

Inchworm Quantum Monte Carlo for Real-Time Dynamics

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[Phys. Rev. Lett. 115, 266802 \(2015\)](#)

[Phys. Rev. B 95, 085144 \(2017\)](#)

[Phys. Rev. B 96, 155126 \(2017\)](#)

[Phys. Rev. B 97, 115109 \(2018\)](#)

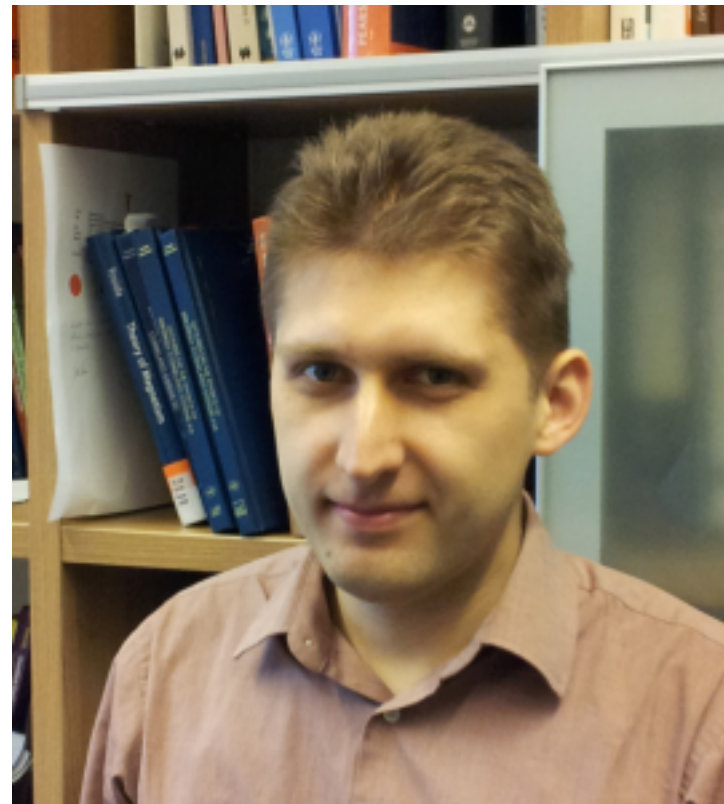
[Phys. Rev. B 98, 115152 \(2018\)](#)

[arXiv:1904.11527](#)

Collaboration



Guy Cohen
TAU

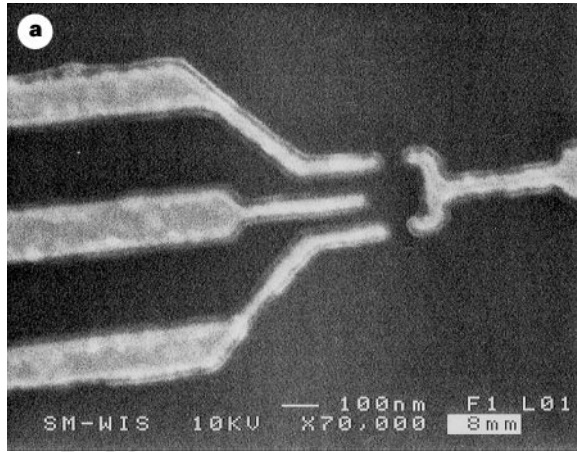


Igor Krivenko

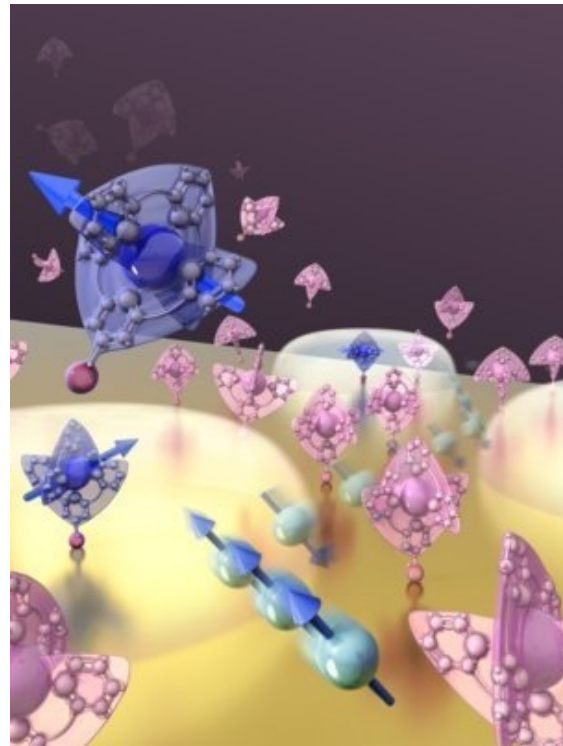


Joe Kleinhenz

The non-equilibrium Kondo problem

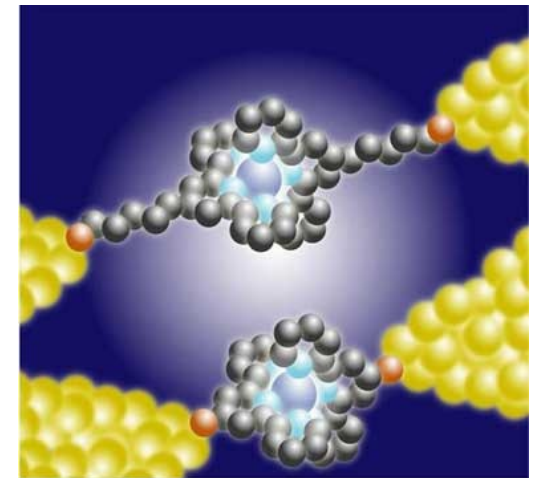


Kondo effect in a single-electron transistor, D. Goldhaber-Gordon *et al*, Nature 391, 156 (1998)



Magnetic impurities in non-magnetic bulk

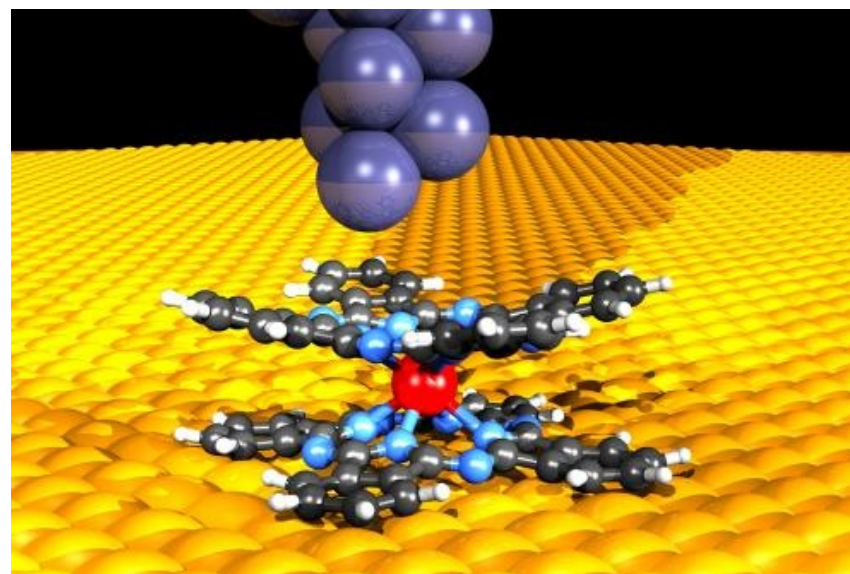
Coulomb blockade and the Kondo effect in single-atom transistors, Park *et al*, Nature 416, 722 (2002)



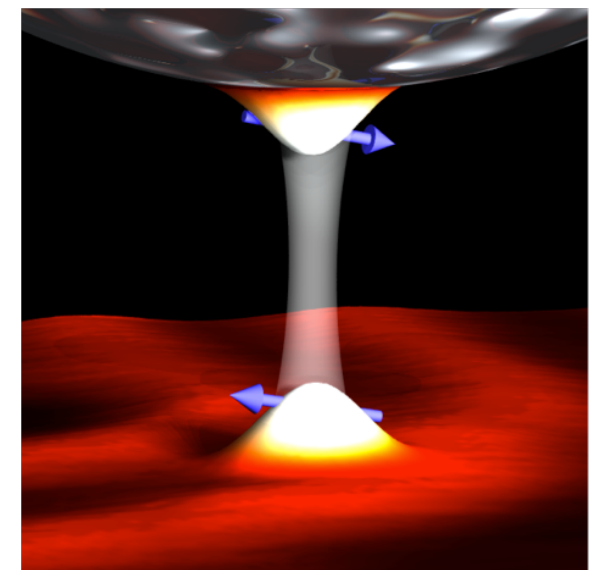
Two-impurity Kondo systems in atomic point contacts: Bork *et al*, Nat. Phys. 7, 901 (2011)



Double quantum dots

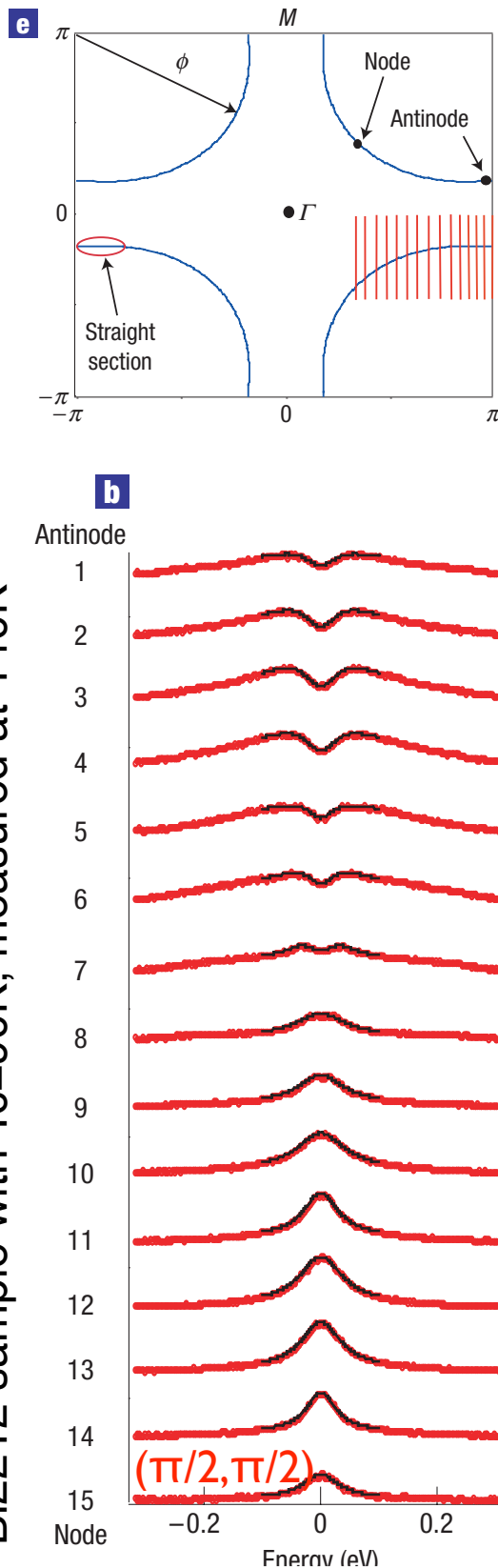


Magnetic molecules adsorbed on surfaces, e.g. Fahrenndorf *et al*, Nature Communications 4, 2425



Spectral function of solids

ARPES: Kanigel *et al.*, Nature Physics 2, 447 - 451 (2006).
Bi2212 sample with $T_c=90\text{K}$, measured at 140K



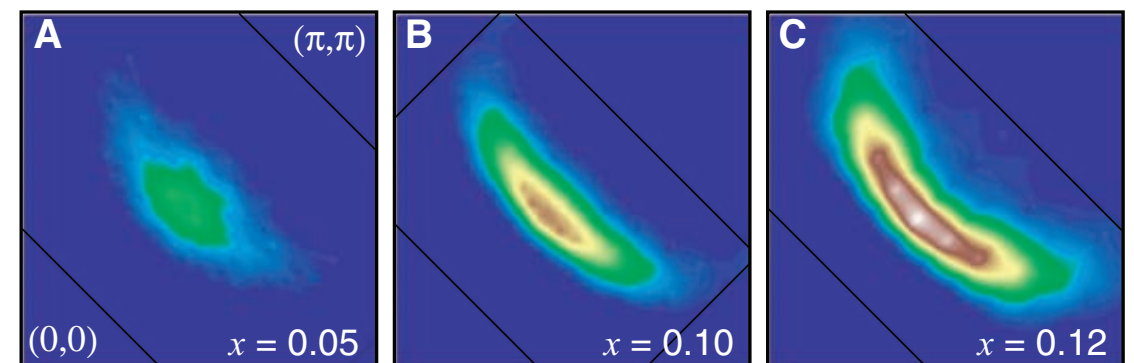
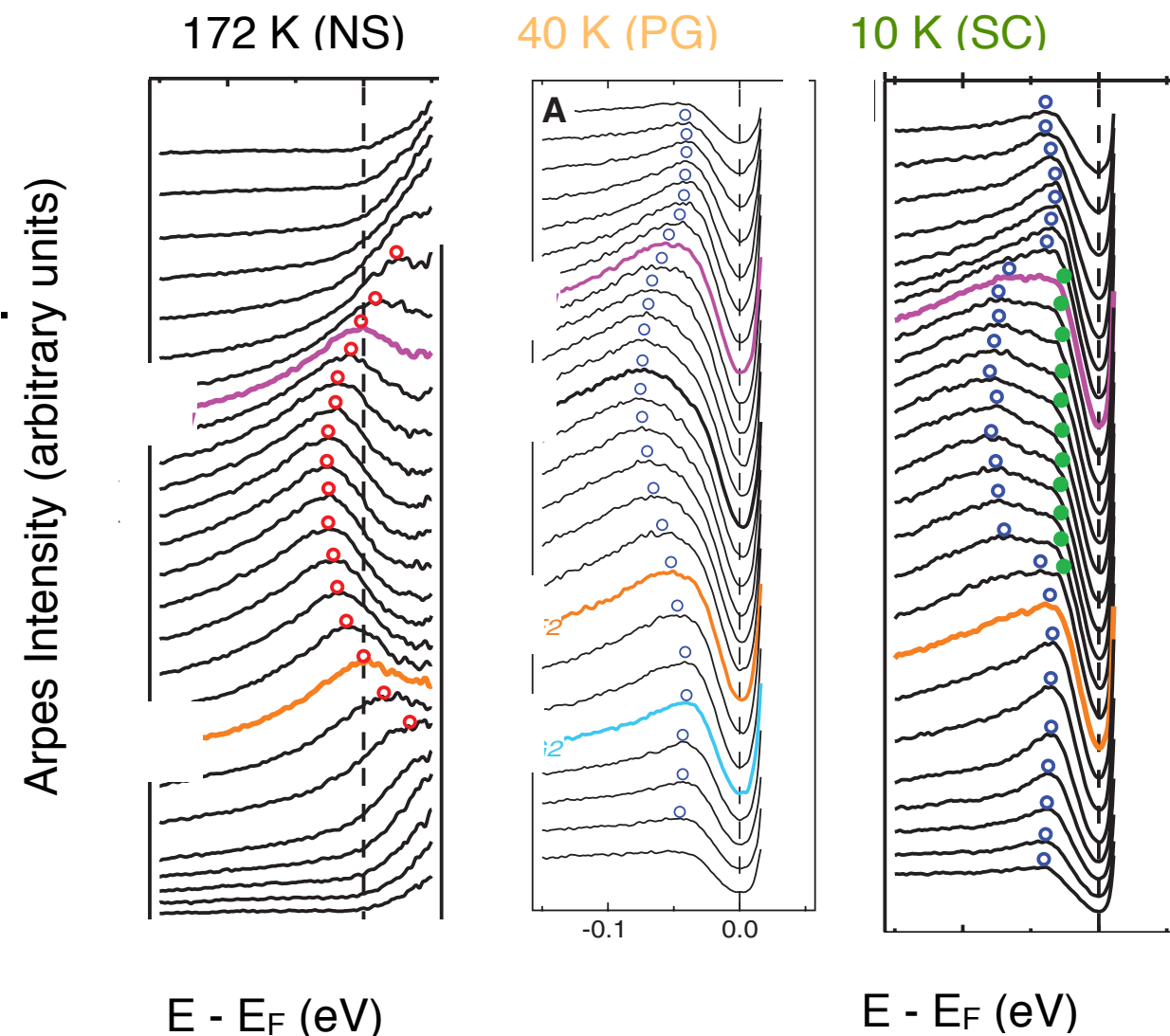
in high- T_c materials:
Electronic spectral
function is **suppressed**
along the BZ face, but
not along **zone diagonal**.

