REAL-FREQUENCY CORRELATION FUNCTIONS OF CORRELATED ELECTRONIC SYSTEMS FROM QUANTUM FIELD THEORY

LMU LUDWIG-MAXIMILIANS-UNIVERSITÄT MÜNCHEN

Nepomuk Ritz
nepomuk.ritz@physik.uni-muenchen.de

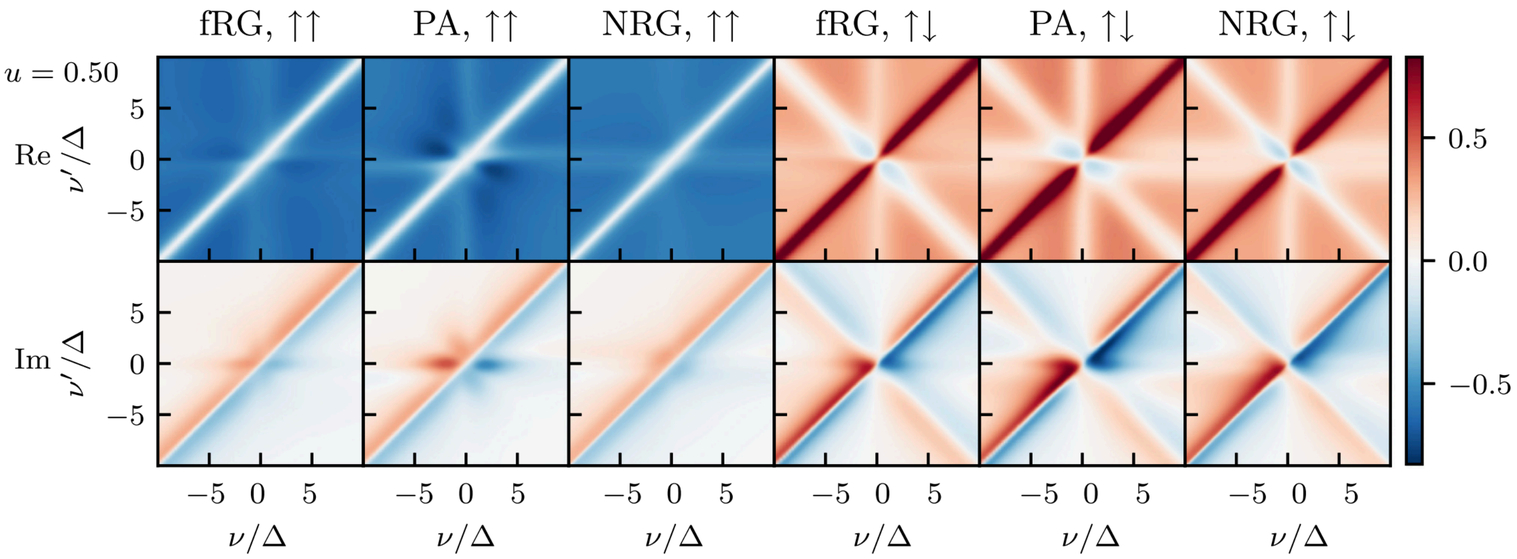
Heidelberg, 12 Nov 2024



Anxiang Ge (LMU) | Jan von Delft (LMU) | Fabian Kugler (CCQ, Flatiron)

Anxiang Ge, NR, Elias Walter, Santiago Aguirre, Jan von Delft, and Fabian B. Kugler
Phys. Rev. B 109, 115128 (2024)

NR, Anxiang Ge, Elias Walter, Santiago Aguirre, Jan von Delft, and Fabian B. Kugler
J. Chem. Phys. 161, 054118 (2024)



- Background: multi-point correlation functions in condensed matter physics
- Field-theory methods for fermionic problems
- Keldysh formalism for computing real-frequency dynamical correlation functions
- fRG vs. parquet study of the Anderson impurity model
- Outlook: Field theory methods + DMFT
- Spectral representation of correlation functions
- Outlook: Quantics Tensor Cross Interpolation

Multi-point correlation functions in condensed matter physics

General theory of interacting fermions:

$$S = -\sum_{1',1} \bar{c}_{1'} [G_0^{-1}]_{1',1} c_1 - \frac{1}{4} \sum_{1',1,2',2} \Gamma_{0;1',2';1,2} \bar{c}_{1'} \bar{c}_{2'} c_2 c_1$$

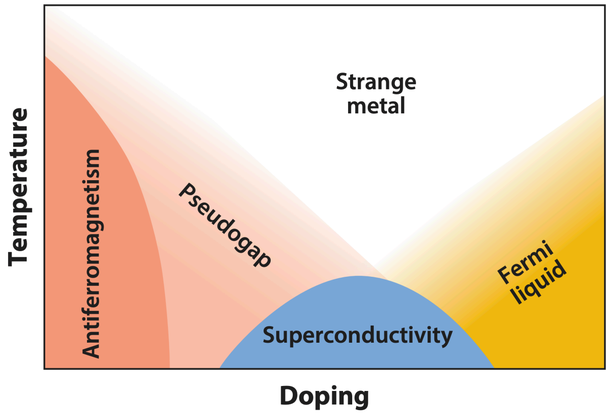
(imaginary) time, momentum, spin, …

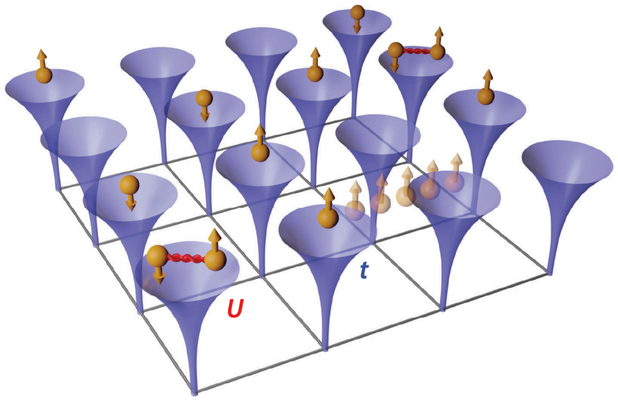
bare propagator

bare interaction vertex

Example: Hubbard model

$$\hat{H} = -t \sum_{\langle ij \rangle \sigma} (\hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} + \text{h.c.}) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{j\downarrow}$$





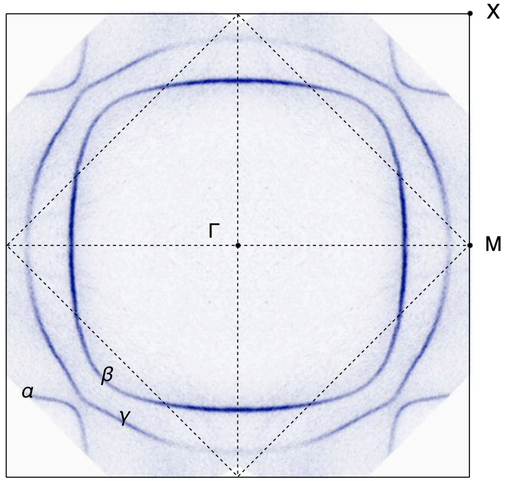
see M.Qin, T.Schäfer, S.Andergassen, P.Corboz, E.Gull, Ann. Rev. Cond. Mat. Phys. (2021)

Correlation functions (= time-ordered expectation values of operators)

$$\langle c_1 \ldots \bar{c}_{1'} \rangle = \frac{1}{Z} \int \mathscr{D}[\bar{c}, c] \, c_1 \ldots \bar{c}_{1'} e^{-S}$$

Two-point functions:

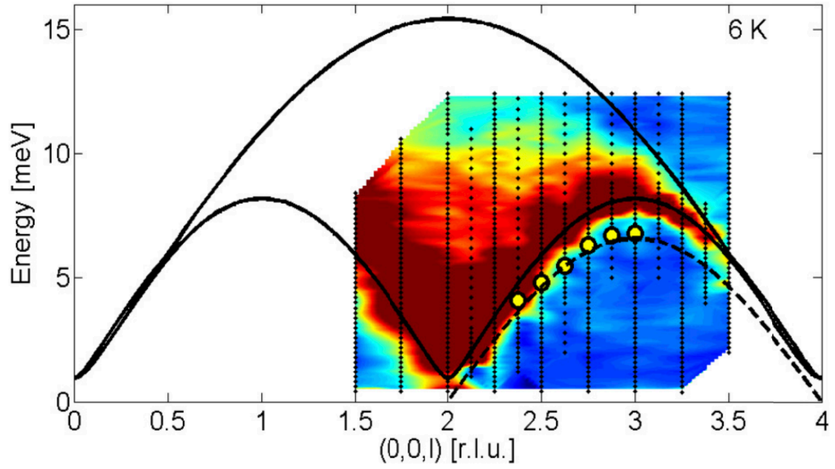
- local density of states
- spectral function
  $A(\omega, \mathbf{k}) = -\frac{1}{\pi} \operatorname{Im} G^R(\omega, \mathbf{k})$
- …



Spectral function of Sr_2RuO_4 from ARPES
A.Tamai et al., PRX (2019)

Four-point functions:

- susceptibilities
- conductivities
- structure factor
  $\sim \langle \mathbf{S}_i(t) \, \mathbf{S}_j(0) \rangle$
- …



Dynamical spin structure factor for $SrCo_2V_2O_8$ from INS
A.K.Bera et al., PRB (2017)

Field theory formulation

Two-point function $G_{1,1'} = -i\langle c_1 \bar{c}_{1'} \rangle$

self-energy Σ **(1PI)**

$$G_{1|1'} = \quad 1 \leftarrow 1' \quad = \quad 1 \xleftarrow[G_0]{} 1' \quad + \quad 1 \xleftarrow[G_0]{} 2' \;\; \Sigma \;\; 2 \xleftarrow[G]{} 1'$$

Four-point function $G^{(4)}_{12|1'2'} = i\langle c_1\, c_2\, \bar{c}_{2'}\, \bar{c}_{1'} \rangle$

vertex Γ

$$\begin{array}{ccc} 2' & & 2 \\ & G^{(4)} & \\ 1 & & 1' \end{array} \quad = \quad \begin{array}{ccc} 2' & & 2 \\ & & \\ 1 & & 1' \end{array} \quad - \quad \begin{array}{ccc} 2' & & 2 \\ \downarrow & & \uparrow \\ 1 & & 1' \end{array} \quad + \quad \begin{array}{ccccc} 2' & & 4 & & 4' & & 2 \\ & & \Gamma & & & & \\ 1 & & 3' & & 3 & & 1' \end{array}$$

needed as function of real frequencies

Four-point vertex $\Gamma_{\sigma_{1'}\sigma_{2'}|\sigma_1\sigma_2}(\omega_1, \omega_2, \omega_3; \mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3)$ **:**

Energy-dependent effective interaction

In thermal equilibrium: Matsubara formalism

looks like time-evolution in imaginary time

$$Z = \mathrm{Tr}\, e^{-\beta \hat{H}} = \int \prod_i (\mathrm{d}\bar{c}_i \mathrm{d}c_i) e^{-\sum_i \bar{c}_i c_i} \langle -c \,|\, e^{-\beta \hat{H}} \,|\, c \rangle$$

$$= \int \mathscr{D}[\bar{c}, c]\, e^{-S} \qquad \textbf{with} \quad S = \int_0^\beta \mathrm{d}\tau \sum_i \bar{c}_i(\tau)\, \partial_\tau\, c_i(\tau) + H[\bar{c}, c]$$

Imaginary times defined on interval $\tau \in [0, \beta)$

→ switch to Matsubara-frequency representation

$$c(\tau) = \frac{1}{\beta} \sum_{\omega_n} c_n\, e^{-i\omega_n \tau} \qquad \textbf{with} \quad \omega_n = \frac{(2n+1)\pi}{\beta}, \quad n \in \mathbb{Z}$$

Convenient to work with:

- **compute correlation functions only at discrete points**
- **no integrations, just summations over Matsubara frequencies**
- **can formally return to real-frequency description by analytic continuation:** $G^R(\nu) = G(i\omega_n \to \nu + i0^+)$

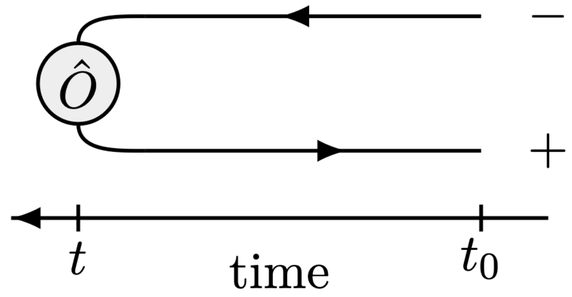
Problem(s):

solved by Ge, Halbinger, Lee, von Delft, Kugler Ann. Phys (2024)

- **How to do this for multi-point functions?**
- **Analytic continuation is numerically ill-conditioned!**

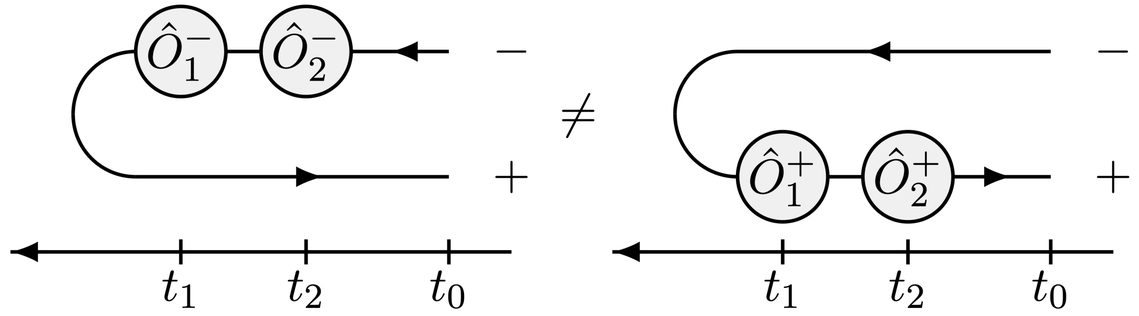
Keldysh formalism

$$\langle \hat{O}(t) \rangle = \mathrm{Tr}\left[\tilde{\mathcal{T}} e^{-i\int_t^{t_0} \mathrm{d}t' H(t')} \hat{O}\, \mathcal{T} e^{-i\int_{t_0}^{t} \mathrm{d}t' H(t')} \rho_0 \right] = \mathrm{Tr}\left[\mathcal{T}_{\mathscr{C}} \left\{ e^{-i\int_t^{t_0} \mathrm{d}t' H^{+}(t')} \hat{O}\, e^{-i\int_{t_0}^{t} \mathrm{d}t' H^{-}(t')} \rho_0 \right\} \right]$$



contour index!

