REAL-FREQUENCY QUANTUM FIELD THEORY APPLIED TO THE SINGLE-IMPURITY ANDERSON MODEL

LMU LUDWIG-MAXIMILIANS-UNIVERSITÄT MÜNCHEN

main paper
PRB (2024)

code publication
JCP (2024)


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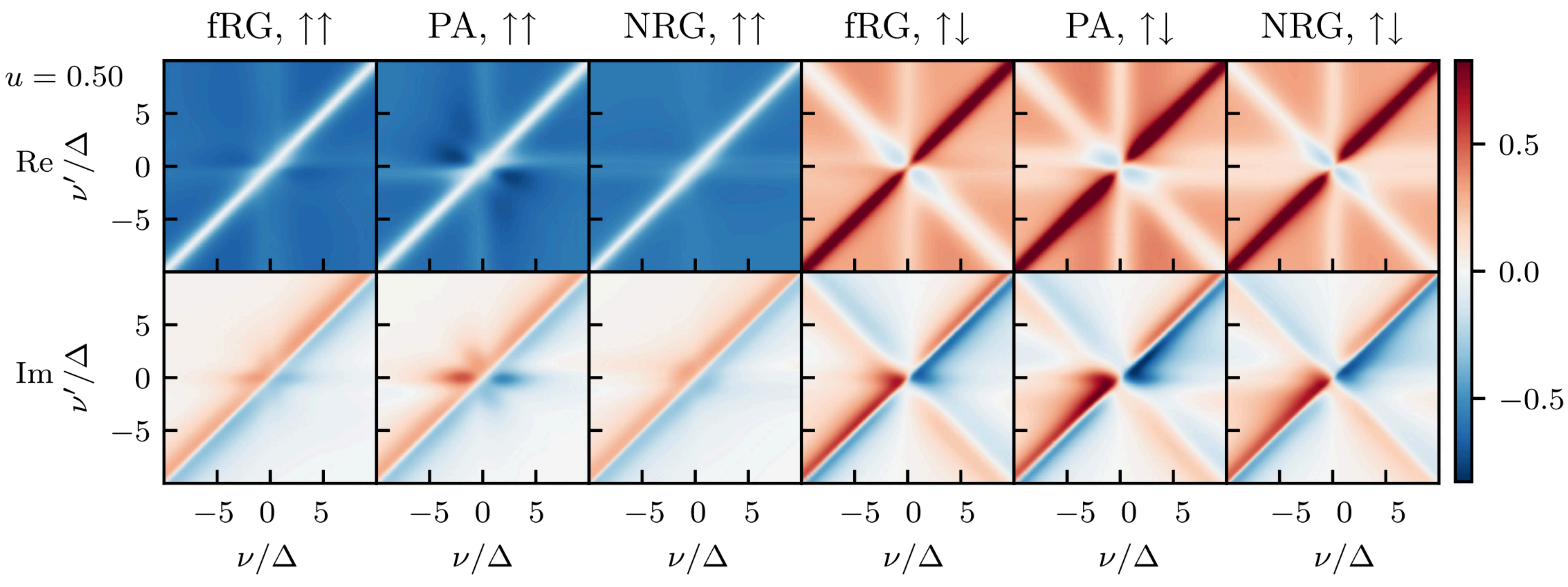
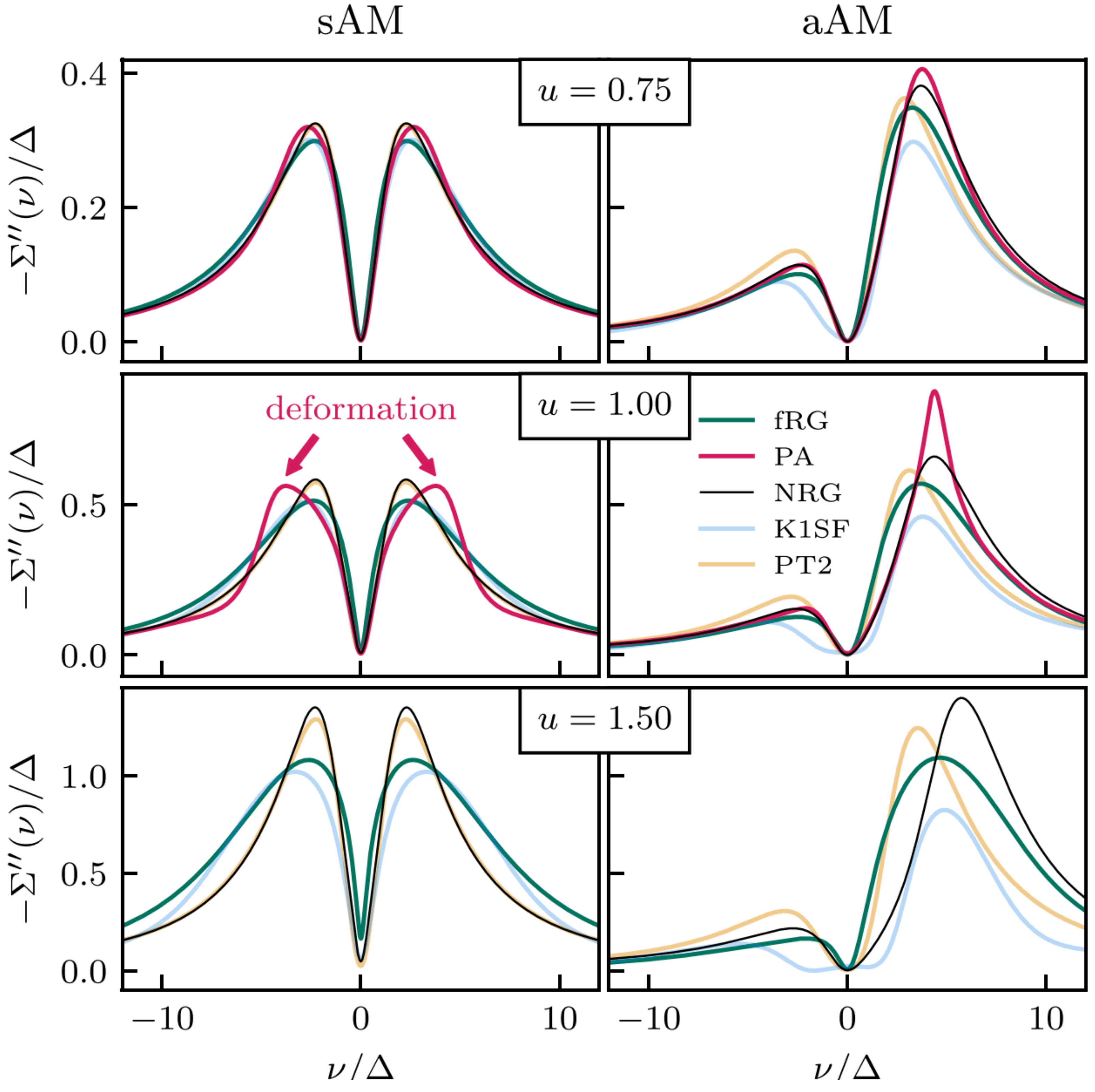
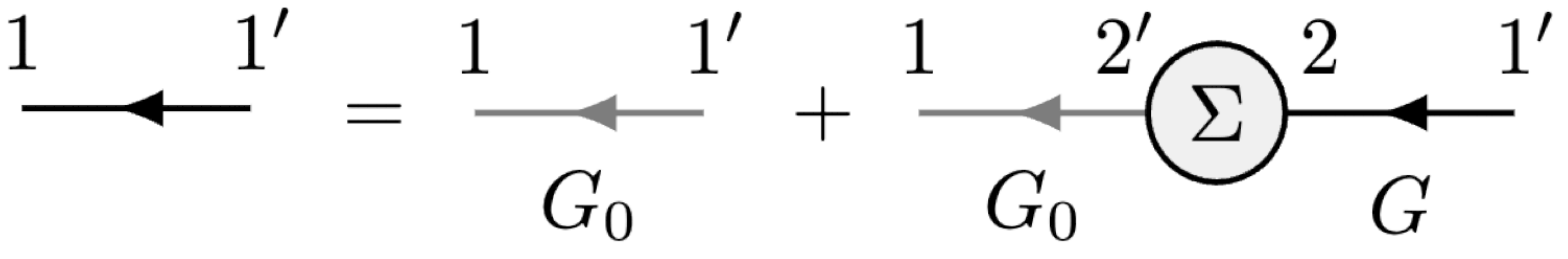