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

Doping dependence of
region with
quasiparticles

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

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



Question to theory

What can we say about non-equilibrium correlation physics?

What can we say about spectral functions of interacting systems?

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

What happens to Kondo physics in non-equilibrium conditions?

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

Model: Anderson Impurity

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

$$H_{\text{loc}} = \sum_{\sigma} \epsilon_{0\sigma} n_{\sigma} + U n_{\uparrow} n_{\downarrow}$$

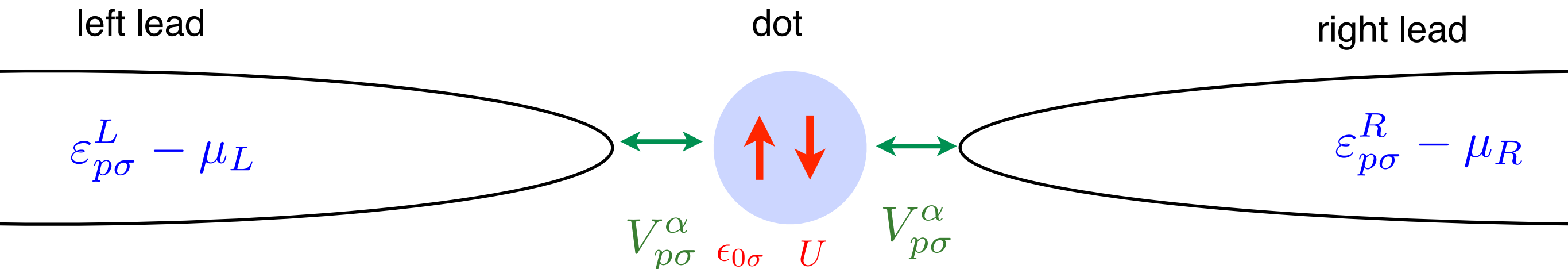
Impurity described by **Coulomb interaction U**, **level energies $\epsilon_{0\sigma}$** .

$$H_{\text{bath}} = \sum_{\alpha=L,R} \sum_{p\sigma} (\epsilon_{p\sigma}^{\alpha} - \mu_{\alpha}) c_{p\sigma}^{\alpha\dagger} c_{p\sigma}^{\alpha}$$

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

$$H_{\text{hyb}} = \sum_{\alpha=L,R} \sum_{p\sigma} V_{p\sigma}^{\alpha} c_{p\sigma}^{\alpha\dagger} d_{\sigma} + h.c.$$

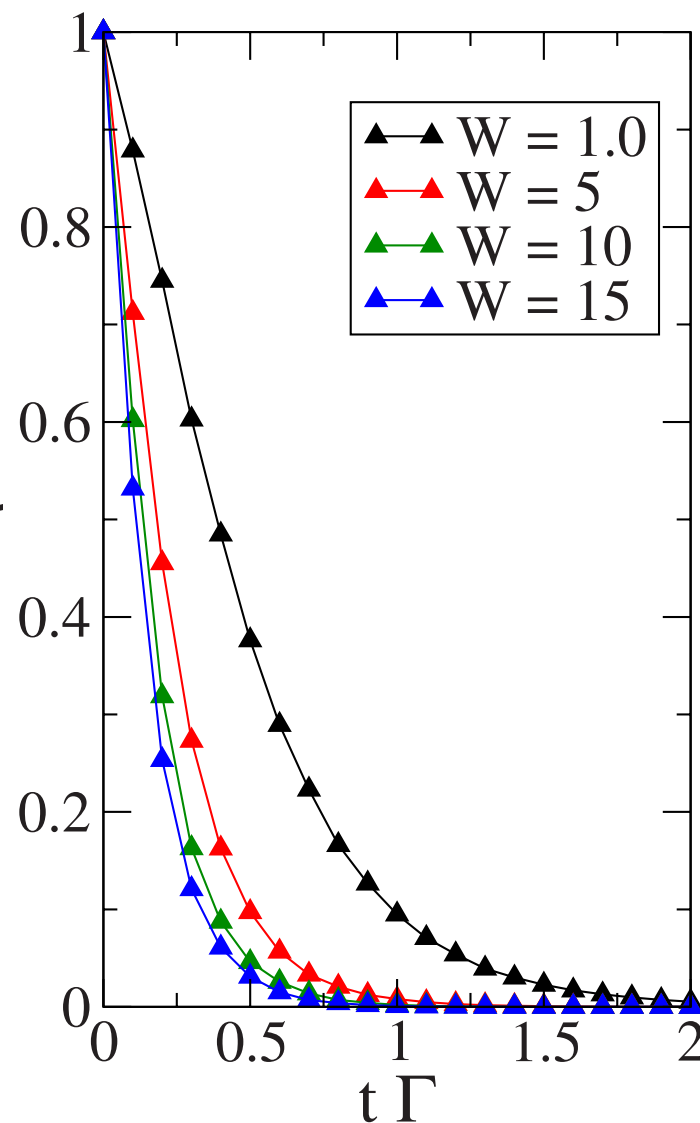
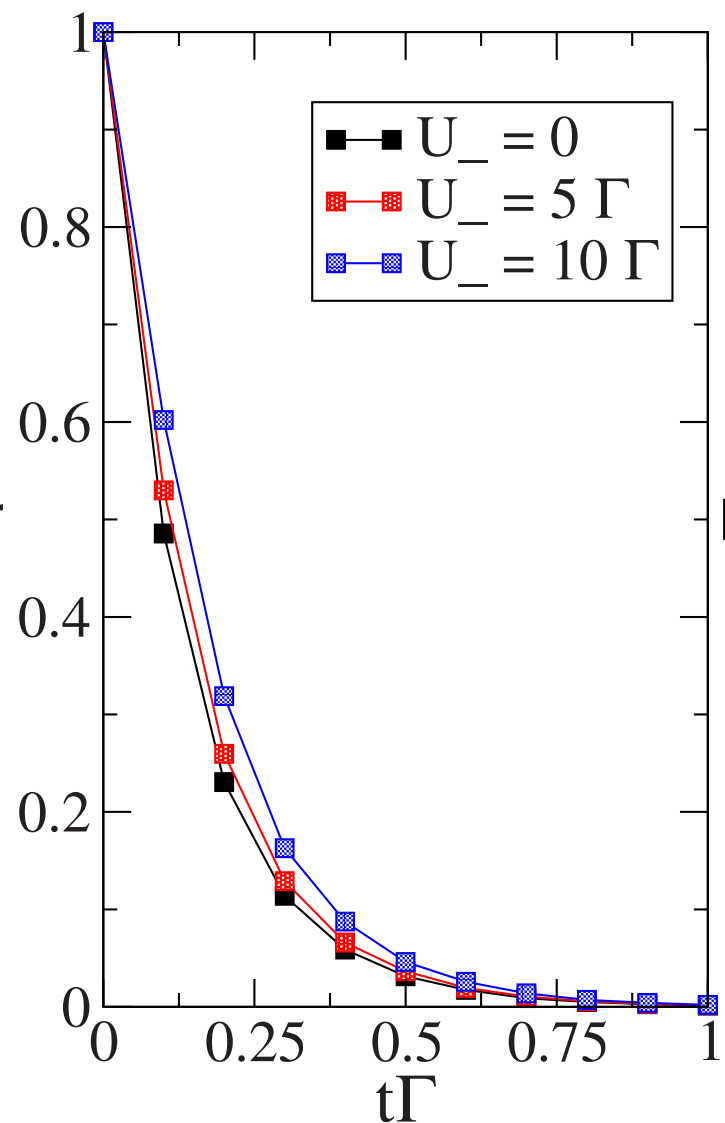
Coupling of dot to lead via '**hybridization strength**' V.



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

CT-QMC out of equilibrium – Motivation for modern MC algorithms

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

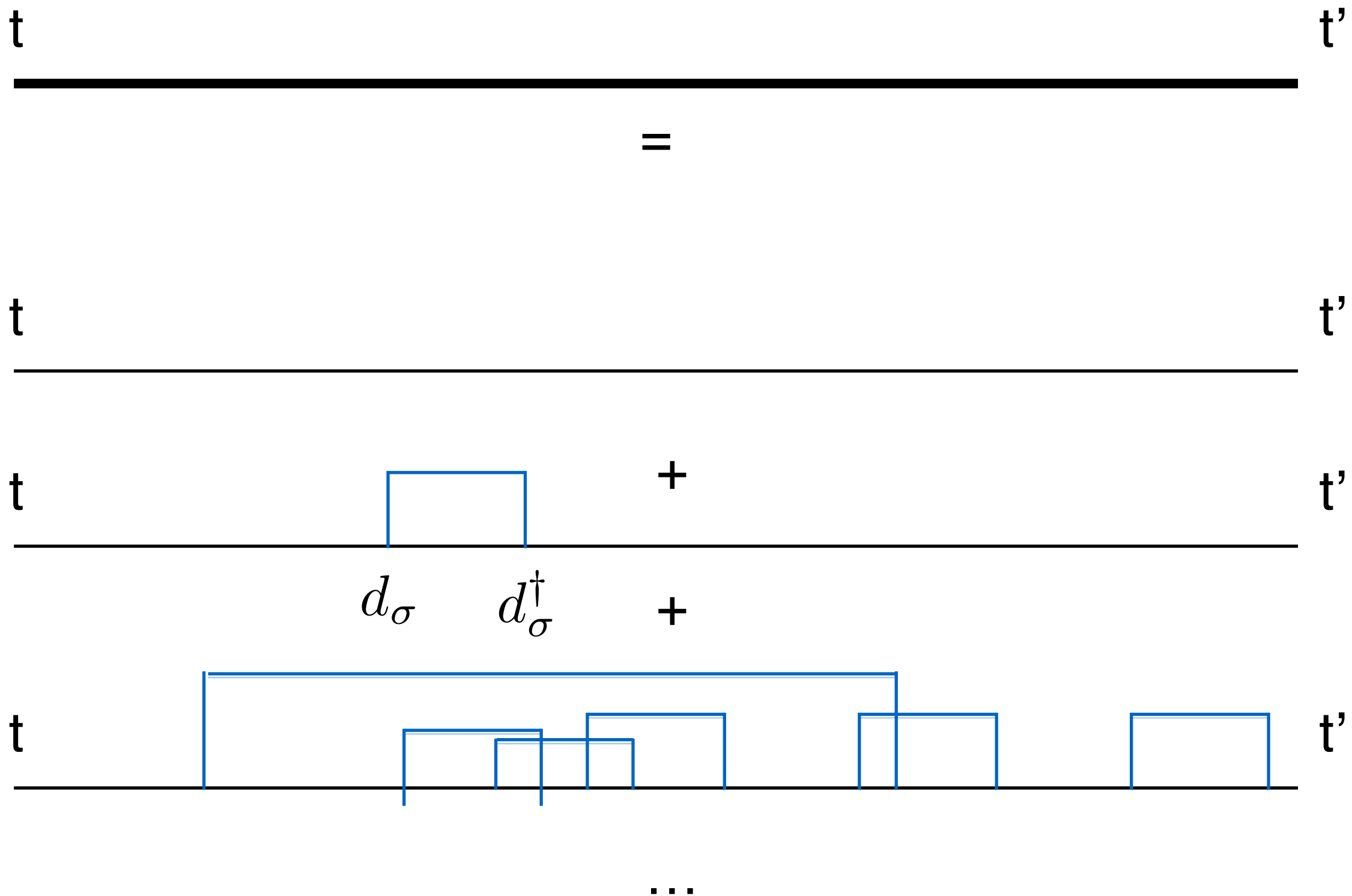
Marco Schiro

[Phys. Rev. B 81, 085126 \(2010\)](#)

[Mühlbacher, Rabani, Phys. Rev. Lett. 100, 176403 \(2008\)](#)

[Werner, Oka, Millis, Phys. Rev. B 79, 035320 \(2009\)](#)

Bare Quantum Monte Carlo



Bold-line Quantum Monte Carlo

t t'

=

=

+



+



semi-analytic partial
summation, coupled
integral equations

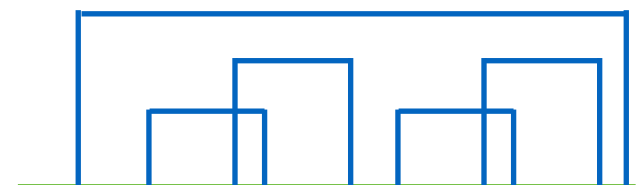
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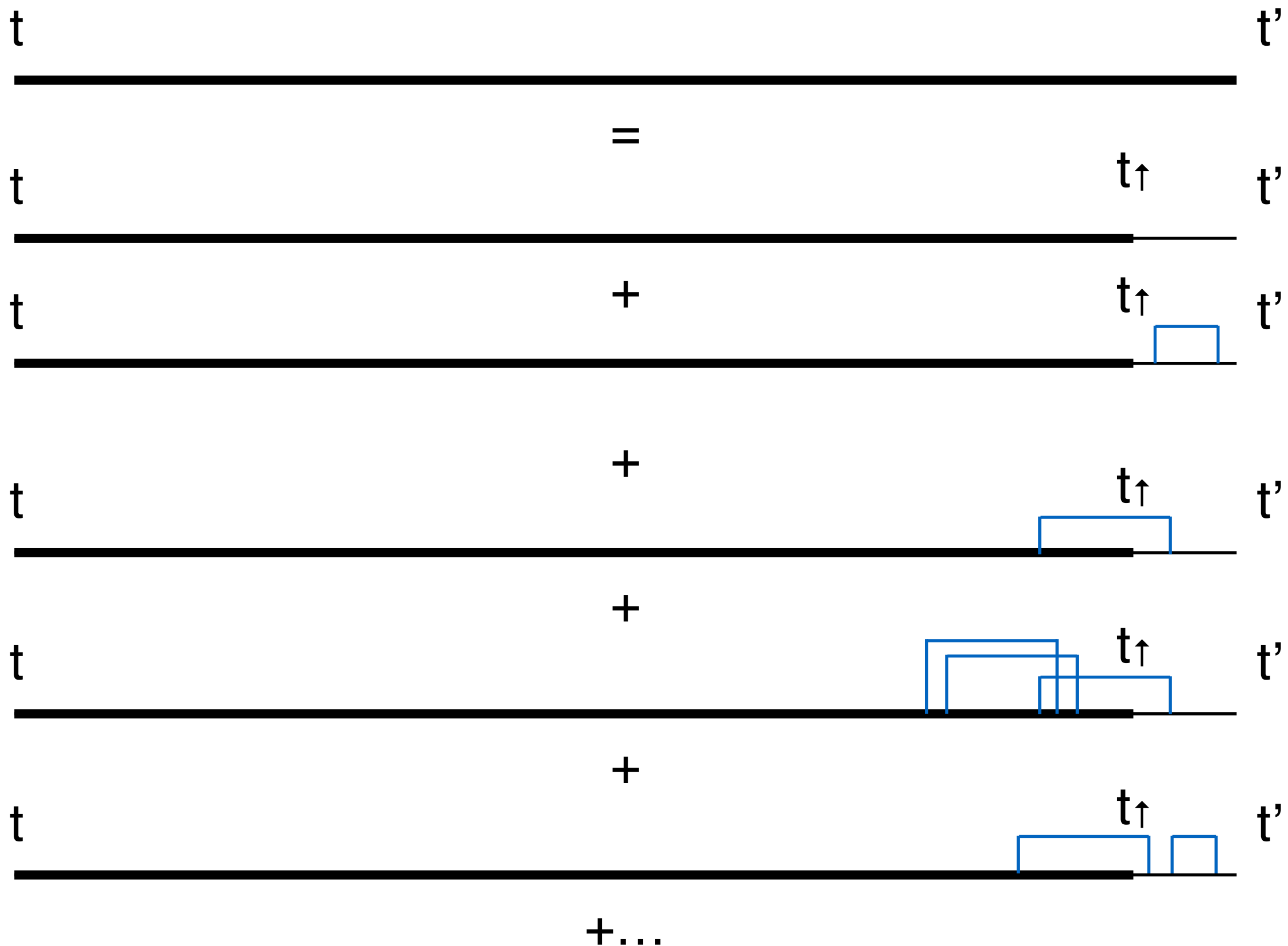
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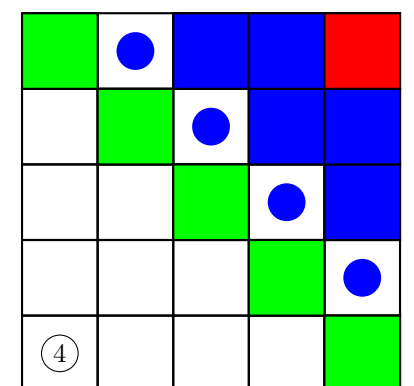
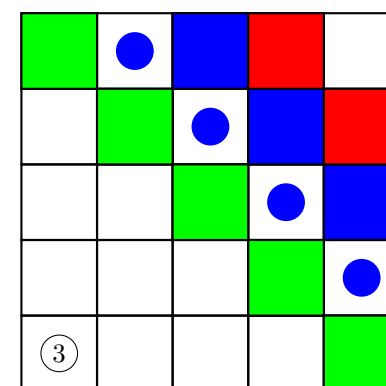
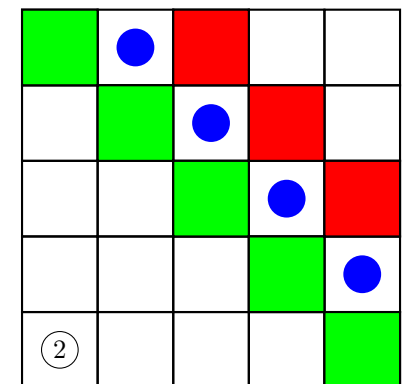
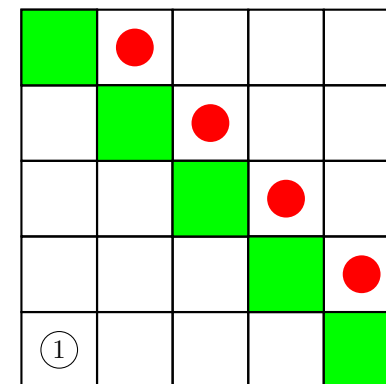
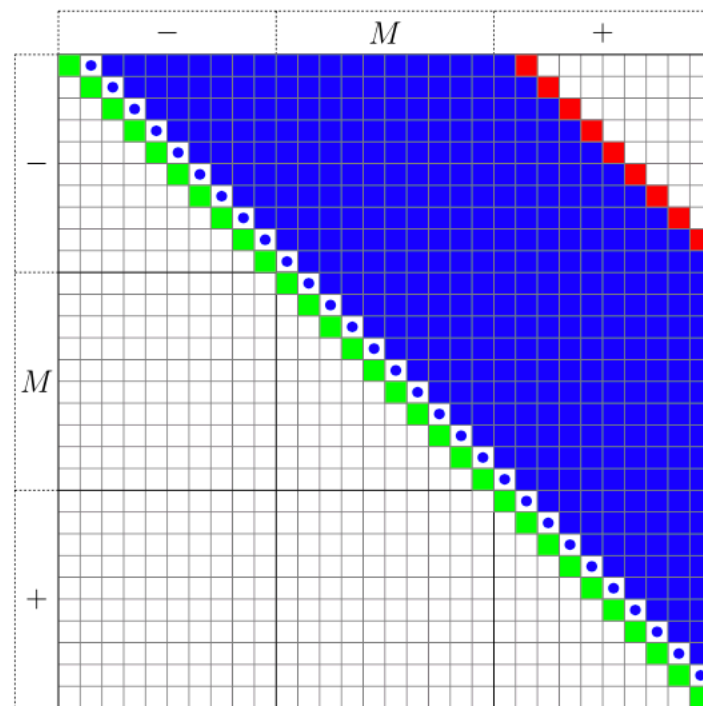
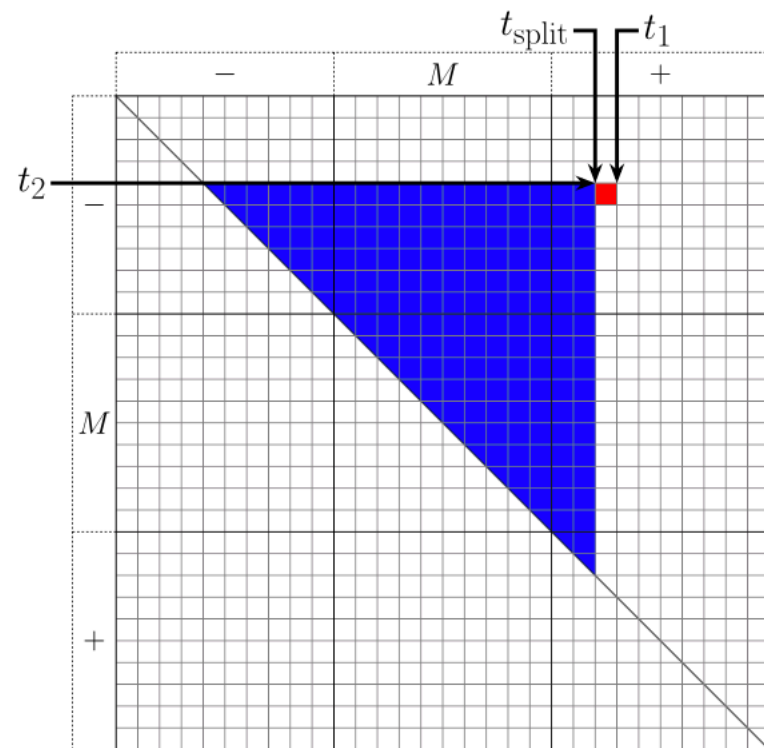


