Equilibrium and non-equilibrium properties of quantum impurities: Insight from diagrammatic Monte Carlo methods on the real-time contour

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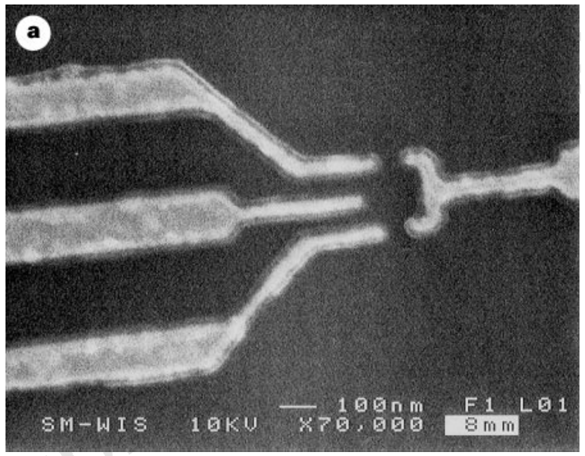
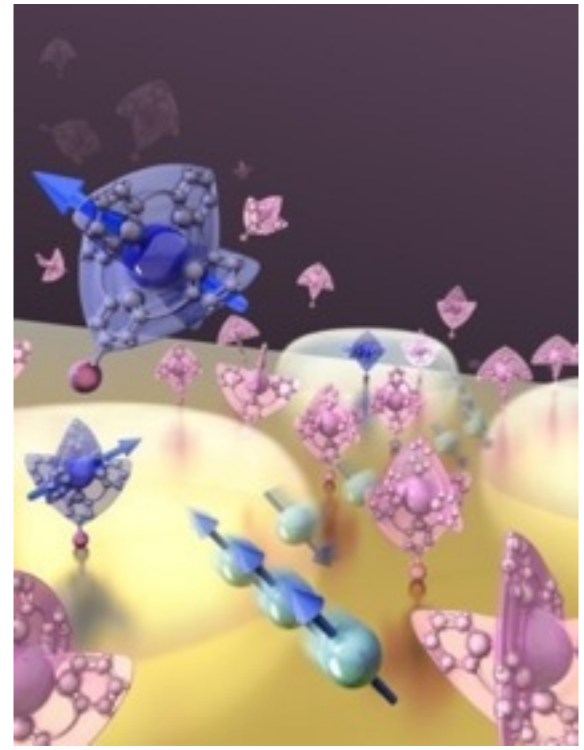
Phys. Rev. B 82, 075109 (2010)
Phys. Rev. B 84, 085134 (2011)
Rev. Mod. Phys 83, 349 (2011)
Phys. Rev. B 87, 195108 (2013)
Phys. Rev. B 89, 115139 (2014)
Phys. Rev. Lett. 112, 146802 (2014)

The non-equilibrium Kondo problem

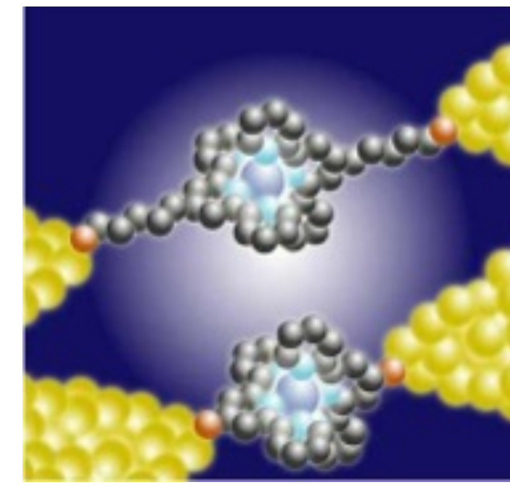


Kondo effect in a single-electron transistor, D. Goldhaber-Gordon et al, Nature 391, 156 (1998)

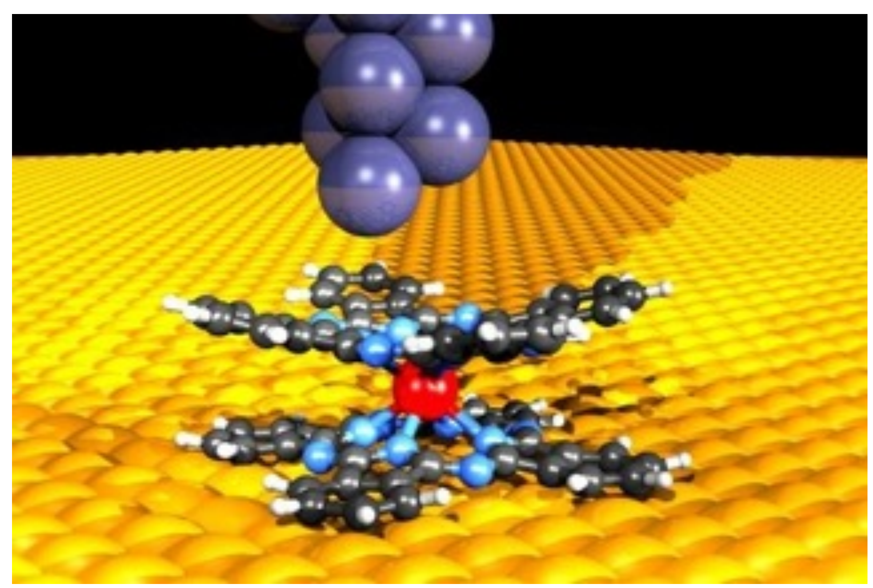


Magnetic impurities in non-magnetic bulk

Coulomb blockade and the Kondo effect in single-atom transistors, Park et al, Nature 416, 722 (2002)

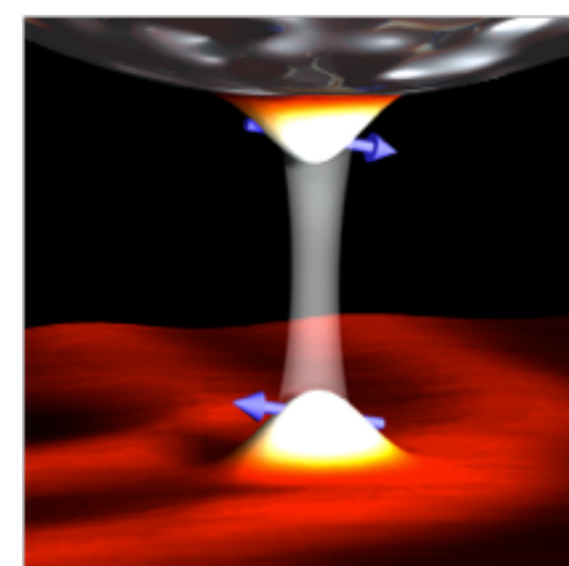


Double quantum dots

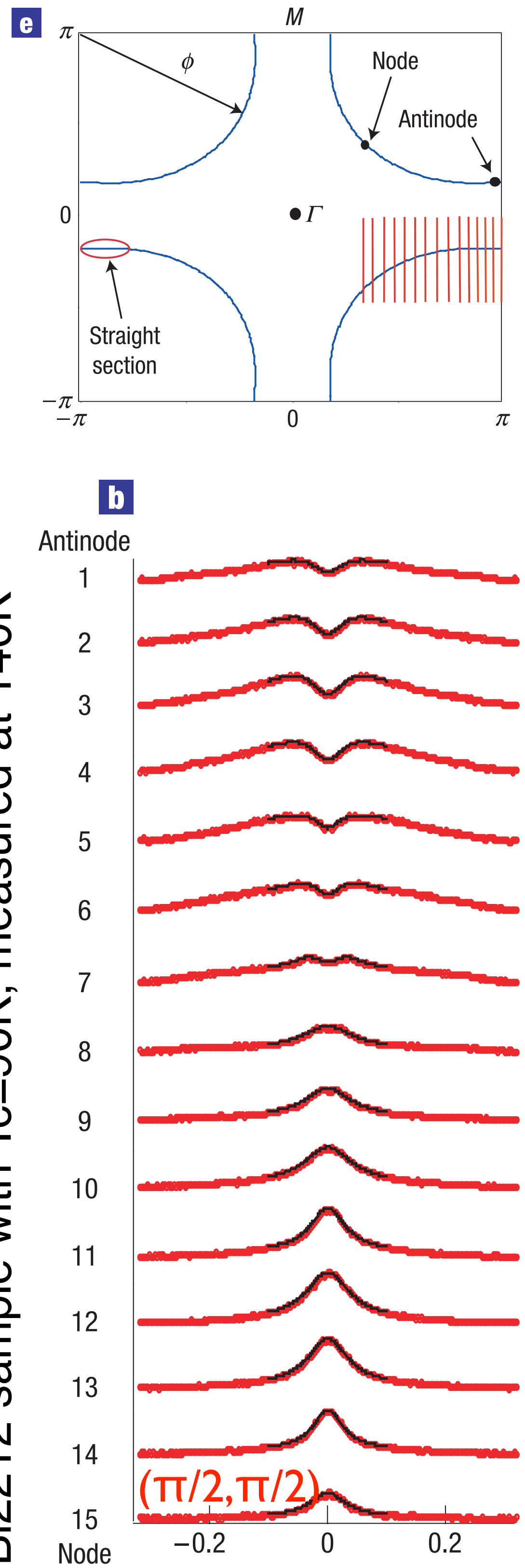


Magnetic molecules adsorbed on surfaces, e.g. Fahrendorf et al, Nature Communications 4, 2425

Two-impurity Kondo systems in atomic point contacts: Bork et al, Nat. Phys. 7, 901 (2011)



ARPES: Spectral function of solids



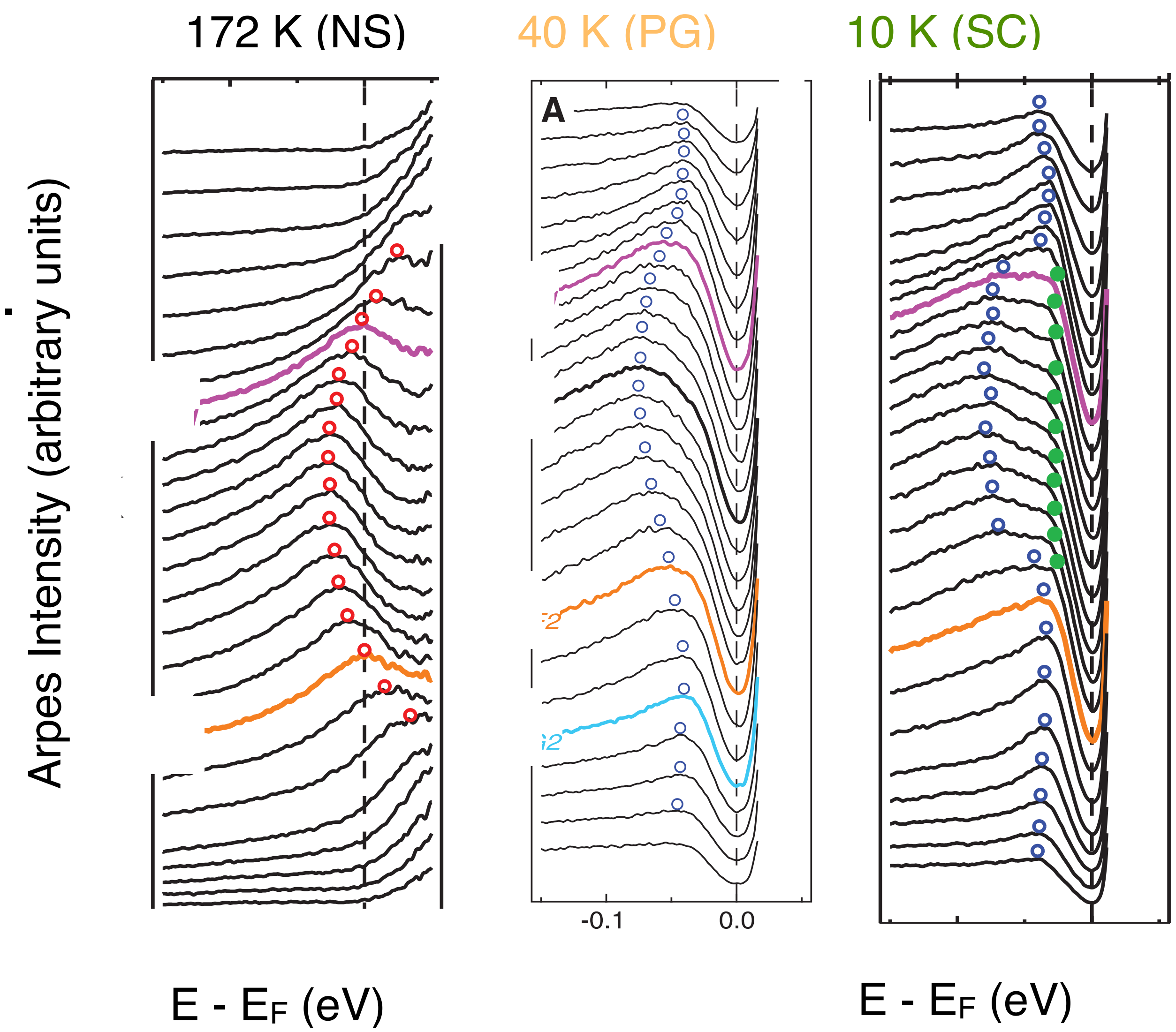
ARPES: Kanigel *et al.*, Nature Physics 2, 447 - 451 (2006).
Bi2212 sample with Tc=90K, measured at 140K

in high-Tc materials: Electronic spectral function is suppressed along the BZ face, but not along zone diagonal.

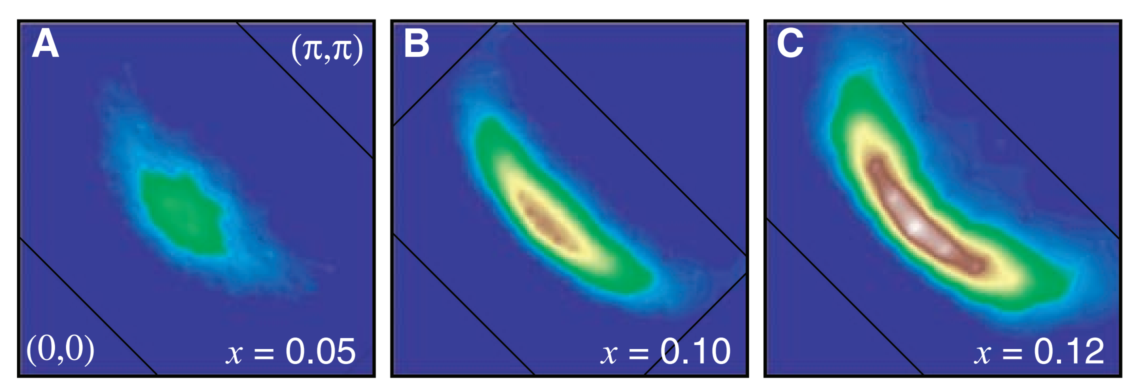
Key physics dependence on momentum around Fermi surface, Difference of spectral function around Fermi surface.

