

Multipoint correlation functions: spectral representation, numerical evaluation, and improved estimators

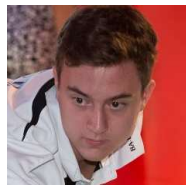
Jan von Delft

Fabian Kugler, Seung-Sup Lee, Jan von Delft, Phys. Rev. X **11**, 041006 (2021)

Seung-Sup Lee, Fabian Kugler, Jan von Delft, Phys. Rev. X **11**, 041007 (2021)

Jae-Mo Lihm, Johannes Halbinger, Jeongmin Shim, Jan von Delft, Fabian Kugler, Seung-Sup Lee, Phys. Rev. B **109**, 125138 (2024)

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



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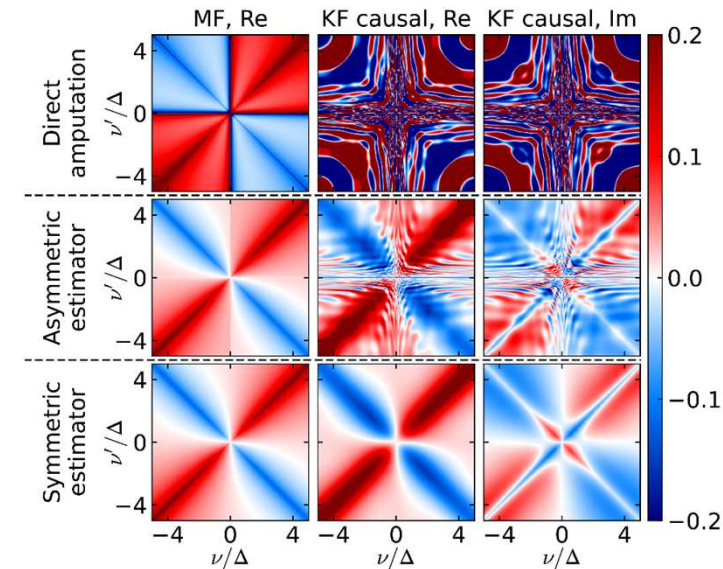
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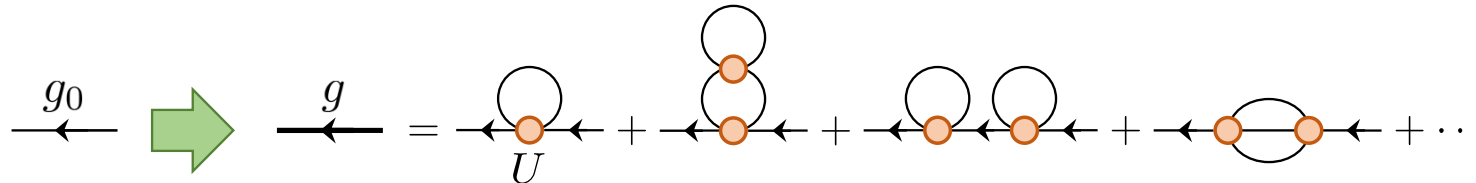
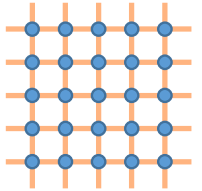


Acknowledgement: many slides are borrowed from Jae-Mo Lihm & Seung-Sup Lee

- Why multi-point functions?
- Limitations of purely field-theoretical approaches for strong-coupling problems
- Spectral representations
- NRG for local multi-point correlators
- Improved estimators for self-energy and 4-point vertices
- Outlook

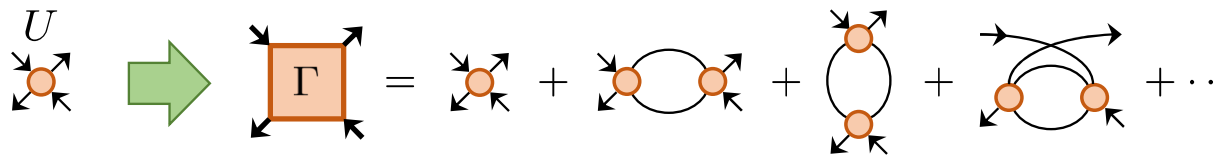
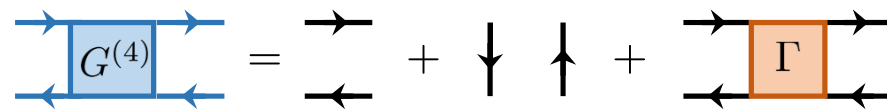
Why multipoint correlation functions?

- Dynamical properties are encoded in correlation functions
- Two-point functions: local density of states, spectral function, ...



- Four-point functions: magnetic susceptibility, conductivity, ...

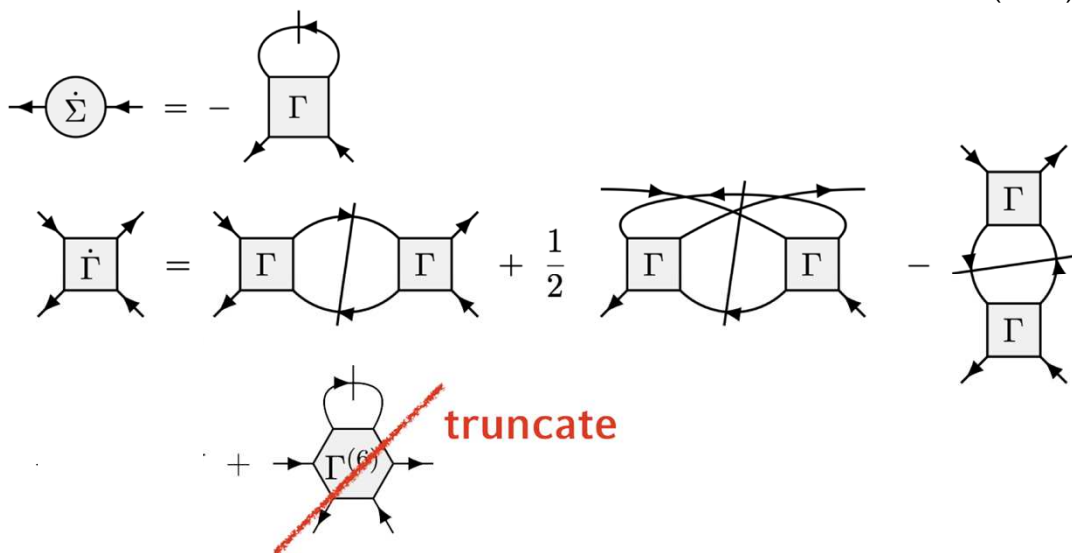
$$\underbrace{\langle c_{\sigma}^{\dagger}(\mathbf{x}_1, t_1^+) c_{\sigma'}(\mathbf{x}_1, t_1) \rangle}_{\mathbf{S}(\mathbf{x}_1, t_1)} \underbrace{\langle c_{\sigma'}^{\dagger}(\mathbf{x}_2, t_2^+) c_{\sigma}(\mathbf{x}_2, t_2) \rangle}_{\mathbf{S}(\mathbf{x}_2, t_2)} \quad \underbrace{\langle c_{\sigma}^{\dagger}(\mathbf{x}_1^+, t_1^+) c_{\sigma'}(\mathbf{x}_1, t_1) \rangle}_{\mathbf{j}(\mathbf{x}_1, t_1)} \underbrace{\langle c_{\sigma'}^{\dagger}(\mathbf{x}_2^+) c_{\sigma}(\mathbf{x}_2, t_2) \rangle}_{\mathbf{j}(\mathbf{x}_2, t_2)}$$



$F_{\sigma\sigma'}(\mathbf{k}_1, \omega_1; \mathbf{k}_2, \omega_2; \mathbf{k}_3, \omega_3)$: 4-point vertex: energy-dependent effective interaction (needed as function of real frequencies)

