Continuous-time quantum Monte Carlo impurity solvers for nonequilibrium dynamics of strongly correlated electronic systems

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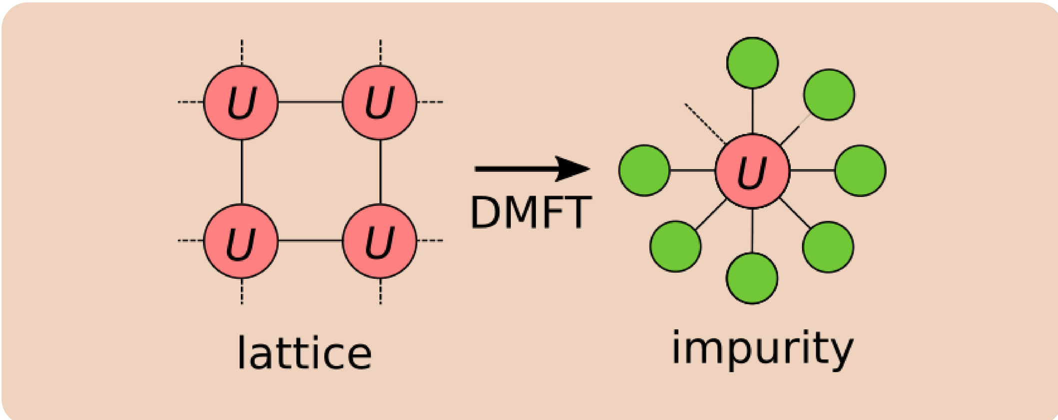
Motivation

Nonequilibrium dynamical mean field theory

- Nonequilibrium dynamical mean field theory (NE-DMFT) provides an approximate solution to an **interacting time-dependent lattice problem** [1].
- NE-DMFT assumes **locality of the electronic self-energy** which is the case for $d = \infty$.
- A lattice problem is mapped onto an **effective time-dependent impurity problem**.



Continuous-time quantum Monte Carlo impurity solvers

- Continuous-time quantum Monte Carlo methods (CT-QMC) offer an **exact solution** to impurity problems (up to stochastic noise) [2].
- However, any fermionic QMC suffers from **fermionic sign problem** as it samples probability amplitudes which can be negative.
- Moreover, any real-time QMC is severely hindered by **dynamical sign problem**, which leads to an exponential rise of observables' error with a simulated time [3, 4].

Hybridization-expansion CT-QMC (CT-HYB-QMC)

Time-dependent Anderson impurity model

$$H(t) = H_{\mathrm{loc}}(t) + H_{\mathrm{bath}}(t) + H_{\mathrm{hyb}}(t) + H^{\dagger}_{\mathrm{hyb}}(t)$$

$$H_{\mathrm{loc}}(t) = \sum_{\sigma} \mathcal{E}_{d\sigma}(t) d^{\dagger}_{\sigma} d_{\sigma} + U(t)\, d^{\dagger}_{\uparrow} d_{\uparrow} d^{\dagger}_{\downarrow} d_{\downarrow}$$

$$H_{\mathrm{bath}}(t) = \sum_{p\sigma}^{N_{\mathrm{bath}}} \varepsilon_{p\sigma}(t)\, c^{\dagger}_{p\sigma} c_{p\sigma}, \quad H_{\mathrm{hyb}}(t) = \sum_{p\sigma}^{N_{\mathrm{bath}}} V_{p\sigma}(t)\, c^{\dagger}_{p\sigma} d_{\sigma}$$

Dynamical partition function on Keldysh-Kadanoff-Baym contour

$$\mathcal{Z}(\beta, t_{\max}) = \mathrm{Tr}\left(e^{-\beta H(0)} \mathcal{T}_{-} e^{-i\int_{t_{\max}}^{0} dt H(t)} \mathcal{T}_{+} e^{-i\int_{0}^{t_{\max}} dt H(t)}\right) \equiv \mathrm{Tr}\left(\mathcal{T}_{\mathcal{C}}\, e^{-i\int_{\mathcal{C}} ds H(s)}\right)$$

