Universität Hamburg
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Diagrammatic theory for correlated electrons out of equilibrium

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Outline

Motivation / physics: see Philipp’s talk

- The Keldysh contour
- Contour-ordered Green’s functions
- The Dyson equation in real time: Kadanoff Baym equations
- Numerical solution of the Kadanoff Baym equations
- Construction of Keldysh Diagrams

NESSi:

A software package to deal with real-time Keldysh Green’s functions

⇨ Basis for diagrammatic perturbation theory in real-time

⇨ Basis for non-equilibrium DMFT

Schüler et al., Computer Phys. Comm. 257, 107484 (2020)

NESSi v1.0.2

The NonEquilibrium Systems Simulation Library

Outline

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NESSi v. 1.0

DFG Deutsche Forschungsgemeinschaft

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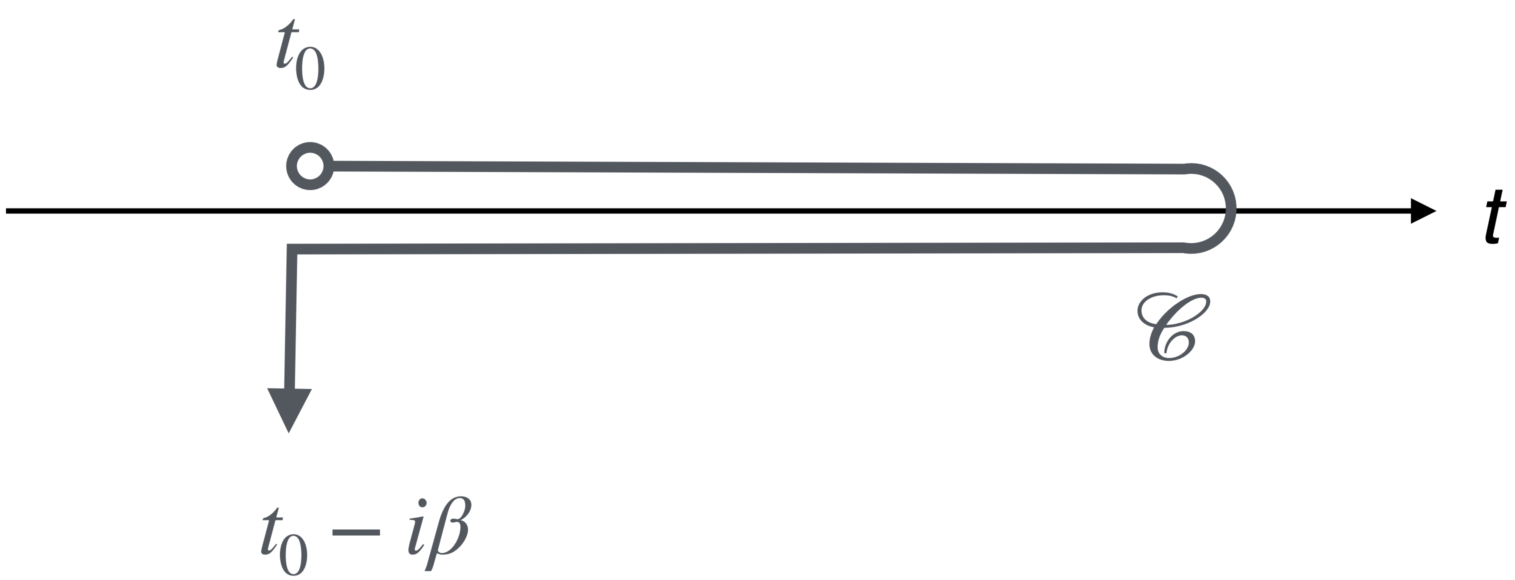
Keldysh Contour



General setting:

- initial state $|\Psi_i\rangle$ or density matrix $\rho = \sum_i w_i |\Psi_i\rangle\langle\Psi_i| = \frac{1}{Z} e^{-\beta H(t_0)}$

- time evolution $|\Psi_i(t)\rangle = \underbrace{\mathcal{U}(t, t_0)}_{\#} |\Psi_i\rangle \quad \# = T_t \exp\left(-i\int_{t_0}^{t} d\bar{t}\, H(\bar{t})\right)$

⇨ time-dependent expectation values?

$$\langle O(t)\rangle = \sum_i w_i \langle\Psi_i(t)|O|\Psi_i(t)\rangle = \mathrm{tr}\left[\rho\, \mathcal{U}(t_0, t)\, O\, \mathcal{U}(t, t_0)\right]$$

Motivation example: Quench in the Hubbard model

$$H = -J \sum_{\langle i,j \rangle,\sigma} c^\dagger_{i,\sigma} c_{j,\sigma} + U(t) \sum_j n_{j,\uparrow} n_{j,\downarrow} \qquad U(t) = \begin{cases} 0 & t < 0 \\ U & t > 0 \end{cases}$$

Initial state $\rho_0 \sim e^{-H(t<0)/T_0}$ … time evolution of closed system

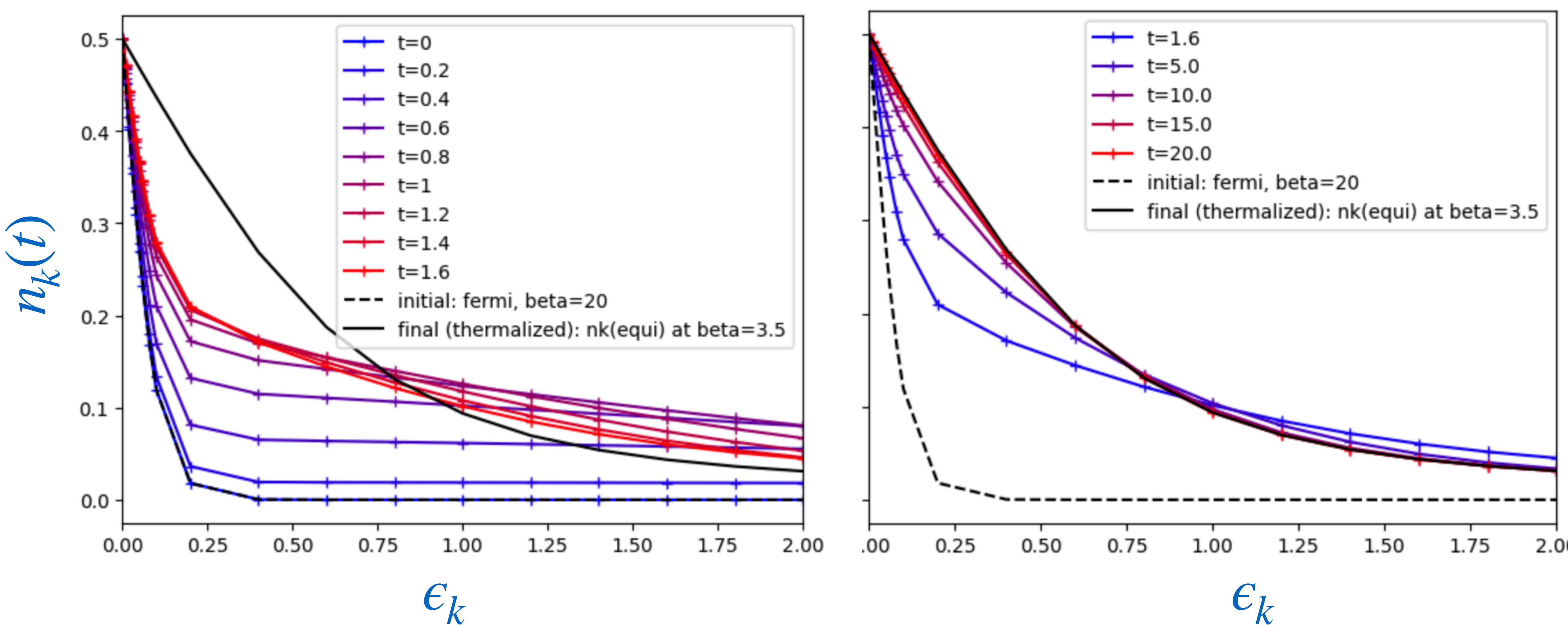
$\Rightarrow$ Thermalization ?

- Final state looks like $\rho_f \sim e^{-H/T_f}$
- T_f conserved energy $\mathrm{tr}(H\rho_0) \overset{!}{=} \mathrm{tr}(H\rho_f)$

Motivation example: Quench in the Hubbard model

Relaxation of the momentum occupation $n_k(t) = \langle c_k^\dagger(t) c_k(t) \rangle$

(J=1, U=2, [time]=$\hbar/J$, Bethe lattice, 2nd order perturbation theory



"Rest of this talk": How to obtain these results

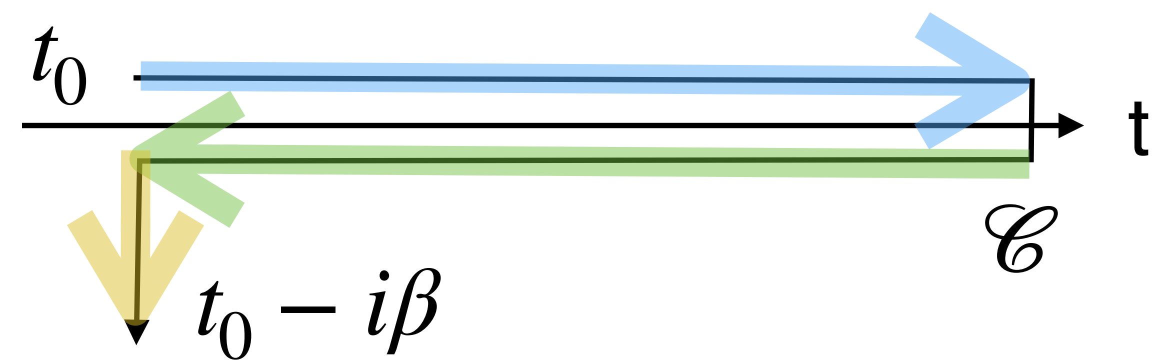
Keldysh contour

$$\langle O(t)\rangle = \mathrm{tr}\Big[\rho\, \mathcal{U}(t_0, t)\, O\, \mathcal{U}(t, t_0)\Big]$$

⇨ Representation as contour-ordered expectation value:

$$= \frac{1}{Z}\mathrm{tr}\Big[\Big(T_\tau\, e^{-\int_0^\beta d\tau\, H(t_0)}\Big)\Big(\bar{T}_t\, e^{-i\int_t^{t_0} d\bar{t}\, H(\bar{t})}\Big) O \Big(T_t\, e^{-i\int_{t_0}^{t} d\bar{t}\, H(\bar{t})}\Big)\Big]$$

$$= \frac{1}{Z}\mathrm{tr}\Big[T_{\mathscr{C}}\, e^{-i\int_{\mathscr{C}} d\bar{t}\, H(\bar{t})}\, O(t)\Big]$$



Contour ordering $T_{\mathscr{C}} A(t)B(t') = \begin{cases} A(t)B(t') & t \text{ later on } \mathscr{C} \\ \pm B(t')A(t) & t \text{ earlier on } \mathscr{C} \end{cases}$

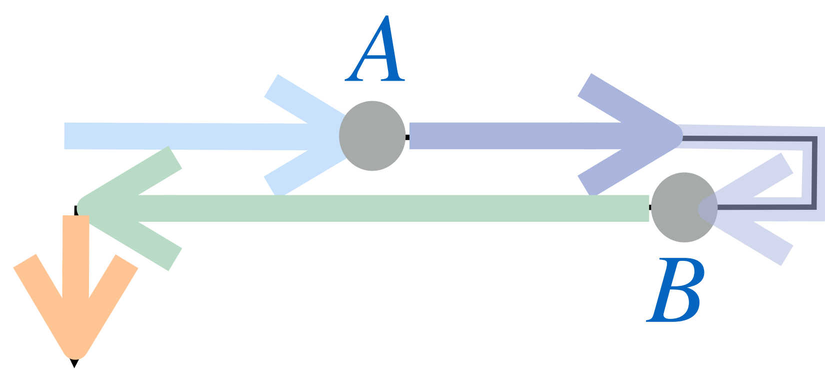
Contour-ordered correlation functions

Analogous: Two- and N-point correlation functions:

$$\langle T_{\mathscr{C}} A(t) B(t') \cdots \rangle \equiv \frac{1}{Z} \mathrm{tr} \left(T_{\mathscr{C}}\, e^{-i \int_{\mathscr{C}} d\bar{t}\, H(\bar{t})}\, A(t) B(t') \cdots \right)$$

e.g., for $t'_- >_{\mathscr{C}} t_+$:

$\langle T_{\mathscr{C}} A(t_+) B(t'_-) \rangle =$



$$= \pm \frac{1}{Z} \mathrm{tr} \left[\rho\, U(t_0, t') B U(t', t) A U(t, t_0) \right]$$

real-time-correlation function

Contour ordering: convenient bookkeeping of different operator orderings

(… which all have different physical significance, see below)

(Anti)periodic boundary condition (cyclic permutation under trace)

$$\langle T_{\mathscr{C}} A(0_+) B(t') \cdots \rangle = \pm \langle T_{\mathscr{C}} A(-i\beta) B(t') \cdots \rangle$$

Keldysh path integral

- Contour-ordered ordered evolution operator on “closed contour” has path integral representation of analogous to imaginary-time contour:

$$\mathrm{tr}\left(T_{\mathscr{C}}\, e^{-i\int_{\mathscr{C}} d\bar{t}\, H(\bar{t})} \,\cdots \right) = \int \mathscr{D}[\bar{c}, c]\, e^{iS_{\mathscr{C}}} \cdots \quad S_{\mathscr{C}} = \int_{\mathscr{C}} dt \left[\bar{c}(t) i\partial_t c(t) - H(t) \right]$$

integrate over all (anti)-periodic path $c(0_+) = \pm\, c(-i\beta)$

- Check: Restriction to imag. time contour: $t = -\, i\tau, \quad \tau \in [0,\beta]$:

$$i\int_{\mathscr{C}} dt \to \int_0^\beta d\tau, \quad \partial_t \to i\partial_\tau \quad \Rightarrow \quad e^{iS_{\mathscr{C}}} \to e^{-\int_0^\beta d\tau \left[\bar{c}\partial_\tau c + H(t) \right]}$$

usual imaginary time action

⇨ Concepts like Wick’s theorem, effective action, diagrammatic perturbation theory, field theoretical tricks like Hubbard Stratonovich transformation … carry over 1:1 to Keldysh formalism

Contour-ordered Green's functions

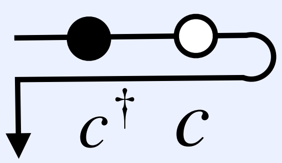
- Contour-ordered Green's functions

$$G(t,x,t',x') = -i\langle T_{\mathscr{C}}\, c_x(t) c^\dagger_{x'}(t')\rangle:$$

x, x': spin/orbital/momentum indices, omitted in the following ⇨ $G(t,t')$ is a matrix in orbital indices

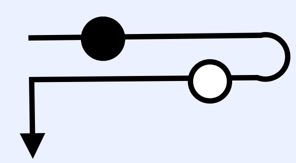
- $\mathscr{C}$-ordering ≡ bookkeeping of operator orderings … here there are 9:

$G(t_+, t'_+) =$



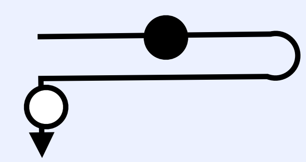
$\equiv G^t(t,t')$

$G(t_-, t'_+) =$



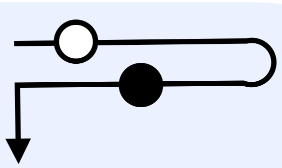
$-i\langle c(t)c^\dagger(t')\rangle \equiv G^>(t,t')$

$G(-i\tau, t_+) =$



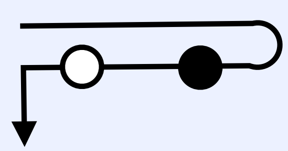
$\equiv G^{vt}(\tau, t')$

$G(t_+, t'_-) =$



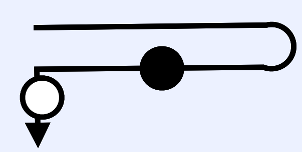
$i\langle c^\dagger(t')c(t)\rangle \equiv G^<(t,t')$

$G(t_-, t'_-) =$



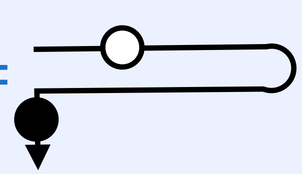
$\equiv G^{\bar{t}}(t,t')$

$G(-i\tau, t_-) =$



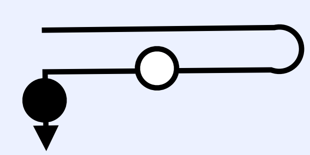
$= G^{vt}(\tau, t')$

$G(t_+, -i\tau) =$



$\equiv G^{tv}(t,\tau)$

$G(t_-, -i\tau) =$

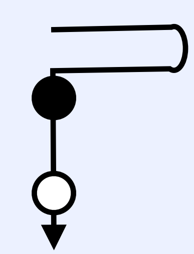


$= G^{tv}(t,\tau)$

$G(-i\tau, -i\tau') =$

$= -i\langle T_\tau c(\tau)c^\dagger(\tau')\rangle$

$= iG^M(\tau - \tau')$

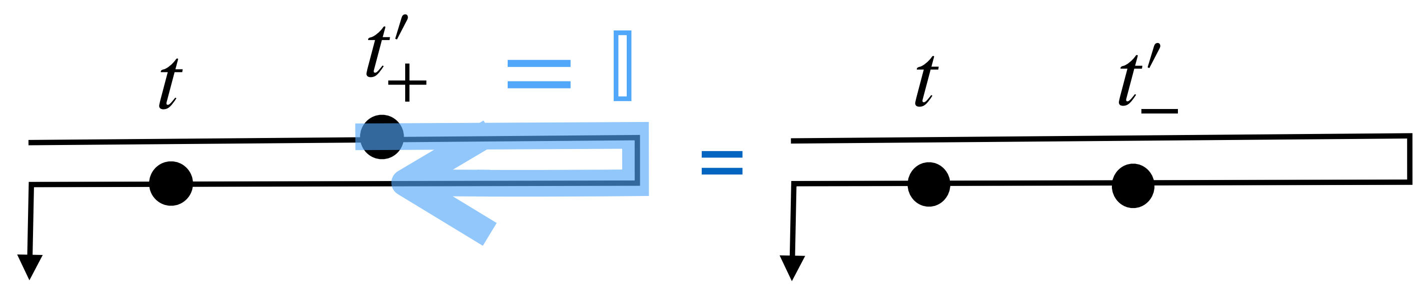


Redundancy among the components of the *G(t,t')*

Causal structure:

"Largest time-argument of any two-time function can be on any contour"

$$t' > t \quad \Rightarrow \quad G(t, t'_+) = G(t, t'_-)$$



⇨ Redundancy:

$$G_{++}(t,t') = \theta(t-t')\underbrace{G_{-+}(t,t')}_{=G^{>}(t,t')} + \theta(t'-t)\underbrace{G_{+-}(t,t')}_{=G^{<}(t,t')}$$

$$G_{--}(t,t') = \theta(t-t')G_{+-}(t,t') + \theta(t'-t)G_{-+}(t,t')$$

$$G_{v+}(\tau,t) = G_{v-}(\tau,t) \quad G_{+v}(t,\tau) = G_{-v}(t,\tau)$$

⇨ Non-redundant parametrization?

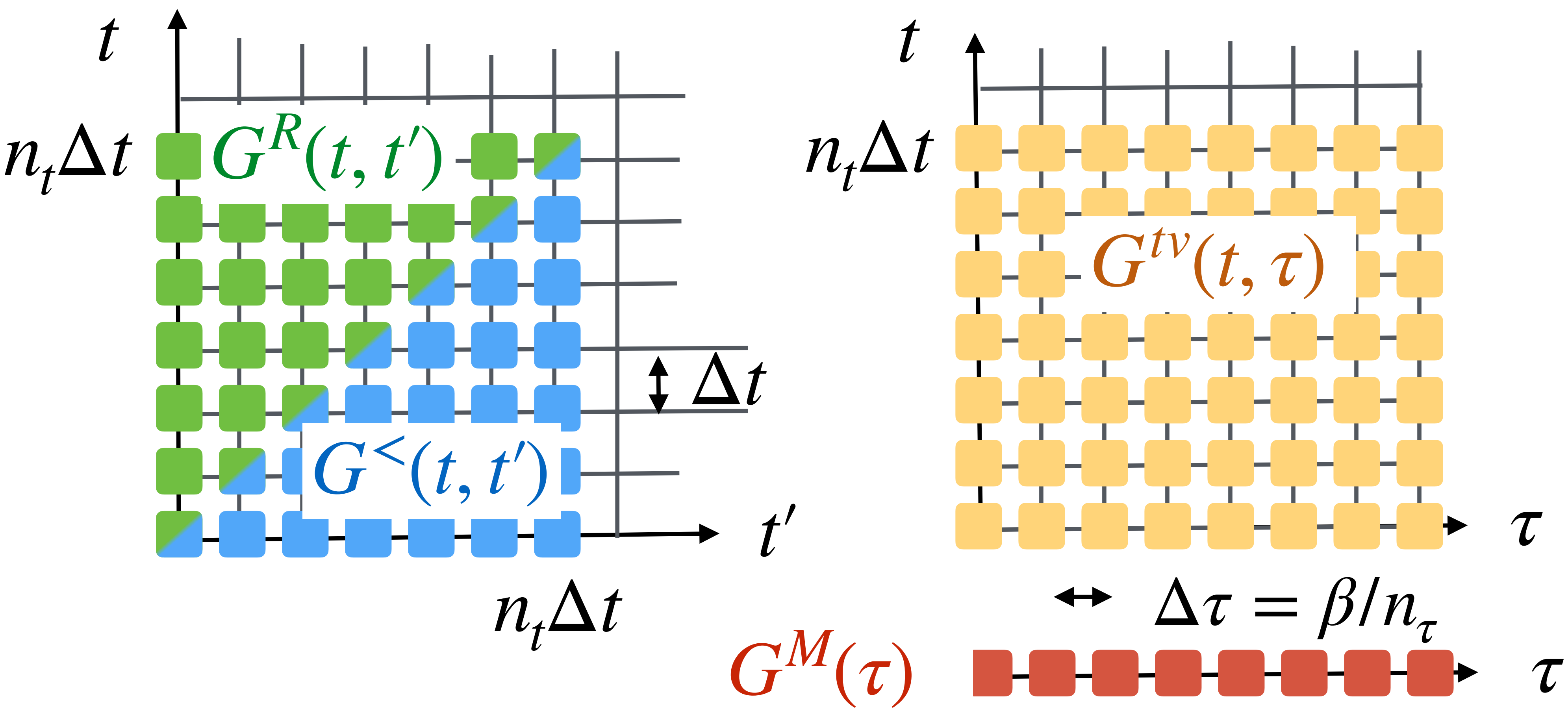
For analytical calculations on two-branch contour: Keldysh matrices

Here: $G^R, G^<, G^{tv}, G^M$

Comeplete set of components (used in NESSi)

Retarded $G^R(t,t') = \theta(t-t')[G^>(t,t') - G^<(t,t')]$, for $t \geq t'$

lesser, mixed, Matsubara



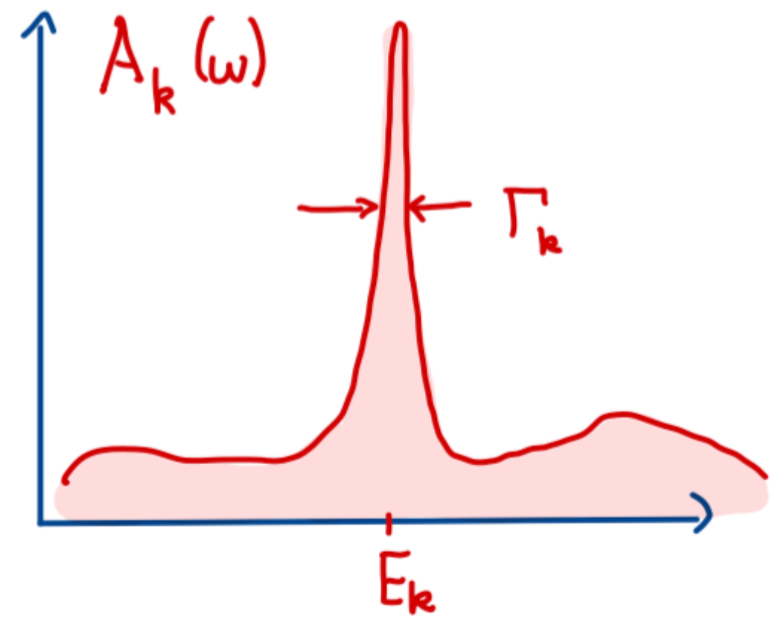
Note: This is only "half of the information" …

But in many cases, $G(t,t')$ has hermitian symmetry:

$$G^<(t,t') = -[G^<(t',t)]^\dagger,\ \ G^>(t,t') = -[G^>(t',t)]^\dagger$$
$$G^{tv}(t,\tau) = \pm[G^{vt}(\beta-\tau,t)]^\dagger$$
$$G^A(t,t') = [G^R(t',t)]^\dagger$$

Equilibrium Green's functions

In equilibrium, i.e., $H(t) = H,\ \rho \sim e^{-\beta H}$:



- $G^R(t-t') = -i\theta(t-t')\langle [c(t), c^\dagger(t')]_+\rangle$

$$= \theta(t-t')[G^>(t-t') - G^<(t-t')]$$

⇨ spectral function: $A(\omega) = -\frac{1}{\pi}\mathrm{Im}\, G^R(\omega + i0)$

- Relation to imag time: $G^M(\tau) = -\int d\omega\, A(\omega) e^{-\omega\tau} f(-\omega)$

- "fluctuation dissipation relations":

$G^<(t-t') = i\langle c^\dagger(t')c(t)\rangle$ hole propagator

⇨ $G^<(\omega) = 2\pi i A(\omega) f(\omega)$ "occupied DOS", photoemission

$G^>(t-t') = -i\langle c(t)c^\dagger(t')\rangle$ electron propagator

⇨ $G^>(\omega) = -2\pi i A(\omega)[1 - f(\omega)]$ "unoccupied density of states"

Non-equilibrium Green's functions

Equilibrium:

- Time translational invariance
- All two-point Green's functions related to spectrum and universal distribution function $(e^{\beta\omega} \pm 1)^{-1}$
- Theory formulated in term of one Green's function

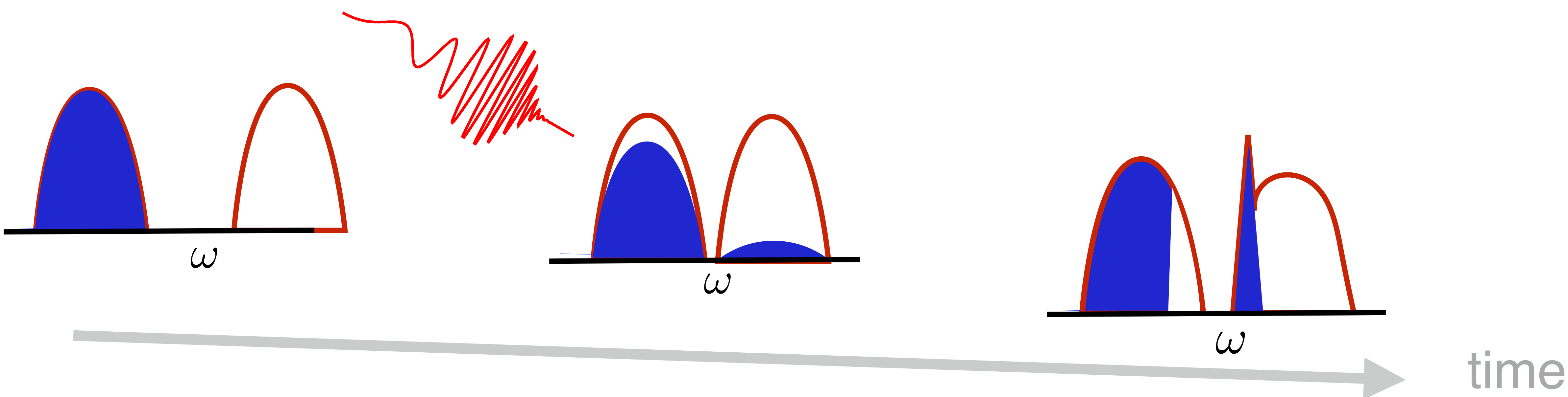
  Matsubara formalism: $G(\tau)$ … $A(\omega)$ from analytical continuation

Out of equilibrium:

- breaking of time-translational invariance $X(t, t')$ or $X(\omega, t)$
- non-universal distribution F: e.g., $G^{<}(\omega, t) = 2\pi i A(\omega, t) F(\omega, t)$

Non-equilibrium Green's functions

Keldysh formalism: Equations for contour-ordered Green's function ≡ coupled equations for time-dependent spectrum and occupation



⇨ Basis for many "standard" approximations:

- Quantum Boltzmann equations: differential equation for $F(\omega, t)$, $A(\omega, t)$
- Semiclassical approximations

see, e.g., A. Kamenev, Field theory of non-equilibrium systems

⇨ NESSi: Evaluation of real-time diagrammatic perturbation theory for contour-ordered Green's functions in (t, t') representation

From equations of motion to the Dyson equation

Free particles: Equation of motion

Free particles: $H = h(t)c^\dagger c$:

⇨ Closed Heisenberg equations of motion $i\partial_t c(t) = h(t)c(t)$:

⇨ Equation of motion for G

$$G(t,t') = -i\theta_{\mathscr{C}}(t,t')\langle c(t)c^\dagger(t)\rangle + i\theta_{\mathscr{C}}(t',t)\langle c(t)c^\dagger(t)\rangle:$$

$$\Rightarrow \quad i\partial_t G(t,t') = \underbrace{\partial_t\theta_{\mathscr{C}}(t,t')}_{\equiv\delta_{\mathscr{C}}(t,t')}\langle[c,c^\dagger]_+\rangle + h(t)G(t,t')$$

$$\int_{\mathscr{C}} dt'\delta_{\mathscr{C}}(t,t')g(t') = g(t)$$

$$\Rightarrow \quad [i\partial_t - h(t)]G(t,t') = \delta_{\mathscr{C}}(t,t')$$

Check: Restricted to imag branch $[-\partial_\tau - h]G(\tau) = \delta(\tau)$ ✔

Free particles: Equation of motion

- Inverse operator notation: $G^{-1}(t,t') = \delta_{\mathscr{C}}(t,t')[i\partial_t - h(t)]$

$$G^{-1} * G = \mathbb{1} \quad \Leftrightarrow \quad \underbrace{\int_{\mathscr{C}} dt_1\, G^{-1}(t,t_1) G(t_1,t')}_{[i\partial_t - h(t)]G(t,t')} = \delta_{\mathscr{C}}(t,t')$$

convolution (the $*$)

Equation has unique solution with (anti)-periodic boundary condition
$\leftrightarrow$ inverse operator well-defined for (anti)-periodic functions

- Read off inverse G from Keldysh action:

$$iS_{\mathscr{C}} = i \int_{\mathscr{C}} dt\, \bar{c}(t)\left(i\partial_t - h\right) c(t)$$

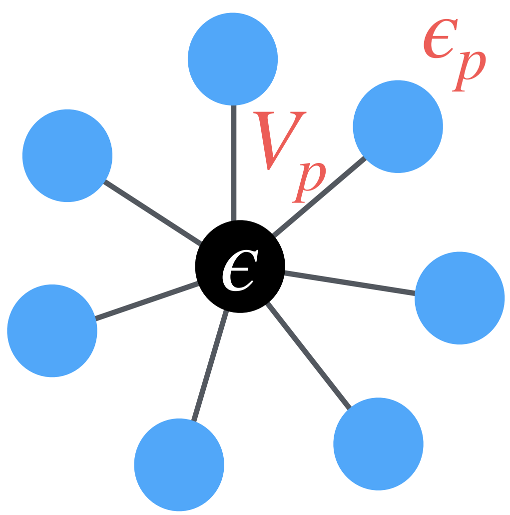
$$= i \int_{\mathscr{C}} dt dt'\, \bar{c}(t) \underbrace{\left(\delta_{\mathscr{C}}(t,t')[i\partial_t - h(t)]\right)}_{G^{-1}(t,t')} c(t') \quad = -\,\bar{c} * (-iG^{-1}) * c$$

$$= i\bar{c} * (G^{-1}) * c$$

$\ldots \langle c(t)\bar{c}(t')\rangle_S = (-iG^{-1})^{-1}(t,t') = iG(t,t')$ from Gauss-integral

Embedding self-energy

$$H = \epsilon\, c^\dagger c + \underbrace{\sum_p \epsilon_p a_p^\dagger a_p}_{\text{bath}} + \sum_p \left(V_p(t) a_p^\dagger c + h.c. \right)$$



GF of isolated site

$$S = \bar{c} * (g_c^{-1}) * c + \sum_p \left[\bar{a}_p * (g_p^{-1}) * a_p - \bar{a}_p * (c V_p) - (\bar{V}_p \bar{c}) * a_p \right]$$

⇨ Integrate out bath: $iS_{eff}[\bar{c}, c] = i\bar{c} * (g_c^{-1} - \Delta) * c$

$$\Delta(t,t') = \sum_p \bar{V}_p(t) g_p(t,t') V_p(t')$$

⇨ $$G^{-1}(t,t') = g_c^{-1}(t,t') - \Delta(t,t')$$

Alternative: derivation from coupled equations of motion for G

Dyson equation on $\mathscr{C}$

$$G^{-1}(t,t') = g_c^{-1}(t,t') - \Delta(t,t')$$

$$\Rightarrow \; G^{-1} * G = \mathbb{1} \quad \equiv \quad [i\partial_t - \epsilon]G(t,t') - [\Delta * G](t,t') = \delta_{\mathscr{C}}(t,t')$$

Integral-differential equation on $\mathscr{C}$

Solution: Projection on individual components

$$[-\partial_\tau - \epsilon]G^M(\tau) - [\Delta * G]^M(\tau) \qquad = \delta(\tau)$$

$$\Leftrightarrow \; [i\omega_n - \epsilon - \Delta(i\omega_n)]G^M(i\omega_n) = 1$$

$$[i\partial_t - \epsilon]G^{<,>}(t,t') - [\Delta * G]^{<,>}(t,t') = 0$$

$$[i\partial_t - \epsilon]G^R(t,t') - [\Delta * G]^R(t,t') = \delta(t-t')$$

$$[i\partial_t - \epsilon]G^{tv}(t,\tau) - [\Delta * G]^{tv}(t,\tau) = 0$$

Properties of convolution?

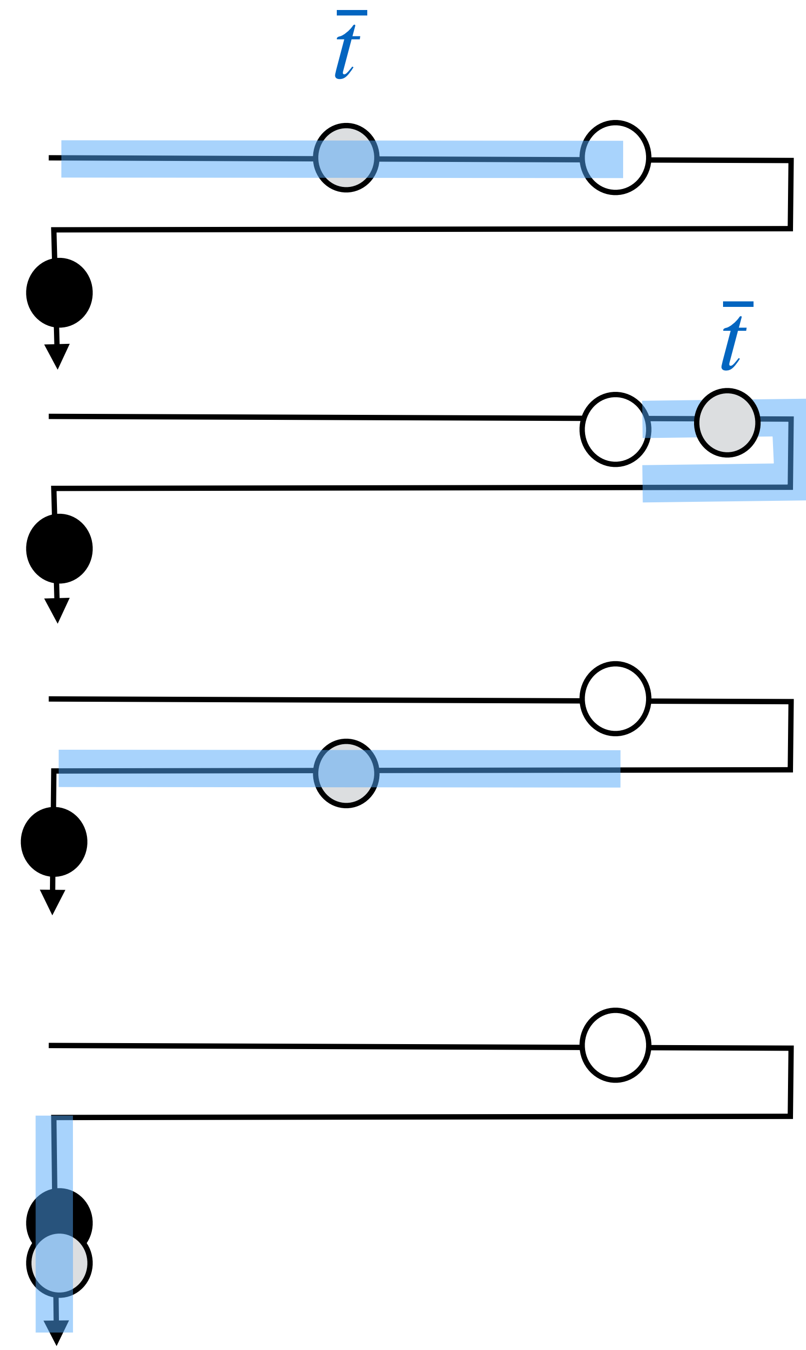
E.g.: Component $C^{tv} = [A * B]^{tv}$

$$C(t_+, -i\tau) = + \int_0^t d\bar{t}\, \underbrace{A(t_+, \bar{t}_+)}_{A(t_-,\bar{t}_+)=A^>(t,\bar{t})} \underbrace{B(\bar{t}_+, -i\tau)}_{B^{tv}(\bar{t},\tau)}$$

$$+0$$

$$-\int_0^t d\bar{t}\, \underbrace{A(t_+, \bar{t}_-)}_{A^<(t,\bar{t})} \underbrace{B(\bar{t}_-, -i\tau)}_{B^{tv}(\bar{t},\tau)}$$

$$-i\int_0^\beta d\bar{\tau} \underbrace{A(t_+, -i\bar{\tau})}_{A^{tv}(t,\bar{\tau})} \underbrace{B(-i\bar{\tau}, -i\tau)}_{iB^M(\bar{\tau}-\tau)}$$



Causality !

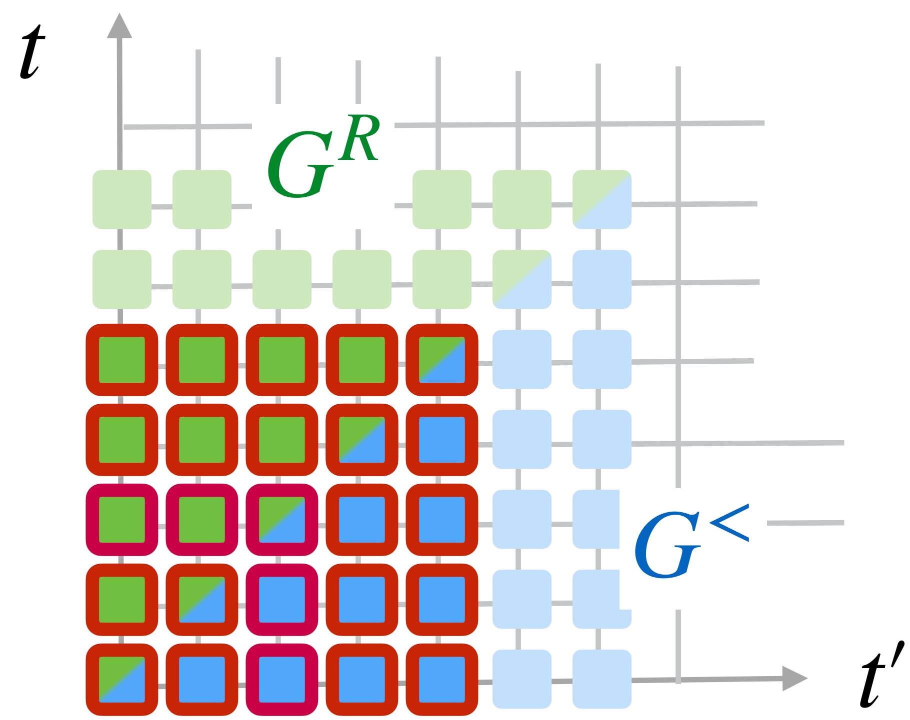
$$= \int_0^t d\bar{t}\, A^R(t,\bar{t}) B^{tv}(\bar{t},\tau) + \int_0^\beta d\bar{\tau}\, A^{tv}(t,\bar{\tau}) B^M(\bar{\tau}-\tau)$$

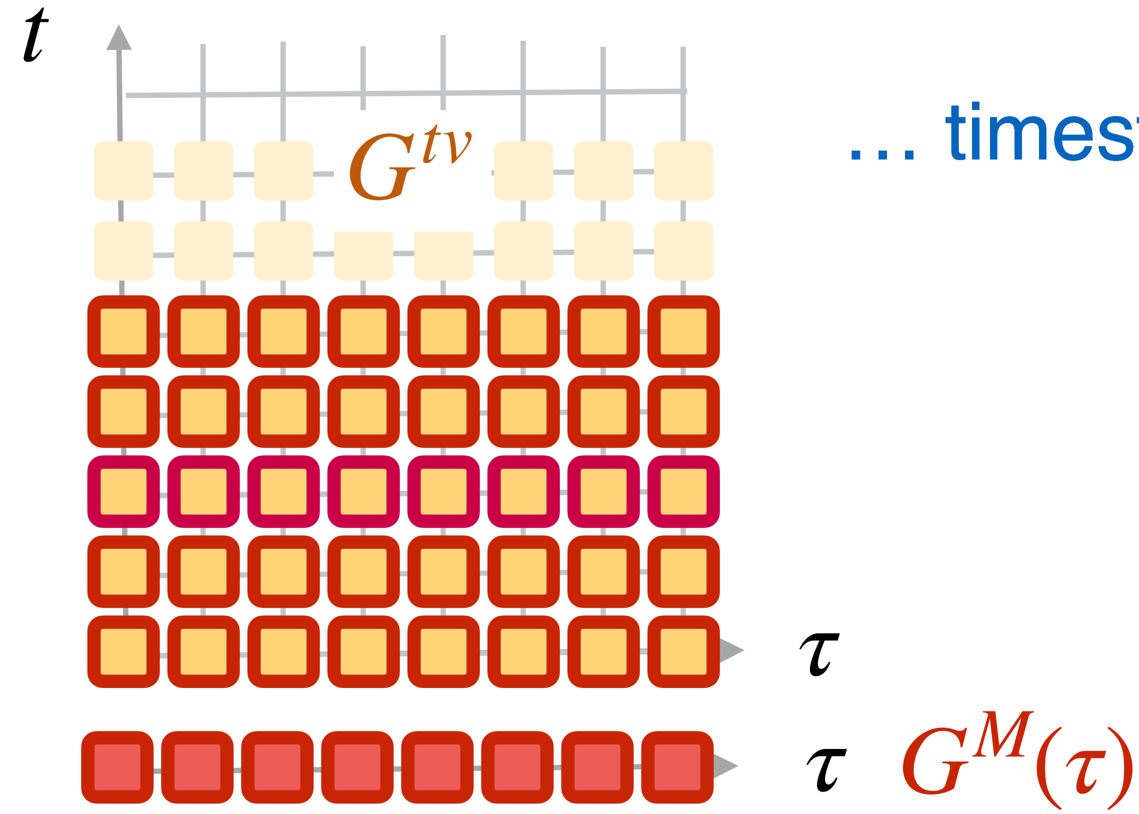
Causality in convolution:

Most important property of convolution, following from causality:

$C = A * B$ on "timeslice n" depends on
A and B only on timeslice $m \leq n$

Timeslice:





… timestep 1

Langreth rules

Dyson equation, broken down to components:

- $[-\partial_\tau - \epsilon]G^M(\tau) - \underbrace{[\Delta * G]^M(\tau)}_{\Delta^M * G^M} = \delta(\tau)$
- $[i\partial_t - \epsilon]G^R(t,t') - \underbrace{[\Delta * G]^R(t,t')}_{\Delta^R * G^R} = \delta(t-t')$
- $[i\partial_t - \epsilon]G^{tv}(t,\tau) - \underbrace{[\Delta * G]^{tv}(t,\tau)}_{\Delta^R * G^{tv} + \Delta^{tv} * G^M} = 0$
- $[i\partial_t - \epsilon]G^<(t,t') - \underbrace{[\Delta * G]^<(t,t')}_{\Delta^R * G^< + \Delta^< * G^A + \Delta^{tv} * G^{vt}} = 0$

independent of real time part, Solution in frequency $i\omega_n$

causal integral equations, solutions timestep by timestep

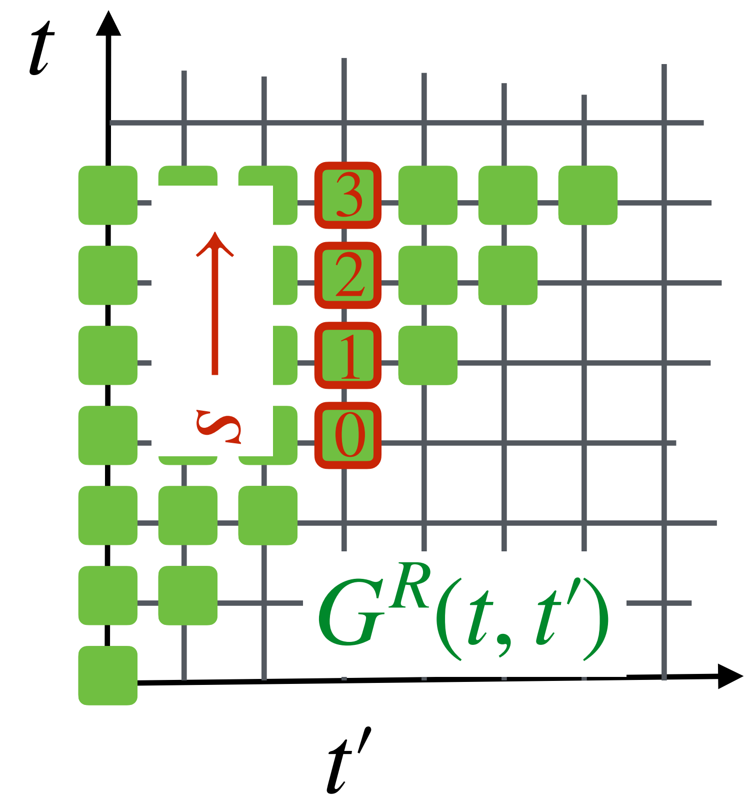
"Kadanoff Baym equations"

Real-time Dyson equation

Example: Retarded component:

$$[i\partial_t - \epsilon]G^R(t,t') - \int_{t'}^{t} dt_1 \Delta^R(t,t_1)G^R(t_1,t') = \delta(t,t')$$

given t': $y(s) \equiv G^R(t'+s,t')$



⇨ Volterra integral/differential equation:

$$[i\partial_s - \epsilon]y(s) - \int_0^s ds' K(s,s')y(s') = q(s)$$

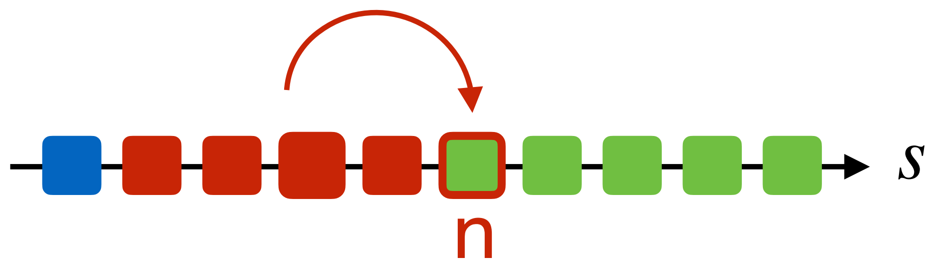
$$y(0) = -i$$

Volterra equation

$$[i\partial_s - \epsilon(s)]y(s) - \int_0^s ds' K(s,s')y(s') = q(s), \quad y(0) = y_0$$

⇨ Implicit scheme: Derivative / Integral at s=$n\Delta t$ in terms of $y_{m\leq n}$:

initial state y_0



Integrators based on
Brunner & van Houwen, 1986

e.g. $\frac{i(y_n - y_{n-1})}{\Delta t} + \epsilon_n y_n - \Delta t \left[\frac{1}{2} K_{n,n} y_n + K_{n,n-1} y_{n-1} + \cdots K_{n,1} y_1 + \frac{1}{2} K_{n,0} y_0 \right] = q_n$

Integration scheme with accuracy $\mathcal{O}(\Delta t^{k+1})$:

⇨ kth order accurate derivative requires $y_n, \ldots, y_{n-k}$ (same for integral)

⇨ First k steps must be solved simultaneously together
(linear equation for $(y_1, \ldots, y_k)$)

Interacting Green's functions and perturbation theory

Wick's theorem for $\mathscr{C}$ ordered functions

Noninteracting fermions (quadratic action)

$$Z = \int \mathscr{D}[\bar{c}, c]\, e^{iS_{\mathscr{C}}} \qquad iS_{\mathscr{C}} = -\sum_{j,j'} \bar{c}_j(-iG_0^{-1})_{jj'} c_j$$

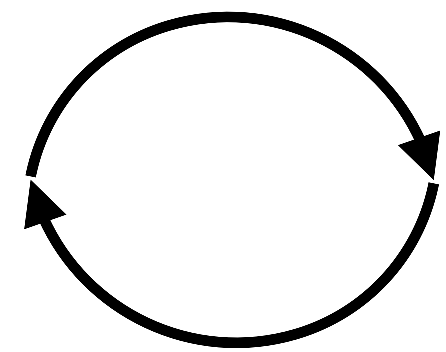
⇨ Factorization of contour-ordered correlation functions:

$$\langle T_{\mathscr{C}} c(t_1) \cdots c(t_n) c^\dagger(t_{n'}) \cdots c^\dagger(t_{1'}) \rangle = \langle c_1 \cdots c_n \bar{c}_{n'} \cdots c_{1'} \rangle_S$$

$$= \det \begin{pmatrix} \langle c_1 \bar{c}_{1'} \rangle_S & \cdots & \langle c_1 \bar{c}_{n'} \rangle_S \\ \vdots & & \vdots \\ \langle c_n \bar{c}_{1'} \rangle_S & \cdots & \langle c_n \bar{c}_{n'} \rangle_S \end{pmatrix} \qquad = \det \begin{pmatrix} iG_{1,1'} & \cdots & iG_{1,n'} \\ \vdots & & \vdots \\ iG_{n,1'} & \cdots & iG_{n,n'} \end{pmatrix}$$

Wick's theorem for $\mathscr{C}$ ordered functions

Wick's theorem for density-density correlation function



$$\chi(t,t') = -i\left[\langle T_{\mathscr{C}} c^\dagger(t)c(t)c^\dagger(t')c(t')\rangle - \langle n(t)\rangle\langle n(t')\rangle\right]$$

$$= -i\,\underbrace{\langle T_{\mathscr{C}} c^\dagger(t)c(t')\rangle}_{-iG(t',t)}\,\underbrace{\langle T_{\mathscr{C}} c(t)c^\dagger(t')\rangle}_{iG(t,t')} = -iG(t,t')G(t',t)$$

Response function: $\chi^R(t,t') = -i\theta(t-t')\langle[n(t),n(t')]\rangle$

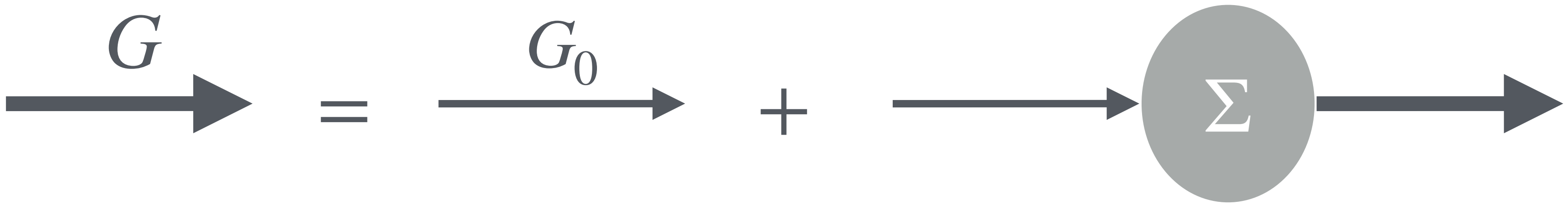
$$\chi^R(t,t') = \chi(t_-,t'_+) - \chi(t_+,t'_-) = -i\,\underbrace{G(t_-,t'_+)}_{G^>(t,t')}\,\underbrace{G(t'_+,t_-)}_{G^<(t',t)} + i\,\underbrace{G(t_+,t'_-)}_{G^<(t,t')}\,\underbrace{G(t'_-,t_+)}_{G^>(t',t)}$$

~ Usual analytical representation of response functions in equilibrium

$$\text{Im}\chi^R(\omega) \sim \int \frac{d\omega}{2\pi} A(\omega_1)A(\omega_2)[\bar{f}(\omega_1)f(\omega_2) - \bar{f}(\omega_2)f(\omega_1)]\delta(\omega - \omega_1 + \omega_2)$$

Perturbation theory

Derivation of perturbation theory for $\mathscr{C}$-ordered Green's functions analogous to imag time ordered Green's functions



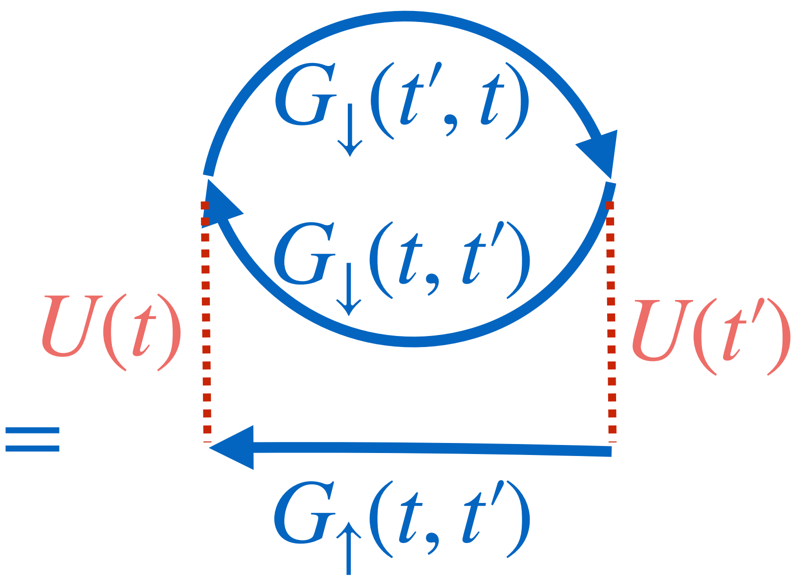
$$G^{-1} = G_0^{-1} - \Sigma$$

⇨ same rules in diagrammatic perturbation theory (apart from factors i)

e.g., second order PT in the Hubbard model:

$$H' = U(t) n_\uparrow n_\downarrow$$

$$\Sigma_\uparrow(t, t') =$$



$$\underbrace{\Sigma(\tau)}_{-i\Sigma(-i\tau, -i\tau')} = -U^2 \times \underbrace{G(\tau)}_{-iG(-i\tau, -i\tau')} \times \underbrace{G(\tau)}_{-iG(-i\tau, -i\tau')} \times \underbrace{G(-\tau)}_{-iG(-i\tau', -i\tau)}$$

⇨ $$\Sigma(t, t') = -i^2 U(t) U(t') G(t, t') G(t, t') G(t', t)$$

Example:
Interaction quench in the Hubbard model

Example: Quench in the Hubbard model

$$H = -J \sum_{\langle i,j \rangle, \sigma} c^\dagger_{i,\sigma} c_{j,\sigma} + U(t) \sum_j n_{j,\uparrow} n_{j,\downarrow} \qquad U(t) = \begin{cases} 0 & t < 0 \\ U & t > 0 \end{cases}$$

2nd order PT solution:

- Dyson for each k: $G_k^{-1} = i\partial_t - \epsilon_k - \Sigma \quad (G_k \equiv G_{\epsilon_k})$
- Local GF: $G = \sum_k G_k = \int d\epsilon_k D(\epsilon_k) G_{\epsilon_k}$

Here "Bethe lattice" : $D_0(\omega) = \sqrt{4 - \omega^2}/2\pi$

- Self-energy (local approximation)

$$\Sigma(t, t') = -i^2 U(t) U(t') G(t, t') G(t, t') G(t', t)$$

Self-consistent approximation (energy conserving)

$$\Sigma(t, t') = -i^2 U(t) U(t') G_0(t, t') G_0(t, t') G_0(t', t)$$

bare PT

Example: Quench in the Hubbard model

Code: (C++)