1-loop fRG

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



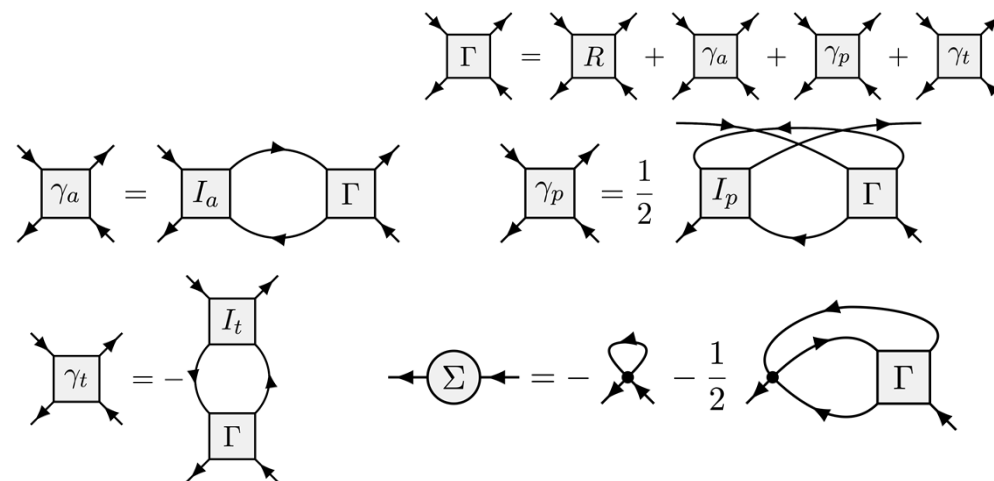
fRG flow:

$$G_0 \rightarrow G_0^\Lambda, \quad \Lambda_{\text{initial}} \rightarrow \Lambda_{\text{final}}$$

$$\Sigma^R|_{\Lambda=\infty} = \Sigma_{\text{Hartree}}, \quad \Gamma|_{\Lambda=\infty} = \Gamma_0$$

Parquet formalism

Review: Bickers (2004)



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

- **multi-loop fRG**: ensures that $\dot{\Gamma}$ = total derivative; integrating flow yields regulator-independent results; sums up all parquet diagrams in parquet approximation

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



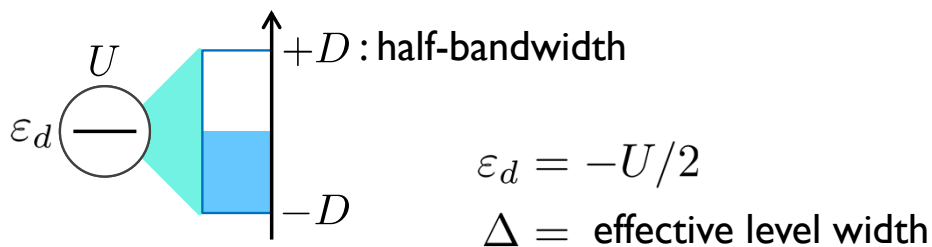
Fabian Kugler

Benchmark study of 1-loop fRG vs. parquet approximation (PA) vs. NRG

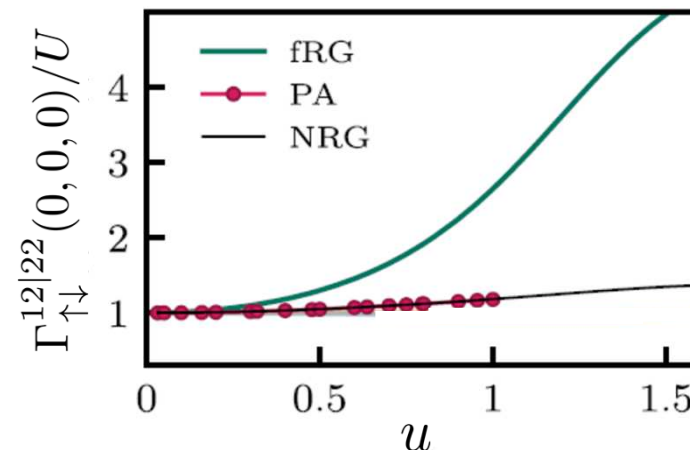
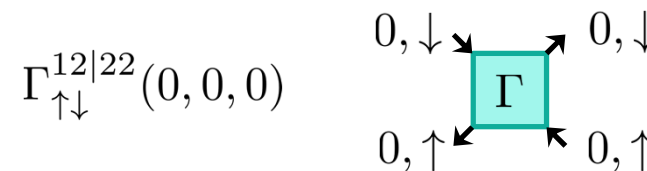
Ge, Ritz, Walter, Aguirre, von Delft, Kugler, PRB **109**, 115128 (2024)

Single-impurity Anderson model

$$H = \sum_{\sigma} \varepsilon_d d_{\sigma}^{\dagger} d_{\sigma} + U d_{\uparrow}^{\dagger} d_{\uparrow} d_{\downarrow}^{\dagger} d_{\downarrow} + \sum_{k\sigma} \varepsilon_k c_{k\sigma}^{\dagger} c_{k\sigma} + \sum_{k\sigma} v (d_{\sigma}^{\dagger} c_{k\sigma} + c_{k\sigma}^{\dagger} d_{\sigma})$$



Kondo temperature: $T_K = \sqrt{\Delta U/2} \exp[-\pi (\frac{U}{8\Delta} + \frac{\Delta}{U})]$



vary $u = U/(\pi\Delta)$ at fixed $T/U = 0.01$

- Low-energy properties of this model can be computed essentially exactly using the numerical renormalization group (NRG)
- Use fRG / PA / NRG to compute $\Gamma_{\uparrow\downarrow}^{12|22}(\nu = 0, \nu' = 0, \omega = 0)$
- Conclusion: 1-loop fRG and parquet both fail for $u > 1$
- both 1-loop fRG and parquet approximation do not yield non-perturbative results

Dynamical mean field theory (DMFT)

treat local correlations exactly
by solving self-consistent impurity model

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



extensions of DMFT

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

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

Examples:

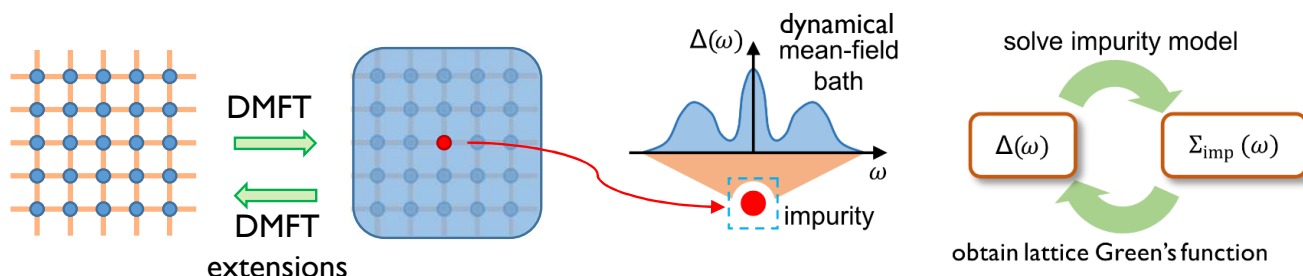
dynamical vertex approximation Held et al. (2008)

dual fermions Havermann et al. (2008)

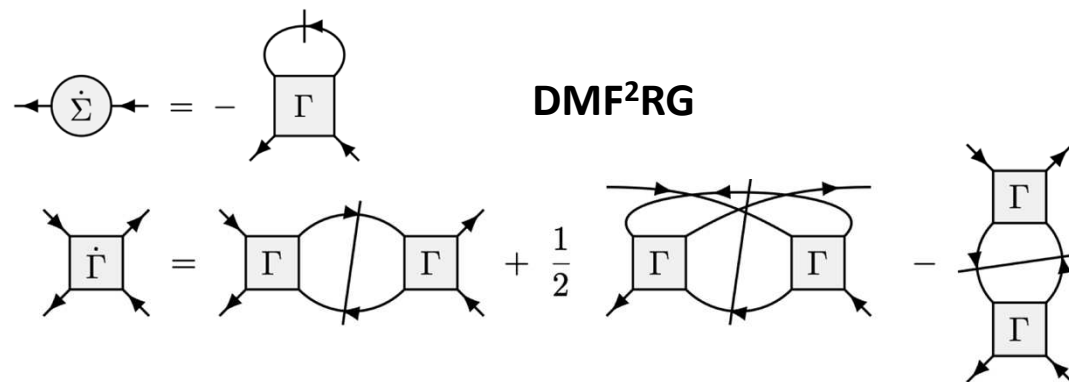
DMF²RG Taranto et al. (2014), Vilardi et al. (2019), poster by Marcel Schäfer

self-consistent parquet Lihm et al. (to be published)

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



Review: Rohringer et al, RMP (2018), Benchmark: Schäfer et al, PRX (2021)