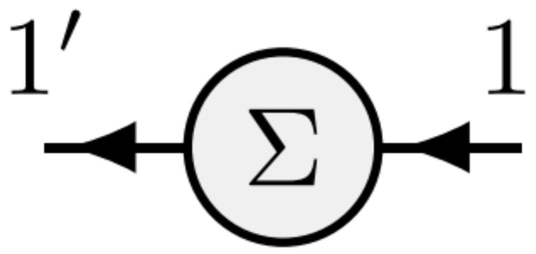


MCQST
Munich Quantum Valley
CeNS Center for NanoScience | LMU
MUNICH QUANTUM CENTER
Studienstiftung des deutschen Volkes
DFG
FLATIRON INSTITUTE
RUTGERS
Alexander von HUMBOLDT STIFTUNG

$G_{1|1'} =$

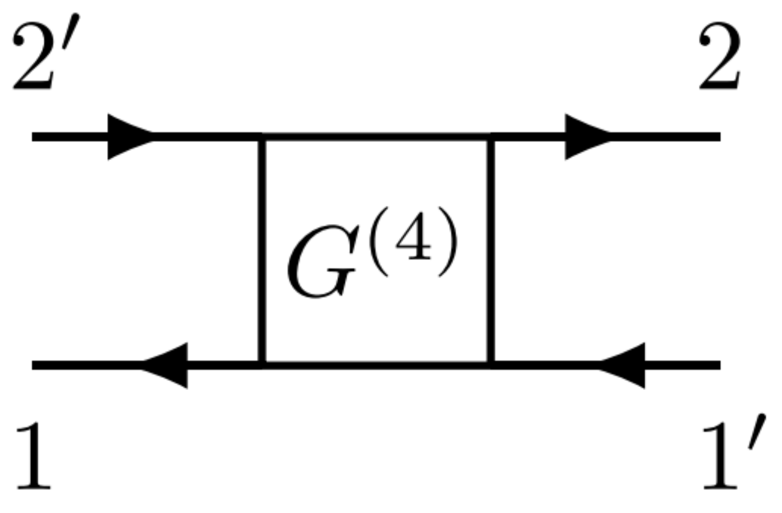


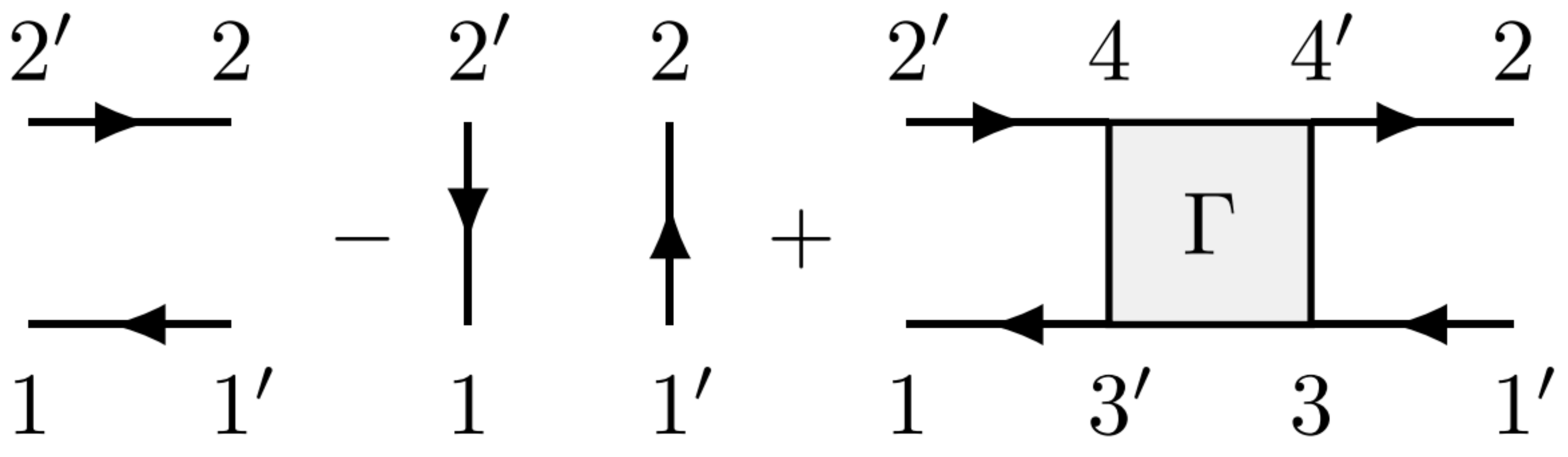
$\Sigma_{1'|1} =$



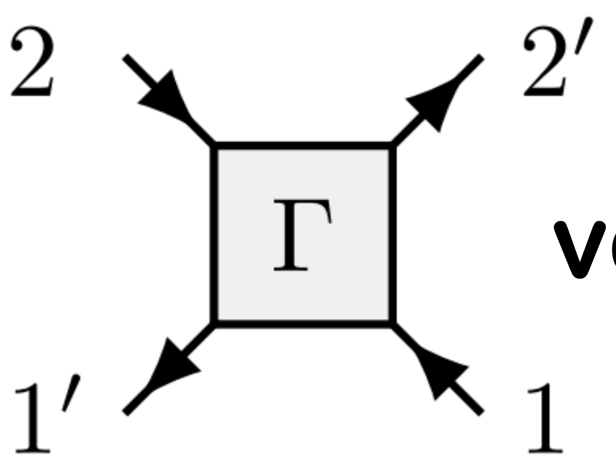
self-energy

$G^{(4)}_{12|1'2'} =$





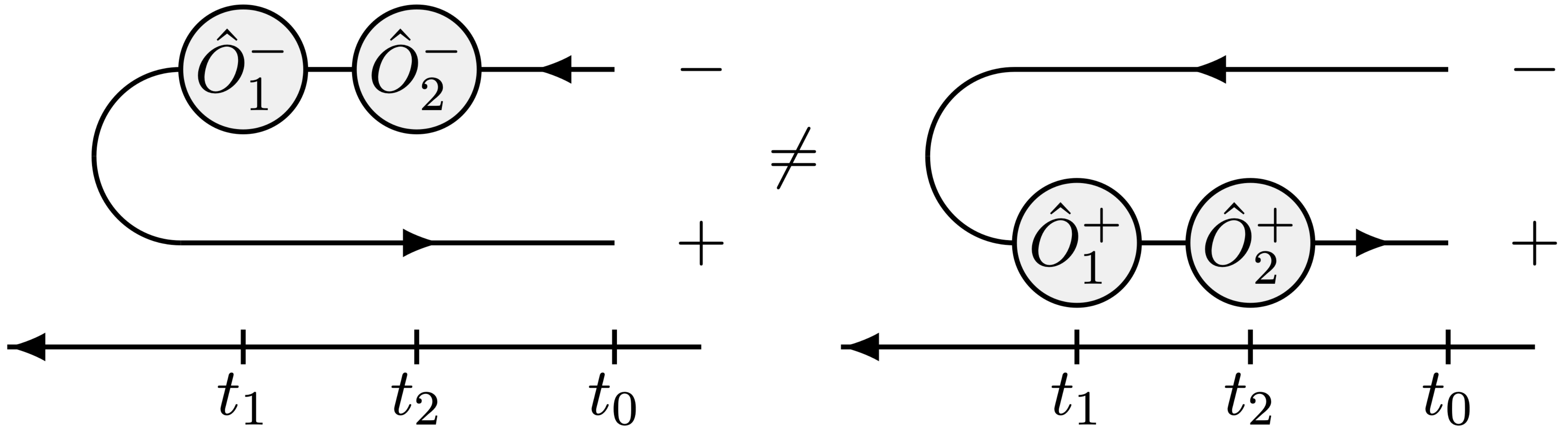
$\Gamma_{1'2'|12} =$



vertex

16 Keldysh components!

3 frequency arguments!



