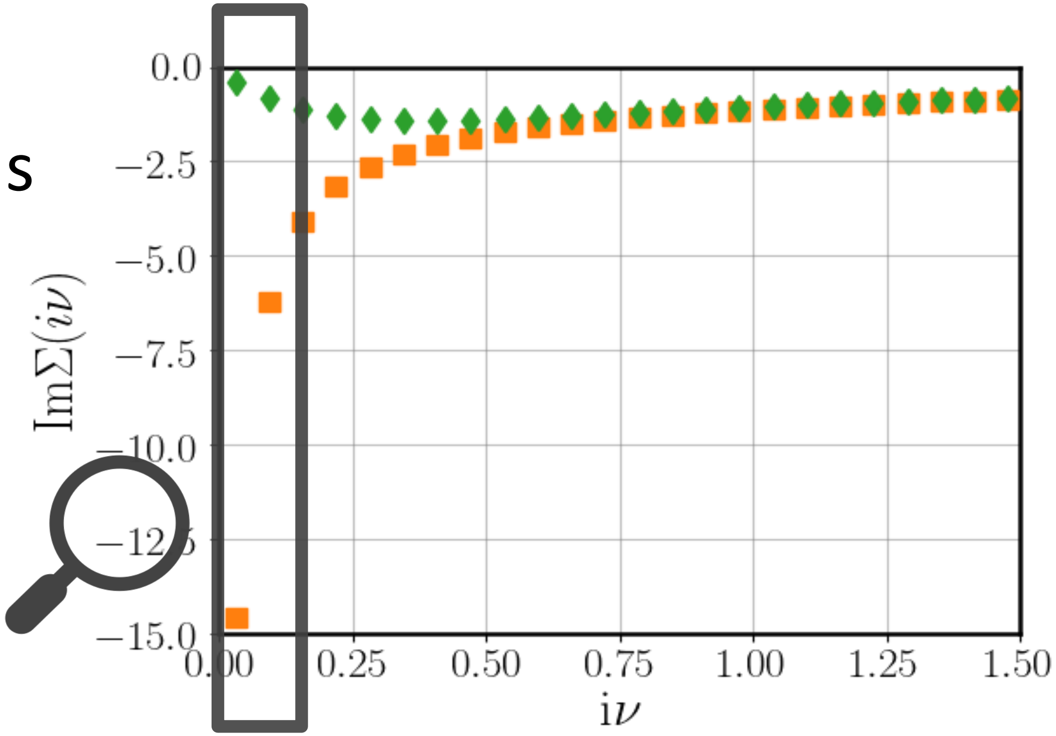
- **Surprising IMPLICATIONS** for the non-local properties !

How to „read“ the physics ... as we can do at the „1P level“

- 1P – Dyson equation



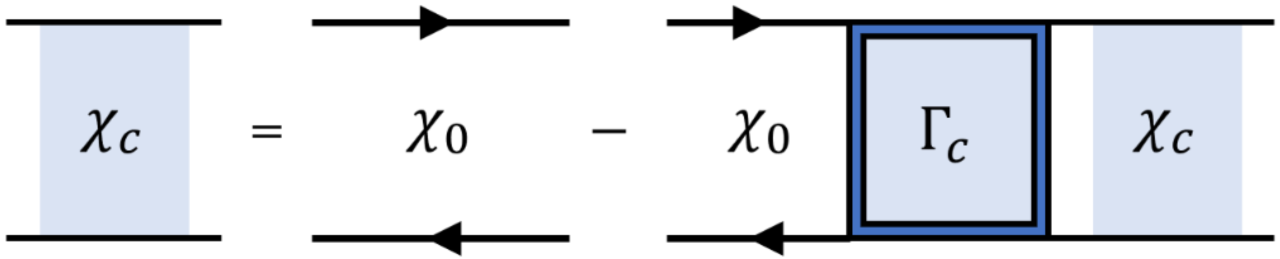
Metallic vs.
Insulating solutions



Low frequencies
$\rightarrow Z, \gamma, A(\nu)$

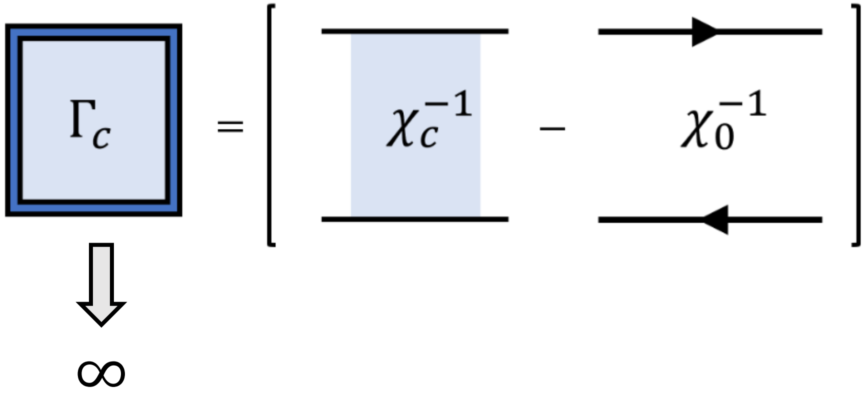
Going at the 2P level

- (local) **B**ethe **S**alpeter **E**quation (BSE)



$$\chi_c^{\nu\nu'} = \chi_{c,0}^{\nu\nu'} - \frac{1}{\beta^2}\sum_{\nu_1,\nu_2} \chi_{c,0}^{\nu\nu_1}\Gamma_c^{\nu_1\nu_2}\chi_c^{\nu_2\nu'}$$

- Irreducible vertex

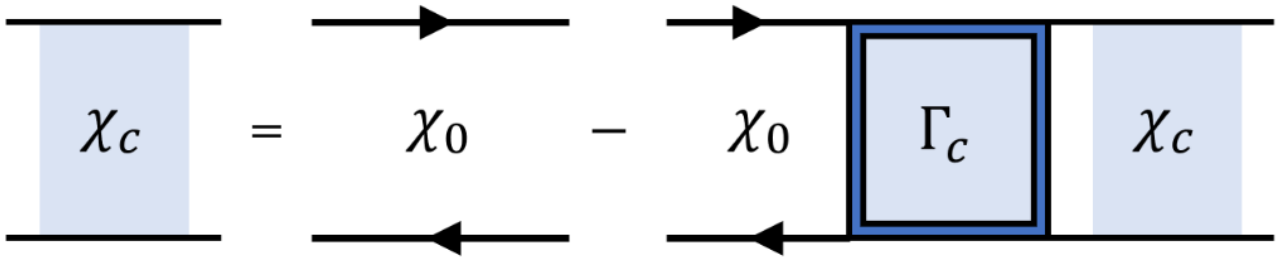


$$[\chi_c]^{-1}_{\nu\nu'} = \sum_i (V^c_{i,\nu'})^*(\lambda_i)^{-1}V^c_{i,\nu}$$

0

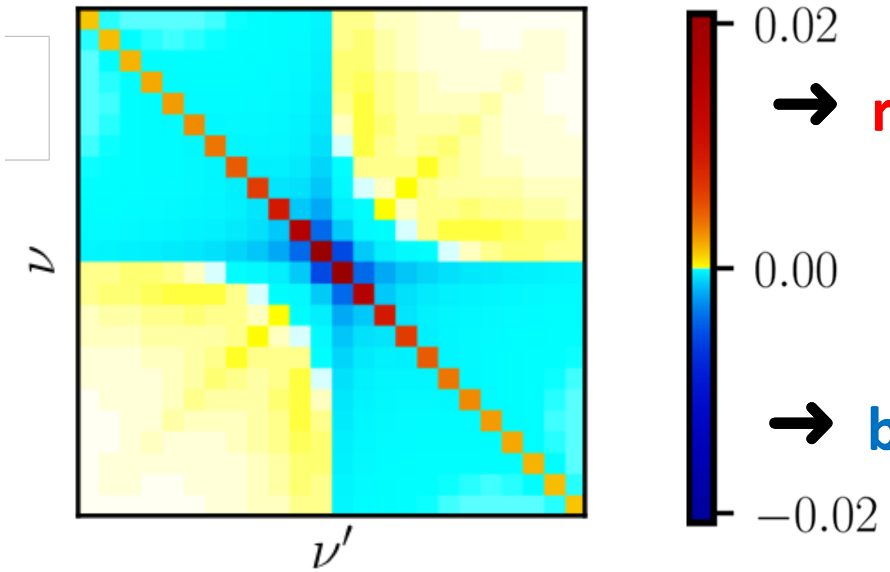
Relation to the physics?

- (local) **B**ethe **S**alpeter **E**quation (BSE)



$$\boxed{\chi_c^{phys} = \frac{1}{\beta^2}\sum\nolimits_{\nu\nu\prime} \chi_c^{\nu\nu\prime}}$$

$$\chi_c^{phys} = \frac{1}{\beta^2}\sum\nolimits_{\nu\nu\prime}$$

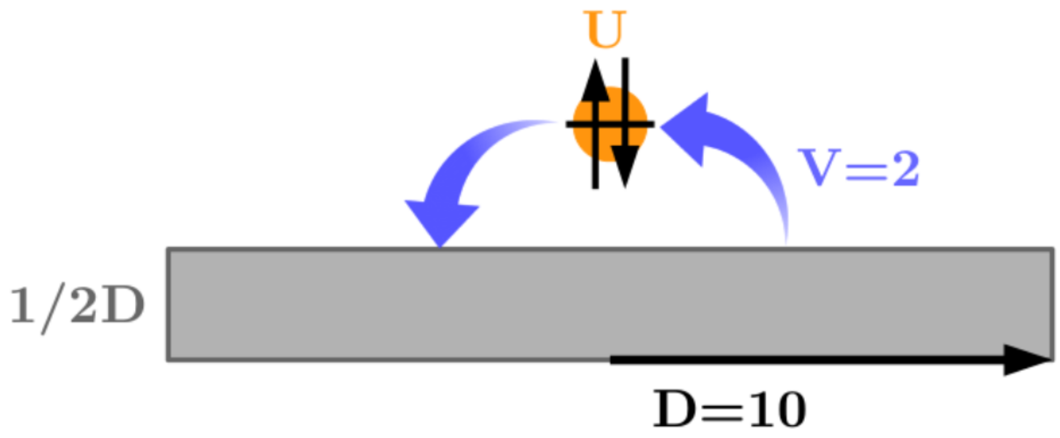


→ **red** = **positive values**

→ **blue** = **negative values**

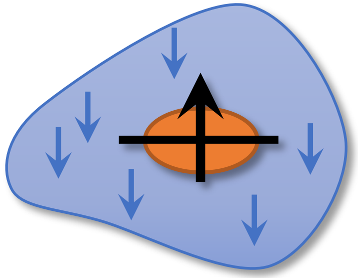
Anderson Impurity Model

- wide-band limit, half-filling



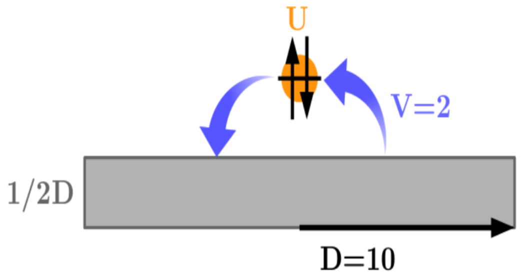
Main physical ingredients:

local magnetic moment



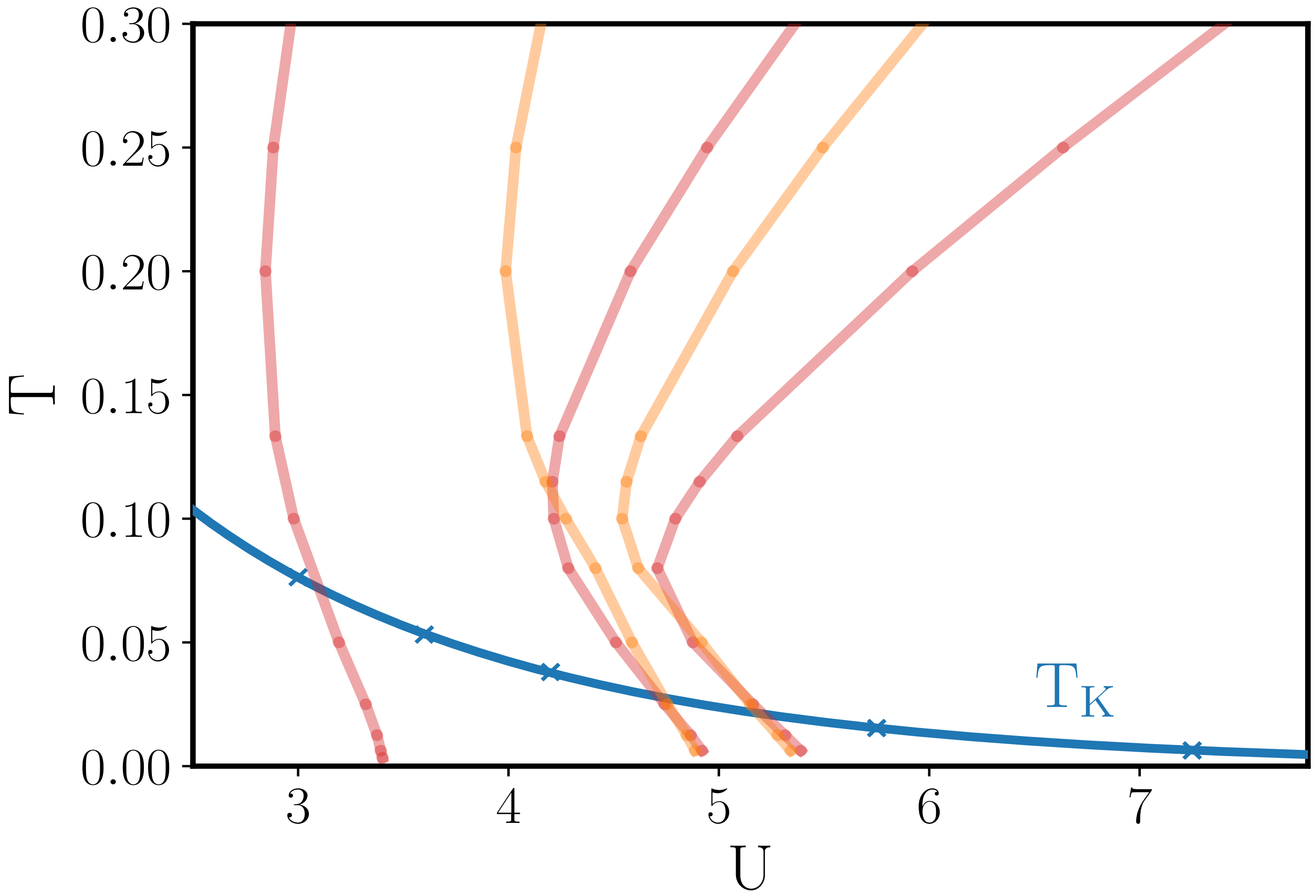
Kondo screening

… where vertex divergences have also been found !



- Solved by means of w2dynamics – CT-HYB

lines where $\boldsymbol{\Gamma}_c$ **diverges**



*) **red** lines:

$\Gamma_c = \infty$

*) **orange** lines:

$\Gamma_c = \Gamma_{pp} = \infty$

❖ *P. Chalupa, P. Gunacker, T. Schäfer, K.Held, and A.T., PRB* **97**, 245136 (2018)

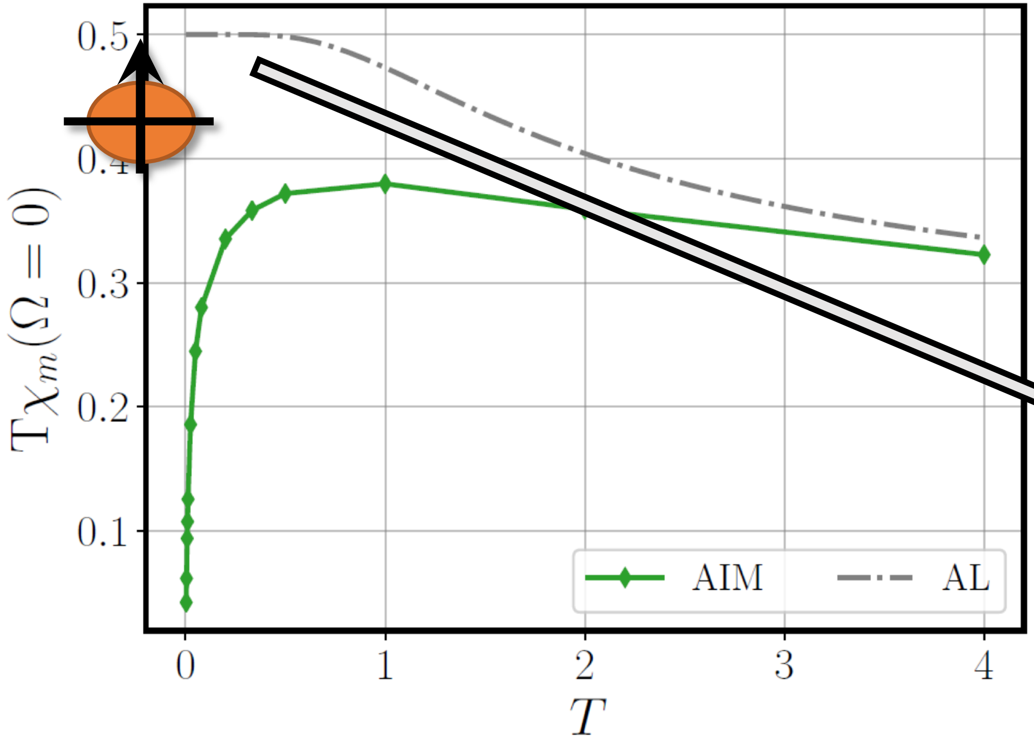
Physical response of the AIM

- w2dynamics – CT-HYB

M.Wallerberger, *et.al*, CPC **235,** 388 (2019)