Doping dependence of region with quasiparticles

He *et al.*, Science 331, 1579 (2011)



ARPES: Shen *et al.*, Science 307, 901 (2005)



Question to theory

Can we say something about non-equilibrium correlation physics?

Can we say something about spectral functions of interacting materials?

Can we make these statements robust and reliable? (and what does that even mean?)

Does a voltage split the Kondo peak?

How well does dI/dV measure A(omega)?

…………we will present a potential answer in this talk………

Theory: Anderson Impurity Model

Quantum dot coupled to a non-interacting environment (‘leads’ or ‘bath’):

$$H_{\mathrm{loc}} = \sum_{\sigma} \varepsilon_{0\sigma} n_{\sigma} + U n_{\uparrow} n \downarrow$$

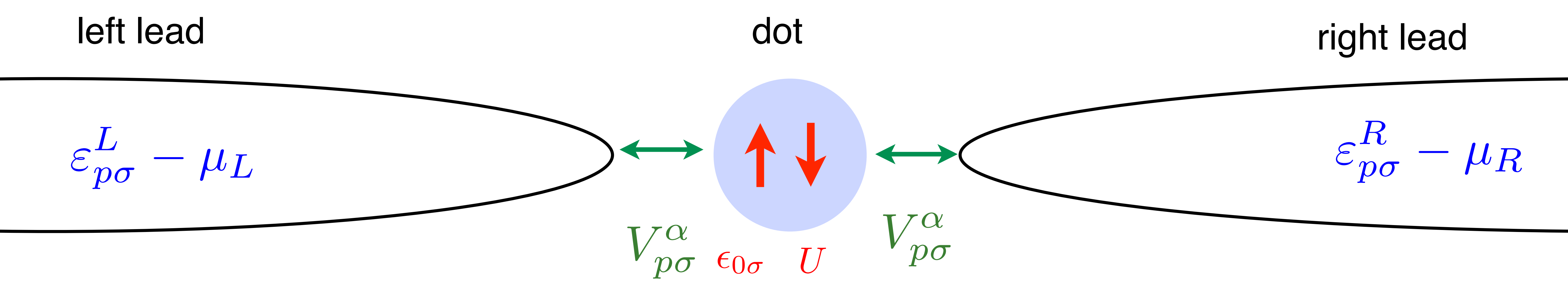
Impurity described by **Coulomb interaction U**, **level energies $\varepsilon_{0\sigma}$**.

$$H_{\mathrm{bath}} = \sum_{\alpha=L,R} \sum_{p\sigma} (\varepsilon^{\alpha}_{p\sigma} - \mu_{\alpha}) c^{\alpha\dagger}_{p\sigma} c^{\alpha}_{p\sigma}$$

Leads described by **bath dispersion, chemical potential**, non-interacting.

$$H_{\mathrm{hyb}} = \sum_{\alpha=L,R} \sum_{p\sigma} V^{\alpha}_{p\sigma} c^{\alpha\dagger}_{p\sigma} d_{\sigma} + h.c.$$

Coupling of dot to lead via ‘**hybridization strength**’ V.



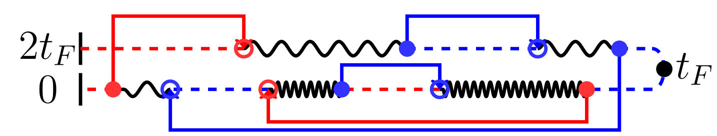
How much of the physics on the previous slides can we address with this setup?

Rev. Mod. Phys 83, 349 (2011)

Technique: Perturbation theory

Interaction representation: $H = H_a + H_b$

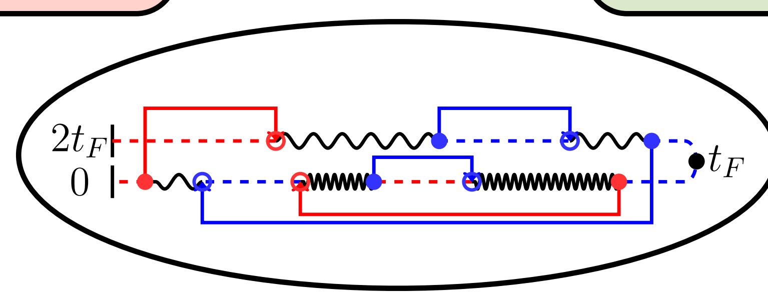
Perturbation theory, **Diagrammatic** expansion:



Diagrams on the real-time contour.
Prep the system in an initial state, let go & simulate transients and steady state

Finite (low) order perturbative expansions, performed analytically

Semi-analytic infinite partial summations



‘Diagrammatic’ or ‘Continuous-Time’ quantum Monte Carlo methods

Phys. Rev. B **82**, 075109 (2010)

'Traditional' techniques

Finite order perturbative expansions

- Obvious advantage where higher order terms are small.
- **Simple**, but
- **Not able to capture a 'correlated' regime**

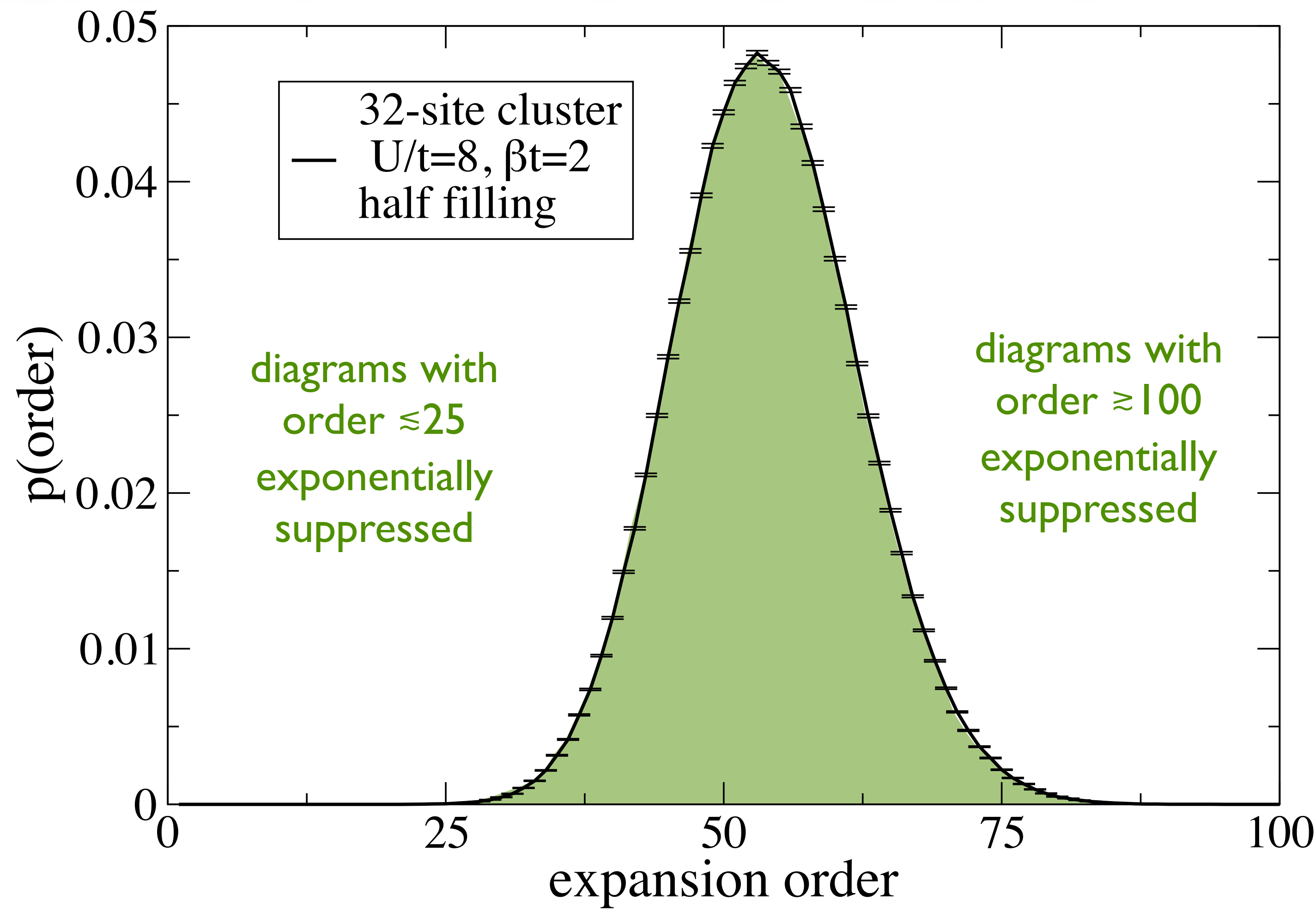
Semi-analytic infinite partial summations

Partial summation of infinite series of terms (diagrams) of a certain type.

- Good answers (hopefully) where resummed diagrams are relevant.
- Comparatively cheap to compute
- In wide use: RPA, non-crossing approximation, FLEX, GW, …
- However: **Uncontrolled**!

Rev. Mod. Phys 83, 349 (2011)

Continuous-Time Quantum Monte Carlo



General idea:

- Identify a convergent diagrammatic expansion.
- Realize that it is just a high order integral.
- Define a Monte Carlo importance sampling procedure for diagrams.
- Sample **all** diagrams stochastically.

Advantages:

- As long as all diagrams are sampled, the only error is a stochastic sampling error.
- Stochastic sampling errors converge like 1/sqrt(N)
- Perfect control over results.

Perceived limitation:

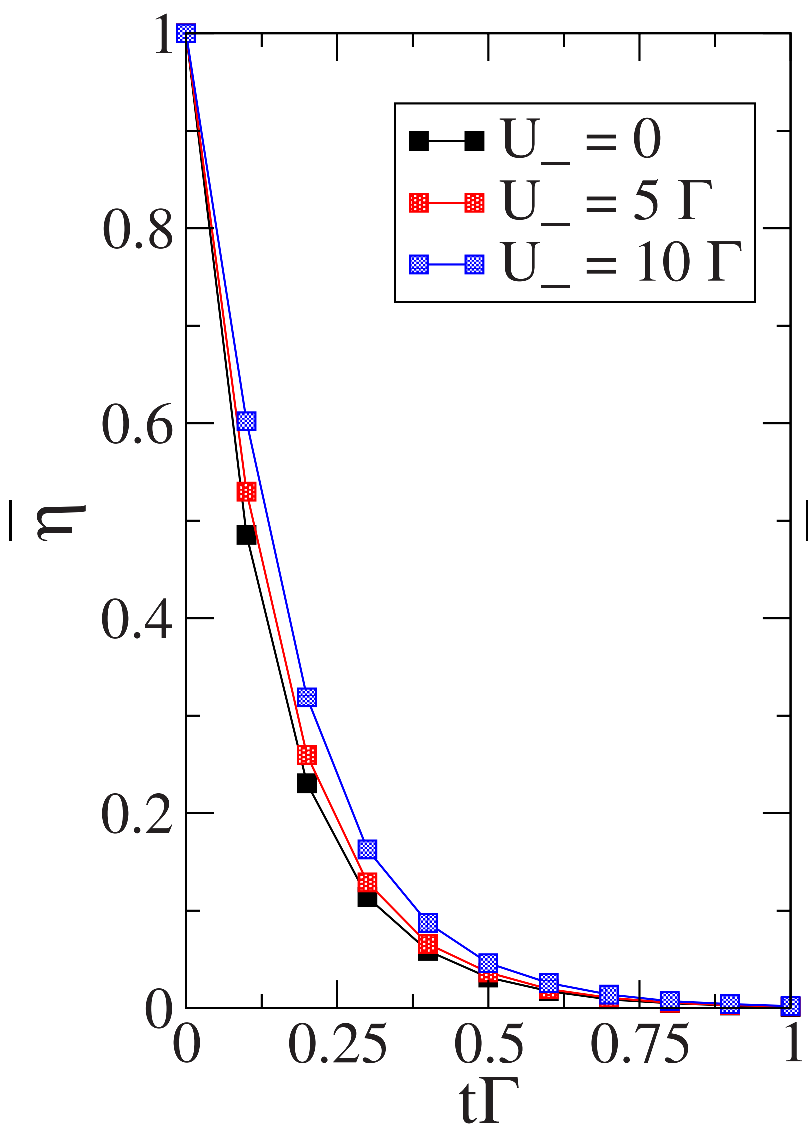
- There are very many diagrams and an infinite dimensional space?
- Luckily the dimensionality of the space does not enter Monte Carlo estimates.