contour index!

$$G^{c|c'}(t\,|\,t') = -i\langle \mathcal{T}_{\mathscr{C}}\, \psi^{c}(t)\psi^{\dagger c'}(t')\rangle = \begin{pmatrix} G^{\mathcal{T}} & G^{<} \\ G^{>} & G^{\tilde{\mathcal{T}}} \end{pmatrix}$$

Thermal equilibrium:

$$G(t_1\,|\,t_2) = G(t_1 - t_2) \quad \rightarrow \quad G(\nu) = \int \mathrm{d}t\, e^{i\nu t}\, G(t)$$

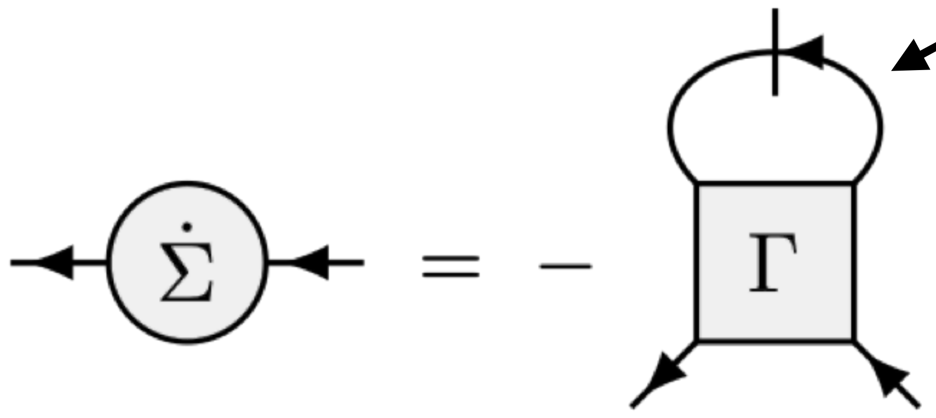
continuous, real frequency

$$G^{K}(\nu) = 2i \tanh\left(\frac{\nu}{2T}\right) \mathrm{Im}\, G^{R}(\nu)$$

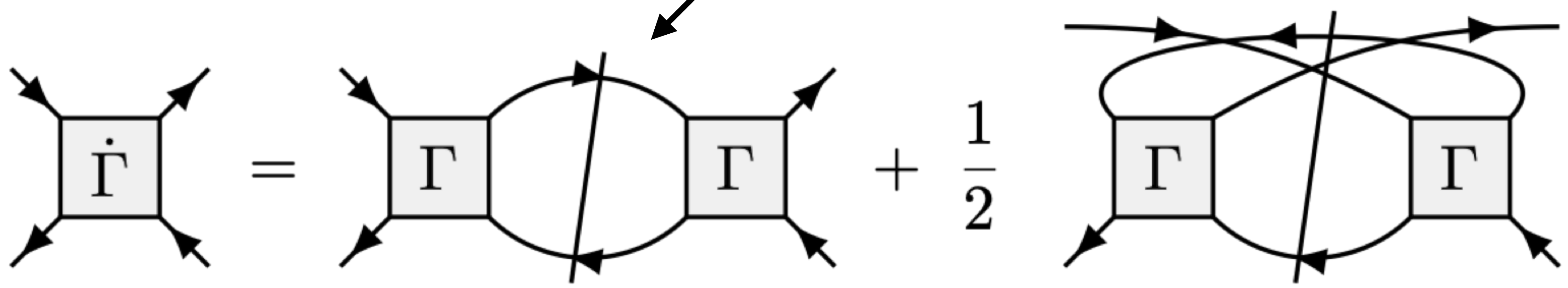
Fluctuation-Dissipation Relation

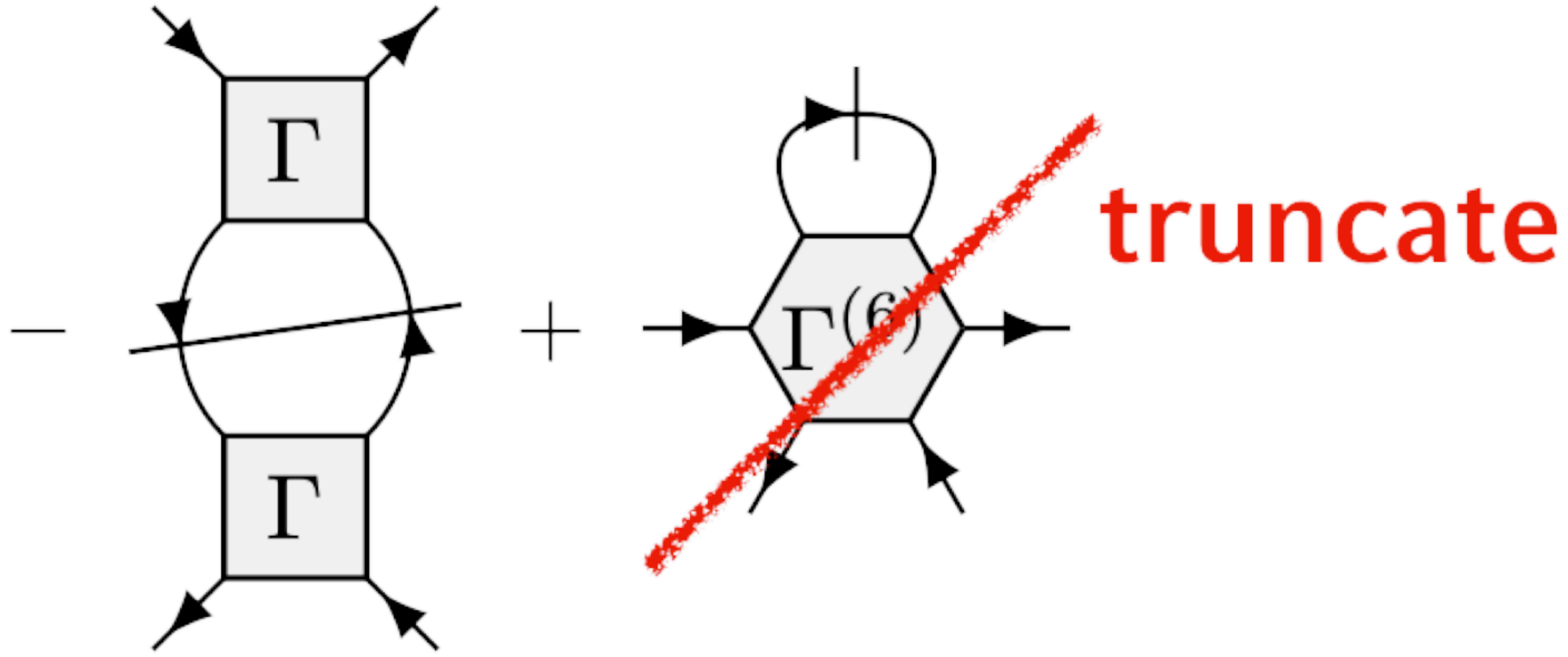
fRG

$S^R(\nu) = \partial_\Delta G^R(\nu)\Big|_{\Sigma=\text{const.}}$



$\dot{\Pi} = \dot{G}G + G\dot{G}$ **(Katanin)**





fRG flow:

$G_0 \to G_0^\Lambda, \quad \Lambda_{\text{initial}} \to \Lambda_{\text{final}}$ **Here:** $\Lambda = \Delta$ **(hybridization)**

