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Hierarchy of Pure States and Tree Tensor Networks

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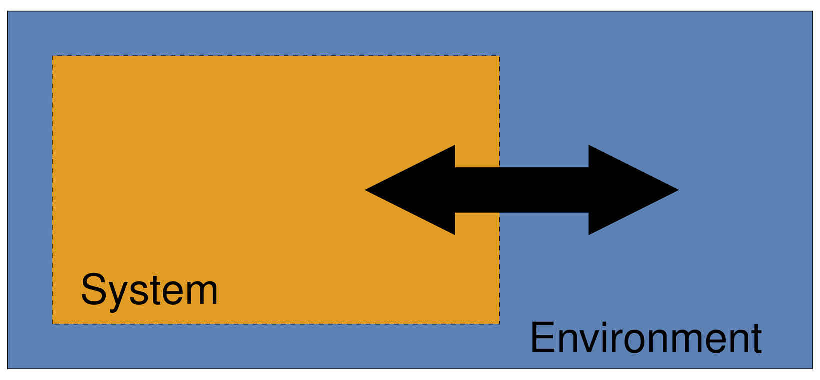
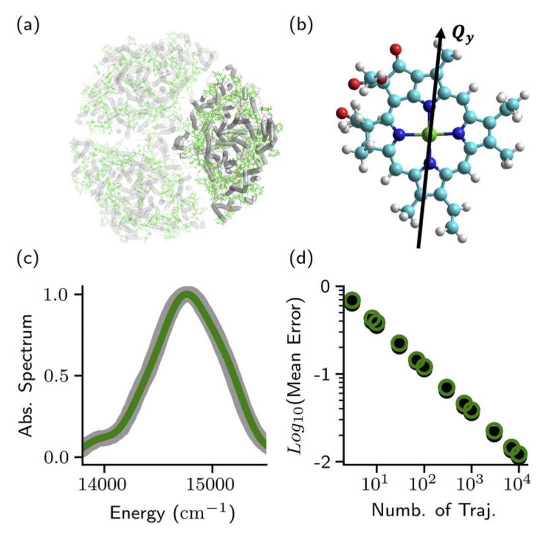
Motivation

- $H_{\text{tot}} = H_{\text{System}} + H_{\text{Environment}} + H_{\text{Interaction}}$
- Strong coupling & finite environment
- Memory effects & environment back reaction
- Breakdown of Markovian assumption

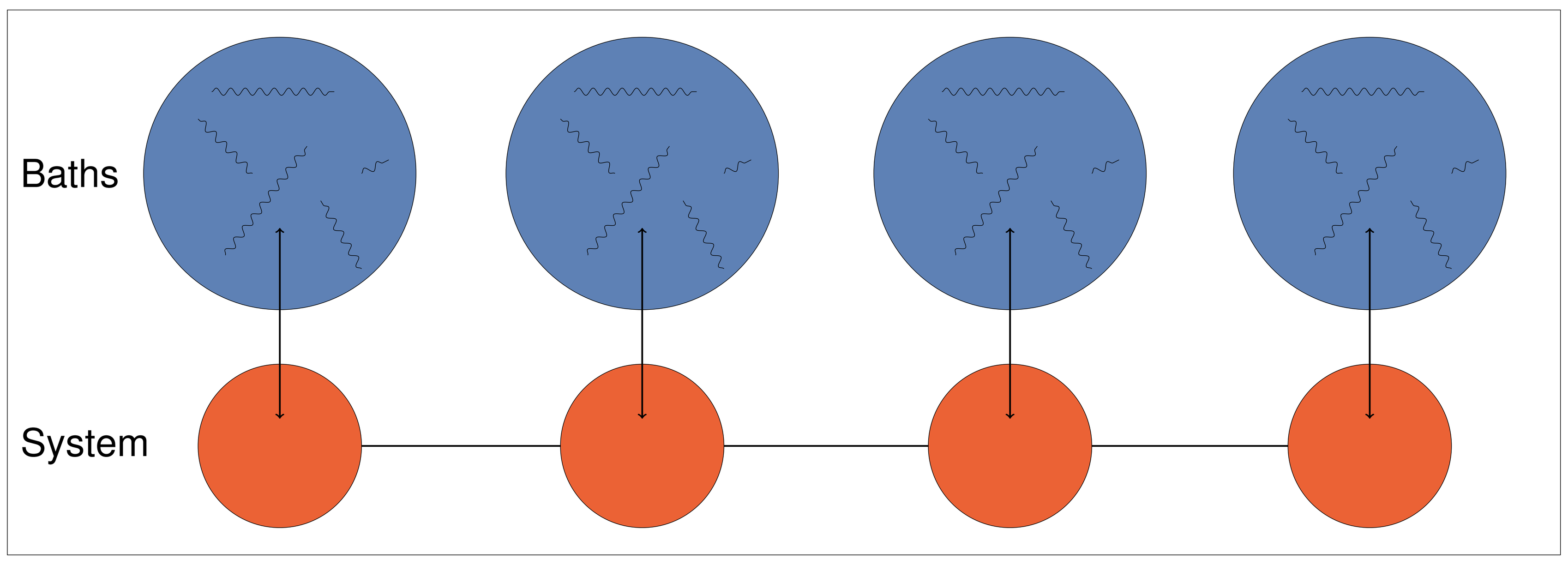


- Few analytical solutions
- Numerical approach: **H**ierarchy **o**f **p**ure **s**tates (HOPS) [1]
- Hierarchy ≙ save many quantum states
- Matrix product state reduce memory requirement [2]
- Increased accuracy, but limited principal system dimension
- Tree tensor networks allow many-body principal systems
- Examples: Photosynthesis & errors in quantum hardware



[3]

Hierarchy of Pure States



$$\rho(t) = \mathbb{E}\left[|\psi_t^{(0)}(Z_t)\rangle\langle\psi_t^{(0)}(Z_t)|\right],$$

where $Z_t = (z_n)_{n=1}^L$ such that

$$\mathbb{E}\left[z_n(t) z_n^*(s)\right] = \alpha_n(t-s) \quad \text{and} \quad \mathbb{E}\left[z_n(t) z_n(s)\right] = \mathbb{E}\left[z_n(t)\right] = 0$$

with the bath correlation functions $\alpha_n(\tau) = \sum_{j=1} g_{n,j} e^{-w_{n,j}\tau}$

⇒ Hierarchy of pure states equations of motion

$$\partial_t |\psi_t^{(K)}\rangle = \left(-iH_S + \sum_n z_n^*(t) L_n + \sum_{n,j} K_{n,j} w_{n,j}\right)|\psi_t^{(K)}\rangle + \sum_{n,j}\left(\sqrt{K_{n,j}}\frac{g_{n,j}}{\sqrt{|g_{n,j}|}} L_n |\psi_t^{(K+E^{(n,j)})}\rangle - \sqrt{(K_{n,j}+1)|g_{n,j}|}\, L_N^\dagger |\psi_t^{(K-E^{(n,j)})}\rangle\right)$$

Introduce $|\Psi_t\rangle = \sum_K C_K(t) |\psi_t^{(K)}\rangle |K\rangle$

$$\Rightarrow H_{\text{eff}} = H_S + i\sum_n z_n^*(t) L_n + i\sum_{n,j} \mathcal{N}_{n,j} w_{n,j} + i\sum_{n,j}\left(\frac{|g_{n,j}|}{\sqrt{g_{n,j}}} L_n \otimes b_{n,j}^\dagger - \sqrt{|g_{n,j}|} L_n^\dagger b_{n,j}\right)$$

with $b^\dagger$, b, and $\mathcal{N}$

- Bath Correlation Function

$$\alpha(\tau) = \frac{1}{\pi}\int_0^\infty d\omega\, J(\omega)\left[\coth\left(\frac{\omega}{2T}\right)\cos(\omega\tau) - i\sin(\omega\tau)\right]$$

- Non-Markovian Quantum State Diffusion Equation

$$\partial_t |\psi_t\rangle = -iH_S|\psi_t\rangle + \sum_n\left(L_n z_n^*(t)|\psi_t\rangle - L_n^\dagger\int_0^t ds\, \alpha(t-s)\frac{\delta|\psi_t\rangle}{\delta z_n^*(t)}\right)$$

- Box-Muller-Wiener algorithm: Random numbers $\chi_1, \chi_2 \in [0,1]$ into z_t, the complex stochastic variable
- Debye spectral density $S(\omega) = \eta\frac{\omega\gamma}{\omega^2+\gamma^2}$
- Evolve via RK4, TEBD, TDVP

References:

1. D. Suess, A. Eisfeld, and W. T. Strunz, *Hierarchy of Stochastic Pure States for Open Quantum System Dynamics*, Phys. Rev. Lett., vol. 113, no. 15, p. 150403, 2014.
2. X. Gao, J. Ren, A. Eisfeld, and Z. Shuai, *Non-Markovian stochastic Schrödinger equation: Matrix-product-state approach to the hierarchy of pure states*, Phys. Rev. A, vol. 105, no. 3, p. L030202, 2022.
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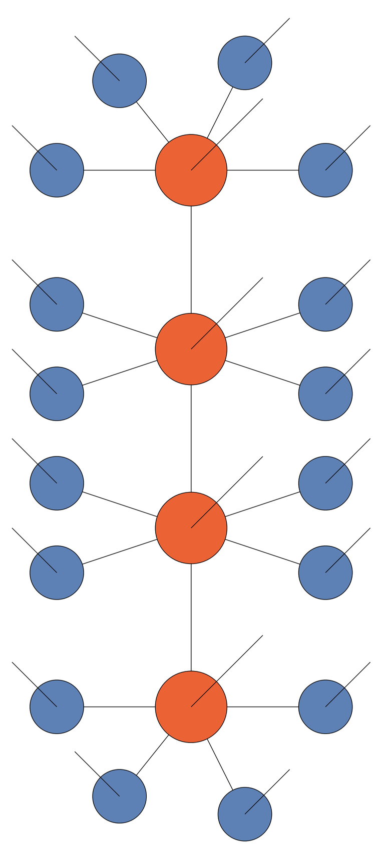
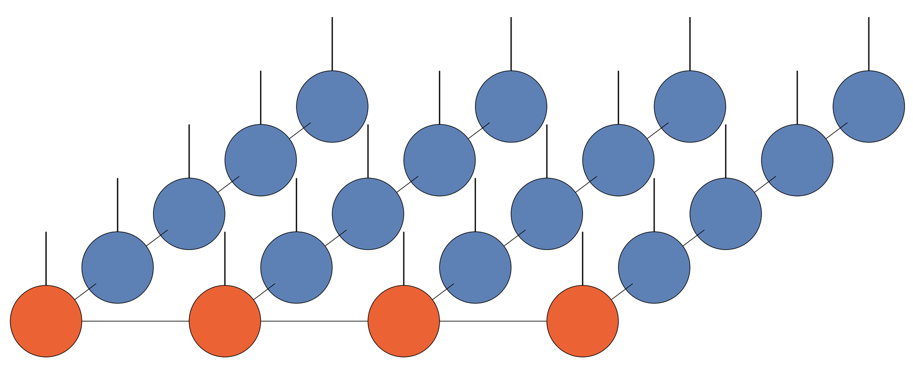
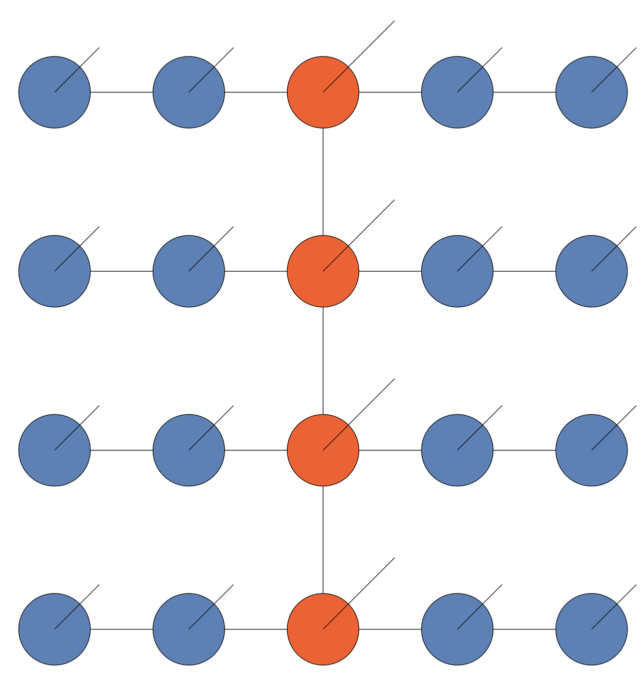
Tree Tensor Networks



Star Tree State



Fork Tensor Product State (FTPS)



Symmetric Tree State

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