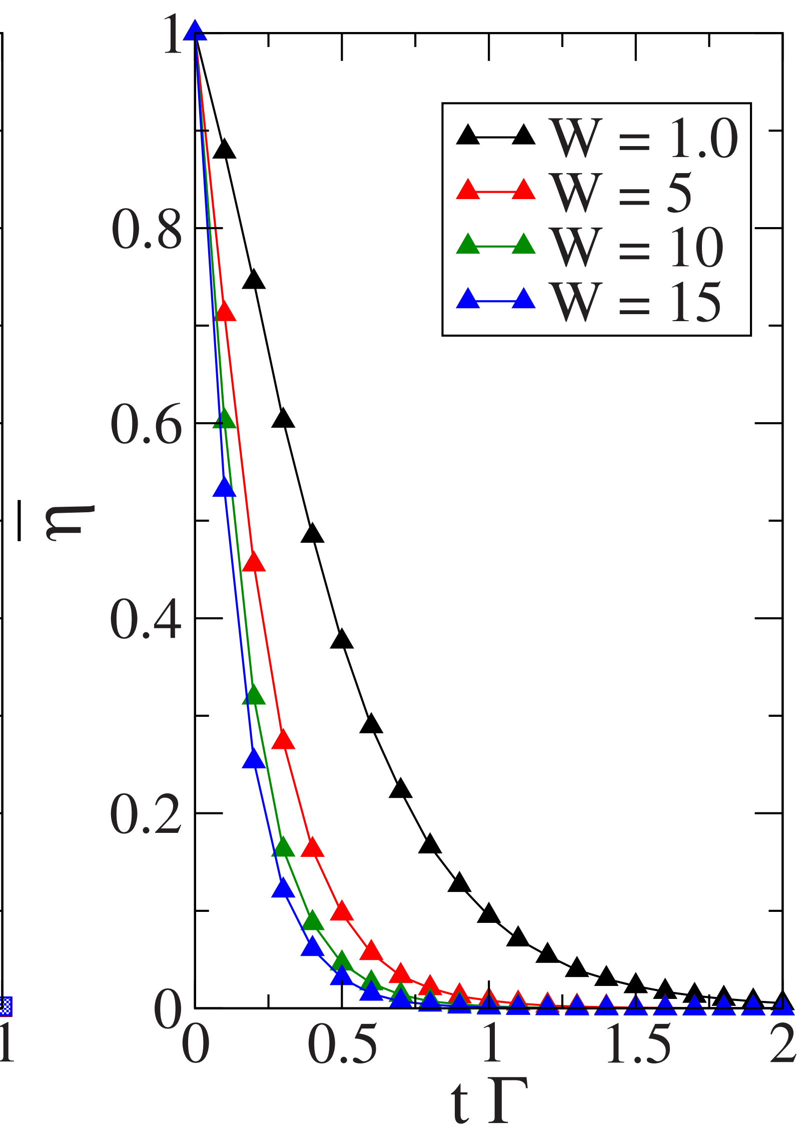
Actual Limitation:

- Sampling in diagram space may be inefficient ('sign/phase problem').

Limitations of CT-QMC out of equilibrium – Motivation for diagrammatic bold-line MC

Limiting factor with CT-QMC out of equilibrium: Complex sign (phase) problem!





Dynamic sign problem: direct consequence of oscillation of real time propagation

'bare' CT-QMC: average sign decays exponentially as a function of real time.

Hard cutoff in times that can be reached, exponential cost for longer times

Marco Schiro
Phys. Rev. B 81, 085126 (2010)

Mühlbacher, Rabani, Phys. Rev. Lett. 100, 176403 (2008)
Werner, Oka, Millis, Phys. Rev. B 79, 035320 (2009)

Phys. Rev. B **82**, 075109 (2010)

Bold-line Monte Carlo

Semi-analytic infinite partial summation

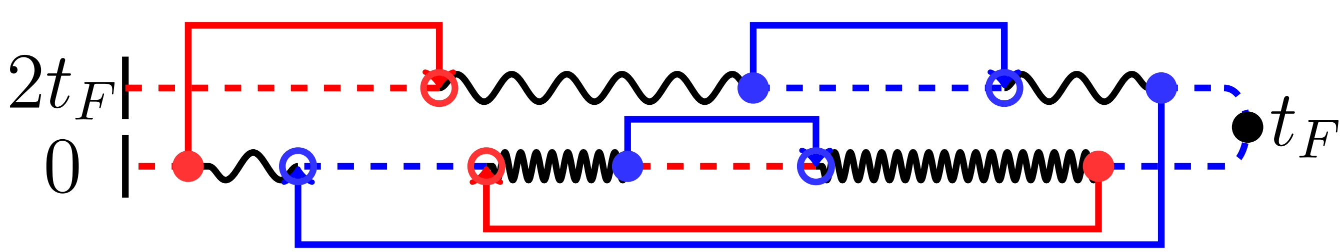
‘Diagrammatic’ or ‘Continuous-Time’ quantum Monte Carlo methods

General idea:

- Two-step procedure
  - First step: run a semi-analytic infinite partial summation
  - Second step: Stochastically sample all corrections to the partial summation

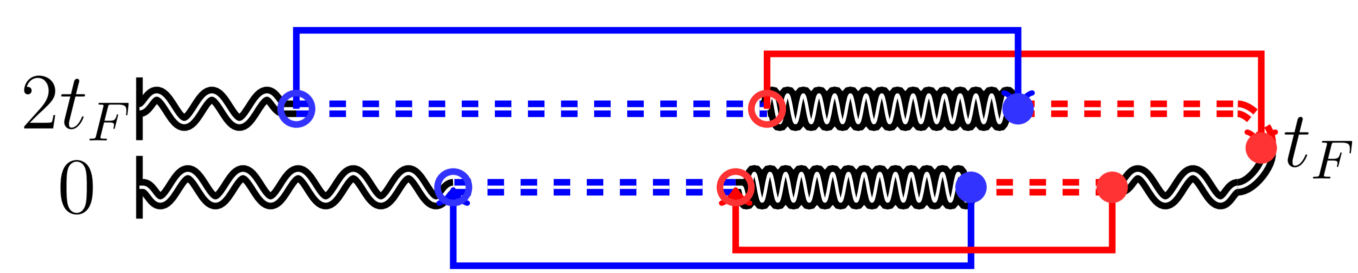
Consequences:

- Numerically exact! (all diagrams are considered)
- Closer starting guess reduces sign problem, size of relevant configuration space
- Observable estimates more precise.



‘bare’ diagram

‘bold’ diagram



See also related iterative bold-line MC method, Prokof’ev and Svistunov, PRL 99, 250201 (2007)

Phys. Rev. B **82**, 075109 (2010)

Bold Expansion

In this talk:

- Underlying partial summation: **Non-crossing approximation (NCA).**
  - See Martin Eckstein's talk later today
- Bold-line Monte Carlo expansion: **BoldNCA method based on the non-crossing approximation**

Summing up all 'crossing' corrections stochastically makes the method **numerically exact**.

Phys. Rev. B **82**, 075109 (2010)

Bold Diagrammatics – Bold NCA

Semianalytic infinite partial summations

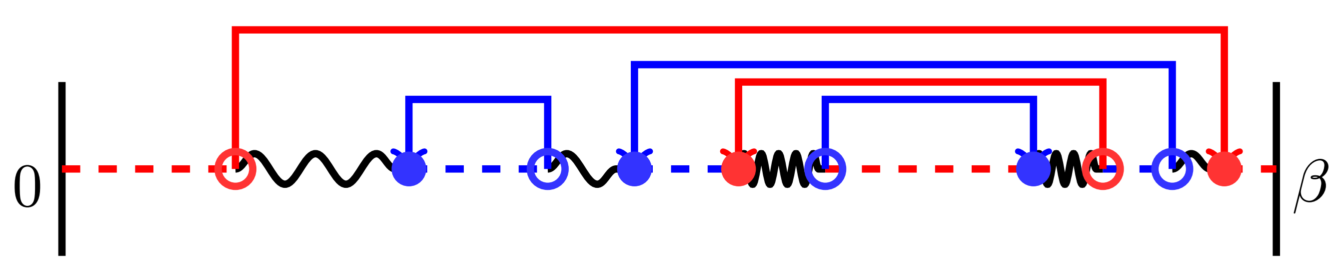
‘Diagrammatic’ or ‘Continuous-Time’ quantum Monte Carlo methods

1.Use the non-crossing approximation to sum up **all non-crossing hybridization lines** (using coupled integral equations)

$$
\begin{aligned}
\Sigma_{|0\rangle}(\tau) &= G_{|\uparrow\rangle}(\tau)\Delta_{\uparrow}(\tau) + G_{|\downarrow\rangle}(\tau)\Delta_{\downarrow}(\tau),\\
\Sigma_{|\sigma\rangle}(\tau) &= G_{|0\rangle}(\tau)\Delta_{\sigma}(-\tau) + G_{|\uparrow\downarrow\rangle}(\tau)\Delta_{-\sigma}(\tau),\\
\Sigma_{|\uparrow\downarrow\rangle}(\tau) &= G_{|\uparrow\rangle}(\tau)\Delta_{\downarrow}(-\tau) + G_{|\downarrow\rangle}(\tau)\Delta_{\uparrow}(\tau).
\end{aligned}
$$

$$
G_{|j\rangle} = G^0_{|j\rangle} + G^0_{|j\rangle}\Sigma_{|j\rangle}G_{|j\rangle}
$$

Obtain NCA propagators and self-energies.



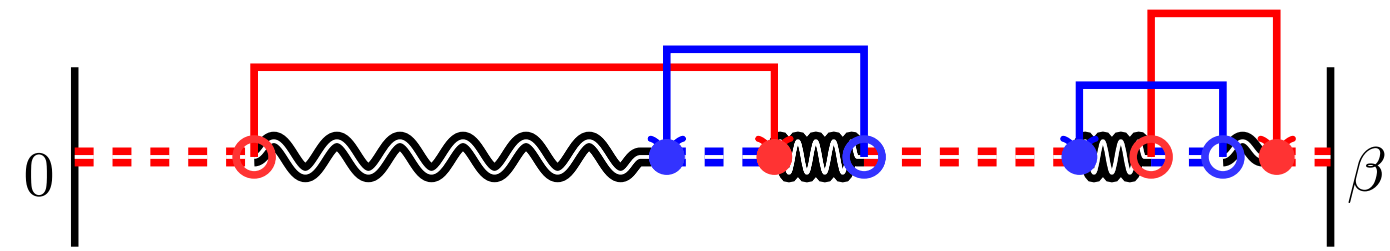
Phys. Rev. B **82**, 075109 (2010)

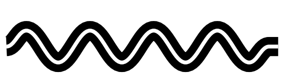
Bold Diagrammatics – Bold NCA

Semianalytic infinite partial summations

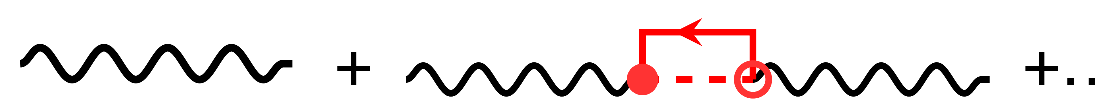
'Diagrammatic' or 'Continuous-Time' quantum Monte Carlo methods

2.Use a continuous-time quantum Monte Carlo algorithm to sum up all crossing terms stochastically, **replacing bare propagators with NCA propagators**

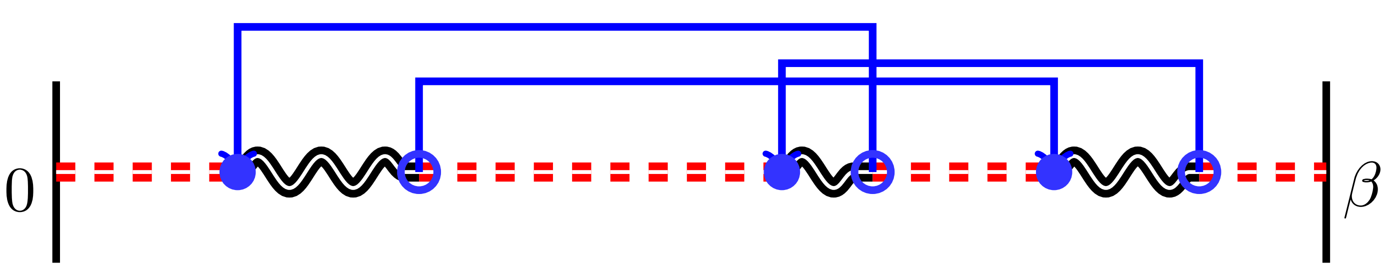




Bold NCA propagator: stands for:



Includes all non-crossing diagrams (to all orders)



Each bare diagram uniquely associated with a diagram that contains only crossing parts. All these crossing diagrams summed up stochastically.

Perform continuous-time QMC algorithm: Insert / remove hybridization lines, measure Green's functions,...

Phys. Rev. B **82**, 075109 (2010)