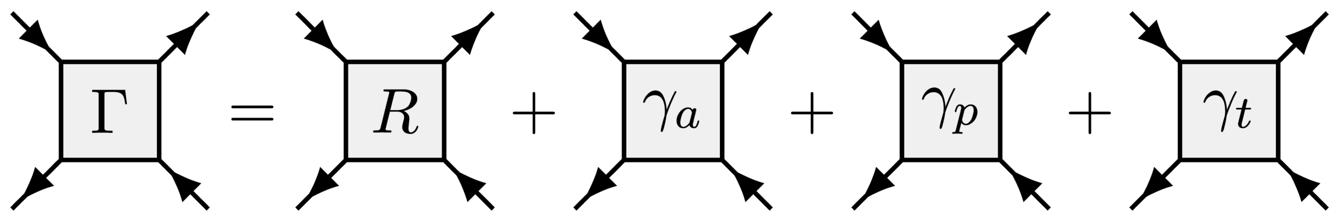
$\Gamma\Big|_{\Delta=\infty} = \Gamma_0, \qquad \Sigma^R\Big|_{\Delta=\infty} = \Sigma_{\mathrm{H}} = U\langle n_\sigma \rangle$

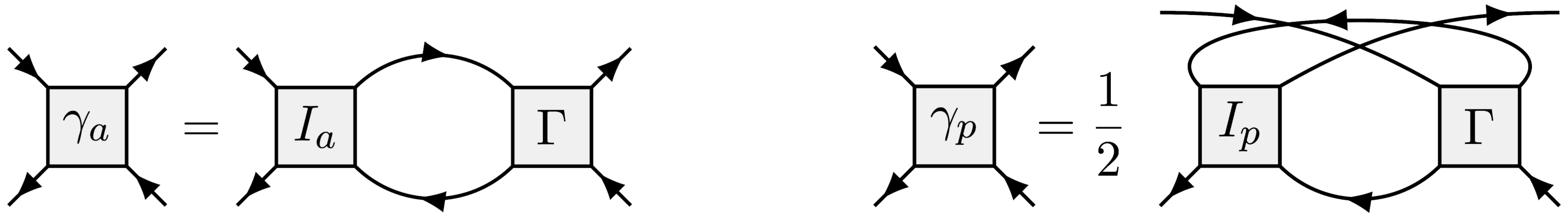
Use a solver with adaptive step-size control!

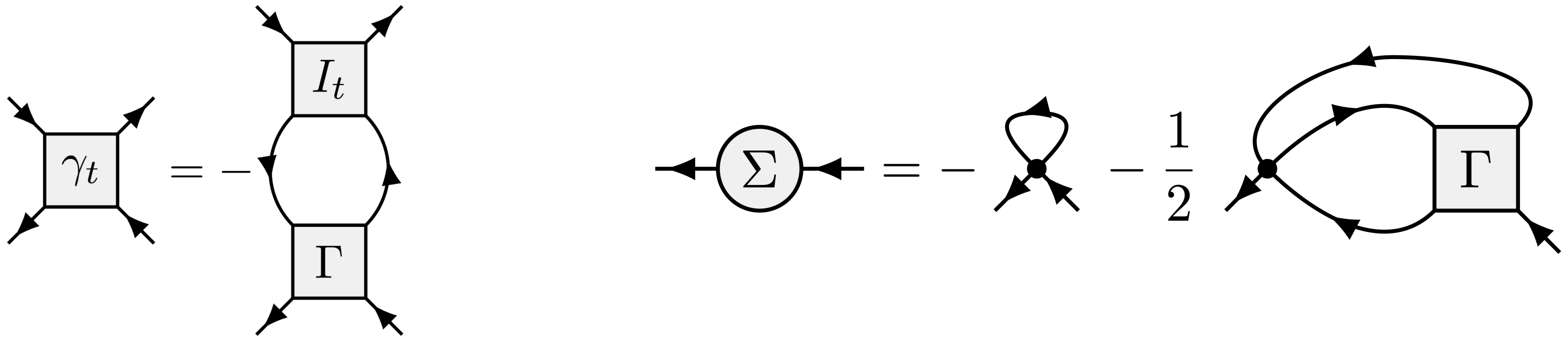
Here: Cash-Karp method with $\epsilon_{\text{rel}} = 10^{-6}$

e.g. Metzner et al., RMP (2012)

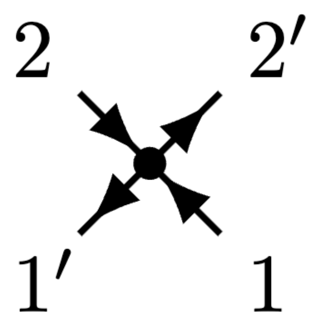
Parquet formalism







Parquet approximation: $R = \Gamma_0 + \mathcal{O}[(\Gamma_0)^4] \approx \Gamma_0 =$



Fixed-point equation: $\Psi = f_{\text{PA}}(\Psi) \qquad \Psi = (\Sigma, \Gamma)$

stabilize with partial update: $\Psi \leftarrow (1-m)\cdot\Psi + m\cdot f_{\text{PA}}(\Psi)$

$0 < m \leq 1$

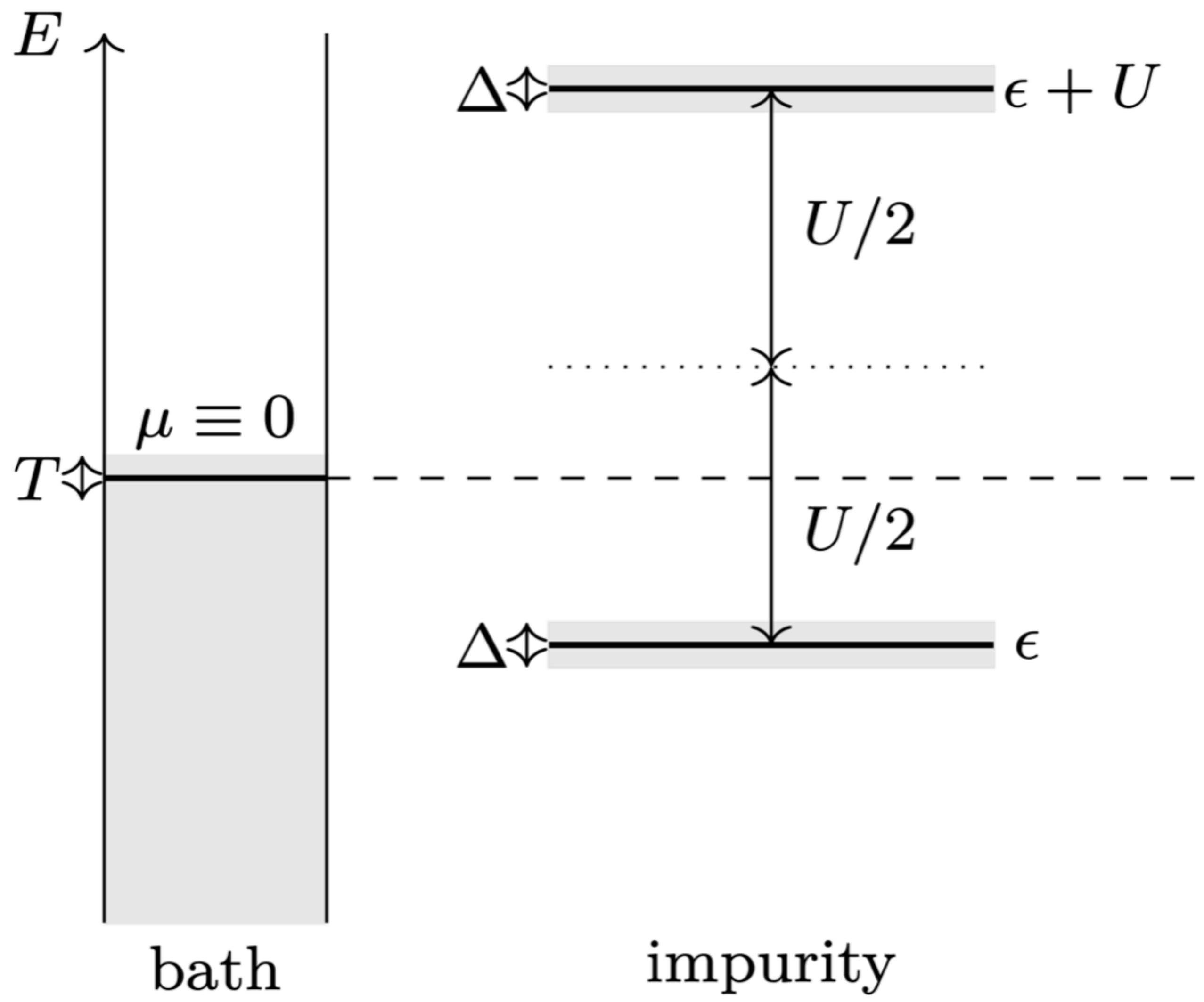
faster convergence using Anderson acceleration

e.g. Bickers (2004)