Inchworm Quantum Monte Carlo



Inchworm Quantum Monte Carlo

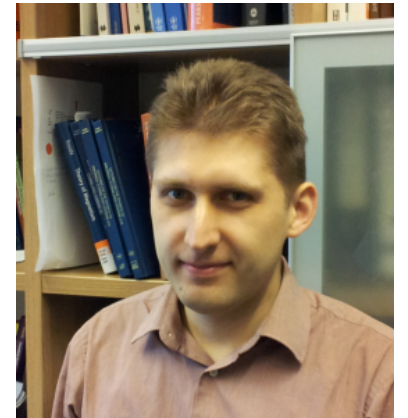
- Build algorithm intrinsically based on causality.
- Only sample corrections to exact solution at smaller times.
- Lots of small but interdependent Monte Carlo simulations



Runtime Systems

- Standard parallelization scheme: **Message Passing Interface**. Send (or broadcast) messages explicitly from node to node.
 - Within a box: **OpenMP** for threading (in scientific applications), threading libraries (pthreads etc) for general purpose
- **Runtime systems** for dealing with many independent tasks that all have different runtimes, different complexities, different data dependencies.
 - Legion (<https://legion.stanford.edu/>)
 - HPX (High Performance ParallelX) <https://github.com/STELLAR-GROUP/hpx>

HPX

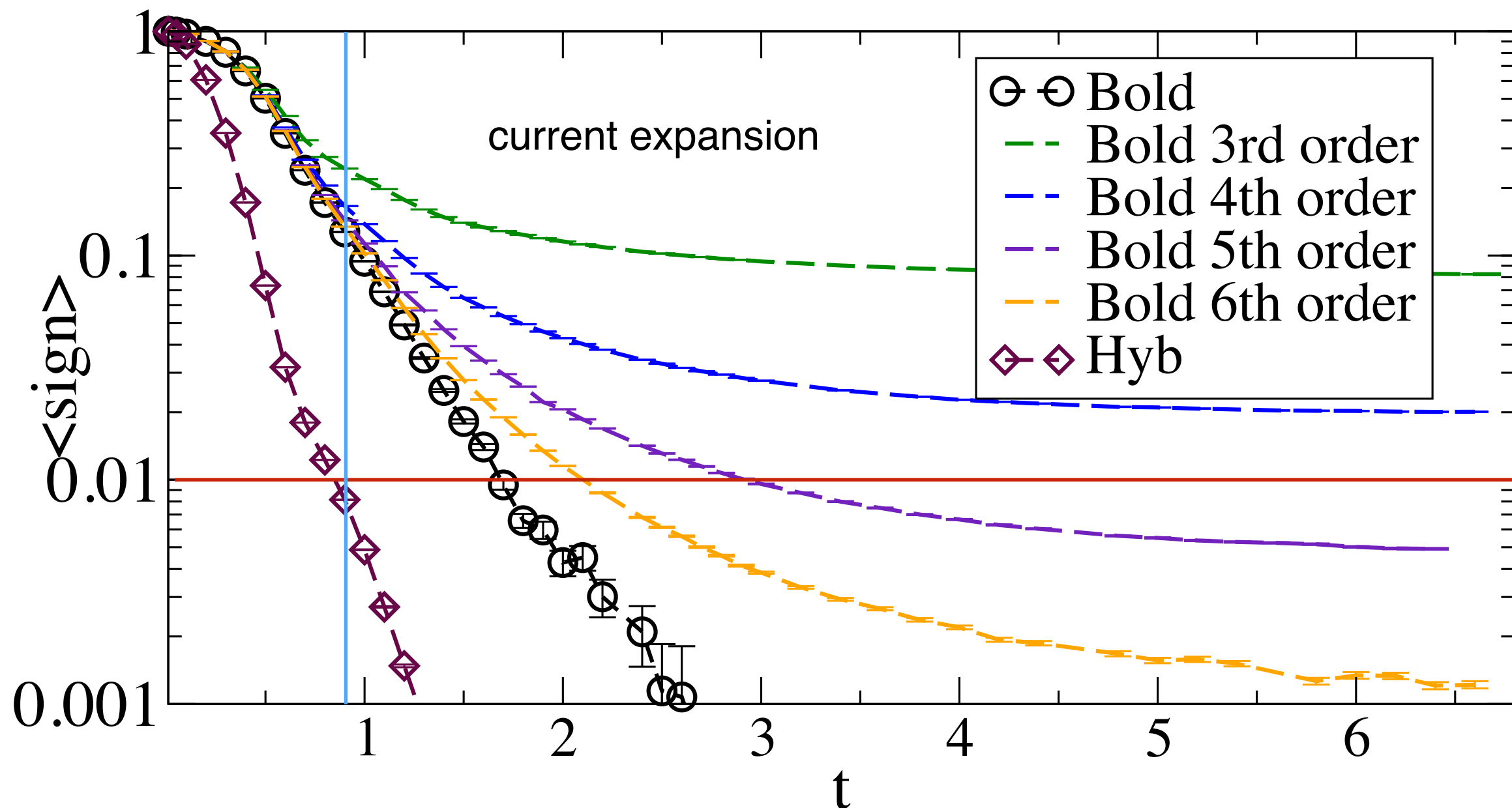


```
int myfunc(int n) {  
    // ... takes 10 minutes to finish ...  
    return 42;  
}  
  
// For now, we restrict ourselves to one locality (one cluster node)  
hpx::naming::id_type locality_id = hpx::find_here();  
  
// Schedule asynchronous evaluation of the result  
// hpx::async() will return immediately  
hpx::future<int> promised_result = hpx::async(myfunc, locality_id, 3);  
  
// A lot of code that does something else...  
  
// Get access to the promised value  
// get() will block and wait until myfunc() finishes  
int result = promised_result.get();
```

```
// Schedule asynchronous evaluation of the result  
hpx::future<eigensystem_t> eigensystem_f =  
    hpx::async(diagonalize_action(), locality_id, block);  
  
// Schedule continuations of eigensystem_f  
hpx::future<weights_t> weights_f =  
    eigensystem_f.then(compute_weights_action());  
hpx::future<a_element_t> a_elements_f =  
    eigensystem_f.then(compute_psiApsi_action());  
// ...  
  
weights_f.get();  
a_elements_f.get();
```

- task that needs to be executed (e.g. an inchworm run)
- localities to execute it on (all the cores on a cluster)
- schedule an asynchronous task
- wait until the job is done
- make tasks dependent on earlier tasks... runtime system will run them whenever resources become available
- automatic distribution to available localities is experimental. We use a round robin scheme for balancing between localities

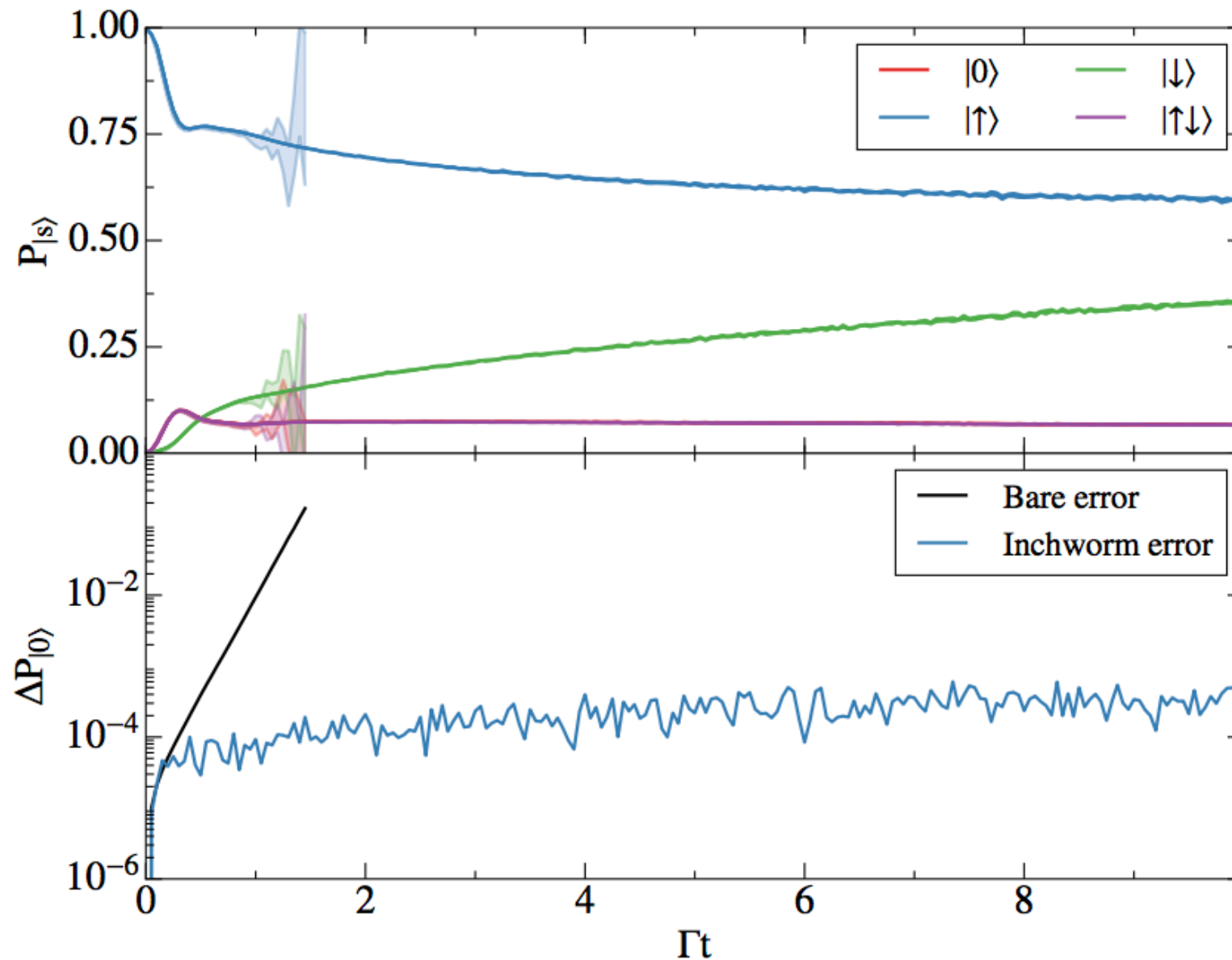
From bare to bold



Bold vs bare:

- Sign better by 1 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.

... to inchworm



inchworm vs bare/bold:

- Monte Carlo error plateaus as a function of time. That means the dynamical sign problem has been overcome.
- Data available to arbitrary time at $O(N^2)$ cost.