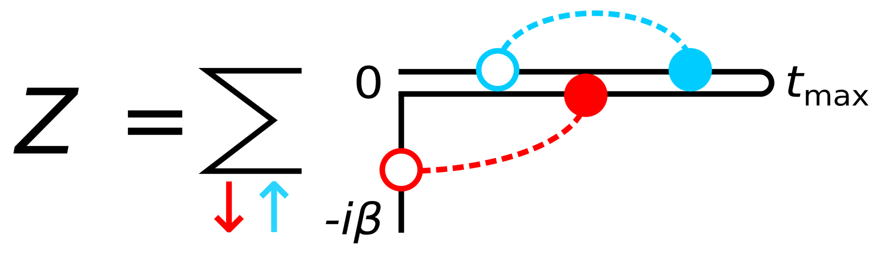
Perturbative expansion in hybridization Hamiltonian

$$\mathcal{Z}(\beta, t_{\max}) = \mathrm{Tr}\left(\mathcal{T}_{\mathcal{C}}\, e^{-i\int_{\mathcal{C}} ds (H_{\mathrm{loc}}+H_{\mathrm{bath}})} e^{-i\int_{\mathcal{C}} ds (H_{\mathrm{hyb}}+H^{\dagger}_{\mathrm{hyb}})}\right)$$

$$= \sum_{k=0}^{\infty} (-1)^k \int_{0_+}^{-i\beta} ds_1 \cdots \int_{s_{k-1}}^{-i\beta} ds_k \int_{0_+}^{-i\beta} ds'_1 \cdots \int_{s'_{k-1}}^{-i\beta} ds'_k$$

$$\mathrm{Tr}\left(\mathcal{T}_{\mathcal{C}}\, e^{-i\int_{\mathcal{C}} ds (H_{\mathrm{loc}}+H_{\mathrm{bath}})} H^{\dagger}_{\mathrm{hyb}}(s_k) \ldots H^{\dagger}_{\mathrm{hyb}}(s_1) H_{\mathrm{hyb}}(s'_k) \ldots H_{\mathrm{hyb}}(s'_1)\right) \equiv \sum_{c} w(c)$$

Pictorial representation of hybridization-expansion configurations



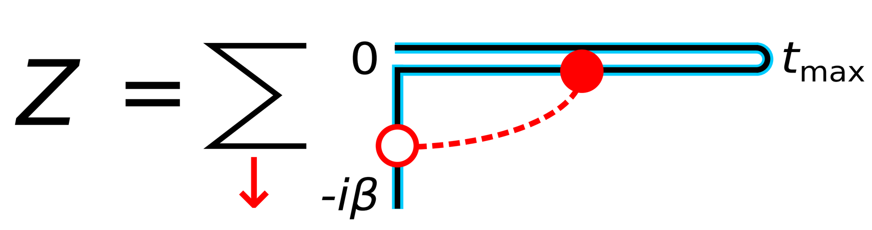
Observables within Monte Carlo: need for positive configuration weights

$$\langle \mathcal{O}(t) \rangle = \frac{1}{\mathcal{Z}} \mathrm{Tr}\left(\mathcal{T}_{\mathcal{C}}\, e^{-i\int_{\mathcal{C}} ds H(s)} \mathcal{O}(t)\right) = \underbrace{\frac{\sum_c \langle \mathcal{O}(t)\rangle_c \,\mathrm{sgn}(w(c))\, |w(c)|}{\sum_c |w(c)|}}_{\text{MC average of } \langle \mathcal{O}(t)\rangle_c \mathrm{sgn}(w(c))} \cdot \underbrace{\frac{\sum_c |w(c)|}{\sum_c \mathrm{sgn}(w(c))\, |w(c)|}}_{\text{inverse average sign}}$$

- Well established method for equilibrium calculations.
- Works for an **infinite bath** and **multiorbital** impurity.
- Computational complexity $\sim \mathcal{O}\left(\langle k \rangle^2_{\text{CT-HYB}} \cdot M^3\right)$ where $\langle k \rangle_{\text{CT-HYB}}$ is the average CT-HYB expansion order and M is the size of the local Hilbert space.
- Average sign $\sim e^{-\alpha t_{\max}}$ where $\alpha > 0$.

