Simulation of long-range quantum spin systems using tree tensor networks

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Problem of interest

Consider the one-dimensional quantum systems consisting of D distinguishable d-level particles undergoing Markovian open quantum dynamics. The density matrix evolves through the differential equation

$$\dot{\rho}(t) = \mathcal{L}[\rho(t)] := -i[H, \rho(t)] + \mathcal{D}[\rho(t)] \,, \tag{1}$$

where H is a long-range Hamilton operator and $\mathcal{D}$ a dissipator of the form

$$H = \Omega \sum_{k=1}^{D} \sigma_x^{(k)} + \Delta \sum_{k=1}^{D} n^{(k)} + \frac{V}{2c_\alpha} \sum_{k \neq h=1}^{D} \frac{n^{(k)} n^{(h)}}{|k-h|^\alpha} \,, \tag{2}$$

$$\mathcal{D}[\rho] = \sum_\mu \left(J_\mu \rho J_\mu^\dagger - \frac{1}{2} \left\{ \rho, J_\mu^\dagger J_\mu \right\} \right) \,, \tag{3}$$

with jump operators J_μ encoding how the environment affects the dynamics.

Tree tensor networks

Let $\bar{\tau} \in \mathcal{T}$ be a fixed tree with d leaves. To each leaf we associate a basis matrix $\mathbf{U}_l$ and to each subtree $\tau \leq \bar{\tau}$ a connection tensor C_τ. We define a tensor $X_{\bar{\tau}}$ with a tree tensor network (TTN) recursively as follows:

- ❶ For each leaf $\tau = l \in \mathcal{L}$, we set
$$X_l := \mathbf{U}_l^\top \in \mathbb{C}^{r_l \times n_l} \,.$$
- ❷ For each subtree $\tau = (\tau_1, \dots, \tau_m)$ (for some $m \geq 2$) of $\bar{\tau}$, we set $n_\tau = \prod_{i=1}^m n_{\tau_i}$ and $\mathbf{I}_\tau$ the identity matrix of dimension r_τ, and
$$X_\tau := C_\tau \times_0 \mathbf{I}_\tau \mathsf{X}_{i=1}^m \mathbf{U}_{\tau_i} \in \mathbb{C}^{r_\tau \times n_{\tau_1} \times \dots \times n_{\tau_m}},$$
$$\mathbf{U}_\tau := \mathbf{Mat}_0(X_\tau)^\top \in \mathbb{C}^{n_\tau \times r_\tau} \,.$$

  The subscript 0 in $\times_0$ and $\mathbf{Mat}_0(X_\tau)$ refers to the mode 0 of dimension r_τ in $\mathbb{C}^{r_\tau \times r_{\tau_1} \times \dots \times r_{\tau_m}}$.

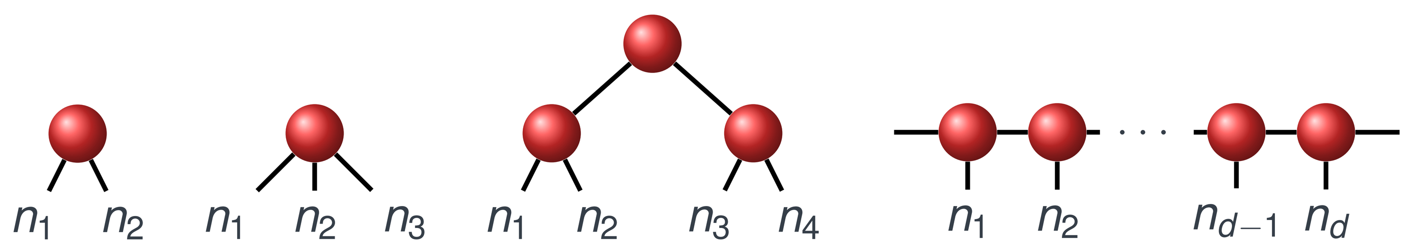

Figure: Different examples for TTN's (from left to right): matrix, Tucker tensor, binary TTN, matrix product state.

The red balls encode a connecting tensor of matching order, while the nodes n_l encode a basis matrix/leaf $\mathbf{U}_l$.