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



Redundancy: $G^{<} + G^{>} - G^{\mathcal{T}} - G^{\tilde{\mathcal{T}}} = 0$

Simplification by Keldysh rotation:

$$G^{k|k'} = D^{kc} G^{c|c'} (D^{-1})^{c'k'} = \begin{pmatrix} G^{1|1} & G^{1|2} \\ G^{2|1} & G^{2|2} \end{pmatrix} = \begin{pmatrix} 0 & G^{A} \\ G^{R} & G^{K} \end{pmatrix}$$

$$D = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}, \qquad D^{-1} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$$

$$G^{R}(t_1, t_2) = -i\,\Theta(t_1 - t_2)\langle\{c(t_1), c^{\dagger}(t_2)\}\rangle$$

$$G^{A}(t_1, t_2) = [G^{R}(t_2, t_1)]^{*}$$

Thermal equilibrium: $\rho_0 = \frac{1}{Z} e^{-\beta H}$

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

continuous, real frequency

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

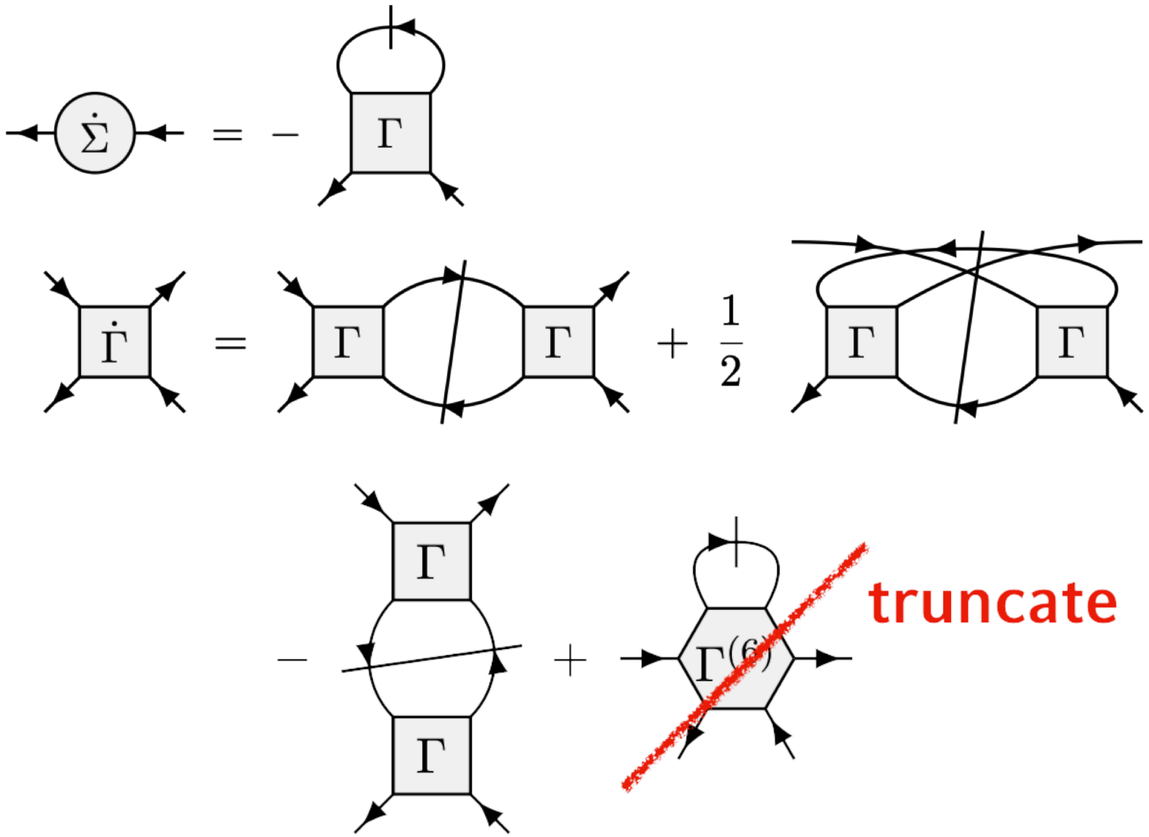
Fluctuation-Dissipation Relation

only explicit occurrence of temperature

Field theory methods

1 Functional Renormalization Group

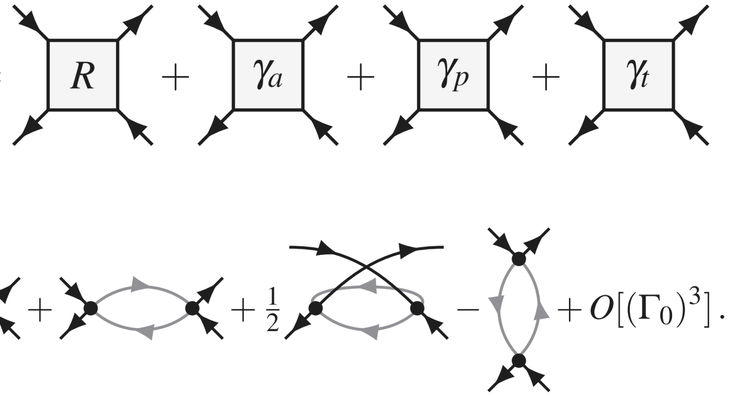
Start from vertex expansion of Wetterich's equation.
Flow equations:



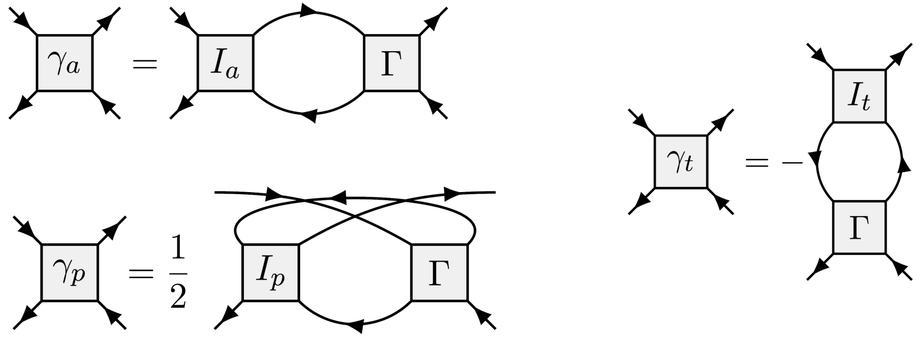
Use single-particle flow parameter Λ to interpolate between $\Lambda_{\text{initial}} \to \Lambda_{\text{final}}$. Theory at Λ_{initial} should be under control.

Review: Metzner, Salmhofer, Honerkamp, Meden, Schönhammer, RMP (2012)

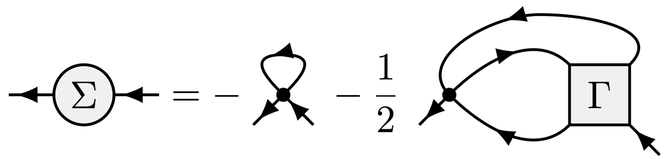
2 Parquet formalism



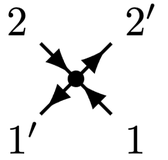
Bethe-Salpeter equations:



Schwinger-Dyson equation:



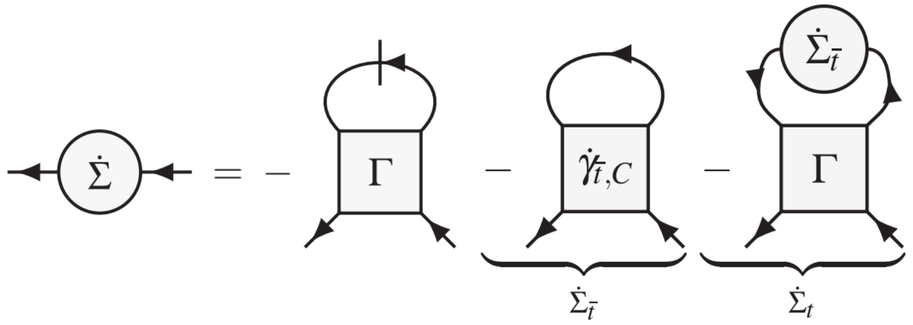
Parquet approximation: $R = \Gamma_0 + \mathcal{O}[(\Gamma_0)^4] \approx \Gamma_0 =$

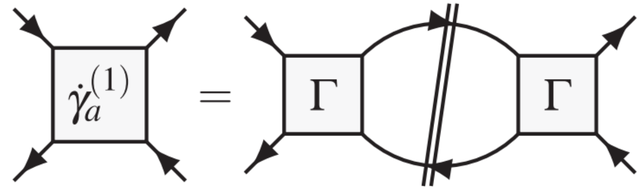


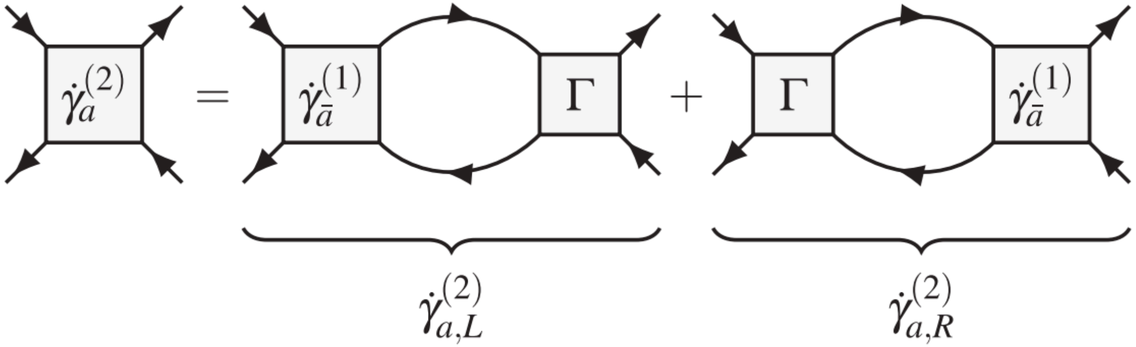
Review: Bickers (2004)

Connection: multi-loop fRG Add the 2PR-contributions of $\Gamma^{(6)}$ to $\dot{\Gamma}$ iteratively, organized by loop-order.

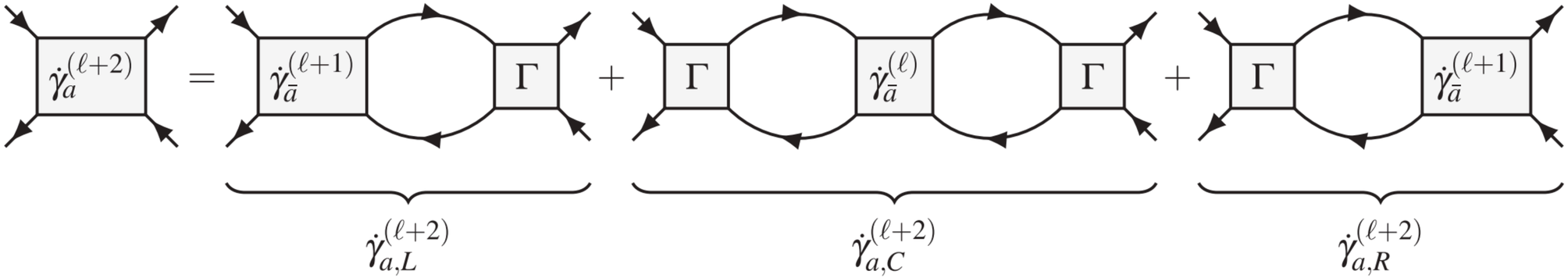
$$\dot{\Gamma} = \sum_{r\in\{a,p,t\}} \dot{\gamma}_r\,, \qquad \dot{\gamma}_r = \sum_{\ell=1}^{\infty} \dot{\gamma}_r^{(l)}$$



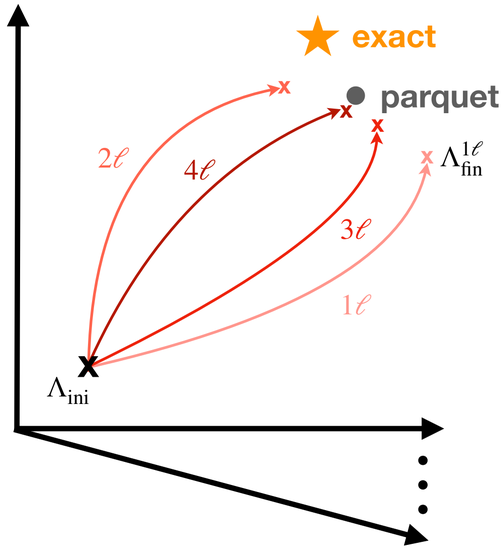




- Ensures that $\dot{\Gamma}$ = total derivative
- integrating flow yields regulator-independent results
- sums up all parquet diagrams



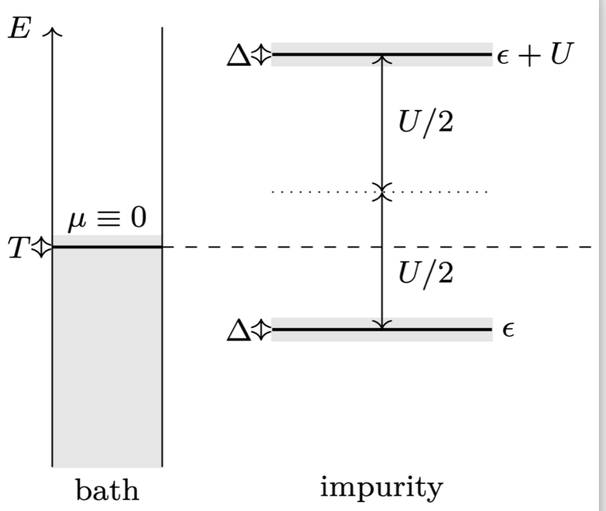
Kugler, von Delft
PRL (2018), PRB (2018), NJP (2018)



[Related work for bosonic theory: Blaizot, Pawlowski, Reinosa, PLB 696, 523 (2011)]

Application: 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)

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

particle-hole symmetry

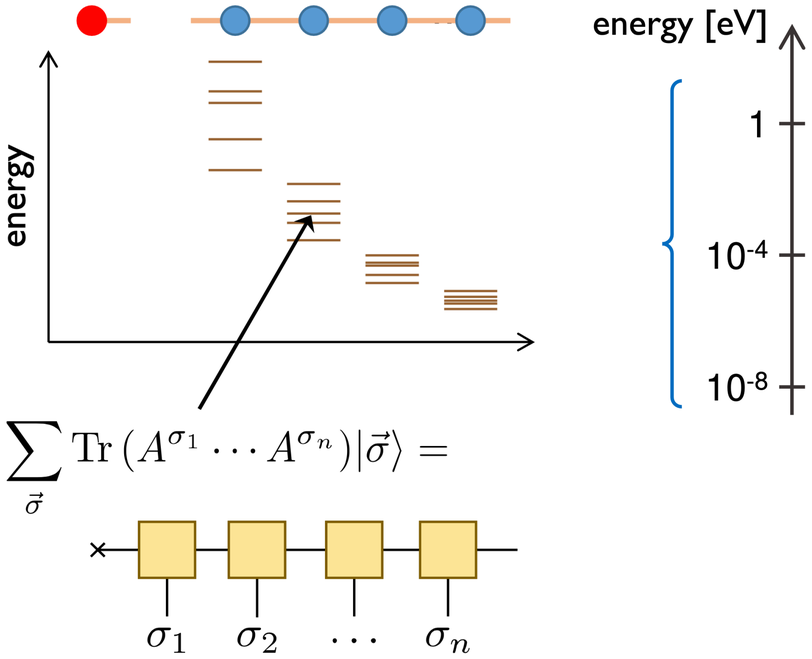
$\epsilon_d \in \{-U/2,\, 0\}$ **impurity level shift**