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

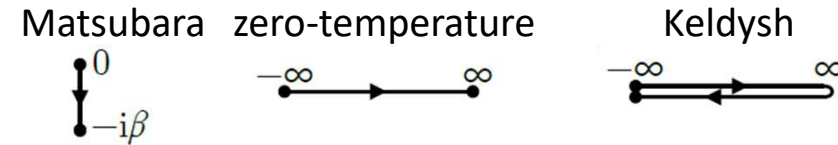
needed: local 2- and 4-point correlators
(full frequency dependence!)

this talk →

General multipoint functions $\langle O^1(t_1) \dots O^\ell(t_\ell) \rangle$: spectral representations

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

- General & unifying: any ℓ , all frequency formalisms
- **Ex:** ℓ -point (ℓp) correlator, real-freq. zero-temp. formalism



$$\mathcal{G}(t) = (-i)^{\ell-1} \left\langle \mathcal{T} \prod_{i=1}^{\ell} O^i(t_i) \right\rangle$$

$$= \sum_p (\pm 1)^p \prod_{i=1}^{\ell-1} [-i\theta(t_{p(i)} - t_{p(i+1)})] \left\langle \prod_{i=1}^{\ell} O^{p(i)}(t_{p(i)}) \right\rangle$$

convolution theorem:

Fourier trafo.

$$\mathcal{G}(\omega) = 2\pi\delta(\omega_{1\dots\ell}) \sum_p (\pm 1)^p \int d^{\ell-1}\omega'_p K(\omega_p - \omega'_p) S[\mathcal{O}_p](\omega'_p)$$

$\omega_{1\dots\ell} = \omega_1 + \dots + \omega_\ell$

convolution kernel

formalism-dependent

system-independent

partial spectral function (PSF)

formalism-independent

system-dependent, has Lehmann representation through eigenstates, eigenenergies of Hamiltonian

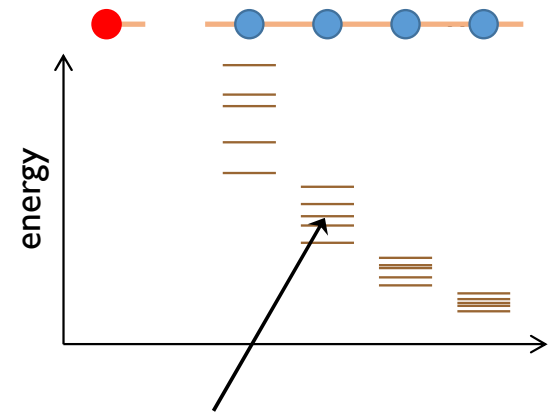


Fabian Kugler

- Two-stage computation: (1) compute PSF; (2) convolve PSF with kernels

→ Different formalisms or frequencies: same PSF, only change kernels

Quantum impurity models: Numerical renormalization group (NRG)



■ Logarithmic discretization: Wilson chain Wilson, *RMP* (1975); Bulla, Costi, Pruschke, *RMP* (2008)

■ Iterative diagonalization: complete basis of energy eigenstates Anders, Schiller, *PRL* (2005)

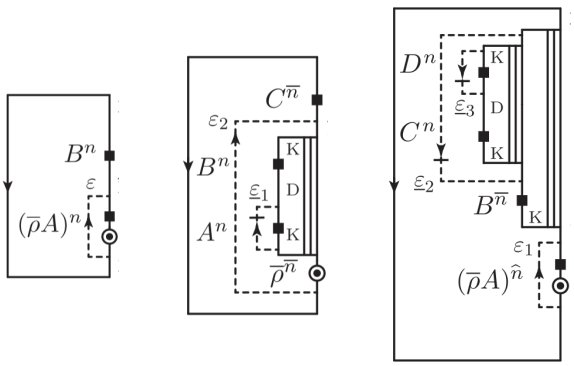
■ Tensor network formulation: many-body states as matrix product states (MPS) Weichselbaum, *PRB* (2012)

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

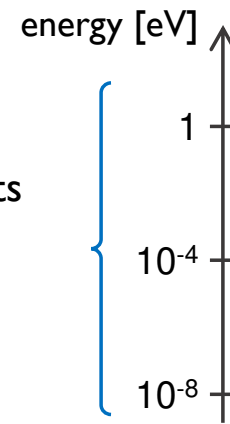
■ (Partial) spectral functions:

two-point: { Peters, Pruschke, Anders, *PRB* (2006)
Weichselbaum, von Delft, *PRL* (2007)

multipoint: Lee, Kugler, von Delft, *PRX* 11, 041007 (2021)



ε_i : PSF arguments
 ν, ν', ω : frequencies
 T : temperature



Andreas Weichselbaum



Seung-Sup Lee

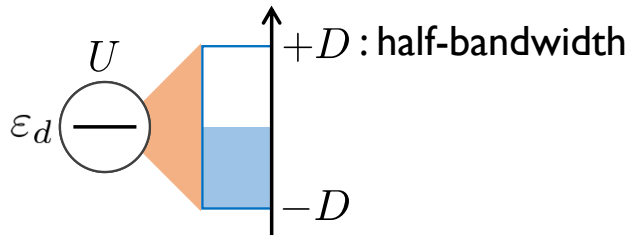
Vertex of Anderson impurity model (AIM)

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



Seung-Sup Lee

$$H = \sum_{\sigma} \varepsilon_d d_{\sigma}^{\dagger} d_{\sigma} + U d_{\uparrow}^{\dagger} d_{\uparrow} d_{\downarrow}^{\dagger} d_{\downarrow} + \sum_{k\sigma} \varepsilon_k c_{k\sigma}^{\dagger} c_{k\sigma} + \sum_{k\sigma} v (d_{\sigma}^{\dagger} c_{k\sigma} + c_{k\sigma}^{\dagger} d_{\sigma})$$



