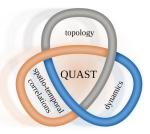
Electronic correlation at the 2P-level:

An intro to diagrammatic extensions of DMFT with applications of DΓA (spin fluctuations, pseudogap, superconductivity)







Alessandro Toschi

7th International Summer School on Computational Quantum Materials

Jouvence Resort, Canada 29.05.2024

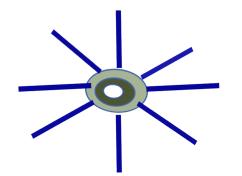


- 1. Intro: DMFT as a starting point
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- 3. How *nonperturbative* information is ``encoded'' in the DMFT vertex functions
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- 5. Pedagogical discussion of relevant results

Conclusions & Outlook

DMFT in a nutshell



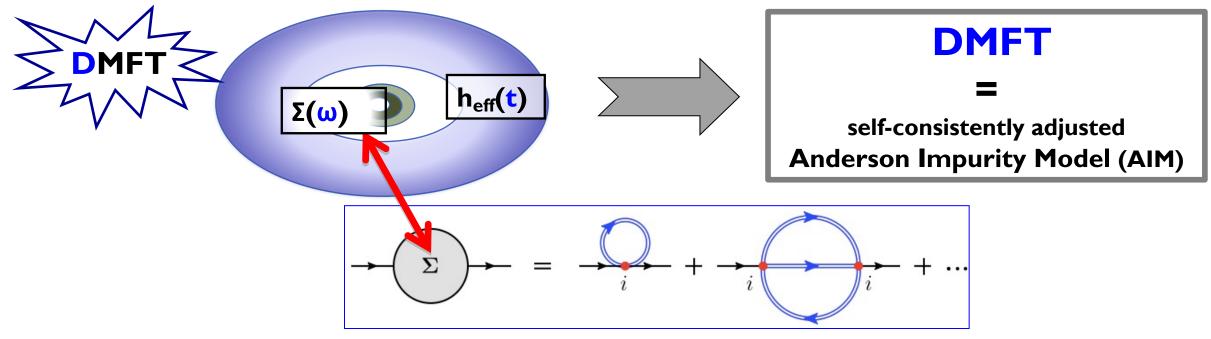
$$\underbrace{\Sigma}_{i} = i = \delta_{ij} \Leftrightarrow \Sigma(\vec{k}, \omega) = \Sigma(\omega)$$

the self-energy is **local !!**

high connectivity/dimensions

* W. Metzner & D. Vollahardt, PRL (1989)

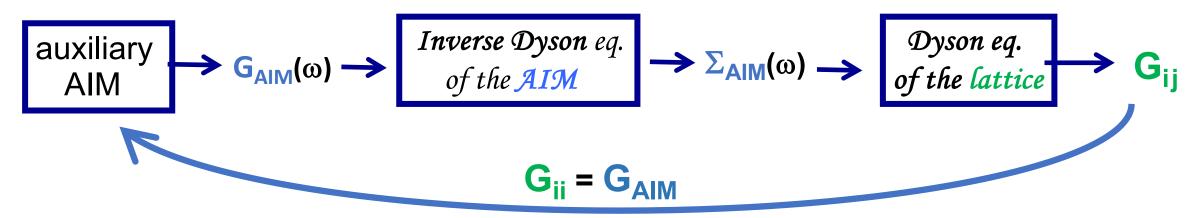
✤ A.Georges & G. Kotliar, PRB (1992)

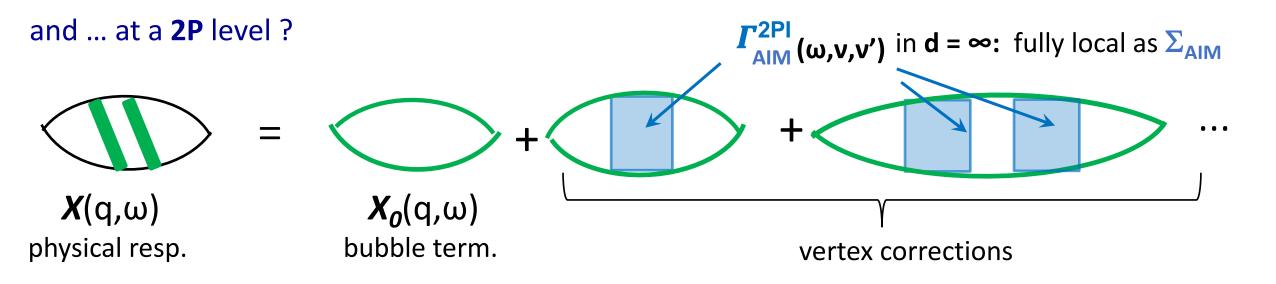


→ local, but all orders included!! → non perturbative in U!!

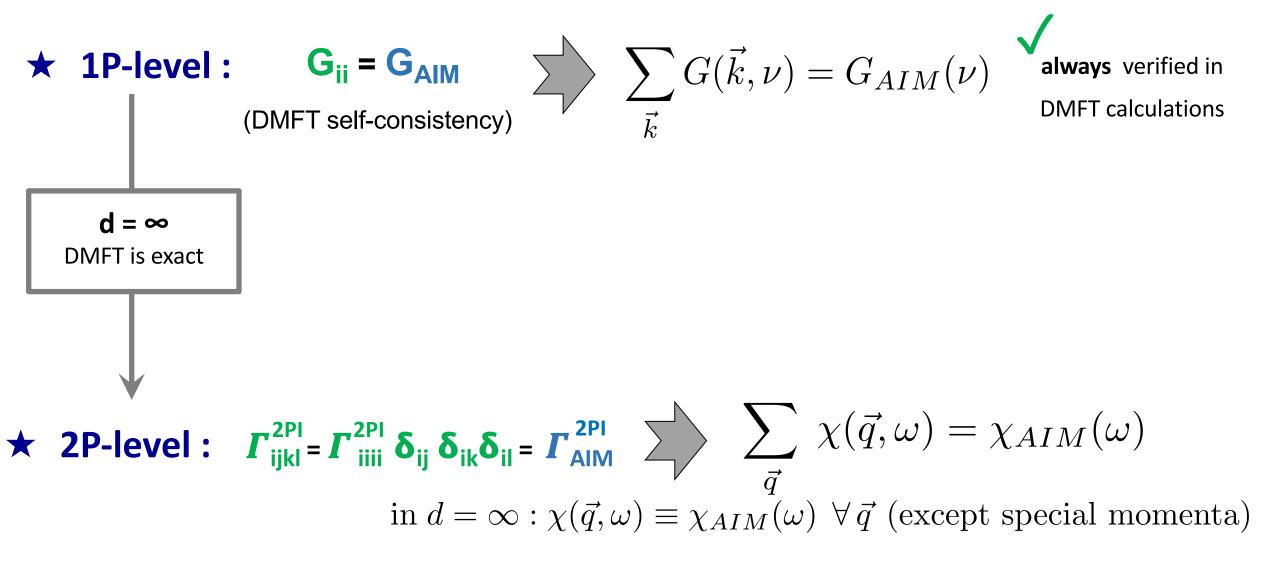
DMFT algorithm: Self-consistency at the 1P level

★ starting point :

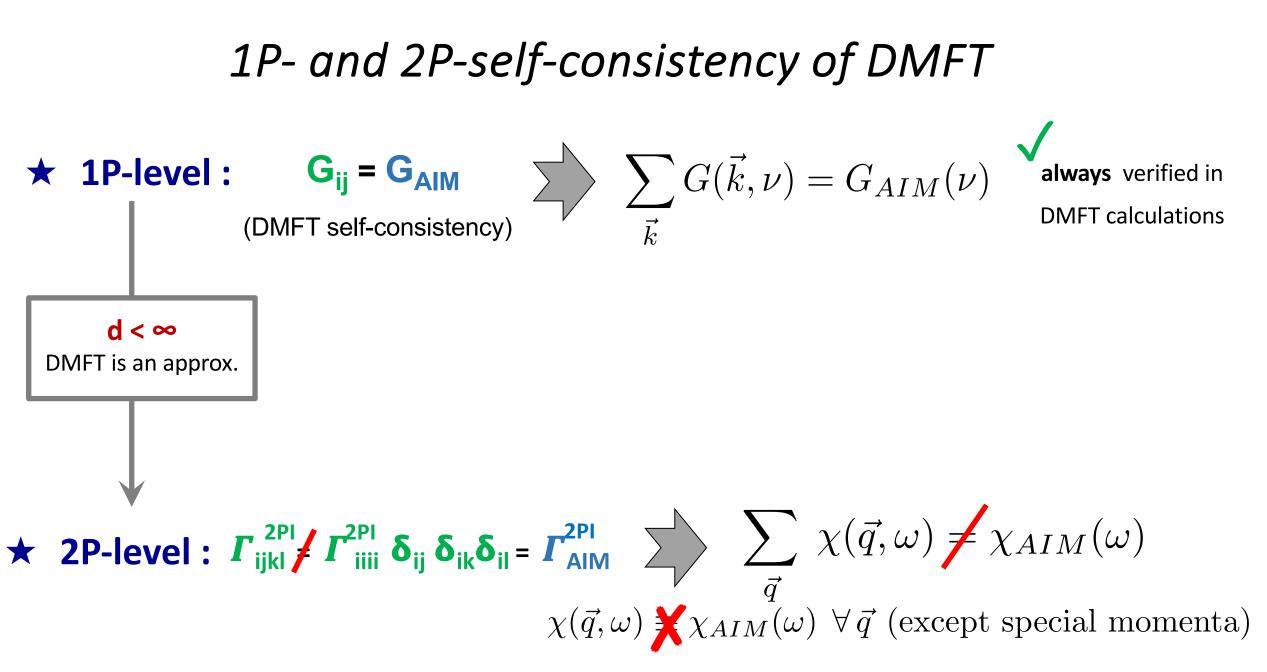




1P- and 2P-self-consistency of DMFT

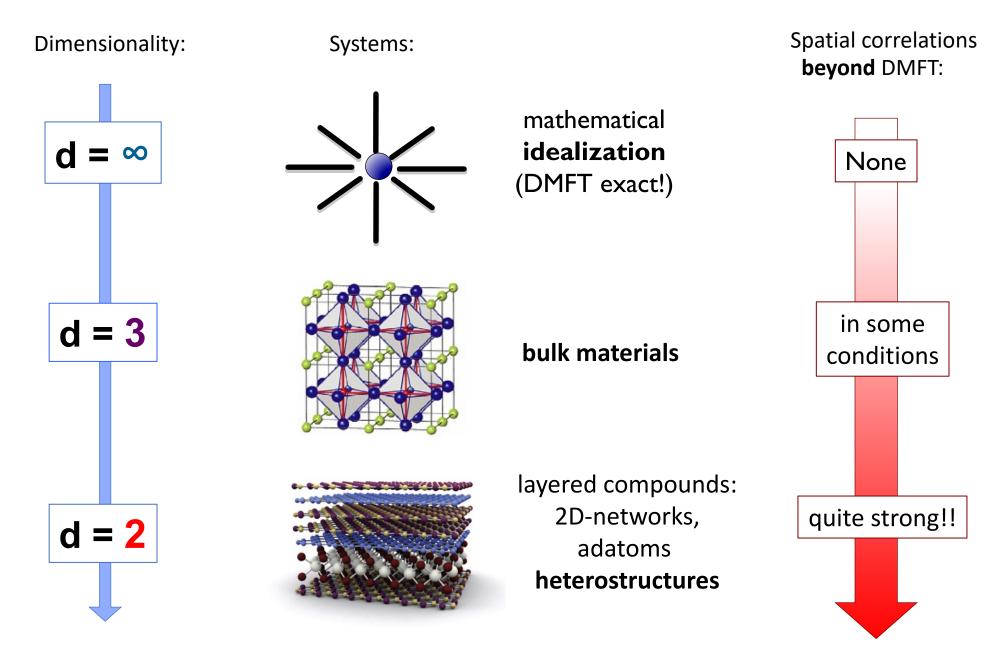


✤ A. Georges et al. RMP (1996)