Δ **effective level width ("hybridization")**

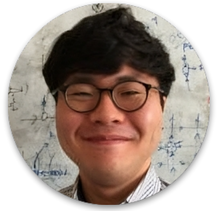
$$T_{\text{K}} = \sqrt{\Delta U/2}\, \exp\left[-\pi \left(\frac{U}{8\Delta} + \frac{\Delta}{U} \right) \right]$$

Kondo temperature

Benchmark: Numerical Renormalization Group (NRG)



$$\sum_{\vec{\sigma}} \text{Tr}\left(A^{\sigma_1} \cdots A^{\sigma_n} \right) |\vec{\sigma}\rangle =$$



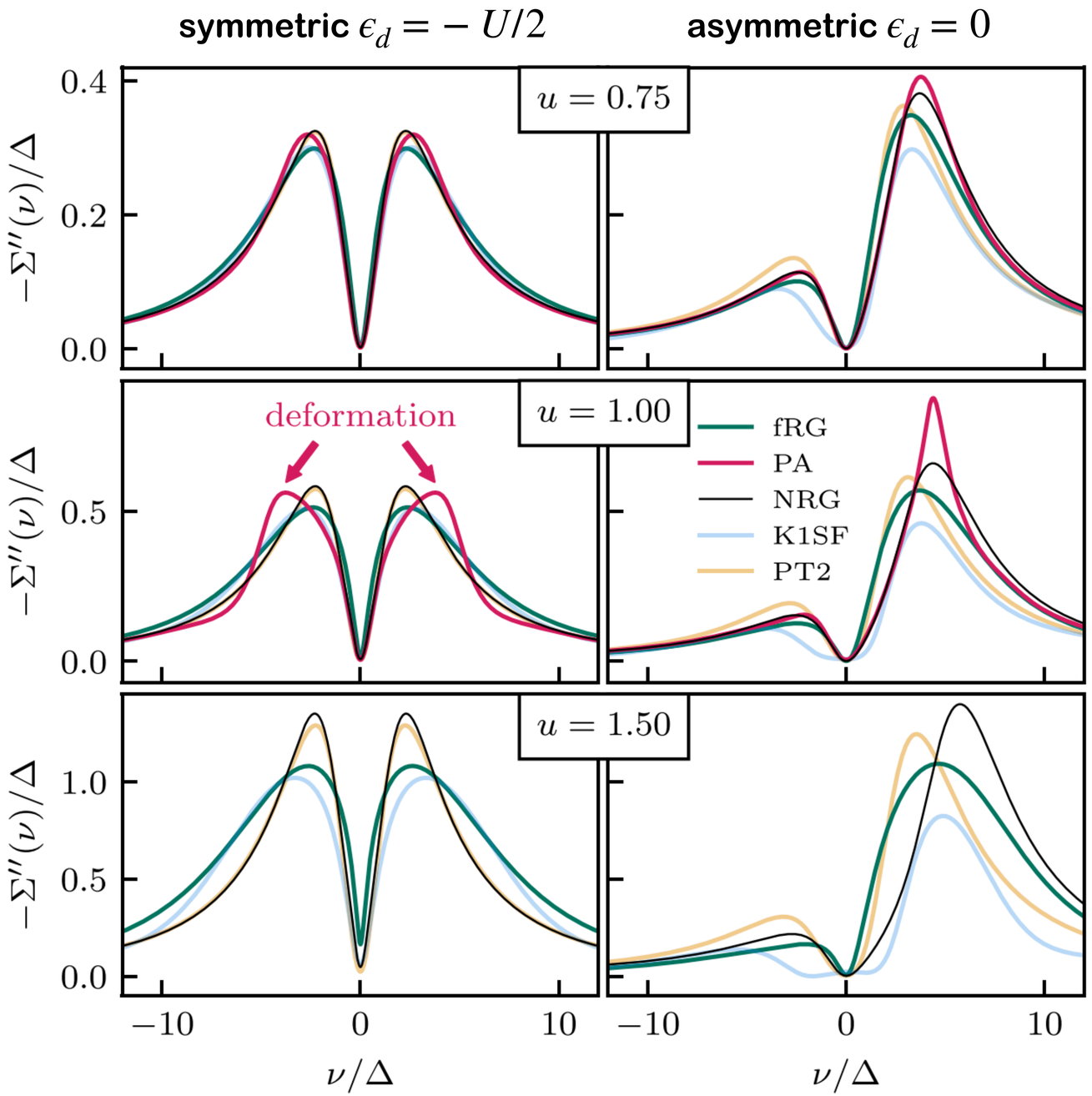
S.S.B. Lee
(Seoul N.U.)

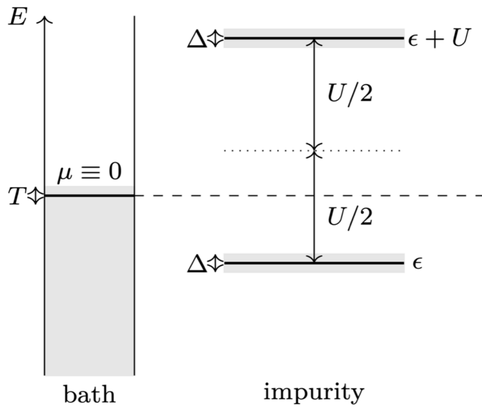
A. Weichselbaum
(Brookhaven)

- **Logarithmic discretization of the bath: Wilson chain**
  Wilson, RMP (1995); Bulla, Costi, Pruschke, RMP (2008)
- **Iterative diagonalization: complete basis of energy eigenstates**
  Anders, Schiller, PRL (2005)
- **Tensor network formulation: many-body states as matrix product states**
  Weichselbaum, PRB (2008)
- **Correlation functions from (partial) spectral functions**
  Peters, Pruschke, Anders, PRB (2006)
  Weichselbaum, von Delft, PRL (2007)
  Lee, Kugler, von Delft, PRX (2021)

fRG & parquet treatment

Anxiang Ge, NR, Elias Walter, Santiago Aguirre, Jan von Delft, and Fabian B. Kugler
Phys. Rev. B 109, 115128 (2024)





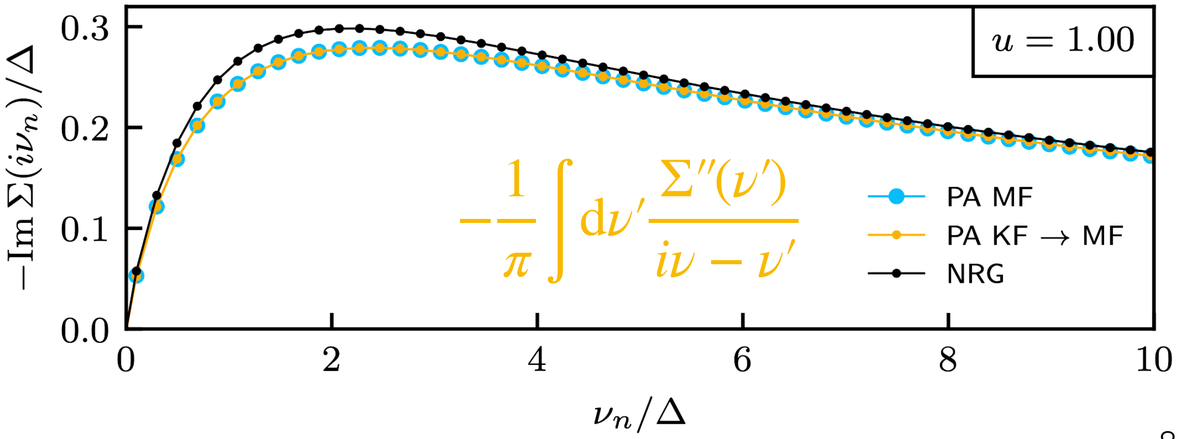
temperature: $T/U = 0.01$

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

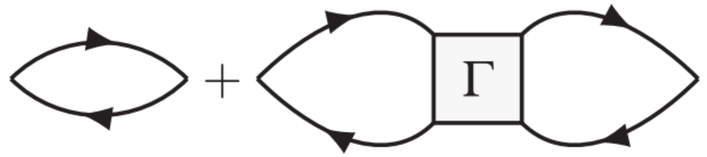
- **NRG:** Numerical exact benchmark
- **K1SF:** Previous state-of-the-art by S. Jakobs, V. Meden, H. Schoeller (RWTH Aachen)

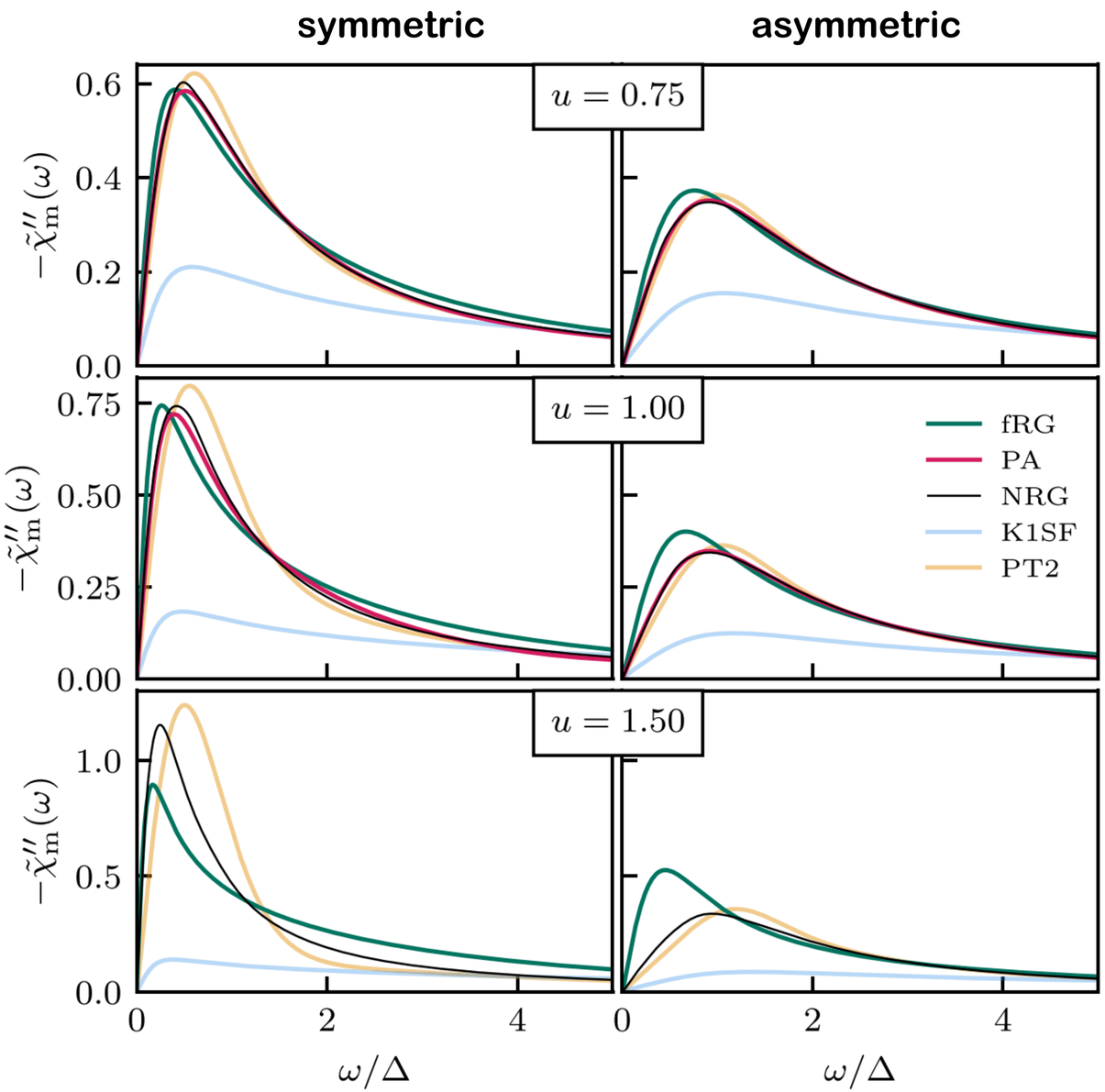
$\gamma(\omega, \nu, \nu') \approx \gamma(\omega)$ → only "static feedback" from other channels

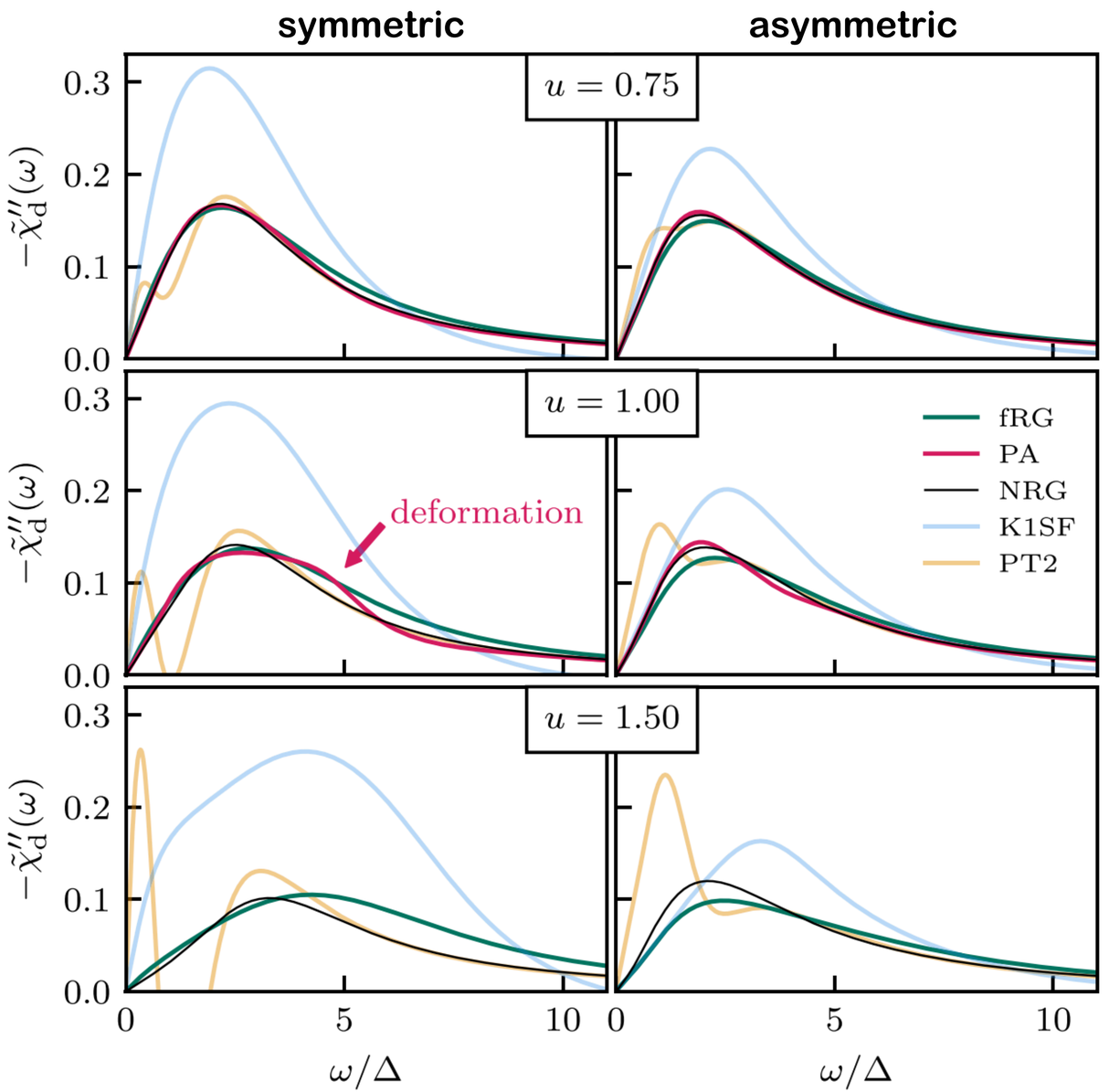
- **PT2:** Second-order perturbation theory