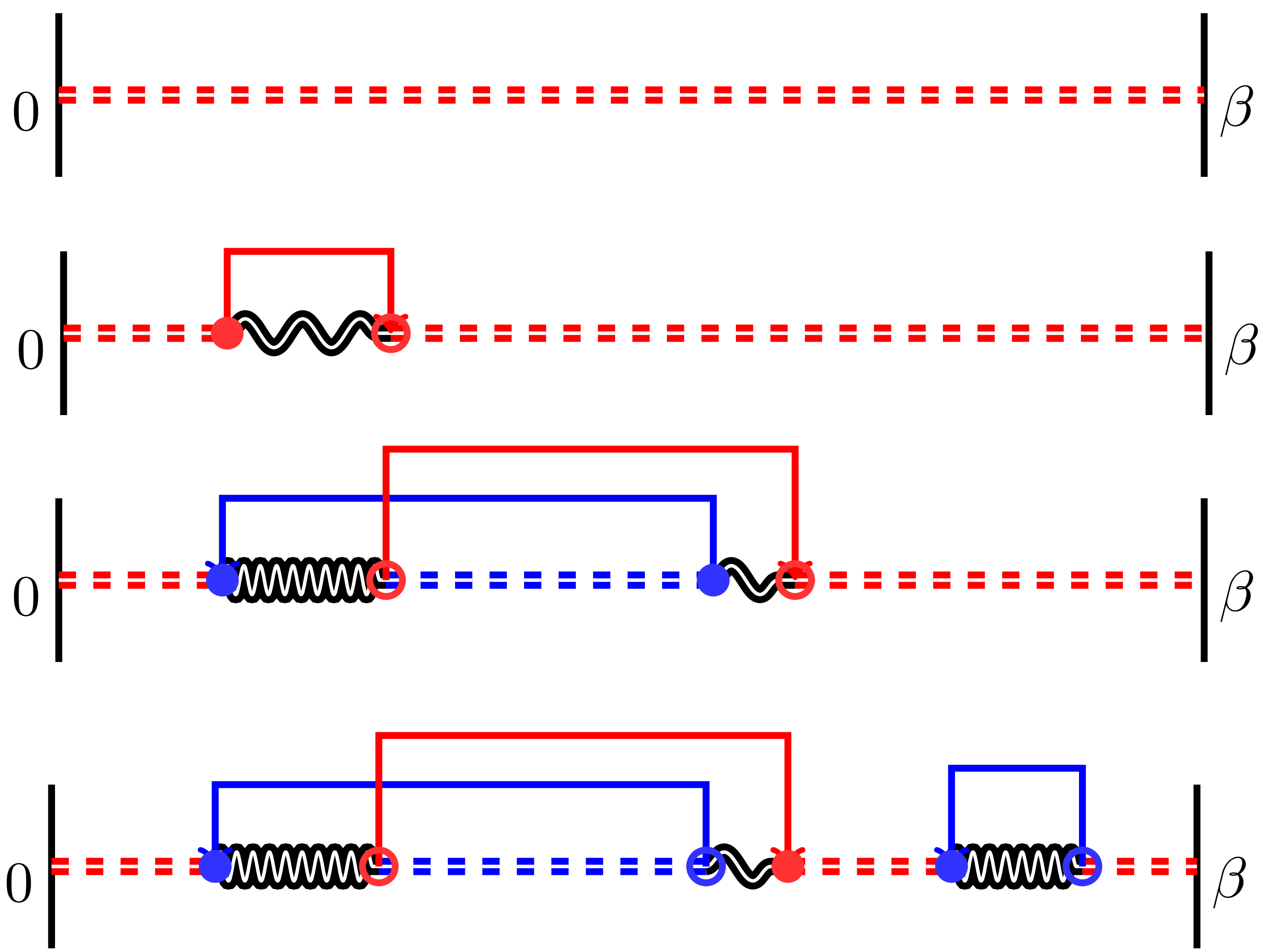
Bold Diagrammatics – Bold NCA

Semianalytic infinite partial summations

'Diagrammatic' or 'Continuous-Time' quantum Monte Carlo methods

Diagrams

weight



$G_{|\uparrow\rangle}(\beta)$ — NCA propagator for 'up' state, for time β

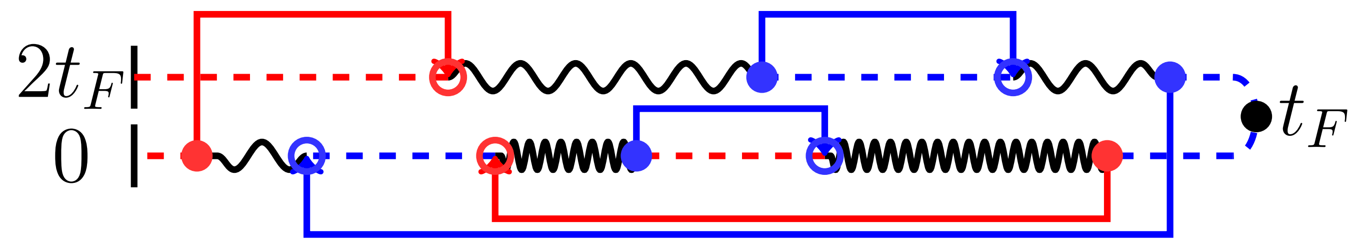
0 — Contained in NCA, diagram rejected

$$G_{|\uparrow\rangle}(\tau_1)G_{|\uparrow\downarrow\rangle}(\tau_2-\tau_1)G_{|\downarrow\rangle}(\tau_3-\tau_2)$$
$$G_{|0\rangle}(\tau_4-\tau_3)G_{|\uparrow\rangle}(\beta-\tau_4)$$
$$\times\Delta_{\downarrow}(\tau_3-\tau_1)\Delta_{\uparrow}(\tau_4-\tau_2)$$

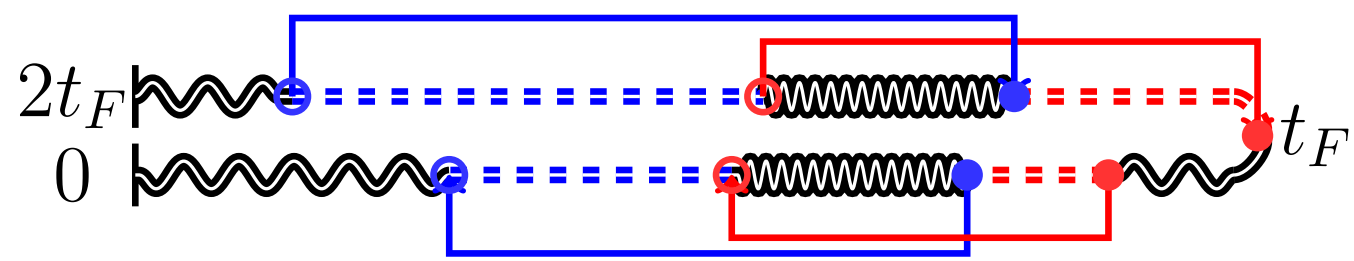
0 — Contains a non-crossing part, diagram rejected

Perform random walk in bold diagram space. Exact: each bare diagram can be uniquely decomposed into crossing and non-crossing parts. Diagrams that contain crossings are not sampled.

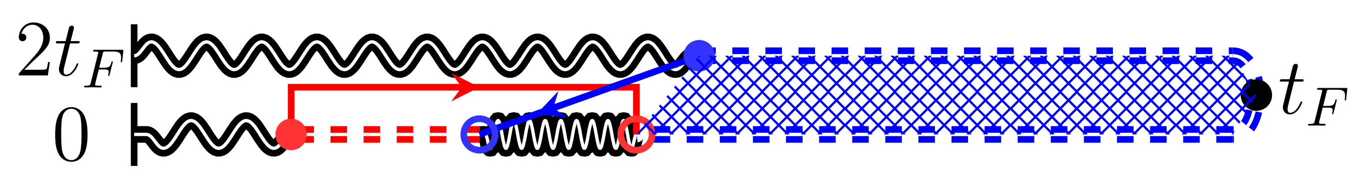
Bold NCA – The Keldysh Contour



NCA equations in real time sum up non-crossing diagrams on double contour.



Bold Method sums up terms not treated by the NCA, replaces bare by bold propagators.

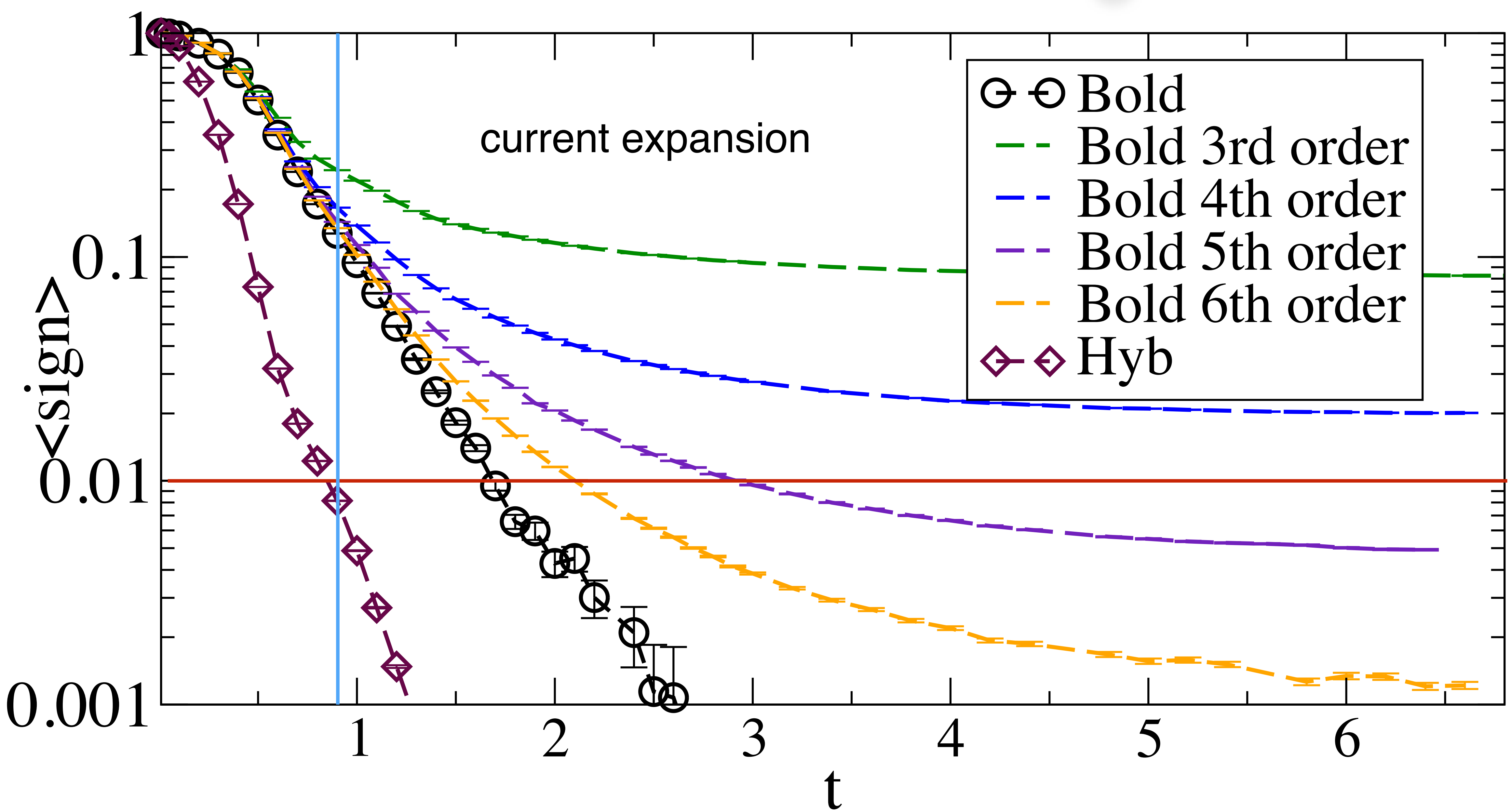


Consider analytically computed vertex functions to sum additional diagrams connecting upper and lower contour.

Phys. Rev. B **84**, 085134 (2011)

Phys. Rev. B **84**, 085134 (2011)

Real Time Bold NCA – Sign Problem

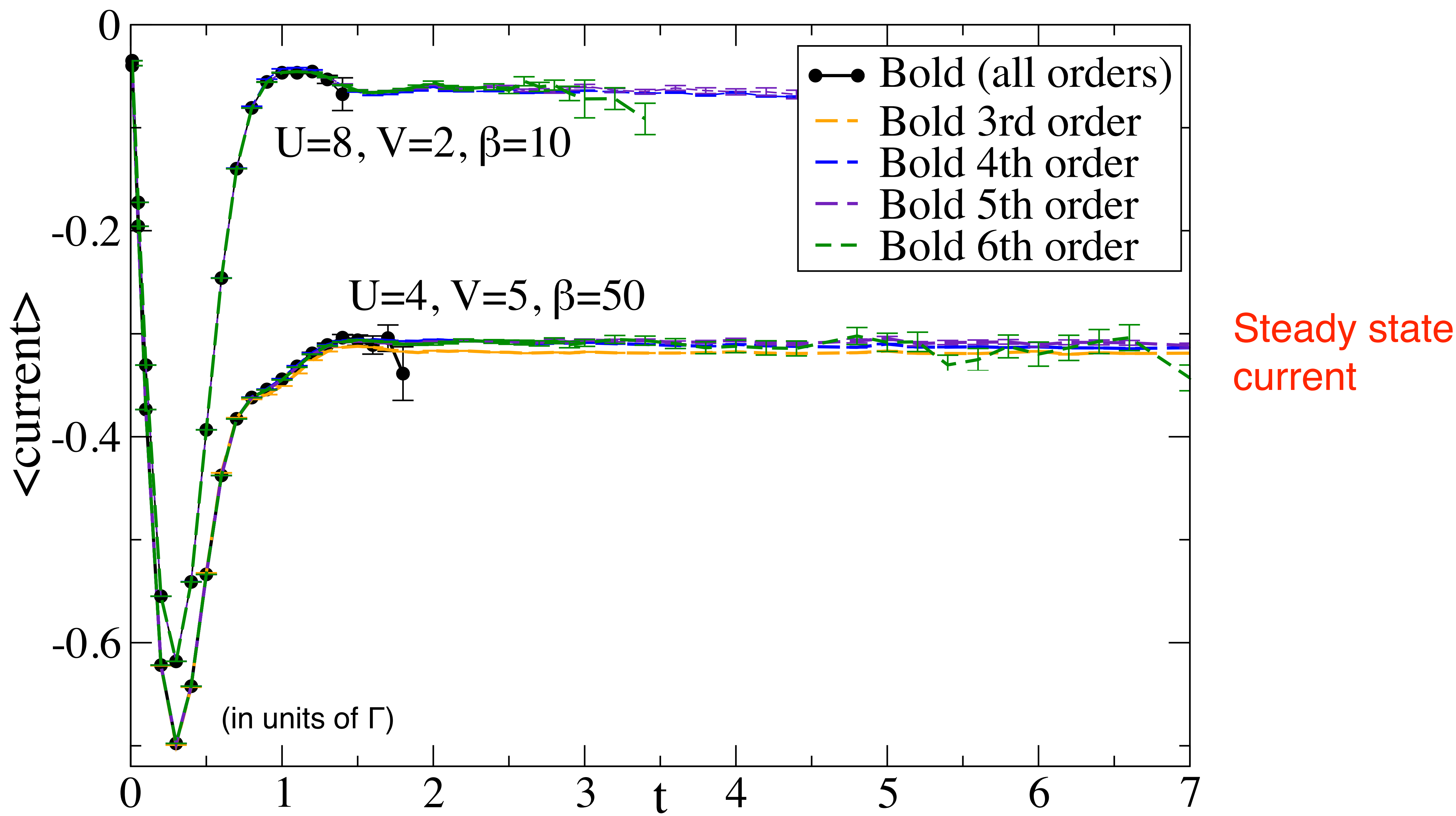


Bold vs bare:

- Sign better by order of magnitude (blue line).
- For same sign: twice longer time accessible (red line).
- If bold expansion is truncated at a fixed order (3rd, 4th, 5th, 6th order): sign problem plateau, arbitrarily long times accessible if converged.