An adaptive integrator for TTN's

We present a integrator for TTNs which is adaptive in the bond dimension and extends the work of [2]. Suppose we have a TTN

$$X_\tau^0 = C_\tau^0 \times_0 \mathbf{I}_\tau \mathsf{X}_{i=1}^m \mathbf{U}_{\tau_i}^0$$

at time t_0. The idea is to first update all the basis matrices $\mathbf{U}_{\tau_i}^0$ in parallel (subflow $\Phi_\tau^{(i)}$) and then update the connecting tensor C_τ^0 (subflow Ψ_τ), i.e.

$$\widehat{X}_\tau^1 = \Psi_\tau \circ (\Phi_\tau^{(1)}, \dots, \Phi_\tau^{(m)})(X_\tau^0).$$

All the ranks of $\widehat{X}_\tau^1$ are (usually) doubled. To get the approximation $X_{\bar{\tau}}^1$ at time t_1 we apply a truncation θ with a given tolerance ϑ, i.e. $X_{\bar{\tau}}^1 = \theta(\widehat{X}_{\bar{\tau}}^1)$. The subflow $\Phi_\tau^{(i)}$ applied to a TTN solves a small matrix ODE if the i-th subtree is a leaf, otherwise it is applied recursively.

begin
- $Y_{\tau_i}^0 = X_\tau^0 \times_0 S_{\tau_i}^{0,\top}$, with $\mathbf{Mat}_i(C_\tau^0)^\top = Q_{\tau_i}^0 S_{\tau_i}^{0,\top}$
- **if** $\tau_i = l$ *is a leaf* **then**
  - solve $\dot{Y}_l = F_l(t, Y_l(t))$, $Y_l(t_0) = Y_l^0$
  - set $\widehat{\mathbf{U}}_l$ as an ONB of the range of $(Y_l(t_1)^\top, \mathbf{U}_l^0) \in \mathbb{C}^{n_l \times \hat{r}_l}$, $\hat{r}_l \leq 2r_l^0$
  - set $\widehat{M}_l = \widehat{\mathbf{U}}_l^* \mathbf{U}_l^0$
- **else**
  - $[\widehat{Y}_{\tau_i}^1, \widehat{C}_{\tau_i}^0] =$ rank-adapt-TTN-integrator $(\tau_i, Y_{\tau_i}^0, F_{\tau_i}, t_0, t_1)$
  - set $\widehat{Q}_{\tau_i}$ as an ONB of the range of $(\mathbf{Mat}_0(\widehat{C}_{\tau_i}^1)^\top, \mathbf{Mat}_0(\widehat{C}_{\tau_i}^0)^\top)$
  - set $\widehat{\mathbf{U}}_{\tau_i} = \mathbf{Mat}_0(\widehat{X}_{\tau_i}^1)^\top$, where $\widehat{X}_{\tau_i}^1$ is obtained from $\widehat{Y}_{\tau_i}^1$ by replacing the connecting tensor with $\widehat{C}_{\tau_i} = Ten_0(\widehat{Q}_{\tau_i}^\top)$
  - set $\widehat{M}_{\tau_i} = \widehat{\mathbf{U}}_{\tau_i}^* \mathbf{U}_{\tau_i}^0$

The subflow Ψ_τ solves a small tensor ODE, which can be interpreted as a Galerkin method on the updated subspace.

begin
- set $\widehat{C}_\tau^0 = C_\tau^0 \mathsf{X}_{i=1}^m \widehat{M}_{\tau_i}$
- solve the tensor ODE
$$\dot{\widehat{C}}_\tau(t) = F_\tau(t, \widehat{C}_\tau(t) \mathsf{X}_{i=1}^m \widehat{\mathbf{U}}_{\tau_i}) \mathsf{X}_{i=1}^m \widehat{\mathbf{U}}_{\tau_i}^*, \quad \widehat{C}_\tau(t_0) = \widehat{C}_\tau^0$$
- set $\widehat{C}_\tau^1 = \widehat{C}_\tau(t_1)$

Mathematical properties

- ❶ Let $A(t)$ be the exact and $X_{\bar{\tau}}^n$ the numerical solution at time $t_0 + nh$ and ϵ be the projection error onto the manifold of TTNs. Then the following error bound holds
$$||A(t_n) - X_{\bar{\tau}}^n|| = \mathcal{O}(h + \epsilon + \vartheta).$$
- ❷ For Schrödinger-type systems the integrator is energy and norm preserving up to the truncation error ϑ.

Results

We apply the integrator to the open quantum system (1) and look at the stationary behavior of the density $\langle n \rangle$ as a function of Ω/γ. In the following figure we see convergence to the mean-field result for $\alpha = 0$ and a persistence of the phase transition for all $\alpha < 1$.