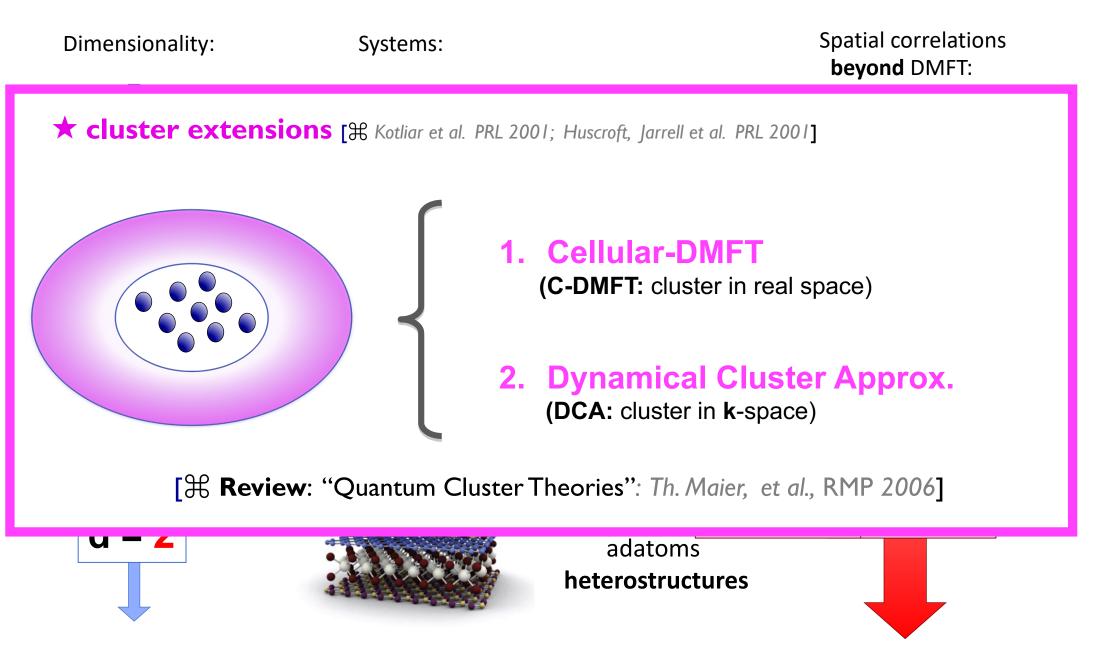


A. Georges et al. RMP (1996); A. Katanin et al. PRB (2009); G. Rohringer & AT, PRB (2016); L. Del Re & AT, PRB (2021)

From ∞ dimensions to ... "reality" !



From ∞ dimensions to ... "reality" !



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Diagrammatic extensions of DMFT

\star Dynamical Vertex Approximation (D Γ A)

[**# AT**, Katanin, Held, PRB (2007)]

★ Dual Fermion (DF) & Dual Bosons (DB)

[₩ Rubtsov, Lichtenstein ..., PRB (2008); Ann. Phys (2012)]

★ I Particle Irreducible approach

[# Rohringer, AT et al., PRB (2013)]

★ DMF²RG

[# Taranto, ...,& AT; PRL (2014); Vilardi , Taranto & Metzner, PRB (2019)]

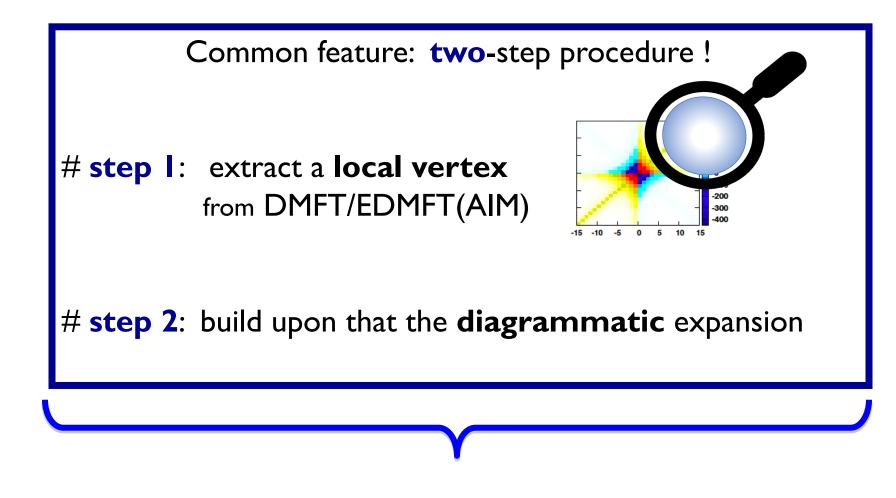
★ TRILEX, QUADRILEX

[# Ayral & Parcollet, PRB 2015; PRB (2016)]

REVIEWS OF MODERN PHYSICS, VOLUME 90, APRIL-JUNE 2018

Diagrammatic routes to nonlocal correlations beyond dynamical mean field theory

Diagrammatic extensions of DMFT



REVIEWS OF MODERN PHYSICS, VOLUME 90, APRIL–JUNE 2018

Diagrammatic routes to nonlocal correlations beyond dynamical mean field theory

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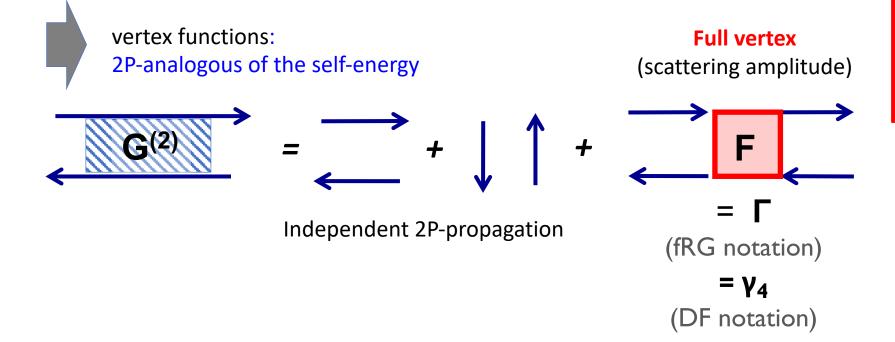
Conclusions & Outlook

2P-Feynman diagrams: (local) Green's & vertex functions

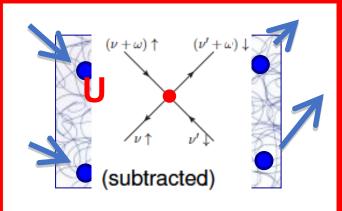
2P-Green's function: $G^{(2)}_{\sigma_1,\sigma_2,\sigma_3,\sigma_4}(\tau_1,\tau_2,\tau_3,0) = \langle \hat{c}_{\sigma_1}(\tau_1)\hat{c}^{\dagger}_{\sigma_2}(\tau_2)\hat{c}_{\sigma_3}(\tau_3)\hat{c}^{\dagger}_{\sigma_4}(0) \rangle$ **Its Fourier Transform:** $G^{(2)}_{\sigma_1\sigma_2\sigma_3\sigma_4}(\omega,\nu,\nu') = \int_0^\beta d\tau_1 \, d\tau_2 \, d\tau_3 \, e^{i\nu\tau_1} e^{-i(\nu+\omega)\tau_2} e^{i(\nu'+\omega)\tau_3} \, G^{(2)}_{\sigma_1\sigma_2\sigma_3\sigma_4}(\tau_1,\tau_2,\tau_3,0)$

\rightarrow computable for AIM

single band: **ED** & **NRG** [*Kugler et al. PRX, (2021)*] general multi-band case: **CTQMC** [*TRIQS, w2dynamics, ALPS,*]



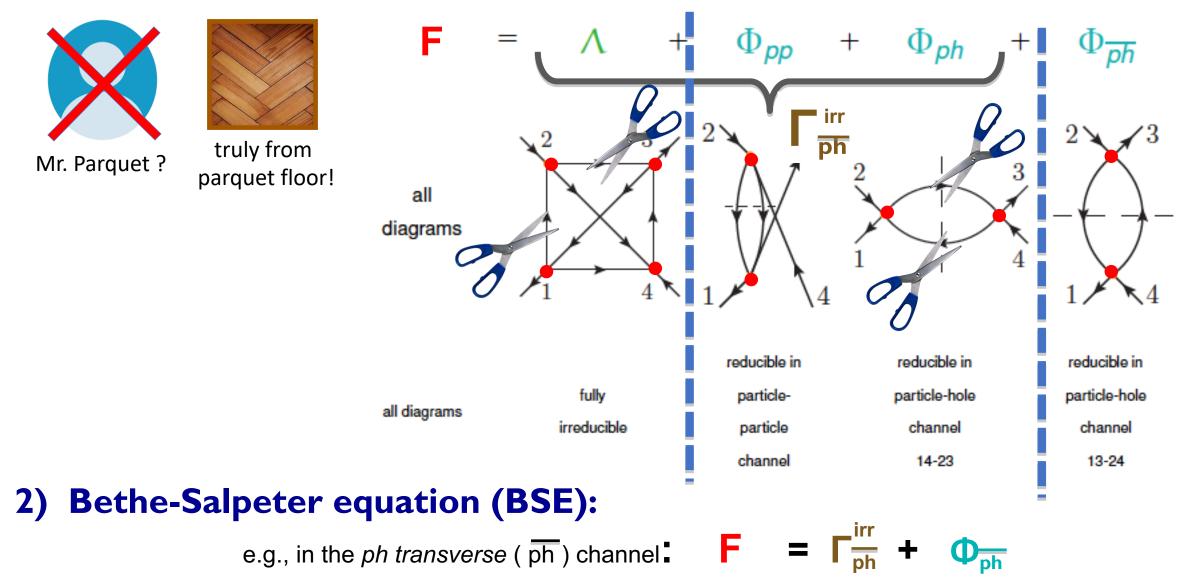
the lowest order :