$$\varepsilon_d = -U/2$$

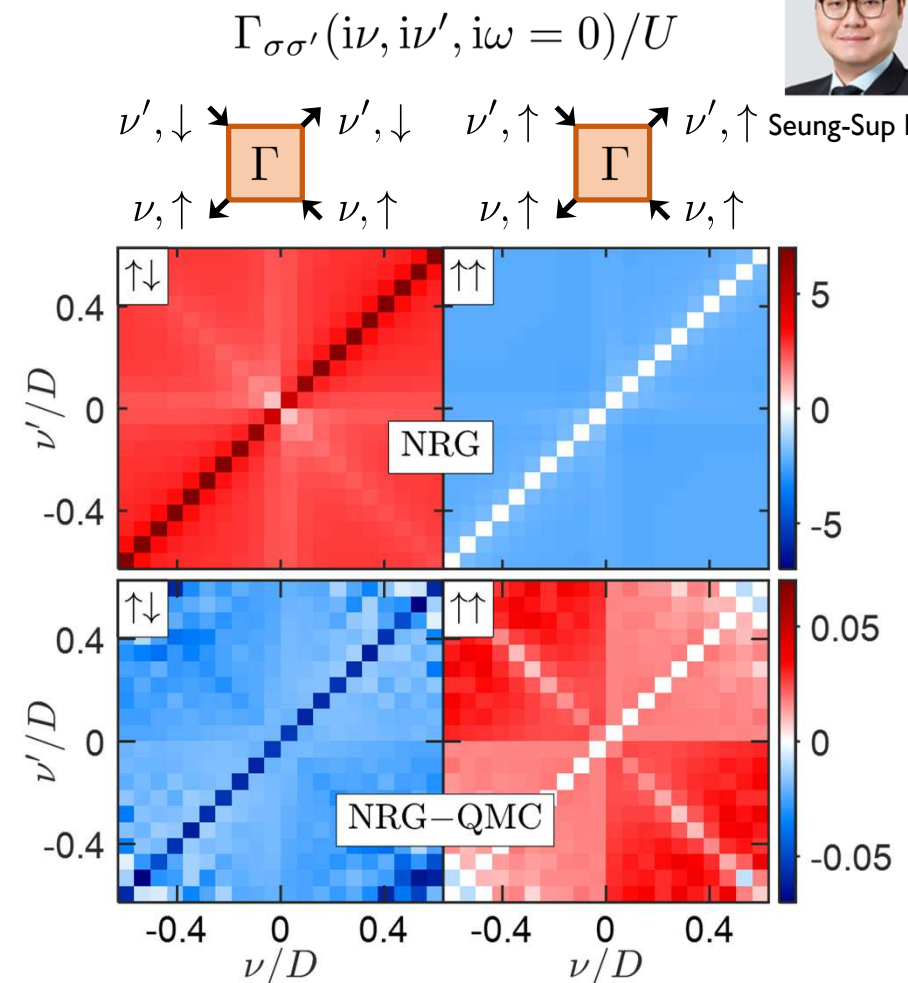
$$U = 0.2D$$

$$\Delta = 0.04D$$

Kondo temperature: $T_K \simeq 5 \times 10^{-3} D$

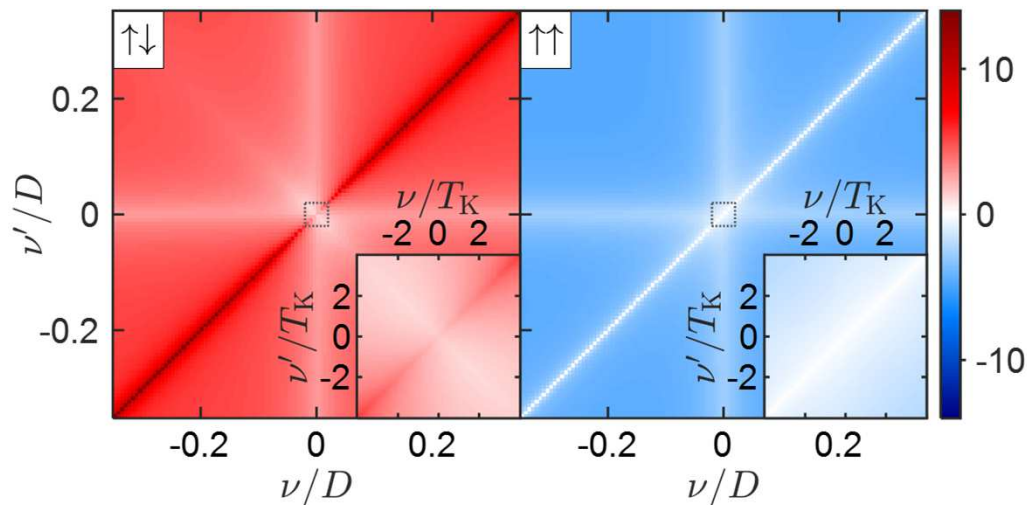
- Benchmark imaginary-frequency vertex against quantum Monte Carlo (QMC) by Toschi group (TU Wien) $T = 0.01D > T_K$ Chalupa et al, *PRB* (2018); *PRL* (2021)

	QMC	NRG
imaginary frequency	○	○
accuracy against statistical noise	△	○
low temperature	×	○
real frequency	×	○

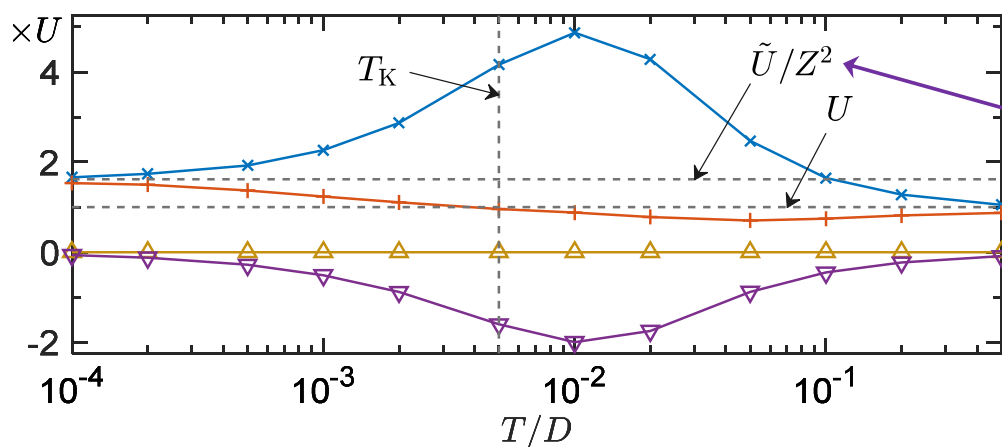


Vertex of Anderson impurity model (AIM)

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



$\times \Gamma_{\uparrow\downarrow}(\pm 1, \pm 1, 0)$
 $+\Gamma_{\uparrow\downarrow}(\pm 1, \mp 1, 0)$
 $\triangle \Gamma_{\uparrow\uparrow}(\pm 1, \pm 1, 0)$
 $\nabla \Gamma_{\uparrow\uparrow}(\pm 1, \mp 1, 0)$



$$T = 10^{-4} D$$

Kondo temperature: $T_K \simeq 5 \times 10^{-3} D$

- stronger features at higher freq.;
reduced at lower freq.
- $T \gg U$: bare vertex $U\delta_{\bar{\sigma}\sigma'}$
- $T \simeq T_K$: most pronounced correlation effects
- $T \ll T_K$: Fermi liquid

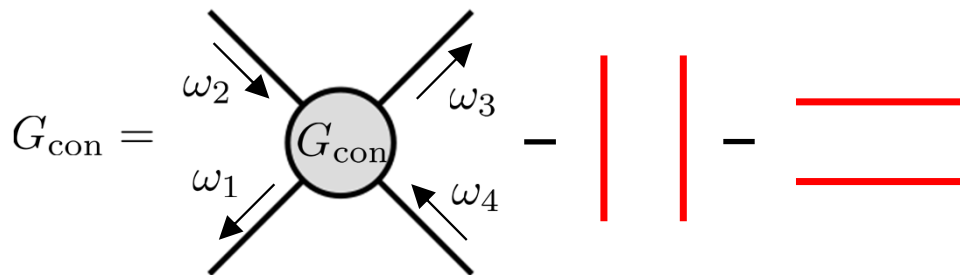
Renormalized perturbation theory (RPT) parameters:
 $\tilde{U} \simeq 0.20U, Z \simeq 0.36$

**From strongly interacting particles to
weakly interacting quasiparticles!**

Challenges when calculating 4-point vertex $G = \langle \mathcal{T} d(t_1)d^\dagger(t_2)d(t_3)d^\dagger(t_4) \rangle$

$$g(\omega) = G[d, d^\dagger](\omega)$$

- Subtraction of the disconnected part

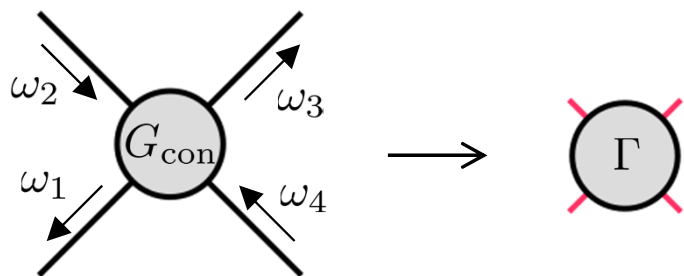


$$G_{\text{con}}(\omega_1, \omega_2, \omega_3, \omega_4) = G_{\text{tot}}(\omega_1, \omega_2, \omega_3, \omega_4) - ig(\omega_1)g(\omega_3)[\delta(\omega_1 + \omega_4) - \delta(\omega_1 + \omega_2)]$$

in the non-interacting limit: $G_{\text{tot}} = G_{\text{dis}}$
 $G_{\text{con}} = 0$

requires numerically delicate cancellations

- Amputation of external legs



$$\Gamma(\omega_1, \omega_2, \omega_3, \omega_4) = \frac{G_{\text{con}}(\omega_1, \omega_2, \omega_3, \omega_4)}{g(\omega_1)g(-\omega_2)g(\omega_3)g(-\omega_4)}$$

large-frequency limit $\sim \frac{U/\omega^4}{1/\omega^4} = U \quad (\omega \gg 1)$

requires numerically delicate cancellations

Remedy: use improved estimators!