Figure 2. Top panel: population dynamics of the Anderson impurity model in the Kondo regime following a coupling quench from a fully magnetized state at $U = -2\varepsilon = 8\Gamma$ and $\beta\Gamma = 50$. The bare hybridization expansion result (Fig. 1(a)) is shown for times $\Gamma t < 1.5$, along with the Inchworm result (Fig. 1(c)) up to $\Gamma t = 10$. Bottom panel: Error estimate of data in upper panel showing an exponential increase of the error as a function of time due to the dynamical sign problem in the bare method, and a roughly constant error in the inchworm method.

currents

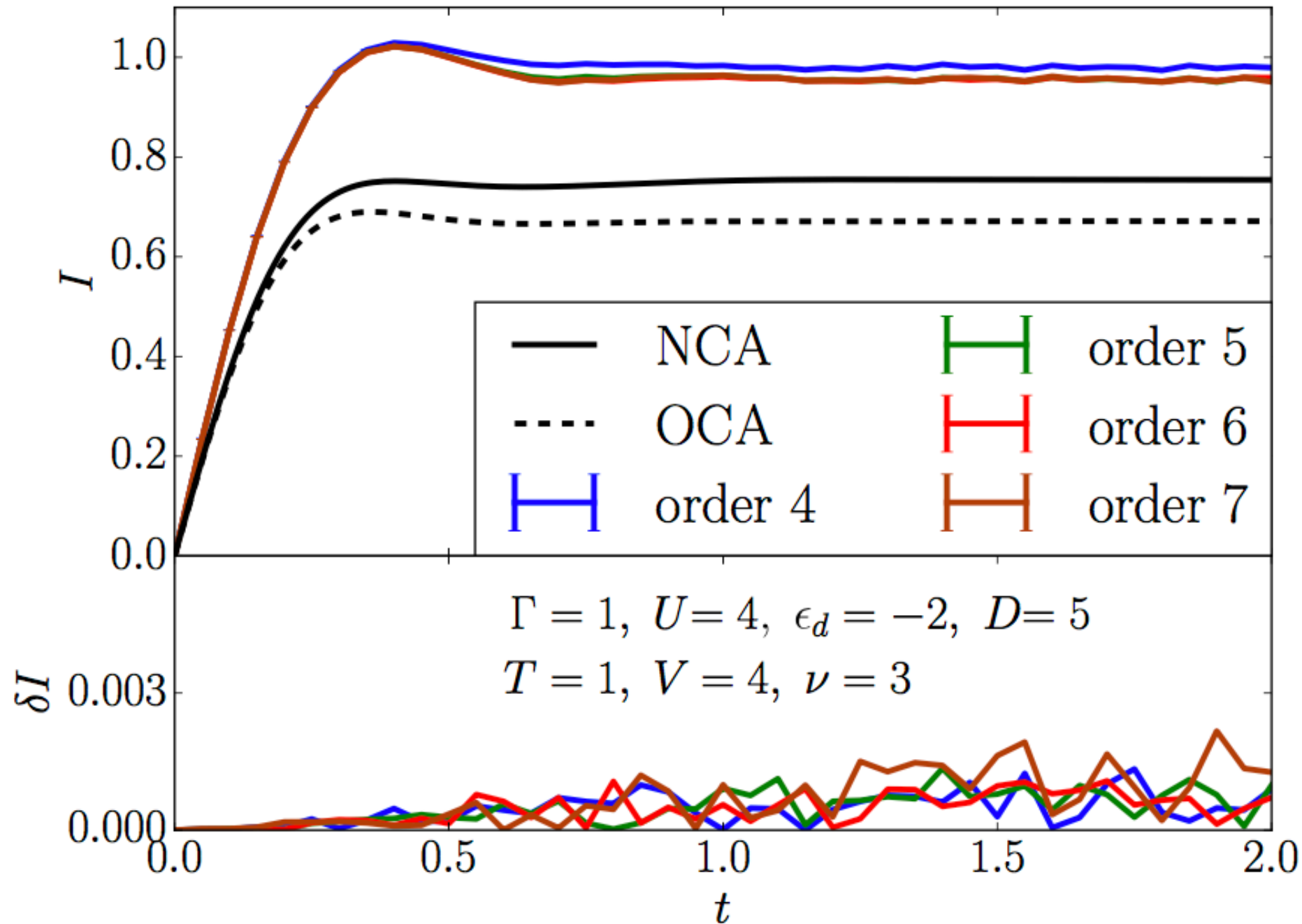


FIG. 8. (Top) The current dynamics after a voltage quench with $\Gamma = 1, U = 4, \epsilon_d = -2, D = 5, T = 1$, and $V = 4$. The inchworm results with different orders converge as maximum-order increases. (Bottom) Error estimates of inchworm data obtained by averaging eight independent calculations. Errors increase as a function of time but avoid the exponential amplification seen in bare calculations.

Extension to Green's functions and DMFT

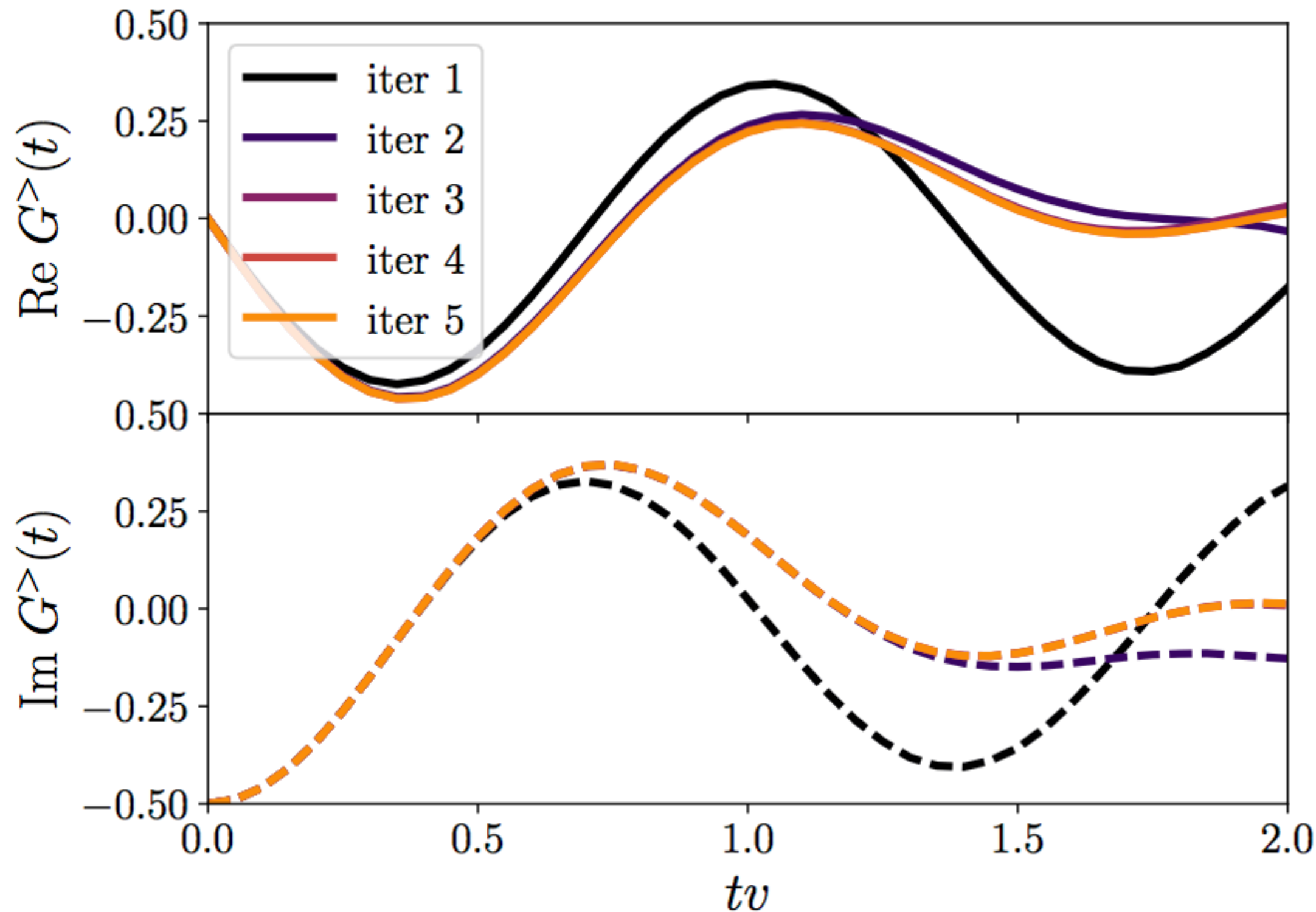


FIG. 1. Real and imaginary parts of the greater dynamical mean field Green's function $G^>(t)$ as a function of real time t up to a maximum time of $t\nu = 2$. $U/v = 4$, $T/v = 0.05$, equilibrium. Shown is the convergence with DMFT iteration.

Extension to Green's functions and DMFT

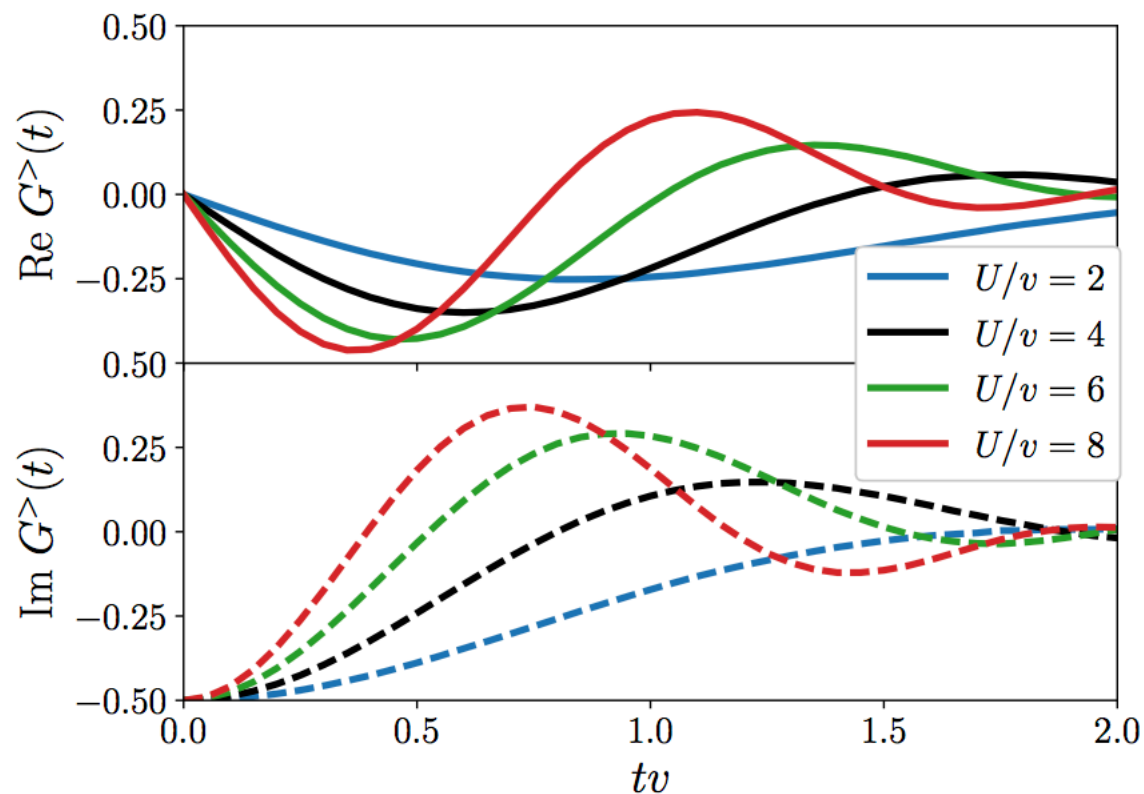
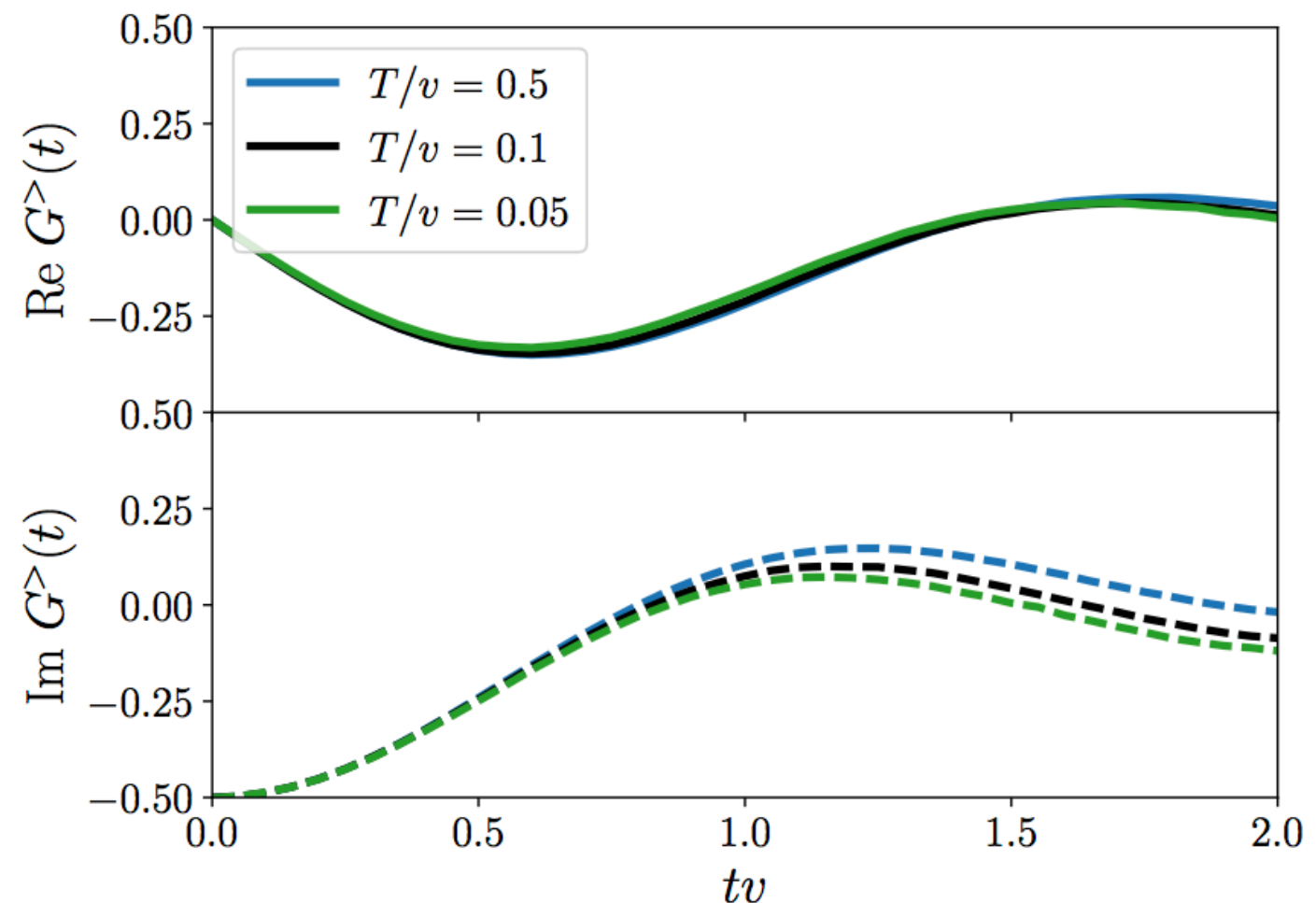


FIG. 2. Real and imaginary parts of the greater DMFT Green's function $G^>(t)$, for times up to $tv = 2$, with $T/v = 0.5$, half filling, equilibrium, at on-site interaction strengths $U/v \in \{2.0, 4.0, 6.0, 8.0\}$.