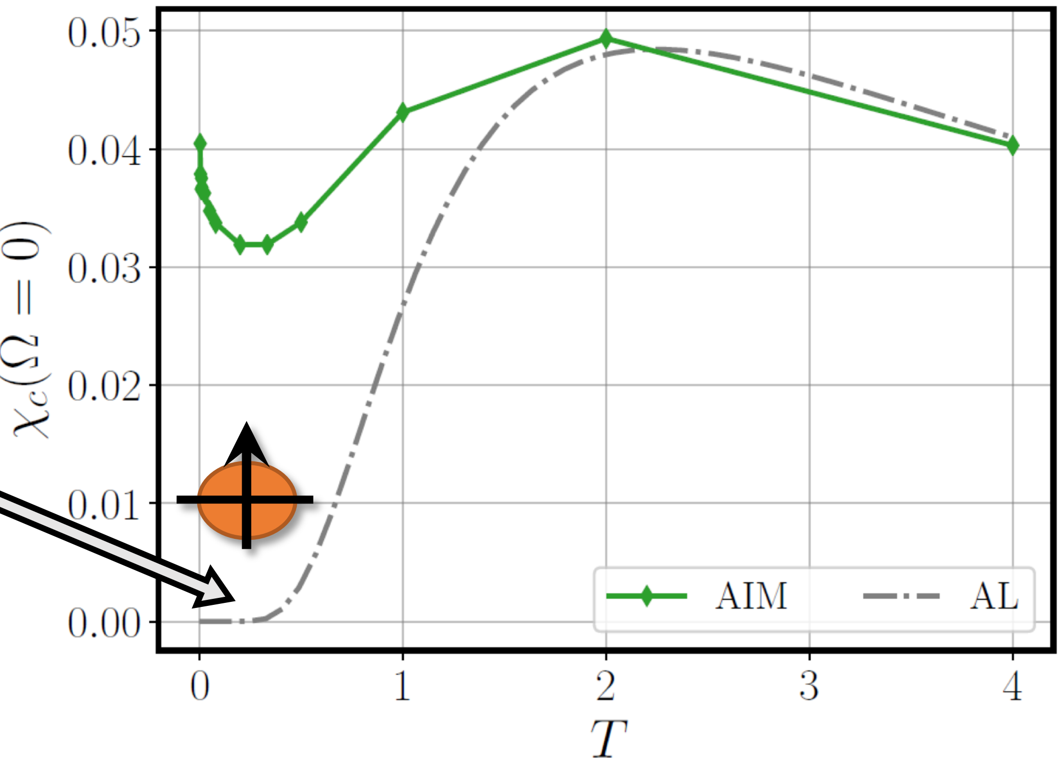
magnetic response

$$\chi_m^{phys} = \frac{1}{\beta^2}\sum_{\nu\nu'}\chi_m^{\nu\nu'}$$



charge response

$$\chi_c^{phys} = \frac{1}{\beta^2}\sum_{\nu\nu'}\chi_c^{\nu\nu'}$$



❖ *P. Chalupa, T. Schäfer, M. Reitner, D. Springer, S. Andergassen, and A.T., PRL* ***126*** *056403 (2021)*

Physical response of AL & AIM

- w2dynamics – CT-HYB

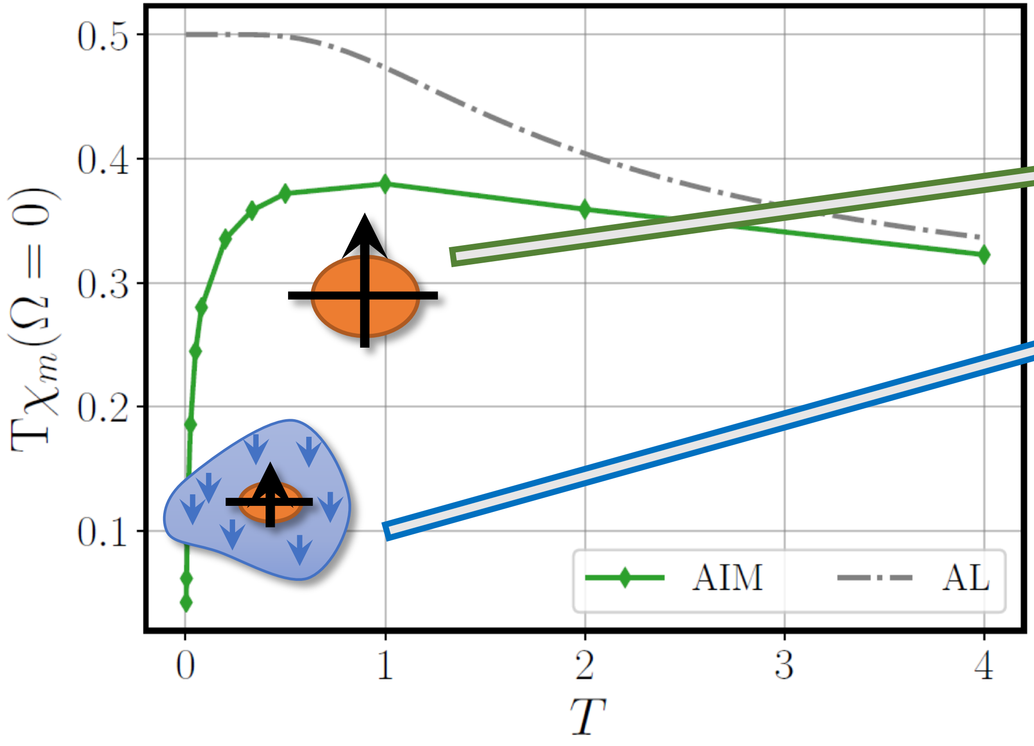
M.Wallerberger, *et.al*, CPC **235,** 388 (2019)

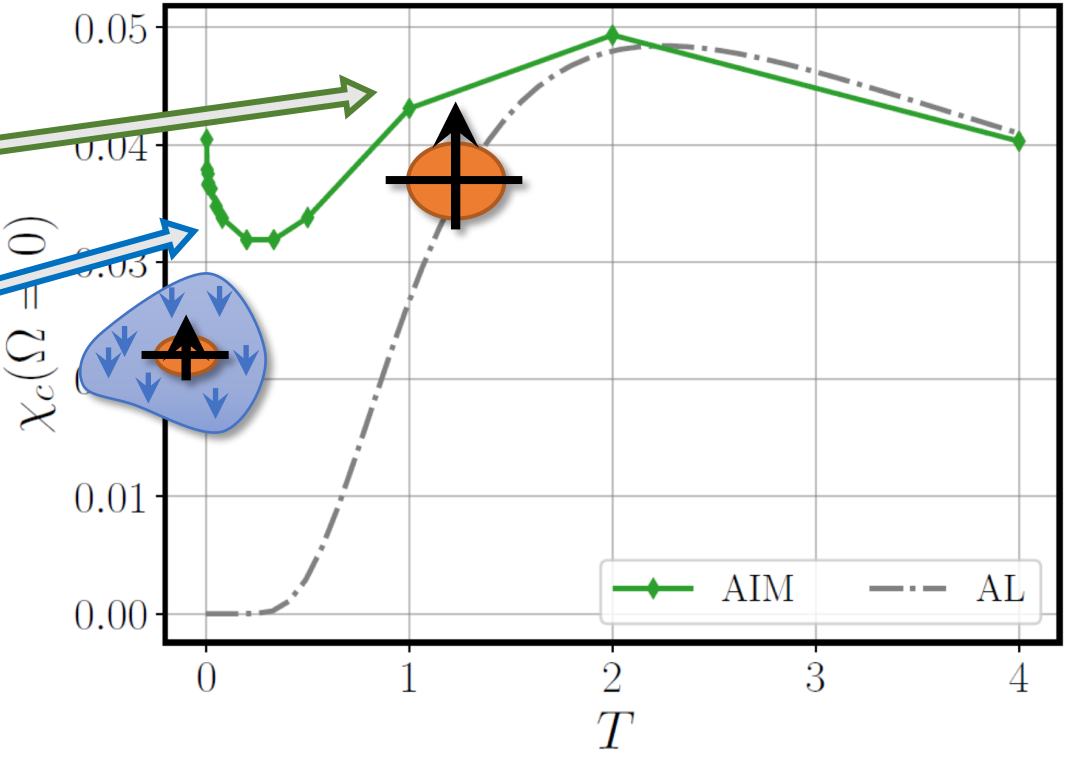
magnetic response

$$\chi_m^{phys} = \frac{1}{\beta^2}\sum_{\nu\nu'}\chi_m^{\nu\nu'}$$

charge response

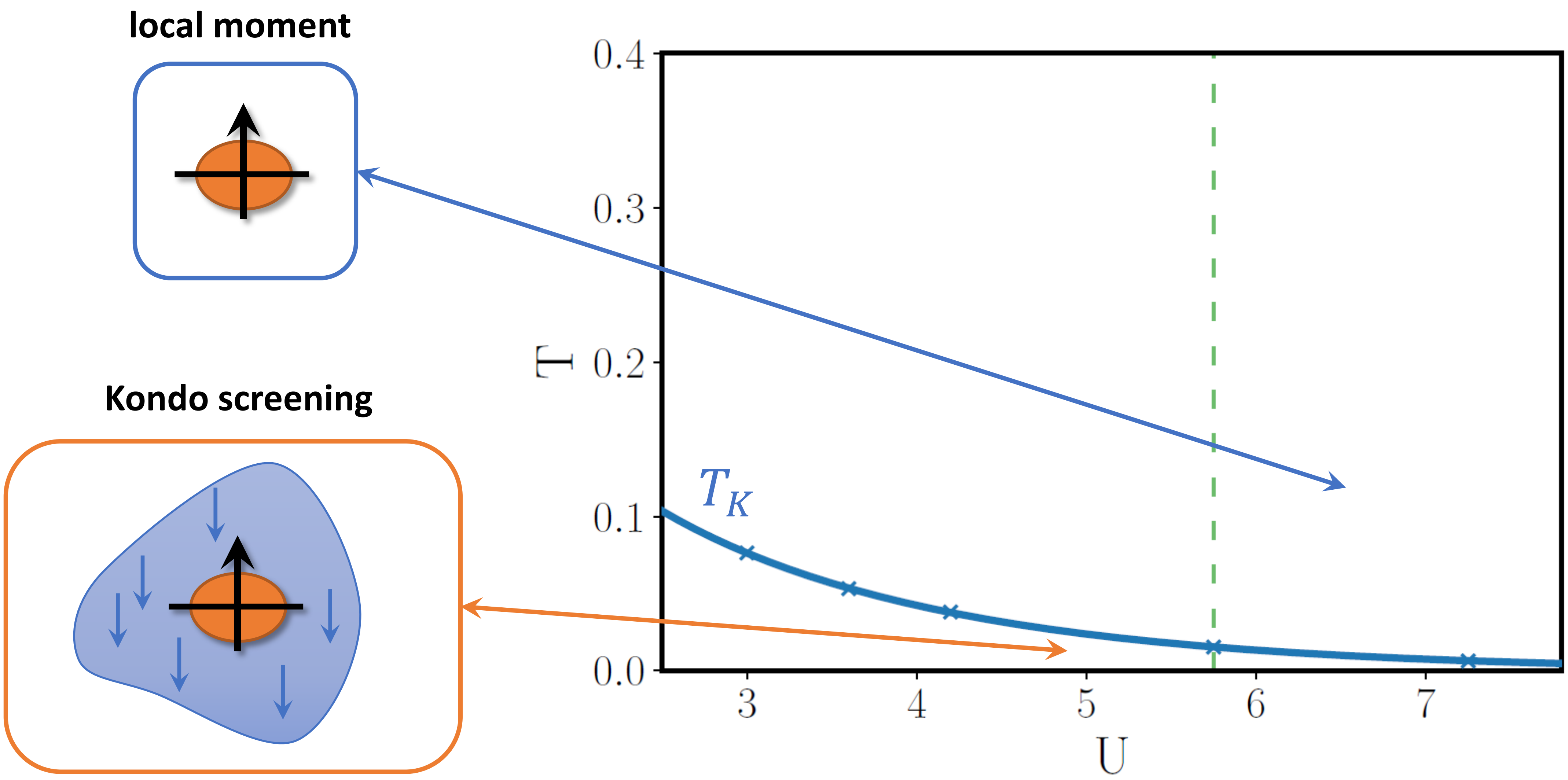
$$\chi_c^{phys} = \frac{1}{\beta^2}\sum_{\nu\nu'}\chi_c^{\nu\nu'}$$



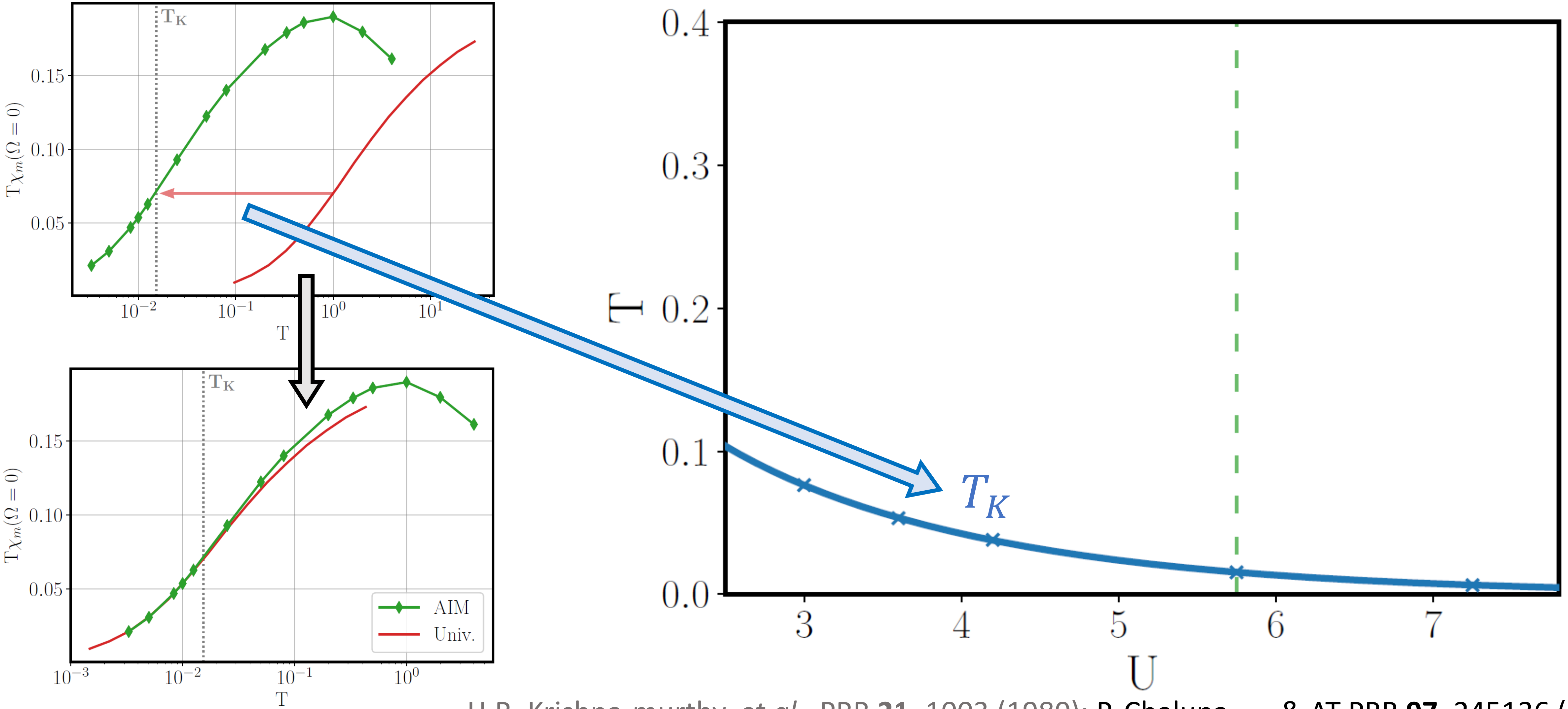


❖ *P. Chalupa, T. Schäfer, M. Reitner, D. Springer, S. Andergassen, and A.T., PRL **126** 056403 (2021)*

AIM phase-diagram



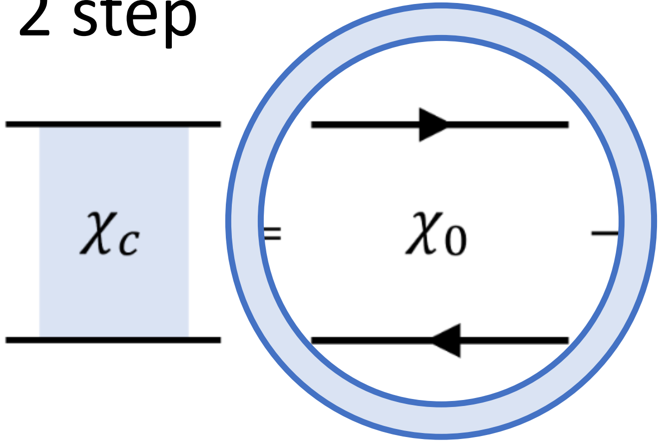
T_K of the AIM - conventional determiation

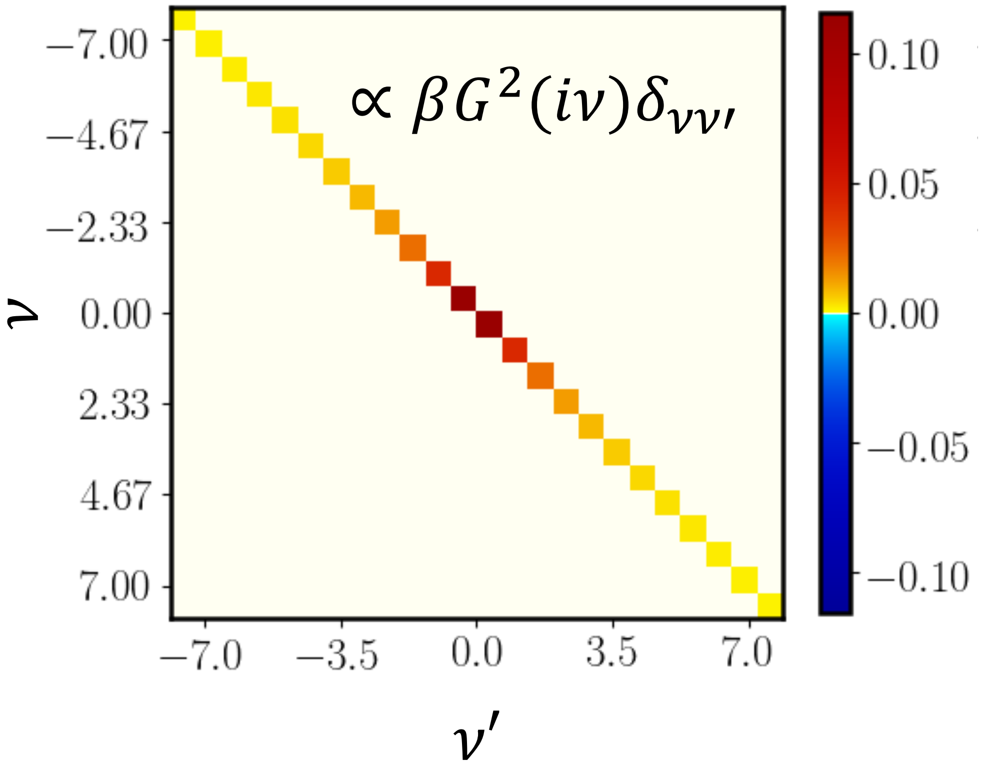


H.R. Krishna-murthy, *et.al.*, PRB **21,** 1003 (1980); P. Chalupa, …, & AT PRB **97**, 245136 (2018)

1.Step: Non interacting case/bubble term

- 2 step

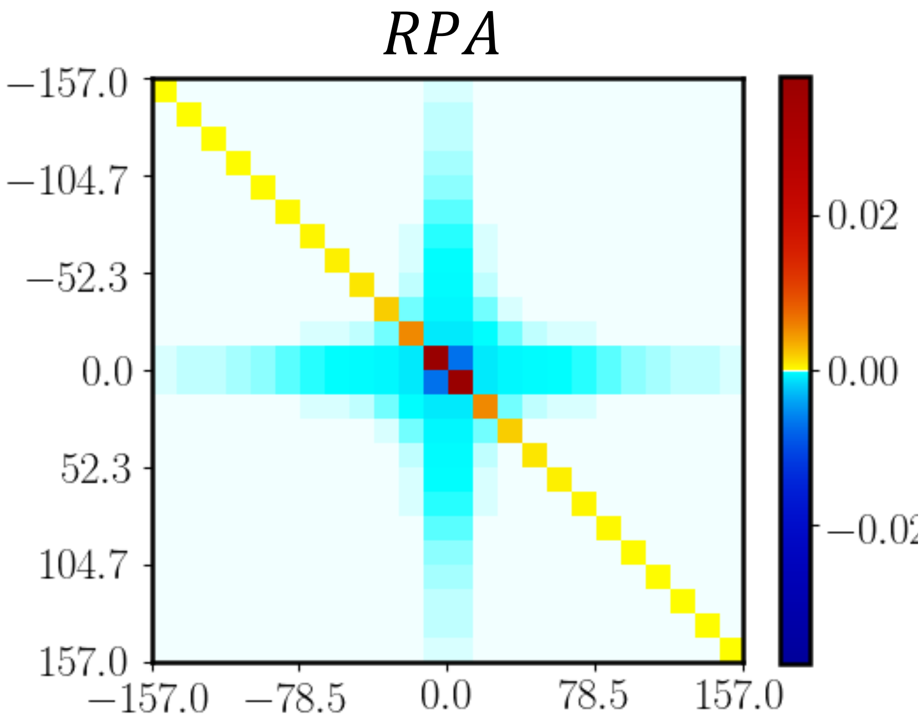




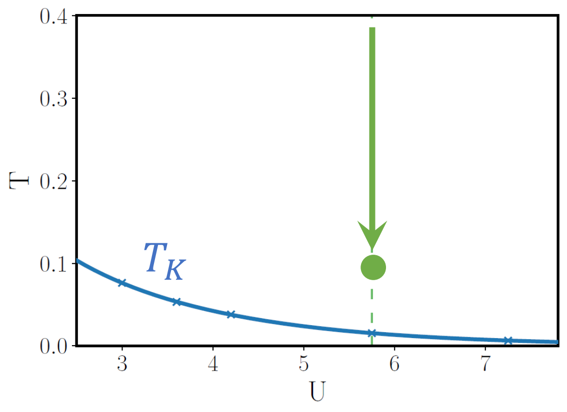
2.Step : Perturbative regime

e.g.: high temperature regime (**ν** = ***π*****T** > **U**)

$$T_{high} = 2.0$$

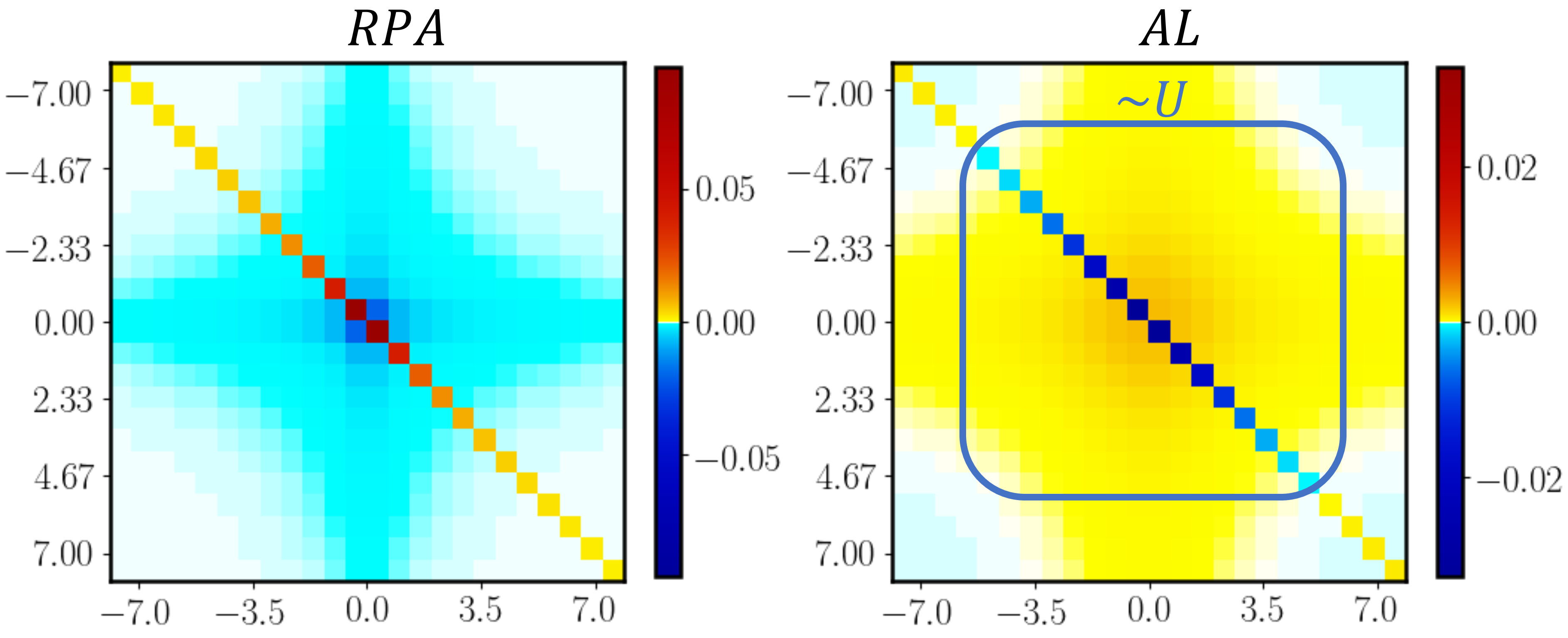


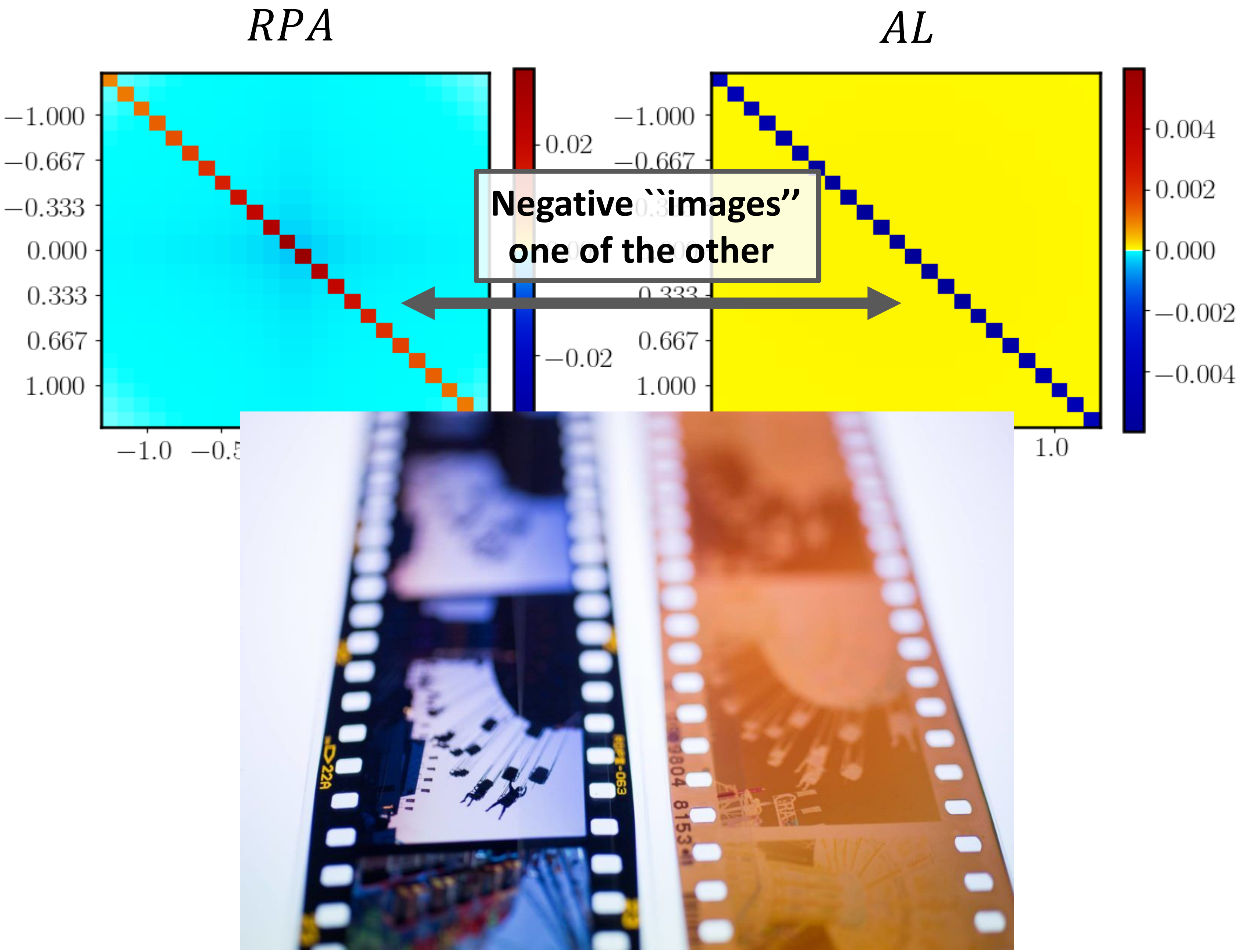
3.Step: Nonperturbative (**local moment**) regime



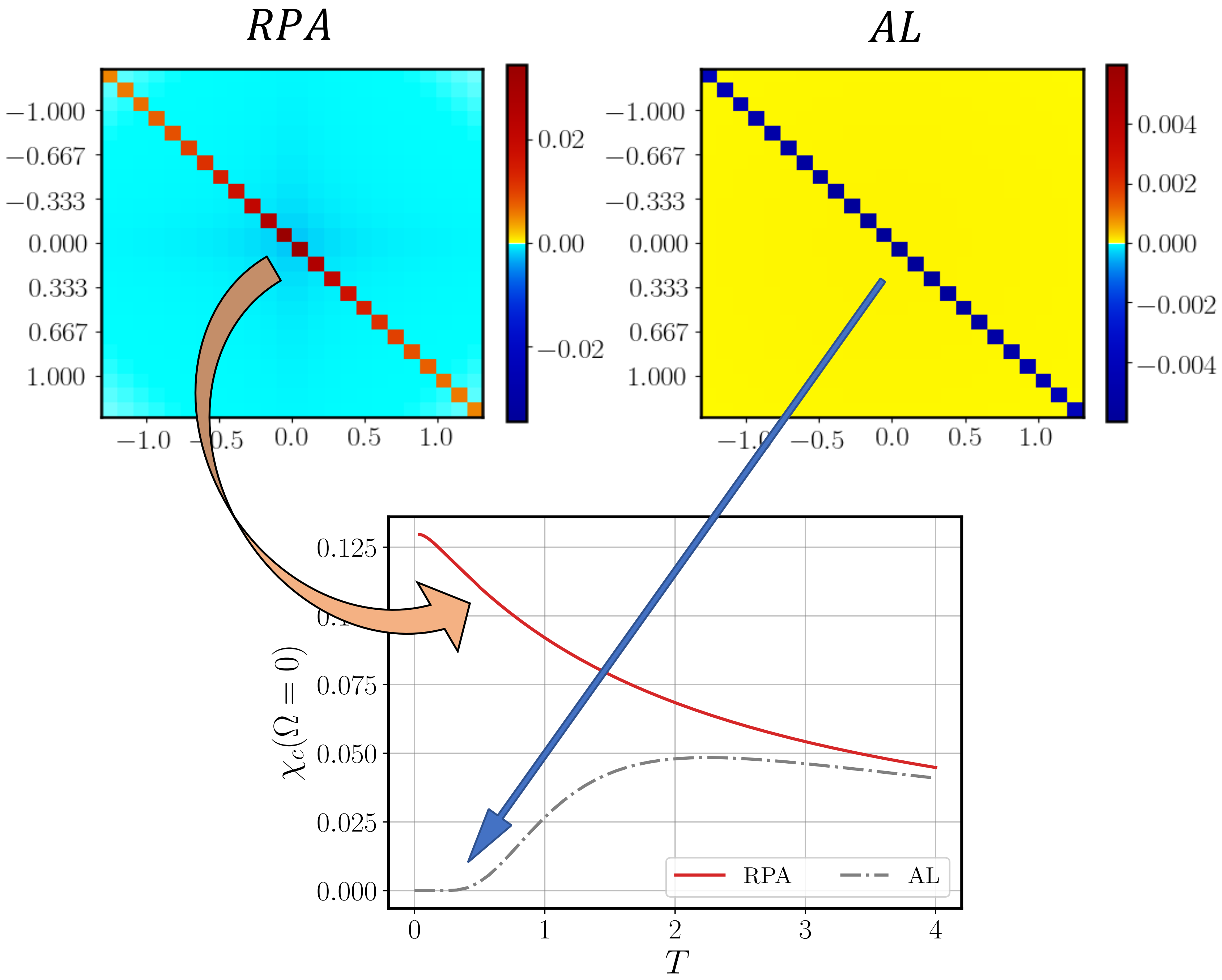
e.g.: intermediate temperature region ($\mathbf{T_K < T \ll U}$)

$T_{int} = 0.1$



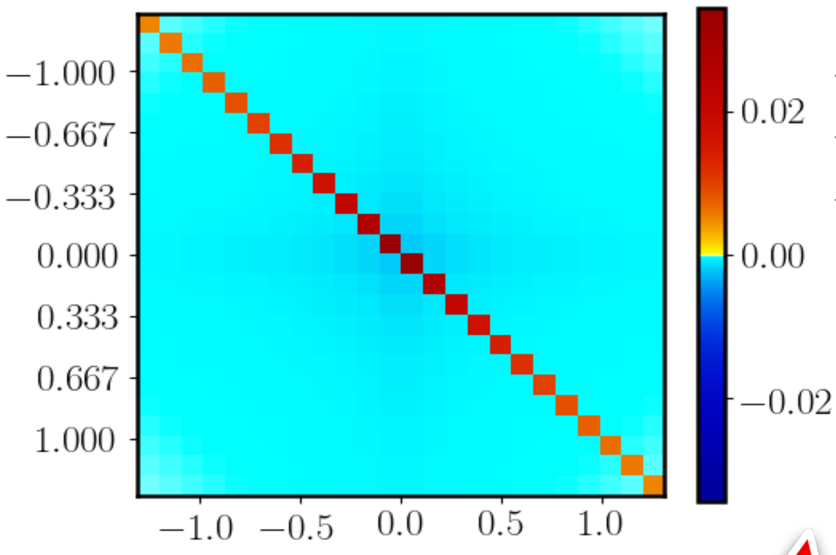


RPA
AL
−1.000
−0.667
−0.333
0.000
0.333
0.667
1.000
−1.0
−0.5
0.02
−0.02
1.0
0.004
0.002
0.000
−0.002
−0.004
Negative ``images'' one of the other

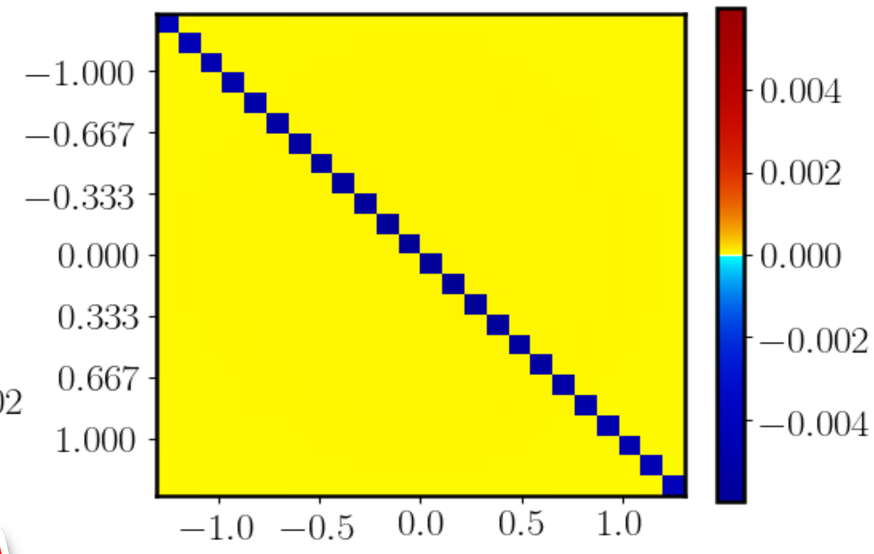


RPA
AL
−1.000
−0.667
−0.333
0.000
0.333
0.667
1.000
−1.0
−0.5
0.0
0.5
1.0
0.02
0.00
−0.02
0.004
0.002
0.000
−0.002
−0.004
$\chi_c(\Omega = 0)$
0.125
0.075
0.050
0.025
0.000
0
1
2
3
4
T
RPA
AL

RPA

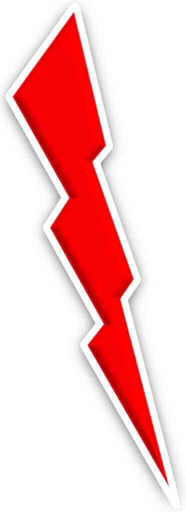


AL



positive diagonal dominates

negative diagonal dominates

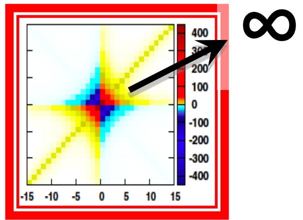


→ all eigevalues **$\lambda > 0$**

→ all low-frequency eigevalues **$\lambda < 0$**

$\lambda = 0$

vertex divergences !!!

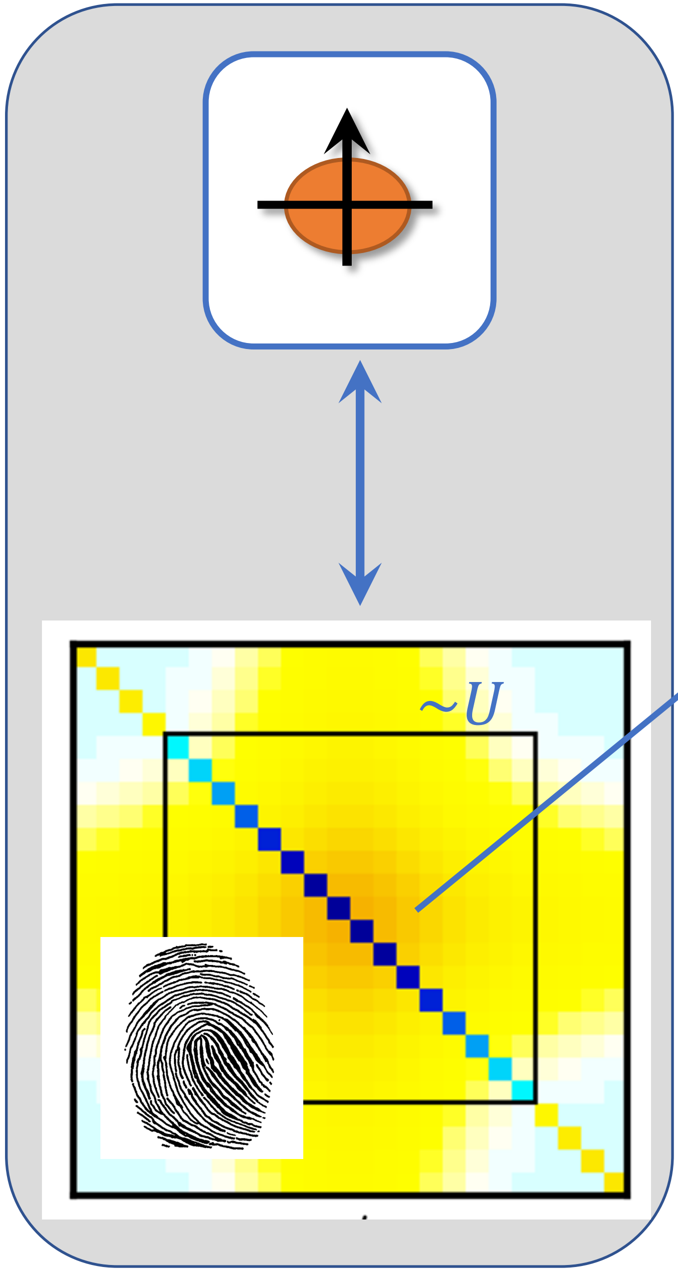


Fingerprints of the local moment !

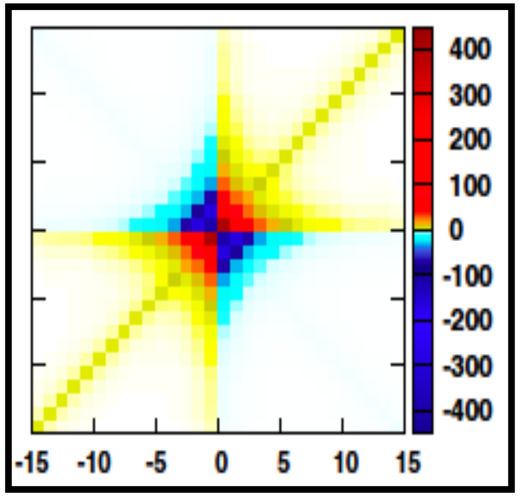
magnetic
$\uparrow\uparrow - \uparrow\downarrow$

$U \rightarrow$ increasing $\uparrow\downarrow$ correlations

charge
$\uparrow\uparrow + \uparrow\downarrow$



vertex divergencies !!

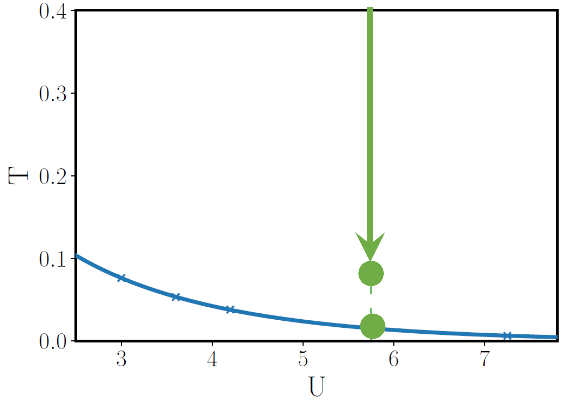


nonpertubative image of **local moment** formation in the **charge** sector

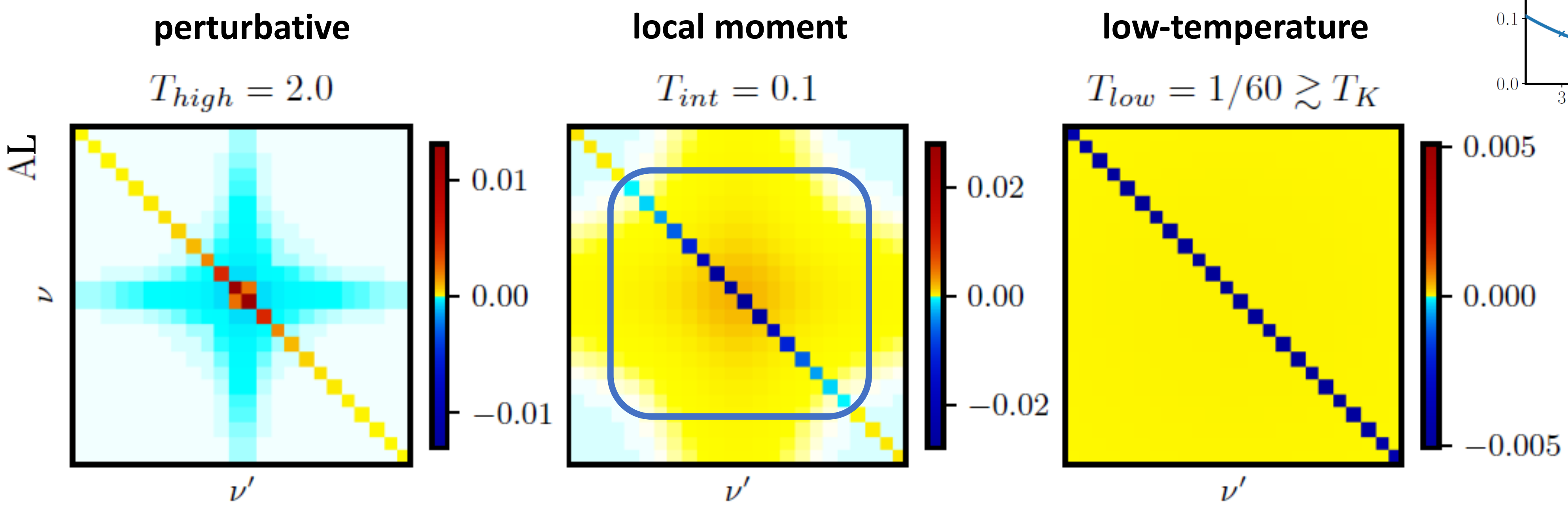
O. Gunnarsson, *et.al.,* PRB **93, 245102** (2016)

P. Chalupa, ..., & AT, PRL **126**, 056403 (2021)

Results AIM

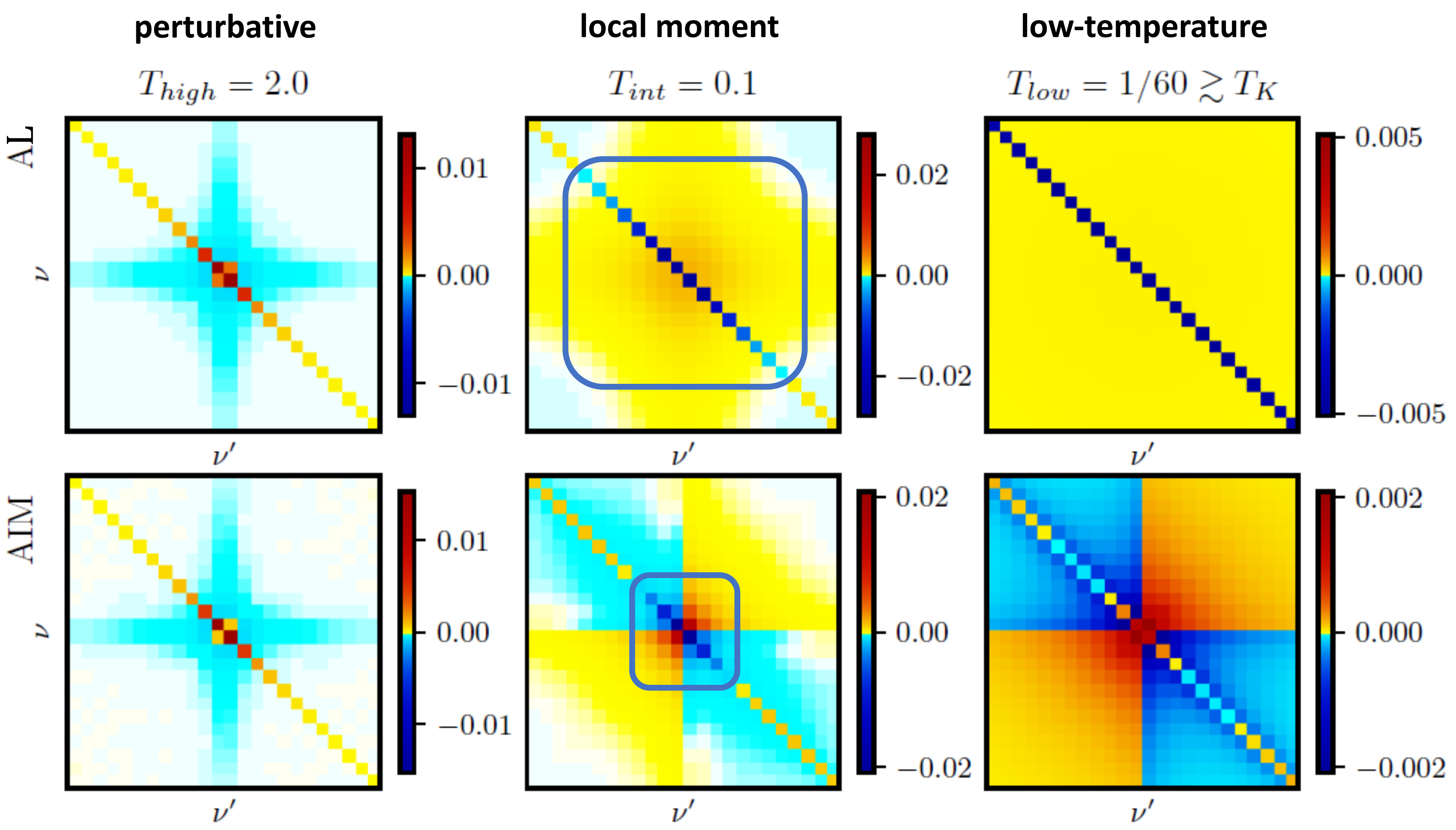


0.4
0.3
0.2
0.1
0.0
T
3
4
5
6
7
U



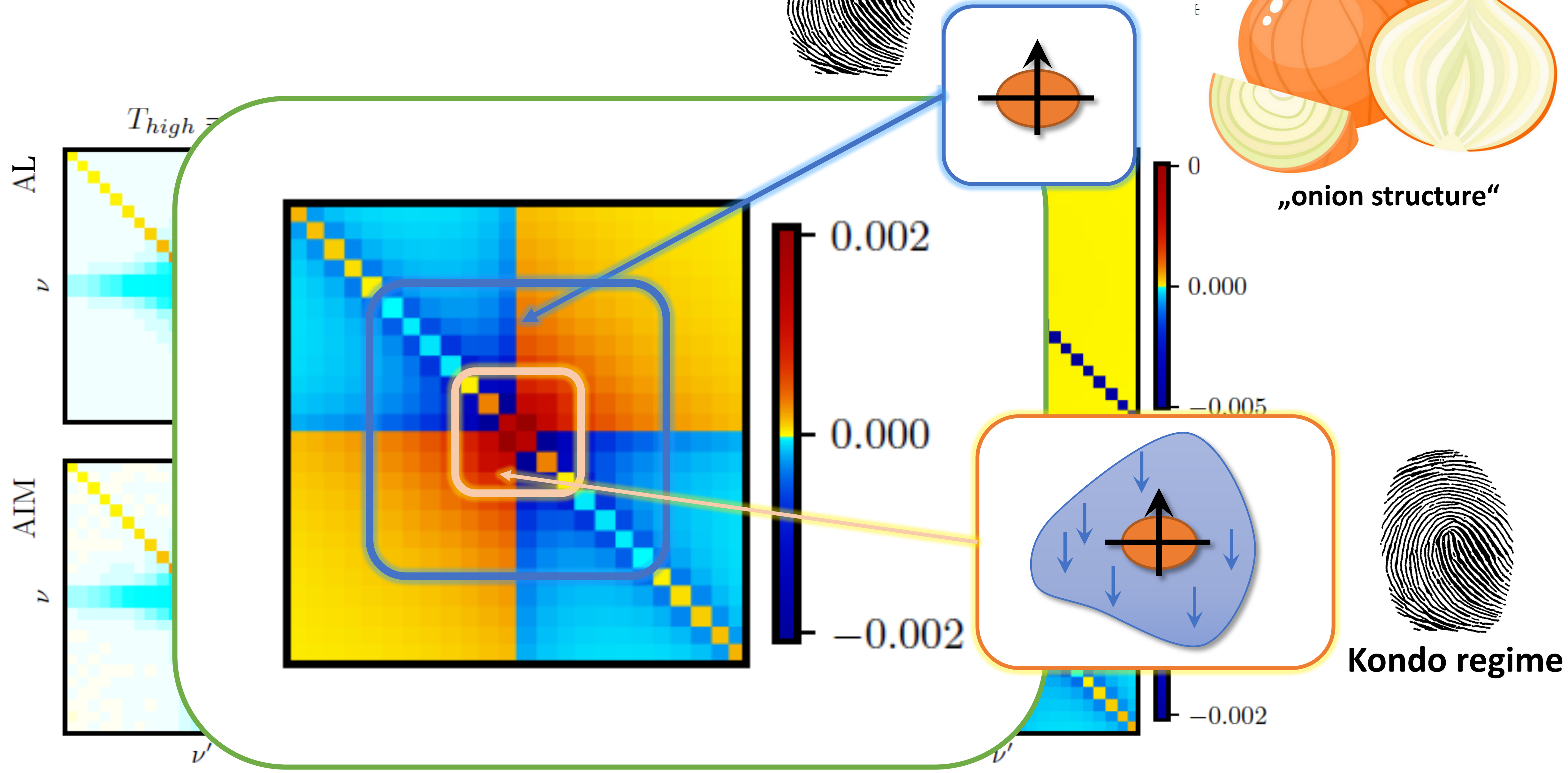
perturbative
$T_{high} = 2.0$
AL
ν
ν'
0.01
0.00
−0.01
local moment
$T_{int} = 0.1$
ν'
0.02
0.00
−0.02
low-temperature
$T_{low} = 1/60 \gtrsim T_K$
ν'
0.005
0.000
−0.005

Results AIM



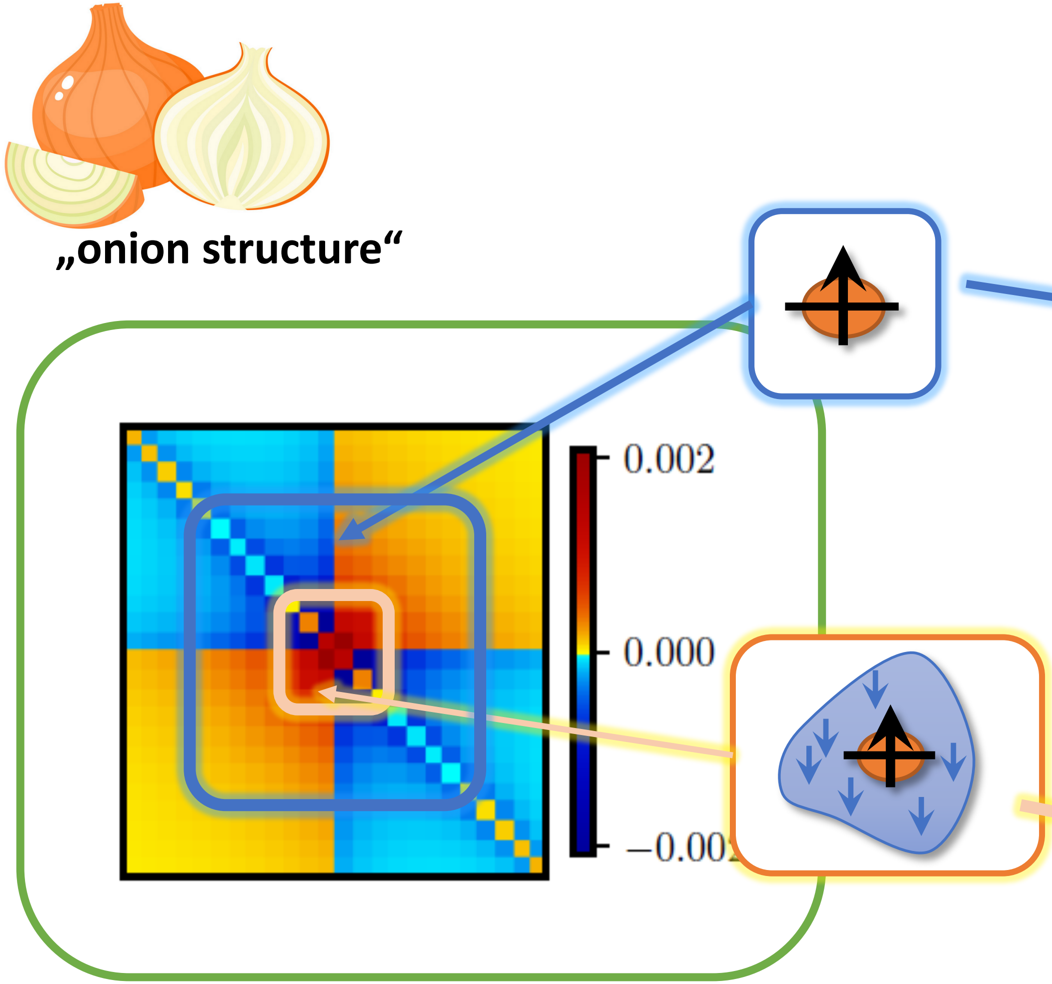
perturbative
local moment
low-temperature
$T_{high} = 2.0$
$T_{int} = 0.1$
$T_{low} = 1/60 \gtrsim T_K$
AL
AIM
ν
ν'
0.01
0.00
-0.01
0.02
0.00
-0.02
0.005
0.000
-0.005
0.002
0.000
-0.002

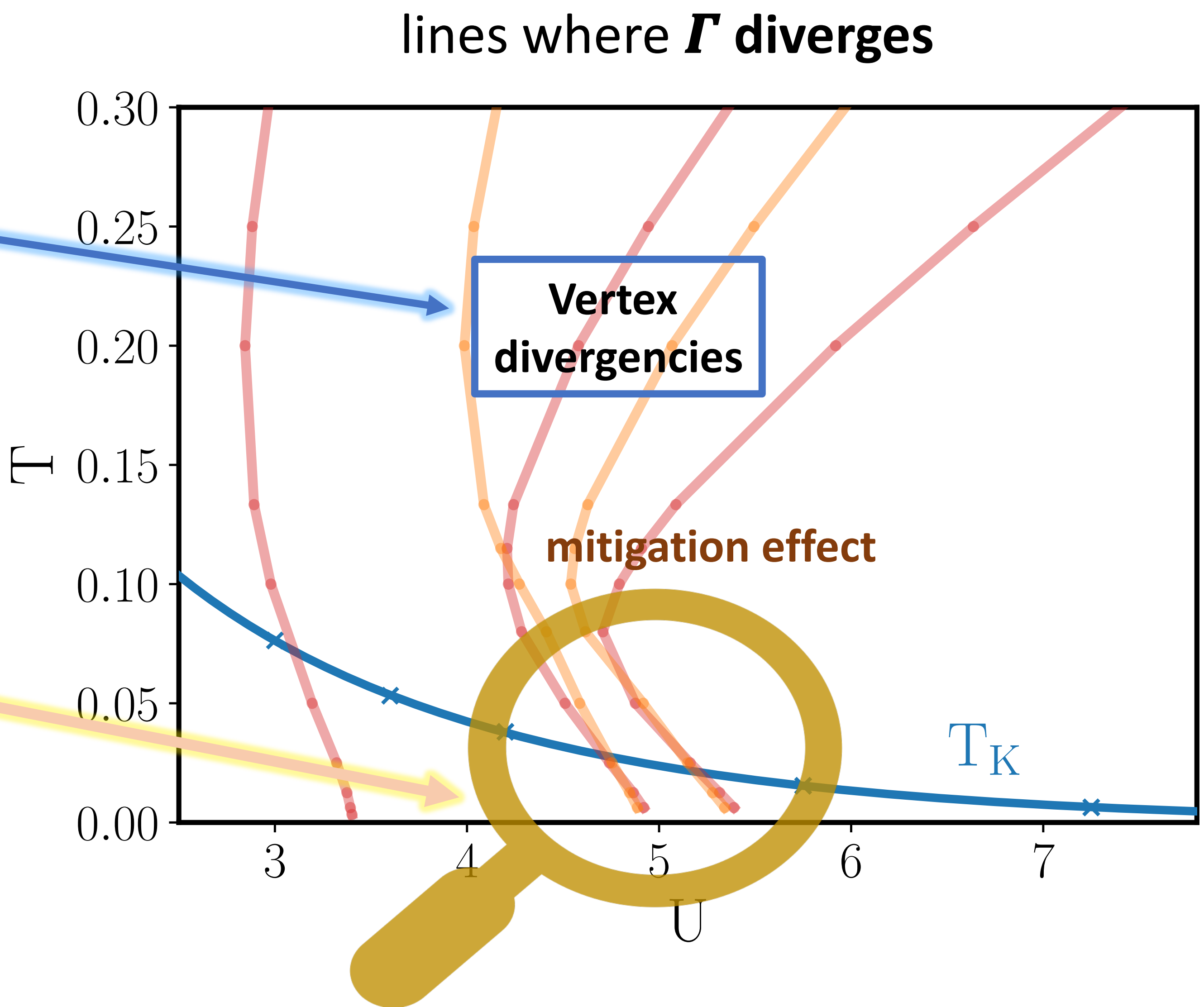
Results AIM



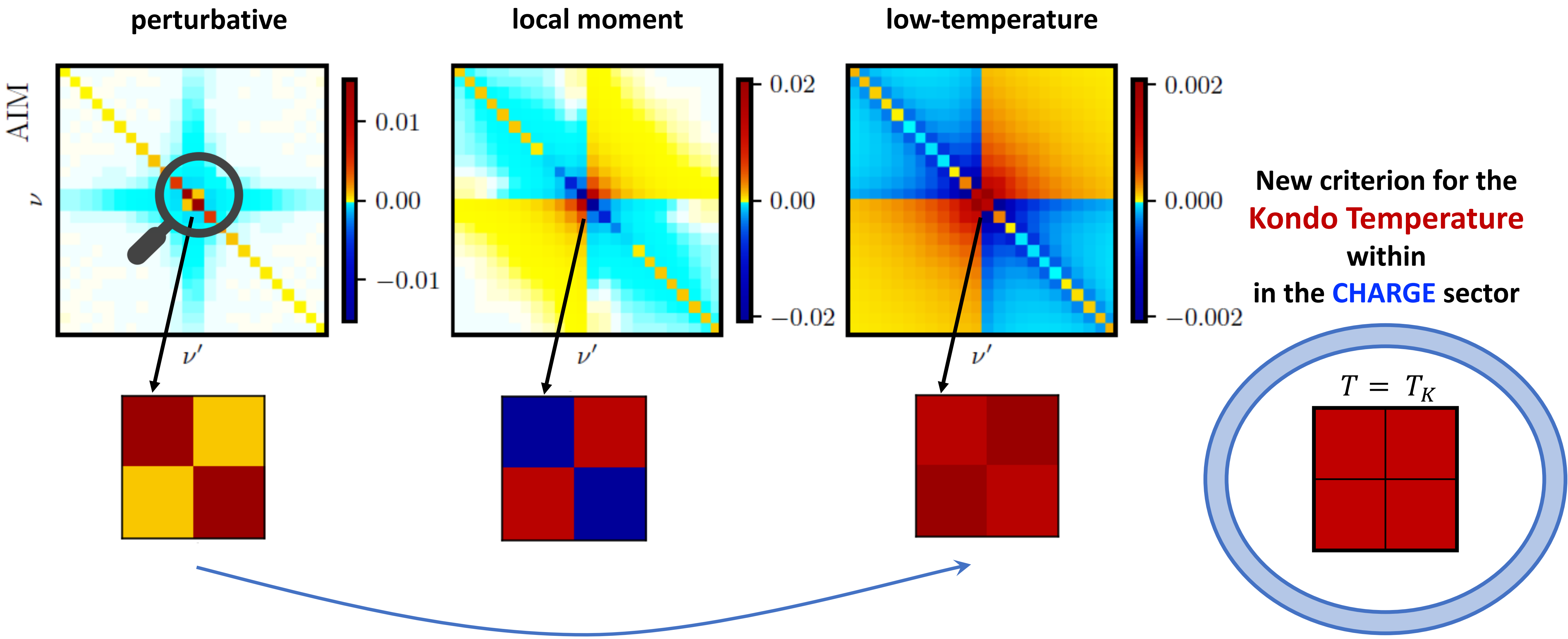
local moment
„onion structure“
Kondo regime
T_{high}
AL
AIM
ν
ν'
0.002
0.000
−0.002
0
0.000
−0.005
−0.002

Effect of the vertex divergencies of the AIM





Results AIM – low frequency regime

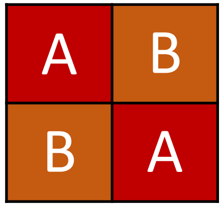


New criterion for the **Kondo Temperature** within in the **CHARGE** sector

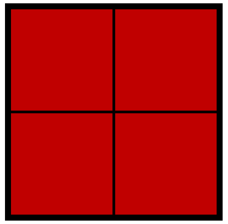
❖ *P. Chalupa, T. Schäfer, M. Reitner, D. Springer, S. Andergassen, and A.T., PRL* ***126*** *056403 (2021)*

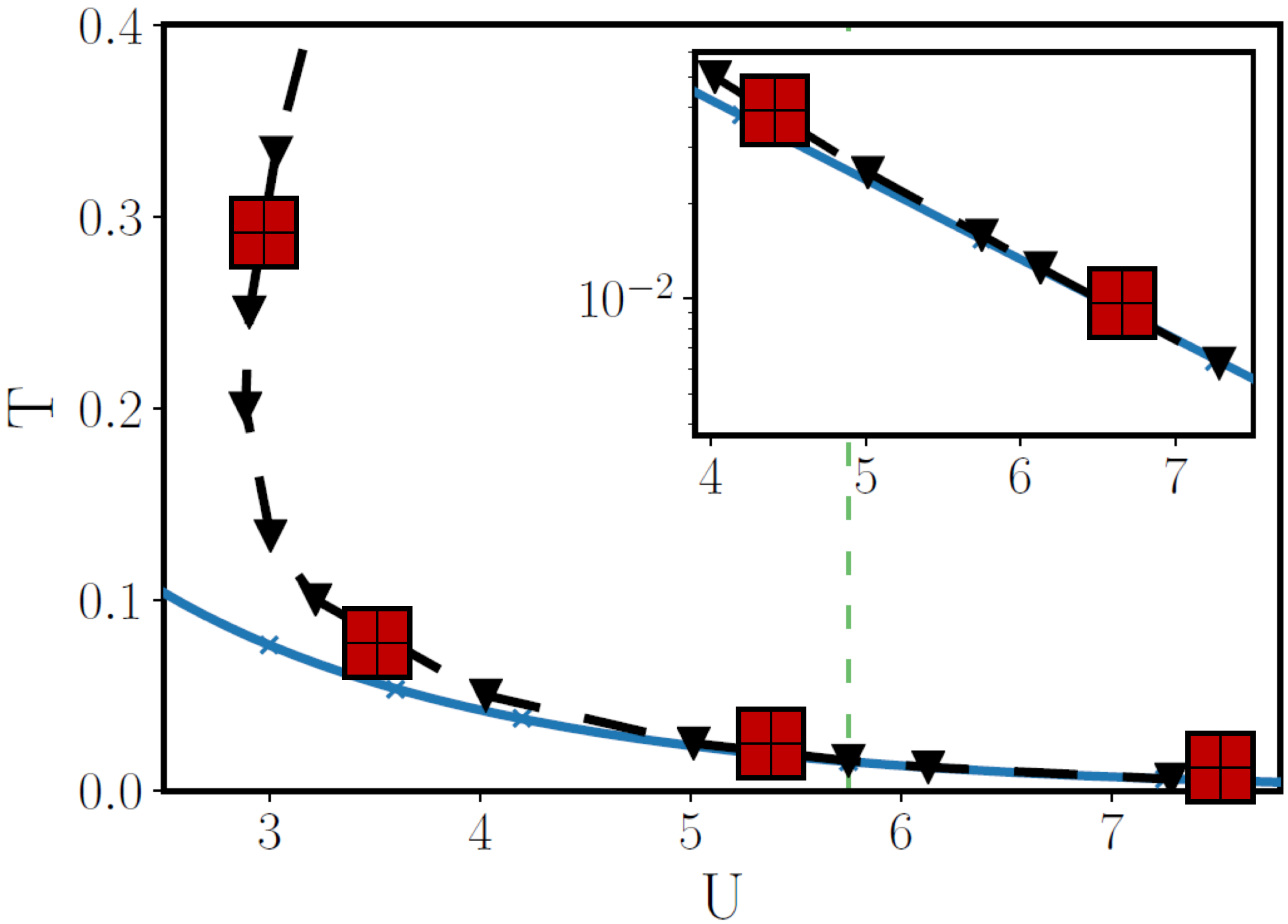
T_K criterion

- Only for one U – what happens at other U?



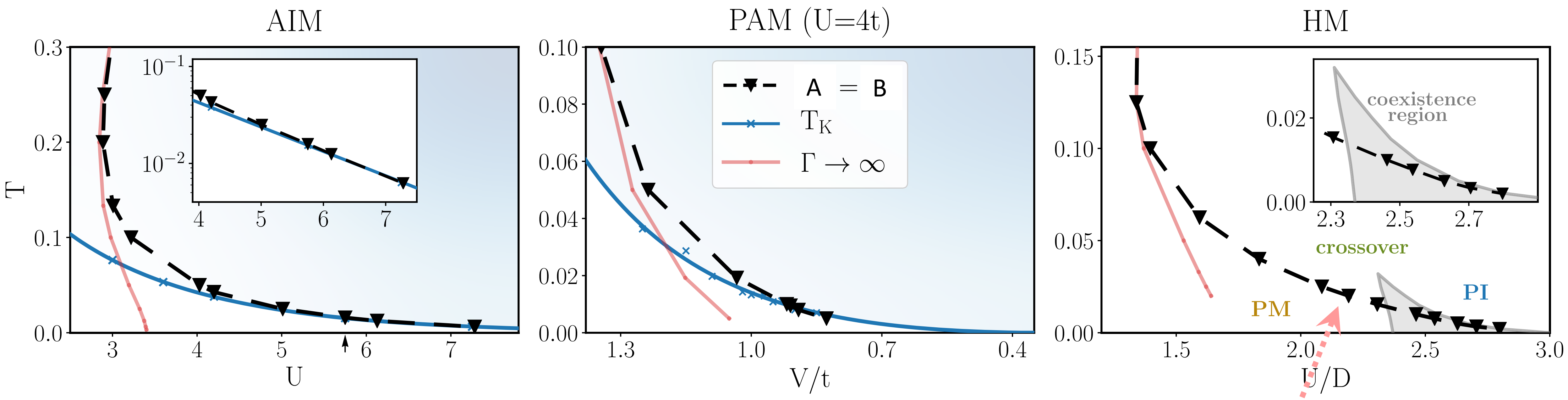
$A = B \leftrightarrow T = T_K$ ▼



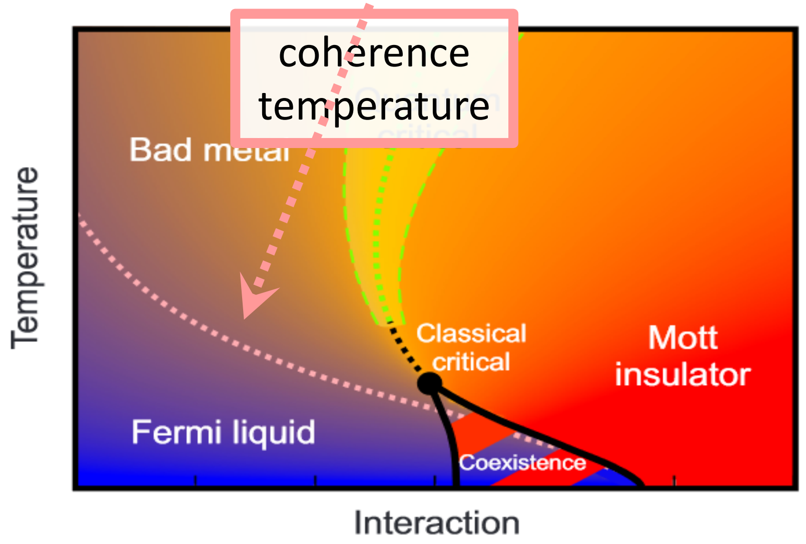


❖ *P. Chalupa, T. Schäfer, M. Reitner, D. Springer, S. Andergassen, and A.T., PRL* ***126*** *056403 (2021)*

Beyond the **single impurity** AIM



❖ *P. Chalupa, T. Schäfer, M. Reitner, D. Springer, S. Andergassen, and A.T., PRL **126** 056403 (2021)*



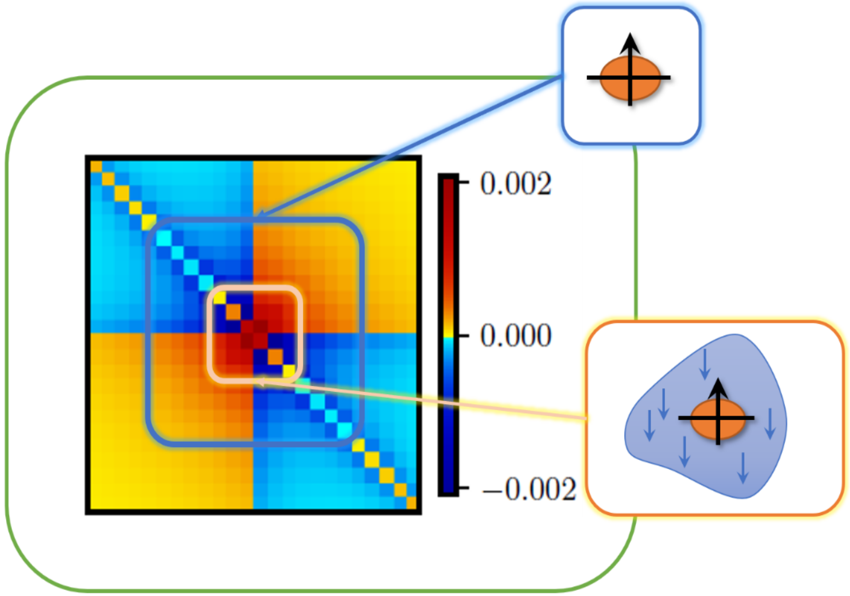
J.Vucicevic,*et.al,* PRB **88**, 075143 (2013)

Our questions

1) What is the **physical ``origin”** for the **breakdown** of the many-body perturbation theories ?

➢ Learn how to read the physics from the 2P quantities

➢ **FINGERPRINTS** of the local moment formation and of its Kondo screening

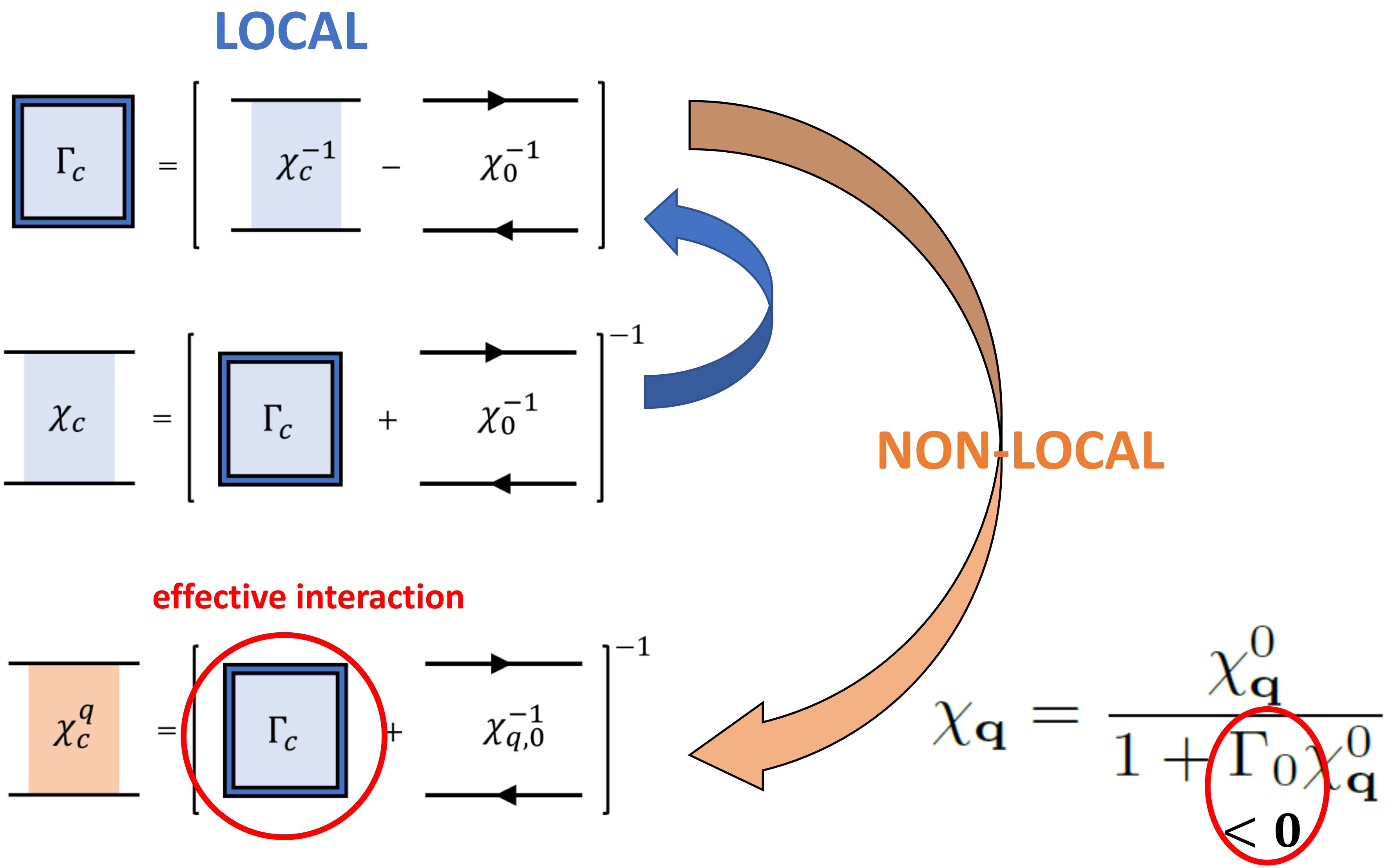


2) Are there relevant **physical consequences?**

➢ **Surprising implications** for the non-local properties !!

Suppression = Vertex Divergences – the whole story?

local moment
&
suppression
of charge response



R. Nourafkan, *et.al.*, PRB **99**, 035161 (2019); M. Reitner, , *et.al.*, PRL **125,** 196403 (2020)

The isothermal **compressibility** (κ) of the **Hubbard model**

$$\kappa = -\frac{1}{V}\frac{\partial V}{\partial p} \propto \begin{cases} \dfrac{\partial n}{\partial \mu} \\ \chi_c^{q=0}(\Omega = 0) \end{cases}$$

$\longleftrightarrow$ **in DMFT**

$$\chi_c^q = \left[\Gamma_c + \chi_{q,0}^{-1} \right]^{-1}$$

Compressibility Divergence and the Finite Temperature Mott Transition

G. Kotliar, *et. al.*, PRL **89** 046401 (2002)

Phase separation in the particle-hole asymmetric Hubbard model

M. Eckstein, *et. al.*, PRB **75** 125103 (2007)

The case of the isothermal **compressibility** κ

eigenvalues of χ_{loc}

weight
(from the
eigenvectors of χ_{loc})

BSEq. in DMFT:

$$\kappa = \chi_c^{q=0} = \frac{2}{\beta^2} \sum_\alpha \left(\frac{1}{\lambda_\alpha} + t^2/\beta \right)^{-1} w_\alpha$$

❖ M. Reitner, P .Chalupa, L. Del Re, D. Springer, S. Ciuchi, G. Sangiovanni, and A.T., PRL **125** 196403 (2020)

The case of the isothermal **compressibility** κ

eigenvalues of $\boldsymbol{\chi}_{\text{loc}}$

BSEq. in DMFT:

$$\boxed{\kappa = \chi_c^{q=0} = \frac{2}{\beta^2}\sum_\alpha \left(\frac{1}{\lambda_\alpha} + t^2/\beta\right)^{-1} w_\alpha}$$

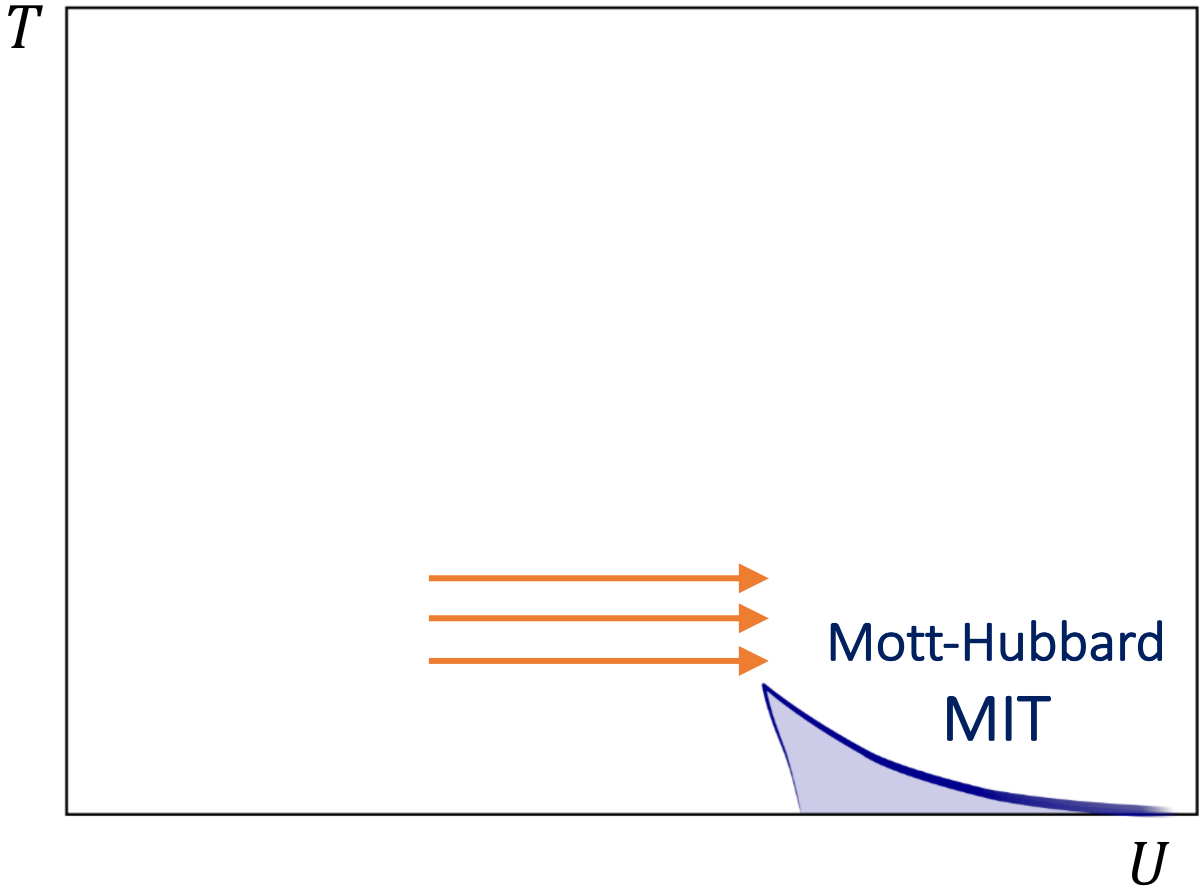
If ${}^1/_{\lambda_\alpha} \approx -t^2/\beta \quad \Rightarrow \; \chi_{q=0} \to \pm\infty \quad$ for $w_\alpha \neq 0$

$\lambda_\alpha < 0$ only after vertex divergence $\lambda_\alpha = 0 \Leftrightarrow \Gamma_{loc} \propto \chi_{loc}^{-1} = \infty$

❖ M. Reitner, P .Chalupa, L. Del Re, D. Springer, S. Ciuchi, G. Sangiovanni, and A.T., PRL **125** 196403 (2020)

κ enhancement? Bethe lattice, half-filling

DMFT phase-diagram of the Hubbard model



❖ M. Reitner, P .Chalupa, L. Del Re, D. Springer, S. Ciuchi, G. Sangiovanni, and A.T., PRL **125** 196403 (2020)

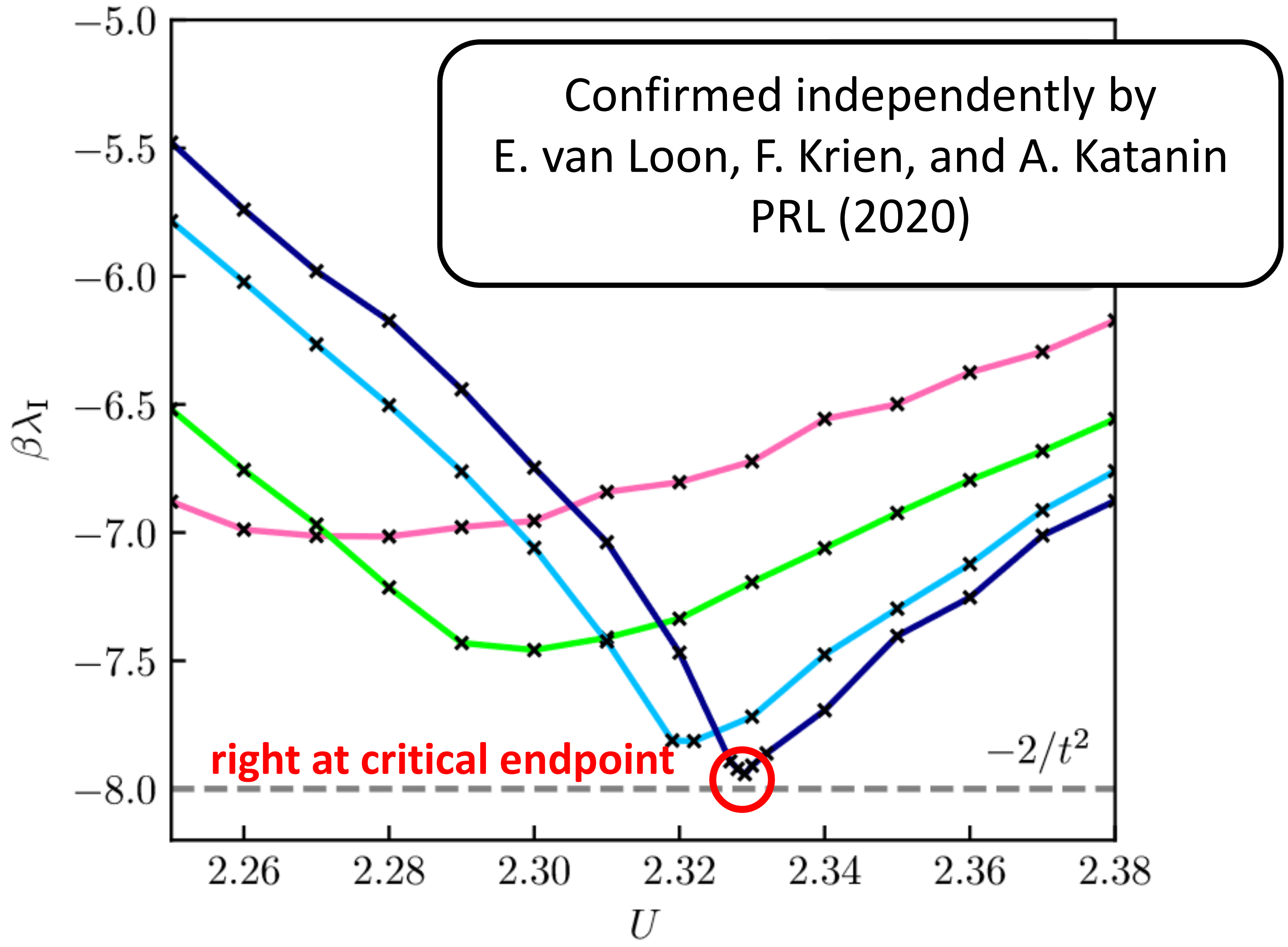
κ enhancement? Bethe lattice, half-filling

condition for lowest λ_α (= $\boldsymbol{\lambda_{\mathrm{I}}}$) fulfilled

$$\underbrace{\left(\frac{1}{\lambda_I} + t^2/\beta\right)^{-1}}_{\to 0} w_I$$

but **no** physical effect !

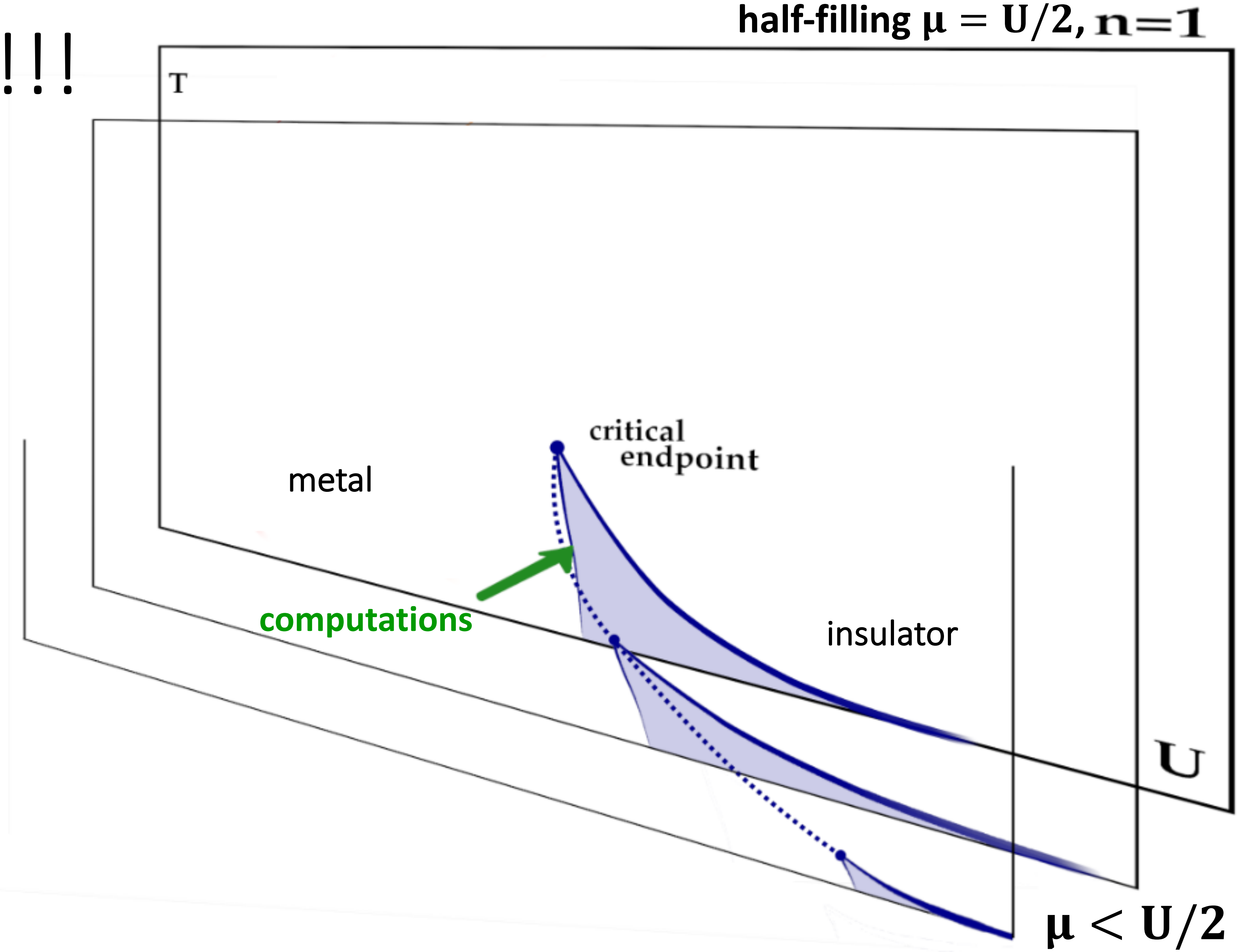
$\boldsymbol{w_I = 0}$ due to perfect **particle-hole** symmetry



❖ M. Reitner, P .Chalupa, L. Del Re, D. Springer, S. Ciuchi, G. Sangiovanni, and A.T., PRL **125** 196403 (2020)

Out-of-half-filling: κ enhancement !!!

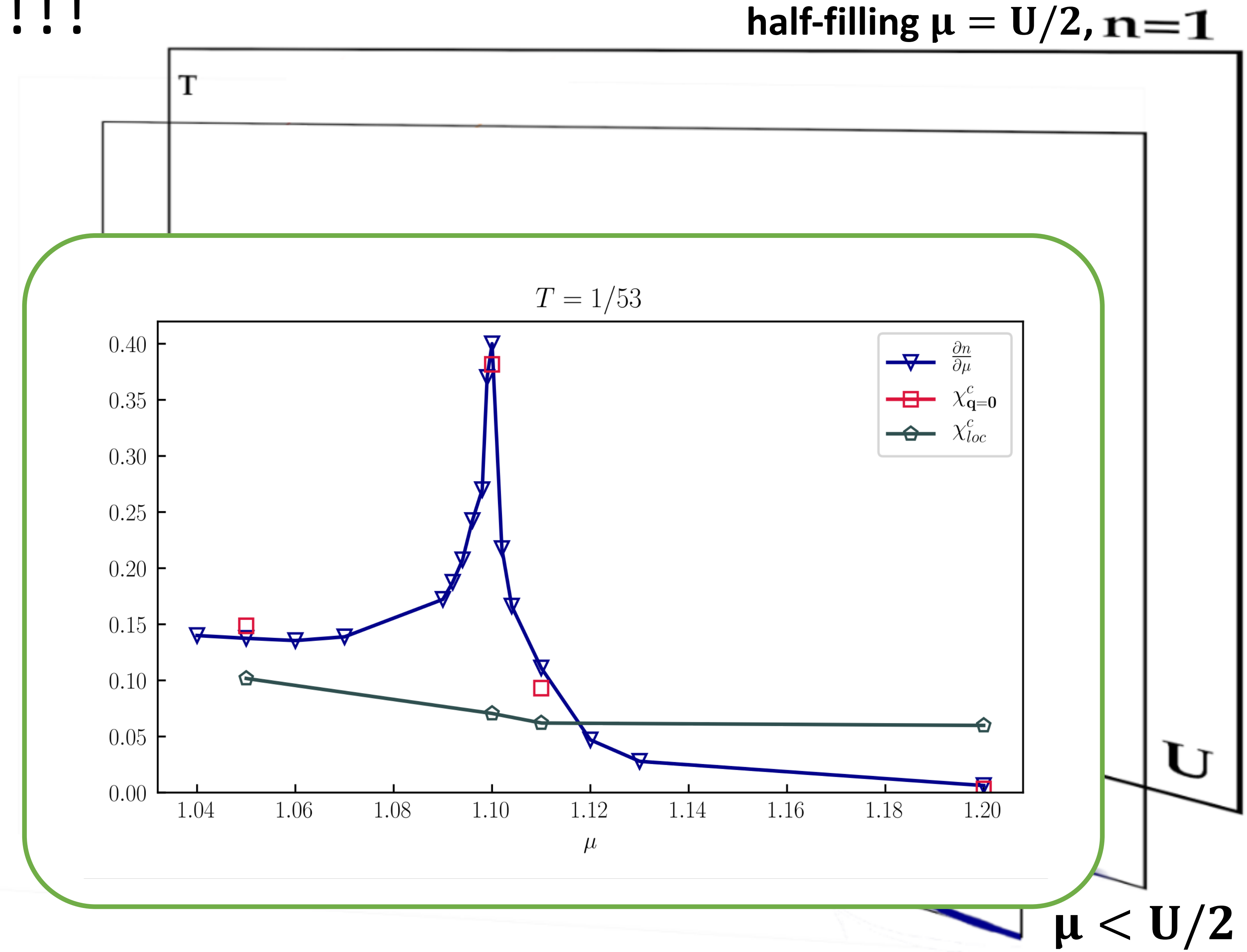
$$\kappa = \begin{cases} \dfrac{\partial n}{\partial \mu} \\ \\ \chi_c^{q=0}(\Omega = 0) \end{cases}$$



M. Reitner, P. Chalupa…., *A.T., PRL* (2020)   G. Kotliar, *et. al.*, PRL **89** 046401 (2002)   M. Eckstein, *et. al.*, PRB **75** 125103 (2007)

κ enhancement !!!

$$\kappa = \begin{cases} \dfrac{\partial n}{\partial \mu} \\ \chi_c^{q=0}(\Omega = 0) \end{cases}$$



M. Reitner, P. Chalupa…., *A.T.*, *PRL* (2020)

G. Kotliar, *et. al.*, PRL **89** 046401 (2002)

M. Eckstein, *et. al.*, PRB **75** 125103 (2007)

Diagnostic of κ

- BSE Eq. in DMFT: $\kappa = \chi_c^{q=0} = \frac{2}{\beta^2} \sum_\alpha \left(\frac{1}{\lambda_\alpha} + t^2/\beta \right)^{-1} w_\alpha$
  - Spectral (=EV) Decomposition

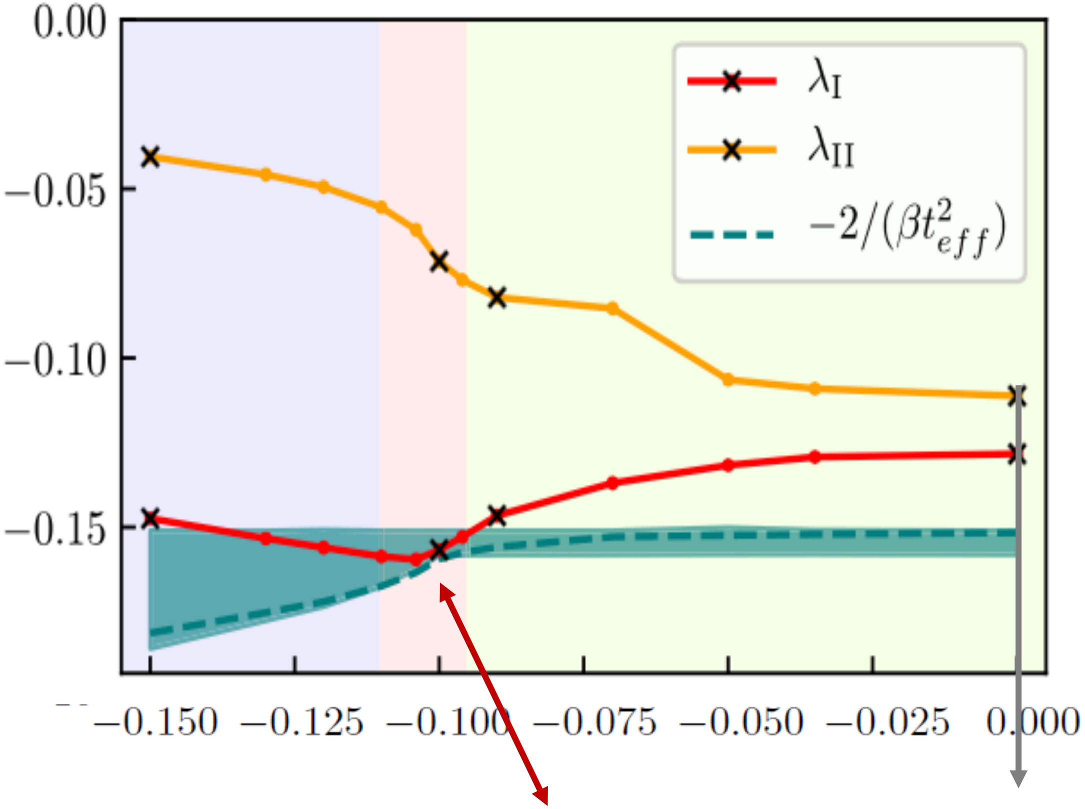
$$\chi_{q=0} = \frac{2}{\beta^2} \left(\frac{1}{\lambda_I} + t^2/\beta \right)^{-1} w_I + \frac{2}{\beta^2} \left(\frac{1}{\lambda_{II}} + t^2/\beta \right)^{-1} w_{II} + \text{rest}$$

$$\chi_{loc} = \frac{2}{\beta^2} \lambda_I w_I + \frac{2}{\beta^2} \lambda_{II} w_{II} + \text{rest}$$

❖ M. Reitner, P .Chalupa, L. Del Re, D. Springer, S. Ciuchi, G. Sangiovanni, and A.T., PRL **125** 196403 (2020)

Diagnostic of κ

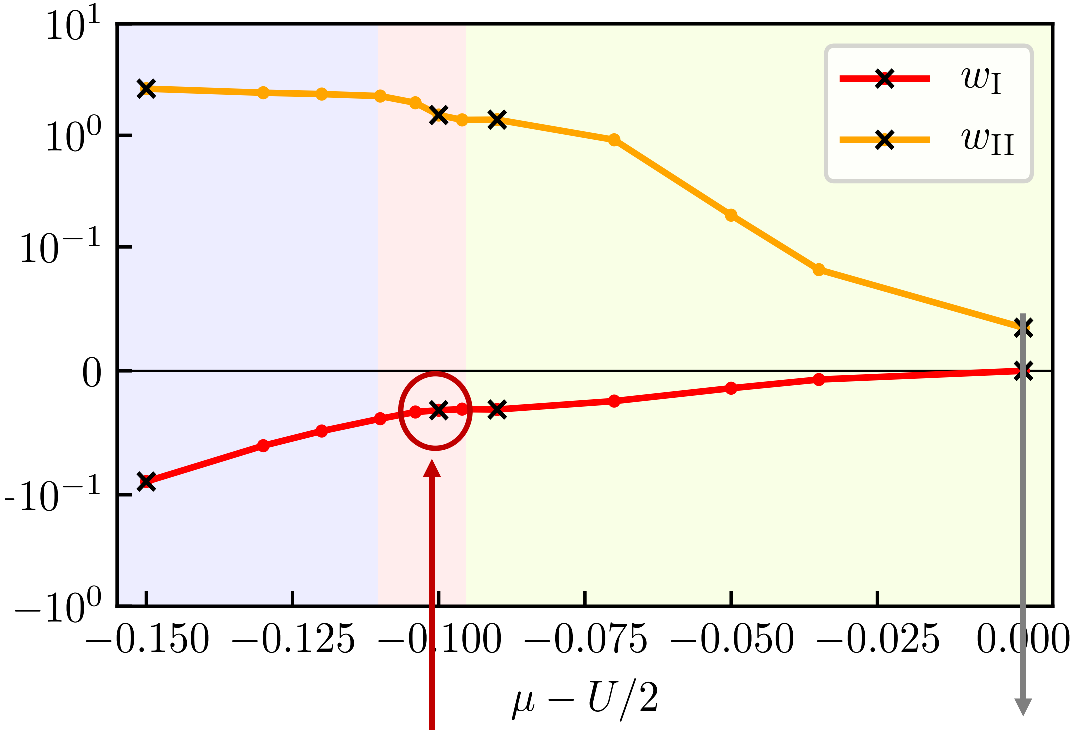
- lowest eigenvalues:



maximum of κ

half-filling

- their eigenweigths:



maximum of κ

half-filling

❖ M. Reitner, P .Chalupa, L. Del Re, D. Springer, S. Ciuchi, G. Sangiovanni, and A.T., PRL **125** 196403 (2020)

Diagnostic of κ

$$\chi_{q=0} = \frac{2}{\beta^2}\left(\frac{1}{\lambda_I} + t^2/\beta\right)^{-1} w_I + \frac{2}{\beta^2}\left(\frac{1}{\lambda_{II}} + t^2/\beta\right)^{-1} w_{II} + \text{rest}$$

$$\Downarrow \qquad \Downarrow \qquad \Downarrow \qquad \Downarrow$$

$$\to -\infty \qquad < 0 \qquad < 0 \qquad > 0$$

$$\chi_{loc} = \frac{2}{\beta^2} \quad \lambda_I \quad w_I + \frac{2}{\beta^2} \quad \lambda_{II} \quad w_{II} + \text{rest}$$

❖ M. Reitner, P .Chalupa, L. Del Re, D. Springer, S. Ciuchi, G. Sangiovanni, and A.T., PRL **125** 196403 (2020)

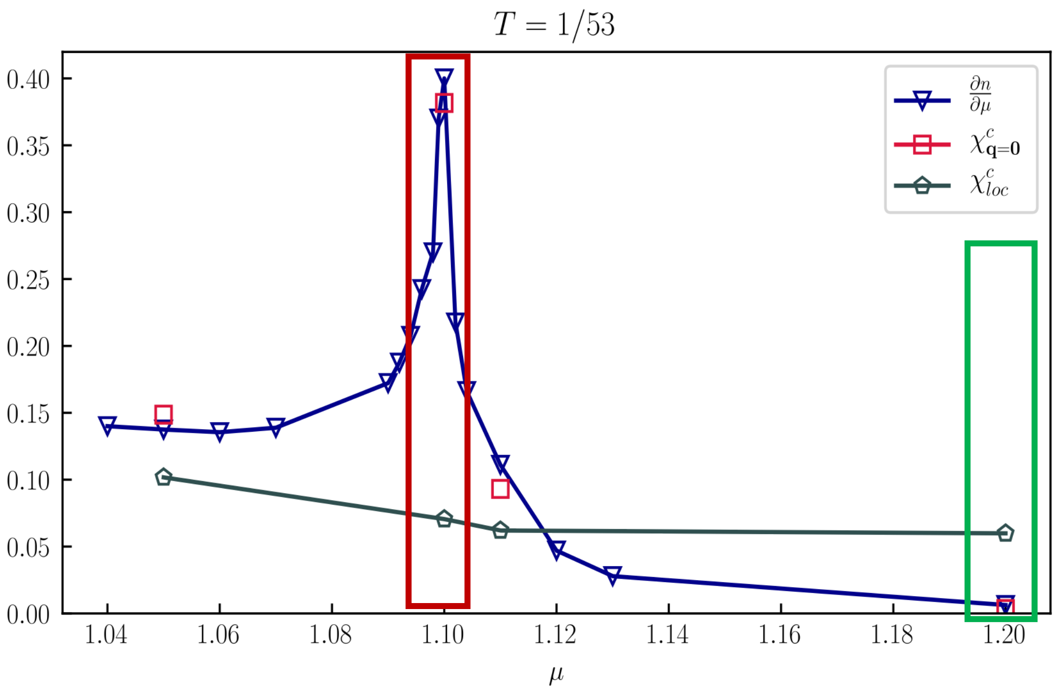
Diagnostic of κ

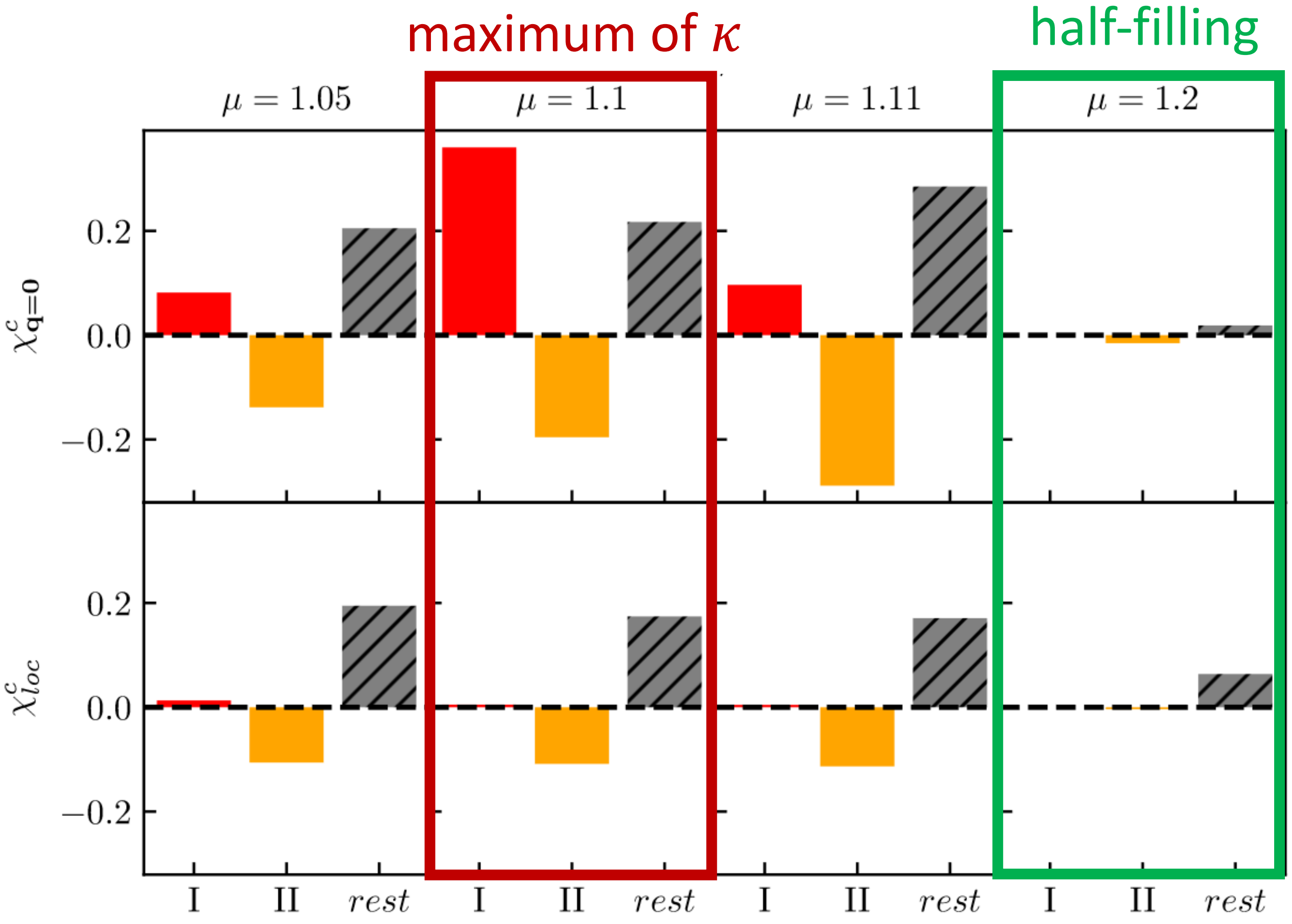
$$\chi_{q=0} = \underbrace{\frac{2}{\beta^2}\left(\frac{1}{\lambda_I} + t^2/\beta\right)^{-1} w_I}_{\text{effective attraction}} + \underbrace{\frac{2}{\beta^2}\left(\frac{1}{\lambda_{II}} + t^2/\beta\right)^{-1} w_{II}}_{\text{effective repulsion}} + \text{rest}$$

$$\chi_{loc} = \underbrace{\frac{2}{\beta^2} \quad \lambda_I \quad w_I}_{\text{effective attraction}} + \underbrace{\frac{2}{\beta^2} \quad \lambda_{II} \quad w_{II}}_{\text{effective repulsion}} + \text{rest}$$

❖ M. Reitner, P .Chalupa, L. Del Re, D. Springer, S. Ciuchi, G. Sangiovanni, and A.T., PRL **125** 196403 (2020)

κ enhancement – the „smoking gun“

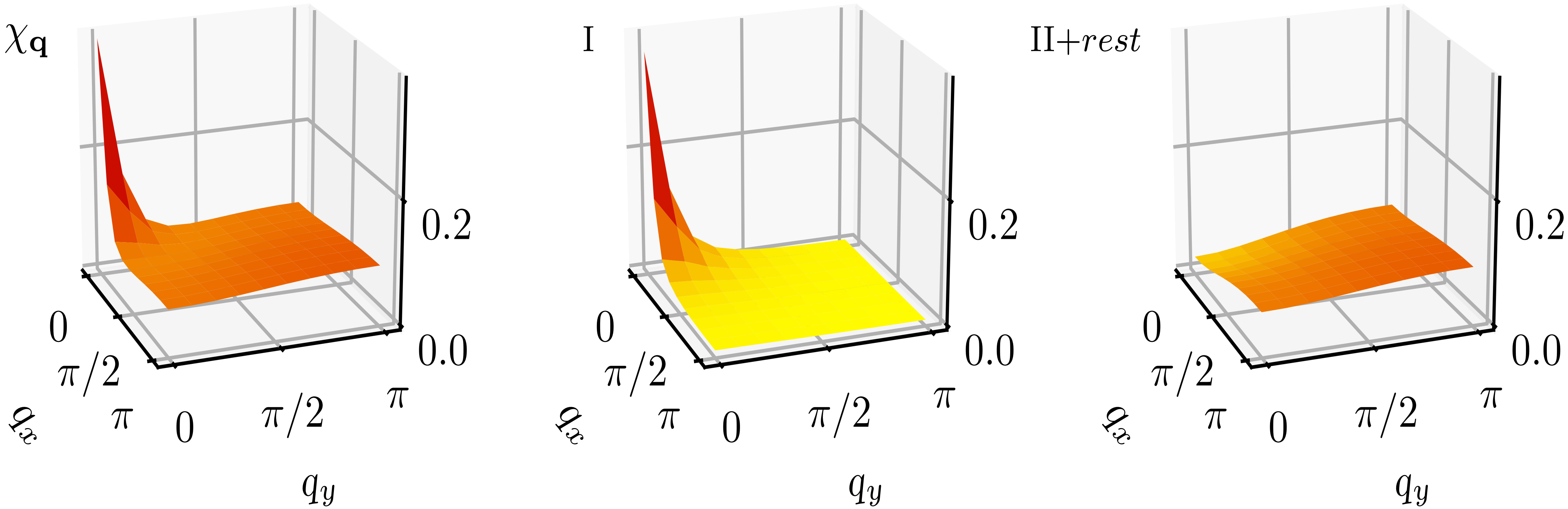




❖ M. Reitner, P .Chalupa, L. Del Re, D. Springer, S. Ciuchi, G. Sangiovanni, and A.T., PRL **125** 196403 (2020)

q-resolved analysis of $\chi_c^q(\Omega = 0)$

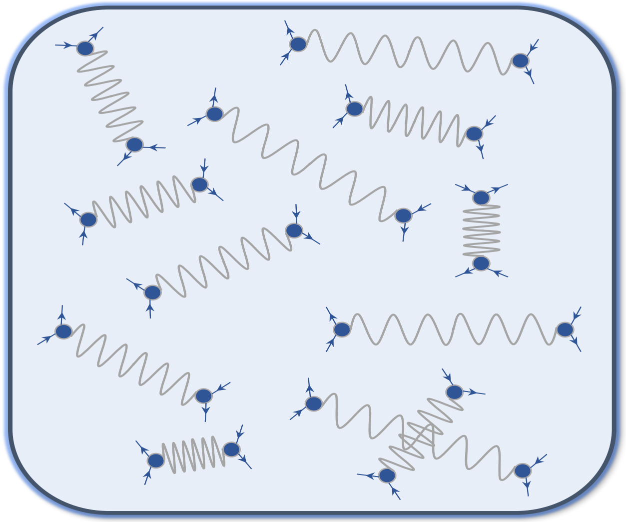
Full DMFT result | **Contribution of the lowest EV** | **All the rest**