Lihm, Halbinger, Shim, von Delft, Kugler, Lee, PRB **109**, 125138 (2024)

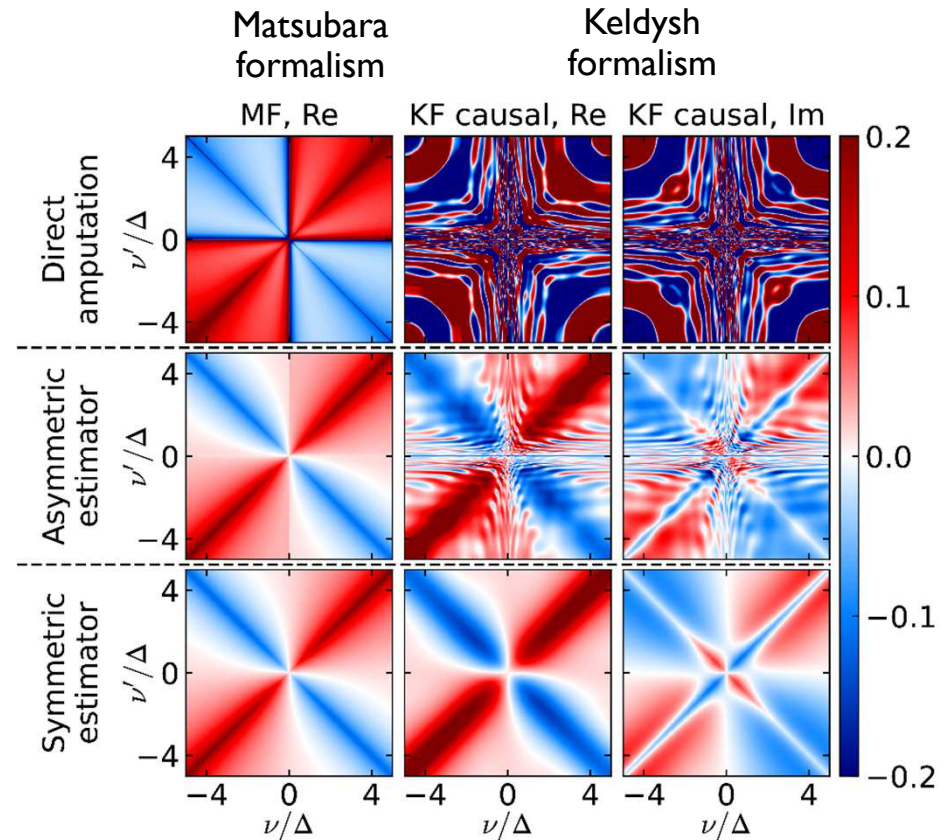
“improved estimator” is formally equivalent to desired function, but yields better cancellation of numerical artifacts;

can be derived using equations of motion (EOM)

amputate external legs by division:

use equation of motion for one operator:

use equations of motion for four operators:



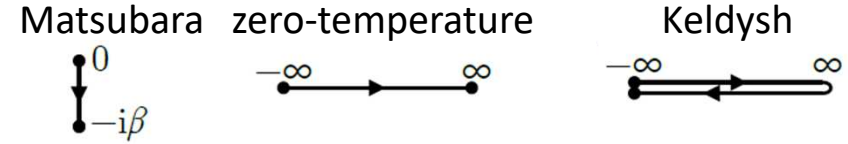
Seung-Sup Lee



Jae-Mo Lihm

EOM for 2-point propagator

$$G[d_1, d_2^\dagger](t_1, t_2) = -i \langle \mathcal{T} d_1(t_1) d_2^\dagger(t_2) \rangle$$



- EOM of a time-ordered correlator: $i \frac{\partial}{\partial t_1} G[d_1, d_2^\dagger](t_1, t_2) = \delta(t_1 - t_2) \delta_{12} + G[[d_1, H], d_2^\dagger](t_1, t_2)$
 $\{d_1, d_2^\dagger\} = \delta_{12}$
- EOM in frequency domain: $\omega G[d_1, d_2^\dagger](\omega) = \delta_{12} + G[[d_1, H], d_2^\dagger](\omega)$

$$H_0 = \sum_{\sigma} \varepsilon_d d_{\sigma}^{\dagger} d_{\sigma} + \sum_{k\sigma} \varepsilon_k c_{b\sigma}^{\dagger} c_{k\sigma} + \sum_{k\sigma} (v_k d_{\sigma}^{\dagger} c_{k\sigma} + \text{H.c.}), \quad H_{\text{int}} = U d_{\uparrow}^{\dagger} d_{\uparrow} d_{\downarrow}^{\dagger} d_{\downarrow}$$

$$\Delta(\omega) = \sum_k \frac{|v_k|^2}{\omega - \varepsilon_k}$$

$$\underbrace{(\omega - \varepsilon_d - \Delta(\omega))}_{(g^0)^{-1}} G[d_{\sigma}, d_{\sigma'}^{\dagger}](\omega) = \delta_{\sigma\sigma'} + G[q_{\sigma}, d_{\sigma'}^{\dagger}](\omega)$$

$$q_{\sigma} = [d_{\sigma}, H_{\text{int}}] = U d_{\sigma} d_{-\sigma}^{\dagger} d_{-\sigma}$$

$$G[d_{\sigma}, d_{\sigma'}^{\dagger}](\omega) = g^0 \delta_{\sigma\sigma'} + g^0 G[q_{\sigma}, d_{\sigma'}^{\dagger}](\omega)$$

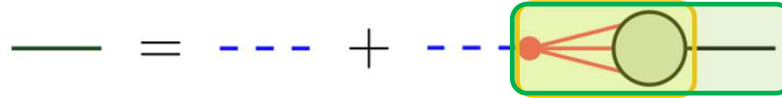


Asymmetric estimator for self-energy

- 1st-order EOM

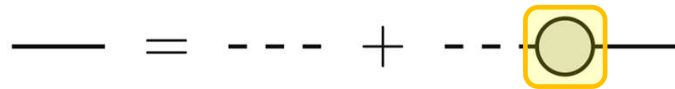
$$g(\omega) = G[d_\sigma, d_{\sigma'}^\dagger](\omega) = g^0 \delta_{\sigma\sigma'} + g^0 \boxed{G[q_\sigma, d_{\sigma'}^\dagger](\omega)}$$

$$\begin{aligned} q_\sigma &= [d_\sigma, H_{\text{int}}] \\ &= U d_\sigma d_{-\sigma}^\dagger d_{-\sigma} \end{aligned}$$

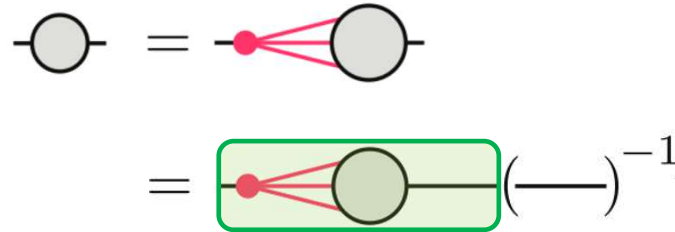


- Dyson equation

$$g = g^0 + g^0 \Sigma g$$



compare:



- Asymmetric improved estimator

(equivalent to the Schwinger-Dyson equation)

$$\Sigma = G[q_\sigma, d_\sigma^\dagger] g^{-1}$$

known as “Bulla trick” in NRG community

Improved estimators for multi-point functions

- We want the improved estimators to be
 - (A) **Symmetric**: symmetric in all indices of the vertex, and
 - (B) **Full**: Involving only full correlators (not the bare ones)

	2-point self-energy $\Sigma(\nu)$	4-point vertex $\Gamma(\nu, \nu', \omega)$
asymmetric, full	Bulla et al. (1998)	Hafermann et al. (2012)
symmetric , bare	Kaufmann et al. (2019)	Kaufmann et al. (2019)
symmetric, full	Kugler (2022)	Lihm et al. (2024)

← our work



Jae-Mo Lihm

(1-leg) EOM for multipoint correlator



Jae-Mo Lihm

2-point correlator:

$$(g^0)^{-1}G[d_1, d_2^\dagger] = \delta_{12} + G[q_1, d_2^\dagger] \quad \{d_1, d_2^\dagger\} = \delta_{12}$$

from differentiation time-ordering theta functions

ℓ -point correlator:

$$G[d_1, O^2, \dots, O^\ell](\mathbf{t}) = (-i)^{\ell-1} \langle \mathcal{T} d_1(t_1) O^2(t_2) \dots O^\ell(t_\ell) \rangle$$

$$(g^0)^{-1}G[d_1, O^2, \dots, O^\ell] = \sum_{n=2}^{\ell} G[O^2, \dots, [d_1, O^n]_{\zeta_n}, \dots, O^\ell] + G[q_1, O^2, \dots, O^\ell]$$