NESSi documentation: http://www.nessi.tuxfamily.org/

NESSi source: https://github.com/nessi-cntr/

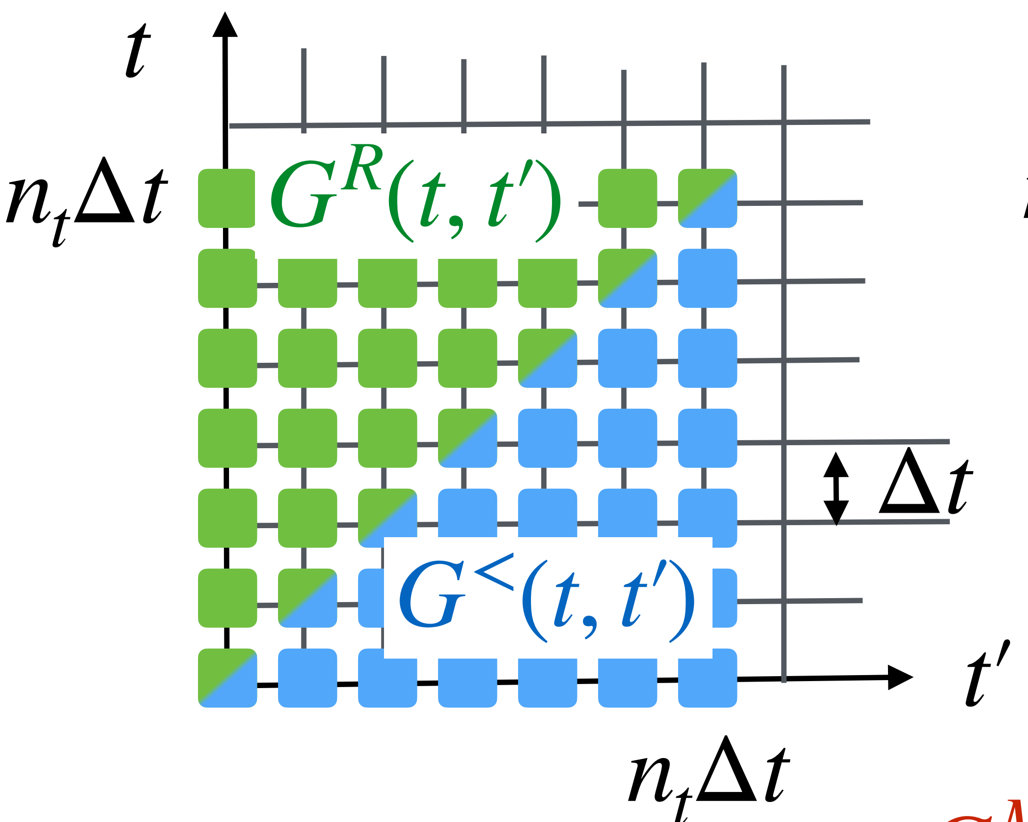
Examples for this lecture: Nessi_demo/

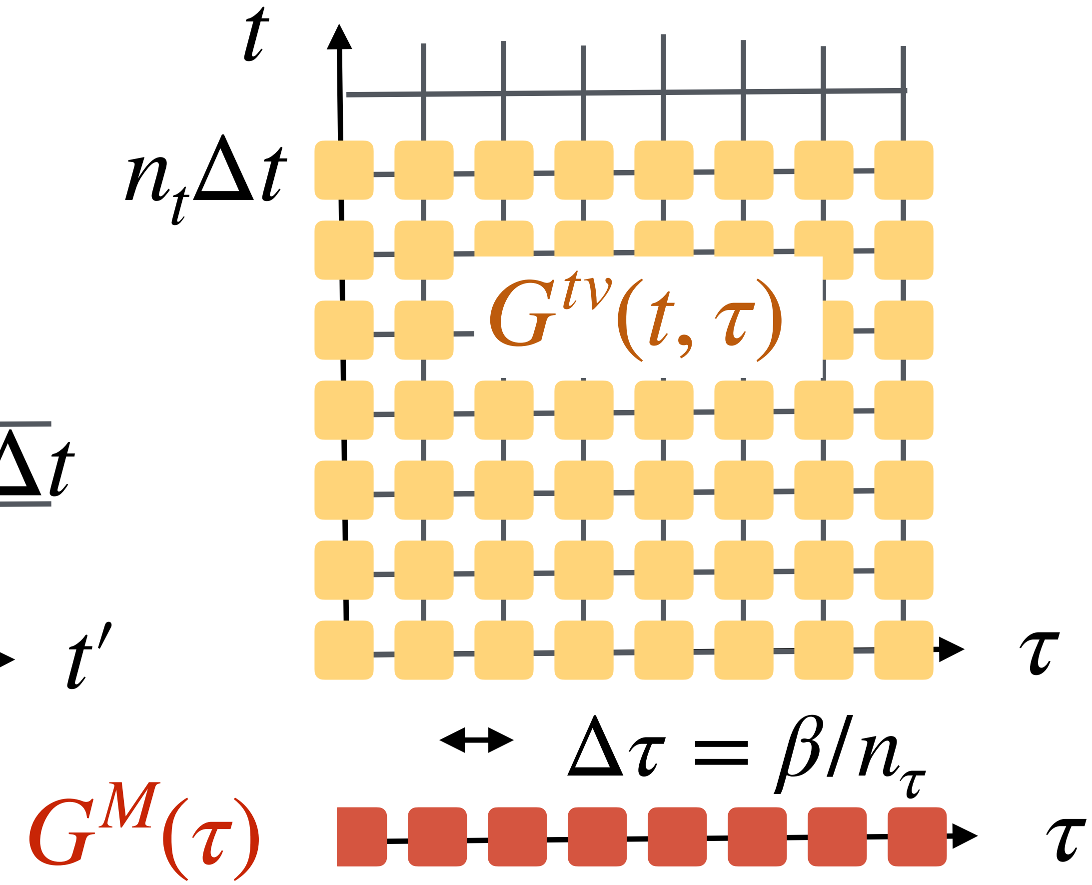
Nessi_demo/programs/	Source code main program
Nessi_demo/python/	Jupyter notebooks for running code

Green's functions in NESSi

Retarded $G^R(t,t') = \theta(t-t')[G^>(t,t') - G^<(t,t')]$, for $t \geq t'$

lesser, mixed, Matsubara





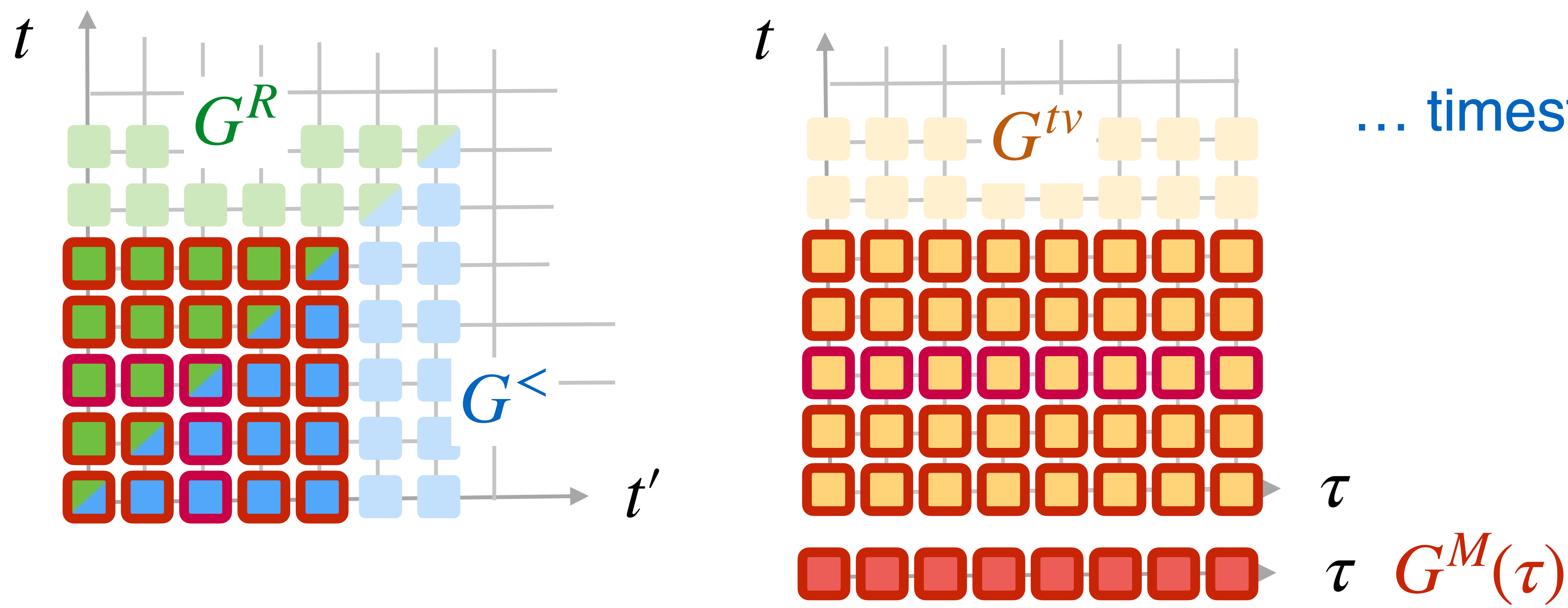
Nc ... ry: ... $t)]^\dagger$

```
int nt=100;       // max. number of real time steps
int ntau=100;  // max. number of imag time steps
int size=1;       // orbital dimension
int sig=-1;       // -1 (FERMION) or +1 (BOSON)

cntr::herm_matrix<double> G(nt,ntau,size,sig);
// natural routines to access matrix elents, input/output ....
```

NESSi Green's functions

Timeslice:



… timestep

Container in NESSi: **cntr::herm_matrix_timestep**

```
int tstp=...;        // >= -1
int ntau=...;       // number of imag time steps
int size=...;       // orbital dimension
int sig=...;        // -1 (FERMION) or +1 (BOSON)
cntr::herm_matrix_timestep<double> tG(tstp,ntau,size,sig);
```

Equilibrium Green's functions: Spectral representation

Equilibrium: All Green functions can be obtained from spectral representation

$$G(t,t') = -i \int d\omega A(\omega) e^{-i\omega(t-t')}[\theta_{\mathscr{C}}(t,t') + \xi F(\omega)]$$

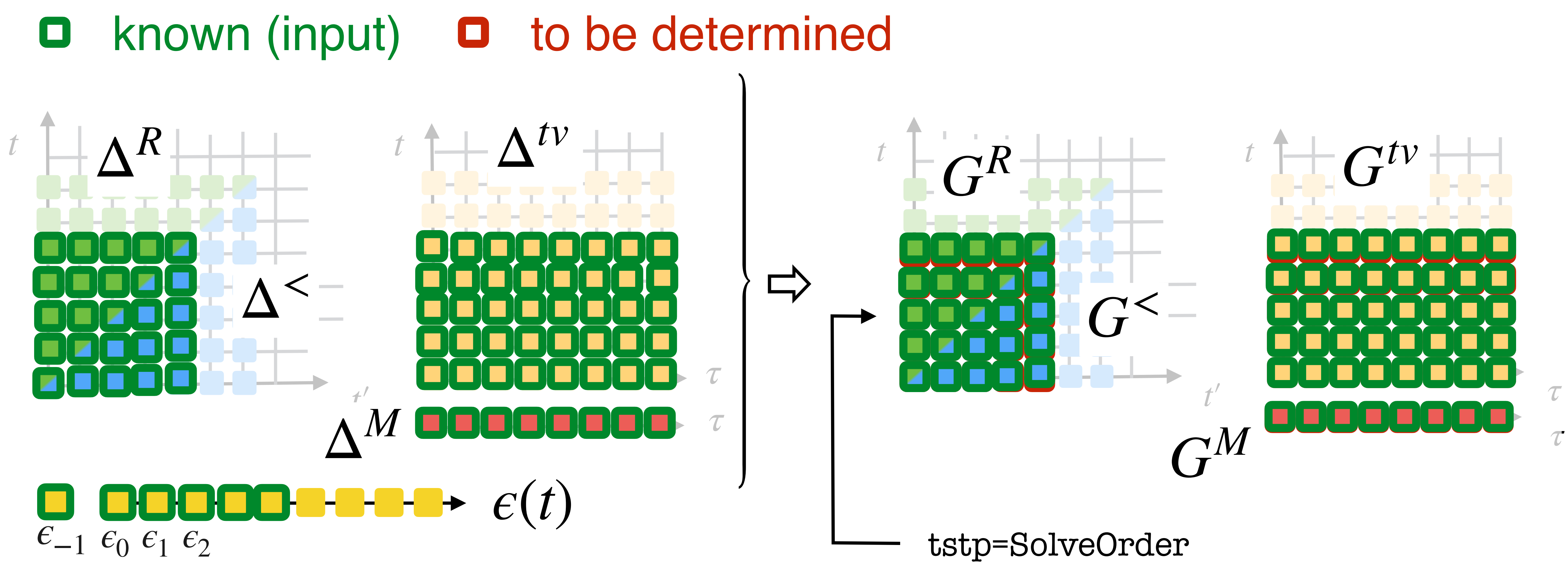
Needed: In particular to explicitly construct bath Green's functions for continuous environment.

NESSi: Some routines provided to construct G from spectrum].

Special example: $A(\omega) = \frac{1}{2\pi}\sqrt{4-\omega^2}$

```
cntr::herm_matrix<double> G(nt,ntau,size,sig);
cntr::green_equilibrium_bethe(G,beta,dt);
```

Time-stepping of Dyson eq. $[i\partial_t - \epsilon]G - [\Delta * G] = \delta_{\mathscr{C}}$




```
double mu=0.0,beta=1.0;dt=0.01;
cntr::herm_matrix<double> Delta(nt,ntau,size,sig);
cntr::herm_matrix<double> G(nt,ntau,size,sig);
cntr::function<double> eps(nt,size); // container for time-dependent function
// initialize D, and eps

int SolveOrder=2;  // integration order, default = 5

cntr::dyson_mat(G,mu,eps,Delta,beta,SolveOrder);  // Matsubara solution (timestep -1)
cntr::dyson_start(G,mu,eps,Delta,beta,dt,SolveOrder); // solution on tstp=0...SolveOrder
for(int tstp=SolveOrder+1; tstp<=nt;tstp++)
   cntr::dyson_timestep(tstp,G,mu.eps,Delta,beta,dt,solveorder);
```

Time-stepping solution of Dyson equation

Self-consistent equation:

$$[i\partial_t - \epsilon[G]]G(t,t') - [\Delta[G] * G](t,t') = \delta_{\mathscr{C}}(t,t')$$

e.g. mean-field potential depending on density $n(t) = iG^<(t,t)$

e.g., self-energy depending on full G

⇨ Iterate on each timestep:

```
// some  guess for Delta and eps on tstp=1

cntr::dyson_mat(G,mu,eps,Delta,beta,SolveOrder);
... // update  Delta and eps from G on timestep -1
```

iterate to convergence

```
cntr::dyson_start(G,mu,eps,Delta,beta,dt,SolveOrder);
... // update  Delta and eps from G on timestep  0...SolveOrder
```

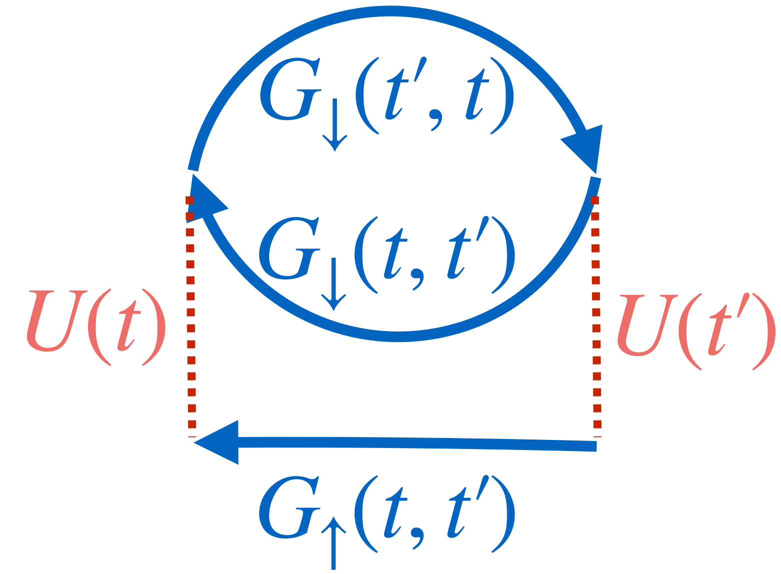
iterate to conv.

```
for(int tstp=SolveOrder+1; tstp<=nt;tstp++)
   cntr::dyson_timestep(tstp,G,mu.eps,Delta,beta,dt,solveorder);
   ... // update  Delta and eps from G on timestep  tstp
```

iterate to conv.

Perturbation theory

$$\Sigma(t,t') = -i^2 U(t)U(t')G(t,t')G(t,t')G(t',t)$$

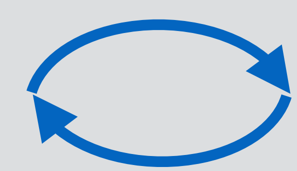


Evaluation in NESSi:

```
cntr::function<double> U(nt,1);
cntr::herm_matrix<double> G(nt,ntau,1,FERMION);
cntr::herm_matrix<double> Sigma(nt,ntau,1,FERMION);
```

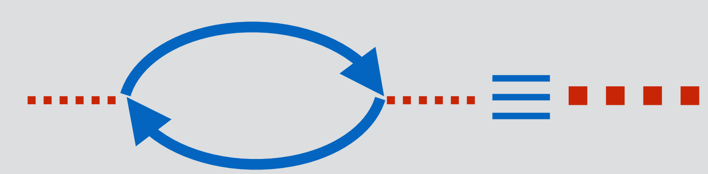
```
/// all following operations performed on given timeslice:
cntr::herm_matrix_timestep<double> Pi(tstp,ntau,1,BOSON);
```

`cntr::Bubble1(tstp,Pi,G,G);` $\Pi(t,t') \to iG(t,t')G(t',t)$



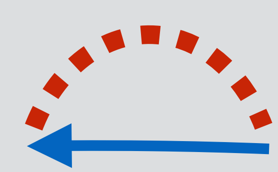
`Pi.left_multiply(tstp,U);` $\Pi(t,t') \to U(t)\Pi(t,t')$

`Pi.right_multiply(tstp,U);` $\Pi(t,t') \to \Pi(t,t')U(t')$



`cntr::Bubble2(tstp,Sigma,Pi,G);` $\Sigma(t,t') \to i\Pi(t,t')G(t,t')$

`Sigma.smul(tstp,-1.0)` $\Sigma(t,t') \to -\Sigma(t,t')$

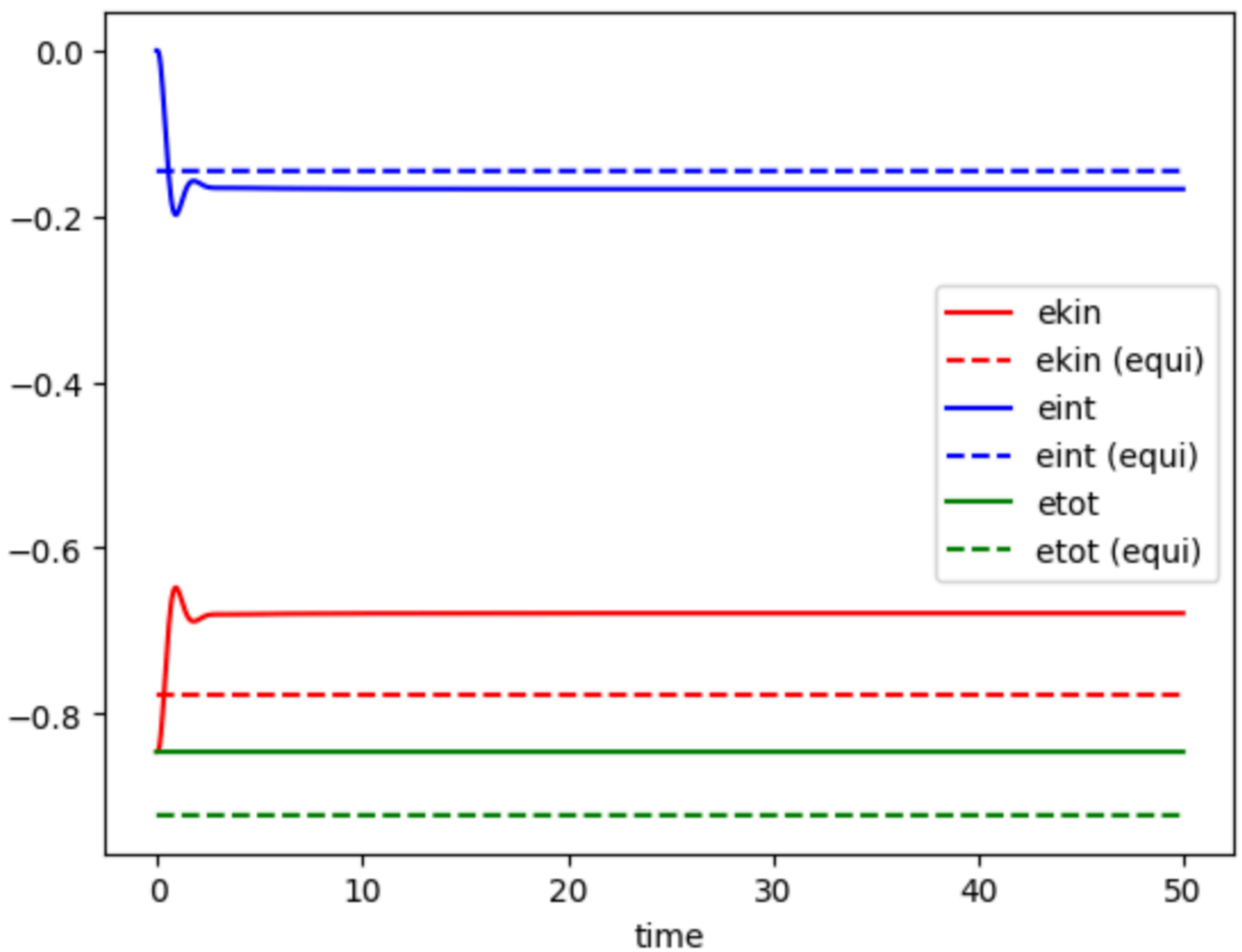


Example: Quench in the Hubbard model

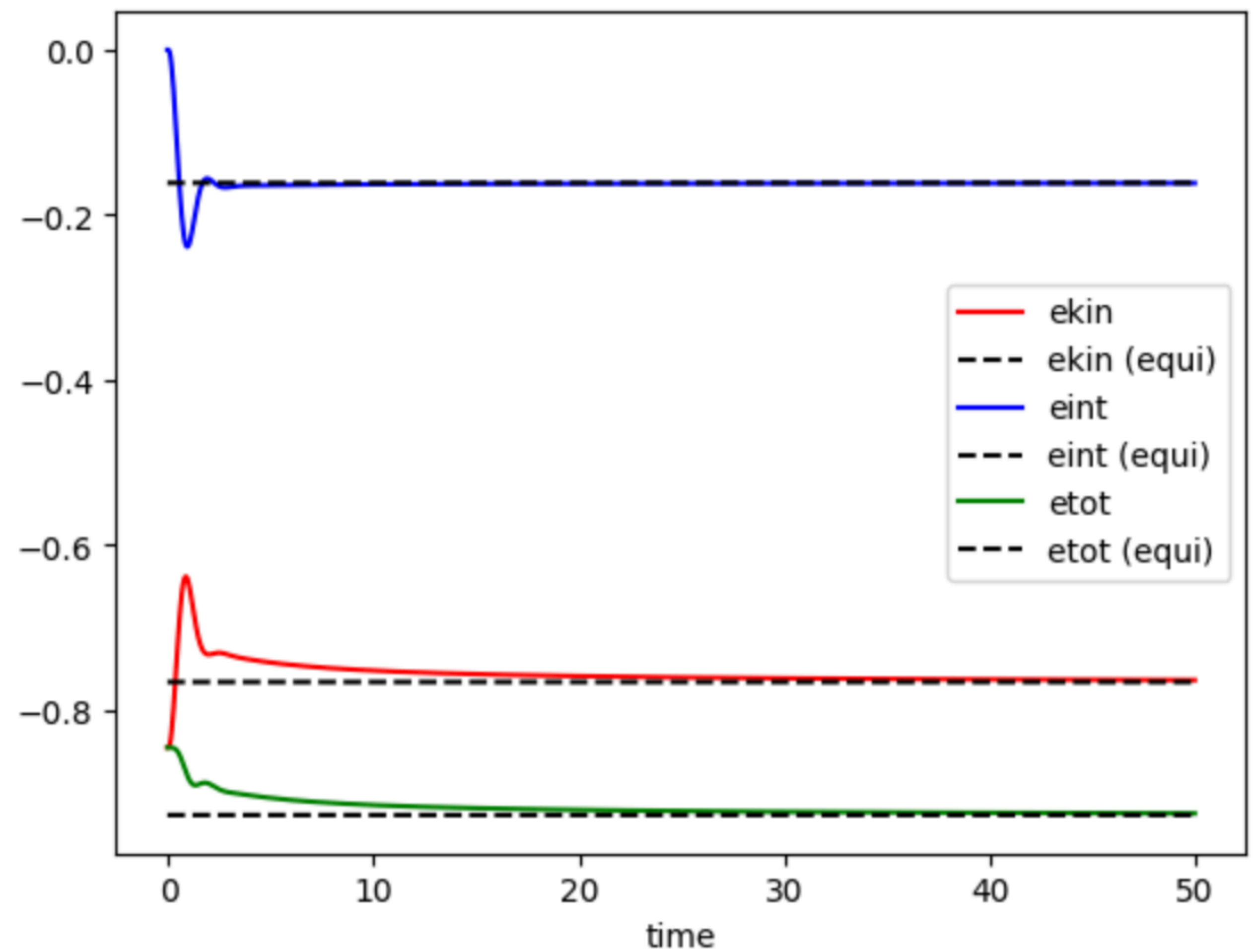
Relaxation of kinetic and potential energy:

$$E_{kin} = \frac{1}{N}\sum_{k,\sigma}\langle c^\dagger_{k,\sigma}c_{k,\sigma}\rangle\epsilon_k, \quad E_{int} = \frac{1}{N}\sum_j U\left\langle n_{j\uparrow}n_{j,\downarrow} - \frac{1}{4}\right\rangle$$

Conserving PT:



Bare PT:

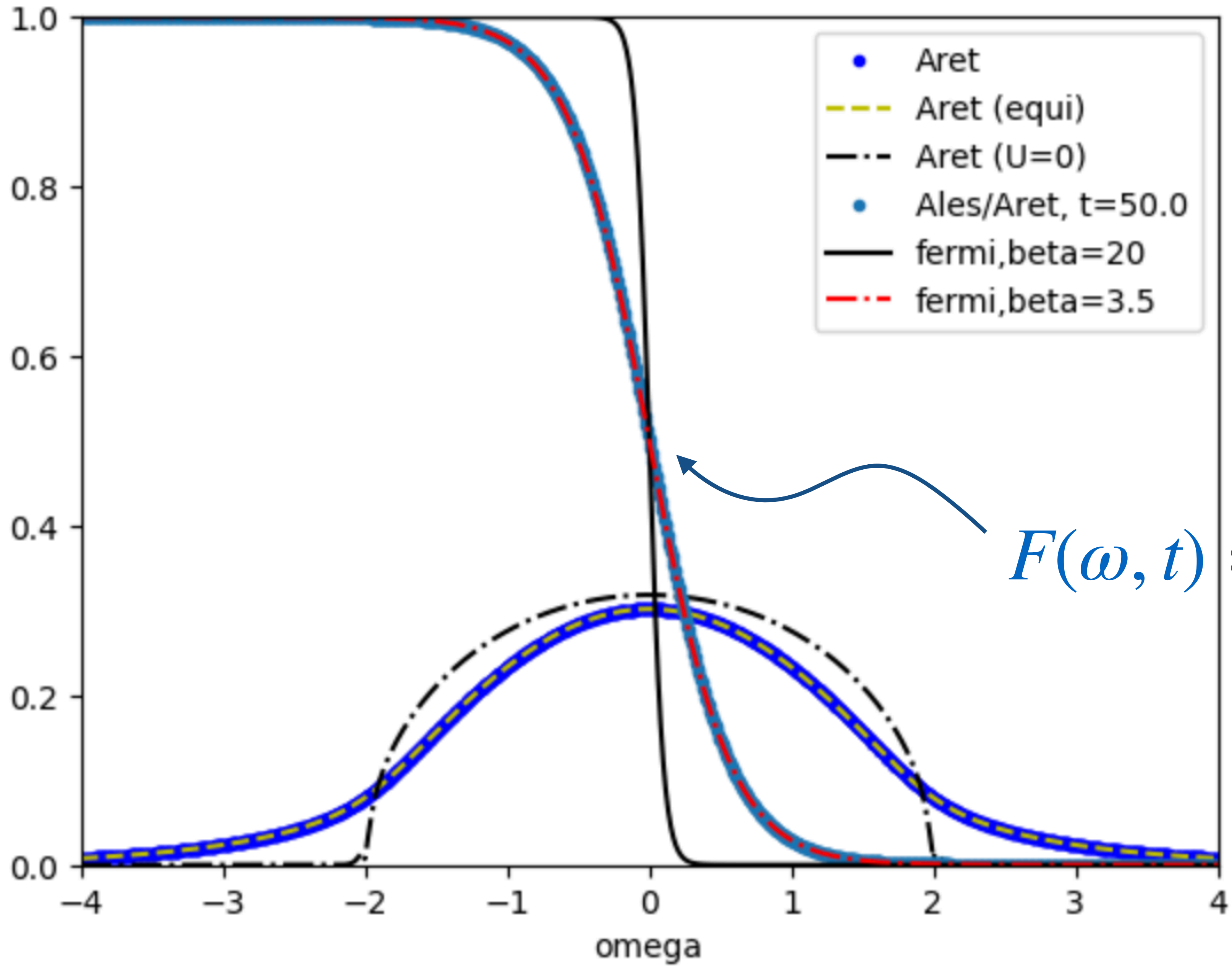


Dashed: Production for interacting system at *initial* temperature

Example: Quench in the Hubbard model

Spectral functions and occupation function:

$$A(\omega, t) = -\frac{1}{\pi}\text{Im}\int_0^t dse^{-\eta s}G^{ret}(t, t-s)e^{i\omega,s}, \quad A^<(\omega, t) = \ldots$$

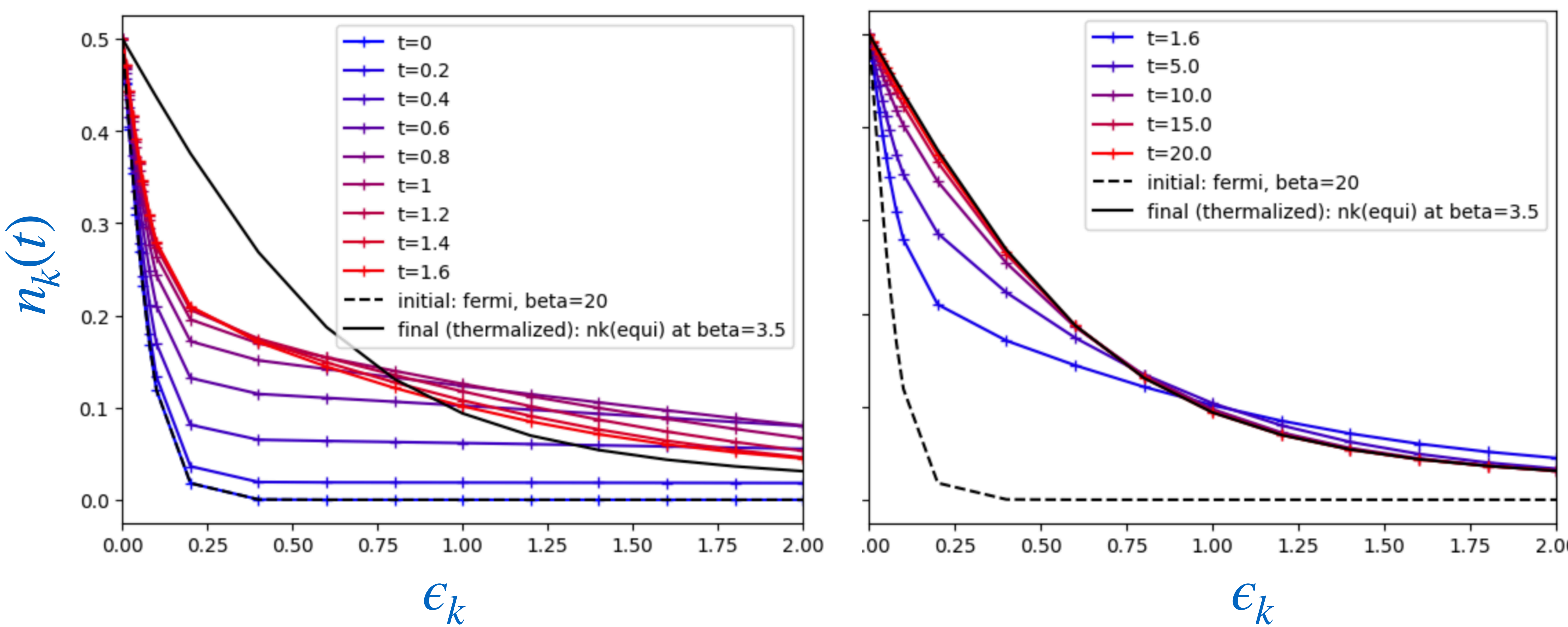


$$F(\omega, t) = A^<(\omega, t)/A(\omega, t)$$

Motivation example: Quench in the Hubbard model

Relaxation of the momentum occupation $n_k(t) = \langle c_k^\dagger(t) c_k(t) \rangle$

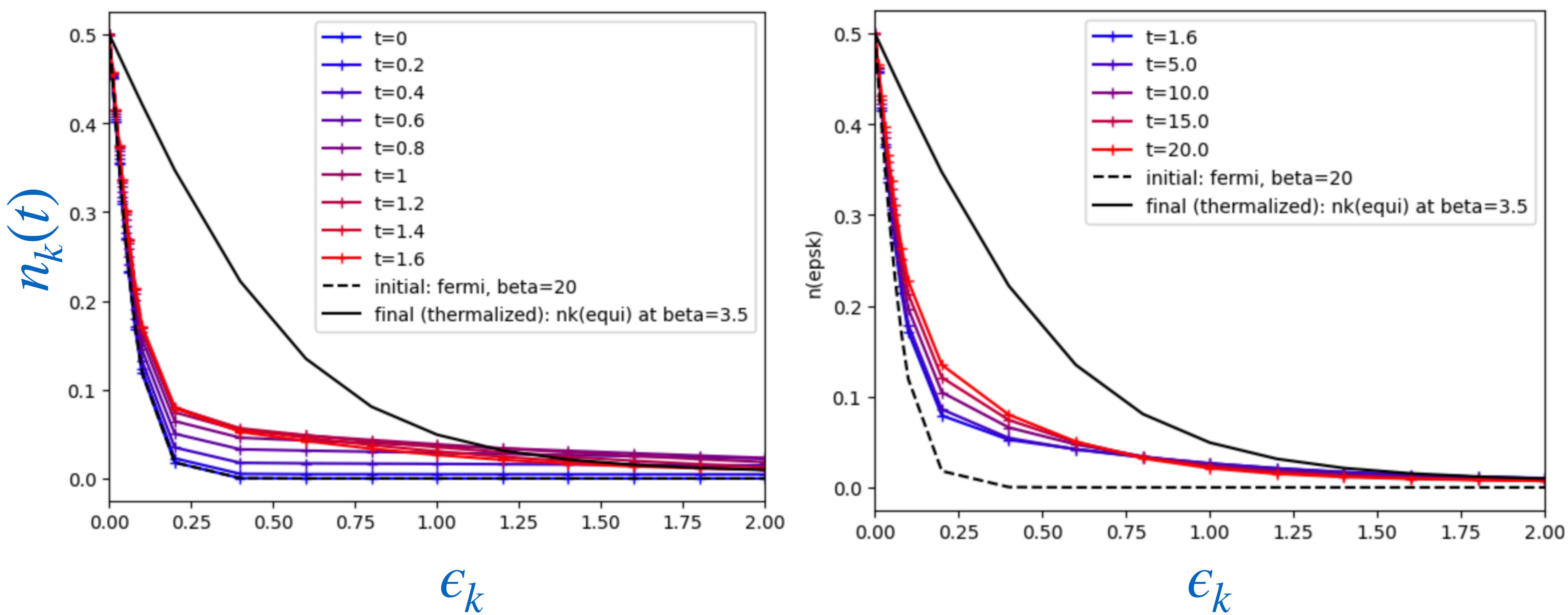
U=2, [time]=$\hbar/J$



Motivation example: Quench in the Hubbard model

Relaxation of the momentum occupation $n_k(t) = \langle c_k^\dagger(t) c_k(t) \rangle$

U=1, [time]=$\hbar/J$



Motivation example: Quench in the Hubbard model

Relaxation of the momentum occupation $n_k(t) = \langle c_k^\dagger(t) c_k(t) \rangle$

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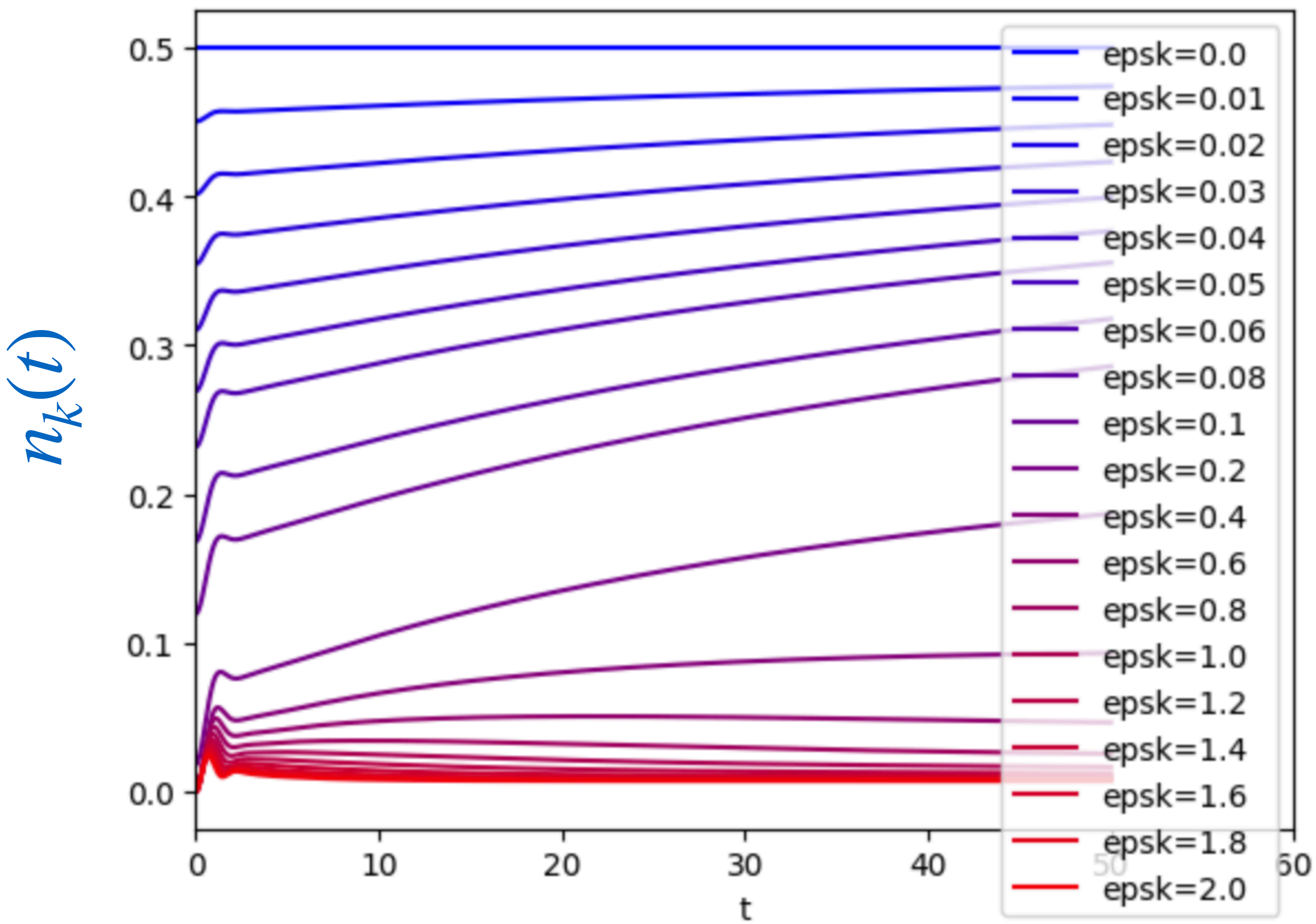


"Prethermalization"

Long times

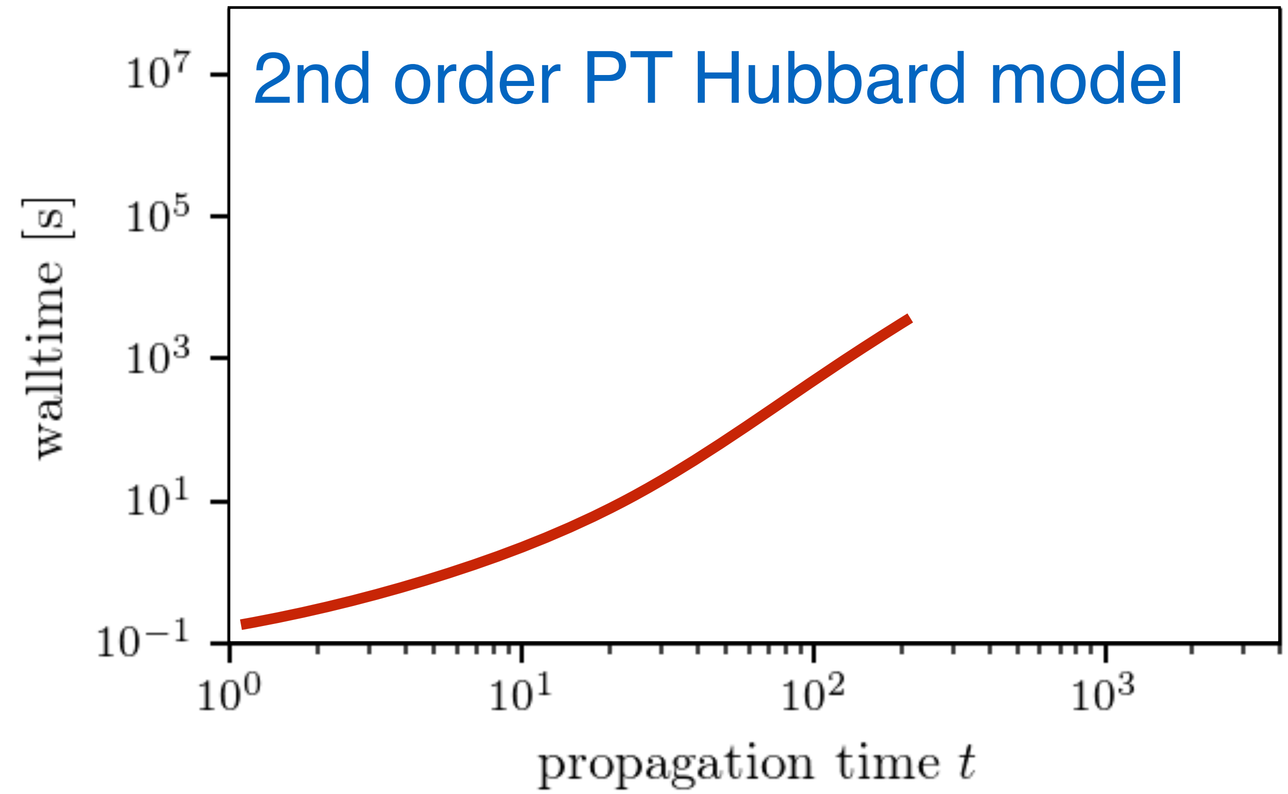
Computational cost / Memory bottleneck

Scaling of numerical cost:

- CPU $\mathcal{O}(N_t^3)$
- memory $\mathcal{O}(N_t^2)$

(OMP parallelisation possible)

more severe …



E.g.: First-principle **multi**-orbital simulations based on standard perturbative approaches?

$L = 10$ orbitals
Energy window 10eV
⇨ $\Delta t \ll 1/\mathrm{eV} = 0.1\mathrm{fs}$)
Simulation time 1000fs

⇨

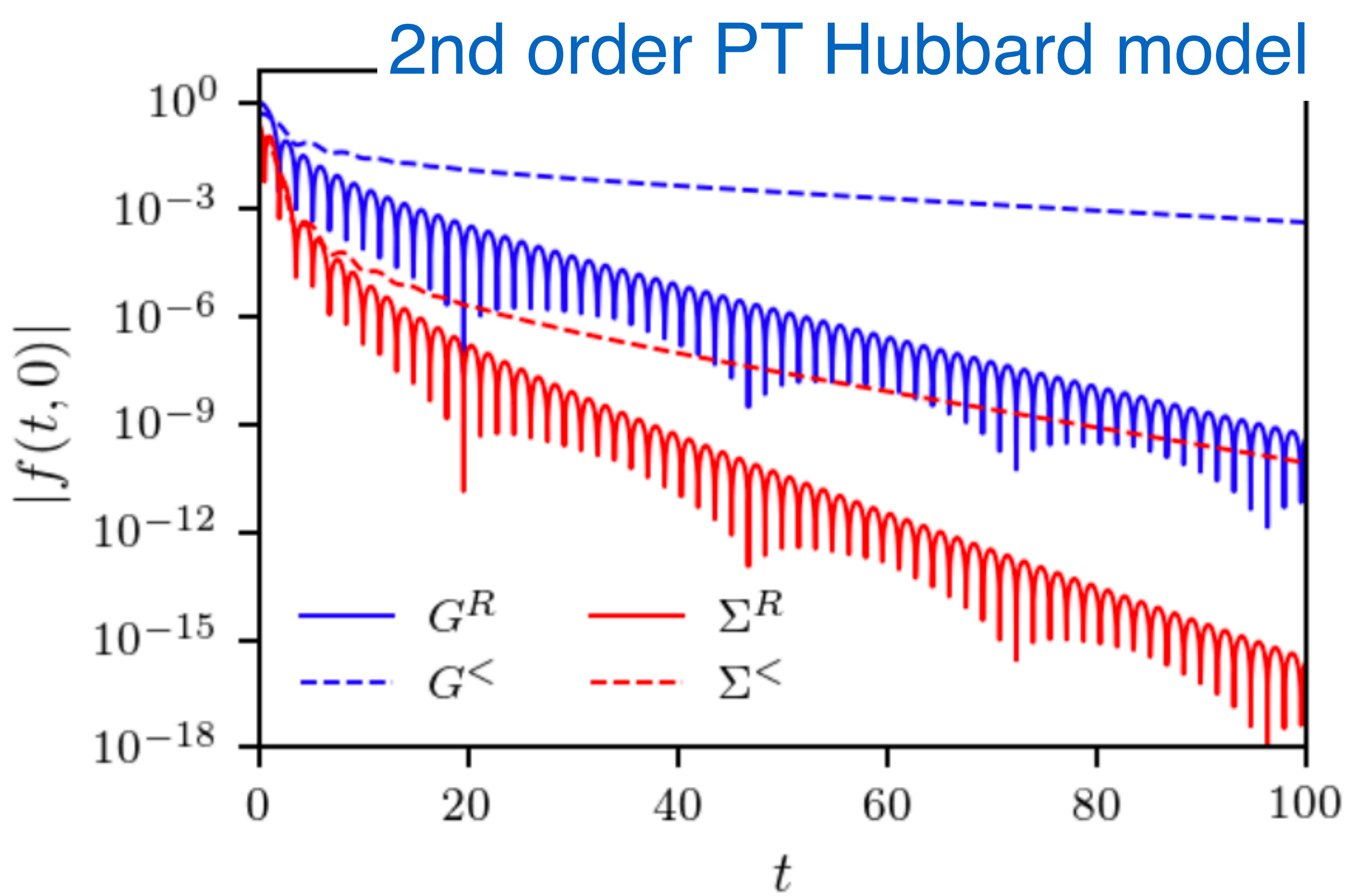
$n_t = 10^4$
Memory $G^<$ and G^R
$n_t^2 \times L^2 = (10^4)^2 \times (10^2) = 10^{10}$
complex numbers

not entirely out of range, but definitely some improvement needed!