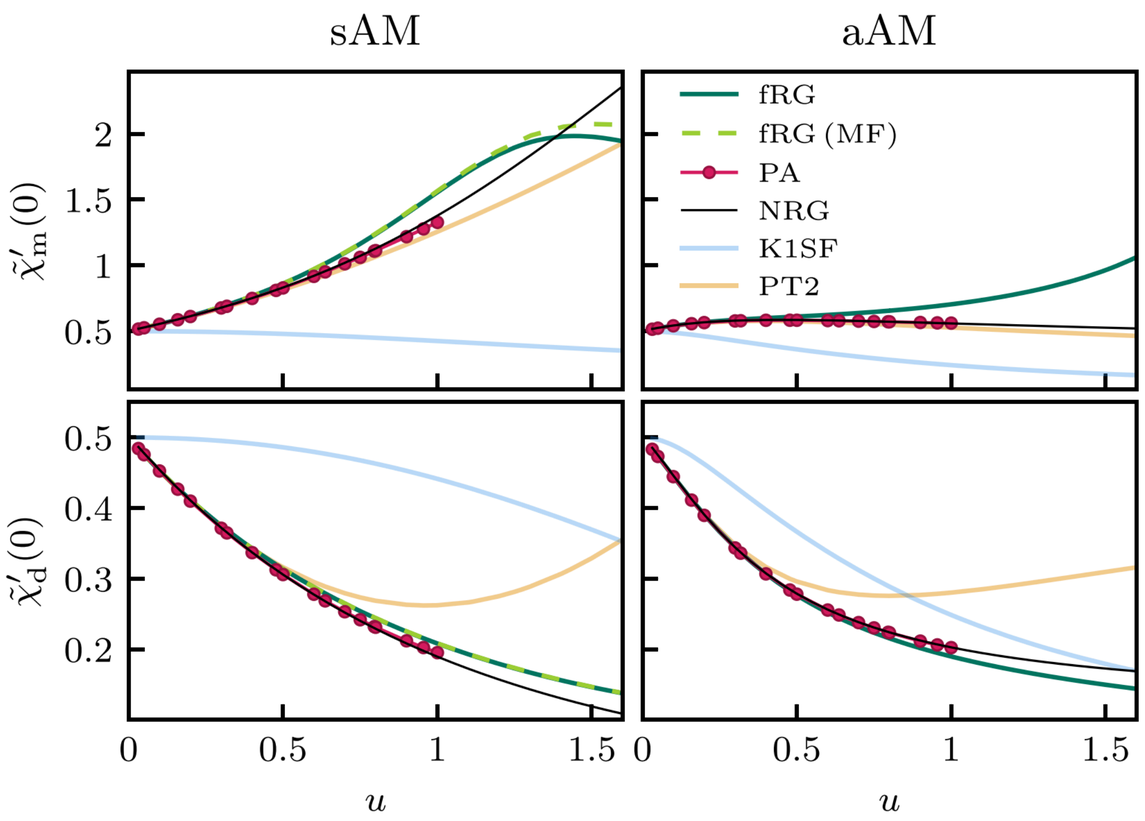
Dynamical Susceptibilities

$\chi_a =$  $+$





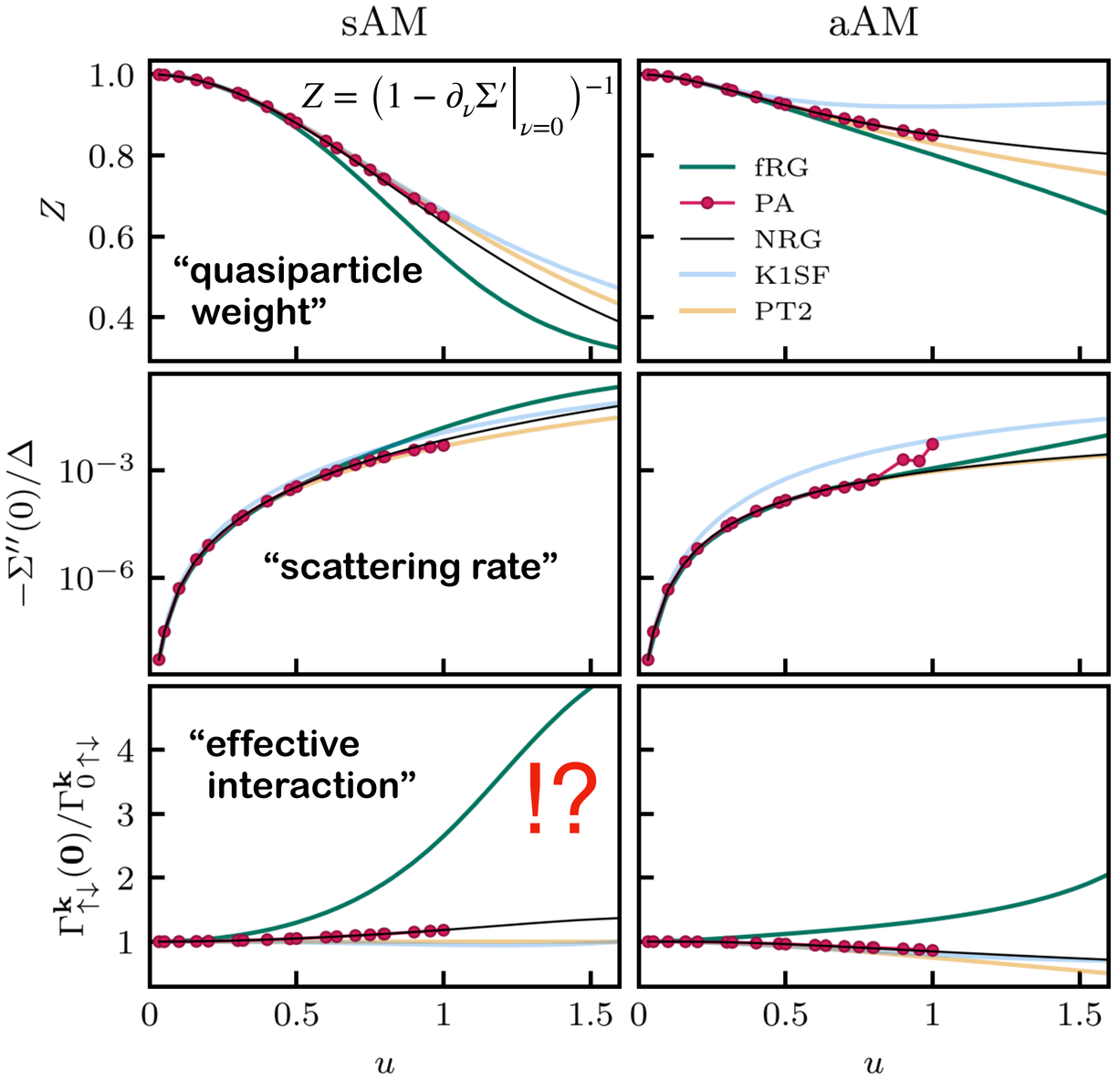
Static quantities



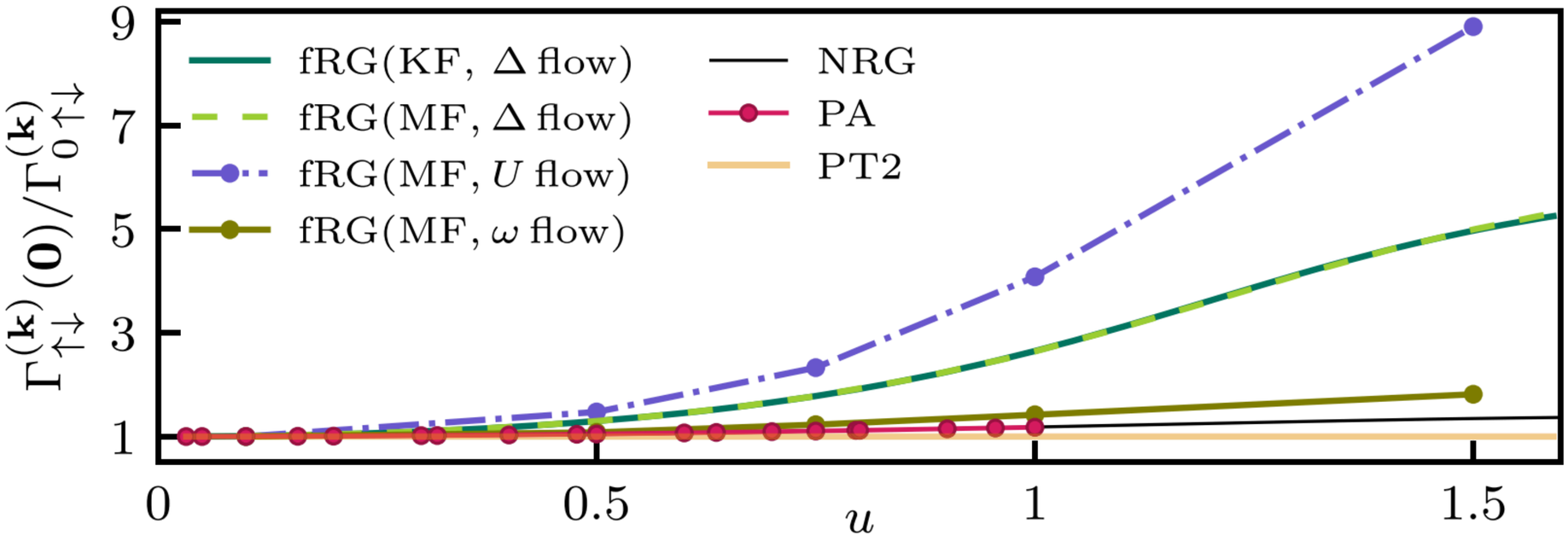
Static susceptibilities:

$$\chi_{\mathrm{m}} = \frac{1}{4}\partial_h \langle n_\uparrow - n_\downarrow \rangle \,|_{h=0}$$

$$\chi_{\mathrm{d}} = \frac{1}{4}\partial_{\epsilon_d} \langle n_\uparrow + n_\downarrow \rangle$$



Regulator dependence in (one-loop) fRG



Flow schemes (Matsubara formalism):

hybridization (Δ) flow: $G_{\Delta}(i\nu) = \dfrac{1}{i\nu - \epsilon_d - \Delta - \Sigma(i\nu)}$

interaction (U) flow: $G_{\Lambda}(i\nu) = \dfrac{\Lambda}{i\nu - \epsilon_d - \Delta - \Lambda\Sigma(i\nu)}$

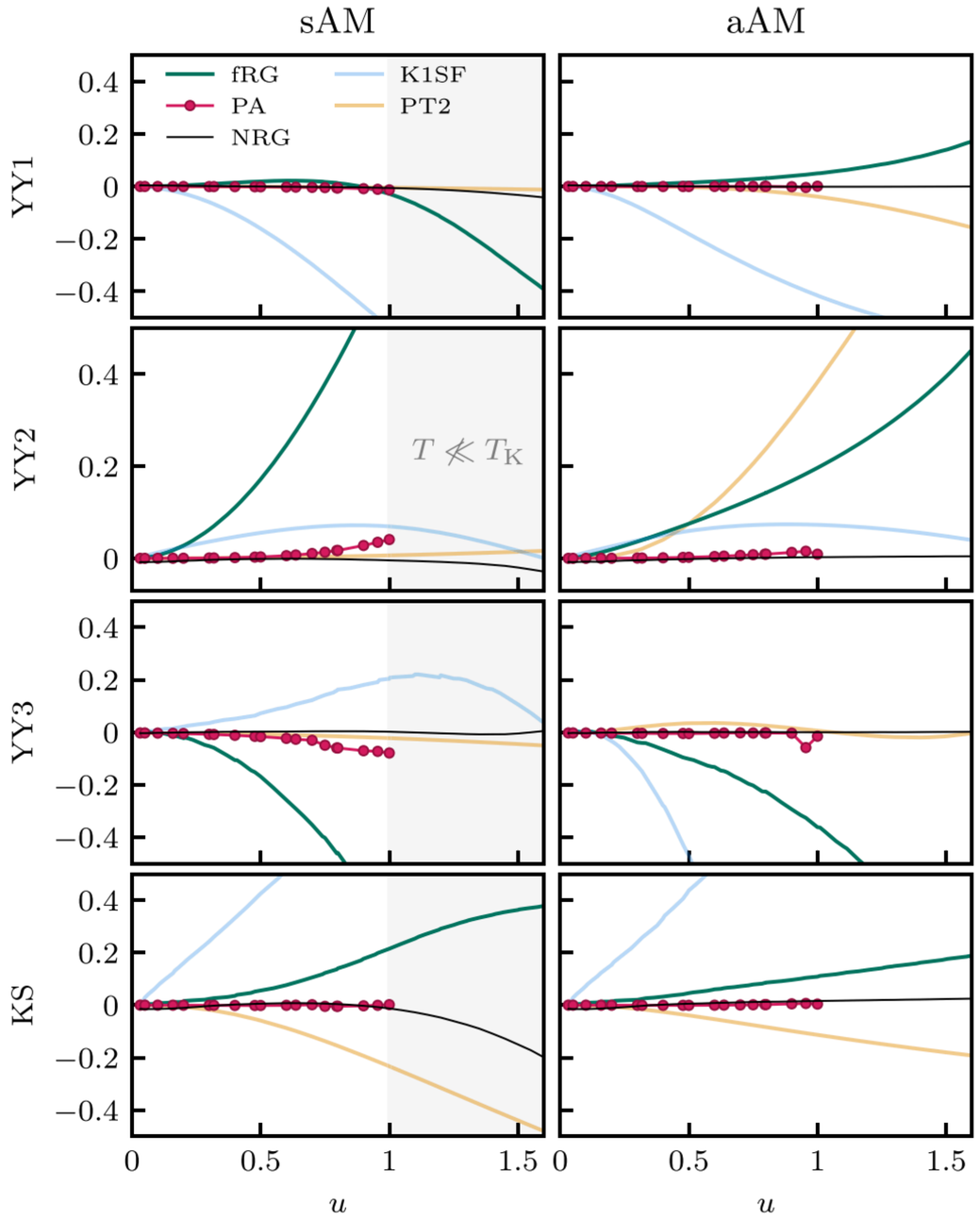
frequency (ν) flow: $G_{\Lambda}(i\nu) = \dfrac{\nu^2}{\nu^2 + \Lambda^2}\dfrac{1}{i\nu - \epsilon_d - \Delta - \Sigma(i\nu)}$

(not possible in Keldysh)

The one-loop truncation in fRG yields highly regulator-dependent results!