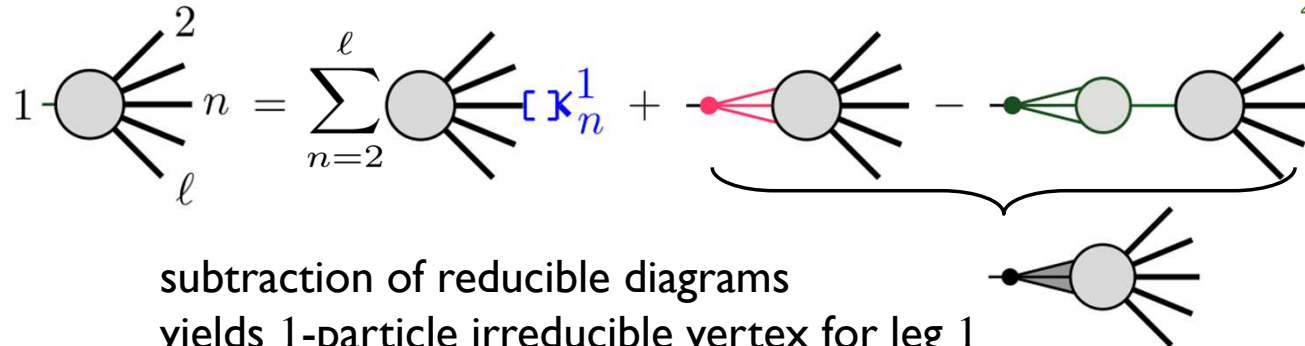
from differentiation time-ordering theta functions

$$(g^0)^{-1} = g^{-1} + \Sigma$$

amputation of one external leg on left side!
(without using $(g^0)^{-1}$ or g^{-1} on right side!)

$$g^{-1}G[d_1, \dots] = \sum_{n=2}^{\ell} G[\dots [d_1, O^n]_{\zeta_n}, \dots] + G[q_1, \dots](\omega) - \Sigma G[d_1, \dots]$$

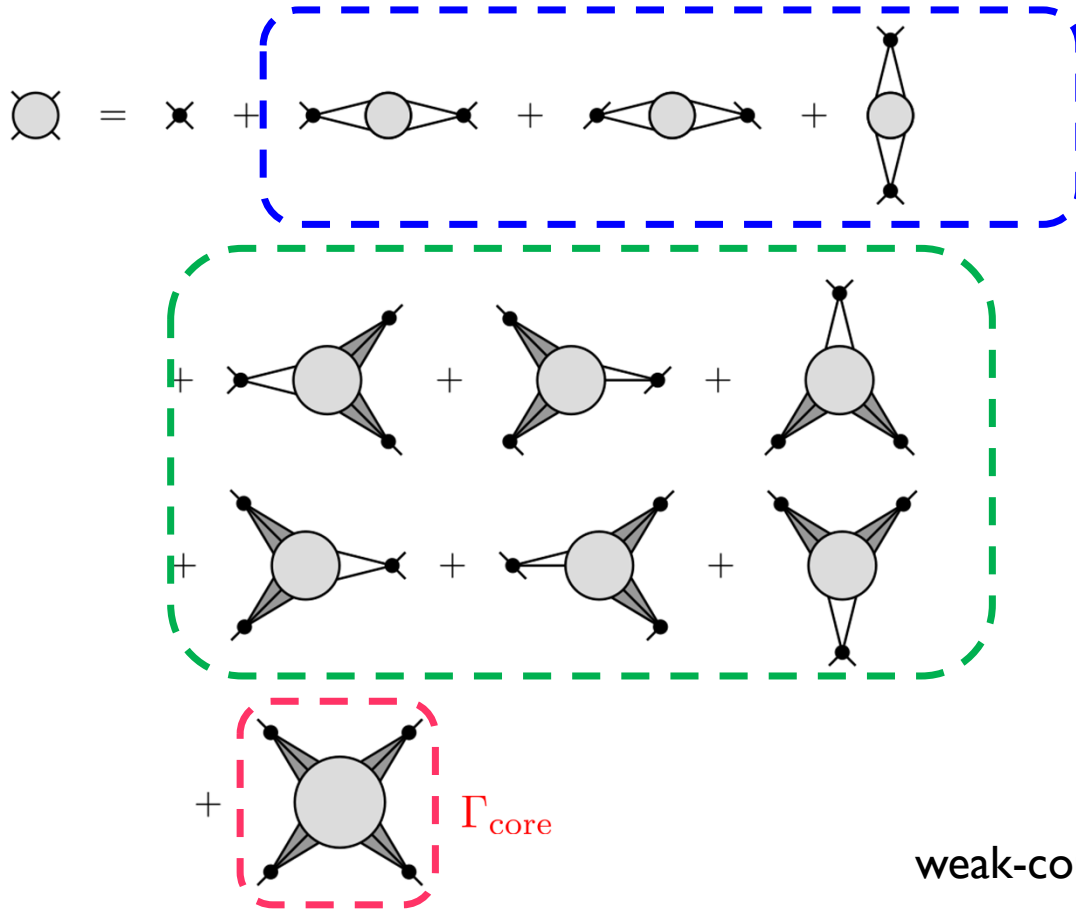
$$\Sigma = G[q_\sigma, d_\sigma^\dagger]g^{-1}$$



subtraction of reducible diagrams yields 1-particle irreducible vertex for leg 1

Symmetric improved estimator for 4-point vertex

$$\Gamma = g_1^{-1} g_3^{-1} G[d_1^\dagger, d_2^\dagger, d_3^\dagger, d_4^\dagger] g_2^{-1} g_4^{-1}$$



$$\Gamma(\nu, \nu'; \omega) = \Gamma_{\text{bare}} + \sum_{r=\text{ph,pp,ph}} \mathcal{K}_1^r(\omega_r)$$

$$+ \sum_{r=\text{ph,pp,ph}} \mathcal{K}_2^r(\nu_r; \omega_r) + \mathcal{K}_{2'}^r(\nu'_r; \omega_r)$$

$$+ \Gamma_{\text{core}}(\nu, \nu'; \omega)$$



Jae-Mo Lihm

asymptotic classes [Wentzell et al. (2020)]

emerge naturally and are computed separately

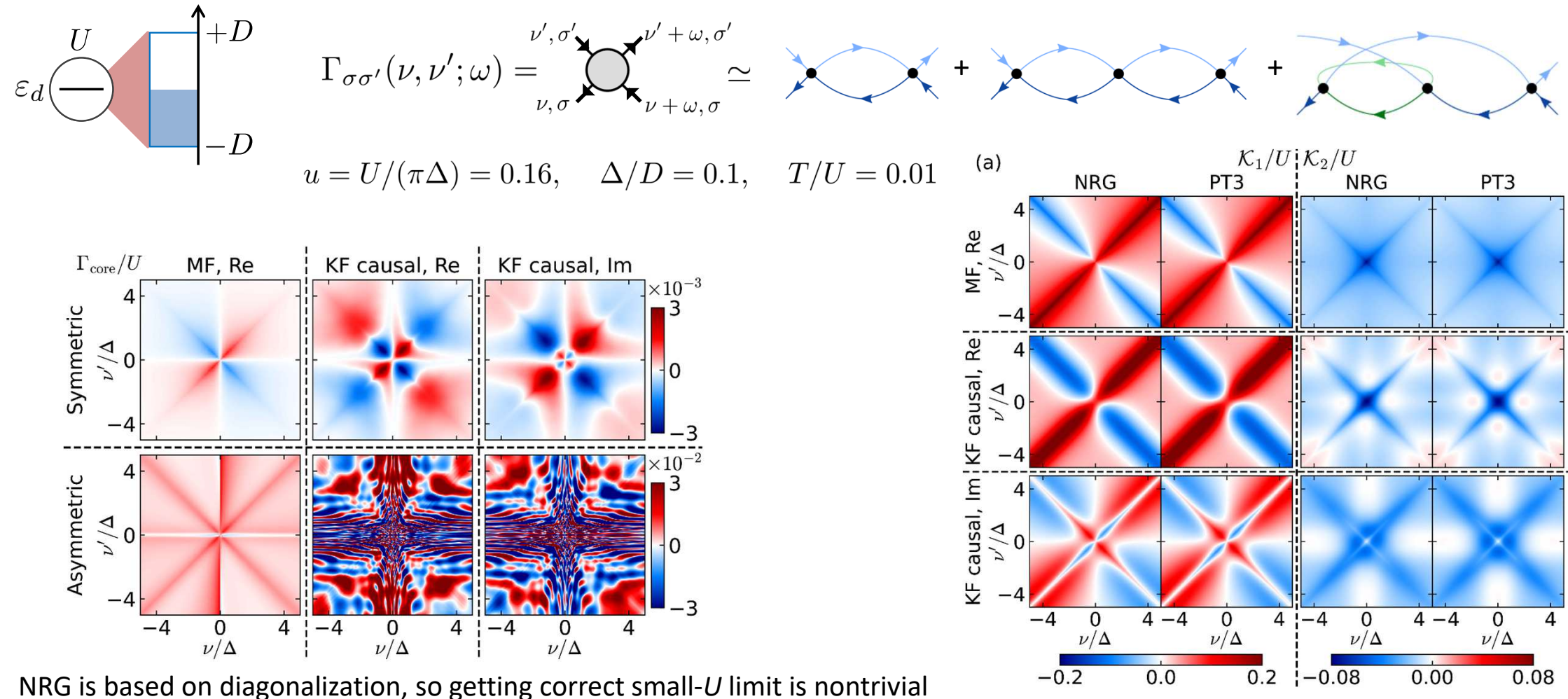
$$\lim_{|\omega| \rightarrow \infty} \mathcal{K}_1(\omega) = 0$$

$$\lim_{|\nu| \rightarrow \infty} \mathcal{K}_2(\nu; \omega) = \lim_{|\omega| \rightarrow \infty} \mathcal{K}_2(\nu; \omega) = 0$$

$$\lim_{|\nu| \rightarrow \infty} \Gamma_{\text{core}} = \lim_{|\nu'| \rightarrow \infty} \Gamma_{\text{core}} = \lim_{|\omega| \rightarrow \infty} \Gamma_{\text{core}} = 0$$