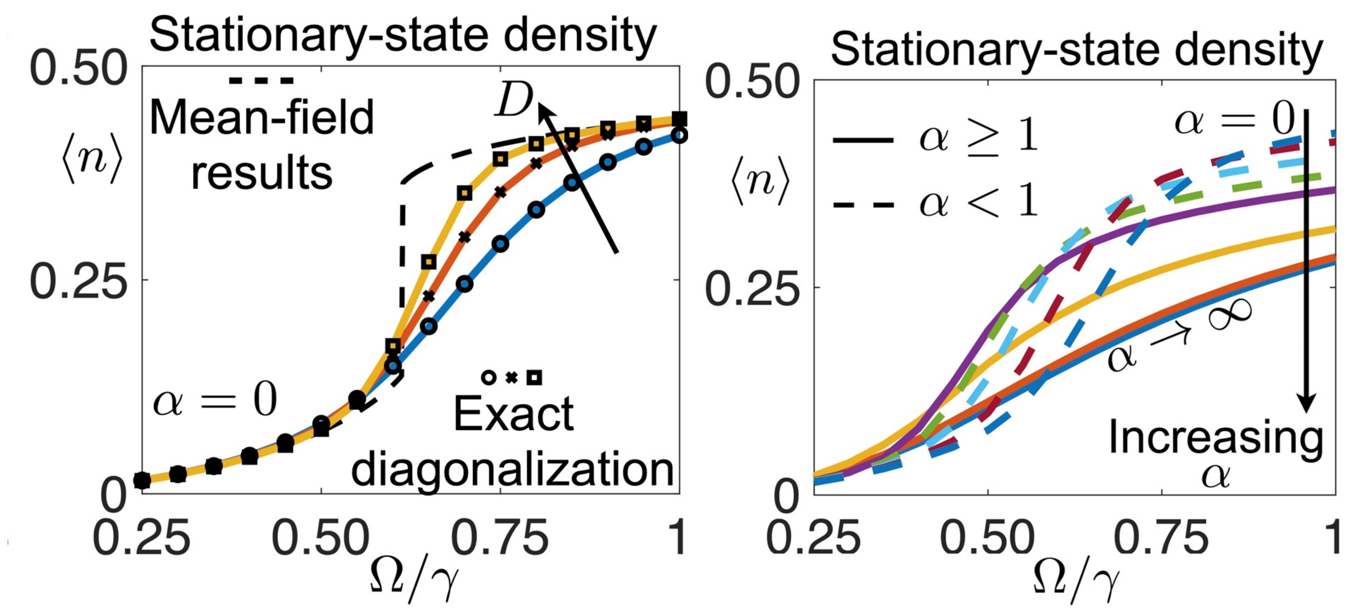

Figure: Left: for $\alpha = 0$ the integrator converges to the mean field limit. Right: the phase transition in α persists for all $\alpha < 1$.

Further we compare how the chosen tree structure affects the bond dimensions of the state over time and the TTN representation of the operator (1), i.e. the TTNO. Note that binary trees and MPS have the same number of nodes. All simulation were done with $\alpha = \gamma = 1$, $\Delta = -2$, $\Omega = 0.4$ and $V = 2$.