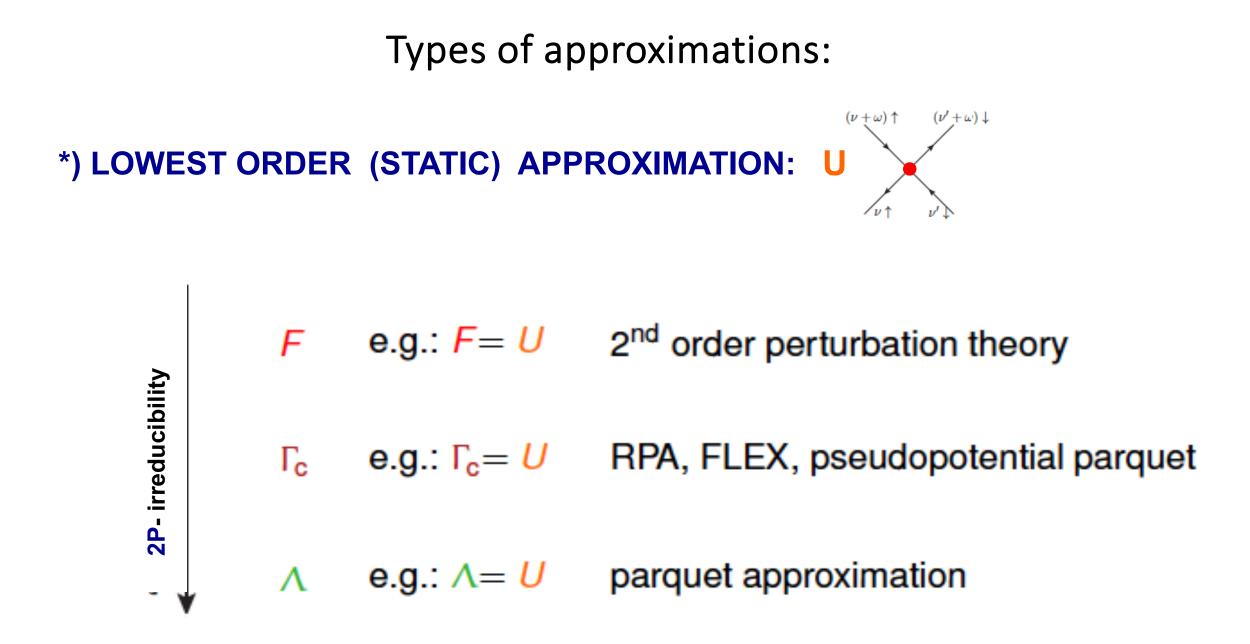


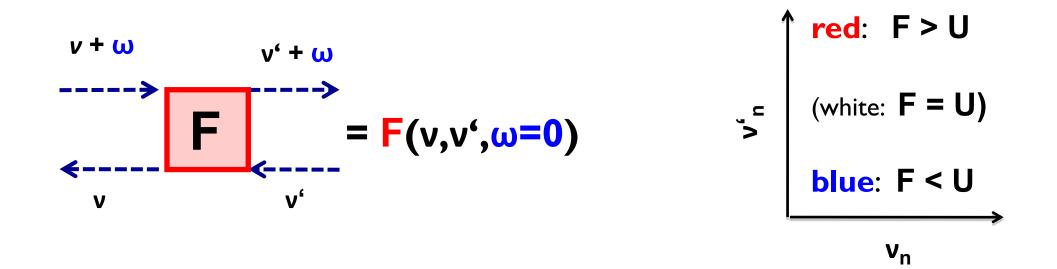


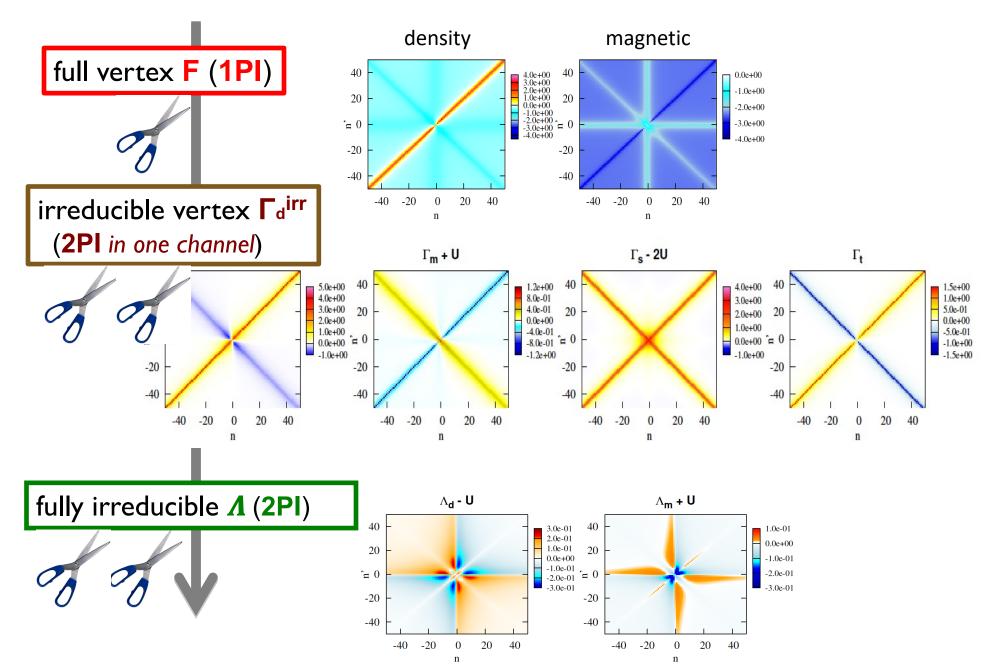
lo fo

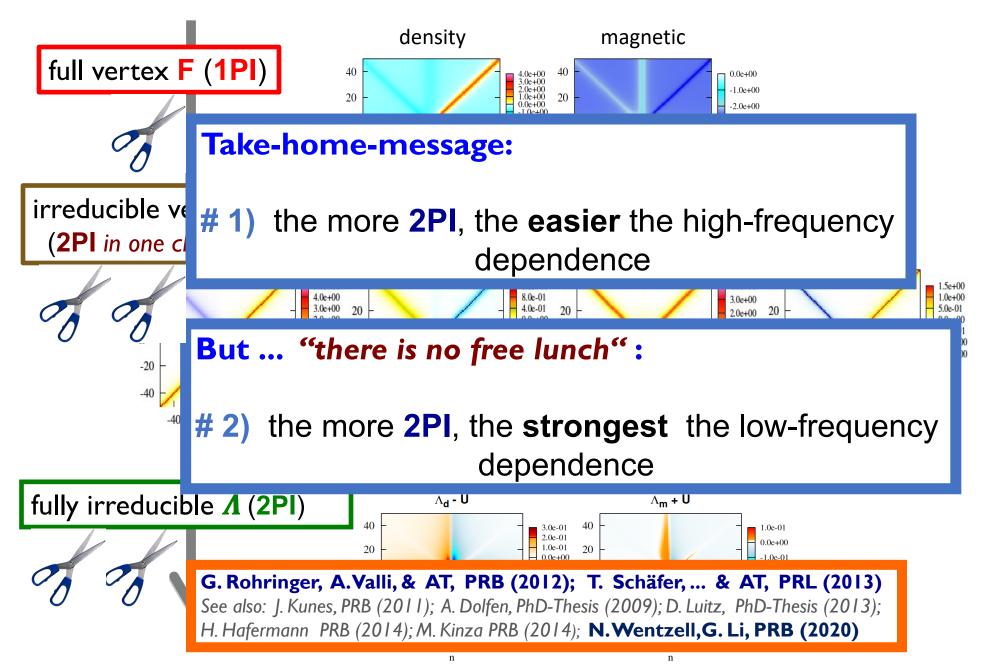
1) parquet equation:

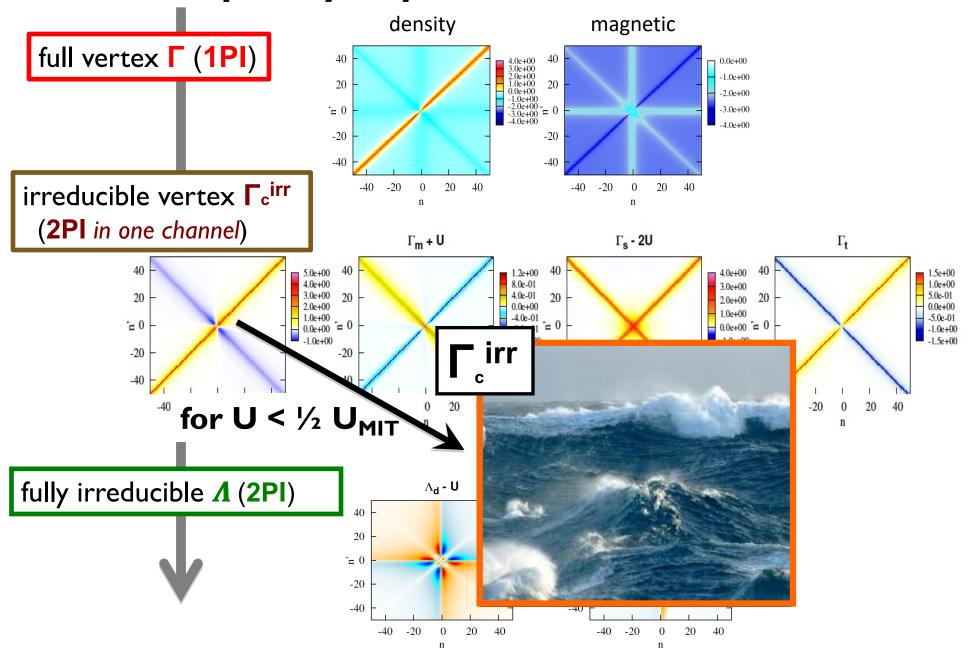






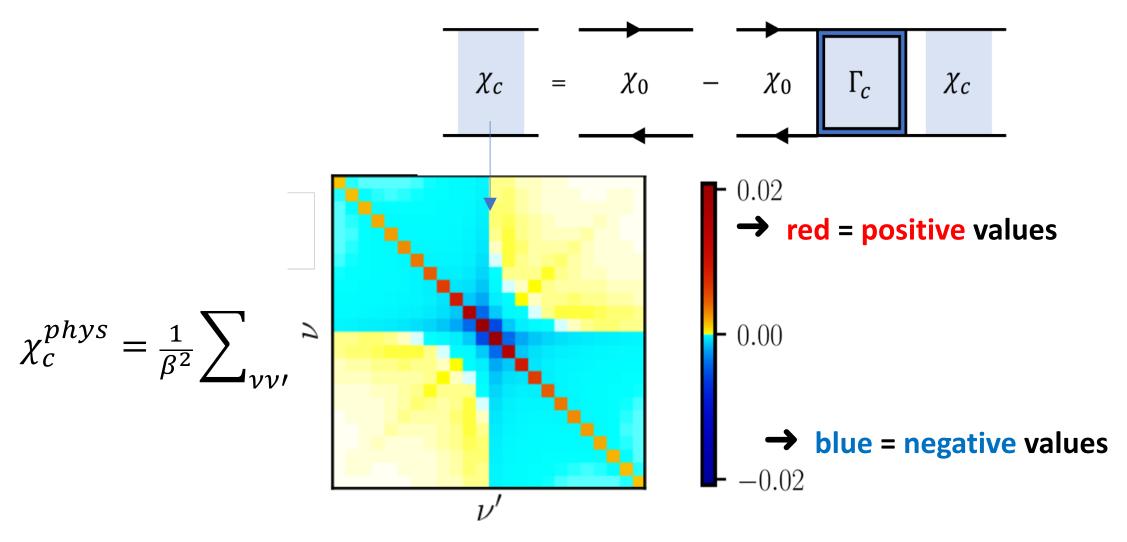






Relation to the physics?

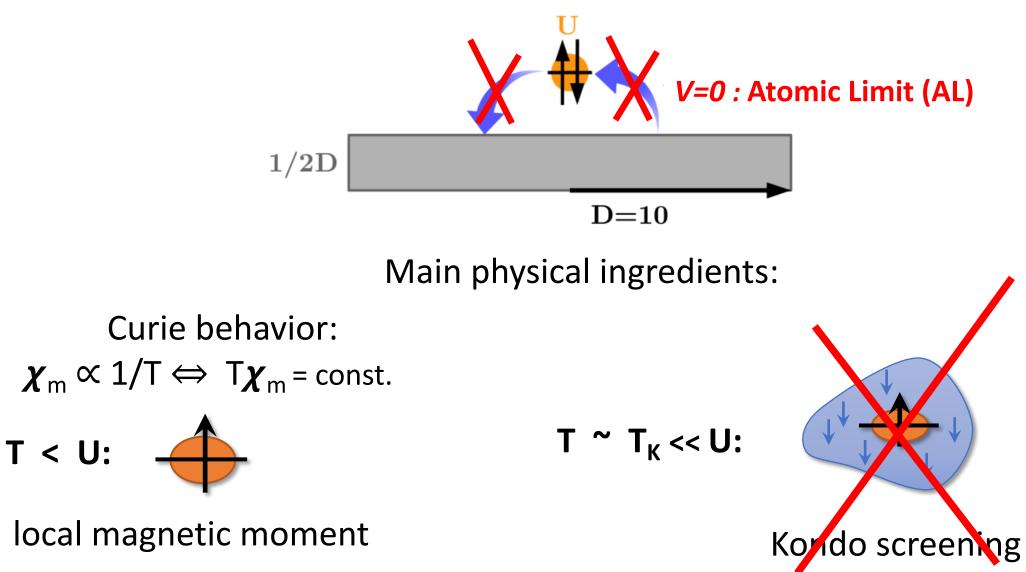
• generalized local charge susceptibility for $i\Omega=0$