Our development: CT-1/2-HYB-QMC

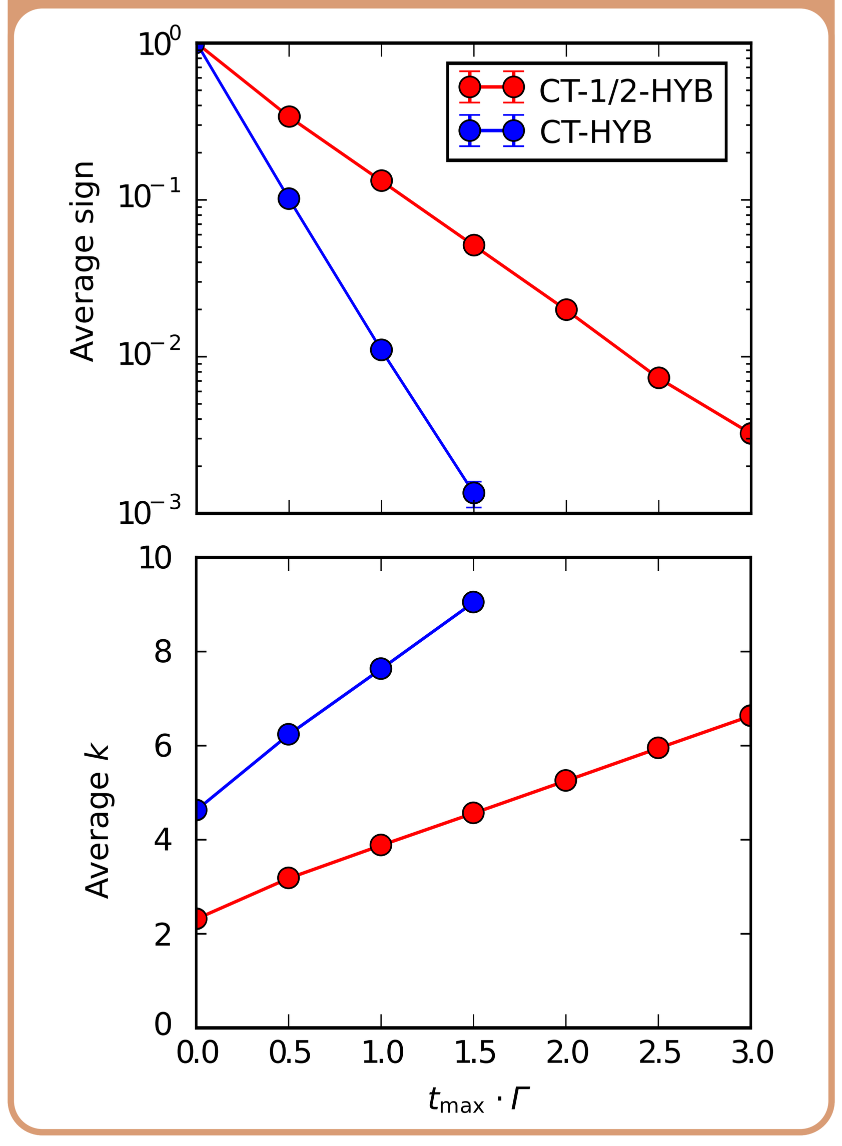
Idea: expand spin-down hybridization only