Kadanoff Baym equations with memory truncation

Dyson equation $[i\partial_t - \epsilon]G(t,t') - [\Sigma * G](t,t') = \delta_{\mathscr{C}}(t,t')$

Σ often decays as function of time difference!



Assume banded memory kernel: $\Sigma^{>,<}(t,t') \approx 0$ for $|t-t'| > t_c$

$\Sigma^{tv}(t,\tau) \approx 0$ for $t > t_c$

Simplifications in equation for G? (Note: G does not decay quickly)

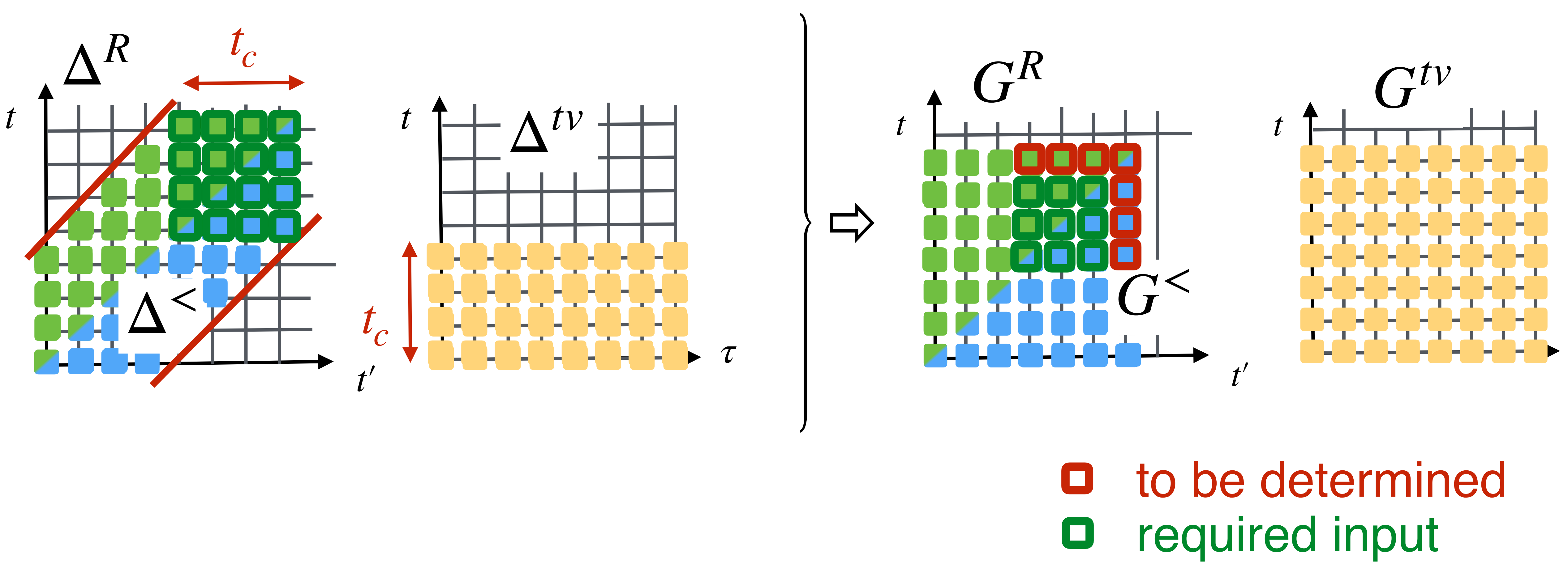
Memory truncation

Banded memory kernel:

$$\Delta^{>,<}(t,t') = 0 \text{ for } |t-t'| > t_c$$
$$\Delta^{tv}(t,\tau) = 0 \text{ for } t > t_c$$

⇨ G does not decay quickly,

but Dyson equation closed on "moving window"



Stahl, Dasari Picano, Li, Werner, Eckstein, PRB **105**, 115146 (2022)

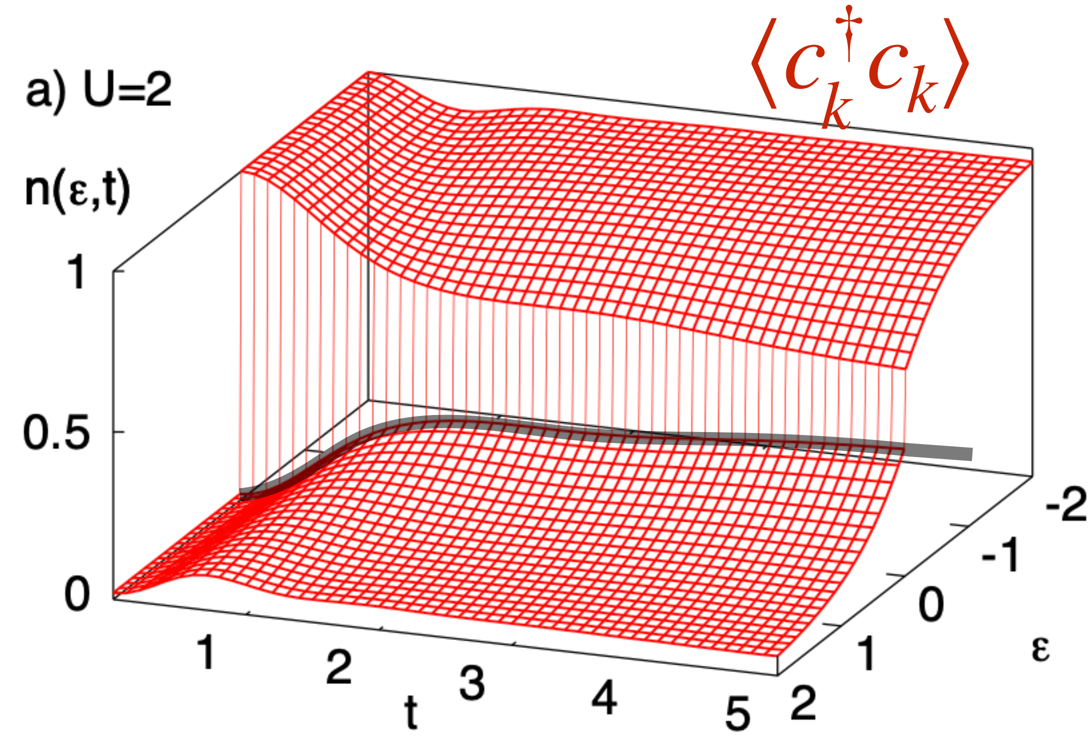
Memory truncation: 2nd order PT Hubbard Model

Hubbard model (Bethe lattice): Interaction quench to U=1 (bandwidth =4)

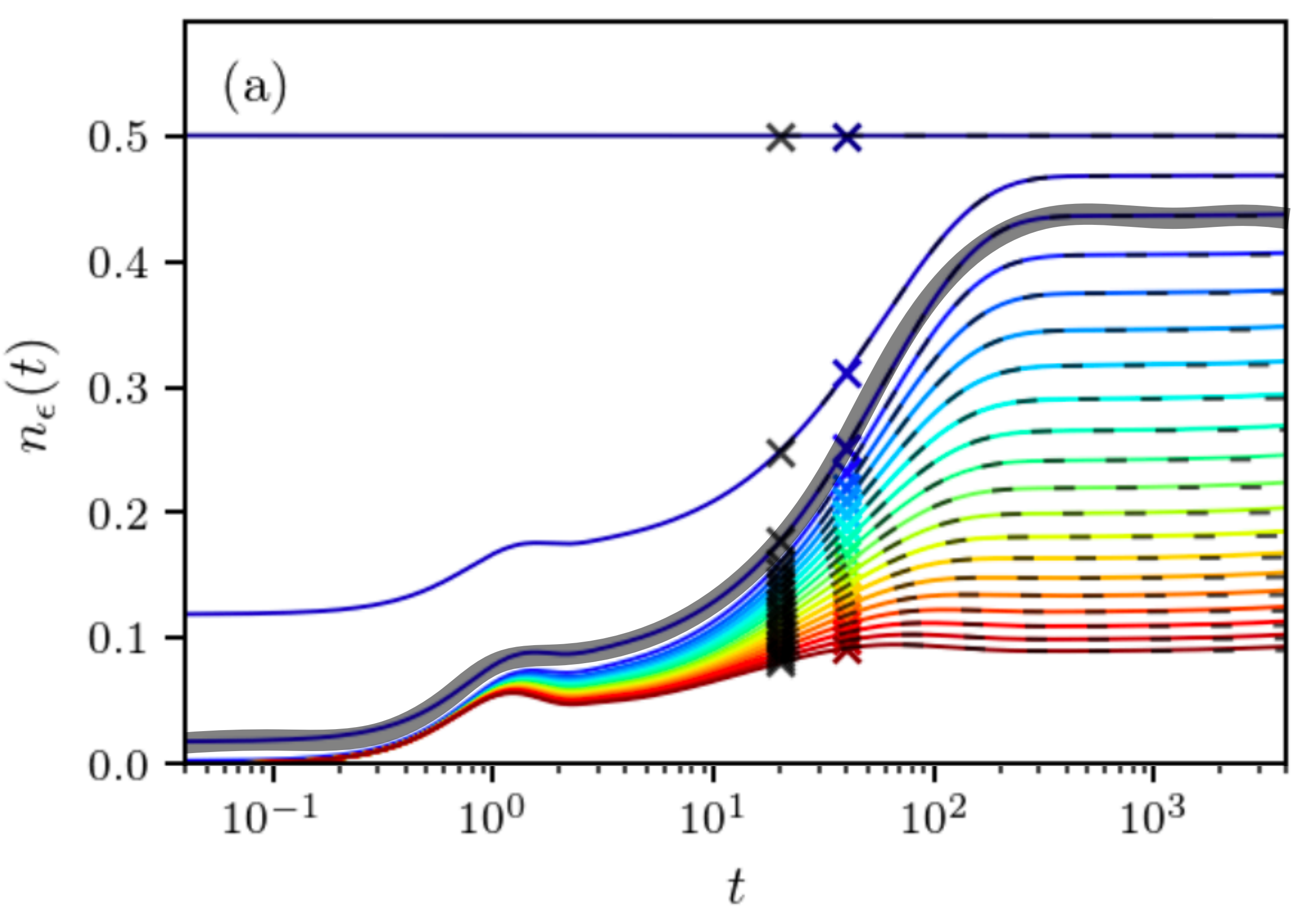
short time (exact CTQMC)

Eckstein, Kollar, Werner (2009)

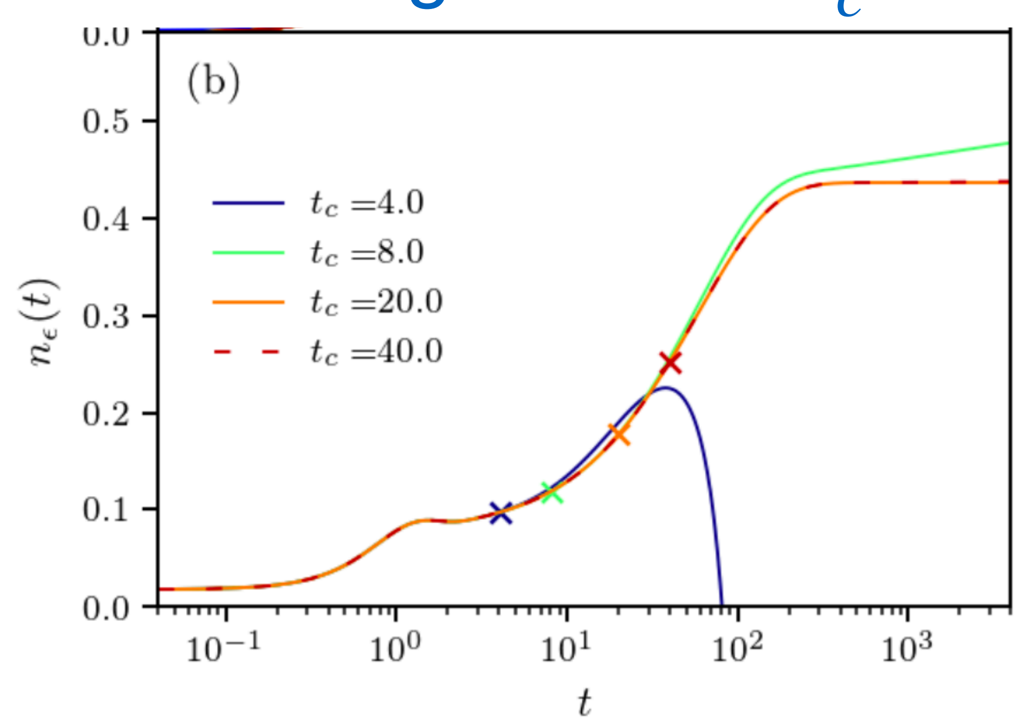
⇨ prethermalization



Long time (2nd oder PT)



Convergence with t_c



Memory bottleneck

Overcoming the memory constraint? … needed for

⇨ simulations with vastly different timescales: electrons & lattice; electrons & collective modes; prethermalization & thermalisation

⇨ first-principle **multi**-orbital simulations based on standard perturbative approaches

- Generalized Kadanoff Baym Ansatz
  Schlünzen, Joost, Bonitz, Phys. Rev. Lett. 124, 076601 (2020)
- Quantum Boltzmann equations
  Picano, Li, Eckstein, Phys. Rev. B **104**, 085108 (2021)

} additional approximations "physical insight"

- Systematic truncation of memory integrals
  Stahl, Dasari Picano, Li, Werner, Eckstein, PRB **105**, 115146 (2022)
- Hierarchical storage of two-time functions
  Kaye and Golez,arXiv:2010.06511

} Reformulation of numerical solutiuoin

Thank you for your attention