P. Chalupa et al., PRL (2021); S.Adler., ..., & AT, SciPost Phys. (2024)

Anderson Impurity Model

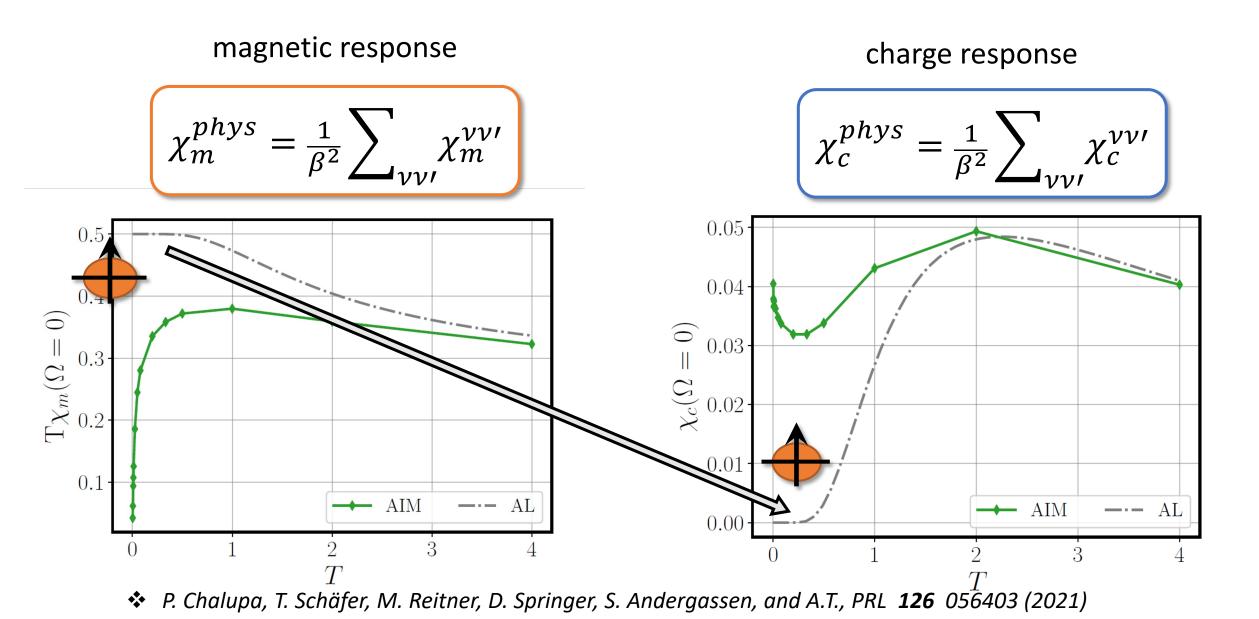
• wide-band limit, half-filling



Physical response of the AIM

• w2dynamics – CT-HYB

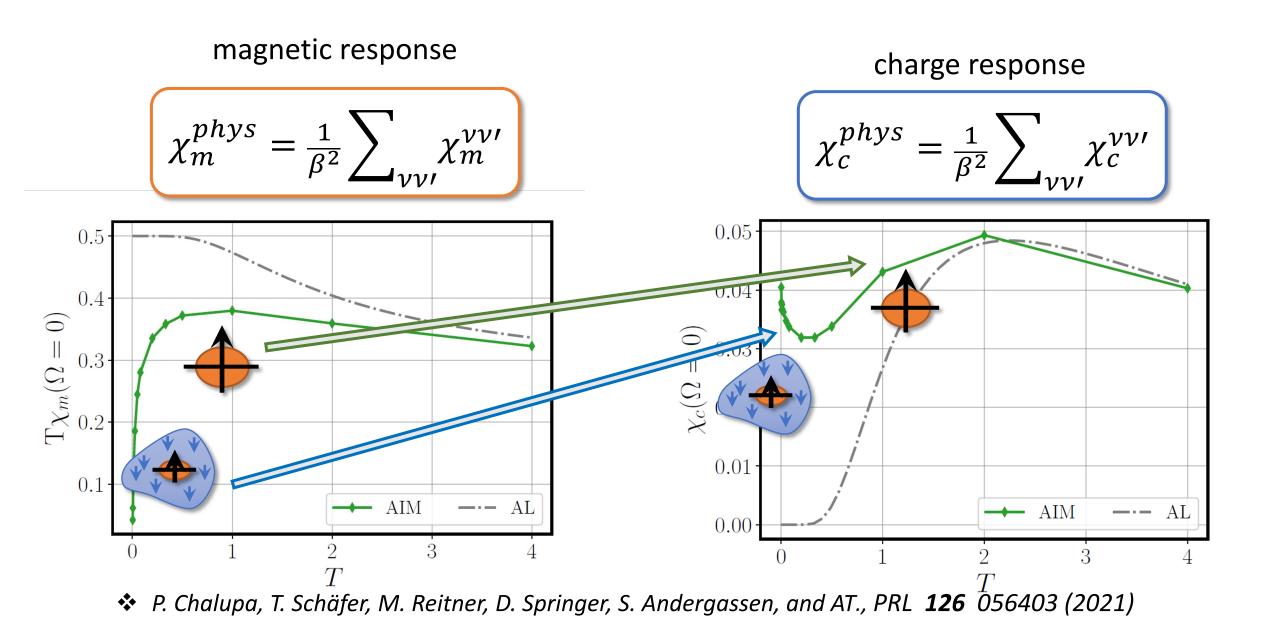
M.Wallerberger, et.al, CPC 235, 388 (2019)



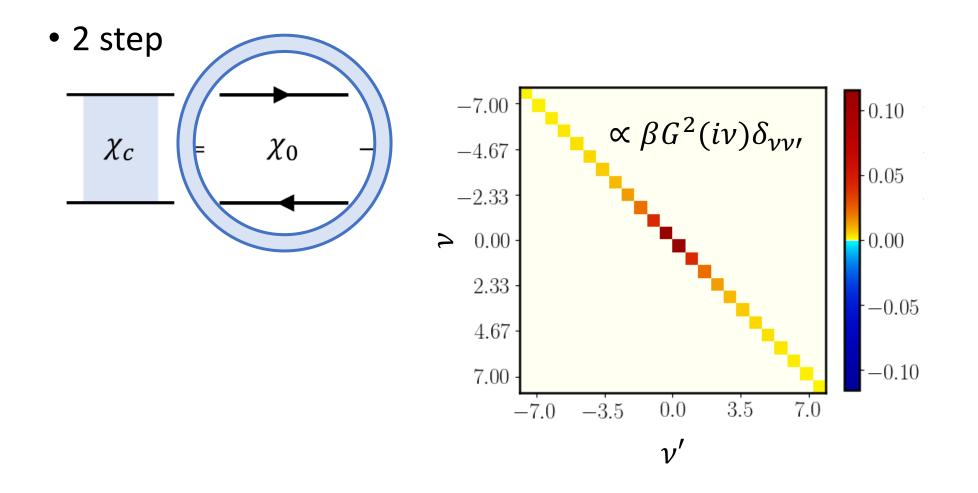
Physical response of AL & AIM

• w2dynamics – CT-HYB

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

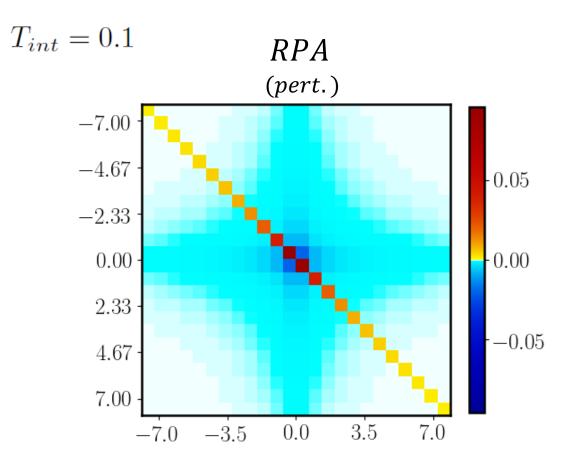


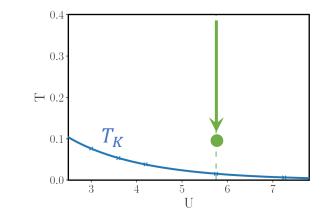
1.Step: Non interacting case/bubble term



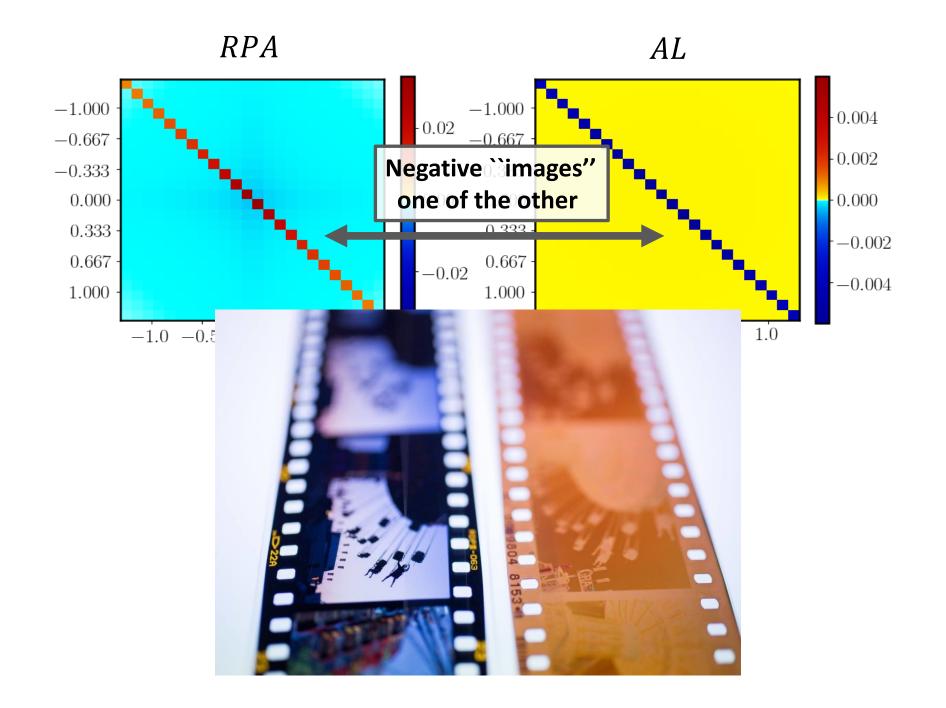
2.Step: weak vs. strong-coupling

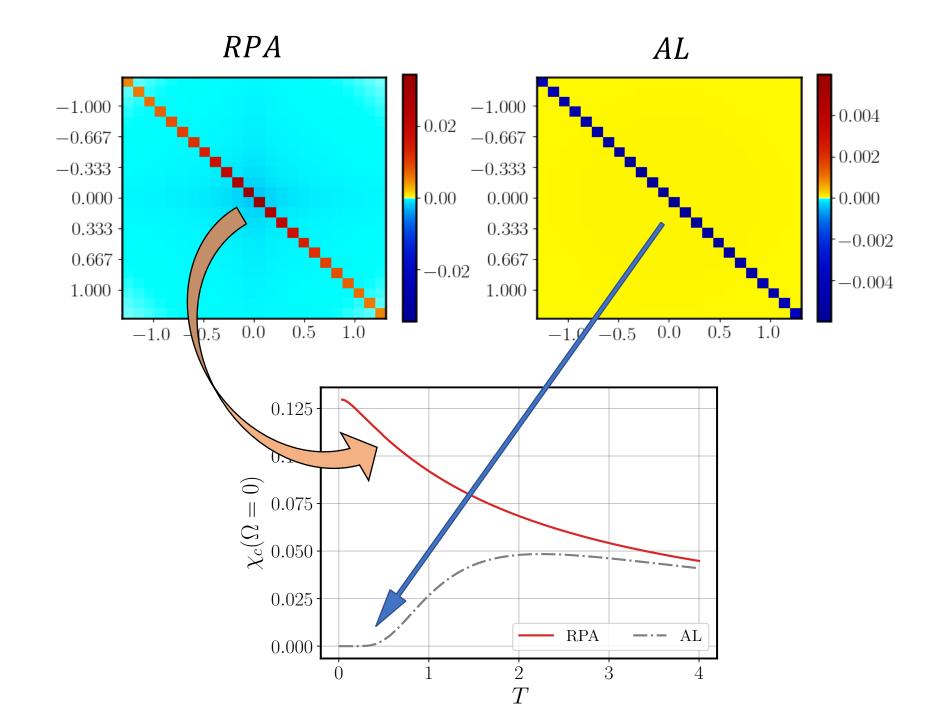
e.g.: intermediate temperature region ($T_{\kappa} < T << U$)