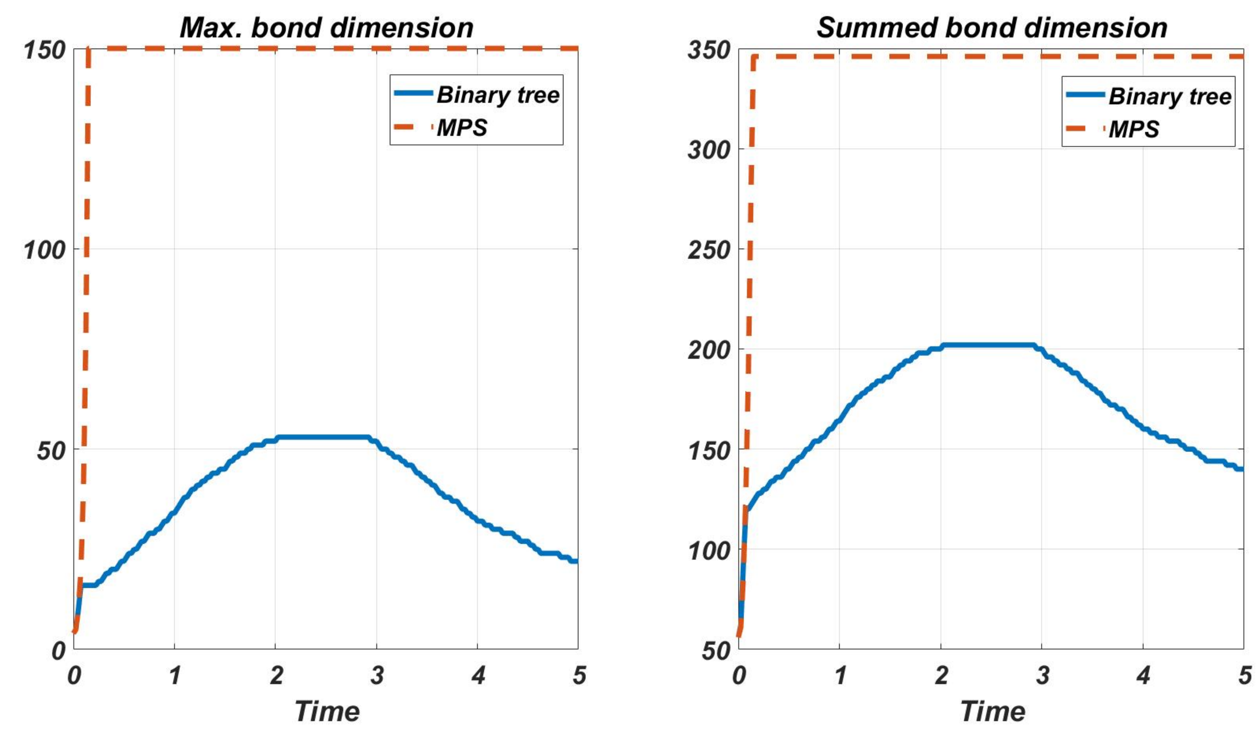

Figure: Simulation for $d = 8$. Left: Max. bond dimension of the state over time. Right: Summed bond dimension of the state over time.

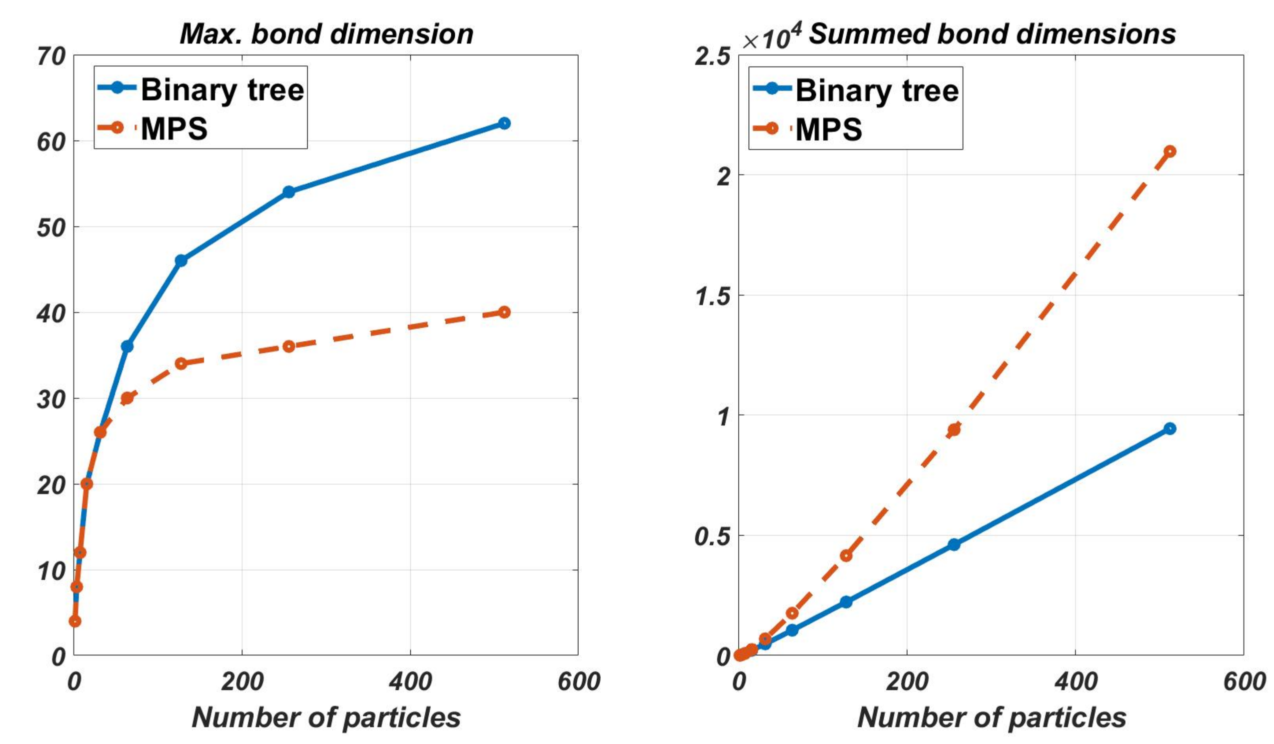

Figure: Left: Max. bond dimension needed for a TTNO representation of the operator. Right: Summed bond dimension needed for a TTNO representation of the operator.

References

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