Connection: Multiloop fRG
Kugler, von Delft (2017-2019)


Single-impurity Anderson model

$$H = \underbrace{\sum_{k,\sigma} \epsilon(k)\, c^\dagger_{k,\sigma} c_{k,\sigma}}_{H_\text{bath}} + \underbrace{\sum_{\sigma} \epsilon_\sigma\, d^\dagger_\sigma d_\sigma + U\, d^\dagger_\uparrow d_\uparrow d^\dagger_\downarrow d_\downarrow}_{H_\text{imp}} + \underbrace{t \sum_{k,\sigma} \left(d^\dagger_\sigma c_{k,\sigma} + \text{h.c.} \right)}_{H_\text{hyb}}$$



Anderson, PR (1961)

$$G^R_\text{H} = \frac{1}{\nu - \epsilon_d + i\Delta - \Sigma_\text{H}} = \frac{1}{\nu + i\Delta}$$

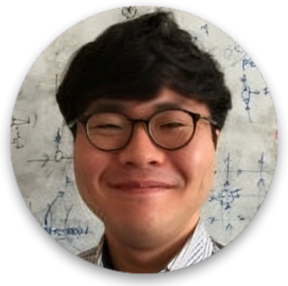
$\epsilon_d \in \{-U/2,\, 0\}$

particle-hole symmetry

temperature: $T/U = 0.01$

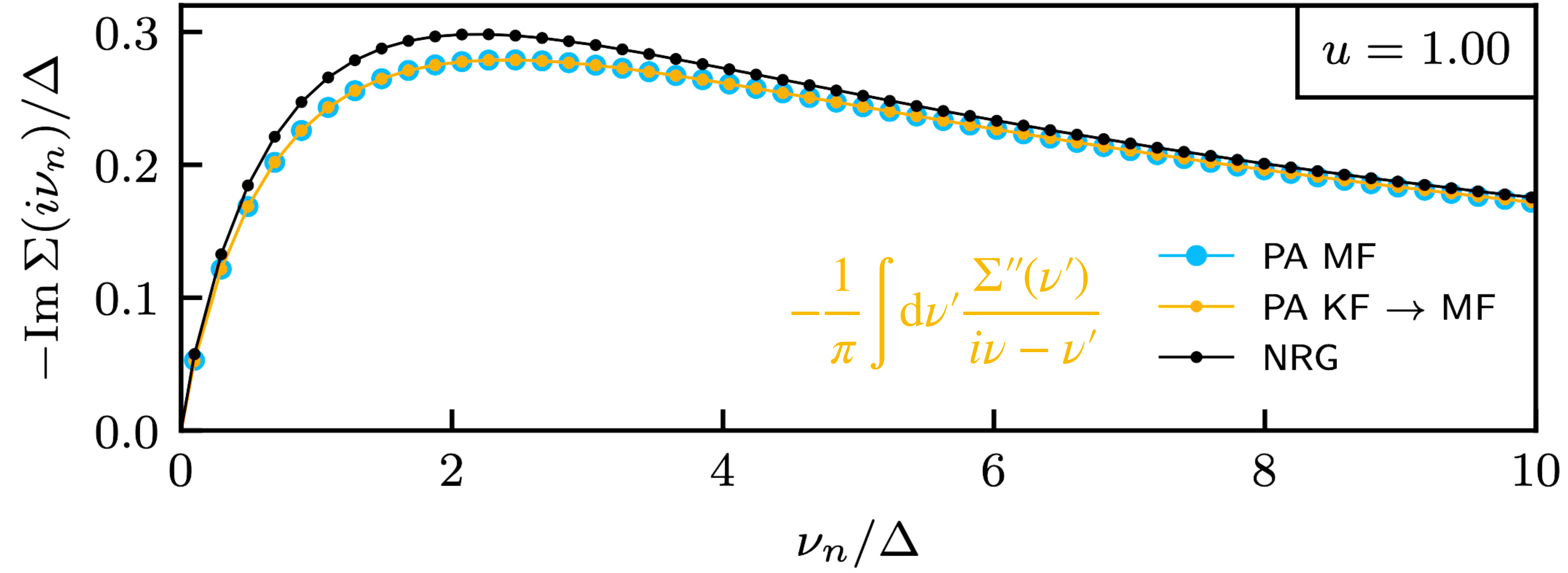
dimensionless interaction strength: $u = U/(\pi\Delta)$

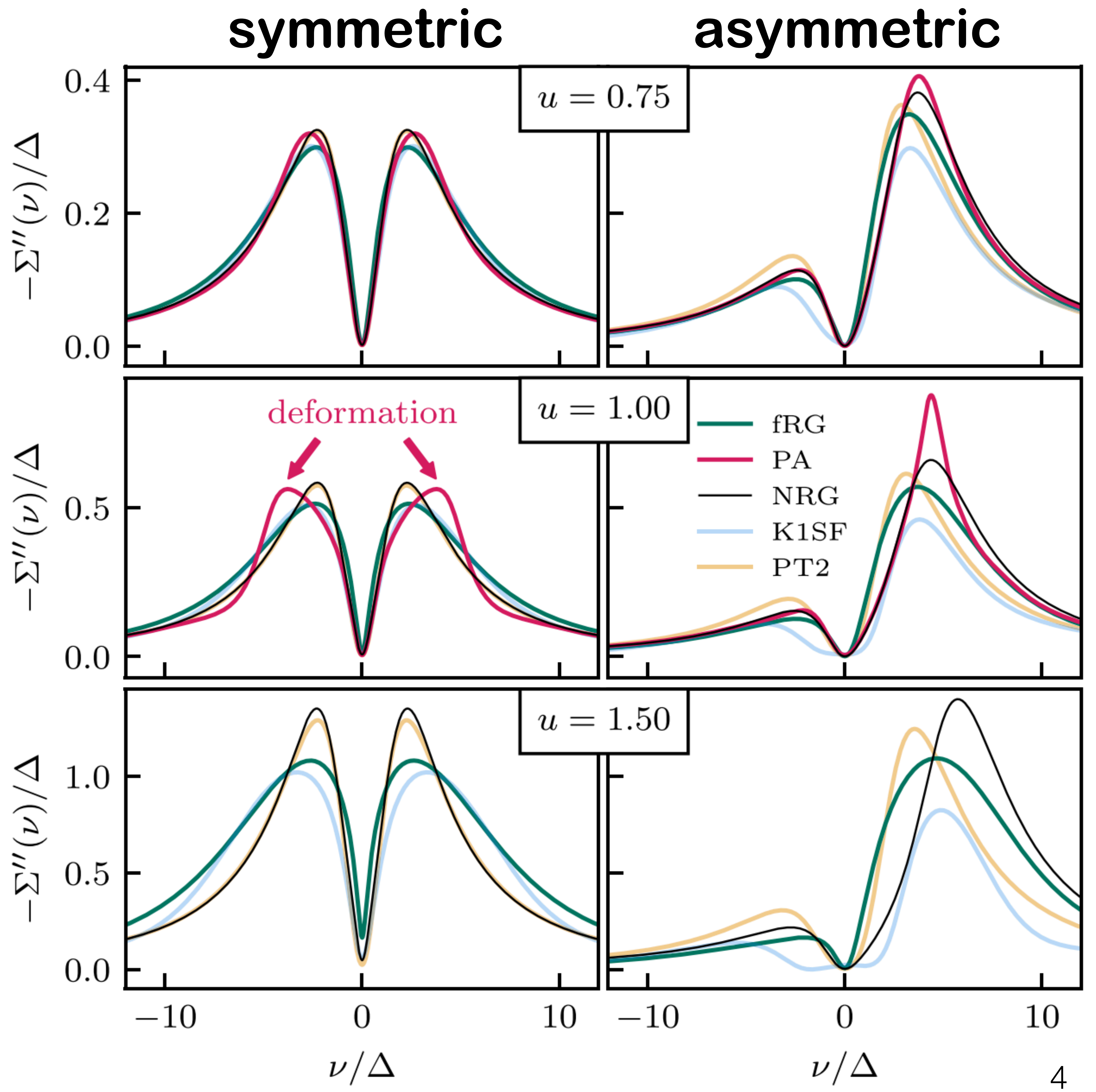
Benchmark: NRG by S.B. Lee and A. Weichselbaum