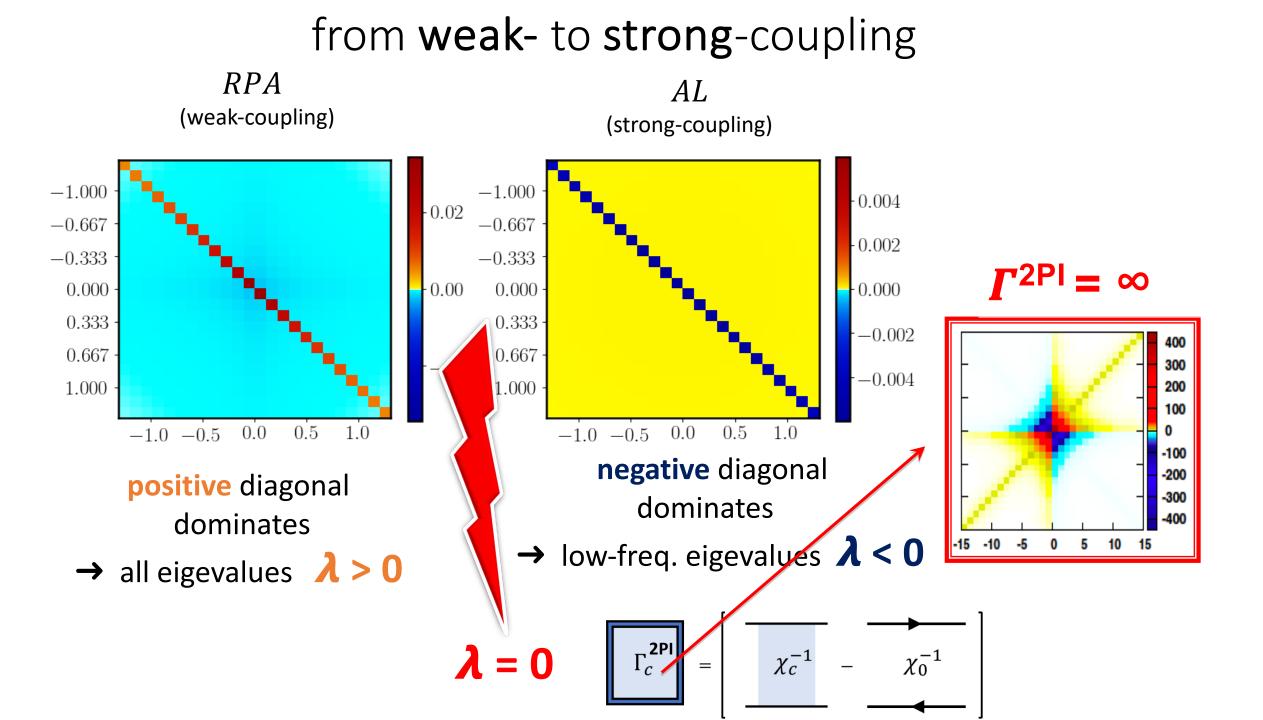




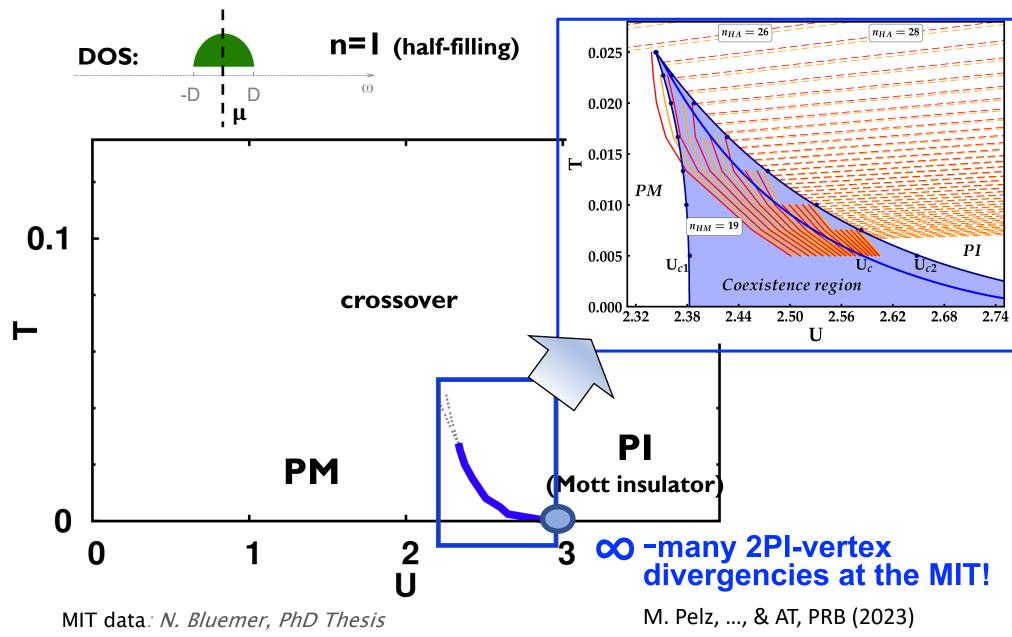
P. Chalupa, T. Schäfer, M. Reitner, D. Springer, S. Andergassen, and A.T., PRL 126 056403 (2021)



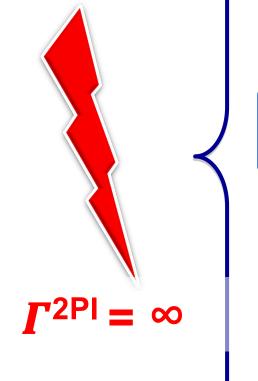




Phase diagram of the Hubbard model



Algorithmic challenges



I. Approaches based on 2PI vertices

parquet-based methods

dynamical vertex approximation (DΓA)

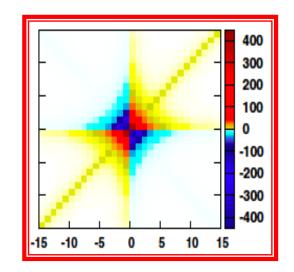
QUADRILEX

 $\overline{\delta^2} \Phi_{LW}$

 $\delta^2 G$

 $\neg 2PI$

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



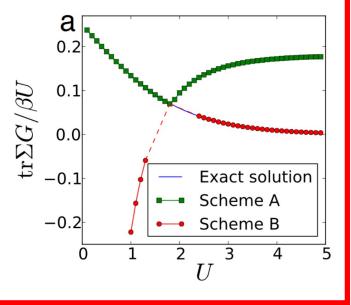
II. Multivaluedness of LW functional

iterative/self-consistent (=``bold'')
Diagrammatic resummation

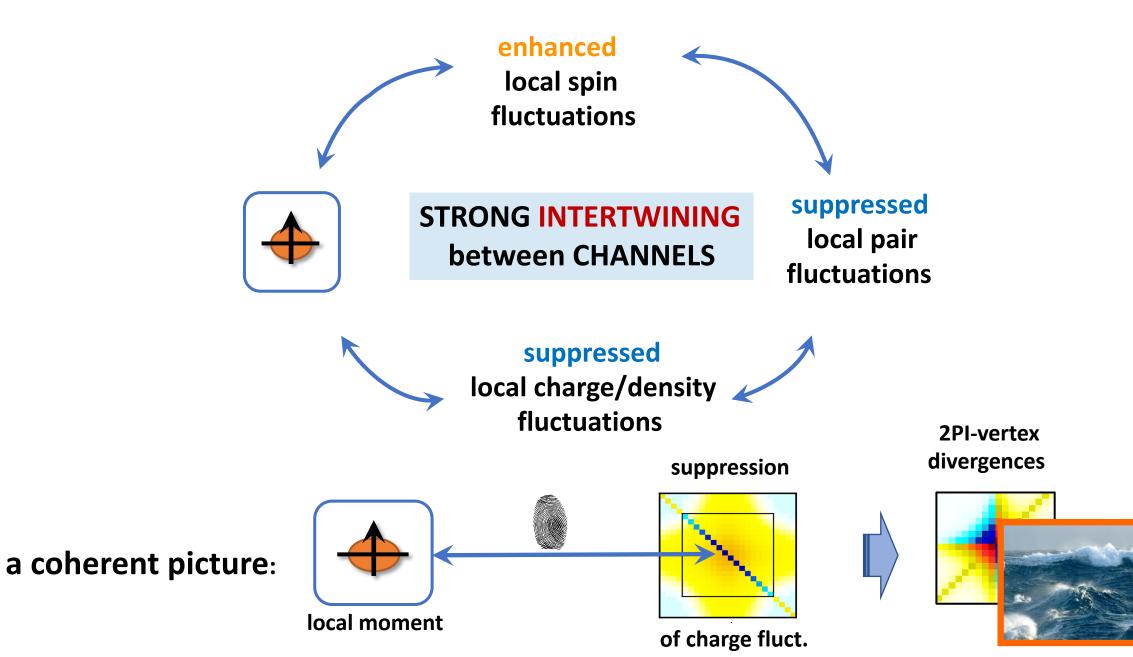
Diagrammatic Monte Carlo

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),]



The underlying physics of the nonperturbative regime



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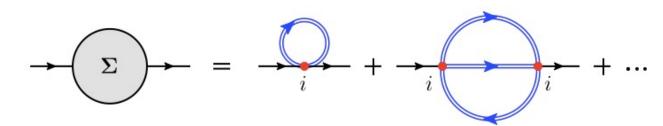
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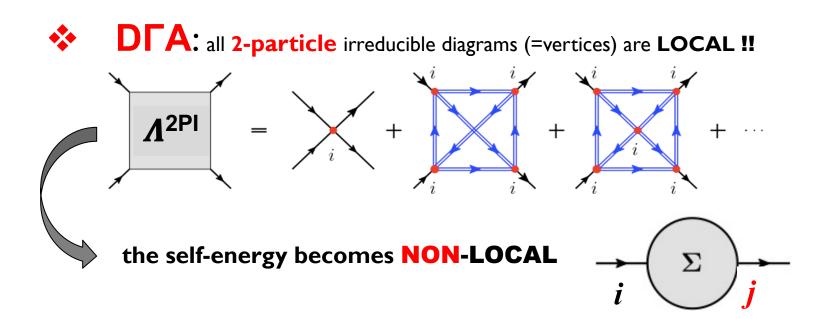
Conclusions & Outlook

the dynamical vertex approximation (DFA): a 2PI-based approach

AT, A. Katanin, K. Held, PRB (2007) See also: PRB (2009), PRL (2010), PRL (2011), PRB (2012), PRB (2015), ... Review: RMP (2018)

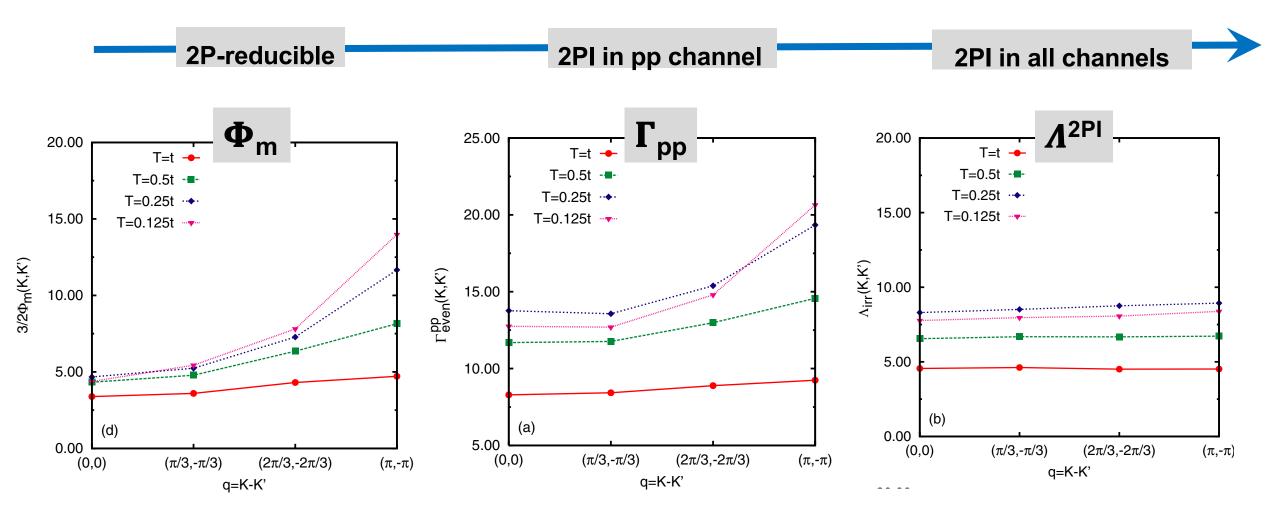
DMFT: all I-particle irreducible diagrams (=self-energy) are LOCAL !!





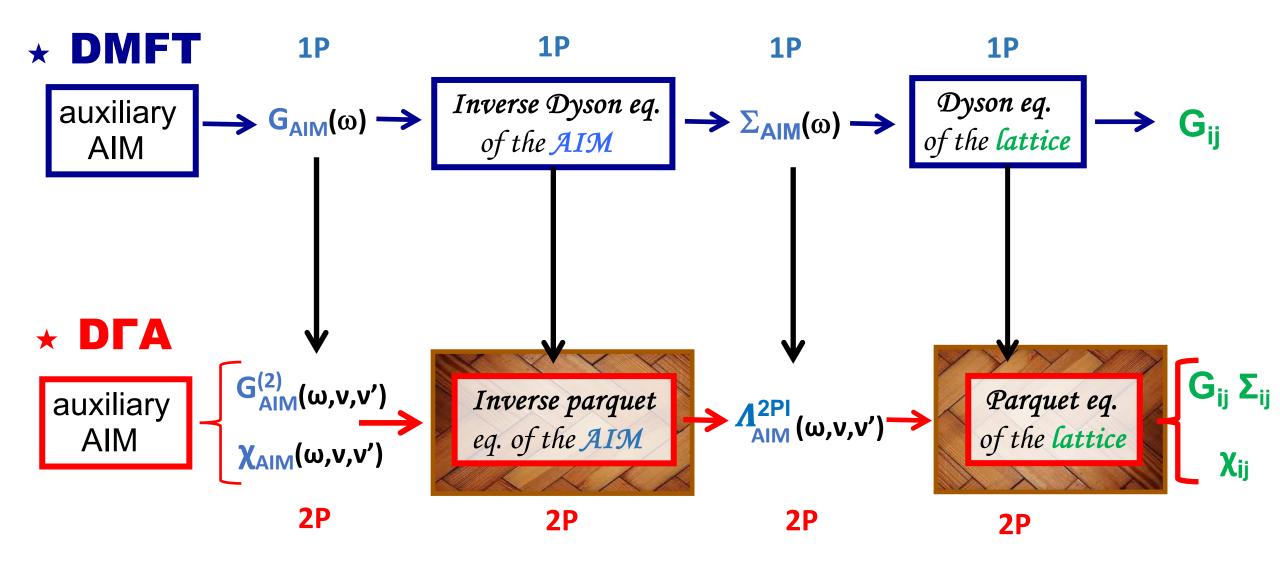
An inspiring example : DCA calculations of k-dependent vertex functions