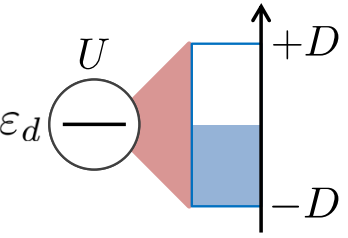
weak-coupling limit: $\mathcal{K}_1 = \mathcal{O}(U^2)$, $\mathcal{K}_2 = \mathcal{O}(U^3)$, $\Gamma_{\text{core}} = \mathcal{O}(U^4)$

SIAM at weak coupling: benchmark NRG vs. 3rd-order perturbation theory (PT3)



NRG is based on diagonalization, so getting correct small- U limit is nontrivial

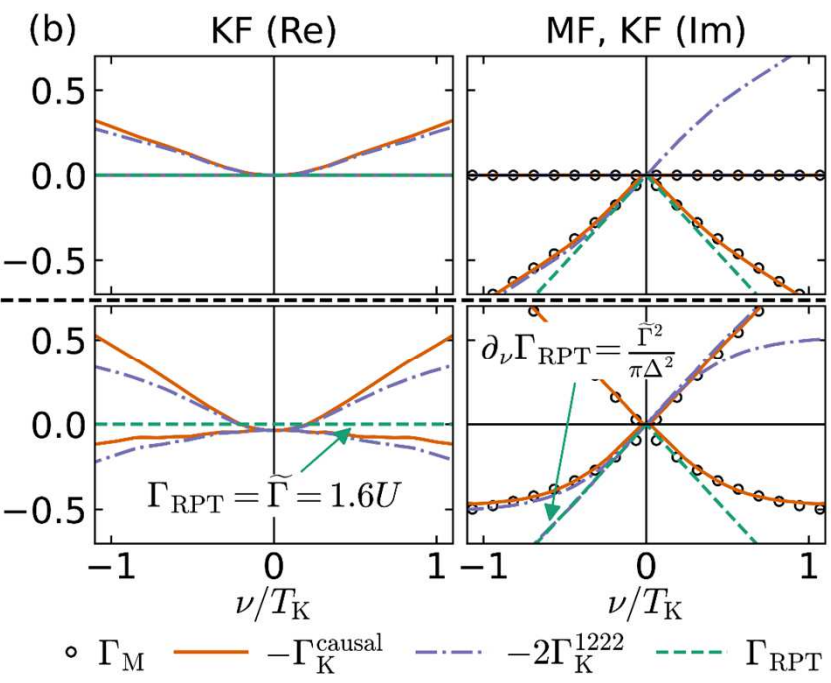
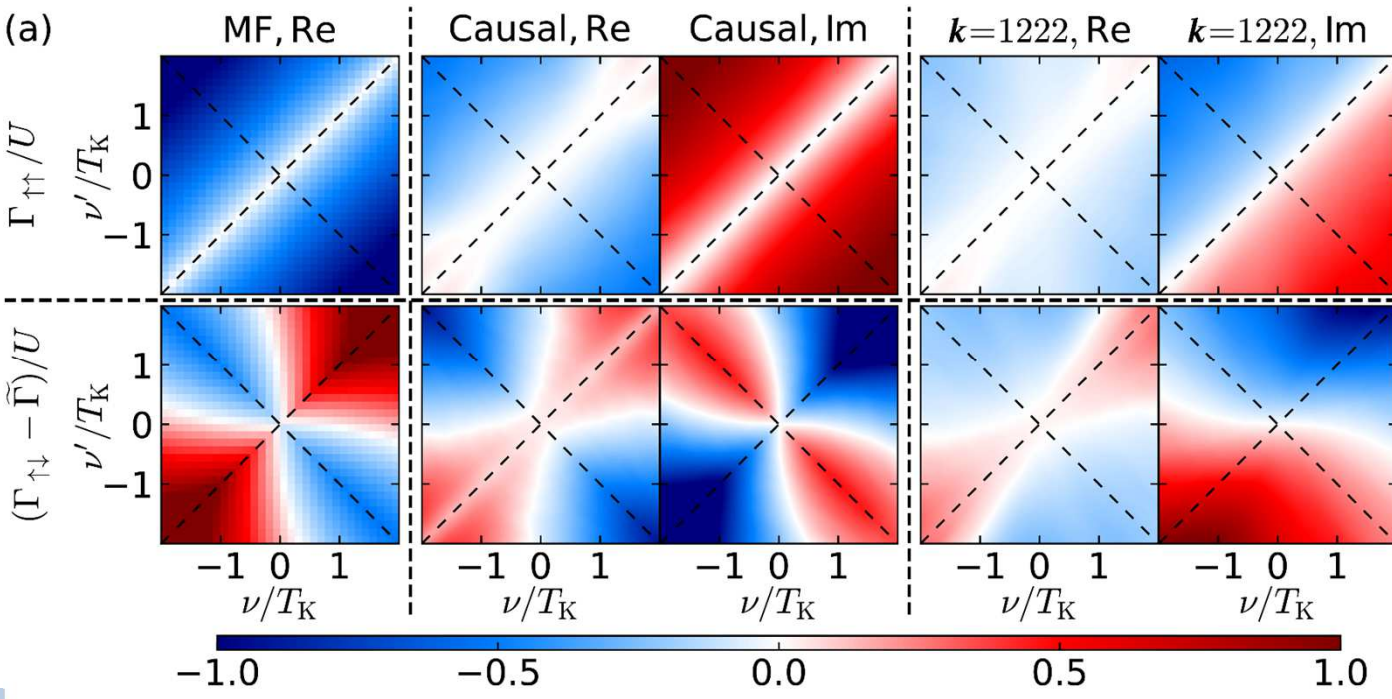
SIAM at strong coupling: benchmark NRG vs. renormalized perturbation theory (RPT)



$$\Gamma_{\sigma\sigma'}(\nu, \nu'; \omega) = \text{diagram}$$

$u = U/(\pi\Delta) = 1.6, \quad \Delta/D = 0.04, \quad T/U = 0.0025$

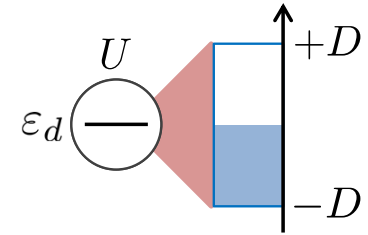
- $T = 0.029T_K$: Fermi-liquid regime
- Low-frequency vertex is consistent with RPT (a Fermi-liquid theory) for both $\Gamma(0,0,0)$ and slope



Ward identity



Nepomuk Ritz



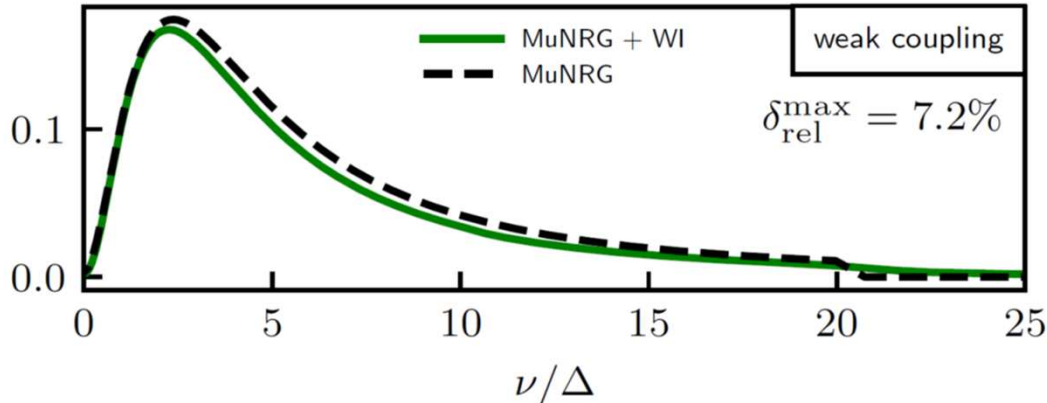
$$\Gamma_{\sigma\sigma'}(\nu, \nu'; \omega) = \text{Diagram of a four-point vertex with incoming lines } (\nu, \sigma) \text{ and } (\nu', \sigma') \text{ and outgoing lines } (\nu + \omega, \sigma) \text{ and } (\nu' + \omega, \sigma')$$

$$u = U/(\pi\Delta) = 0.5, \quad \Delta/D = 0.04, \quad T/U = 0.01$$

Ward identity: $2 \text{Im}\Sigma^R(\nu) = \frac{1}{i\pi} \int_{-\infty}^{\infty} d\tilde{\nu} \text{Im} \Delta^R(\tilde{\nu}) G^R(\tilde{\nu}) G^A(\tilde{\nu}) \left\{ \Gamma_{\uparrow\downarrow+\uparrow\uparrow}^{12|21}(\tilde{\nu}, \nu|\nu, \tilde{\nu}) \right.$

$$\left. - [1 - 2n_F(\tilde{\nu})] \left[\Gamma_{\uparrow\downarrow+\uparrow\uparrow}^{12|22}(\tilde{\nu}, \nu|\nu, \tilde{\nu}) - \Gamma_{\uparrow\downarrow+\uparrow\uparrow}^{22|21}(\tilde{\nu}, \nu|\nu, \tilde{\nu}) \right] \right\}$$

$$-2 \text{Im} \Sigma^R / U$$

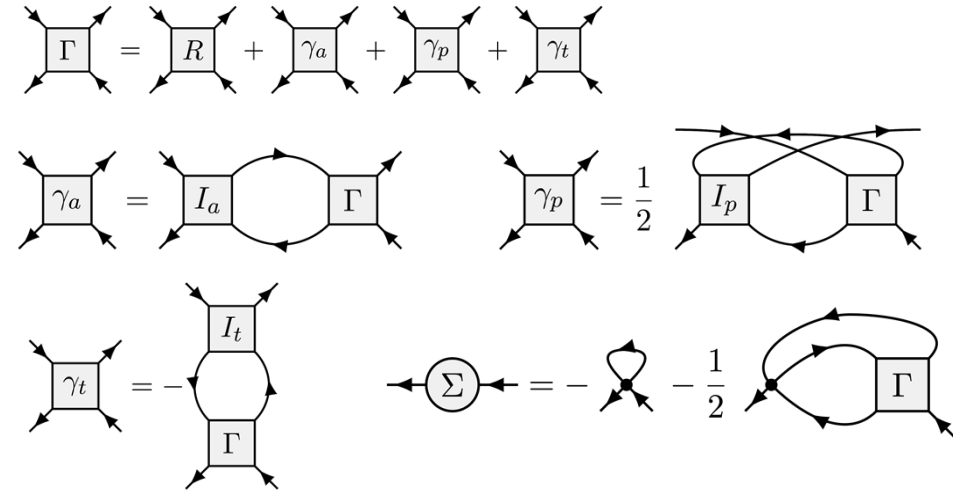


NRG results for self-energy and vertex satisfy Ward identity to within 7% !

This is highly non-trivial consistency check, since Ward identity involves integral over entire frequency axis.

Outlook: Going beyond impurity model – non-local extensions of DMFT

- Main methodological result: full frequency dependence of impurity models is accessible !
- Next steps: tackle non-local extensions of DMFT
- diagrammatic vertex approximation (DΓA)
- or DMF²RG
- parquet formalism
- Input: 4-point vertex of the impurity Hamiltonian



$$R = R_{\text{DMFT}}$$

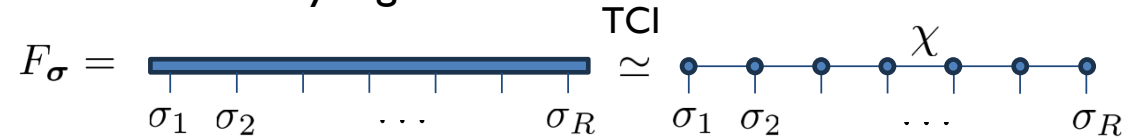
- Major challenge: vertex is “big object”, with huge memory costs. Can it be compressed?

Outlook: Compression via Tensor Cross Interpolation (TCI)

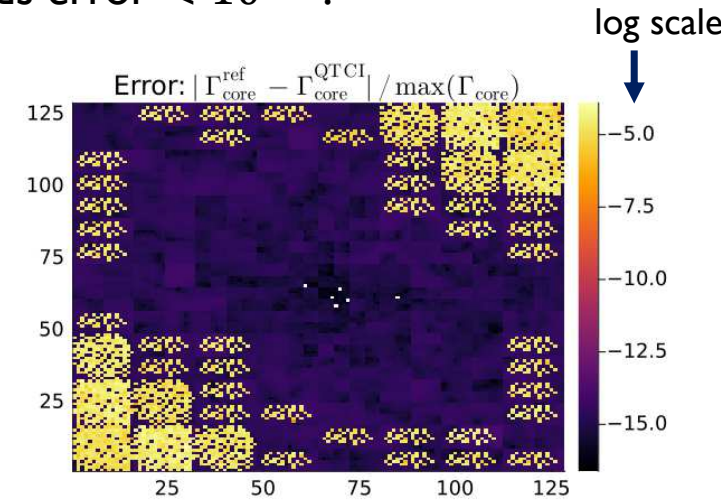
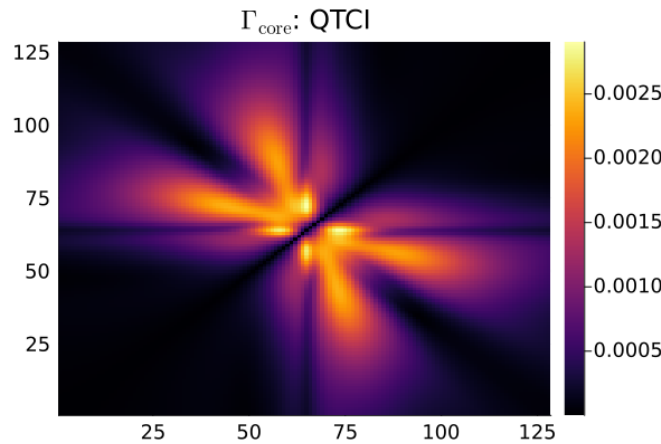
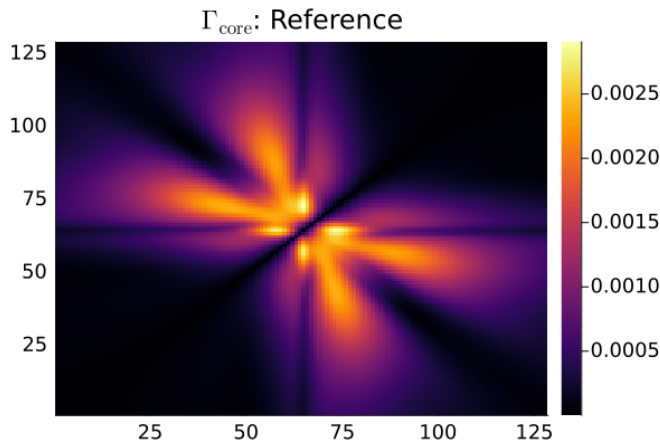
- Discretized functions can be expressed as tensors
- Sometimes, these tensors are compressible
- TCI is efficient scheme for finding compressed representation in form of a tensor train

$$f(x) = f(\sigma_1, \dots, \sigma_R) = F_{\sigma_1, \dots, \sigma_R} \quad \sigma_\ell \in \{0, 1\}$$

binary digits



- Vertices of impurity models are compressible: bond dimension $\chi \leq 500$ yields error $< 10^{-5}$!



- Outlook for DMFT extensions: use TCI representation of vertices !