In Keldysh, the Δ - flow is the method of choice.

Fulfillment of Fermi-liquid identities



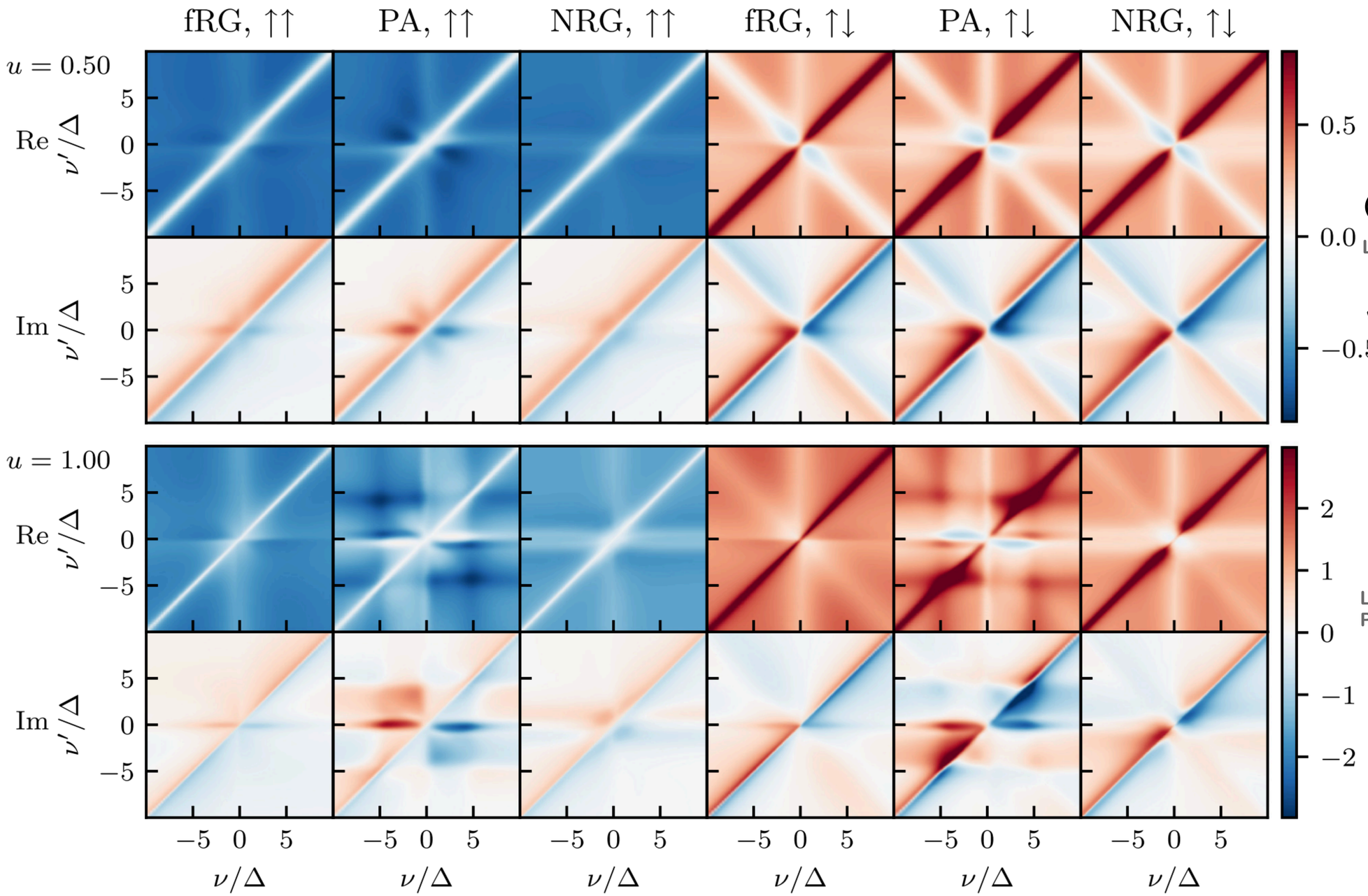
$$Z^{-1} = [\chi_m(0) + \chi_d(0)]/\rho(0) \qquad \rho(0) \equiv A(0)\,|_{T=0}$$

$$-\rho(0)\Gamma_{\uparrow\downarrow}(\vec{0}) = [\chi_m(0) - \chi_d(0)]/\rho(0)$$

$$-\Sigma''(\nu) = \frac{1}{2}\pi\rho(0)^3[\Gamma_{\uparrow\downarrow}(\vec{0})]^2(\nu^2+\pi^2T^2)$$

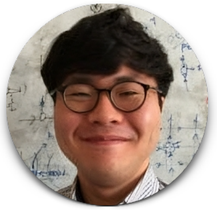
$$\lim_{\omega\to 0}\chi_m''(\omega)/\omega = 2\pi\left[\chi_m'(0)\right]^2$$

Full frequency-dependent vertex $[\Gamma^{\mathbf{k}}_{\sigma\sigma'}(\omega_t = 0, \nu_t = \nu, \nu'_t = \nu') - \Gamma^{\mathbf{k}}_{0,\sigma\sigma'}]/\Gamma^{\mathbf{k}}_{0,\uparrow\downarrow}$ **for** $\mathbf{k} = 12\,|\,22$



Multi-point NRG by

J. Shim
(now at Samsung)



S.S.B. Lee
(Seoul N.U.)

Lee, Kugler, von Delft, PRX (2021)

with symmetric estimators by

J.M. Lihm
(CCQ, Flatiron)

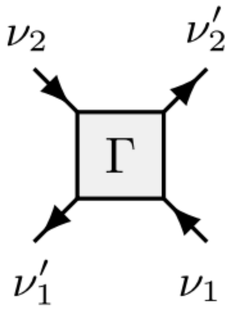
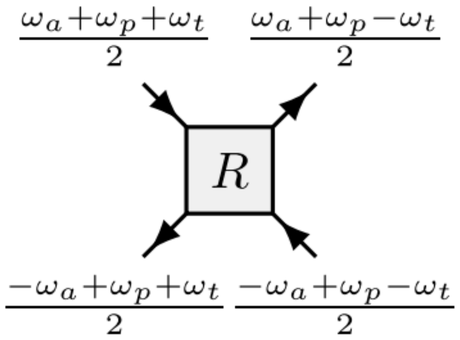
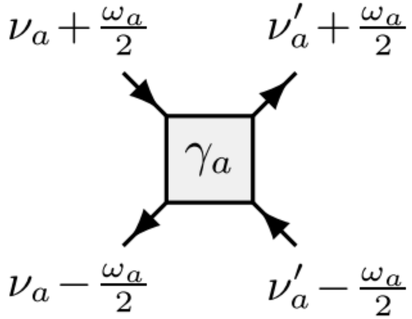
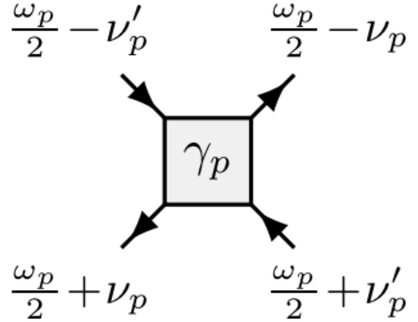
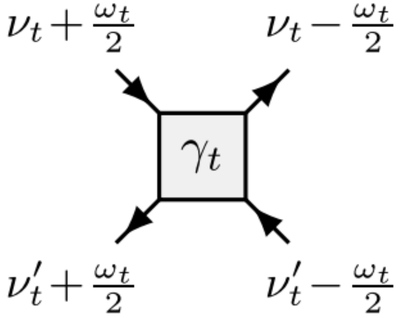
J. Halbinger
(now at BayernLB)

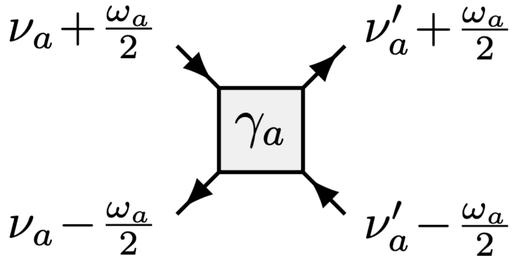
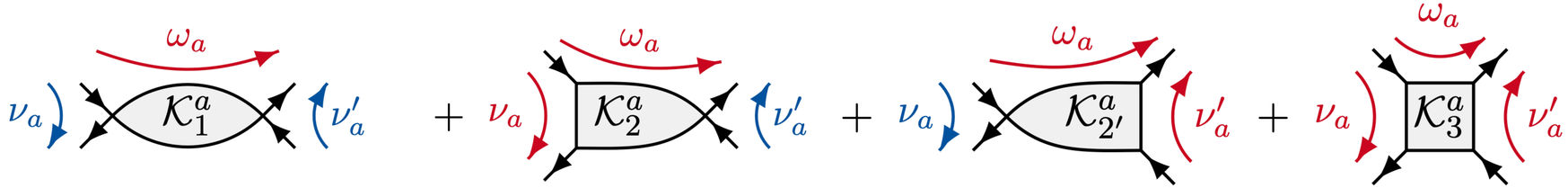
Lihm, Halbinger, Shim, von Delft, Kugler, Lee, PRB (2024)

more on this later…

Details 1: Frequency parametrization

symmetric!

$$\Gamma(\nu_1'\nu_2'|\nu_1\nu_2) =$$  $=$  $+$  $+$  $+$ 

 $=$ 

$$= \mathcal{K}_1^a(\omega_a) + \mathcal{K}_2^a(\omega_a, \nu_a) + \mathcal{K}_{2'}^a(\omega_a, \nu_a') + \mathcal{K}_3^a(\omega_a, \nu_a, \nu_a')$$

similarly for channels p and t

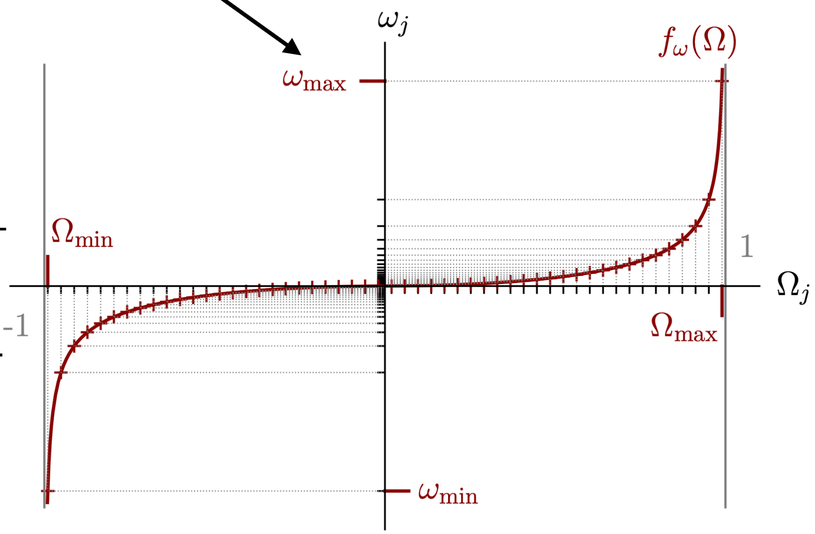
Details 2: Frequency grids and integrations

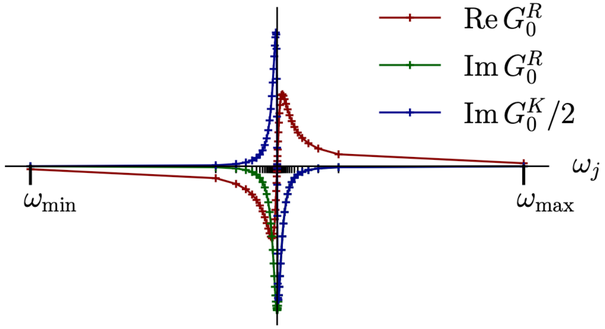
Use a non-linear grid to resolve sharp structures at small frequencies and the slow asymptotic decline.

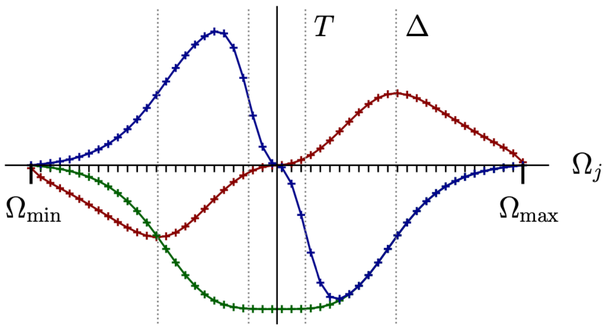
$\propto \Delta$

$$\omega = f_A(\Omega) = \frac{A\Omega\,|\,\Omega\,|}{\sqrt{1-\Omega^2}}$$

$$\Omega = \frac{\omega}{A}\sqrt{\frac{\sqrt{1+\left(\frac{A}{\omega}\right)^2}-1}{2}}$$

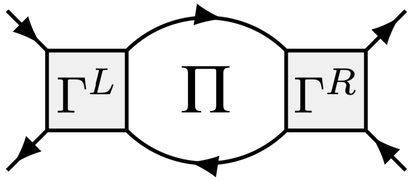






most challenging: bubble-integrations of the type

$$\int \mathrm{d}\nu''\,\Gamma^L(\omega,\nu,\nu'')\Pi(\omega,\nu'')\Gamma^R(\omega,\nu'',\nu')$$



approximate:

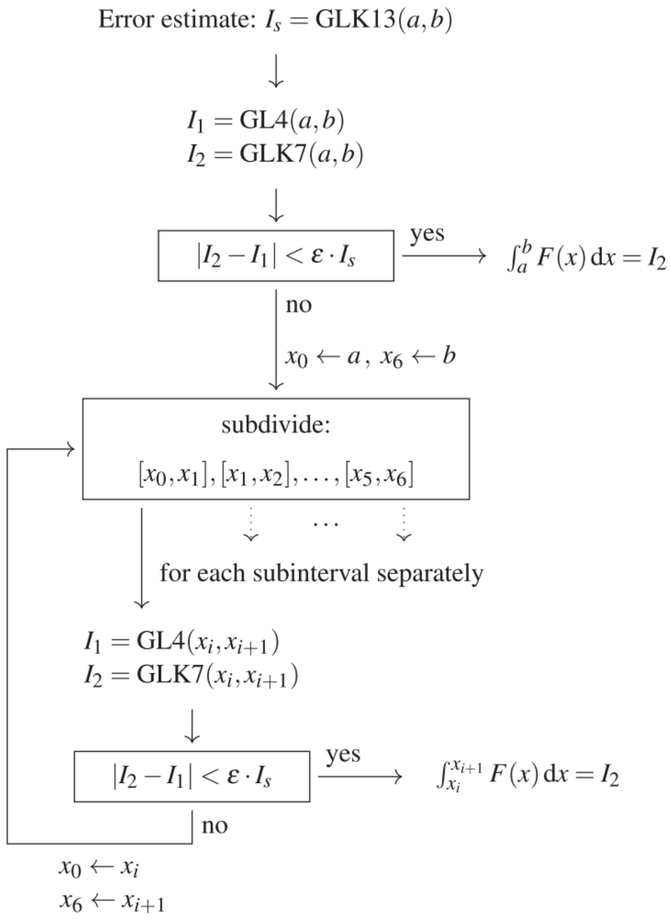
$$\boxed{\int_a^b F(x)\,\mathrm{d}x \approx \sum_{j=1}^{n} F(x_j)\,w_j}$$

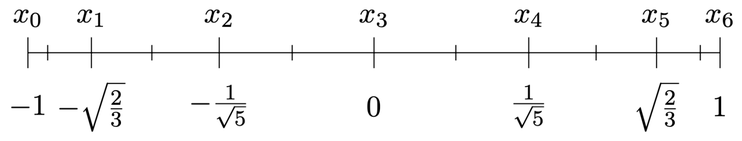
$$\mathrm{GL4}(x_0,x_6) = \sum_{j\in\{0,2,4,6\}} F(x_j)\,w_j$$

4-point Gauss-Lobatto

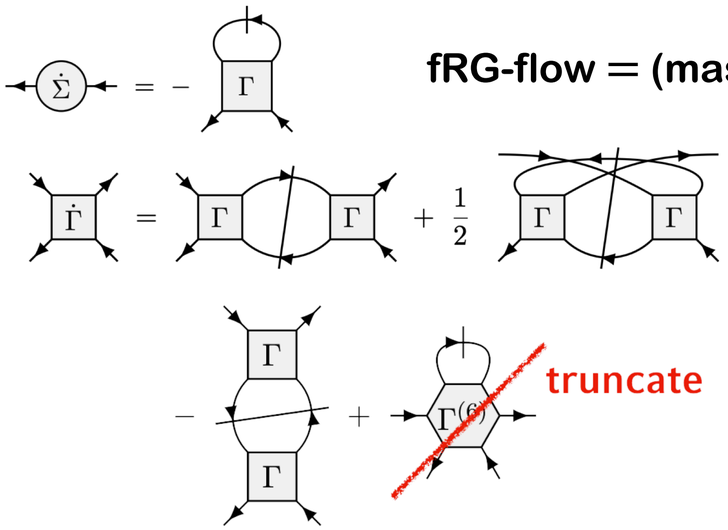
$$\mathrm{GLK7}(x_0,x_6) = \sum_{j=0}^{6} F(x_j)\,w_j$$

4-point Gauss-Lobatto
+ 7-point Kronrod extension





Details 3: Solving the fRG flow equations & self-consistent parquet equations



fRG-flow = (massive) set of coupled ODEs

$$G_0 \to G_0^{\Lambda}$$

$$\Lambda_{\text{initial}} \to \Lambda_{\text{final}}$$

$$\Gamma\Big|_{\Delta=\infty} = \Gamma_0$$

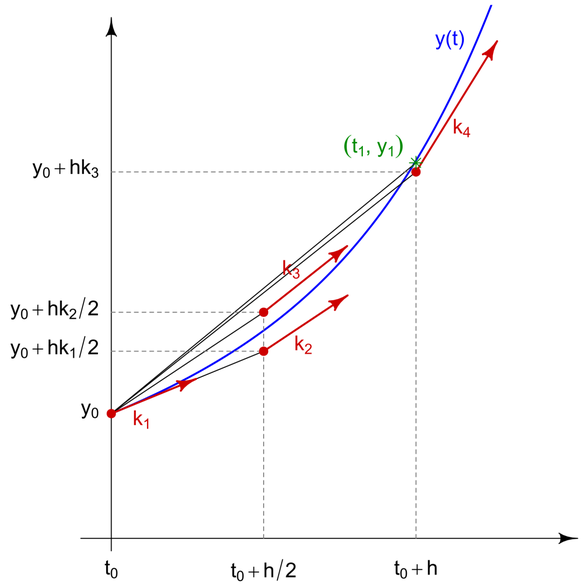
$$\Sigma^R\Big|_{\Delta=\infty} = \Sigma_{\text{H}} = U\langle n_\sigma \rangle$$

Observation: Right-hand sides can vary rapidly w.r.t. Λ

→ crucial to use a solver with adaptive step-size control!

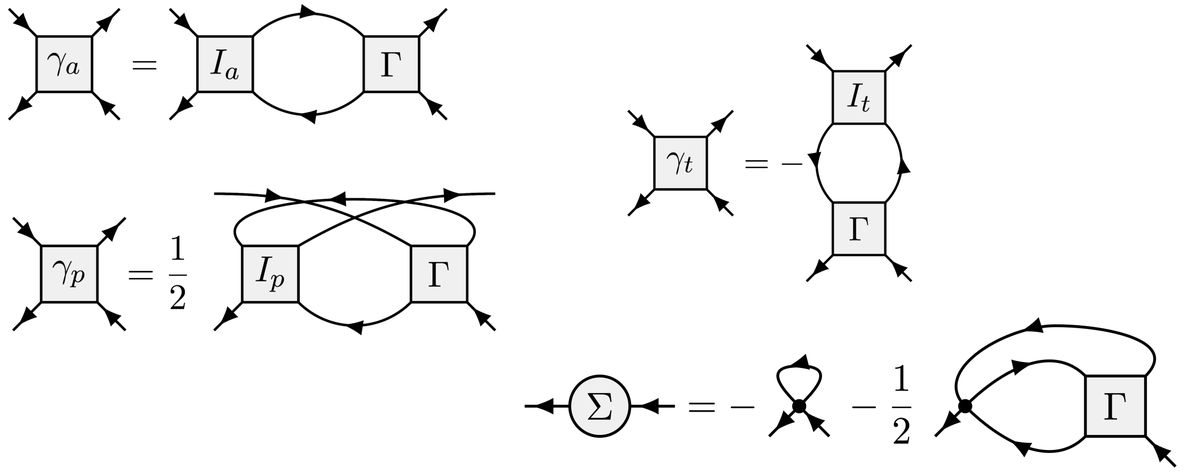
Here: Cash-Karp method with $\epsilon_{\text{rel}} = 10^{-6}$

(4th order Runge-Kutta solver with 5th order error estimate)



Cash, Karp, ACM TMS (1990)
see also Beyer, Goth, Müller, EPJB (2022)

Parquet equations = set of self-consistent equations



Set up as fixed-point equation: $\Psi = f_{\text{PA}}(\Psi)$ $\quad \Psi = (\Sigma, \Gamma)$

Solve iteratively, stabilizing with partial update:

$$\Psi \leftarrow (1-m)\cdot\Psi + m\cdot f_{\text{PA}}(\Psi)$$

$$0 < m \leq 1$$

faster convergence using Anderson acceleration, combining previous evaluations of $f_{\text{PA}}(\Psi)$

Anderson, JACM (1965)

Details 4: Symmetries, Vectorization and Parallelization

crossing symmetry: $\Gamma_{1'2'|12} = -\Gamma_{2'1'|12} = -\Gamma_{1'2'|21} = \Gamma_{2'1'|21}$

complex conjugation: $\Gamma_{1'2'|12} = (-1)^{1+\sum_i k_i}\Gamma^*_{12|1'2'}$

SU(2) symmetry: $\Gamma_{\sigma\sigma|\sigma\sigma} = \Gamma_{\sigma\bar{\sigma}|\sigma\bar{\sigma}} + \Gamma_{\sigma\bar{\sigma}|\bar{\sigma}\sigma}$

$$\Gamma^{k_{1'},k_{2'},k_1,k_2} \mapsto \begin{cases} \Gamma^{(k_{1'},k_2),(k_{2'},k_1)}, & \text{for a} - \text{channel}, \\ \Gamma^{(k_{1'},k_{2'}),(k_1,k_2)}, & \text{for p} - \text{channel}, \\ \Gamma^{(k_{2'},k_2),(k_{1'},k_1)}, & \text{for t} - \text{channel}\,. \end{cases}$$

Keldysh sum ⟶ matrix product

particle-hole symmetry:

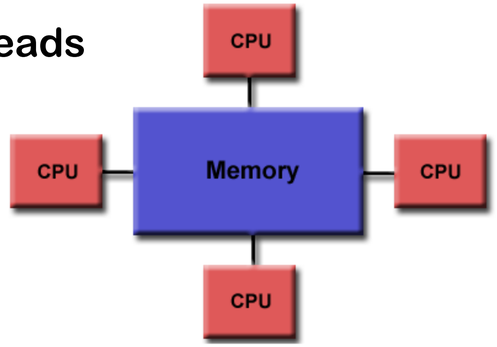
$$\begin{aligned}\Gamma_{1'2'|12}(\nu_1', \nu_2' \,|\, \nu_1, \nu_2) &= \Gamma_{12|1'2'}(-\nu_1, -\nu_2 \,|\, -\nu_1', -\nu_2') \\ &= (-1)^{1+\sum_i k_i}\Gamma_{1'2'|12}(-\nu_1', -\nu_2' \,|\, -\nu_1, -\nu_2)^*\end{aligned}$$

energy conservation: $\nu_1' + \nu_2' = \nu_1 + \nu_2$

Parallelize across multiple threads (OpenMP) and nodes (MPI)

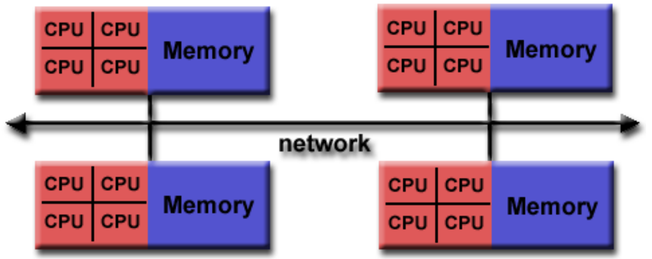
OpenMP:

- parallelization across multiple threads on a single node
- shared memory

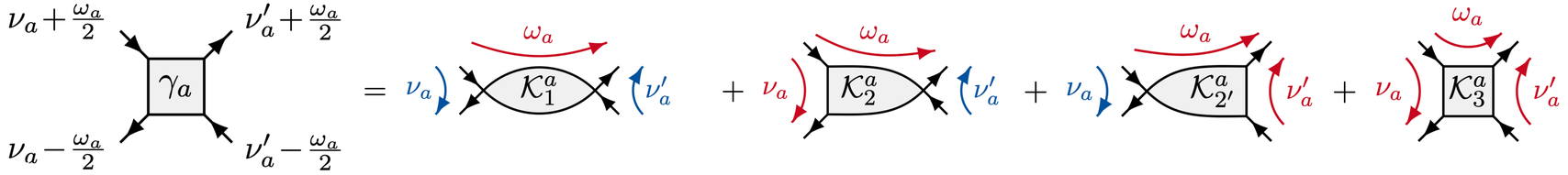


MPI:

- parallelization across multiple nodes running many threads each
- distributed memory

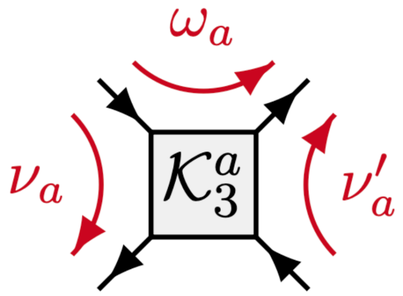


Details 5: Numerical complexity & computational resources



$$= \mathcal{K}_1^a(\omega_a) + \mathcal{K}_2^a(\omega_a, \nu_a) + \mathcal{K}_{2'}^a(\omega_a, \nu'_a) + \mathcal{K}_3^a(\omega_a, \nu_a, \nu'_a)$$

most expensive:



computational cost $\sim \mathcal{O}(N_{K_3}^3)$ up to 125 $\Rightarrow \approx$ 2 million frequency points
— memory & CPU

typical numbers:

	N_{K_1}	N_{K_2}	N_{K_3}
fRG	401	201	101
PA	401	201	51-125
PT2	801	—	—
K1SF	401	—	—

RESEARCH ARTICLE | AUGUST 07 2024

KeldyshQFT: A C++ codebase for real-frequency multiloop functional renormalization group and parquet computations of the single-impurity Anderson model

Special Collection: Algorithms and Software for Open Quantum System Dynamics

Nepomuk Ritz ; Anxiang Ge ; Elias Walter ; Santiago Aguirre; Jan von Delft ; Fabian B. Kugler

Check for updates

J. Chem. Phys. 161, 054118 (2024)
https://doi.org/10.1063/5.0221340

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

fRG more economical
(full parameter sweep)

Leibniz Supercomputing Centre
of the Bavarian Academy of Sciences and Humanities

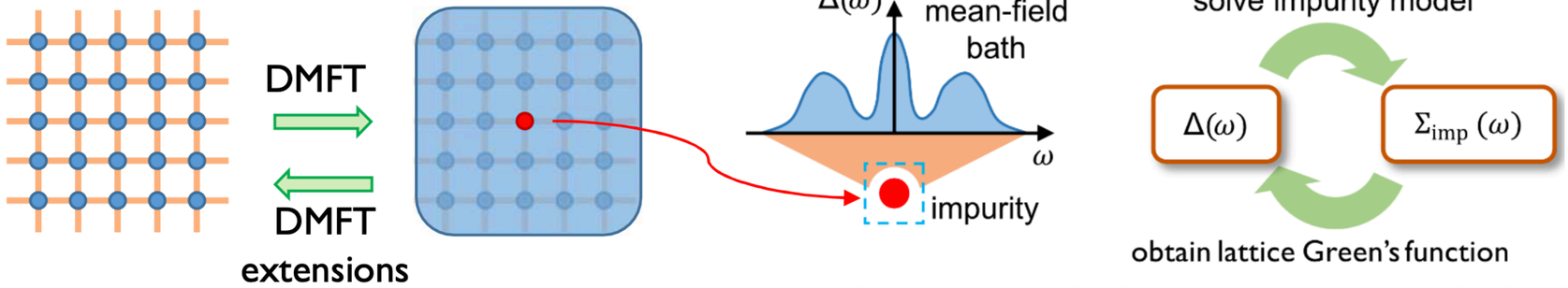
Outlook: Field theory methods + DMFT

Before: 1-loop fRG and parquet approximation fail at large couplings. How to improve?

Dynamical mean field theory (DMFT)

treats local correlations exactly

$$G(\omega, \mathbf{k}) = [\omega - \varepsilon_{\mathbf{k}} - \Sigma(\omega, \mathbf{k})]^{-1}$$



Reviews: Georges et al. RMP (1996); Kotliar et al. RMP (2006)

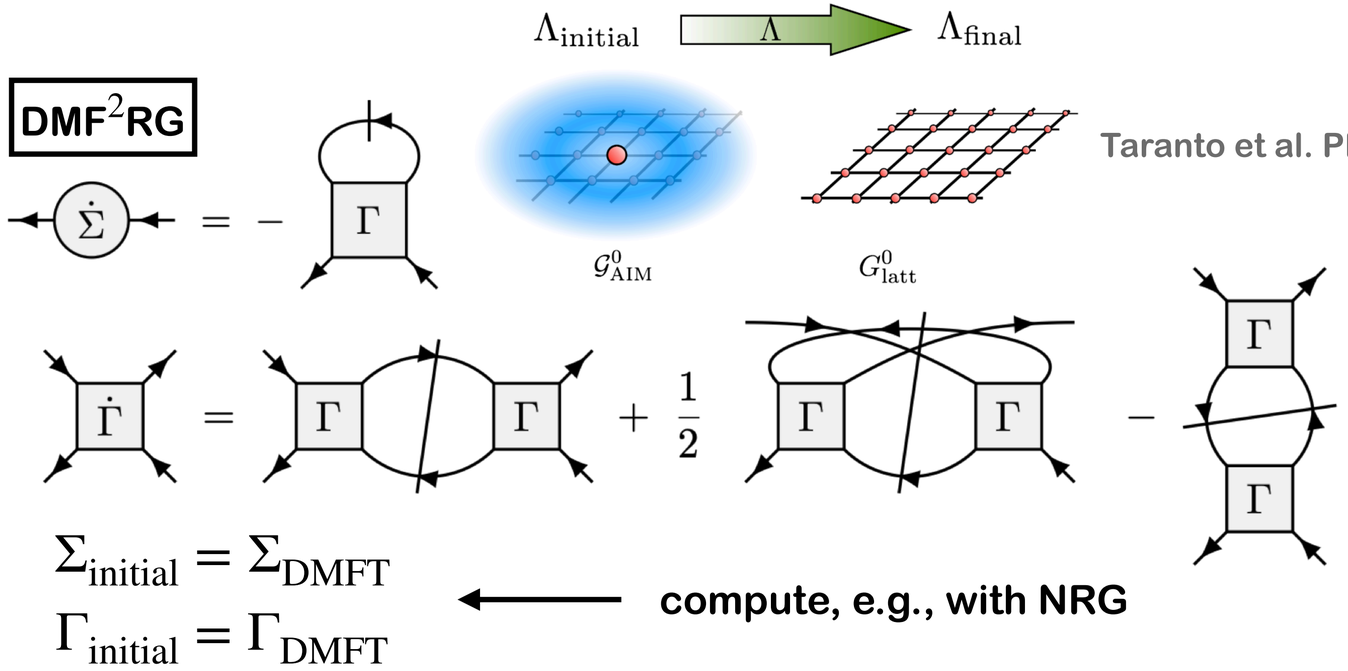
Diagrammatic extensions of DMFT

include non-local correlations
by field-theoretic methods with DMFT input
for local self-energy and 4-point vertex

$$G(\omega, \mathbf{k}) = [\omega - \varepsilon_{\mathbf{k}} - \Sigma(\omega, \mathbf{k})]^{-1}$$

Can use either fRG (→ DMF^{2}RG) or parquet (→DΓA)

Review: Rohringer et al., RMP (2018)



Taranto et al. PRL (2014)

$$\Sigma_{\text{initial}} = \Sigma_{\text{DMFT}}$$
$$\Gamma_{\text{initial}} = \Gamma_{\text{DMFT}}$$

← compute, e.g., with NRG

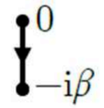
Issues:

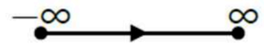
(1) How do we compute Γ with NRG?

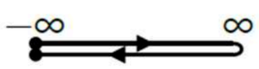
(2) Vertex $\Gamma_{\sigma_1'\sigma_2'|\sigma_1\sigma_2}(\omega_1, \omega_2, \omega_3; \mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3)$ becomes huge due to additional momentum dependence! How to resolve?

(1) Spectral representation of correlation functions $\langle O^1(t_1)\dots O^\ell(t_\ell)\rangle$

Matsubara | Zero temperature | Keldysh







Example: Consider ℓ-point correlator in the real-frequency zero-temperature formalism

$$\mathcal{G}(\mathbf{t}) = (-i)^{\ell-1}\langle \mathcal{T}\prod_{i=1}^{\ell} O^i(t_i)\rangle = \sum_p (\pm 1)^p \prod_{i=1}^{\ell-1}[-i\theta(t_{p(i)} - t_{p(i+1)})]\langle \prod_{i=1}^{\ell} O^{p(i)}(t_{p(i)})\rangle$$

convolution theorem

$$\Rightarrow \quad G(\omega) = 2\pi\delta(\omega_1 + \dots + \omega_\ell)\sum_p (\pm 1)^p \int \mathrm{d}^{\ell-1}\omega'_p \, K(\omega_p - \omega'_p)\, S[\mathbf{O}_p](\omega'_p)$$

convolution kernel — **partial spectral function (PSF)**

Matsubara:

$$K(\tau_p) = \prod_{i=0}^{\ell-1}[-\theta(\tau_{p(i)} - \tau_{p(i+1)})]$$

Zero temperature:

$$K(t_p) = \prod_{i=1}^{\ell-1}[-i\theta(t_{p(i)} - t_{p(i+1)})]$$

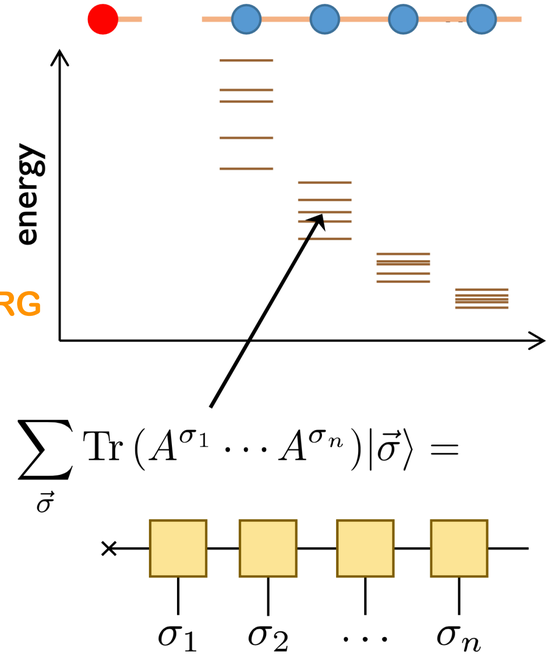
Keldysh:

$$K^{[\eta]}(\mathbf{t}_p) = \prod_{i=1}^{\eta-1}[i\theta(t_{p(i+1)} - t_{p(i)})]\prod_{i=\eta}^{\ell-1}[-i\theta(t_{p(i)} - t_{p(i+1)})]$$

anti-time-ordered (backward branch) | time-ordered (forward branch)

formalism-dependent	formalism-independent
system-independent	system-dependent: Lehmann representation through eigenstates and eigenenergies of the Hamiltonian

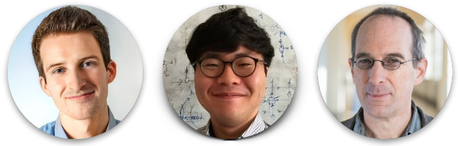
get from NRG



Two-stage computation:

(1) compute PSFs (e.g. using NRG)
(2) convolve PSFs with kernels

Use same PSFs in each formalism, only change kernels.



Kugler, Lee, von Delft, PRX 11, 041006 (2021)

(1) Diagrammatic consistency of NRG

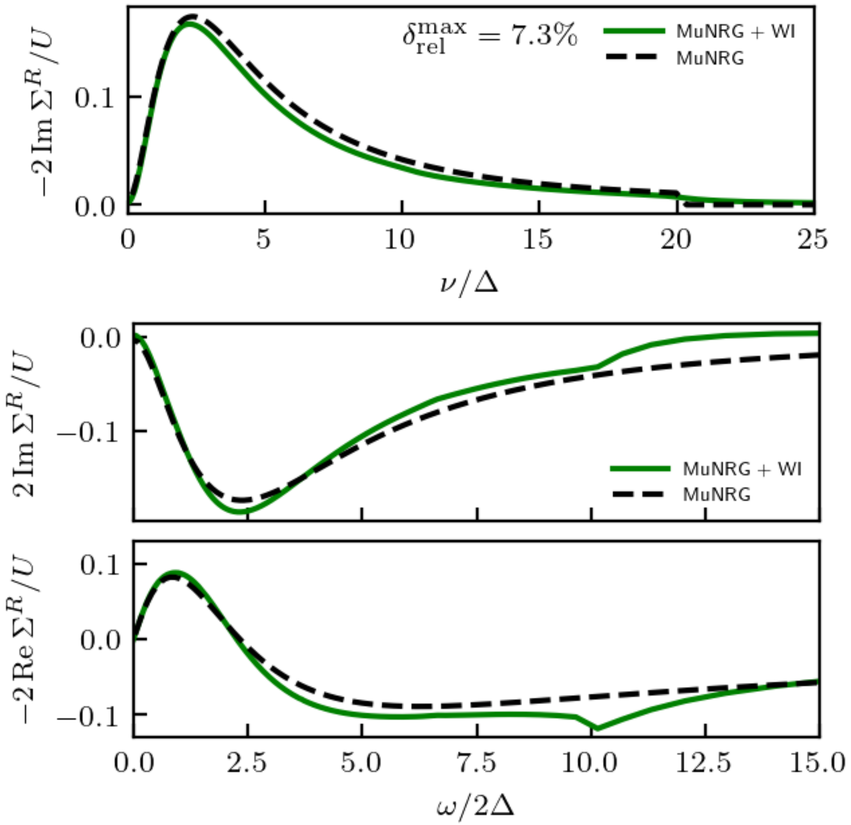
NRG knows nothing about equations from field theory.
Should fulfill them anyway if used as a starting point for diagrammatic calculations.

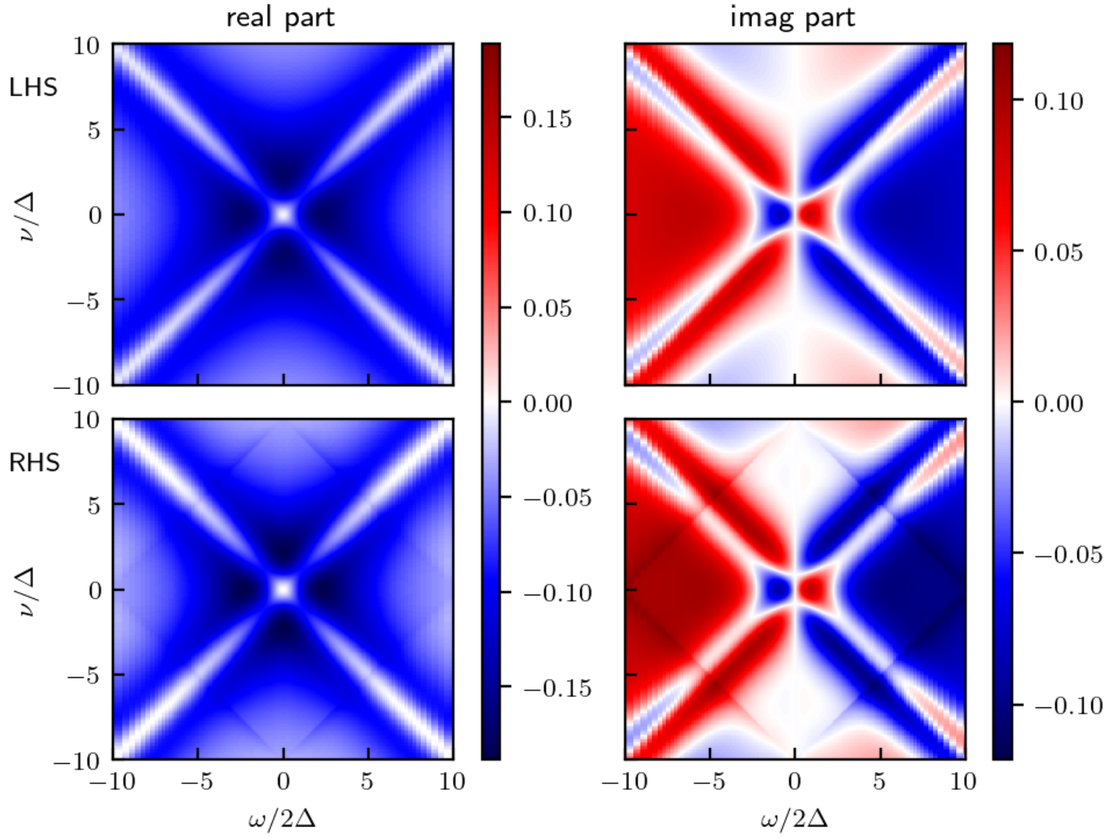
Example: U(1) Ward-identity (related to particle number conservation on the impurity):

PRELIMINARY!

$$i\Sigma^{\alpha_1'|\bar{\alpha}_1}(\nu-\tfrac{\omega}{2}) - i\Sigma^{\bar{\alpha}_1'|\alpha_1}(\nu+\tfrac{\omega}{2}) \stackrel{!}{=} \frac{1}{2\pi}\sum_{\alpha_2'\alpha_2\alpha_{\tilde{2}}}\int d\tilde{\nu}\Big\{\omega\; G^{\alpha_{\tilde{2}}|\alpha_{2'}}(\tilde{\nu}+\tfrac{\omega}{2})\Gamma^{\alpha_1'\alpha_{2'}|\alpha_2\alpha_1}_{\uparrow\uparrow+\overline{\uparrow\downarrow}}(\omega,\nu,\tilde{\nu})G^{\alpha_2|\alpha_{\tilde{2}}}(\tilde{\nu}-\tfrac{\omega}{2})$$
$$-\sum_{\alpha_{\tilde{1}}}\Big[\Delta^{\bar{\alpha}_{\tilde{2}}|\alpha_{\tilde{1}}}(\tilde{\nu}+\tfrac{\omega}{2})G^{\alpha_{\tilde{1}}|\alpha_{2'}}(\tilde{\nu}+\tfrac{\omega}{2})\Gamma^{\alpha_1'\alpha_{2'}|\alpha_2\alpha_1}_{\uparrow\uparrow+\overline{\uparrow\downarrow}}(\omega,\nu,\tilde{\nu})G^{\alpha_2|\alpha_{\tilde{2}}}(\tilde{\nu}-\tfrac{\omega}{2}) - G^{\alpha_{\tilde{2}}|\alpha_{2'}}(\tilde{\nu}+\tfrac{\omega}{2})\Gamma^{\alpha_1'\alpha_{2'}|\alpha_2\alpha_1}_{\uparrow\uparrow+\overline{\uparrow\downarrow}}(\omega,\nu,\tilde{\nu})G^{\alpha_2|\alpha_{\tilde{1}}}(\tilde{\nu}-\tfrac{\omega}{2})\Delta^{\alpha_{\tilde{1}}|\bar{\alpha}_{\tilde{2}}}(\tilde{\nu}-\tfrac{\omega}{2})\Big]\Big\}$$

Choice $\alpha_1 = \alpha_{1'} = 2,\ u = 0.5,\ T/U = 0.01$





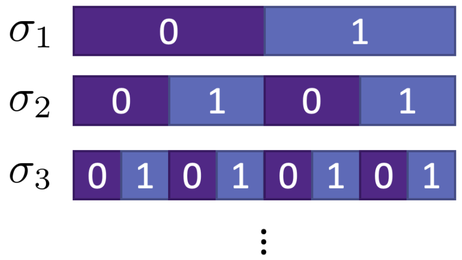
(2) Quantics Tensor Cross Interpolation (QTCI)

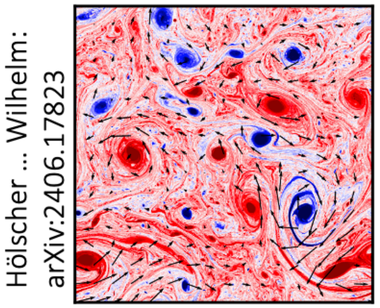
How to resolve $\Gamma_{\sigma_1'\sigma_2'|\sigma_1\sigma_2}(\omega_1, \omega_2, \omega_3; \mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3)$??

Quantics representation:

$$x = \frac{\sigma_1}{2^1} + \frac{\sigma_2}{2^2} + \ldots + \frac{\sigma_R}{2^R}$$

$$f(x) \to f(\sigma_1, \ldots, \sigma_R)$$

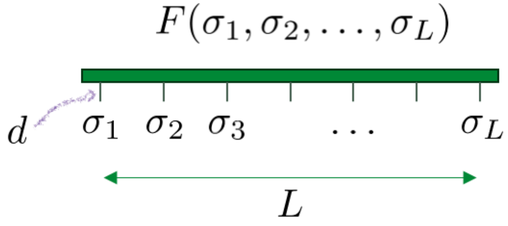




function $f(x_1, x_2, \ldots, x_L)$

discretization

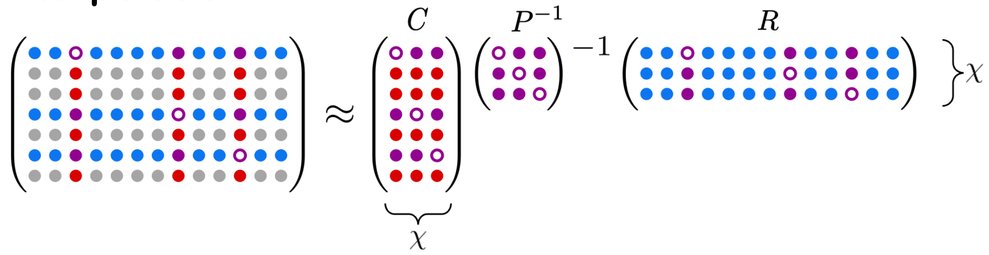
tensor $F(\sigma_1, \sigma_2, \ldots, \sigma_L)$



$O(d^L)$

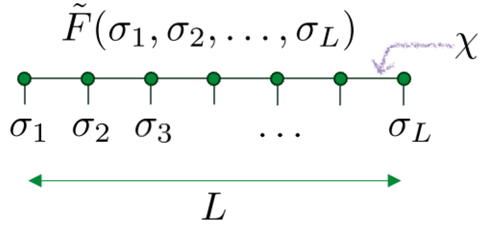
Matrix cross interpolation:

$$A = \left(\quad\right) \approx \left(\quad\right)^{C} \left(\quad\right)^{P^{-1}} \left(\quad\right)^{R}$$



factorization

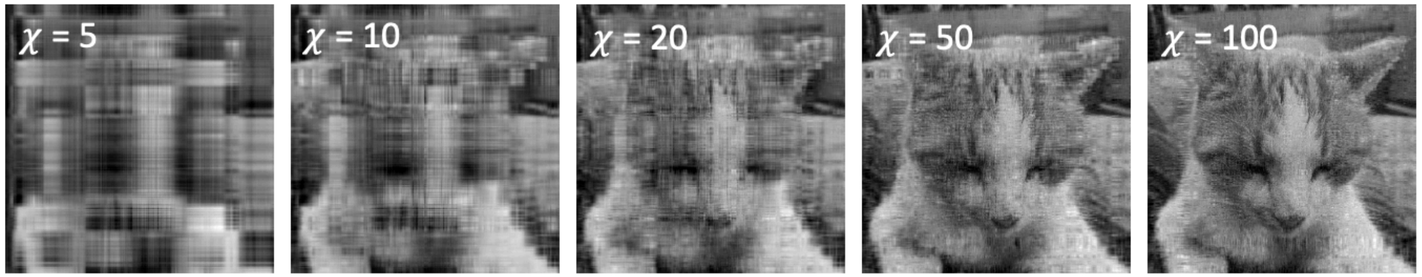
tensor train $\tilde{F}(\sigma_1, \sigma_2, \ldots, \sigma_L)$



$O(d\chi^2 L)$

generalizes to higher dimensions

Can afford exponential resolution at linear cost!
(provided χ is bounded)

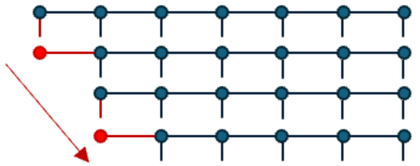


I. V. Oseledets, Dokl Math 2009; B. N. Khoromskij, Constr Approx 2011
Shinaoka, Wallerberger, Murakami, Nogaki, Sakurai, Werner, Kauch, PRX 2023
Ritter, Nuñez Fernández, Wallerberger, von Delft, Shinaoka, Waintal: Phys. Rev. Lett. 132 (2024)

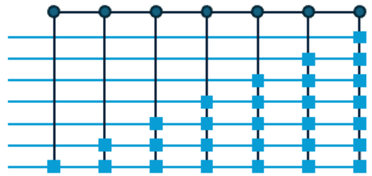
Algorithms

Tensor train construction via TCI: $O(\chi^3 L)$

Integrals $\int_{I^d} \mathrm{d}^d\mathbf{x}\, f(\mathbf{x})$: $O(\chi^2 L)$



Fourier transform: $O(\chi^3 L)$



Integral transform: $O(\chi^4 L)$

$$f(\mathbf{x},\mathbf{z}) = \int_{I^d} \mathrm{d}^d\mathbf{y}\, g(\mathbf{x},\mathbf{y}) h(\mathbf{y},\mathbf{z})$$

Multiplication: $O(\chi^4 L)$

$$f(\mathbf{x},\mathbf{y},\mathbf{z}) = g(\mathbf{x},\mathbf{y}) h(\mathbf{y},\mathbf{z})$$

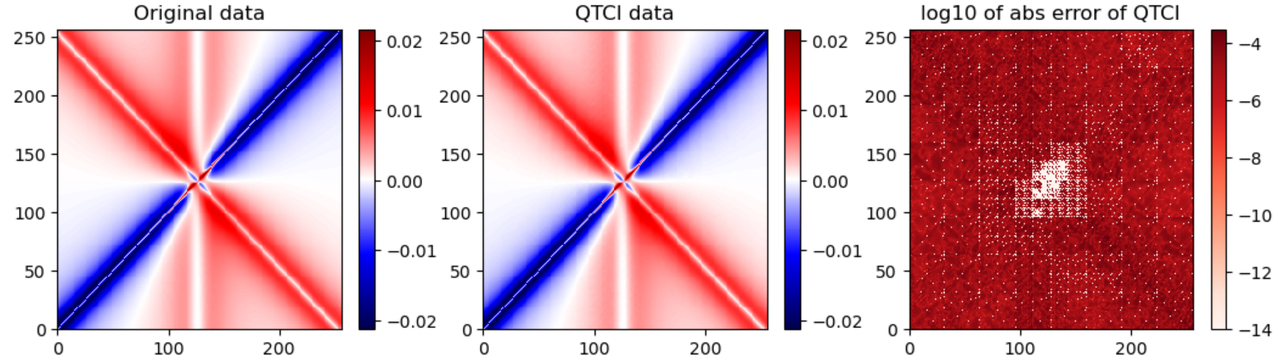
Addition, subtraction, coordinate transform, …

Open-Source Libraries:

https://tensor4all.org

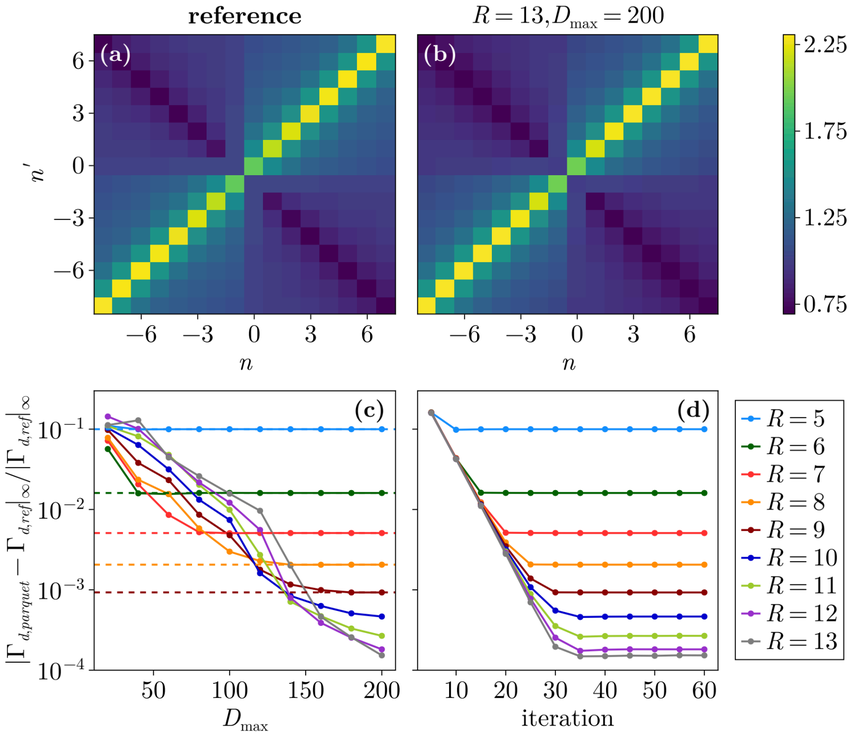
Nuñez Fernández, Ritter, Jeannin, Li, Kloss, Louvet, Terasaki, Parcollet, von Delft, Shinaoka, Waintal: arXiv:2407.02454

Application to the Keldysh vertex (preliminary!)



$\chi \lesssim 70$ **sufficient! (worst case:** $\chi = 4096$**)**

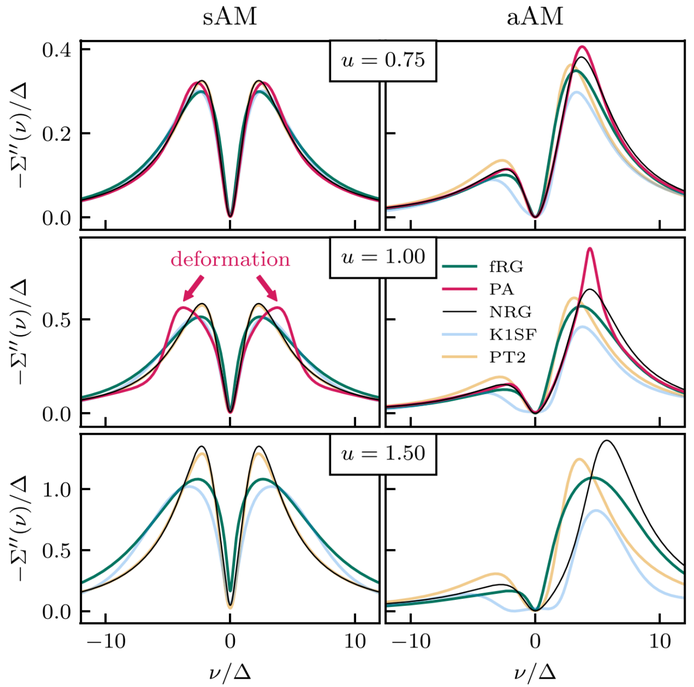
Very recent: Proof-of-principle study on solving the parquet equations (Matsubara formalism)

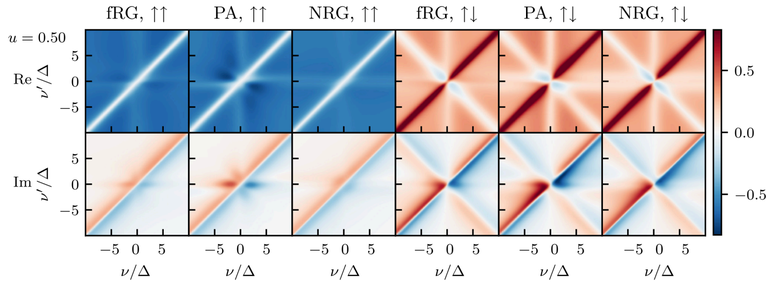


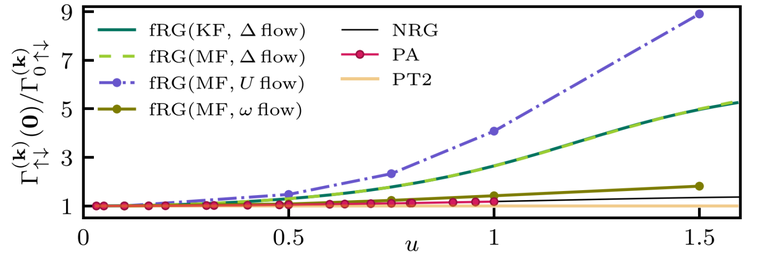
Rohshap, Ritter, Shinaoka, von Delft, Wallerberger, Kauch, arXiv:2410.22975

Summary

- multi-point correlation functions play a crucial role in condensed matter physics
- real-frequency QFT with full frequency resolution of the vertex Γ is feasible
  → full frequency dependence improves accuracy
- PA gives best agreement, where available
- fRG more economical, but less accurate







Next steps

- Combine local calculations from NRG with diagrammatic computations, extended to include non-local correlation effects
- Make sure NRG computations are consistent with diagrammatic equations
- Use compression techniques such as QTCI to keep the required numerical resources in check
- Long-term: Apply to realistic materials!