... of increasing 2P-irreducibility

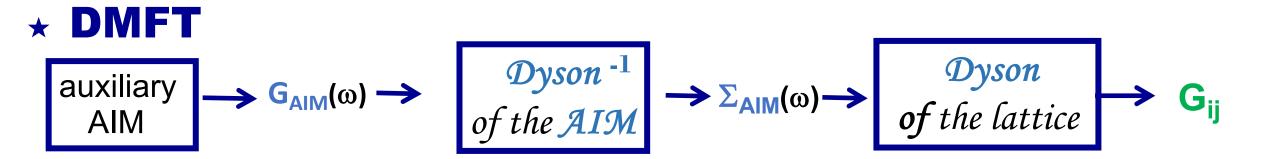


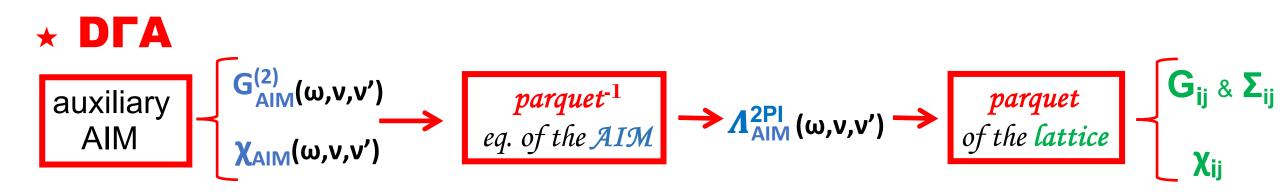
DCA, 2d-Hubbard model, **U**=4t, **n=0.85**, $v=v'=\pi/\beta$, $\omega=0$, s. Th. Maier et al., PRL (2006)

Flowchart of the (full fledged) DΓA algorithm

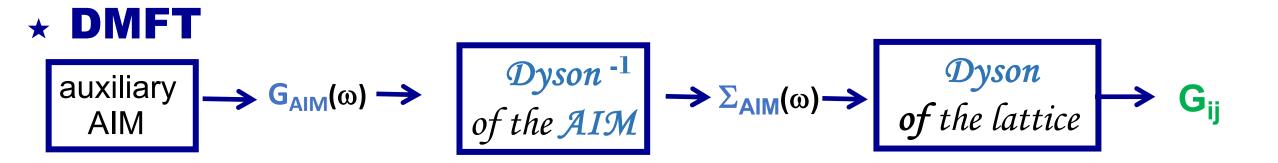


Flowchart of the (full fledged) DΓA algorithm

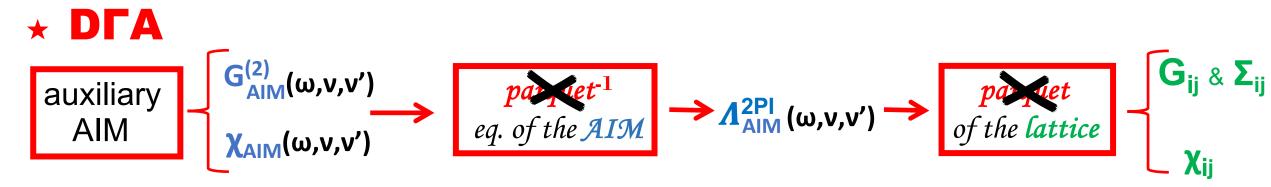




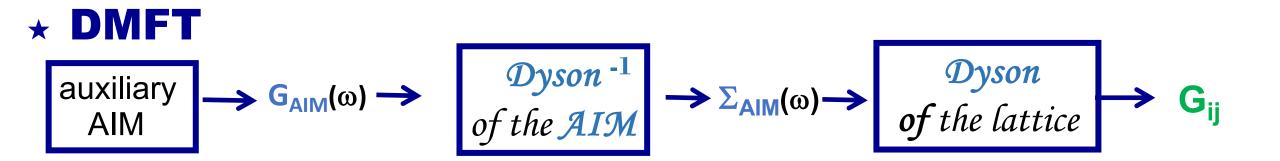
Flowchart of the full fledged DΓA algorithm

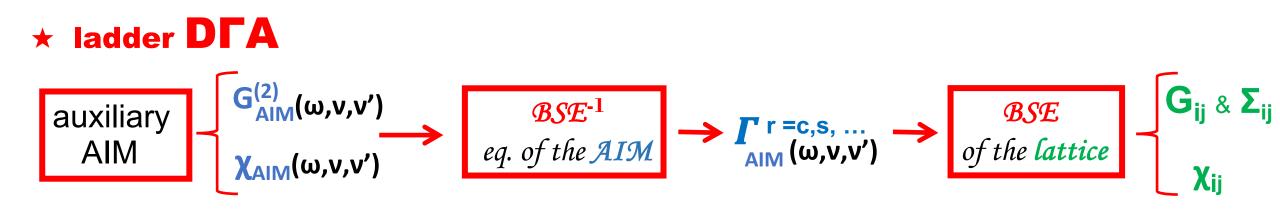


→ Possible simplification, if the nonlocal fluctuation of one channel dominate:

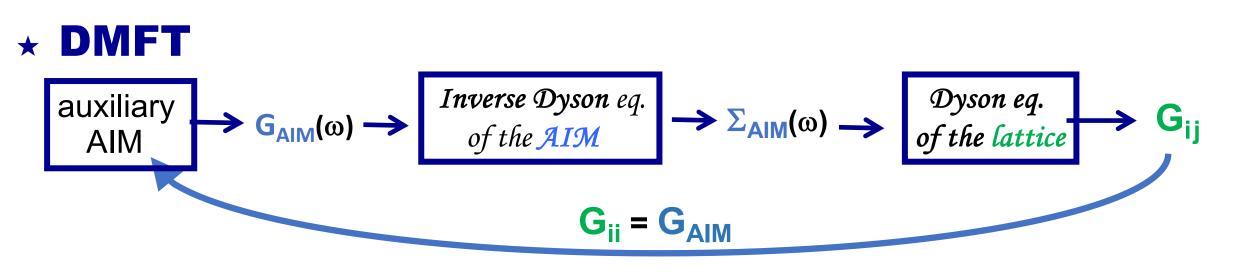


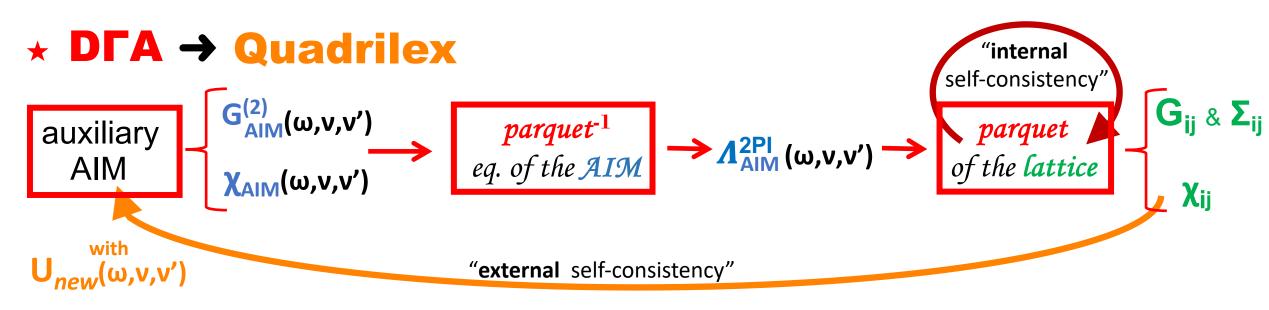
Possible simplification: the ladder DΓA algorithm





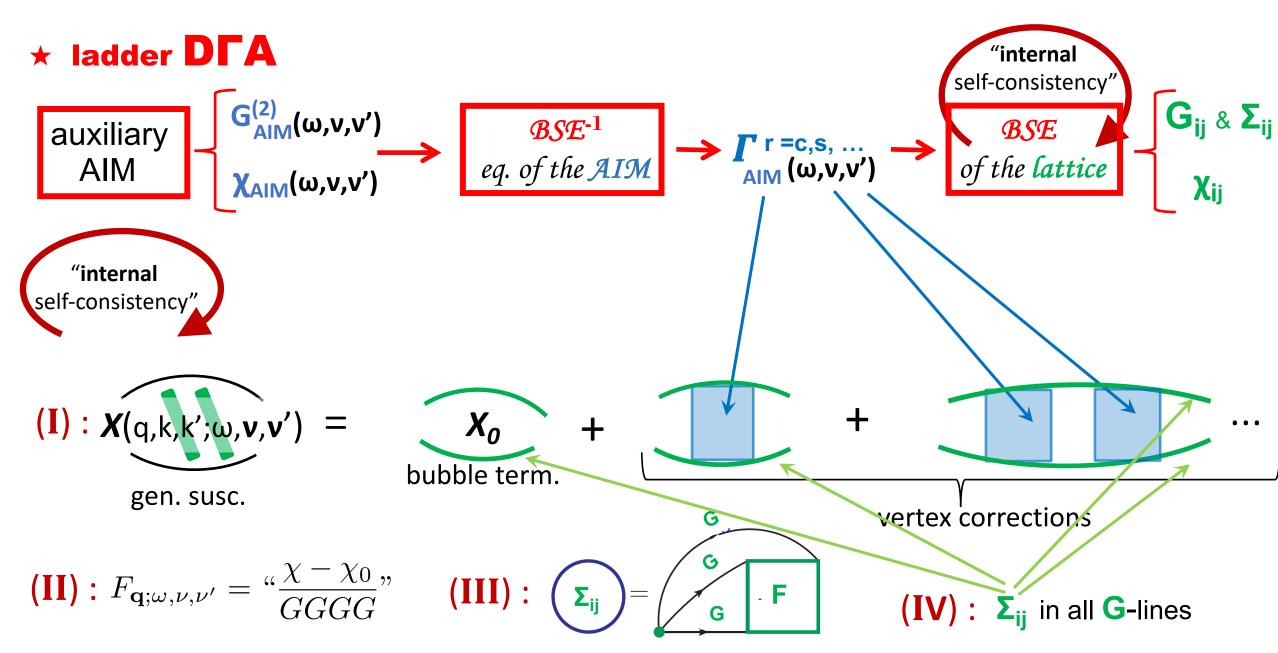
And ... what about self-consistency?



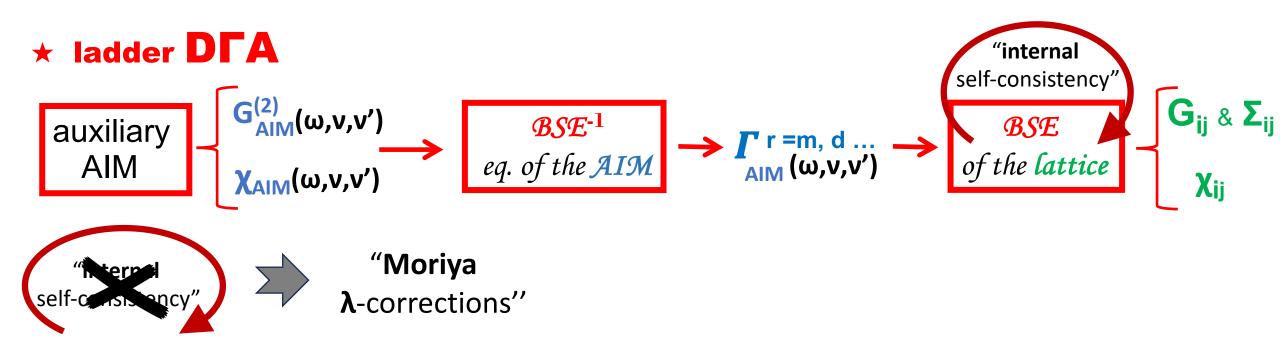


For the theory of the QUADRILEX approach, s. T. Ayral & O. Parcollet, PRB (2016)

Self-consistency of the ladder DFA algorithm



An approximation for the self-consistency: Moriya $D\Gamma A$ or `` λ - $D\Gamma A''$



A. Katanin et al, PRB (2009); G. Rohringer & AT, PRB (2016); J. Stobbe & G. Rohringer, PRB (2023)

Explicit expressions for the Moriya $D\Gamma A$ or `` λ - $D\Gamma A''$

(I):
$$\chi_{q,\omega}^{(\mathbf{q},\omega)} = \chi_{0}^{(\mathbf{q},\omega)} + \chi_{AIM}^{(\mathbf{r},\omega)} + \Gamma_{AIM}^{(\mathbf{r},\omega)} + \Gamma_{AIM}^{(\mathbf{r},\omega)} \cdots$$
bubble term.
in channel r (eg. m, d)
(II):
$$\chi_{r=m,d,\cdots}^{\lambda}(\mathbf{q},\omega) = \left([\chi_{r}(\mathbf{q},\omega)]^{-1} + \chi_{r}^{(\mathbf{r},\omega)} \right)^{-1} + \chi_{r}^{(\mathbf{r},\omega)} + \chi_{mass''}^{(\mathbf{r},\omega)} + \chi_{m,q}^{(\mathbf{r},\omega)} \right) = \frac{n}{2} \left(1 - \frac{n}{2} \right),$$
term correction
(III):
$$\Sigma_{\mathbf{k}}^{\lambda,\nu} = \frac{Un}{2} - U \sum_{\omega \mathbf{q}} \left[1 + \frac{1}{2} \gamma_{d,\mathbf{q}}^{\nu\omega} (1 - U \chi_{d,\mathbf{q}}^{\lambda,\omega}) - \frac{3}{2} \gamma_{m,\mathbf{q}}^{\nu\omega} (1 + U \chi_{m,\mathbf{q}}^{\lambda,m,\omega}) - \sum_{\nu'} \chi_{0,\mathbf{q}}^{\nu'\omega} F_{\mathbf{m}}^{\nu\nu'\omega} \right] G_{\mathbf{k}+\mathbf{q}}^{\nu+\omega},$$

with $\gamma_{r,\mathbf{q}}^{\nu\omega} = \sum_{\nu'} \left(\chi_{0,\mathbf{q}}^{\nu\nu'\omega} \left(1 \pm U \chi_{r,\mathbf{q}}^{\omega} \right) \right)^{-1} \chi_{r,\mathbf{q}}^{\nu\nu'\omega}$ and $\chi_{0,\mathbf{q}}^{\nu\nu'\omega} = -\beta \delta_{\nu\nu'} \sum_{\mathbf{k}} G_{\mathbf{k}}^{\nu} G_{\mathbf{k}+\mathbf{q}}^{\nu+\omega}$, for further details, s. J. Stobbe & G. Rohringer, PRB (2023).

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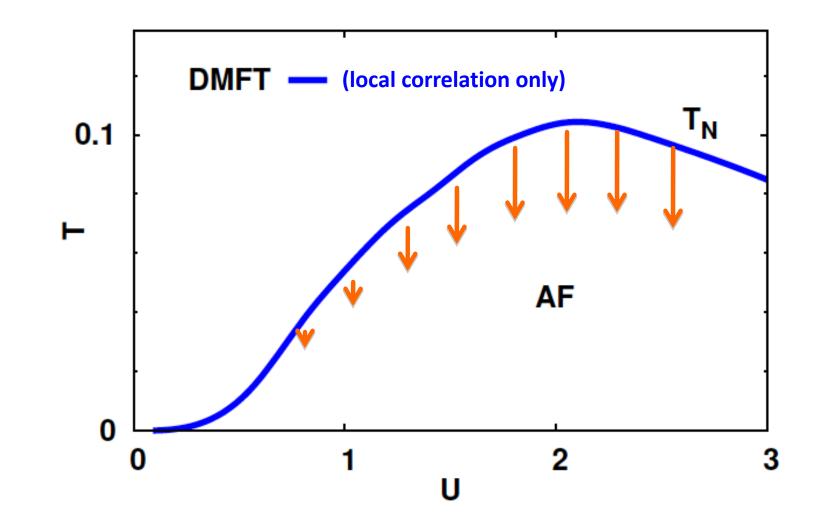
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DΓA (=beyond DMFT) results in 3 dimensions

ν phase diagram computed by λ -DΓA:

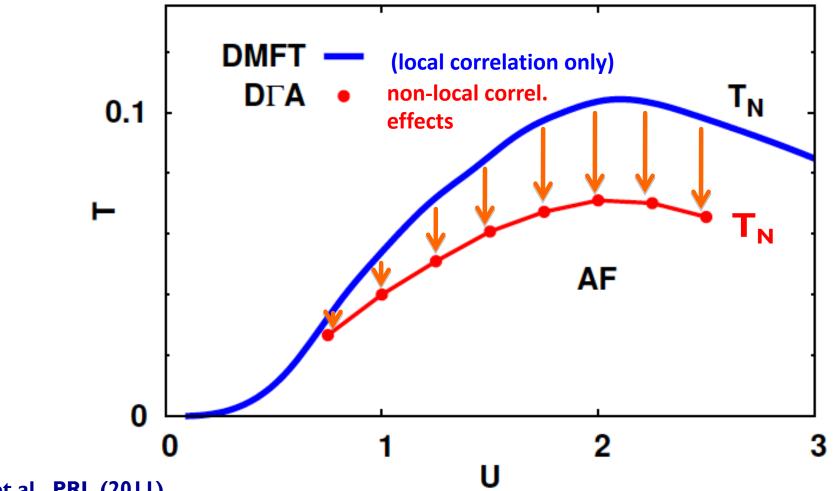
single band **Hubbard model** with nearest neibouring hopping in **d=3** (@ half-filling), in unit of $t = \frac{2}{\sqrt{6}}$



λ -D Γ A results in **3** dimensions

✓ phase diagram: one-band Hubbard model in d=3 (half-filling)

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

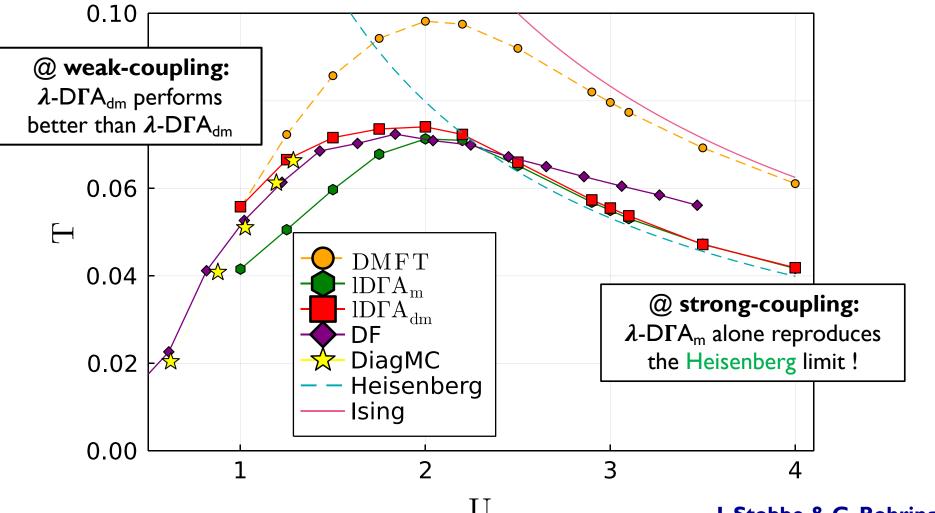


G. Rohringer, AT, et al., PRL (2011)

DFA results in 3 dimensions: a quantitative comparison

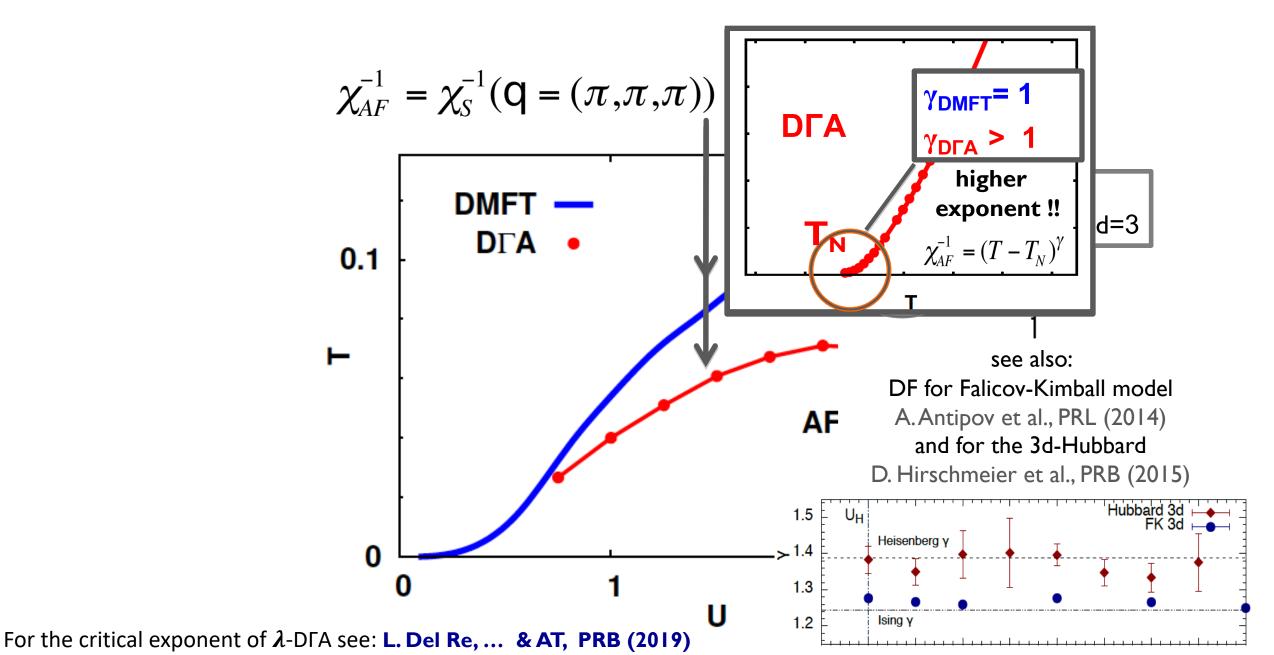
phase diagram computed by λ-DΓA:

single band **Hubbard model** with nearest neibouring hopping in **d=3** (@ half-filling)

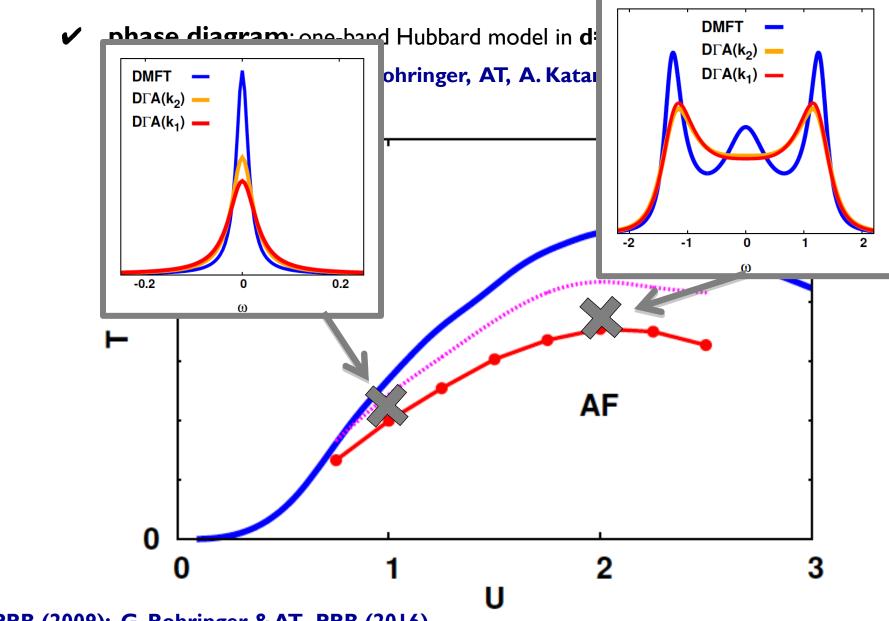


J. Stobbe & G. Rohringer, PRB (2023)

λ -DFA results: the **critical** region

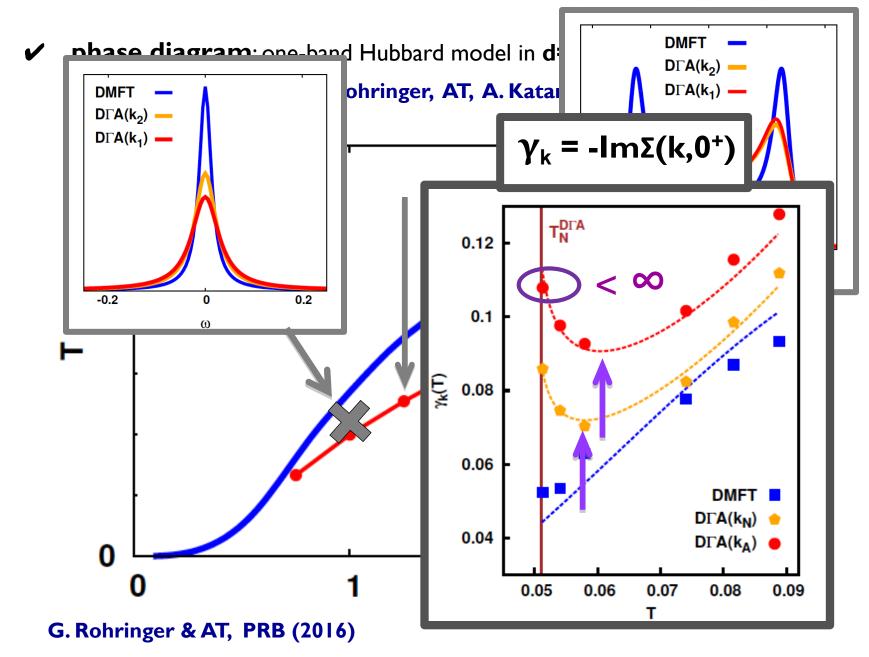


λ -DFA results in 3 dimensions: the spectral properties

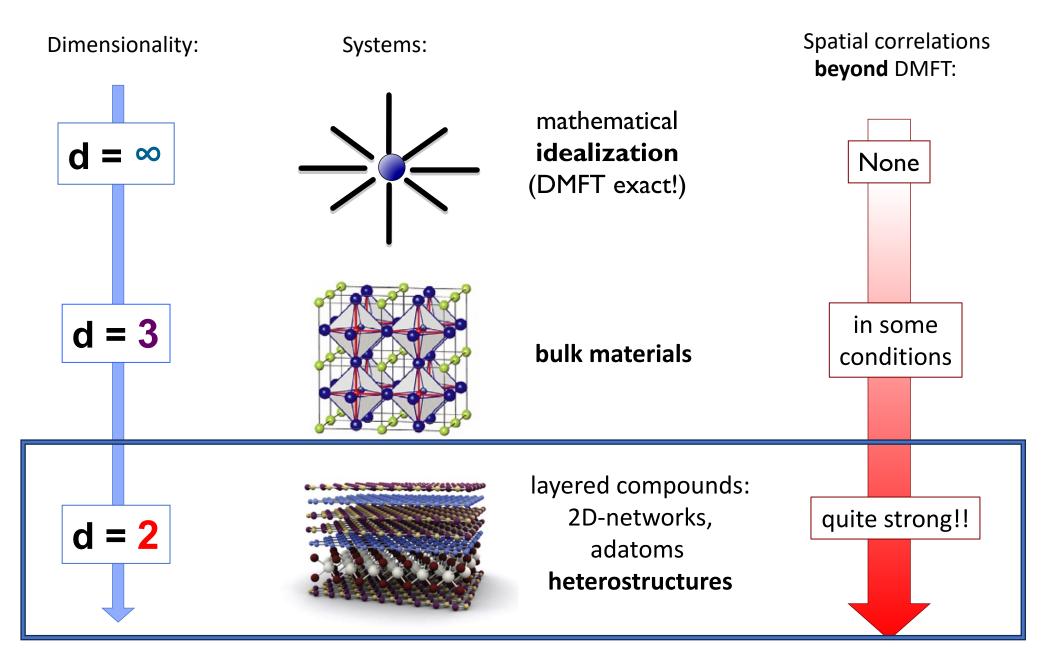


A. Katanin et al, PRB (2009); G. Rohringer & AT, PRB (2016)

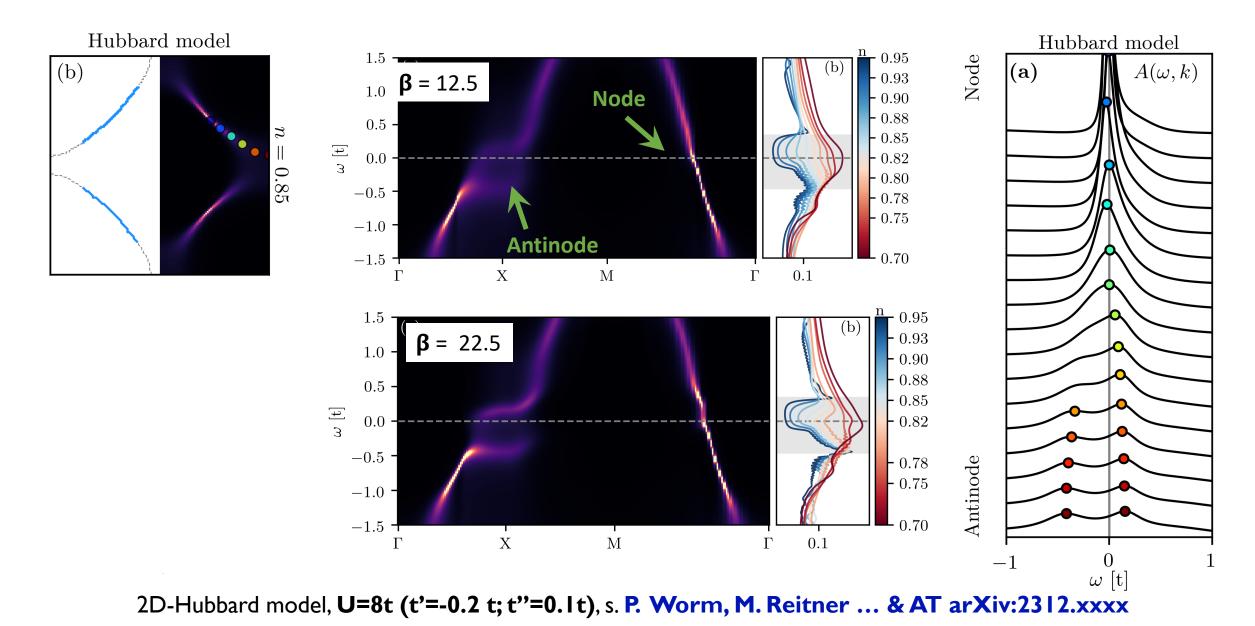
λ -DFA results in **3** dimensions: the spectral properties

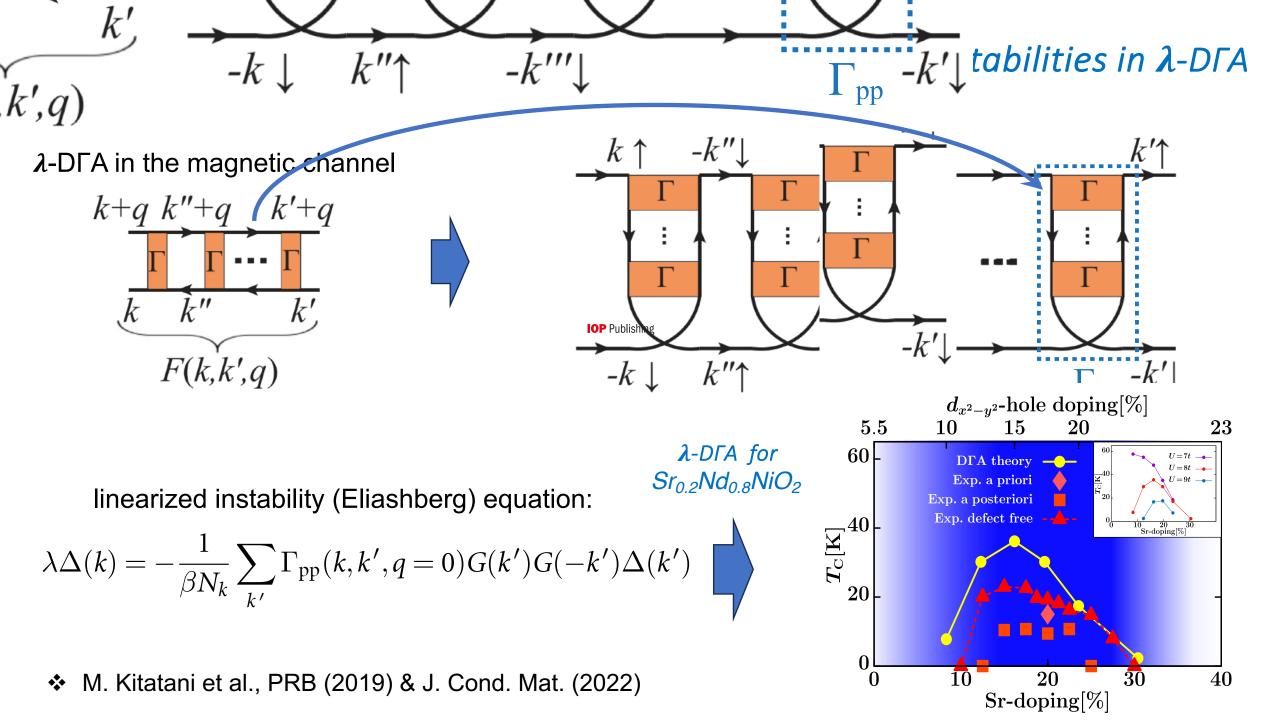


From ∞ dimensions to ... "reality" !

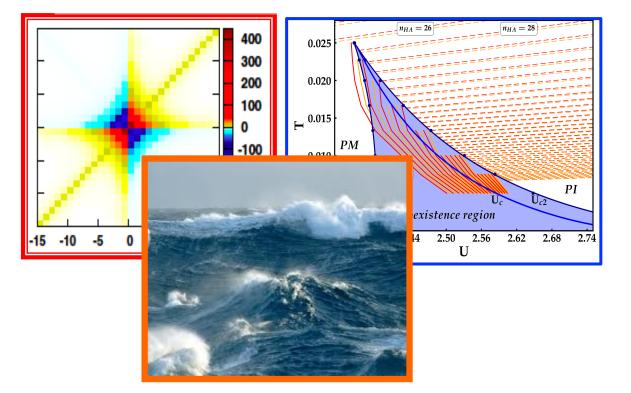


"There is life" ... out of half-filling: λ *-DFA study of the* pseudogap in 2D





A (diverging) elephant in the room (of D ΓA)? $\Gamma^r = \infty$



Should be $D\Gamma A$ called rather ... `` $D \sim A''$?

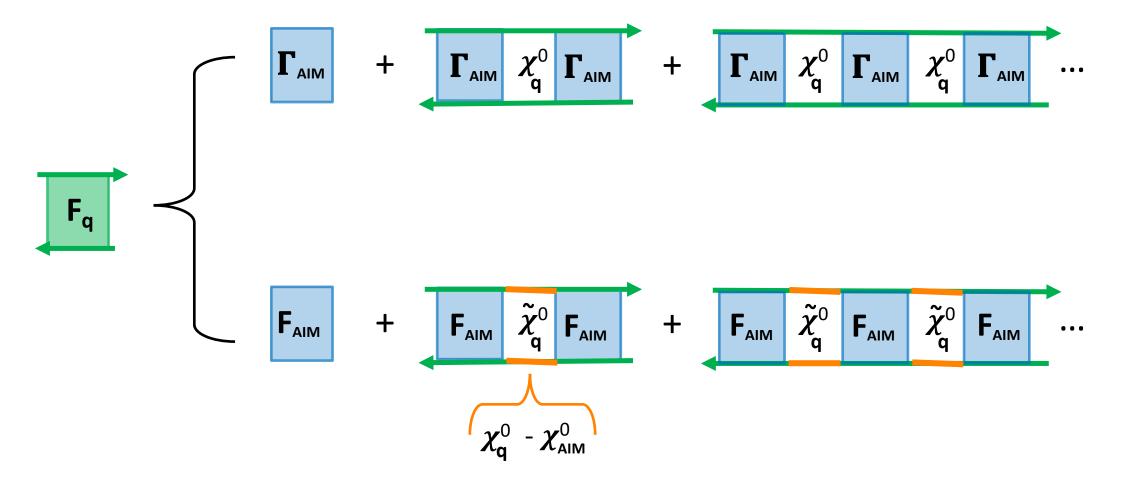
[credit: G. Sangiovanni, 2013]

No, luckly this elephant... is **not** a dangerous one:



Working with 2PI vertices : The (non-problematic) ladder case

By exploiting the following identity the ladder diagrams of DΓA can be **exactly** rewritten ...



... eliminating any explicit appearance of the (possibly dangerous) $\Gamma_{\scriptscriptstyle{
m AIM}}$!

G. Rohringer, AT, et al., PRB (2013); G. Rohringer et al., RMP (2018)

And, remarkably, this works even at the parquet-DFA level !!

✓ Important progress achieved by Jae-Mo Lihm, Seung-Sup Lee, F. Kugler & D. Kiese

(no spoiler here: preprint in preparation)

Conclusions:

