SAND2014-16740PE

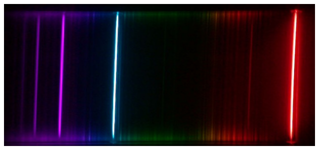
Maximum entropy quantum simulation

Jonathan E. Moussa
@ Sandia National Labs

This work was supported by the Laboratory Directed Research and Development program at Sandia National Laboratories. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Motivation

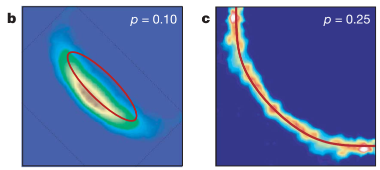
Few-body physics:



H

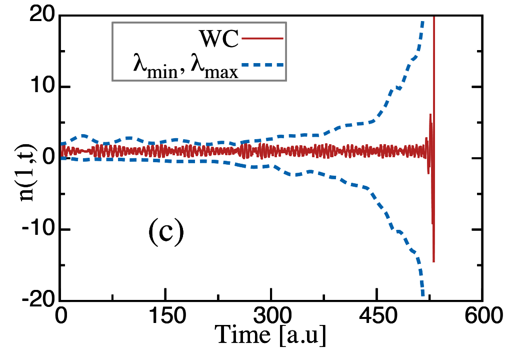
$$\frac{d}{dt}\Psi = \hat{H}\Psi$$

Many-body physics:



$XCuO_2$

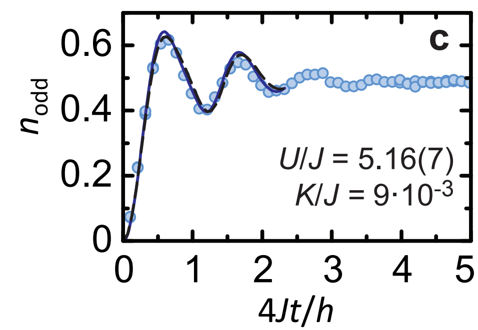
Bias & instability in theories:



4-site fermion Hubbard model

[Akbari, Hashemi, *et al.*, PRB (2012)]

Analog quantum simulators:



1-D boson Hubbard model

[Trotzky *et al.*, Nat. Phys. (2012)]

What are the fundamental limits of approximate classical algorithms & noisy analog quantum simulators?

Q vs. **C**

Future king of quantum simulation = error-corrected quantum computer

Uncertainty-based error model

$$\underbrace{\frac{d}{dt}\rho(t) = [\rho(t), iH]}_{\text{the intended time-evolution}} + \underbrace{R(t, c_j(t))}_{\text{sample variations (noise \& errors)}}$$

the intended time-evolution

sample variations (noise & errors)

$$\underbrace{\frac{d}{dt}\langle X_j\rangle(t) = \langle [iH, X_j]\rangle(t)}_{\text{fine-tuned equations of motion}} = \underbrace{\sum_k h_{j,k}\langle X_k\rangle(t)}_{\text{expectation values}}$$

fine-tuned equations of motion (by adjusting $c_j(t)$, but $R \neq 0$)

expectation values used to verify EOM

Pessimistic assumption: increasing entropy (2nd law) and fast thermalization ($R >> H$)

Maximum entropy time evolution

$$\{X_j | 1 \leq j \leq M\} = \mathcal{E} \cup \mathcal{R} \qquad (\mathcal{E} \cap \mathcal{R} = \{\varnothing\})$$

"important" expectation values

evolved

reconstructed

Time evolve what we can …

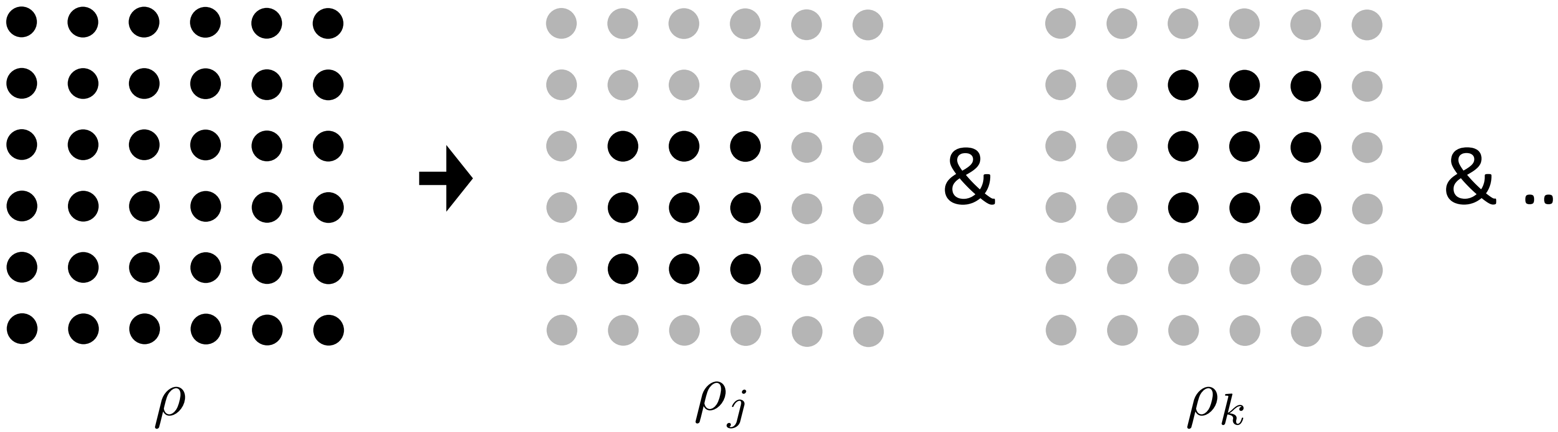
$$\frac{d}{dt}\langle X_j\rangle(t) = \langle [iH, X_j]\rangle(t) = \sum_k h_{j,k}\langle X_k\rangle(t) \qquad X_j \in \mathcal{E}$$

Reconstruct at every moment what we cannot …

$$\langle X_j\rangle(t) \in \underset{\{\langle X_j\rangle | X_j \in \mathcal{R}\}}{\arg\max}\ S(\{\langle X_j\rangle(t) | 1 \leq j \leq M\}) \qquad X_j \in \mathcal{R}$$

Entropy must be approximated …

Cluster decomposition



+ consistency between marginal states

$$S(\rho) \approx \sum_j f_j S(\rho_j)$$

How to choose f_j?

	transferrable	concave	upper bound
Möbius inversion formula	✓	✗	✗
Markov entropy decomposition [Poulin & Hastings, PRL (2011)]	✗	✓	✓

Can we do better?

Test problem

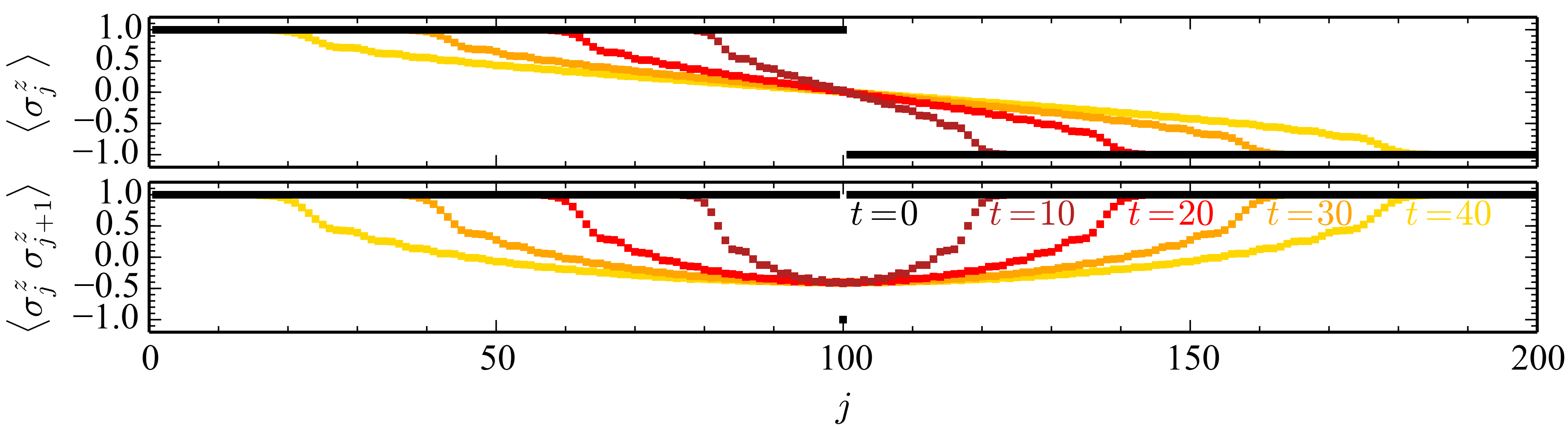
1D Heisenberg *XX* model w/ critical transverse field:

$$H = -\frac{1}{2}\sum_{j=1}^{2N-1} J_j \left(\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y\right) - \sum_{j=1}^{2N} h_j \sigma_j^z \quad (h_j = J_j = 1)$$