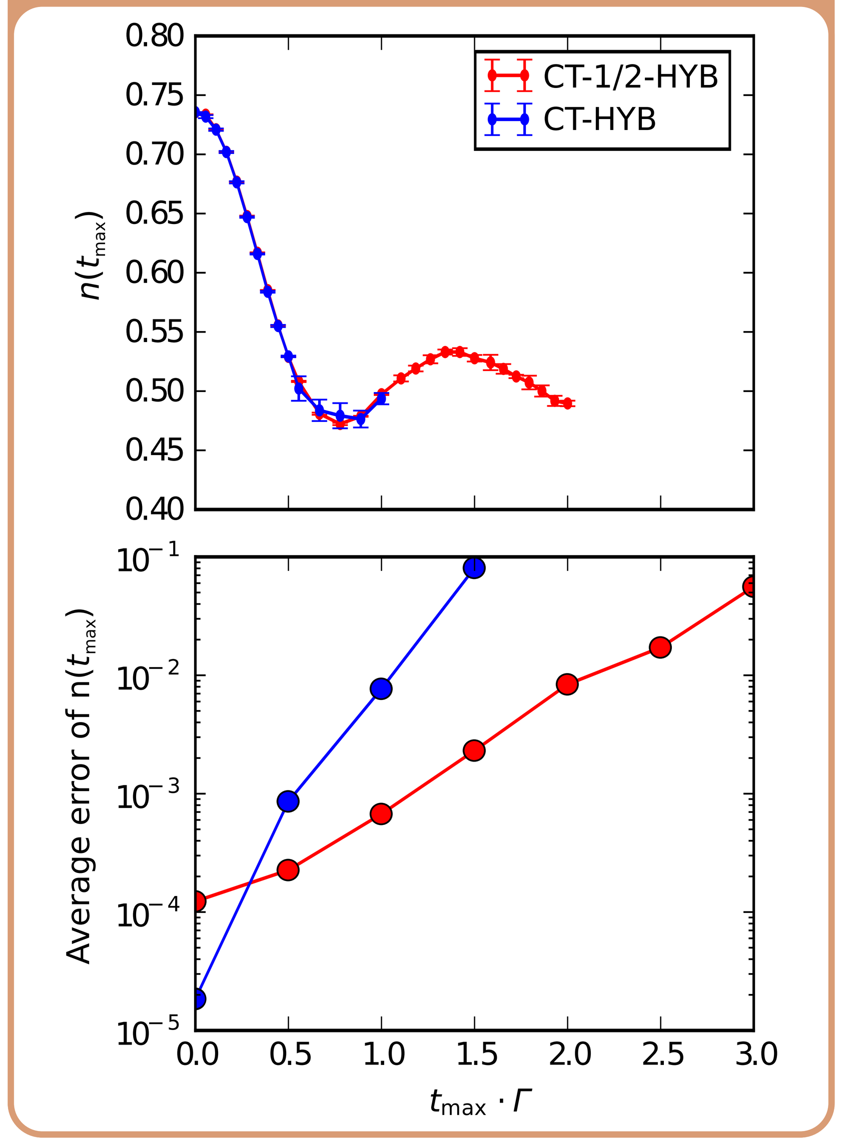
- Spin-up dynamics is solved explicitly since the time-dependent occupation of spin-down impurity level is fixed for a given configuration → **effective single particle problem**.
- Solution of a time-dependent single particle problem possible only for a **finite bath**.
- Method useful only for a **single orbital** impurity.
- Computational complexity $\sim \mathcal{O}\left(\frac{1}{4} \langle k \rangle^2_{\text{CT-HYB}} \cdot (N_{\mathrm{bath}}+1)^3\right) \to \langle k \rangle$ reduced by 2.
- Average sign $\sim e^{-\frac{\alpha}{2} t_{\max}} \to$ **timescales twice as long as in CT-HYB-QMC are accessible**.

Benchmark: impurity level quench

Average sign and expansion order



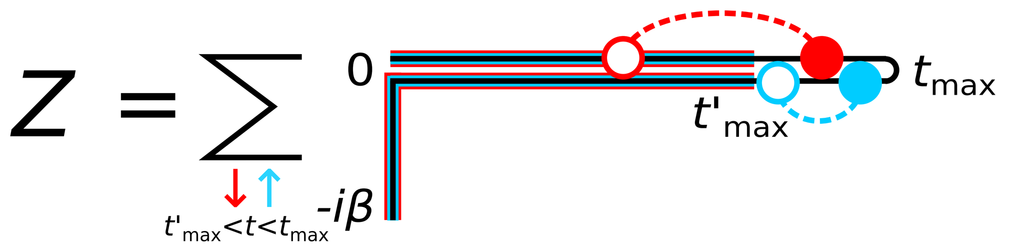
Time-dependent impurity occupancy



$\mathcal{E}_{d\sigma}(0) = -6$, $\mathcal{E}_{d\sigma}(t > 0) = -3$; $U(t) = 6$; $N_{\mathrm{bath}} = 10$; bandwidth $2D = 8$; $\beta = 5$; $\Gamma = \frac{\pi N_{\mathrm{bath}} |V_p|^2}{2D} = 1$

Most promising improvement: Inchworm QMC

Idea: use information gained up to $t'_{\max}$ for a new simulation up to $t_{\max} > t'_{\max}$



Inchworm algorithm [5]

- Start from $t_{\max} = 0$ and perform a series of QMC calculations increasing $t_{\max}$ each time ("inching").
- During each simulation measure propagator $P(t, t')$ which will be used to evaluate QMC configurations in a simulation with an increased $t_{\max}$.
- Propagator $P_{nm}(t, t') = \langle n | \mathcal{T}_{\mathcal{C}}\, e^{-i\int_{t'}^{t} ds H(s)} | m \rangle$ encodes an exact time evolution in impurity's Hilbert space.

- Inchworm QMC belongs to a class of **bold line** QMC solvers, in which bold (i.e. partially resummed) configurations are sampled
- If the "inching" steps are sufficiently small, **the exponential dynamical sign problem does not occur** [6].
- The computational burden scales with the size of $P \sim \mathcal{O}(t^2_{\max})$.
- **Multiorbital** impurities and **infinite** baths possible.
- Efficient implementation very challenging.

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Acknowledgement

The work has been supported by SFB 925 and RNF/DFG 16-42-01057/ LI 1413/9-1.

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