FIG. 3. Real and imaginary parts of the greater DMFT Green's function $G^>(t)$, for times up to $tv = 2$, half filling, equilibrium, for $U/v = 4$, at temperatures $T/v \in \{0.5, 0.1, 0.05\}$.



self-energies

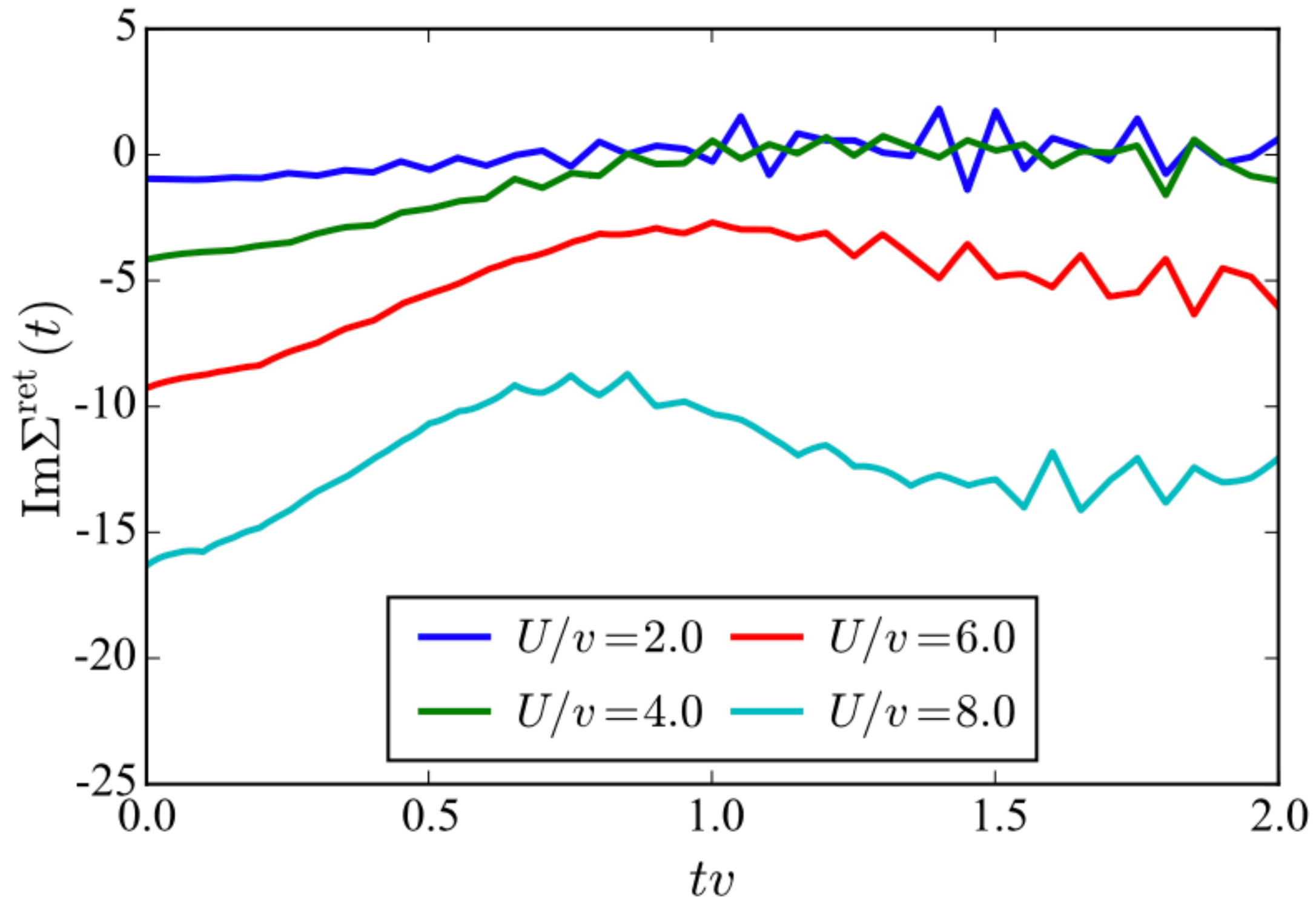


FIG. 5. Retarded component of the imaginary part of the DMFT self-energy for interaction strengths $U/v \in \{2.0, 4.0, 6.0, 8.0\}$ at half-filling and temperature $T/v = 0.5$.

long-time extrapolation (linear prediction)

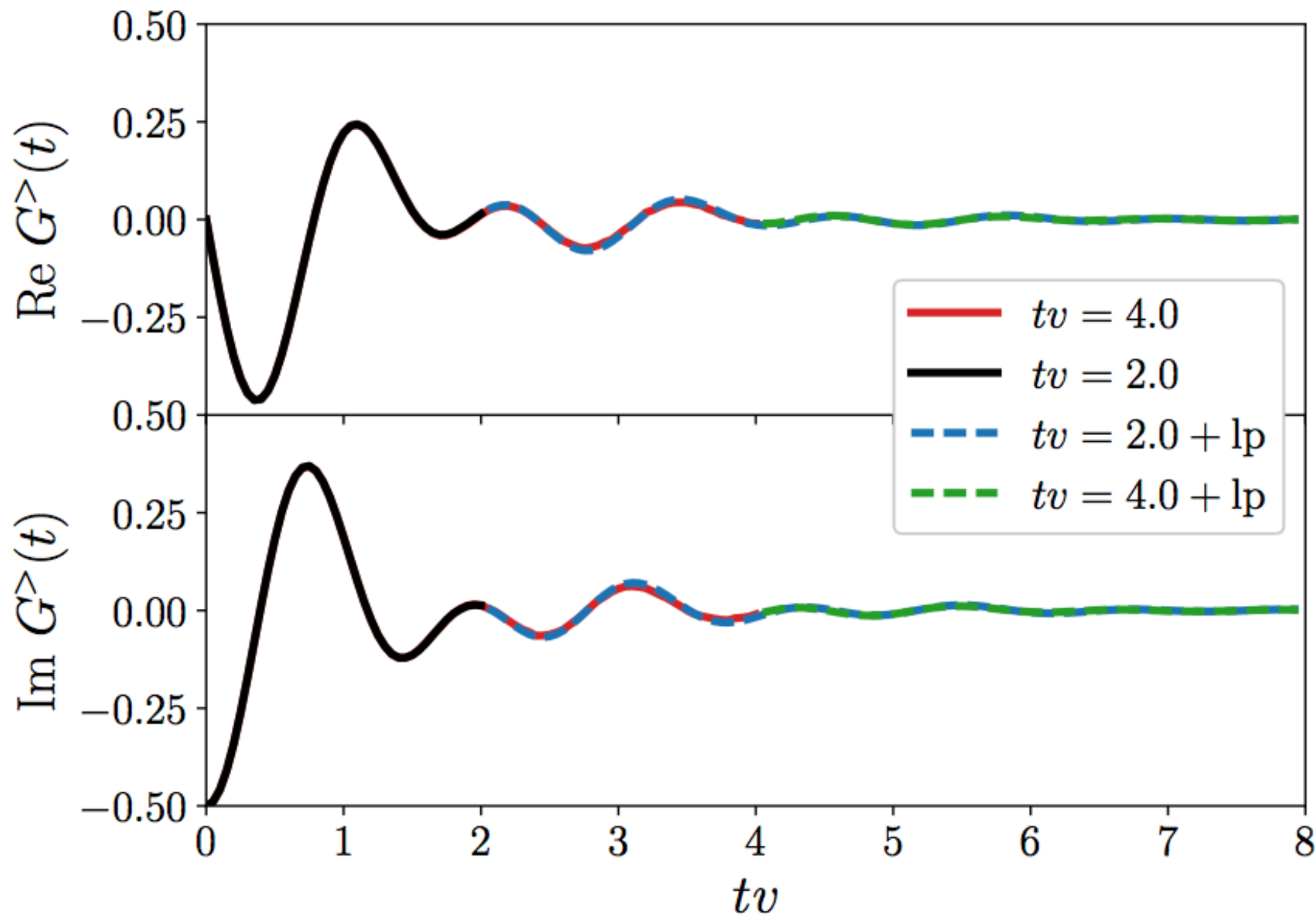


FIG. 7. Comparison of raw Green's function data up to $tv = 2$ (black) and $tv = 4$ (red) with results from linear prediction of the $tv = 2$ data (blue) and $tv = 4$ data (green) for $U/v = 8$, $T/v = 0.5$. For the linear prediction we use $p = 9$, $t_{\text{fit}}v = 1.0$.

naive spectral function

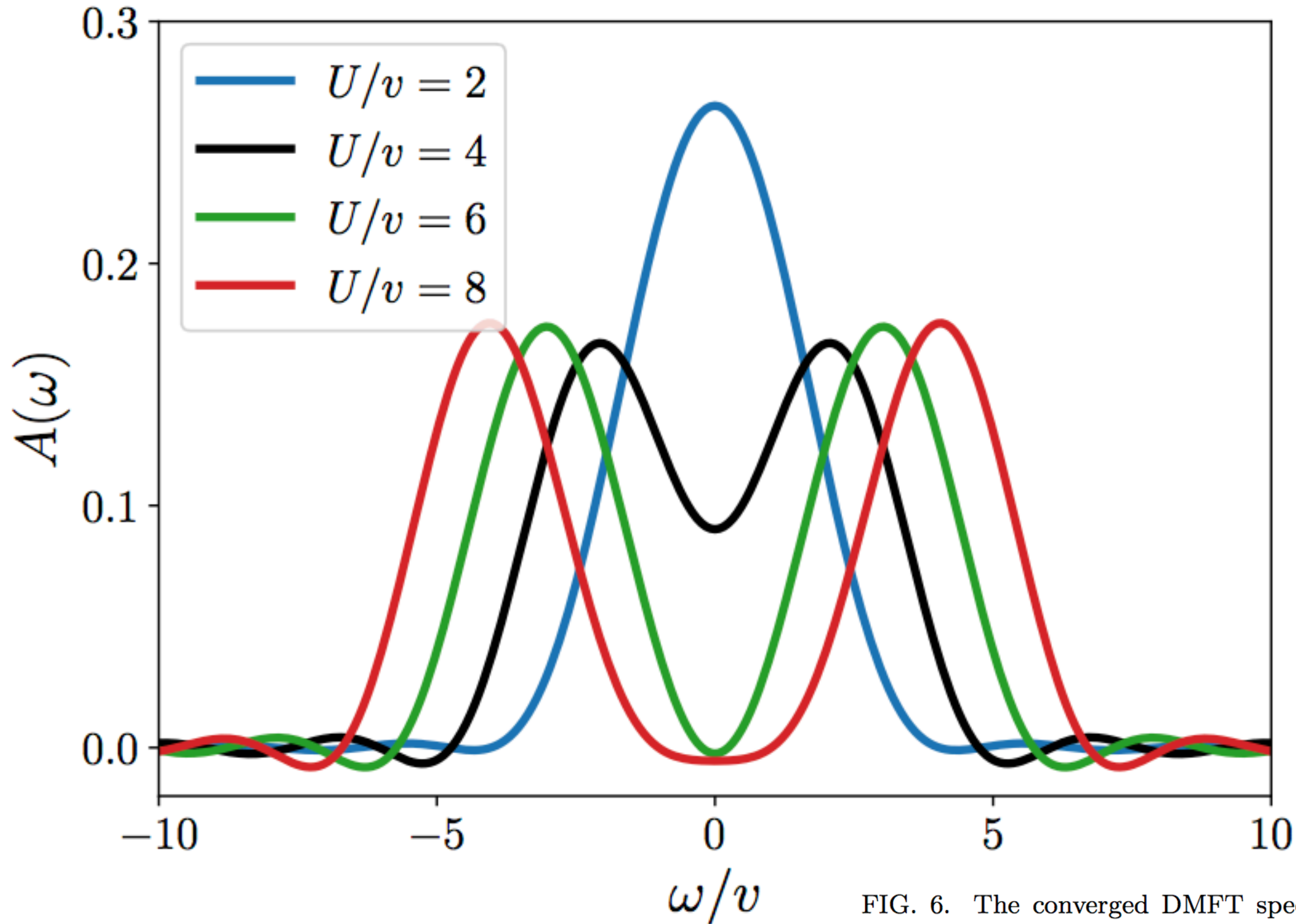


FIG. 6. The converged DMFT spectral function $A(\omega)$ obtained by directly performing the Fourier transform on the real time Green's function with a cutoff at $t_{\max}v = 2$ with $T/v = 0.5$ and at on-site interaction strengths $U/v \in \{2.0; 4.0; 6.0; 8.0\}$.

comparison to linear prediction

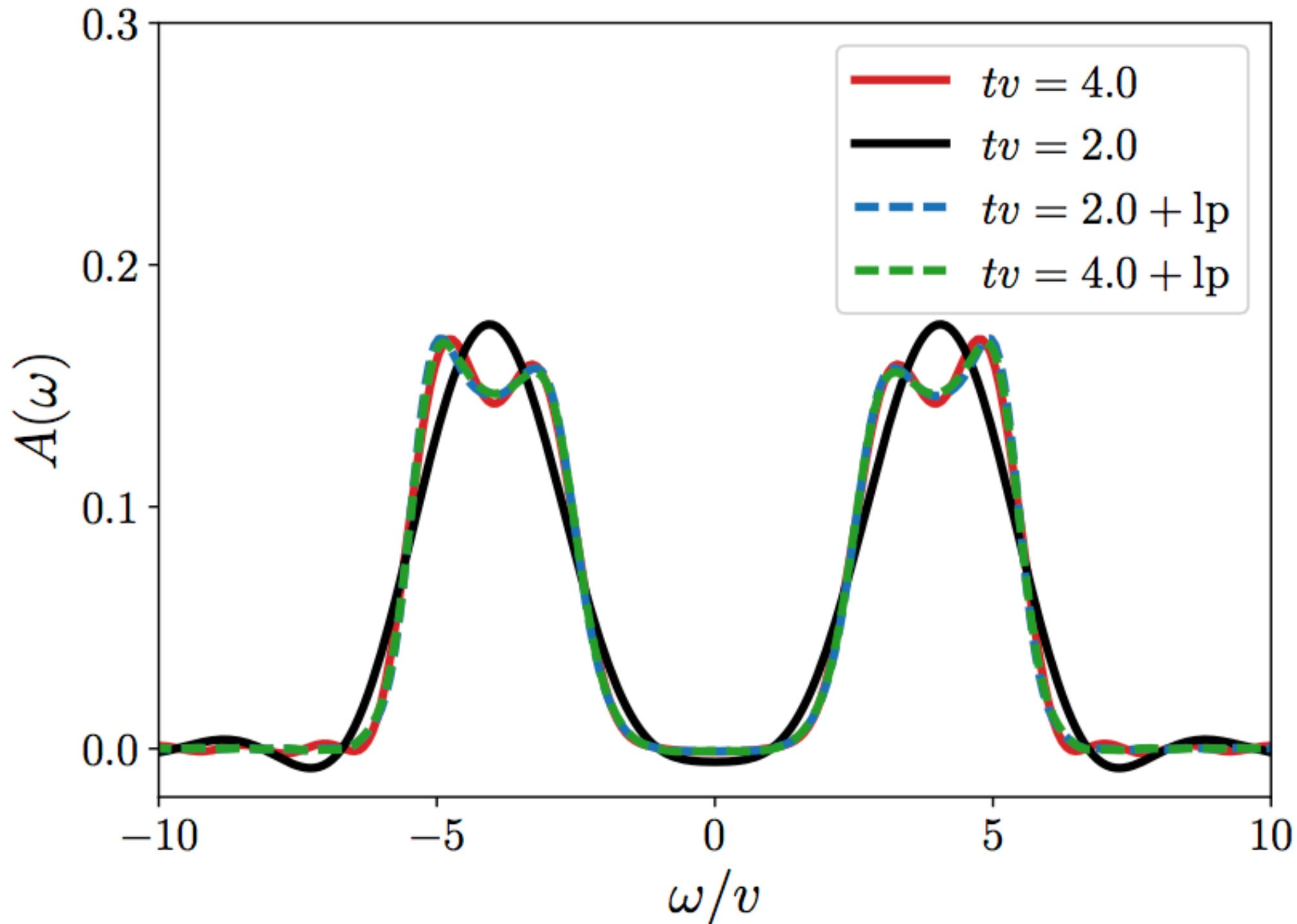
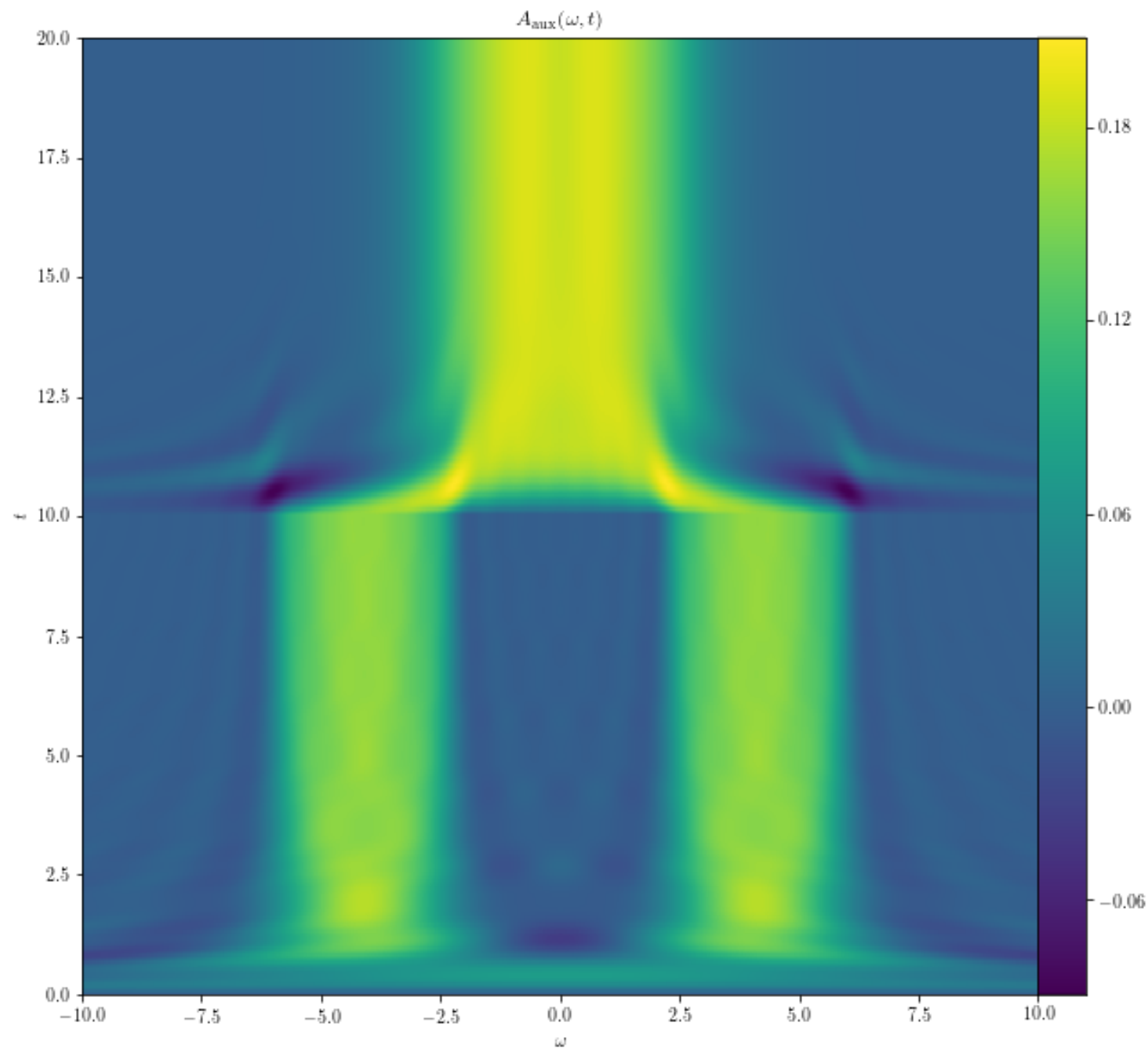
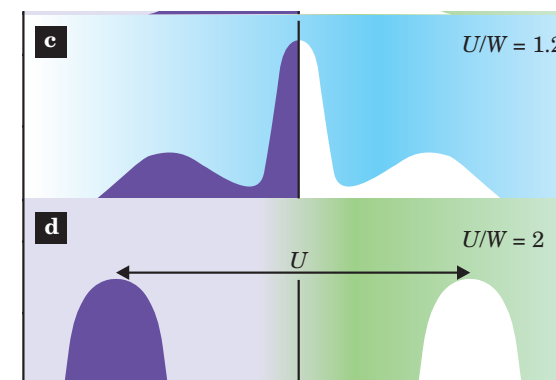


FIG. 8. Comparison of spectral function obtained from raw Green's function data up to $tv = 2$ (black) and $tv = 4$ (red) with results from linear prediction of the $tv = 2$ data (blue) and $tv = 4$ data (green) for $U/v = 8, T/v = 0.5$. For the linear prediction we use $p = 9, t_{\text{fit}}v = 1.0$.

Interaction Quench



- Dynamical mean field theory
- $U=8 \rightarrow U=2$
- Quench applied at $t=10$
- starting from thermal equilibrium state for $U=8$



emergence of a quasiparticle peak

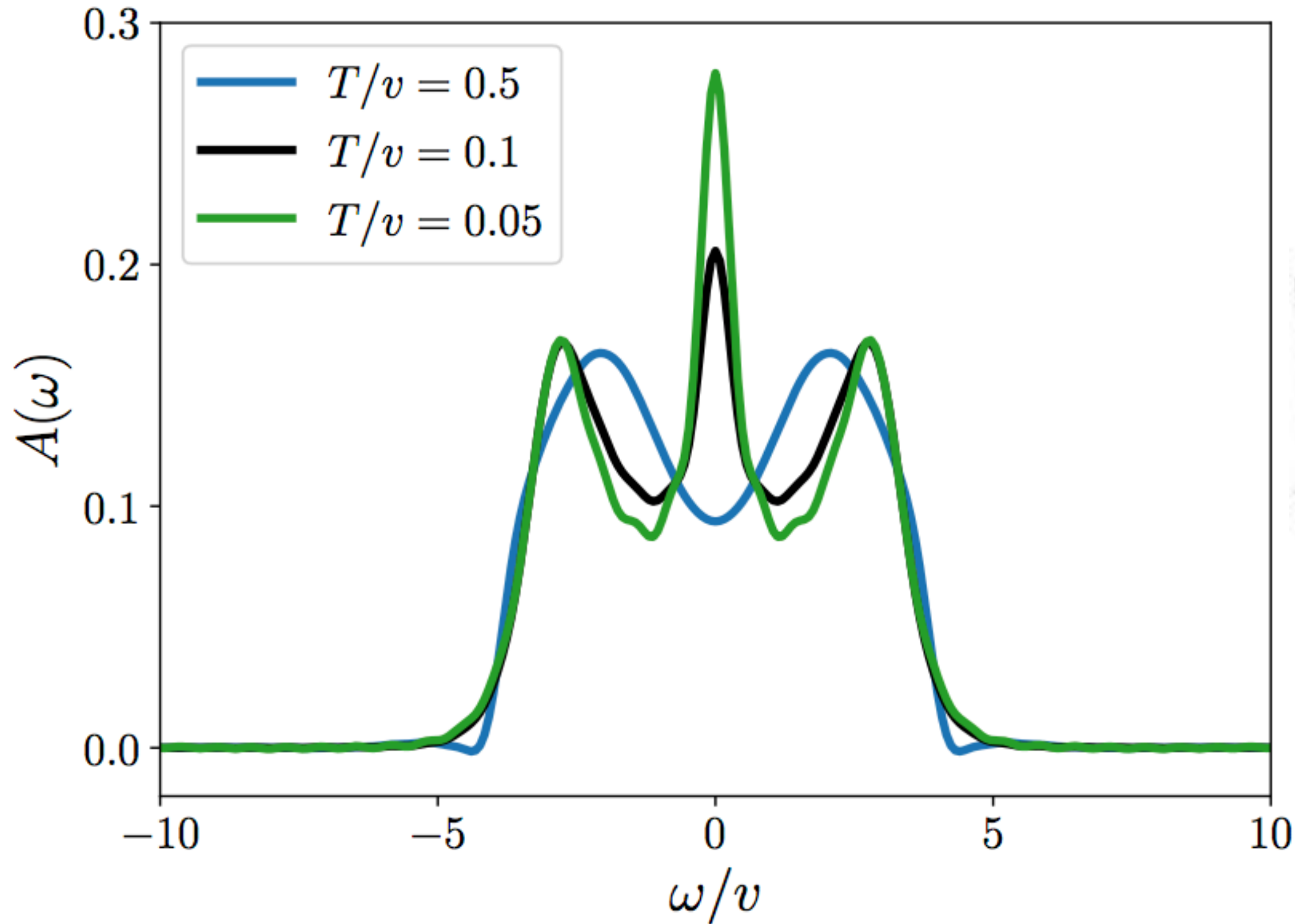
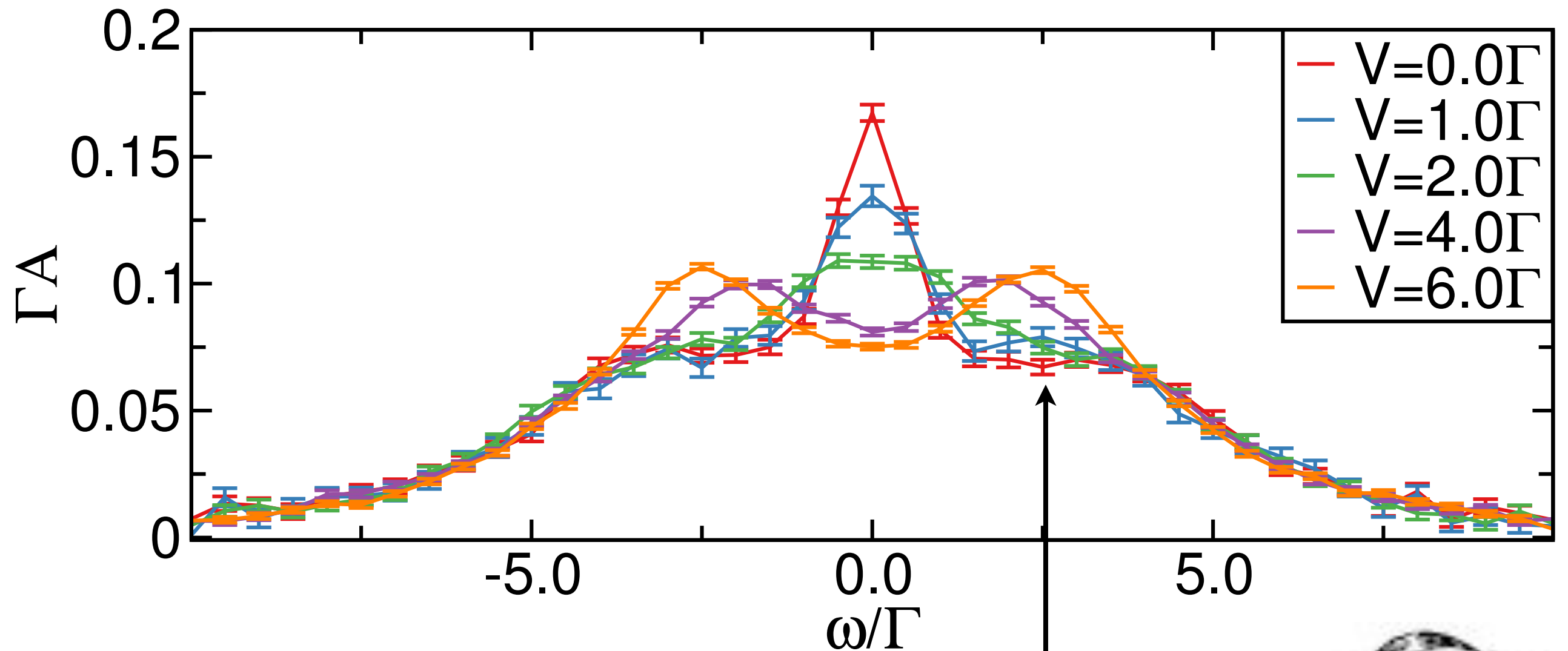


FIG. 10. The converged DMFT spectral function $A(\omega)$ obtained by extrapolating the real-time Green's function from $tv = 2.0$ to $tv = 10.0$ using linear prediction with $p = 9$, $t_{\text{fit}}v = 1.0$ for $U/v = 4$ at temperatures $T/v \in \{0.5, 0.1, 0.05\}$.

Non-equilibrium spectral functions from QMC



Parameters:

$U/\Gamma=6$

$\beta\Gamma=3$

flat band (width 10Γ) with soft cutoff

unbiased error bars on
the spectral functions!



Crossover regime to Kondo

Kondo non-equilibrium spectral functions

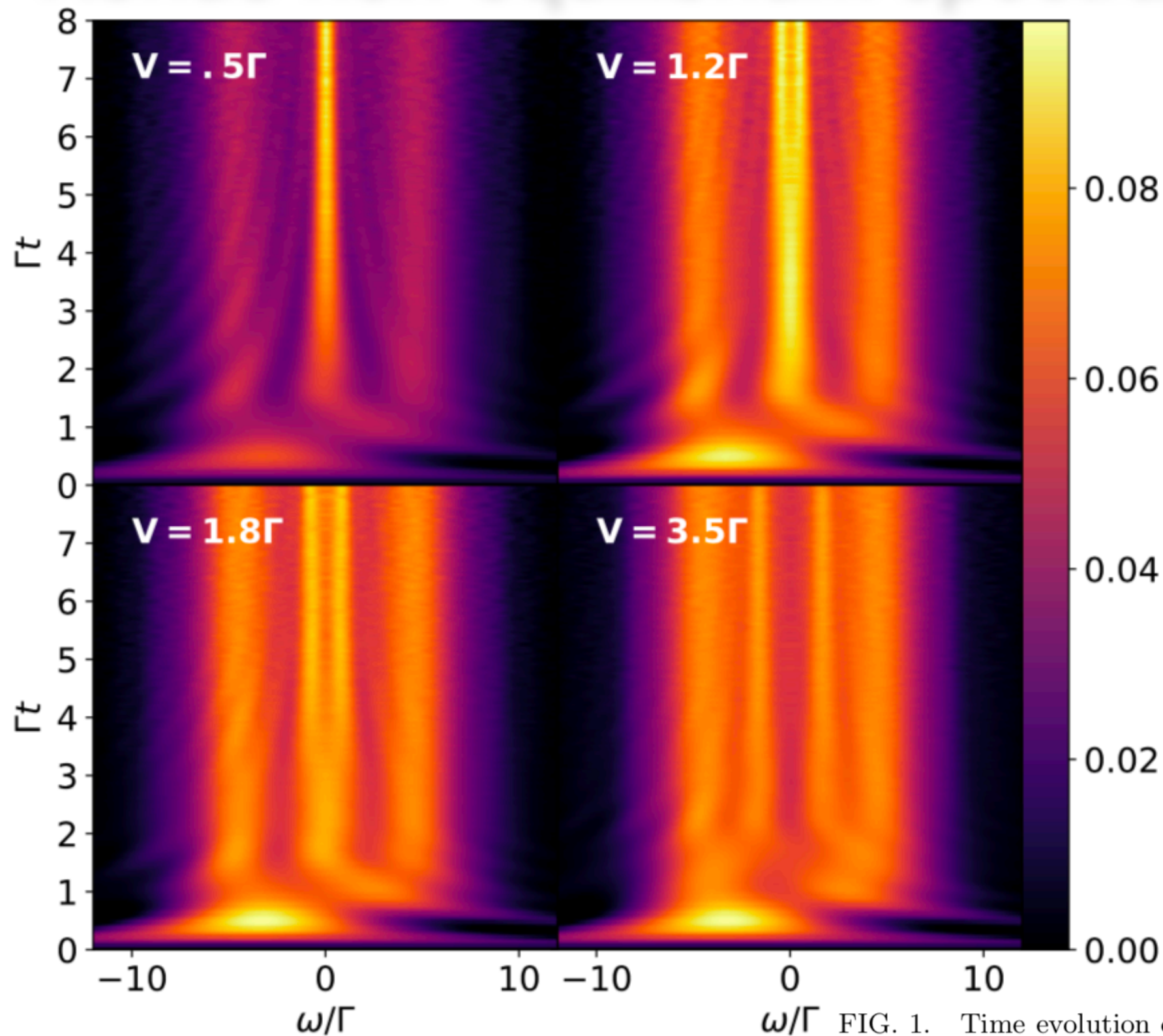
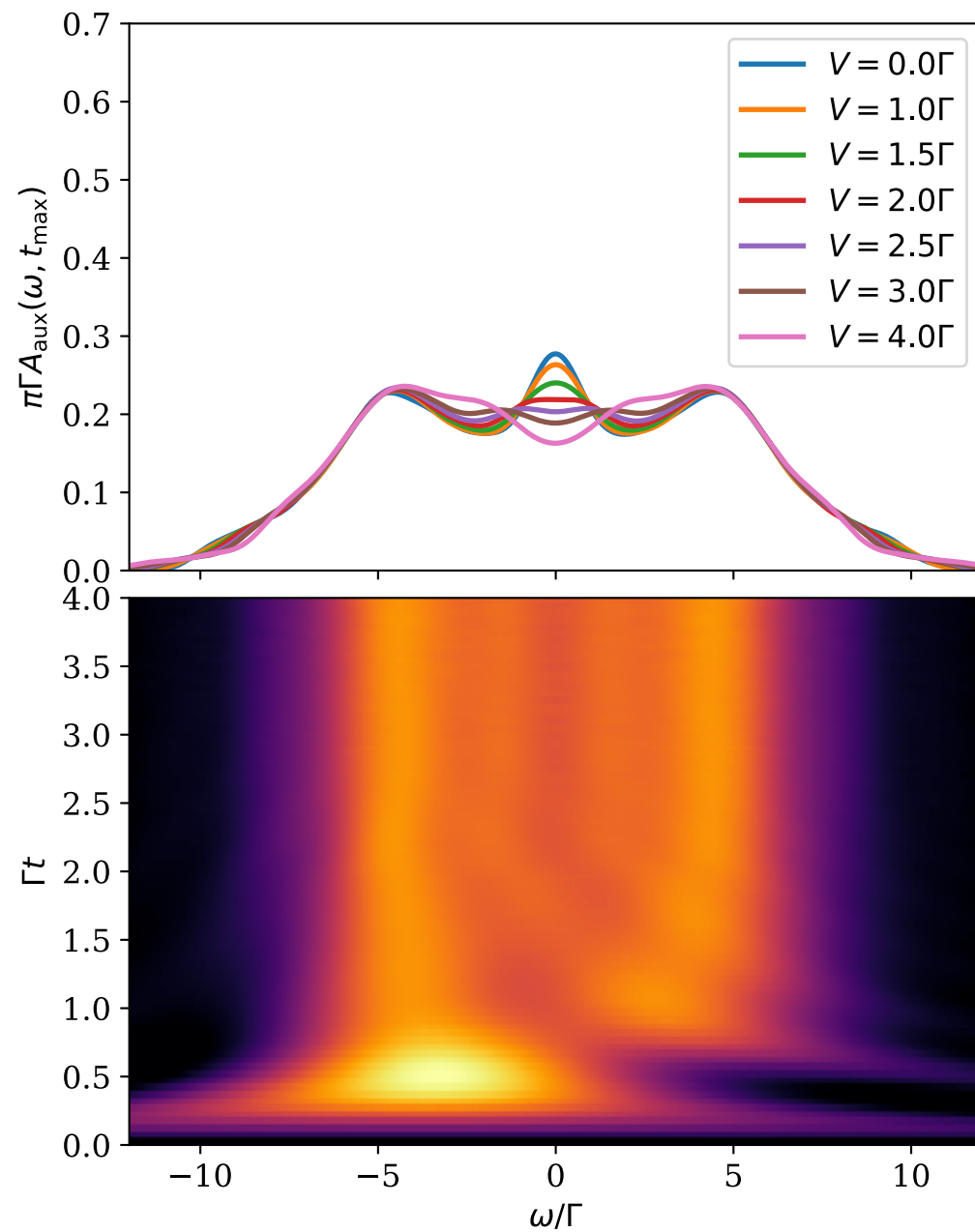
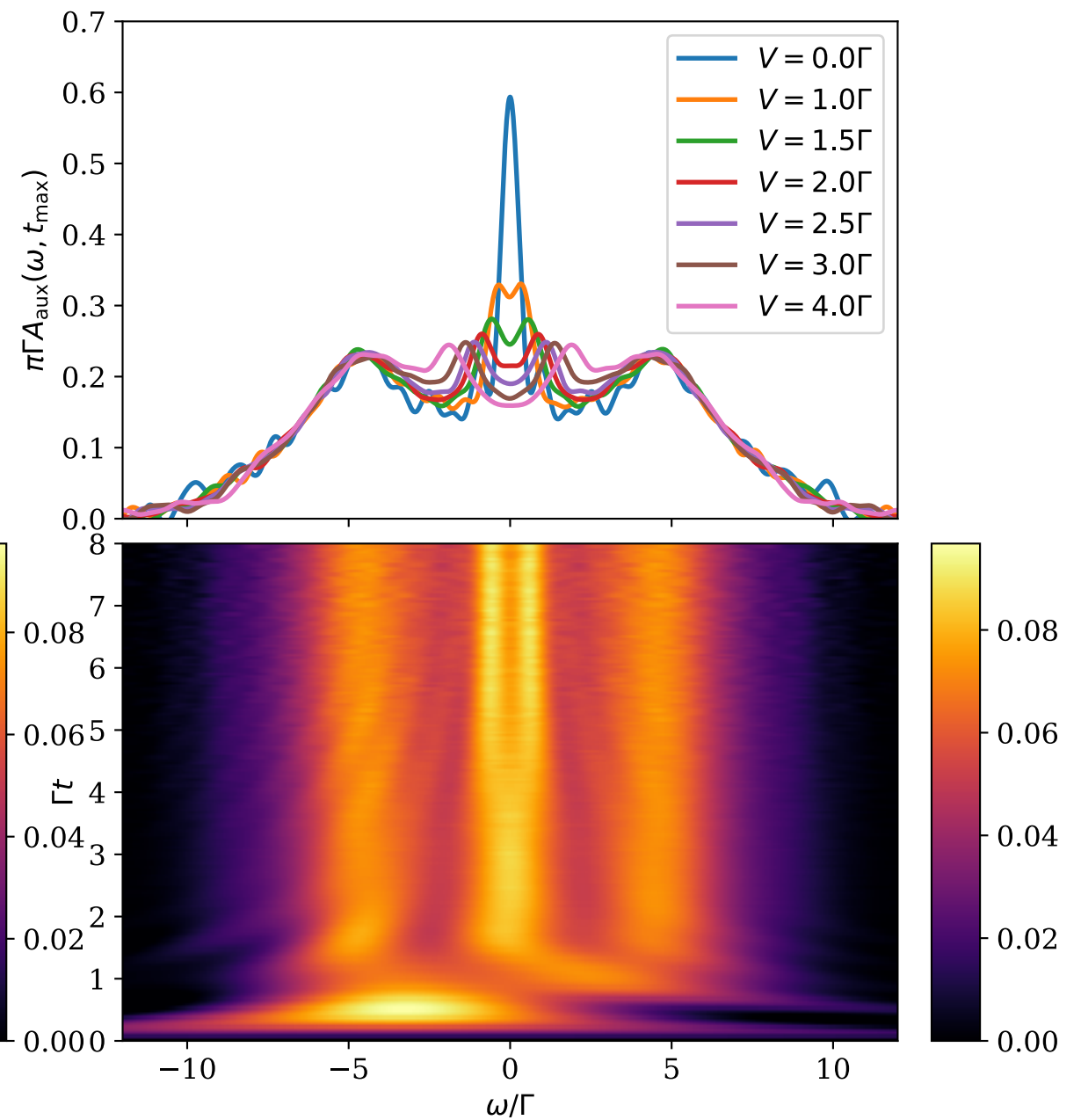


FIG. 1. Time evolution of the QD spectral function after a coupling quench and in the presence of a bias voltage V , at interaction strength $U = 8.0\Gamma$ and temperature $T = 0.02\Gamma \ll T_K$. The voltages are $V = 0.5\Gamma$ (upper left), $V = 1.2\Gamma$ (upper right), $V = 1.8\Gamma$ (lower left) and $V = 3.5\Gamma$ (lower right).

Kondo non-equilibrium spectral functions



Parameters: $U/\Gamma=8$ $\beta\Gamma=2$ $V/\Gamma=3$



Parameters: $U/\Gamma=8$ $\beta\Gamma=50$ $V/\Gamma=1.5$

$$\beta k \sim 9/\Gamma$$

Full Counting Statistics

$P(\Delta n, t)$ Probability that the dot occupancy changed by Δn at time t

P is characterized by a generating function:

$$Z(\lambda, t) \equiv \left\langle e^{i\lambda \Delta \hat{N}} \right\rangle = \sum_{\Delta n \in \mathbb{Z}} P(\Delta n, t) e^{i\lambda \Delta n}.$$

$$P(\Delta n, t) = \int_{-\pi}^{\pi} d\lambda Z(\lambda, t) e^{-i\lambda \Delta n},$$

knowledge of Z gives access to P , as well as to moments, cumulants, waiting time distributions, etc.

Full Counting statistics (FCS) aims to construct Z and, from it, measurable properties.

$$M_k(t) \equiv \left\langle \left(\Delta \hat{N} \right)^k \right\rangle = \lim_{\lambda \rightarrow 0} \frac{\partial^k Z(\lambda, t)}{\partial (i\lambda)^k},$$

$$C_k(t) \equiv \lim_{\lambda \rightarrow 0} \frac{\partial^k \ln Z(\lambda, t)}{\partial (i\lambda)^k}.$$

Full Counting Statistics

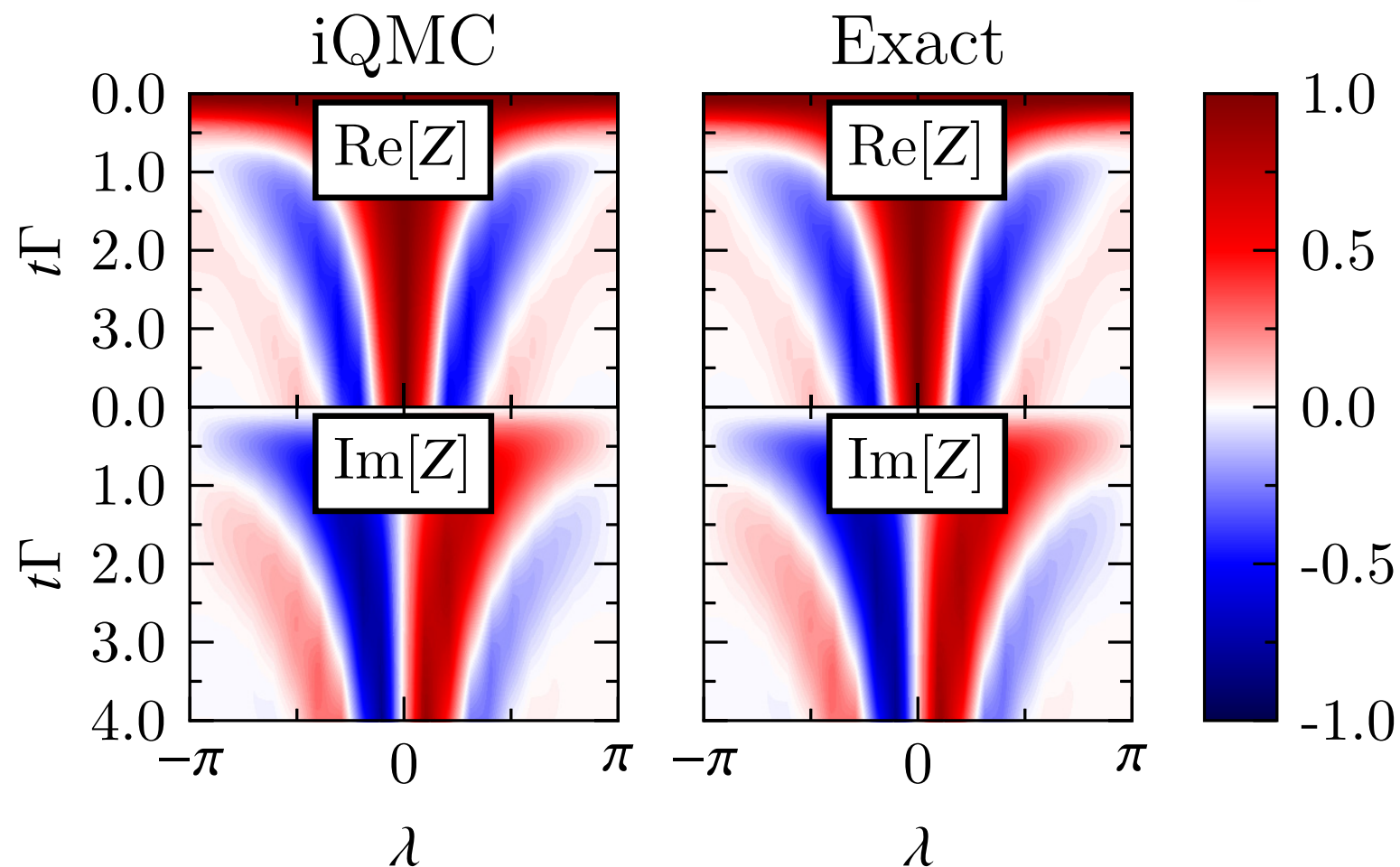


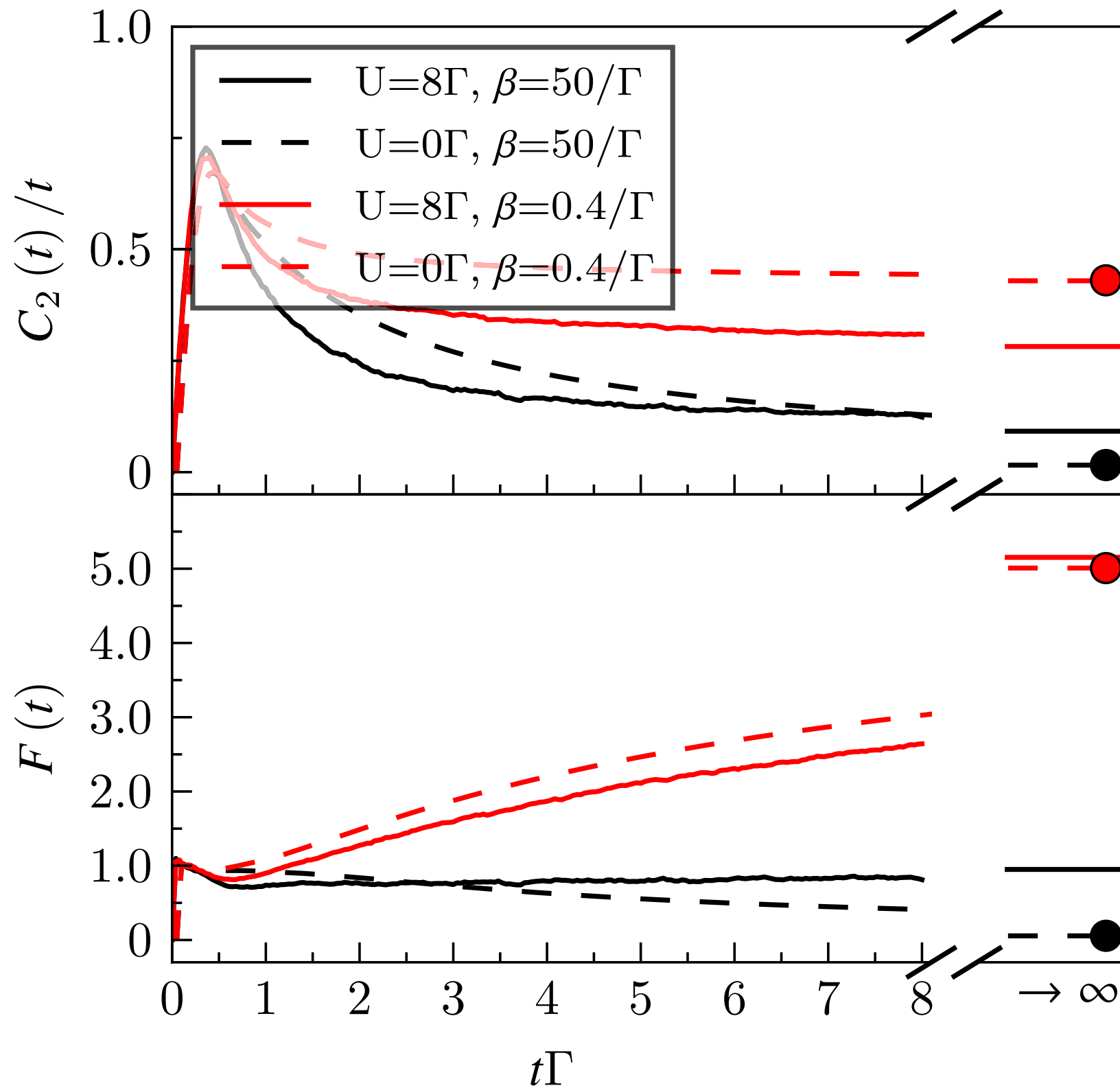
FIG. 6. Real and imaginary parts of the generating function from iQMC (left) compared to the exact result (right) at $U = 0\Gamma$, $V = 10\Gamma$, and $\beta = 50/\Gamma$.

...using the inchworm formalism to compute the FCS in the non-interacting case, where comparison results are available.

For variants of the hybridization expansion (such as this inchworm result), the non-interacting case is a non-trivial test case.

$$Z(\lambda, t) \equiv \left\langle e^{i\lambda\Delta\hat{N}} \right\rangle = \sum_{\Delta n \in \mathbb{Z}} P(\Delta n, t) e^{i\lambda\Delta n}.$$

Full Counting Statistics



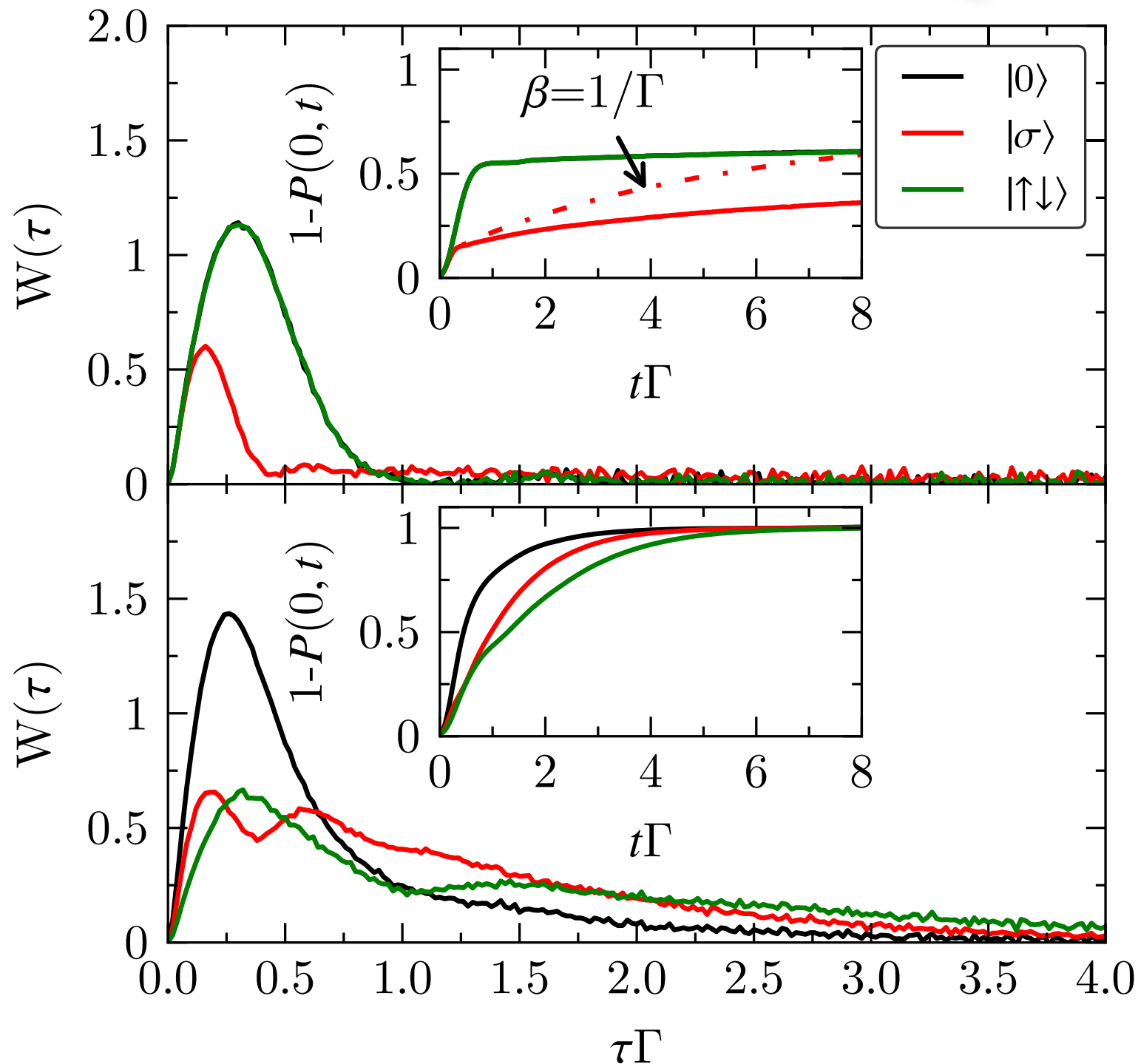
This allows to compute numerically exact FCS for interacting quantum dots.

Second moment $C_2(t)$.

Fano factor $F(t)=C_2(t)/C_1(t)$

FIG. 10. Evolution of $C_2(t)$ (upper panel) and the Fano factor $F(t) = C_2(t)/C_1(t)$ (lower panel) for voltage $V = 1\Gamma$ and initial condition $|0\rangle$. To the right extreme of the plot, we show the asymptotic values of these quantities, obtained from linearly fitting the cumulants at long times. The exact values of the noninteracting noise and Fano factor from Levitov-Lesovik theory are shown as filled circles.

Full Counting Statistics



First passing time distribution: probability distribution of the time separating the initialization of the counting experiment from the first detection of a charge transfer event

$$\Pi(t) \equiv P(0, t) = \int_{-\pi}^{\pi} d\lambda Z(\lambda, t).$$

$$W(t) = -\frac{d\Pi(t)}{dt},$$

FIG. 12. The FPTD $W(\tau)$ at inverse temperature $\beta = 50/\Gamma$ for $U = 8\Gamma$, at $V = 0$ (upper) and $V = 10\Gamma$ (lower). Insets show the integral over the data, with the upper inset also containing a result at higher temperature (dashed line).

Outlook & Open Questions

Very similar time to DMFT equilibrium, 2005:

suddenly have numerically exact impurity solver, can start to ask difficult questions

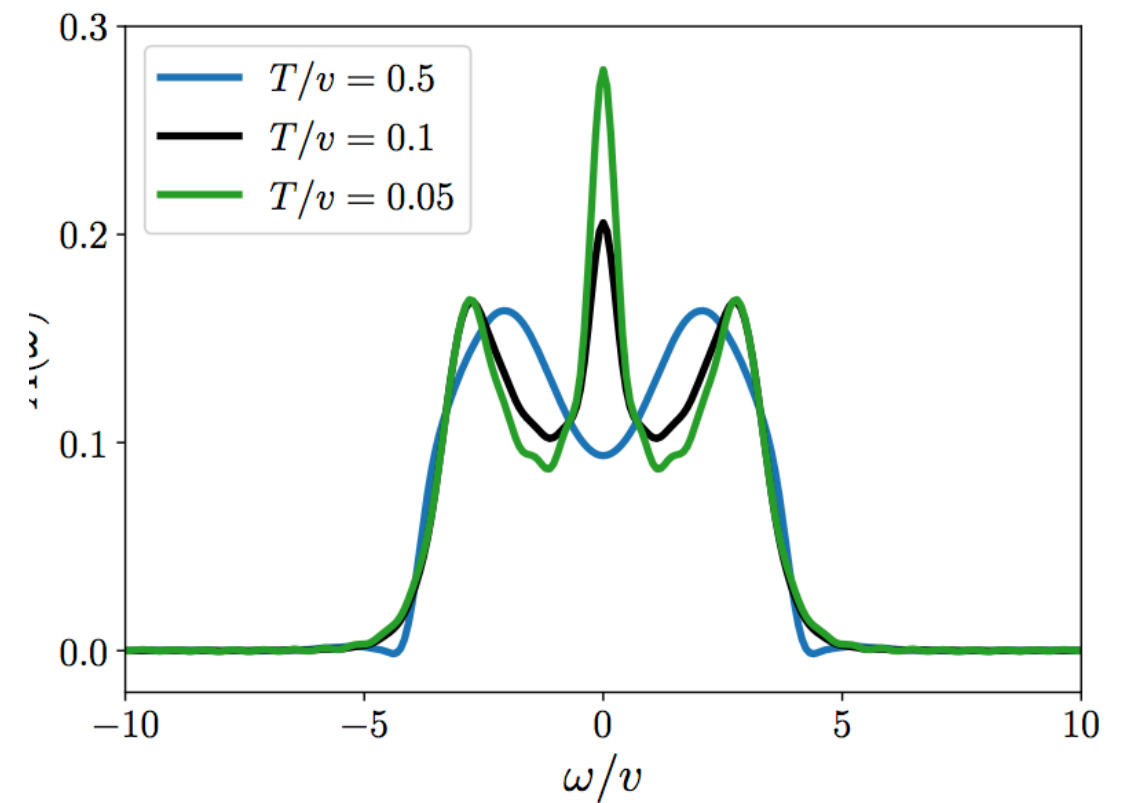
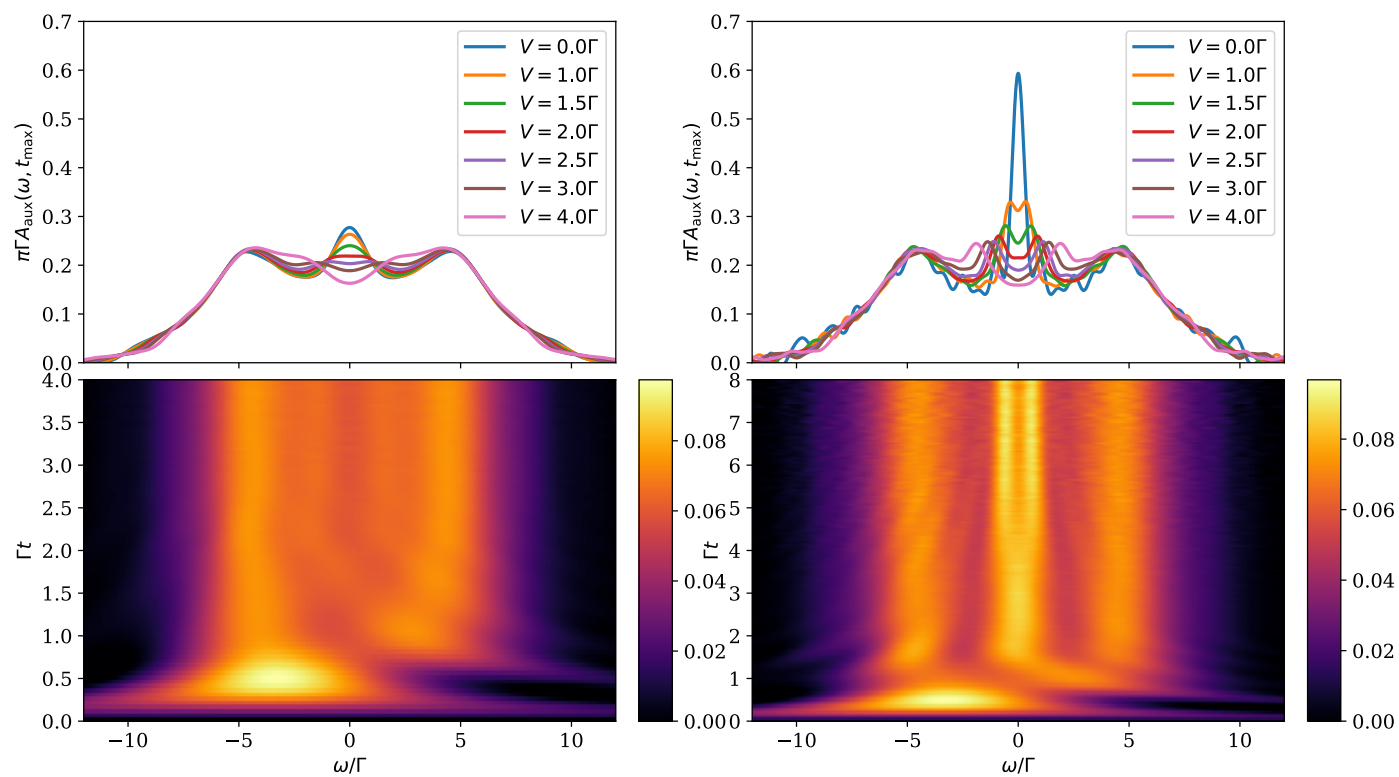
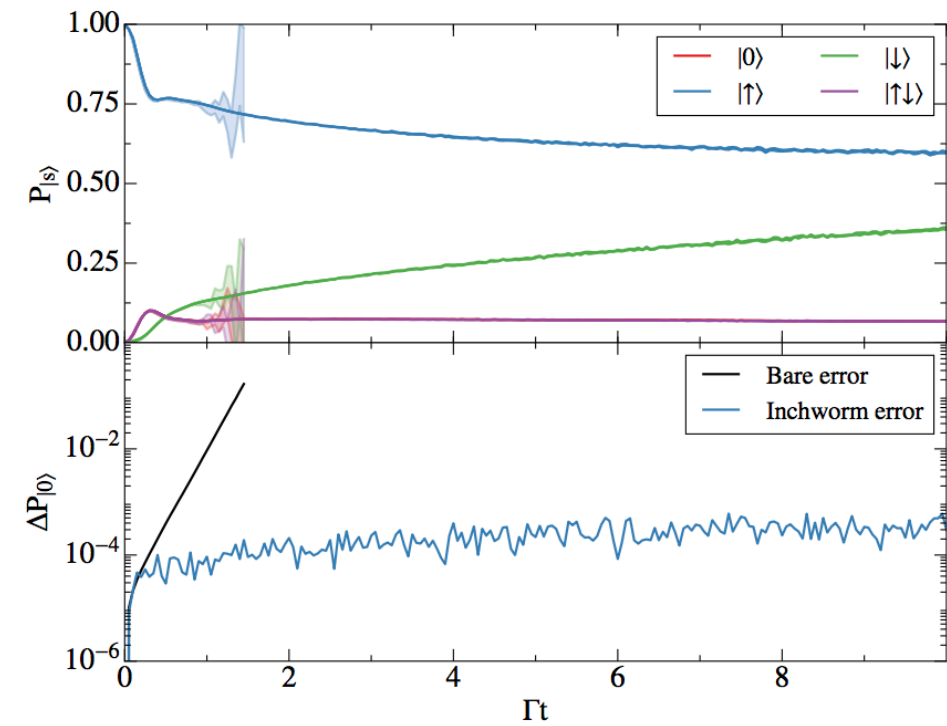
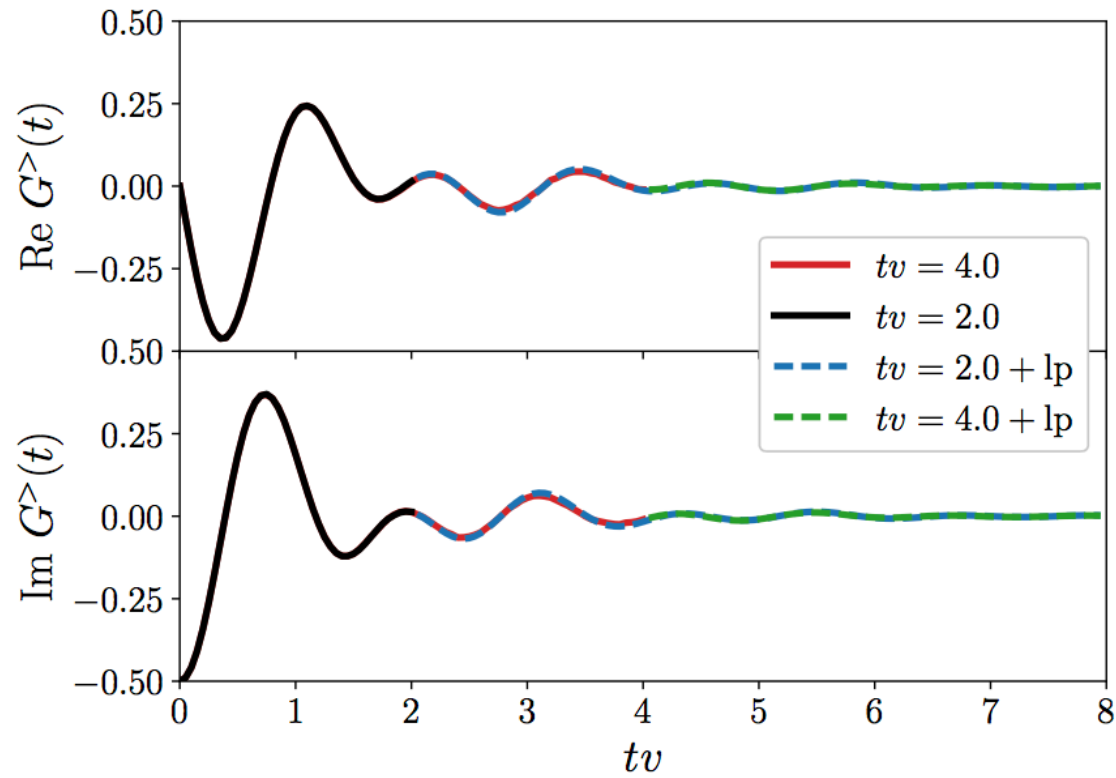
Impurity route: transport and correlations, quantum dots, noise. Replaces established approximate techniques.

Materials route: DMFT, beyond DMFT, more physics, multi-band and multi-site

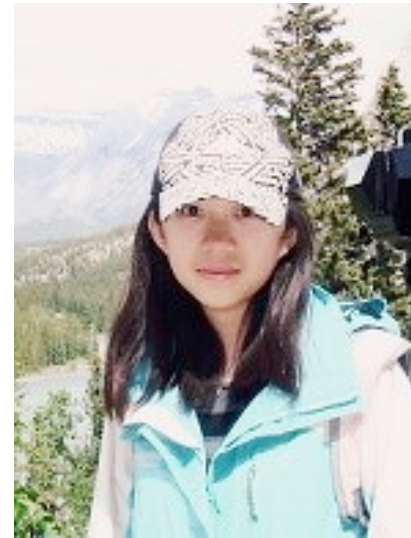
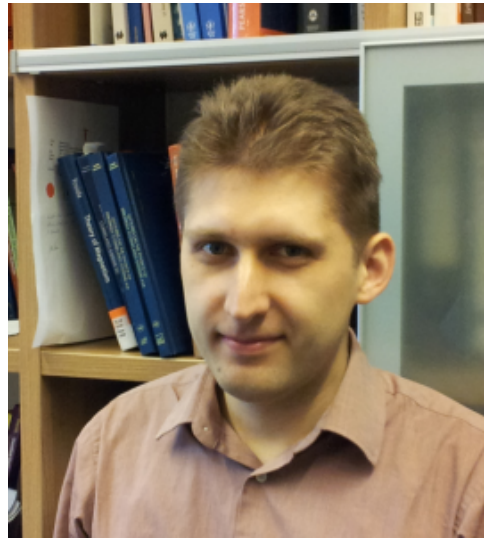
In non-equilibrium, approximate methods are often misleading: wrong relaxation times, wrong qualitative trends, etc.

Much less intuition/‘universality’ available, more materials specificity / experiment specificity needed.

Conclusions



Acknowledgments



**Guy Cohen, Igor Krivenko, Qiaoyuan Dong, and
Joe Kleinhenz**

[Phys. Rev. Lett. 115, 266802 \(2015\)](#)

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[Phys. Rev. B 96, 155126 \(2017\)](#)

[Phys. Rev. B 97, 115109 \(2018\)](#)

[Phys. Rev. B 98, 115152 \(2018\)](#)

[arXiv:1904.11527](#)