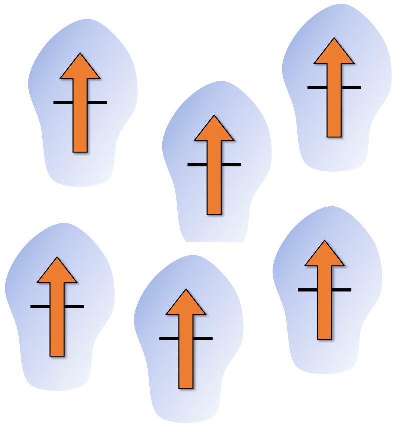
❖ M. Reitner, P .Chalupa, L. Del Re, D. Springer, S. Ciuchi, G. Sangiovanni, and A.T., PRL **125** 196403 (2020)

The *feats* …. of nonperturbativity

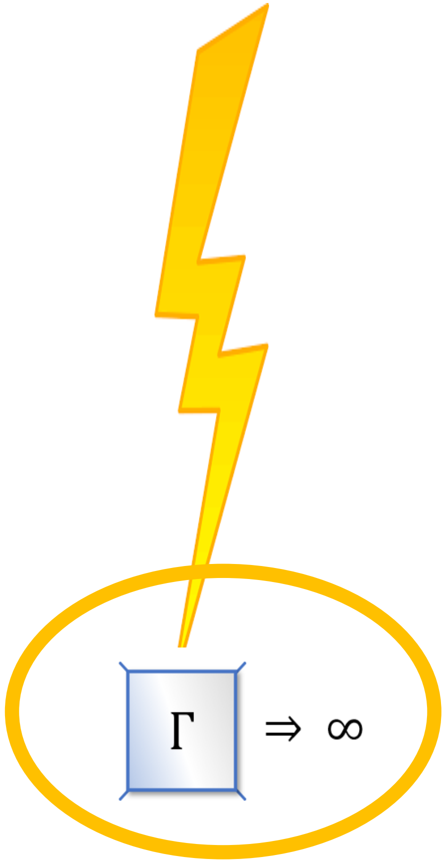
strong repulsion



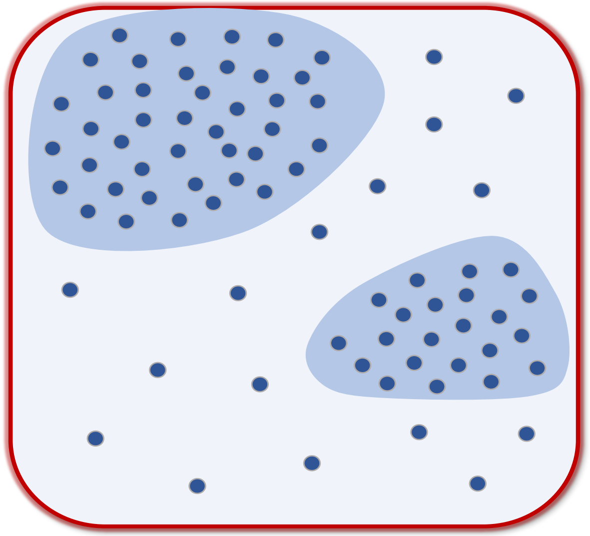
local magnetic moments



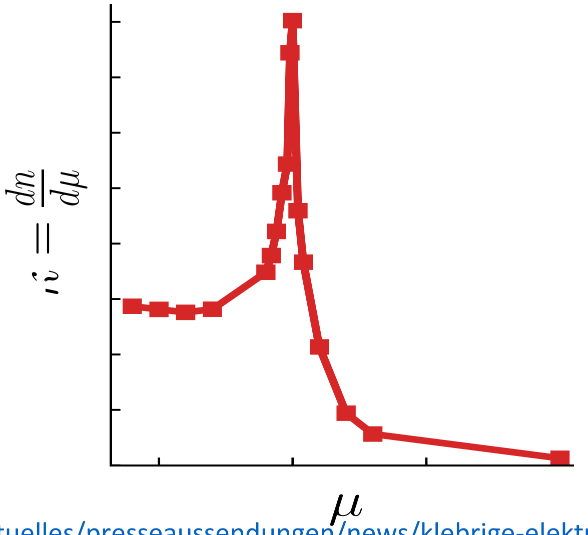
breakdown of perturbation theory



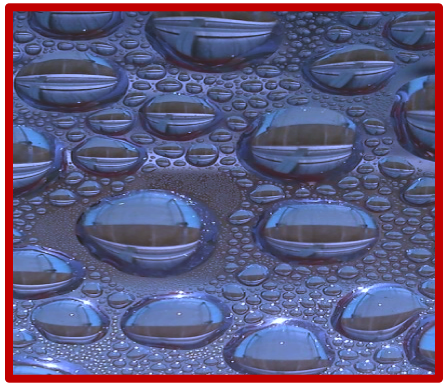
effective attraction



phase separation



As in the case of



the liquid-vapor transition

but **without**

Van Der Waals

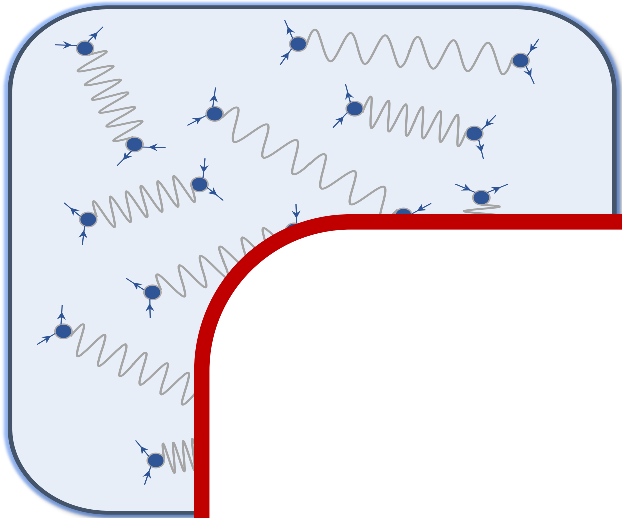
interactions !!

❖ M. Reitner, P. Chalupa, …. & AT, PRL. **125** 084402 (2020)

[https://www.tuwien.at/tu-wien/aktuelles/presseaussendungen/news/klebrige-elektronen-aus-abstossung-wird-anziehung]

The *feats* …. of nonperturbativity

strong repulsion



breakdown
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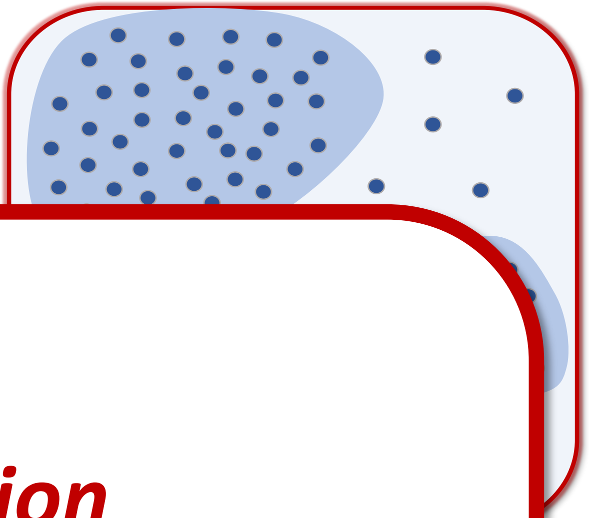
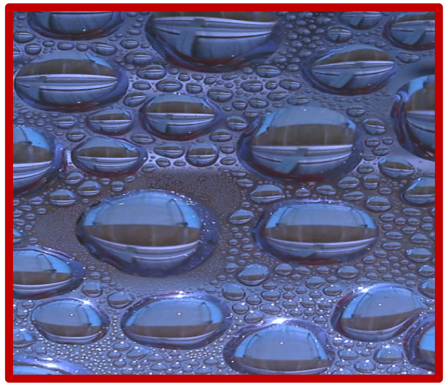


As in the case of



the **liquid-vapor** transition

but **without**

Van Der Waals

interactions!!

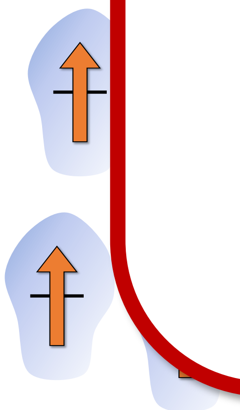
effective *attraction*

in uniform charge response !

BUT what about other channels?

loca

r



μ

❖ M. Reitner, P. Chalupa, …. & AT, PRL. **125** 084402 (2020)

[https://www.tuwien.at/tu-wien/aktuelles/presseaussendungen/news/klebrige-elektronen-aus-abstossung-wird-anziehung]

Phase separation, FM

Charge-density wave, SC (s-wave), AFM

$$\chi_{\mathbf{q=0}} = \frac{2}{\beta^2}\sum_{\alpha}\left(\frac{1}{\lambda_\alpha} + t^2/\beta\right)^{-1} w_\alpha$$

$$\chi_{\mathbf{q=\Pi}} = \chi^{pp}_{\mathbf{q=0}} = \frac{2}{\beta^2}\sum_{\alpha}\left(\frac{1}{\lambda_\alpha} - t^2/\beta\right)^{-1} w_\alpha$$

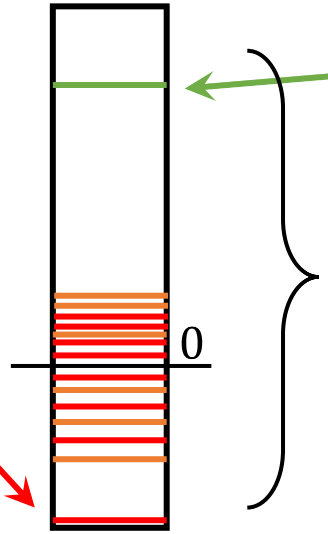
$\Downarrow$

minimal negative λ

$\Downarrow$

maximal positive λ

eigenvalues



$\chi_{loc}^{\nu\nu'}$

nonperturbative
path
to phase-transitions !

❖ M. Reitner, P .Chalupa, L. Del Re, D. Springer, S. Ciuchi, G. Sangiovanni, and A.T., PRL **125** 196403 (2020)

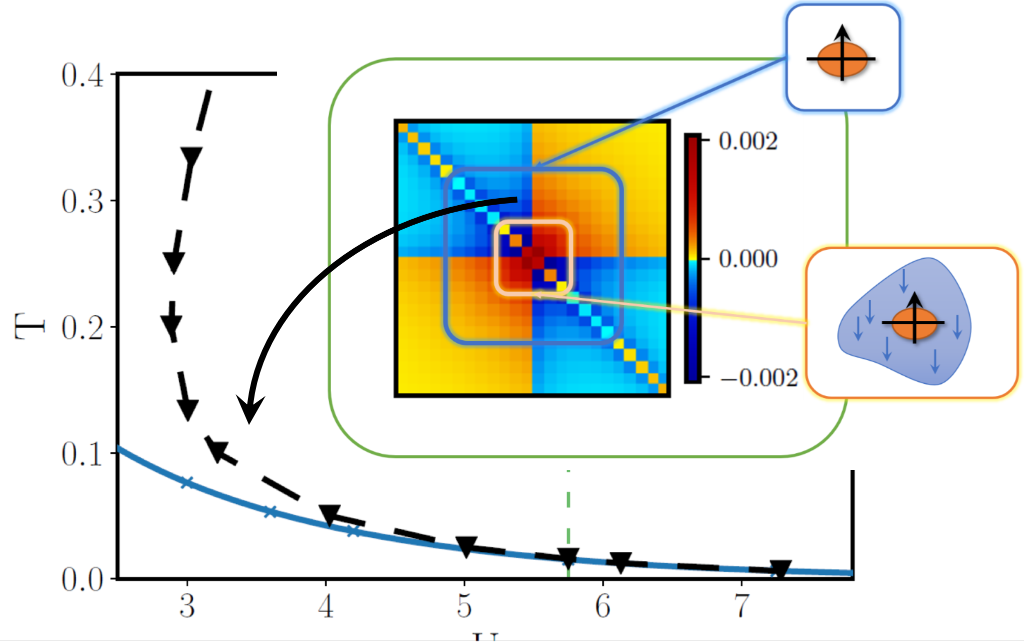
Summary

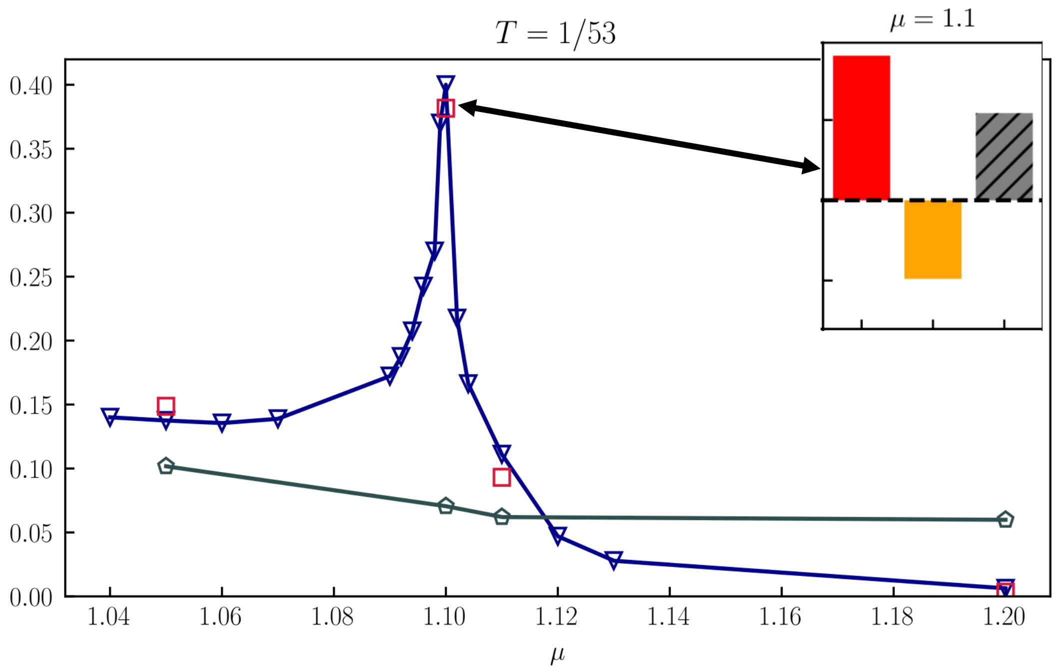
FINGERPRINTS:

Reading fundamental physics in 2P quantities

IMPLICATIONS:

Unveiling the underlying non-perturbative mechanisms





Summary

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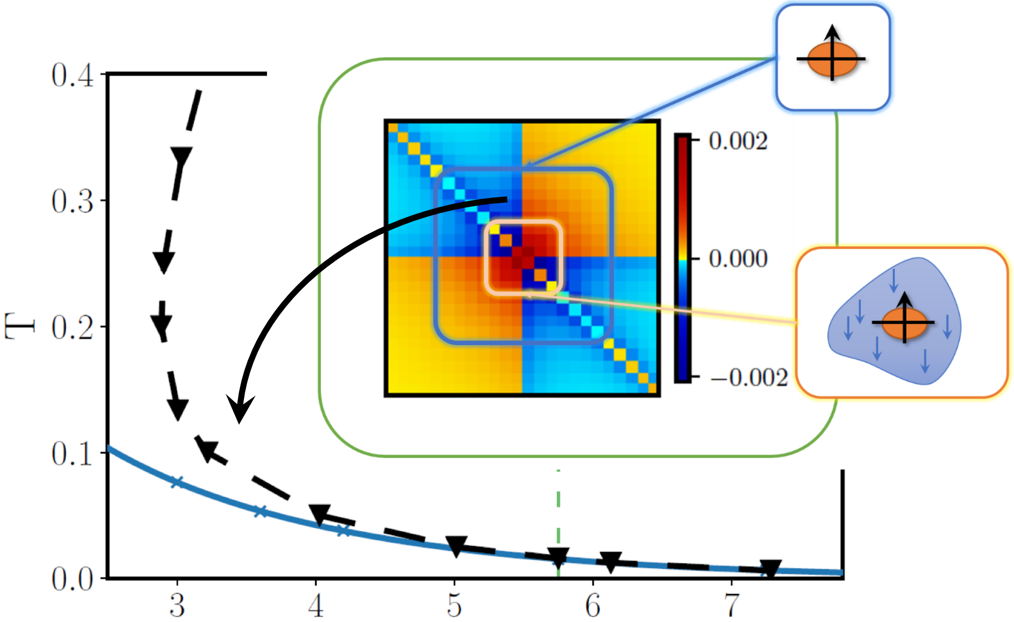

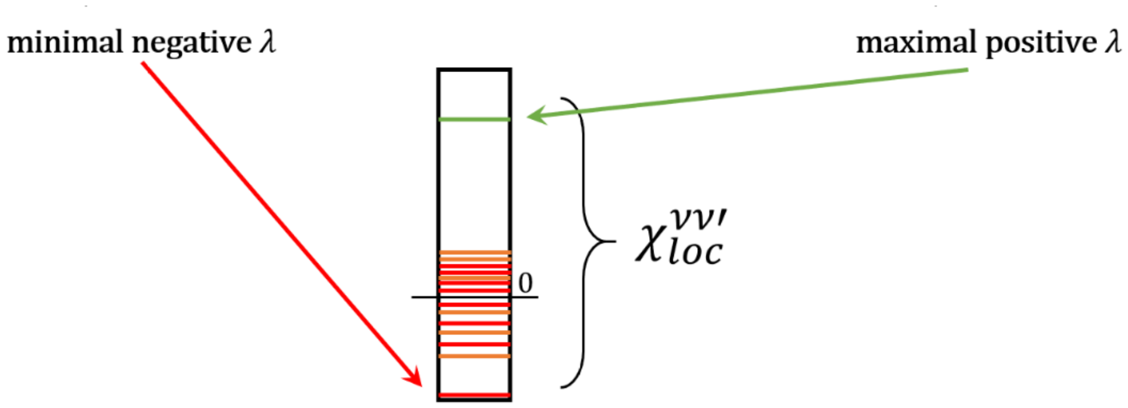

Summary & **Outlook**