Phys. Rev. B **84**, 085134 (2011)

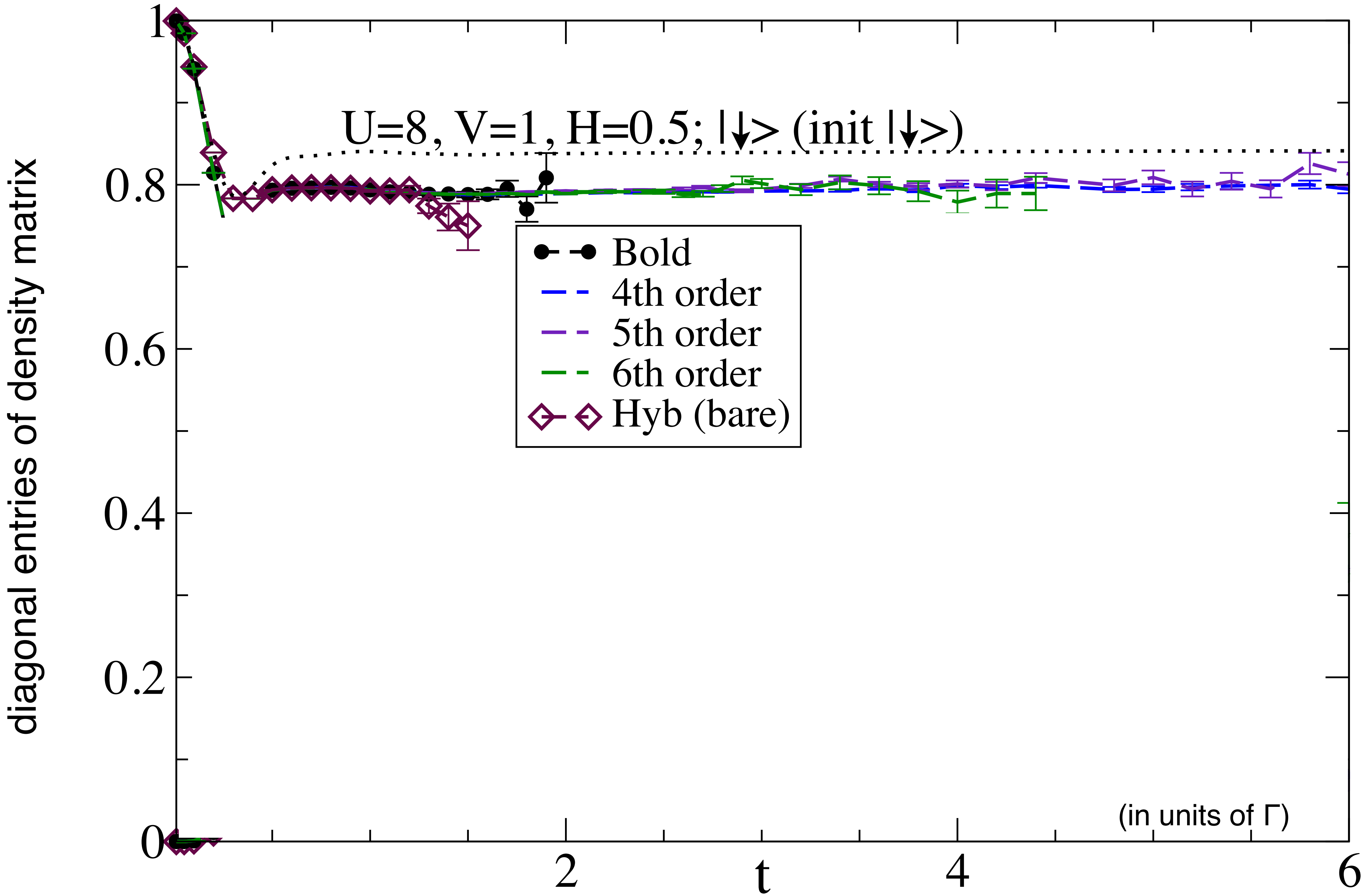
Real Time Bold NCA – Current



Current as a function of time, starting from the empty dot $\hat{\rho}_0 = |0\rangle\langle 0|$. Inset: starting from an NCA density matrix $\hat{\rho}_{\mathrm{NCA}}$.

Phys. Rev. B **84**, 085134 (2011)

Real Time Bold NCA – Density Matrix



Spin- and charge relaxation for various systems and initial conditions: longer times accessible, steady state reachable.

[Phys. Rev. B 87, 195108 (2013)]

Combination with Memory Function Methods

Monte Carlo:

- extremely precise answers for short t
- exponential cost for long t
- Can we use short-t knowledge to obtain long-t behavior?

(exakt) Nakajima Zwanzig Mori equation:

$$i\hbar \frac{d\sigma(t)}{dt} = \mathcal{L}_{H_S}\sigma(t) + \vartheta(t) - \frac{i}{\hbar}\int_0^t d\tau\, \kappa(\tau)\,\sigma(t-\tau)\,.$$

impurity Liouvillian

initial conditions

memory ‘Kernel’

impurity density matrix

This implies:

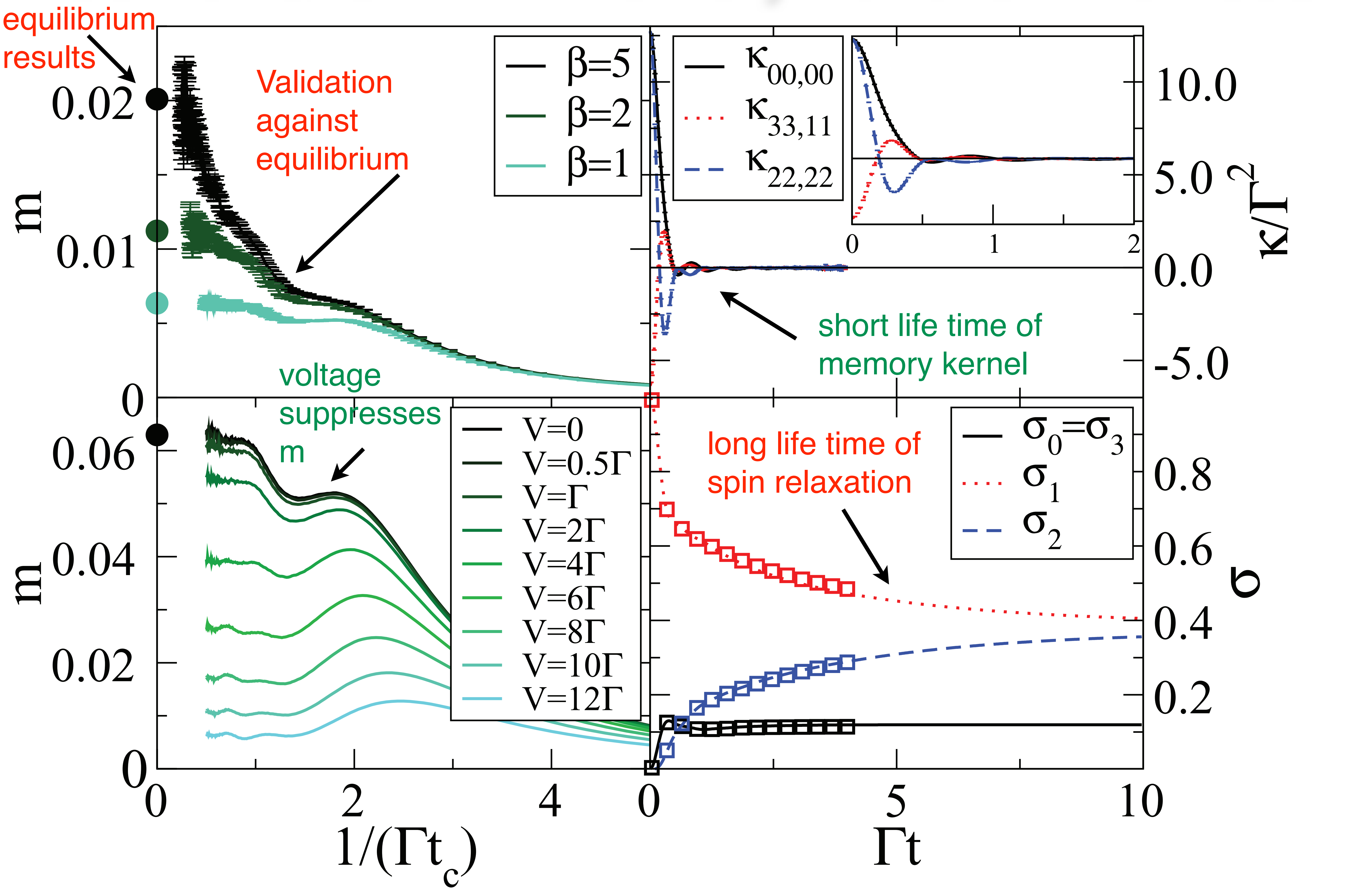
- obtain exact impurity density matrix IF memory kernel is accessible for all times
- If memory kernel goes to zero in short time: obtain exact impurity density matrix for all times using short time simulation

- Memory kernel is a function of current observables – straightforwardly accessible

Plan: Check if memory kernel converges within simulation time, use it to propagate density matrix to steady state: Numerically exact results in the Kondo regime.

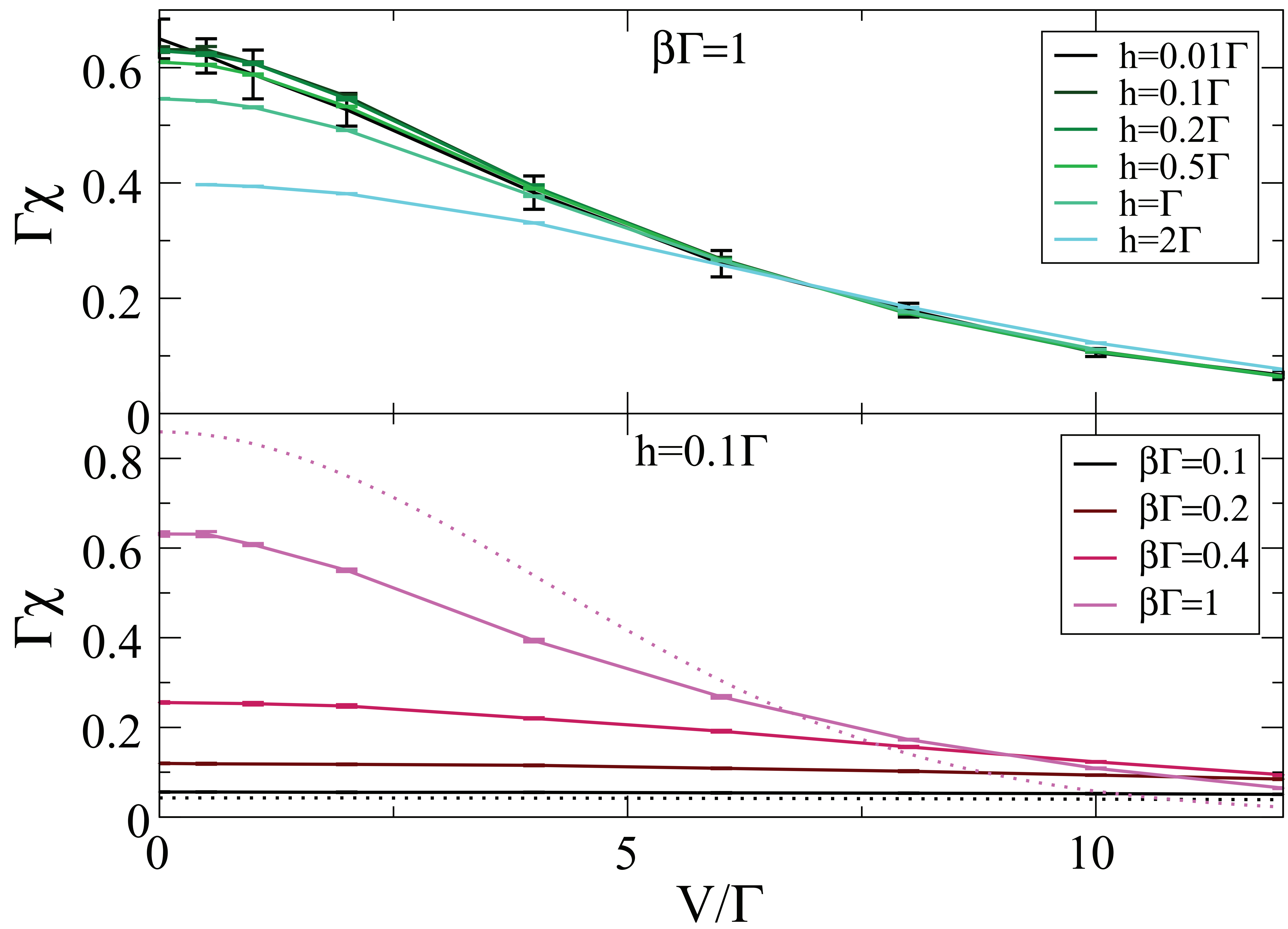
Phys. Rev. B 87, 195108 (2013)

Combination with Memory Function Methods



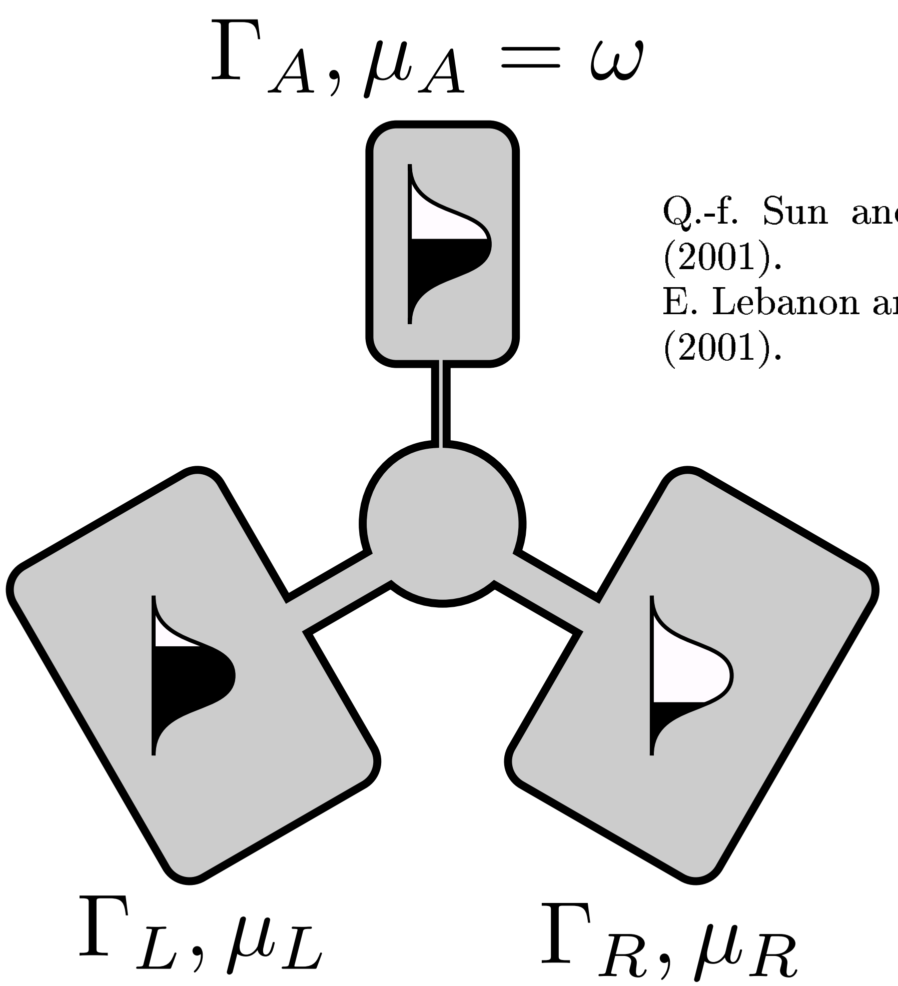
Phys. Rev. B 87, 195108 (2013)

Combination with Memory Function Methods

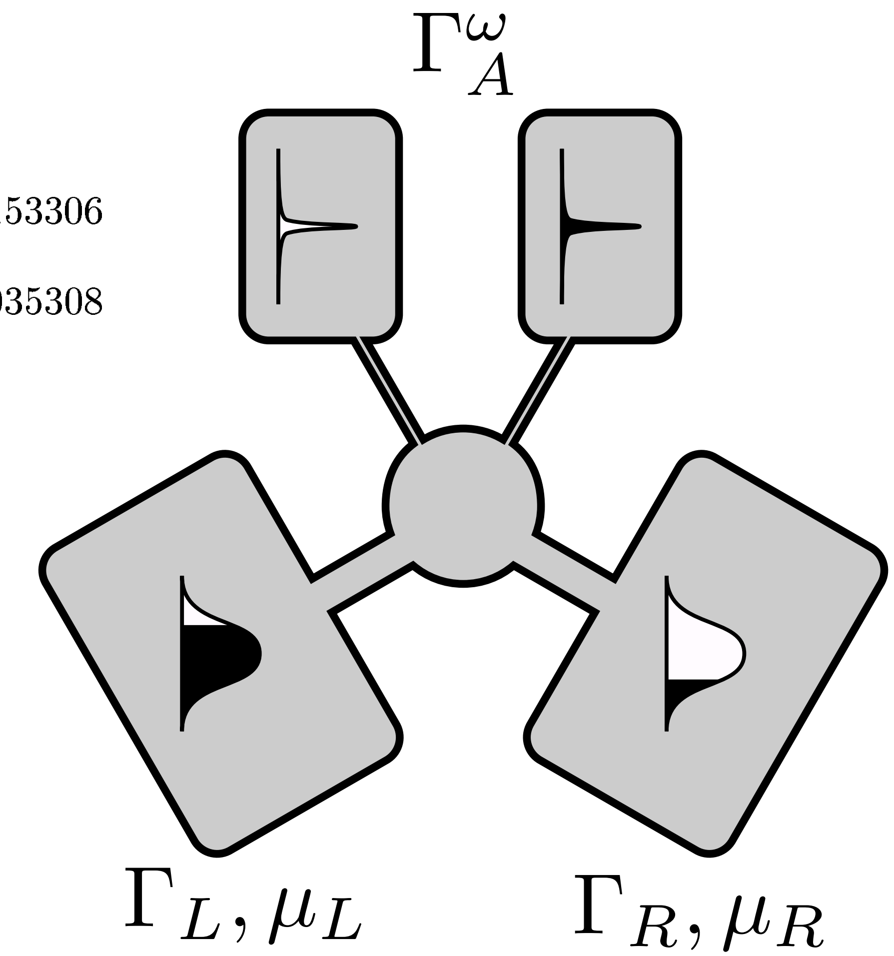


Phys. Rev. B 89, 115139 (2014)

Obtaining spectral functions from QMC



Q.-f. Sun and H. Guo, Physical Review B **64**, 153306 (2001).
E. Lebanon and A. Schiller, Physical Review B **65**, 035308 (2001).



Quantum impurity coupled to two baths, weakly coupled to a an 'auxiliary probe lead'.

Actual QIM setup: symmetrical with empty and filled lead

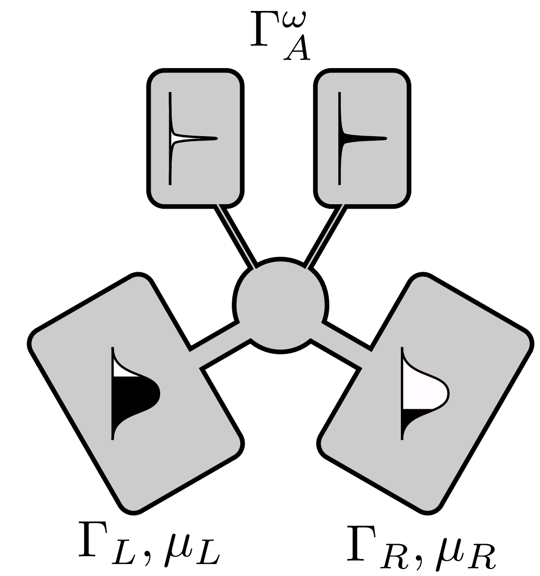
Express spectral function as a current difference

$$A(\omega) = \lim_{\eta \to 0} -\frac{2h}{e\pi\eta}\left[I_A^1(\omega) - I_A^0(\omega)\right].$$

Phys. Rev. B 89, 115139 (2014)

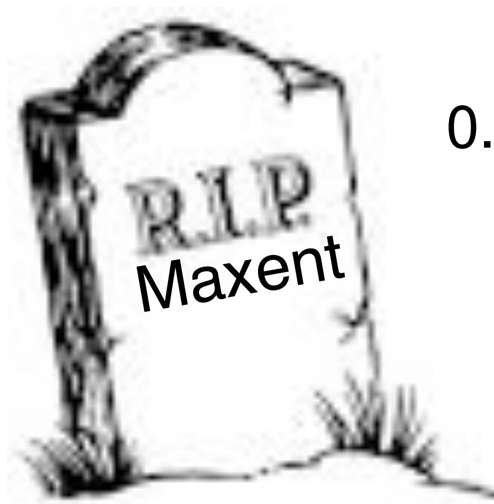
Obtaining spectral functions from QMC

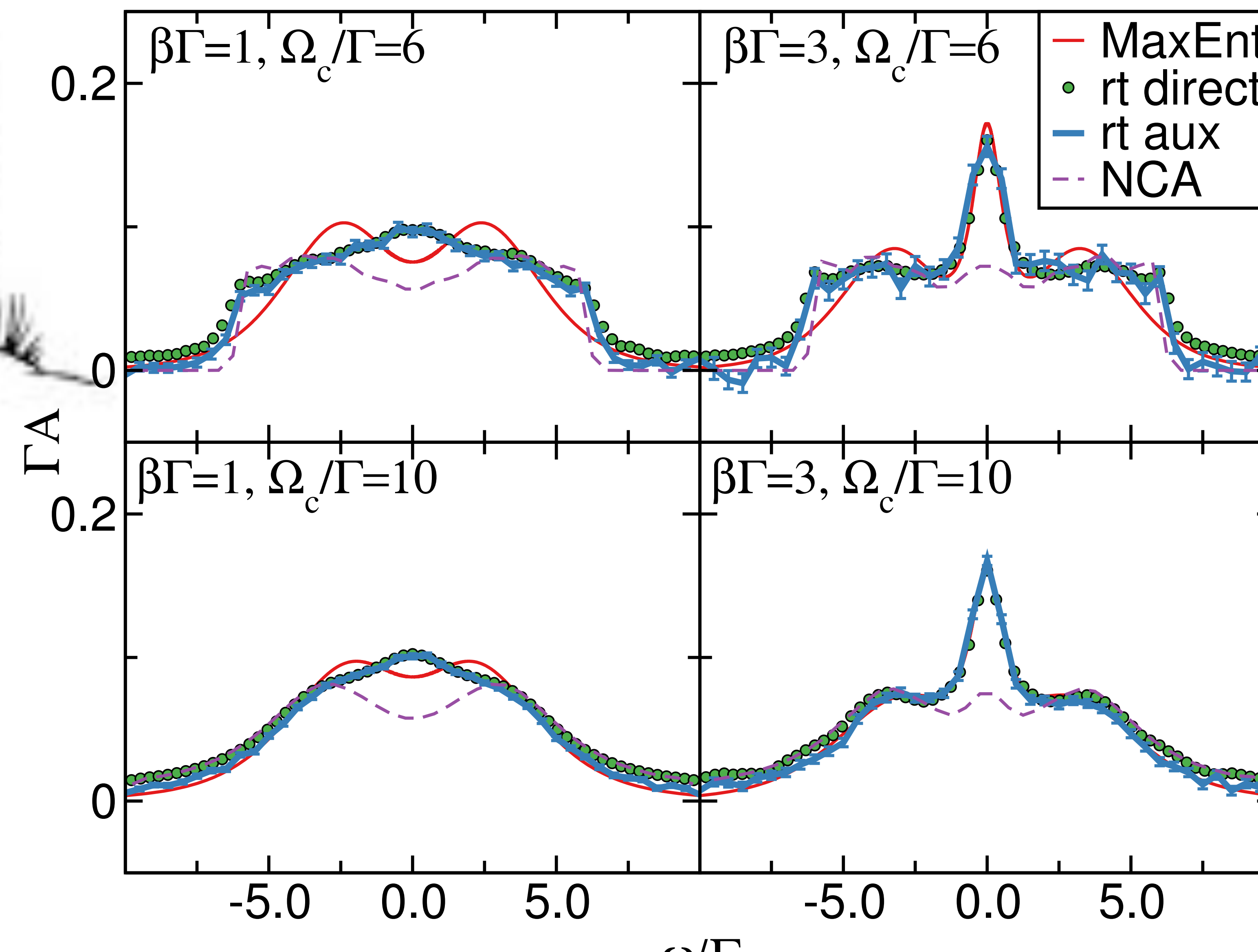
$$A(\omega) = \lim_{\eta \to 0} -\frac{2h}{e\pi\eta}\left[I_A^1(\omega) - I_A^0(\omega)\right].$$



We have error bars on the currents…

…and that implies we have error bars on the spectral functions!



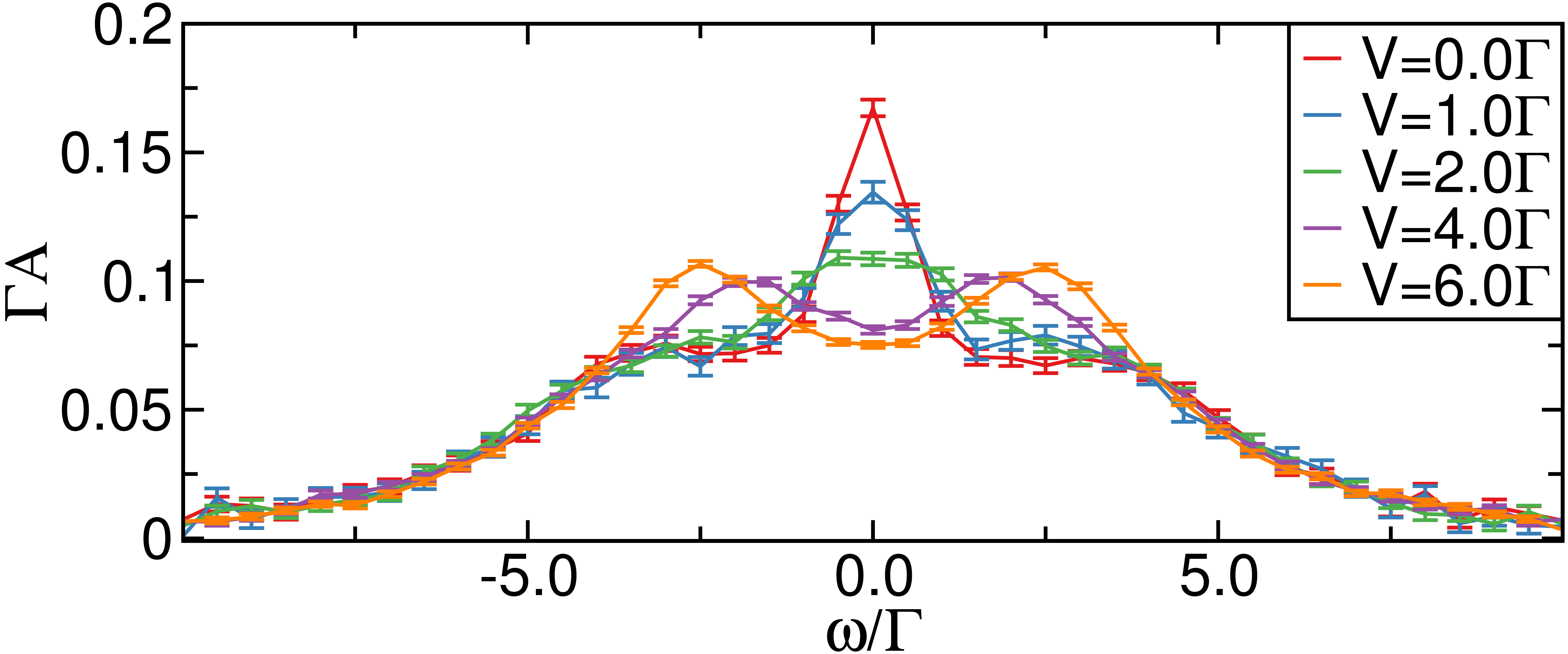


Limitation: have to reach equilibrium current, i.e. long-time behavior!

Convergence to steady state slow in the Kondo regime & at low T -> exponential sign problem barrier

Phys. Rev. B 89, 115139 (2014)

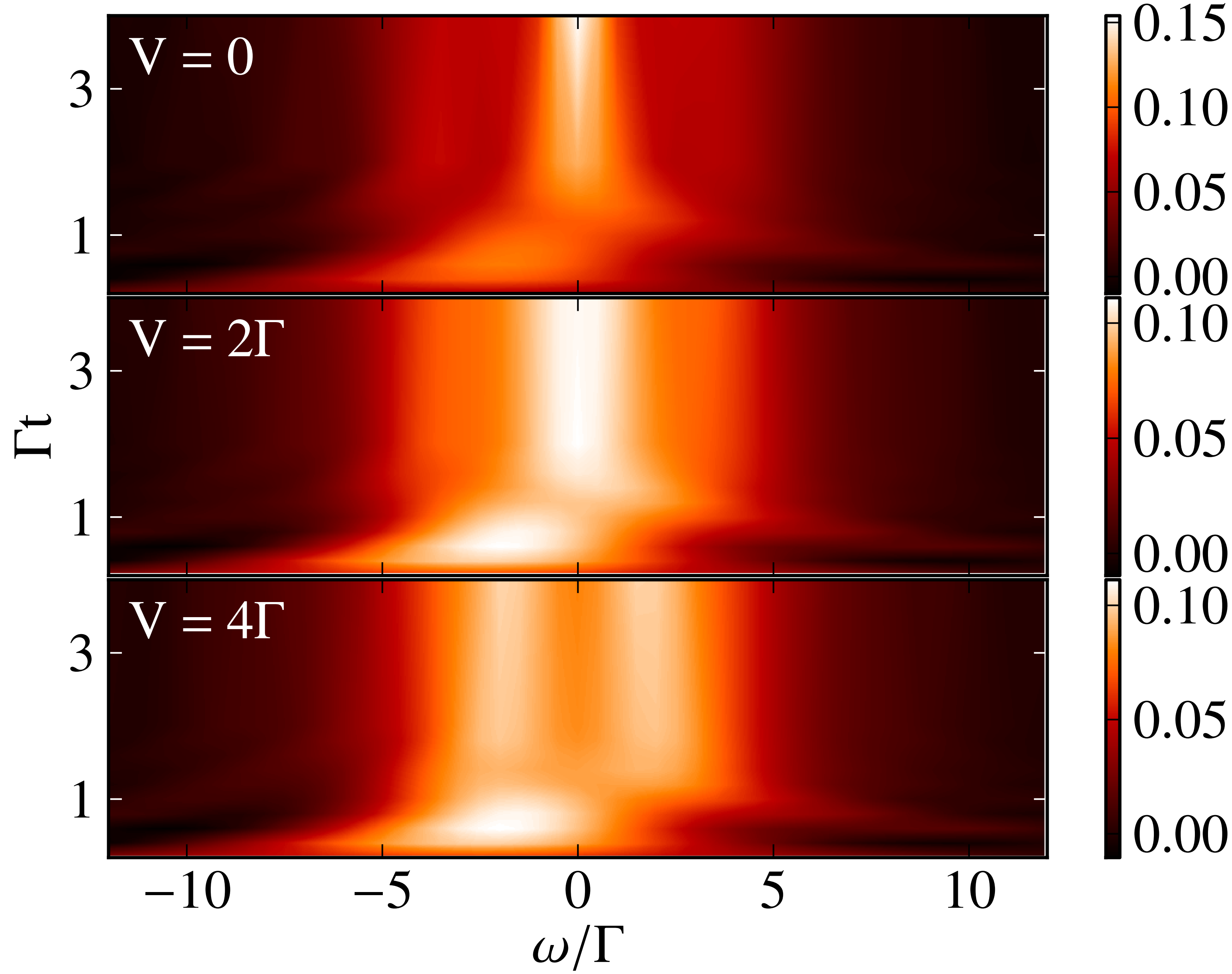
Non-equiliibrium spectral functions from QMC



Parameters:
Voltage V
U/Γ=6
βΓ=3
flat band (width 10Γ) with soft cutoff

Phys. Rev. B 89, 115139 (2014)

Non-equiliibrium spectral functions from QMC



Buildup of Kondo peak

Suppression/ broadening of Kondo peak

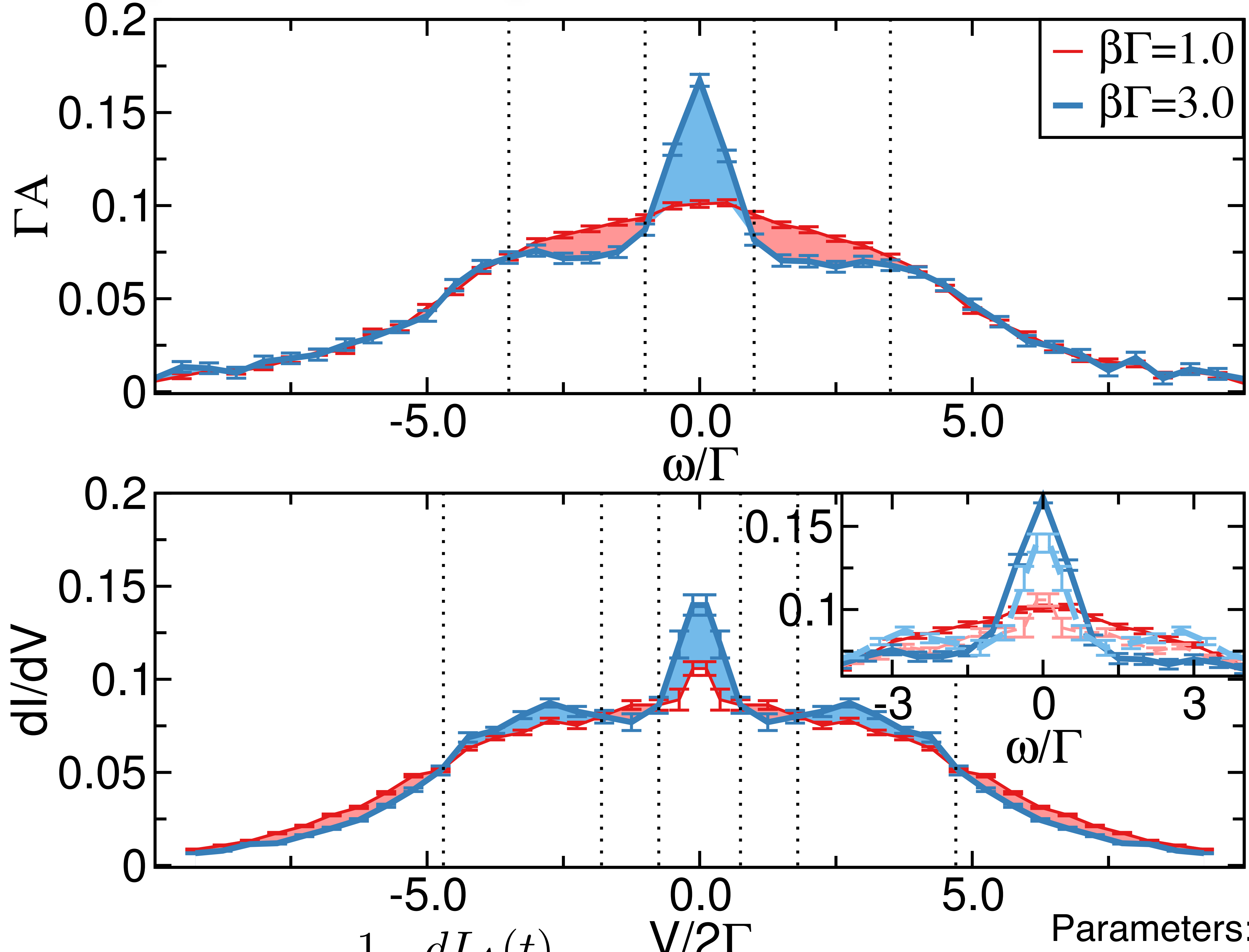
Voltage splitting of Kondo peak

Figure 2. The time evolution of the spectral function $A_{aux}(\omega)$ shown at several voltages, obtained from bold-CTQMC using the double-probe auxiliary lead formalism.

Parameters:
U/Γ=6
βΓ=3
flat band (width 10Γ) with soft cutoff

Phys. Rev. B 89, 115139 (2014)

Non-equiliibrium spectral functions from QMC



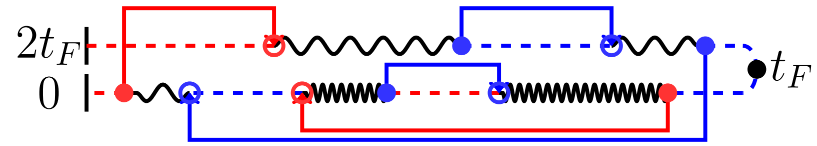
$$A_{aux}(V_A, t) =_{\Gamma_A \to 0} -\frac{1}{\Gamma_A \pi} \frac{dI_A(t)}{dV_a}.$$

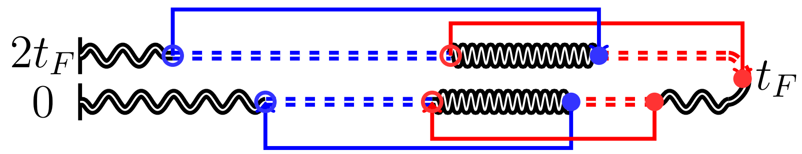
Parameters: U/Γ=6, βΓ=3, flat band (width 10Γ) with soft cutoff

Phys. Rev. B 89, 115139 (2014)

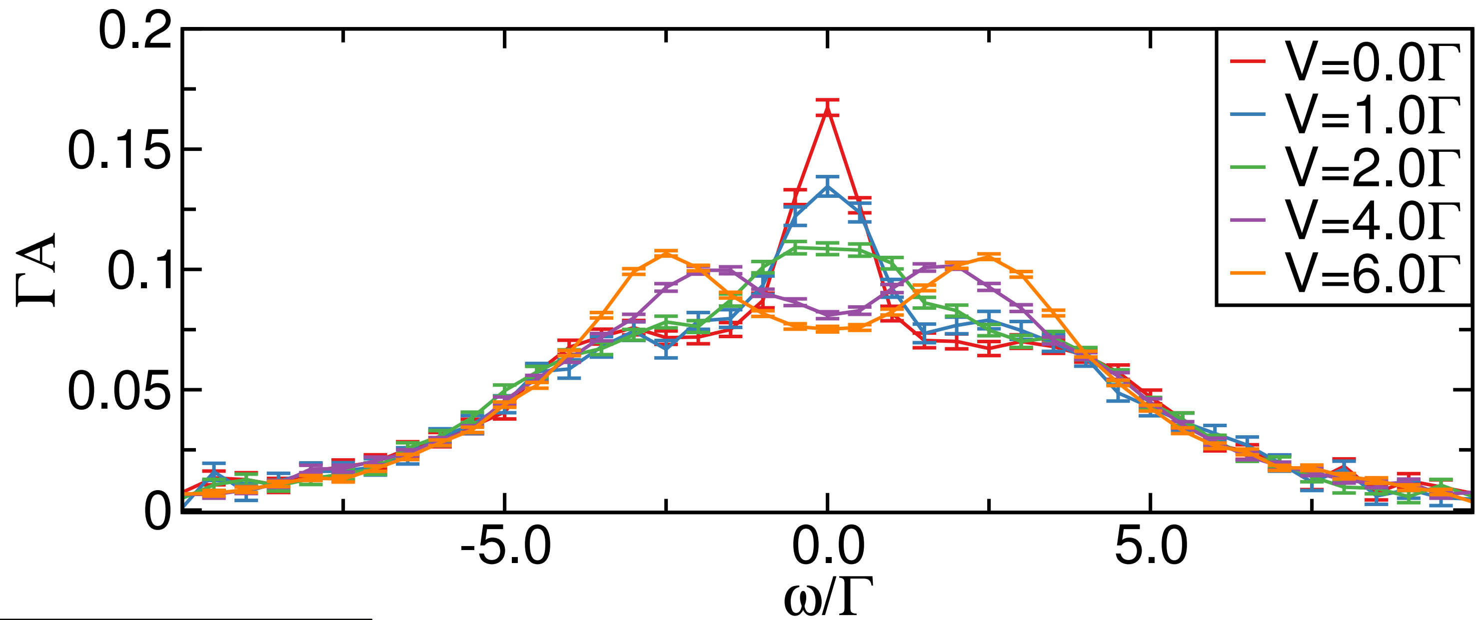
Conclusions

QMC for real-time evolution:



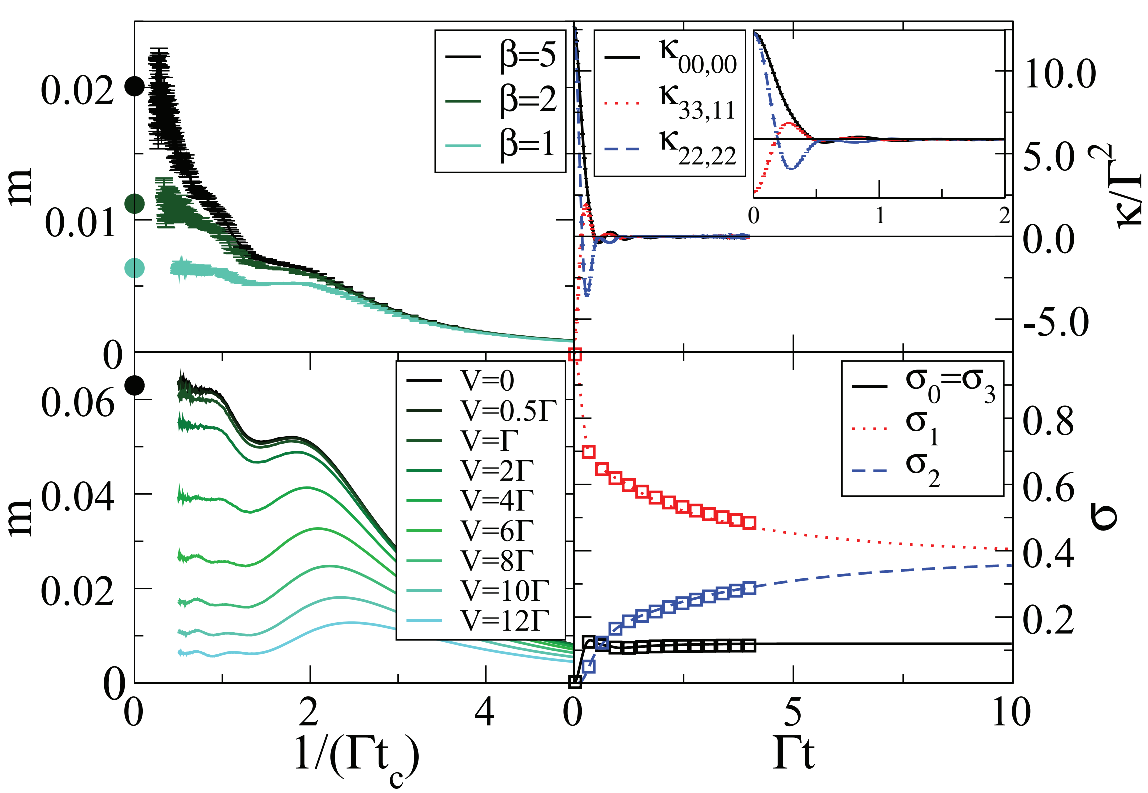


need to combine analytics with numerics to be competitive

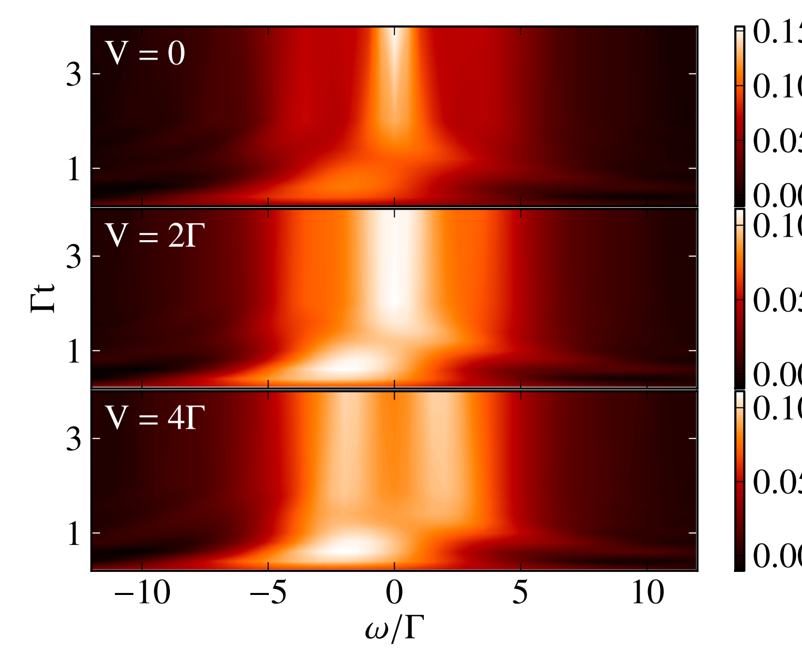


Memory kernel methods: spin and charge relaxation

'true' nonequilibrium spectral functions



equilibrium /steady state spectral functions



Acknowledgments

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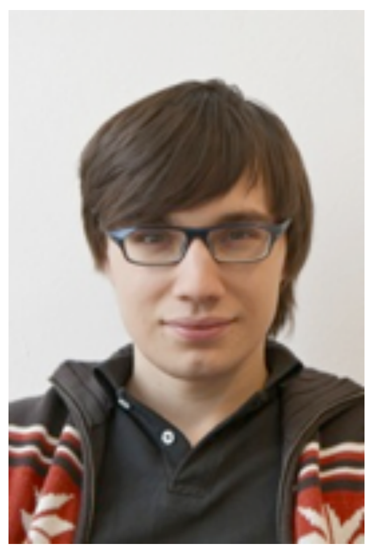


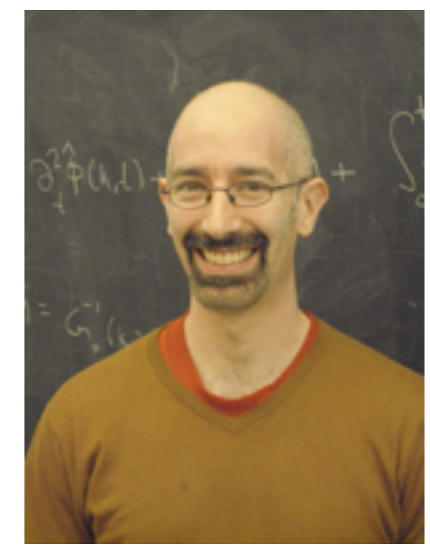

Guy Cohen, A.J. Millis, D. Reichman;
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[Phys. Rev. B 82, 075109 (2010)]
[Phys. Rev. B 84, 085134 (2011)]
[Rev. Mod. Phys 83, 349 (2011)]
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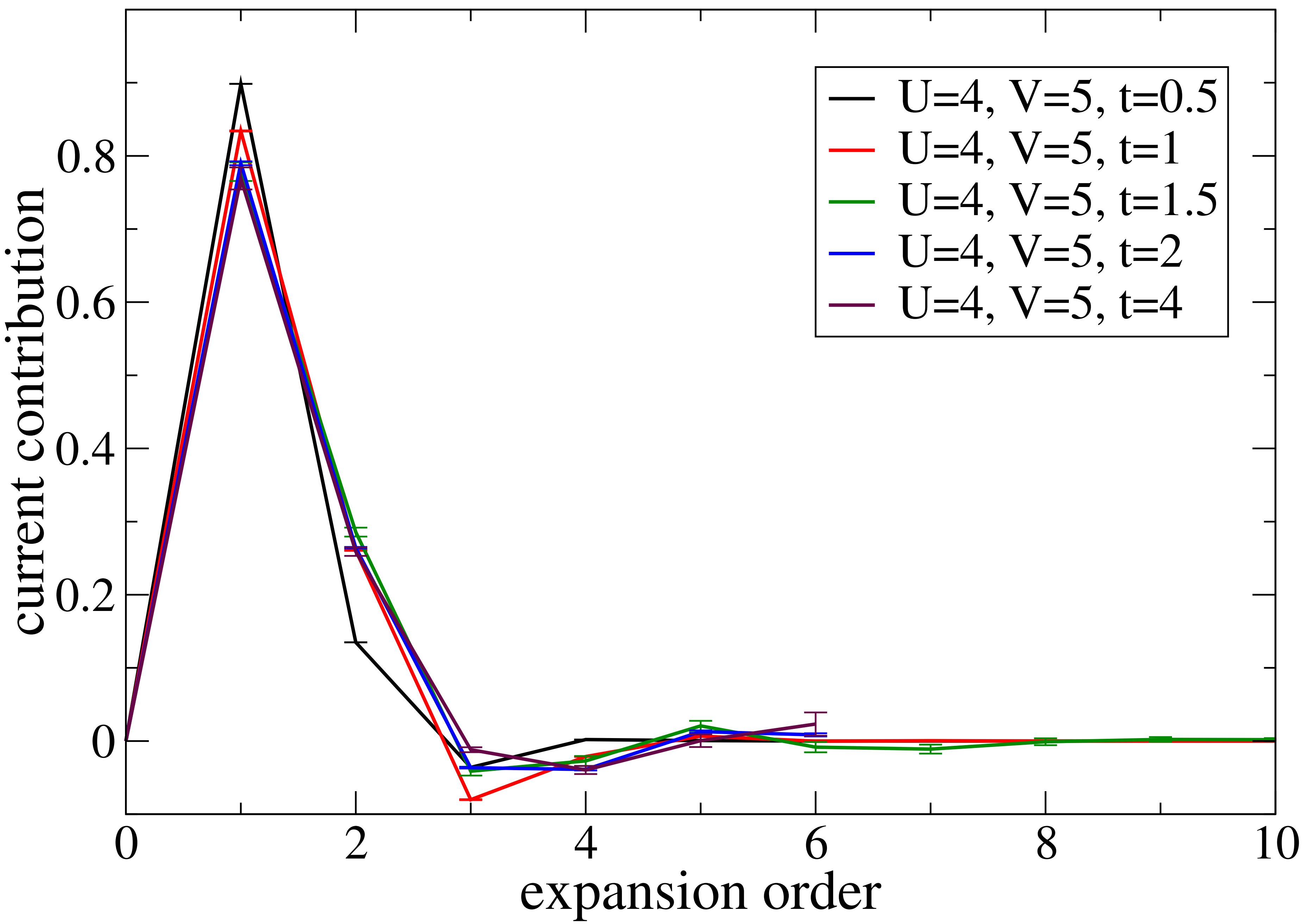
[Phys. Rev. B 89, 115139 (2014)]
[Phys. Rev. Lett. 112, 146802 (2014)]

Phys. Rev. B **84**, 085134 (2011)

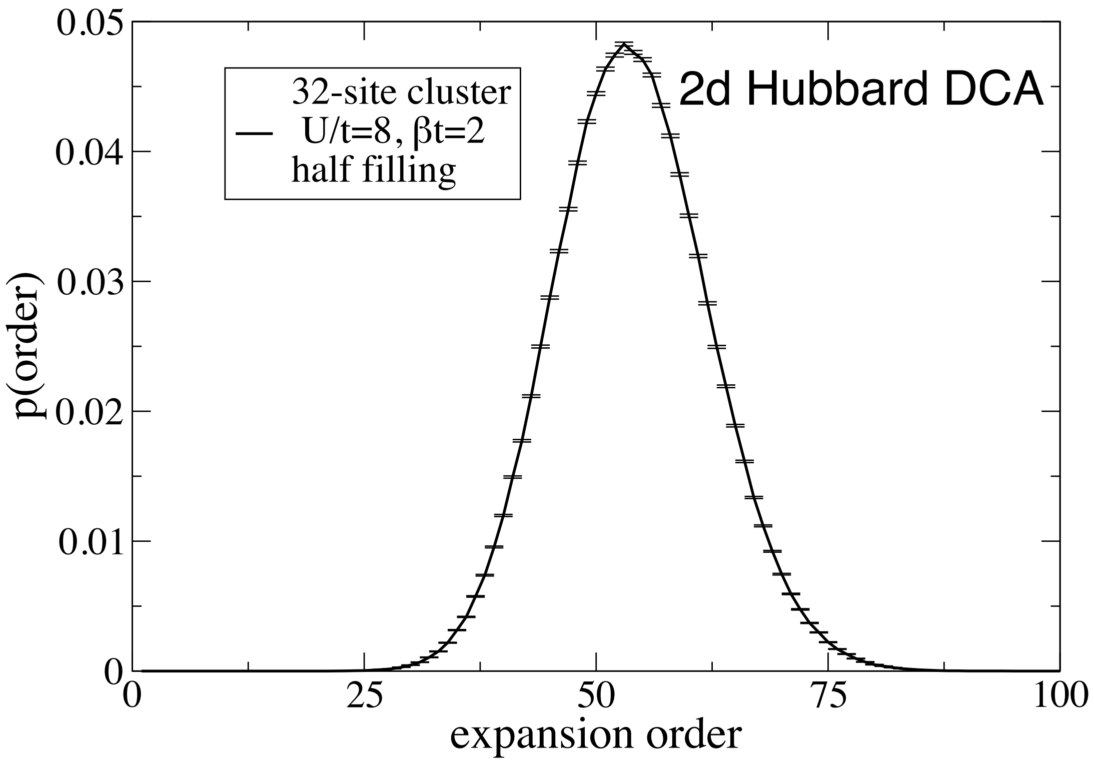
Real Time Bold NCA – Order Contribution

Contribution to the current as a function of expansion order:



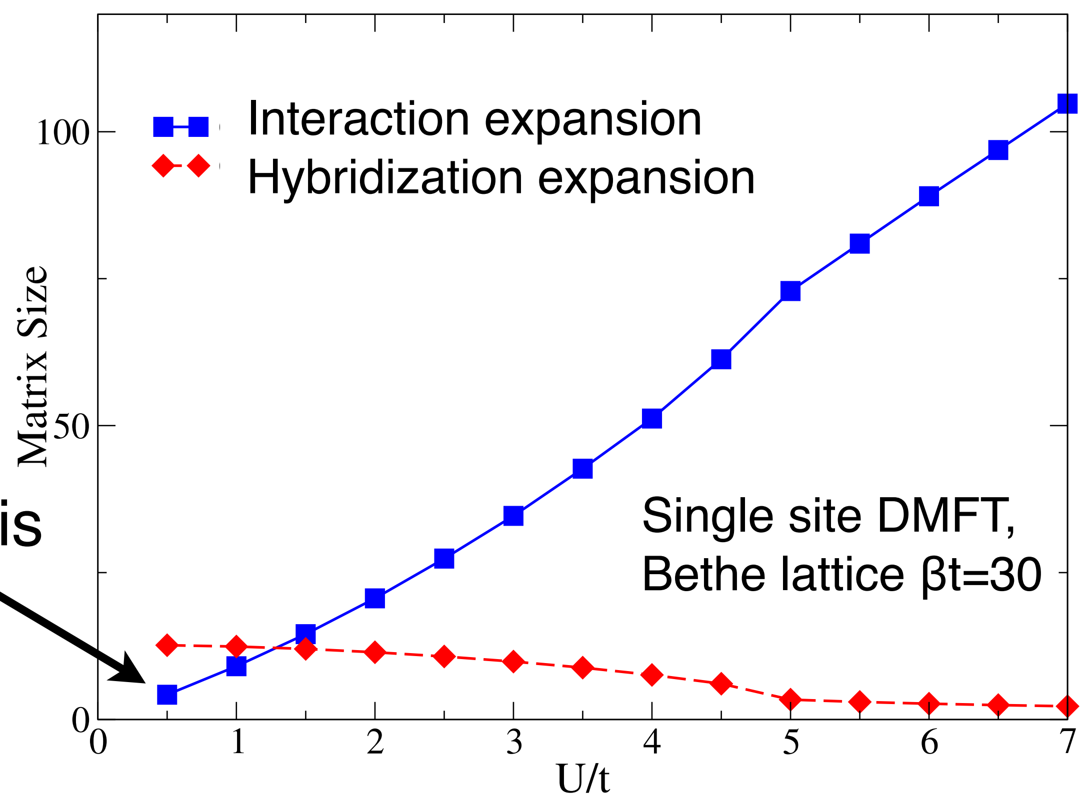
E. Gull, A. Millis, A. I. Lichtenstein, A. N. Rubtsov, M. Troyer, P. Werner, [Rev. Mod. Phys 83, 349 (2011)]

‘Bare’ Continuous-Time algorithms



Expansion order histogram

expansion is convergent, peaked at typical expansion order.



Average expansion order as a function of interaction

Expand in interaction: best when interaction is small

Expand in hybridization: best in insulating phase (few hybridization processes)