Efficient method for quantum impurity problems out of equilibrium

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Quantum systems out of equilibrium



ETH or MBL?

Quantum computing



Quantum advantage?

Dynamical phases



Impurity models



Kondo physics, DMFT, NMR

Real time evolution of local observables



$$\langle O(t) \rangle_{\rho(t=0)=\rho_0}$$
 or $\langle O(0)O(t) \rangle_{\rho_0}$

- Measurable quantity
- Transport properties: (Sub)diffusion vs ballistic
- Localization, Edge modes

Wavefunction based approaches

- Represent the density matrix at different time $\rho(t)$
- Obtain observables by computing $Tr[\rho(t)O]$

Problem:

Complexity grows exponentially with time!



Influence functional approach¹

Idea:

Describe the local subsystem as a quantum system coupled to a bath.



¹Feynman and Vernon Jr 1963.

The numerical power of the Influence matrix approach is limited by **temporal entanglement** instead of spatial entanglement



- Represents the "Memory" of the quantum bath
- Low temporal entanglement \Rightarrow efficient MPS representation
- Examples for low temporal entanglement:
 - Very chaotic systems $U \approx e^{i\frac{\pi}{4}Z_iZ_{i+1}+hZ_i}e^{i\frac{\pi}{4}X_i1}$
 - Close to integrability $U \approx e^{iJ_X X_i X_{i+1} + iJ_y Y_i Y_{i+1} 2}$
 - Dissipative system³
 - Many body localized systems Exact disorder averaging!⁴

¹Lerose, Sonner, and Abanin 2021a.

²Lerose, Sonner, and Abanin 2021b; Giudice et al. 2021; Thoenniss, Lerose, and Abanin 2022.

³Sonner, Lerose, and Abanin 2021; Mi et al. 2022.

⁴Sonner, Lerose, and Abanin 2022.

Obtaining the Influence matrix





¹Lerose, Sonner, and Abanin 2022; Frías-Pérez and Bañuls 2022; Banuls et al. 2009

Model

Single Impurity Anderson model

$$H = \sum_{k,\sigma} \left(\epsilon_{k,\sigma} c_{k,\sigma}^{\dagger} c_{k,\sigma} + V_{k,\sigma} d_{\sigma}^{\dagger} c_{k,\sigma} + h.c. \right) + U(n_{\uparrow} - \frac{1}{2})(n_{\downarrow} - \frac{1}{2})$$

- Impurity with on-site interaction coupled to free fermions
- Bath defined by spectral density $f(\omega) = 2\pi \sum_{k} |V_k|^2 \delta(\epsilon_k \omega)$
- Kondo effect: Effective impurity spin forms singlet with the fermions in the bath
- Quantum embedding approaches



Entanglement barrier²¹



Reflection at the boundary cause high temporal entanglement in finite system IM!

But: thermodynamic IM has low temporal entanglement

¹Calabrese and Cardy 2005.

²Lerose, Sonner, and Abanin 2022.

Algorithm¹

Spectral density



¹Thoenniss, Lerose, and Abanin 2022; Thoenniss et al. 2023.

- Initialize impurity in the $|\uparrow\rangle$ state
- Slow spin relaxation in the Kondo regime
- $\cdot\,$ Competitive with state of the art QMC 1



¹Cohen et al. 2015

²Thoenniss et al. 2023.

Transport²

- Left and right reservoir at different chemical potential
- Small bond dimension $\chi = 32,64$ (!)
- Steady state reachable
- Comparable with QMC ¹





¹Bertrand et al. 2019

²Thoenniss et al. 2023.

Imaginary time - RAMPS¹

Imaginary time Green's function

$$G(\tau) = \operatorname{Tr}(e^{-(\beta-\tau)H}c^{\dagger}e^{-\tau H}c)$$



Benedikt Kloss, Matthew T. Fishman, E. M. Stoudenmire, Olivier Parcollet, Antoine Georges

- Central step for Dynamic mean field theory (DMFT)
- Requires relatively high bond dimension
- Multi-orbital possible, no sign problem!



¹Kloss et al. 2023.

Compute local observables by finding a compressed representation of the large quantum system as a bath (IM)

- Complexity of the IM can be low even in traditionally difficult regimes
- For free fermions there is an efficient algorithm to compute the IM directly
- Natural for impurity problems, DMFT!
- For one dimensional interactive models, we can be efficiently obtain the IM through sequencial contraction¹

¹Lerose, Sonner, and Abanin 2022; Frías-Pérez and Bañuls 2022.