Time evolution from an interface between low- & high-energy states:

$$|\Psi\rangle(t=0) = |0\rangle^{\otimes N} \otimes |1\rangle^{\otimes N}$$

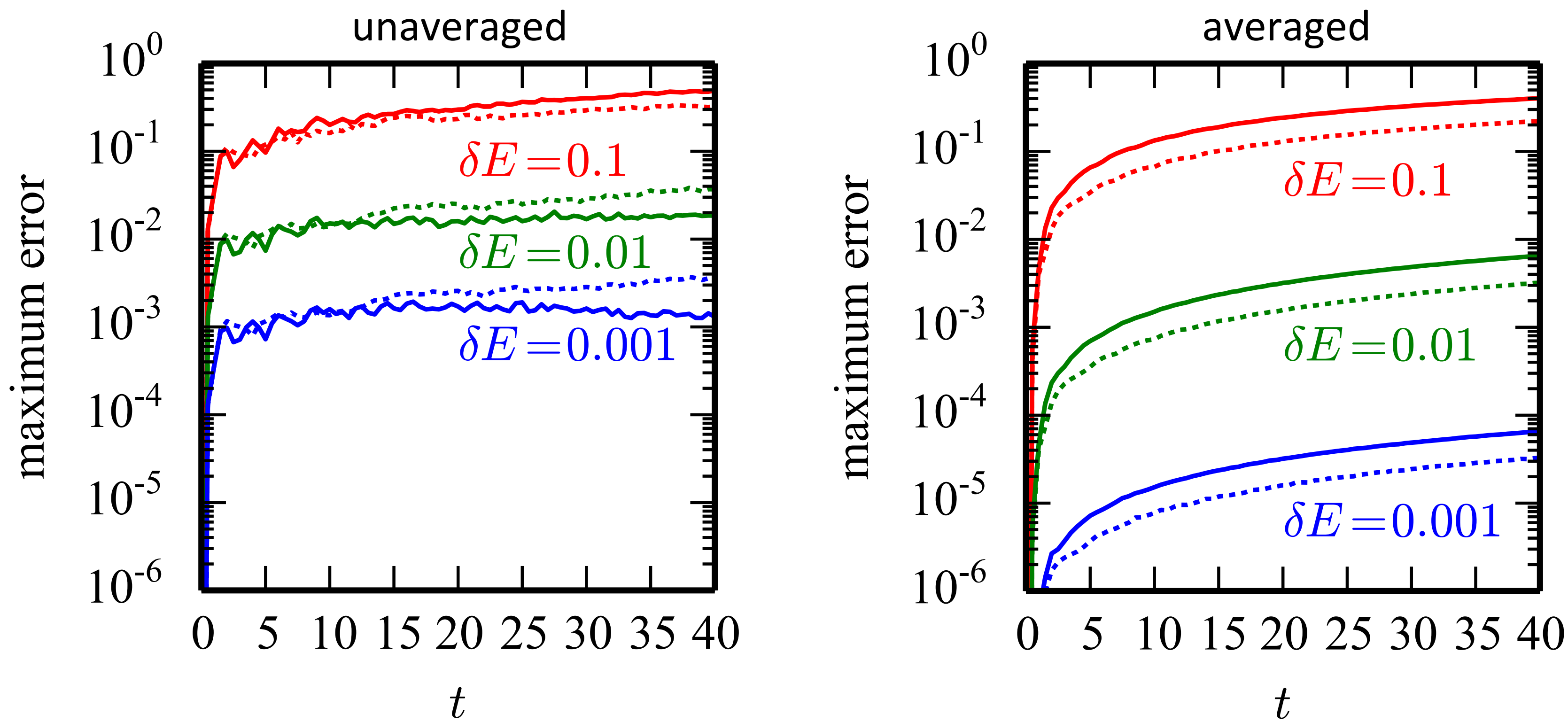
Exact solution w/ Jordan-Wigner transformation:



Noise-based error model

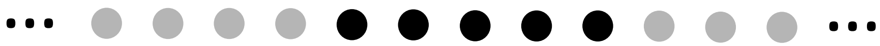
$$H + \delta H \Leftrightarrow (h_j + \delta h_j, J_j + \delta J_j) \qquad \text{i.i.d. } \delta h_j, \delta J_j \in [-\delta E, \delta E]$$

Average over noise realizations to reduce errors:



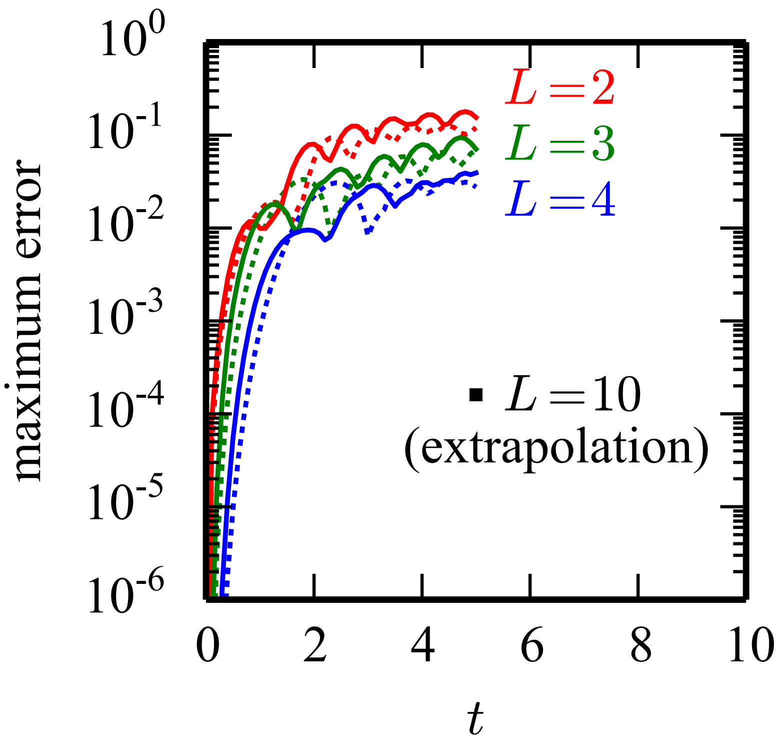
$$\varepsilon \propto |\delta H| t \qquad\qquad \varepsilon \propto |\delta H|^2 t$$

Preliminary numerical results

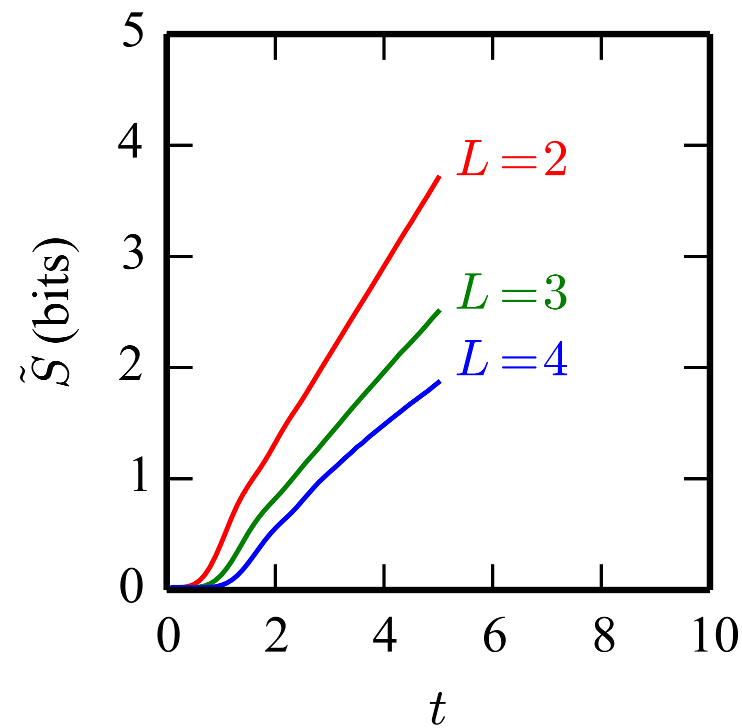


$\rho_{j,j+L}$ marginals on intervals

$$S(\rho) \leq \sum_{j=1}^{2N-L} S(\rho_{j,j+L}) - \sum_{j=2}^{2N-L} S(\rho_{j,j+L-1})$$



$\varepsilon \propto \exp(-cL)t$



linear growth of entropy?

Future work

Short term:

- Preconditioning of entropy maximization
- Compare w/ cumulant reconstruction & tMPS
- Applications (quantum algorithms & D-Wave device)

Long term:

- Examine choice of expectation values
- Develop new entropy approximants:

Efficient optimization of Shannon-type inequalities?

Thermodynamic integration / energy representation?

$$\hat{\rho} = \int w(E)\delta(E - \hat{H})dE$$

- Develop compatible variational states: