Field-Driven Quantum Systems, From Transient to Steady State

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THE Ames Laboratory
Creating Materials & Energy Solutions
U.S. DEPARTMENT OF ENERGY

BERKELEY LAB
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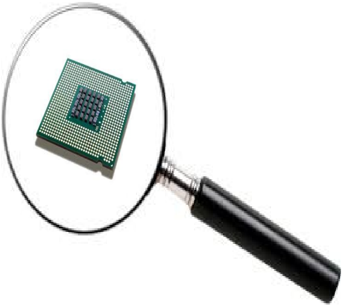
Device Miniaturization

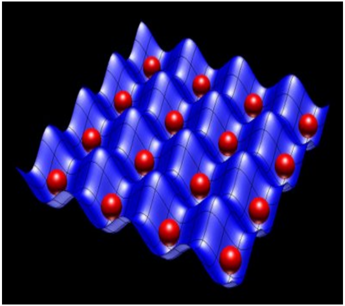


- Small potential difference

$\Downarrow$

- Large electric fields
- Beyond linear response

Ultracold Atoms
Optical Lattices



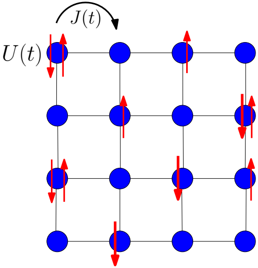
$$|\Psi(t = t_0)\rangle \xrightarrow{?} |\Psi_{SS}(t >> t_0)\rangle$$

Prepared state   Steady state

Thermal State?

Models: Hubbard, Falicov-Kimball

Hubbard,
Falicov-Kimball



F-K: Heavy-light mixture.

$$H_{eq} = -\sum_{<ij>,\sigma} J_{ij\sigma}\left(c^\dagger_{i\sigma}c_{j\sigma} + h.c.\right)$$

$$-\mu\sum_{i\sigma} c^\dagger_{i\sigma}c_{i\sigma} + U\sum_i n_{i\sigma}n_{i\bar{\sigma}}$$

$J_{ij\sigma} = J_{ij\bar{\sigma}} = J \rightarrow$ Hubbard

$J_{ij\downarrow} = 0$ and $J_{ij\uparrow} = J \rightarrow$ F-K

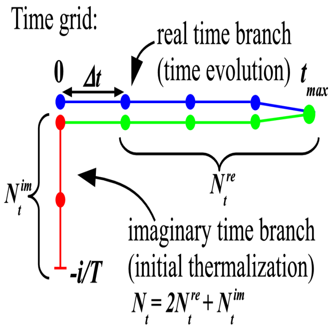
Electric field: $E(t) = E\theta(t - t_0)$

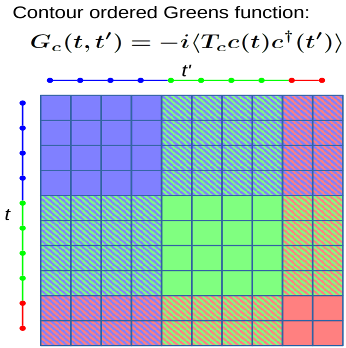
Peierls substitution:

$$J_{ij\sigma} \rightarrow J_{ij\sigma}\mathrm{e}^{\left[-i\int_{\mathbf{R}_i}^{\mathbf{R}_j}\mathbf{A}(\mathbf{r},t)d\mathbf{r}\right]}$$

Methods

Kadanoff Baym Keldysh Schwinger formalism
Two-time contour ordered Green's function



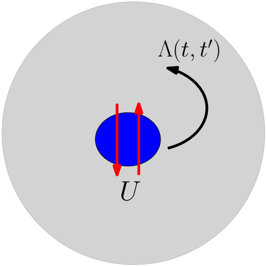


NonEquilibrium DMFT

Need Inpurity Solver

Lattice to Impurity

Exact solution for the Falicov-Kimball model



$$G^c_{imp}(t,t')$$

$$=$$

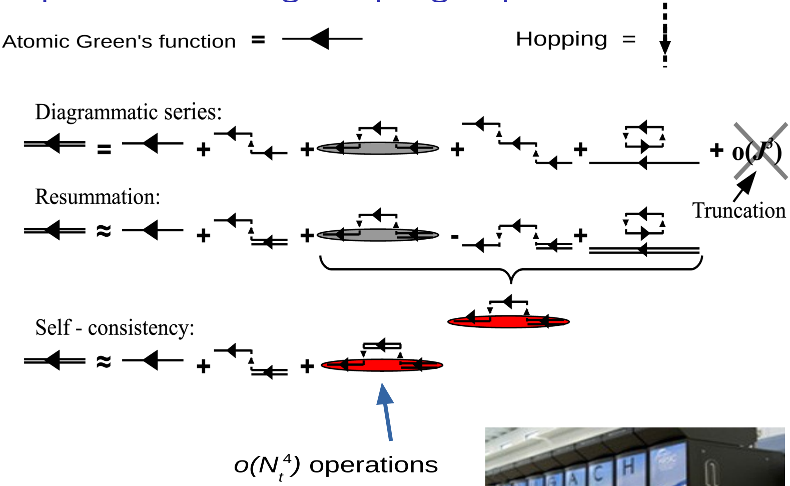
$$(1-\langle w_1\rangle)\left[(i\partial^c_t+\mu)\,\delta_c(t,t')-\Lambda(t,t')\right]^{-1}$$

$$+\quad\langle w_1\rangle\left[(i\partial^c_t+\mu-U)\,\delta_c(t,t')-\Lambda(t,t')\right]^{-1}$$

Half-filling, $\langle w_1\rangle = 0.5$

J. K. freericks, Phys. Rev. B **77**, 075109 (2008)

Nonequilibrium Strong Coupling Expansion



K. Mikelsons, J. K. Freericks, and H. R. Krishnamurthy, Phys. Rev. L **109**, 260402 (2012)

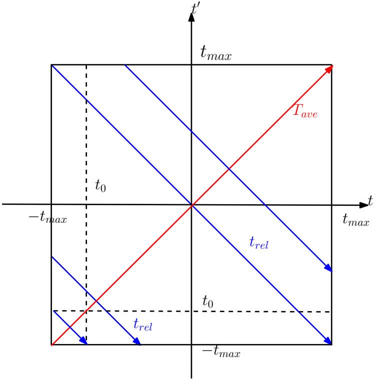
Two-Time Green's Function

$G^{R,<,>}(t,t')$ extracted from contour ordered $G^c(t,t')$

$G^R \Rightarrow$ Density Of States
$G^< \Rightarrow$ Distribution Function

Observables:
$J(t), E_{Kin}(t), E_{Pot}(t), E_{Tot}(t)$

Wigner Coordinates



$T_{ave} = (t + t')/2$
$t_{rel} = t - t'$

$G^{R,<}(T_{ave}, t_{rel})$

$G^R(T_{ave}, \omega) \Rightarrow$ Density Of States at time T_{ave}

$G^<(T_{ave}, \omega) \Rightarrow$ Distribution Function at time T_{ave}

Thermalization

Thermal State:

$$\text{FDT: } G^{<}(T_{ave},\omega) = -2iF_T(\omega) Im G^R(T_{ave},\omega)$$

$$Re G^{<}(T_{ave},\omega) \to 0$$

Joule heating: $\mathbf{J} \cdot \mathbf{E}$

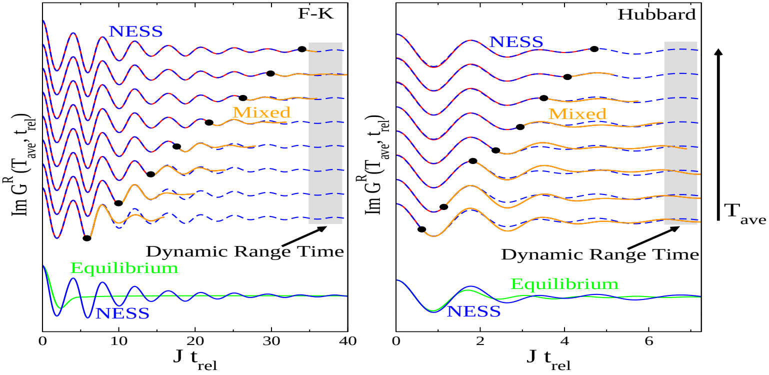
$$T \to \infty \; E_{Kin} = 0, E_{Pot} = E_{Tot} = U/4$$

H.F., K. Mikelsons and J. freericks, Scientific Reports **4**, 4699 (2013)

Density of states

Falicov-Kimball
E=1.0 , U=3.0 , T=0.1.

Hubbard
U/J=24, U/T=4, E/U=(1,1,1)



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Relaxation Scenarios

Using $ReG^{<}$ + Observables ($J(t), E_{kin}(t), E_{Pot}(t), E_{Tot}(t)$)

In both F-K and hubbard models:

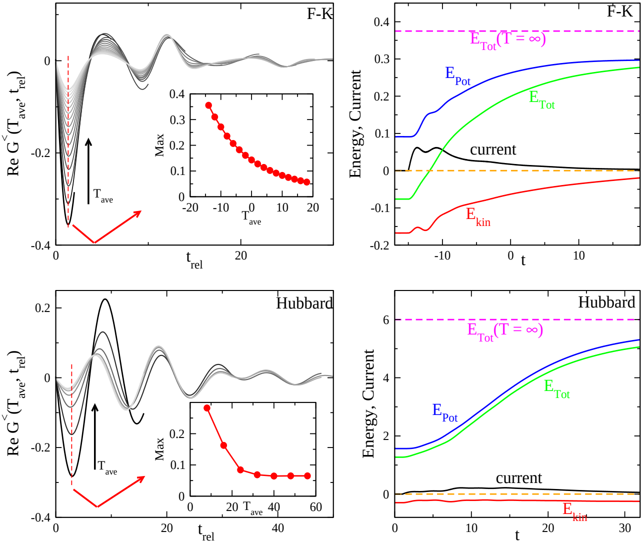
- Monotonic
- Oscillatory
- Thermalization
- No Thermalization

In the Hubbard model:

- A case of persistent oscillations

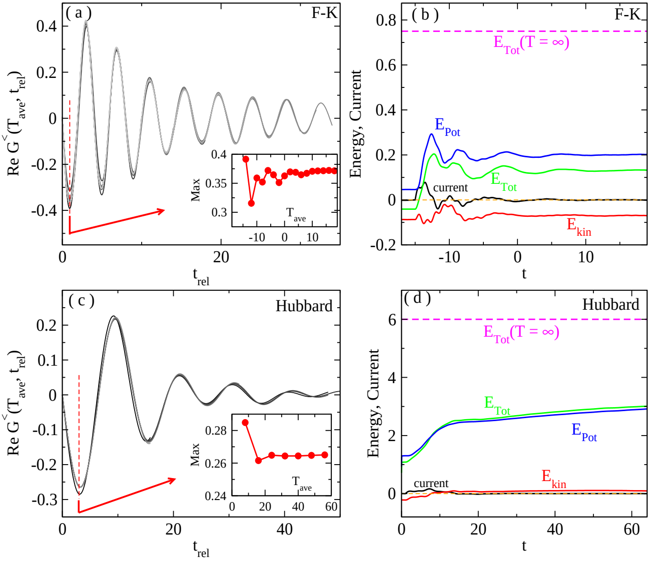
H.F., K. Mikelsons and J. freericks, Scientific Reports **4**, 4699 (2013)

Monotonic thermalization



F-K, E=0.5, U=1.5, T=0.1. Hubbard, U/J=24, E/U=(1,0,0), U/T=4.

Monotonic approach to non-thermal state



F-K, E=2.0, U=3.0, T=0.1. Hubbard, U/J=24, E/U=1.25(1,0,0), U/T=4.

Relaxation Scenarios

Using $ReG^{<}$ + Observables $(J(t), E_{kin}(t), E_{Pot}(t), E_{Tot}(t))$

In both F-K and hubbard models:

- Monotonic
- Oscillatory
- Thermalization
- No Thermalization

In the Hubbard model:

- A case of persistent oscillations

Relaxation Scenarios

Using $ReG^{<}$ + Observables $(J(t), E_{kin}(t), E_{Pot}(t), E_{Tot}(t))$

In both F-K and hubbard models:

- Monotonic
- Oscillatory
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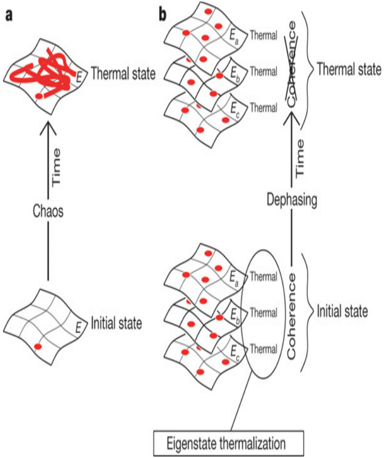
In the Hubbard model:

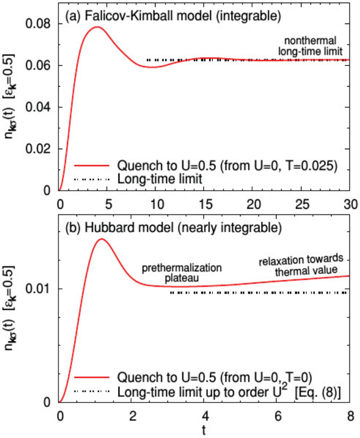
- A case of persistent oscillations

What about integrability?

What about integrability?



ETH, M. Rigol, V. Dunjko and M. Olshanii, Nature **452**, 854 (2008)



M. Kollar, F. A. Wolf, and M. Eckstein, PRB **84**, 054304 (2011)

Distribution Function

- E-field along the diagonal $\mathcal{E} = \mathcal{E}(1, 1, 1, ...)$
- Wigner distribution function $n_k(t)$

$$n_{\mathbf{k}}(t) = -iG^{<}_{\mathbf{k}+\mathbf{A}(t)}(t, t)$$

- Band Energy, Band Velocity

$$E(k) = \lim_{d\to\infty} \tfrac{-J^*}{\sqrt{d}} \textstyle\sum_{i=1}^{d} \cos(k_i)$$
$$V(k) = \lim_{d\to\infty} \tfrac{-J^*}{\sqrt{d}} \textstyle\sum_{i=1}^{d} \sin(k_i)$$

- $n_{\mathbf{k}}(t) \to n_{E(k),V(k)}(t)$
- Isolated system, Joule heating: $\mathcal{J}(t) \cdot \mathcal{E}$
- T $\to \infty$, $n_k(t) \to 0.5$

Time evolution of Wigner distribution function

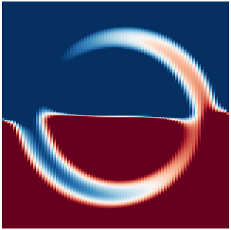
TOF measurements for heavy-light Fermi-Fermi mixtures

Movies produced with Paraview/VTK

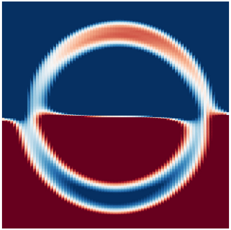
H.F., J. Vicente and J. freericks, Phys. Rev. A. **90** 053630 (2014)

Still Images, E=2.0, U=0.25

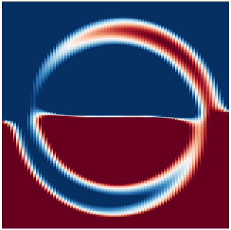
$t_0 + 2\pi/U$



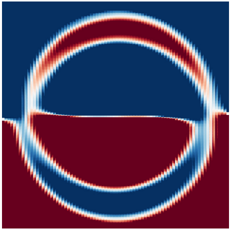
$t_0 + 2\pi/U + 0.5 \times 2\pi/\mathcal{E}$



$t_0 + 2\pi/U + 1.0 \times 2\pi/\mathcal{E}$

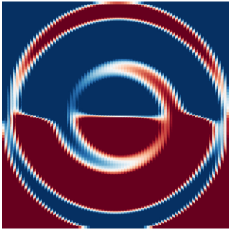


$t_0 + 2\pi/U + 1.5 \times 2\pi/\mathcal{E}$



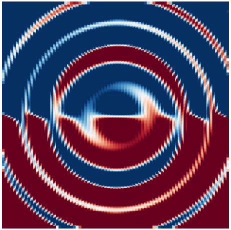
Still Images, E=2.0, U=0.25

$t_0 + 2 \times 2\pi/U$

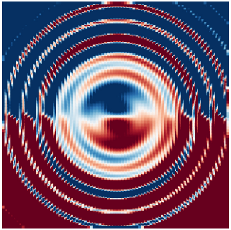


$t_0 + 3 \times 2\pi/U$

$t_0 + 4 \times 2\pi/U$

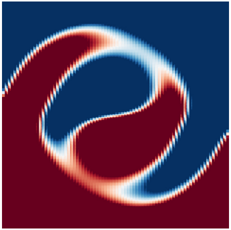


$t_0 + 7 \times 2\pi/U$

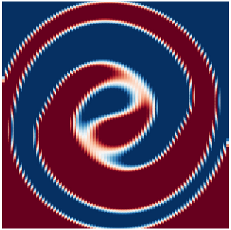


Still Images, E=2.0, U=1.0

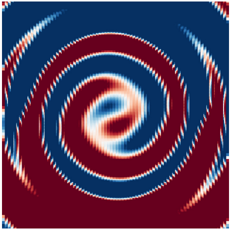
$t_0 + 1 \times 2\pi/U$



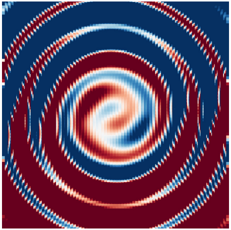
$t_0 + 2 \times 2\pi/U$



$t_0 + 3 \times 2\pi/U$



$t_0 + 3 \times 2\pi/U$



Between the Transient and the steady state

Desire solution from transient to steady state.

The case of field-driven correlated systems

Computational approaches:

- Sign problem in Quantum Monte Carlo
- Poor scaling
- Computational time and memory

What about extrapolation from transient?

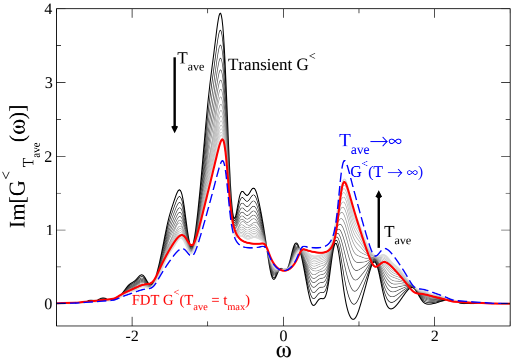
Beyond t_{max}

- Want momentum dependent quantities at longer times
- Increase $t_{max} \rightarrow$ More memory, longer run times
- DMFT: $\Sigma_k(t,t') = \Sigma(t,t')$,
  $G_k(t,t') = \left[G_k^0(t,t')^{-1} - \Sigma(t,t')\right]^{-1}$
- Instead, extrapolate the self-energy $\Sigma(t,t')$
- $\Sigma(t,t')$ also satisfies FDT:
  $\Sigma^<(T_{ave},\omega) = -2iF_T(\omega) Im\Sigma^R(T_{ave},\omega)$
- For FK model, we have an exact solution for the Steady State DMFT.

Monotonic Thermalization

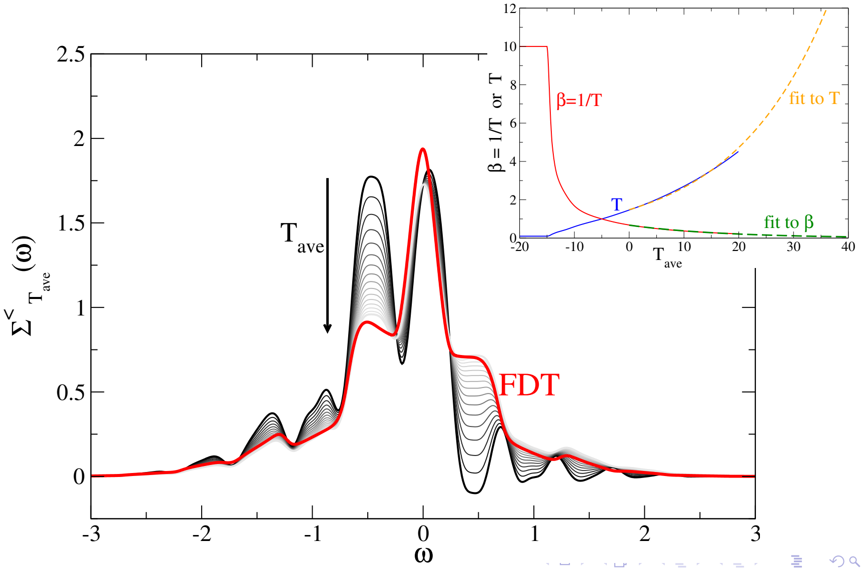
E=0.5, U=1.5, T=0.1.

Monotonic thermalization
System evolves through successive effective temperature states.

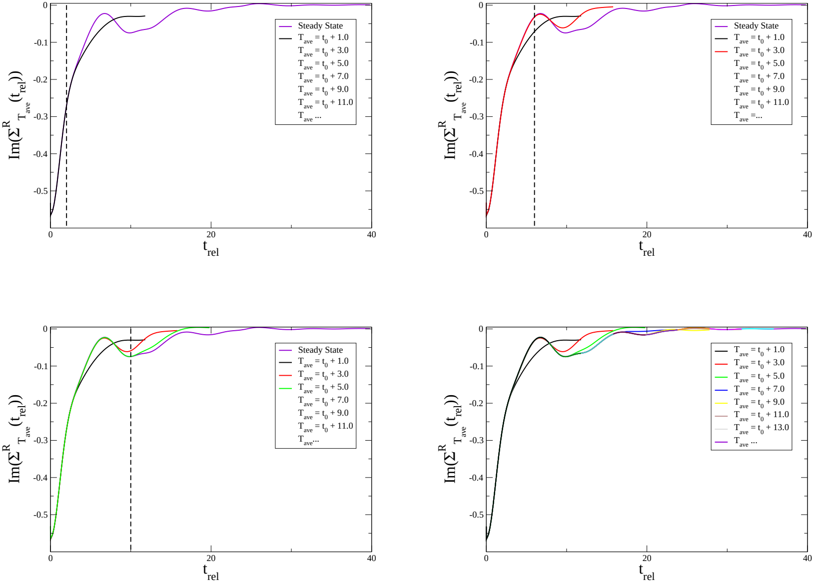


H.F., K. Mikelsons and J. freericks, Scientific Reports **4**, 4699 (2013)

FDT for the Self-energy

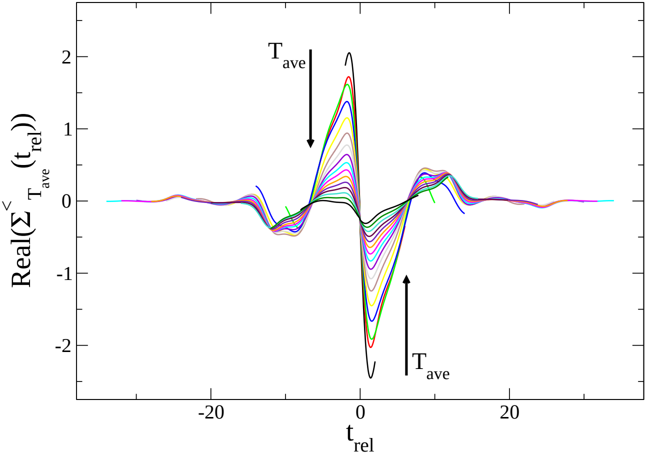


$Im\Sigma^{R,<}_{T_{ave}}(t_{rel})$ completely defined by causality



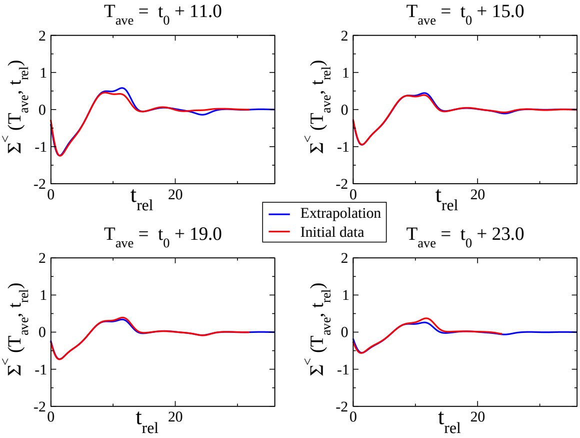
Monotonic Thermalization of Σ

Relaxation completely captured by $Real\Sigma^{<}_{T_{ave}}(t_{rel})$.



Extrapolate Σ to longer T_{ave}...

Extrapolation to longer t_{max}



Can calculate k-dependent quantities to longer t_{max}

Conclusion and outlook

Field-Driven Quantum System

- Different Relaxation scenarios
- What about integrability?
- Frustrated phase separation
- Extrapolation scheme to bridge the gap between transient and steady state
- Can calculate momentum dependent quantities at longer times
- How about oscilatory relaxation?

Thank you!