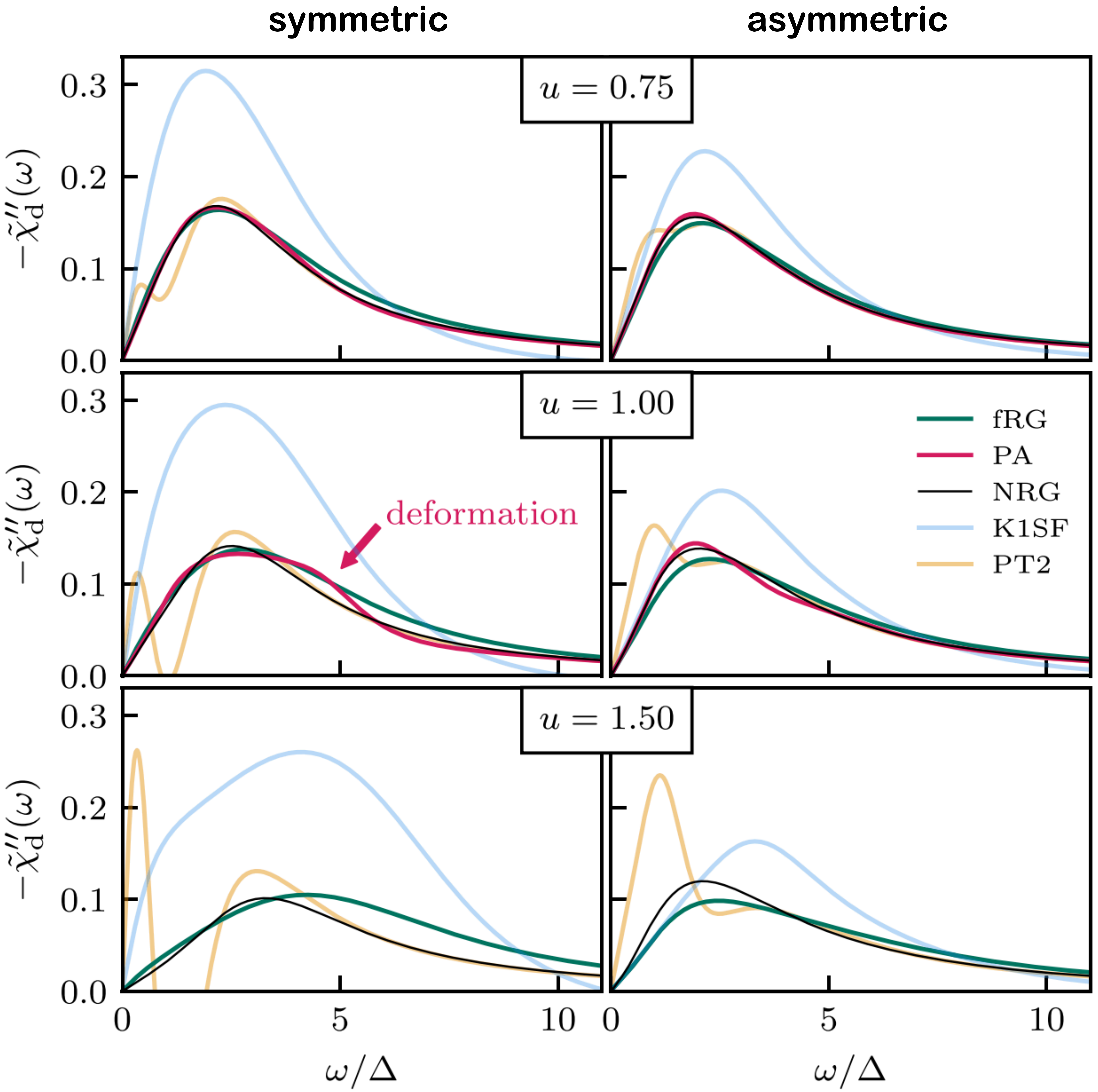
K1SF: Previous state-of-the-art by S. Jakobs, V. Meden, H. Schoeller

$\gamma(\omega, \nu, \nu') \approx \gamma(\omega)$
→ only "static feedback" from other channels

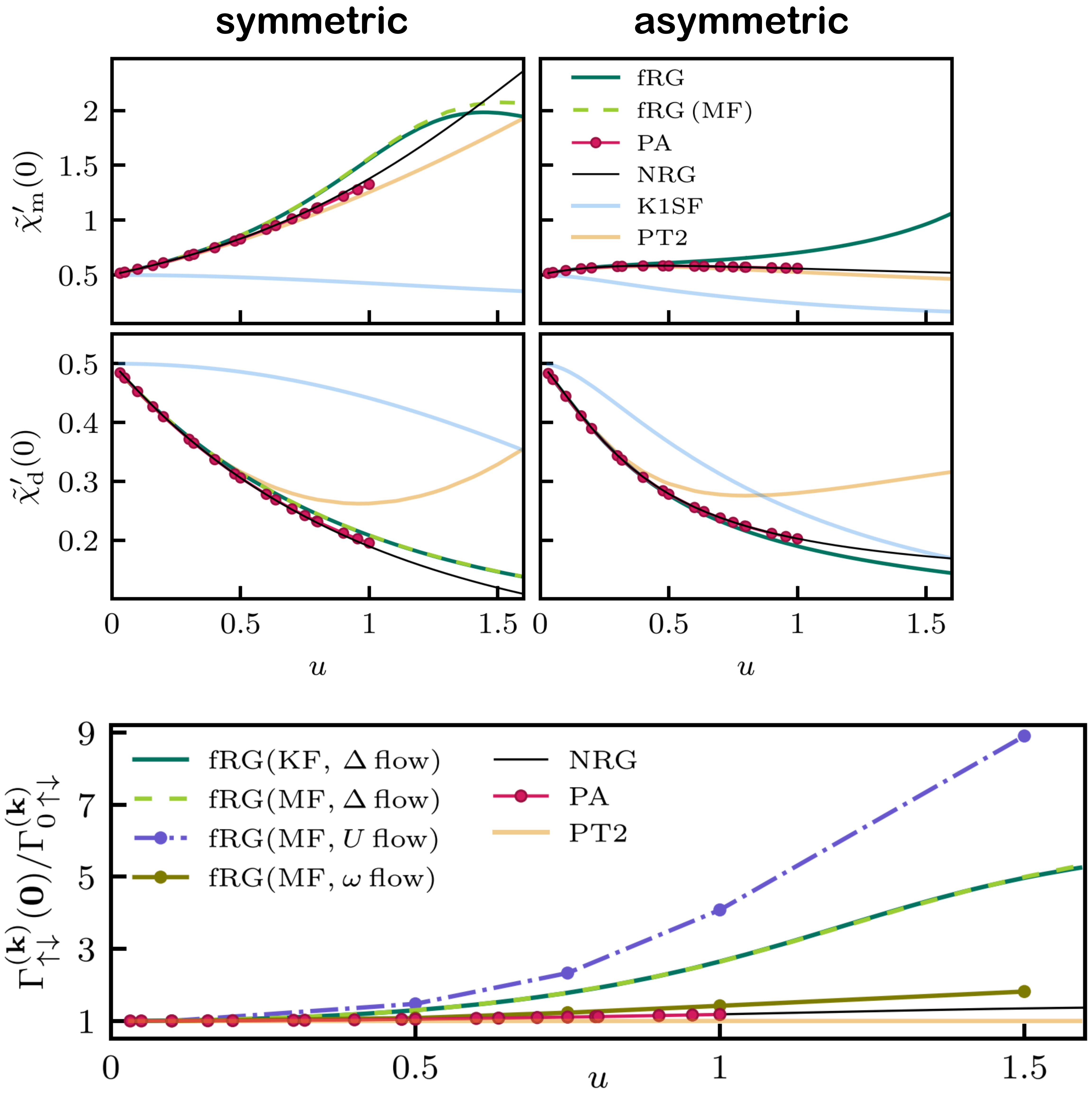




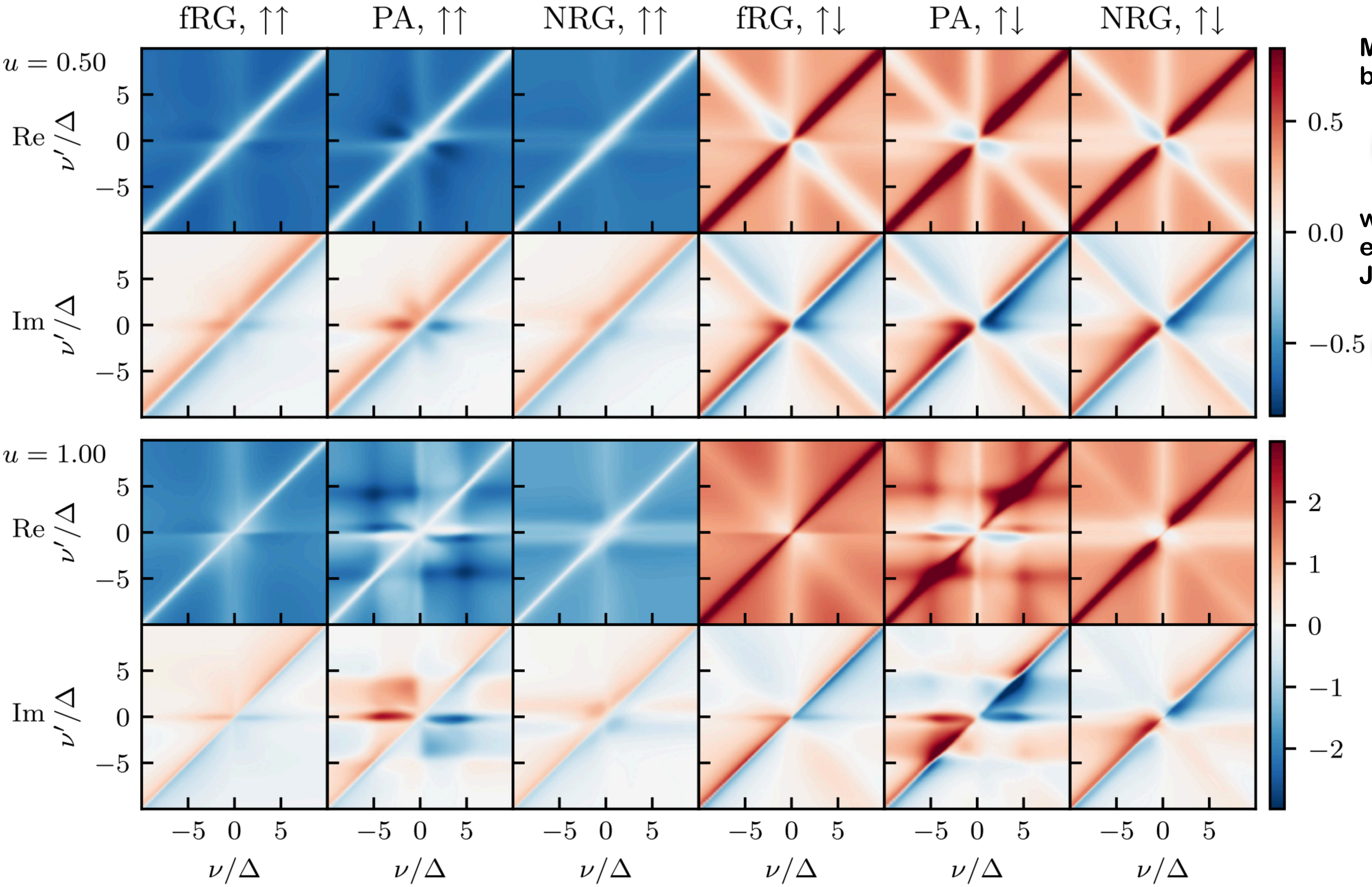
Dynamical density susceptibility



Static quantities



Strong regulator dependence in (one-loop) fRG!



Multipoint NRG
by J. Shim, S.B. Lee

with symmetric estimators by J. Lihm, J. Halbinger

Numerical complexity
& computational resources

$\sim \mathcal{O}(N_\nu^3)$ — memory & CPU

up to 125 $\Rightarrow \approx$ 2 million frequency points

PA @ $u = 1$: 25k CPU h (single data point!)

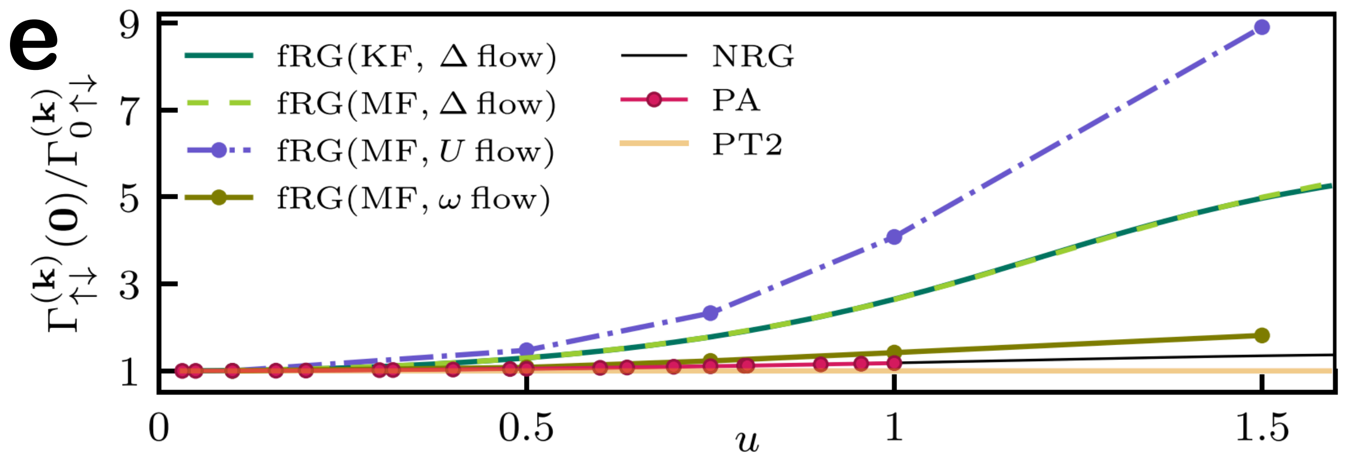
fRG more economical

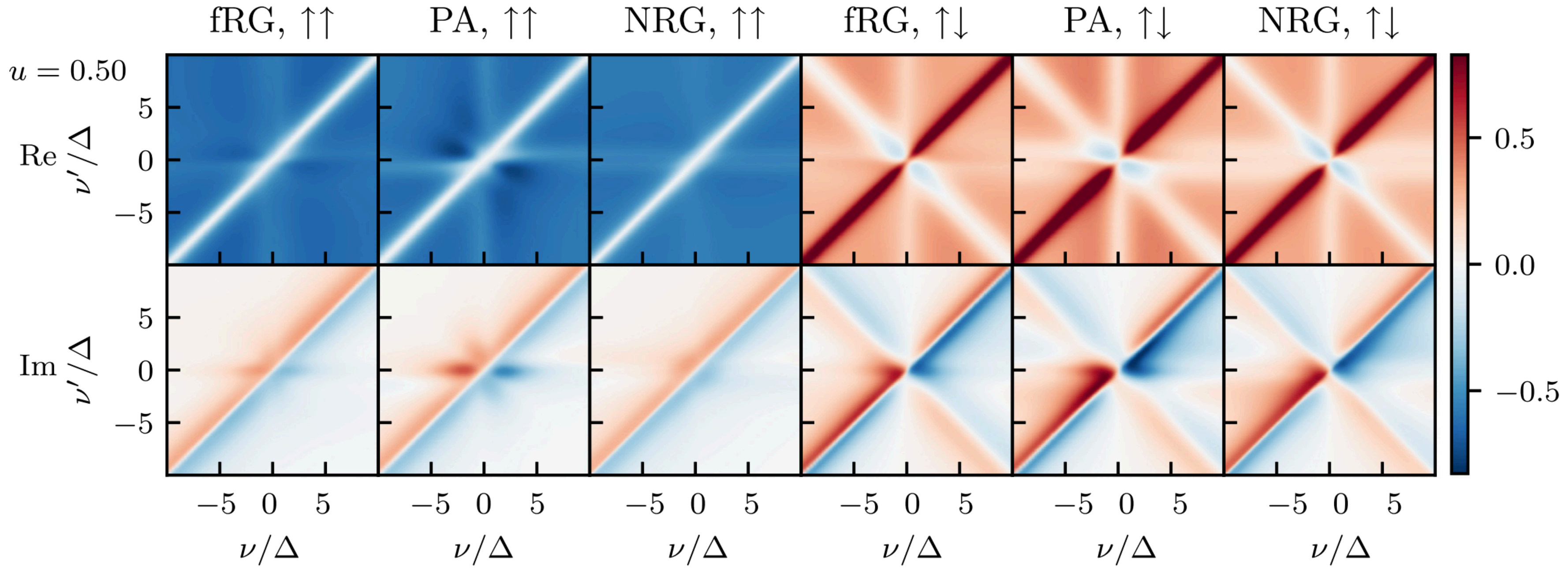
- optimized frequency grids
- efficient integrator
- exploit symmetries
- parallelization
- vectorization

Summary

main paper PRB (2024)
code publication JCP (2024)
repository (github)
documentation

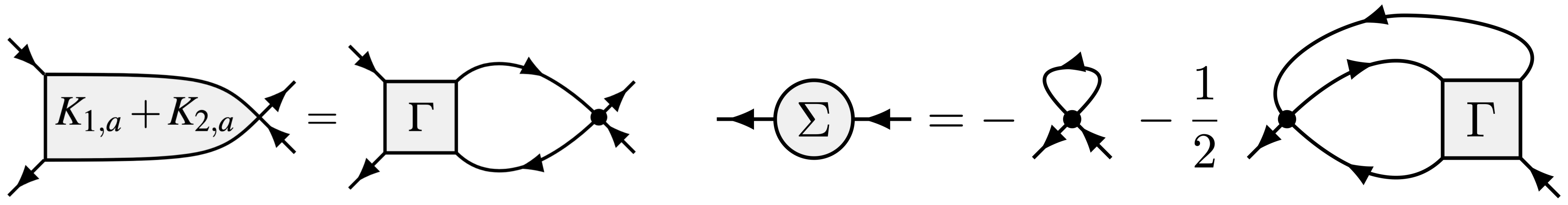
- real-frequency QFT with full frequency resolution is feasible
  - full frequency dependence improves accuracy
- PA gives best agreement, where available
- fRG more economical, but less accurate

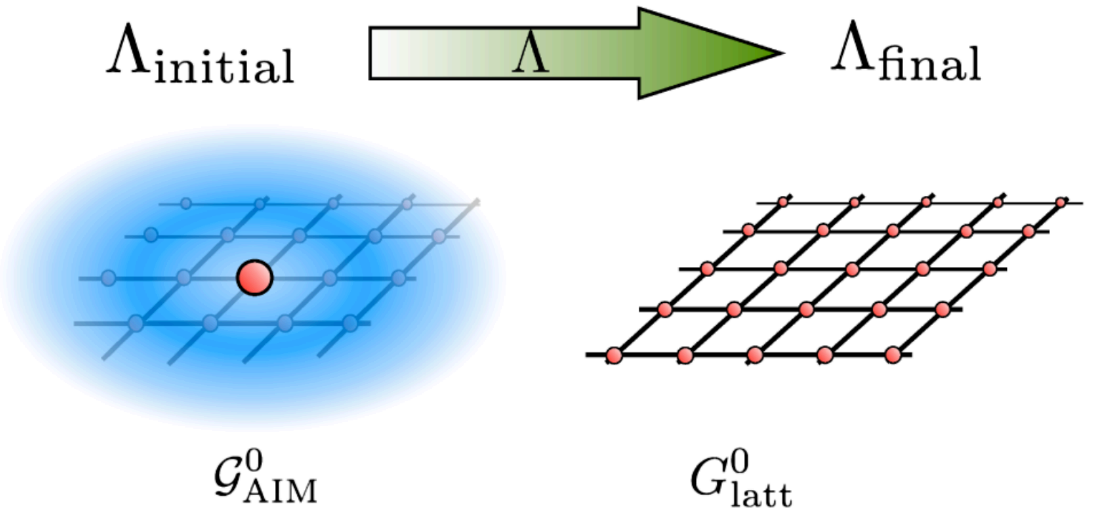




Outlook

- Exact diagrammatic relations fulfilled by NRG results?
  - BSEs, SDE, Ward-Identities, …

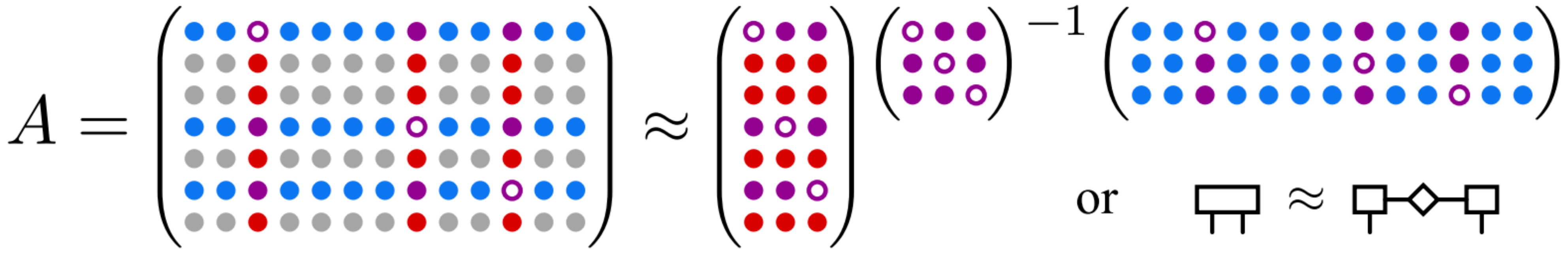




Taranto, Andergassen et al., PRL (2014)

- Real-frequency diagrammatic extensions of DMFT
  - Requires compression of the vertex

  Promising technique: Quantics Tensor Cross Interpolation



Ritter, Fernández et al., PRL (2023)