Preparing Thermal States of Quantum Systems by Dimension Reduction

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Joint work with Sergio Boixo

Outline

Motivation

- Very few quantum systems have analytical solutions.
- Have to resort to numerical simulations in many cases
  - Brute force calculations take $\mathcal{O}(e^N)$ time and memory for N-particle systems.
  - Classical algorithms to approximate solutions (DMRG, PEPS, BP, etc) only work for specific cases.
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Previous work

- Feynman suggested quantum machines to simulate quantum systems.
- Quantum computers are very good at simulating unitary evolutions (Lloyd).
- Initial state preparation is still a difficult problem.
- Several Proposals:
  - Evolving with a bath (Terhal and DiVincenzo)
  - Quantum Metropolis Sampling (Temme *et al.*, Yung and Aspuru-Guzik)
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Main Results

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1D systems	$\mathcal{O}(e^{\alpha N})$	$\mathcal{O}(N^{\beta\|\|h\|\|})$
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Thermalization using QPE

- Given $H = \sum_a E_a |a\rangle\langle a|$, we want $\rho \propto \sum_a e^{-\beta E_a} |a\rangle\langle a|$.

- Now, instead of $|a\rangle$, we input $I = \sum_a |a\rangle\langle a|$

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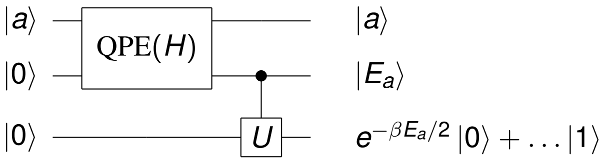

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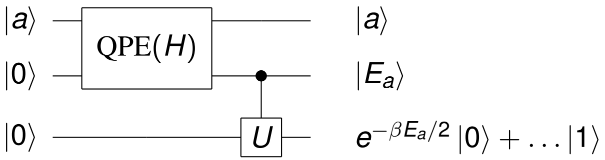

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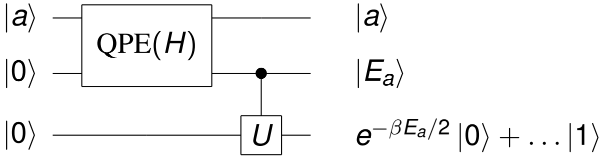

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- Projecting everything in one step costs $\mathcal{O}(e^{\beta||H||}) \sim \mathcal{O}(e^N)$.
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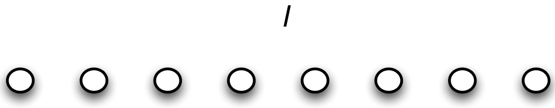

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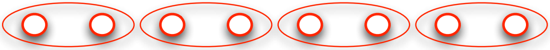

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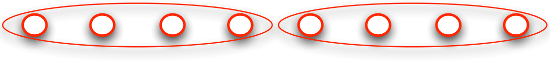

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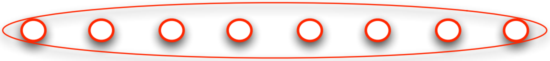

$p \sim e^{-\beta||h||}$, Total cost: $\mathcal{O}(N^{\beta||h||})$

Perturbative Hamiltonian Update

- We need the map $e^{-\beta H} \to e^{-\beta(H+h)}$.
- Defining $\rho^{(\epsilon)} \propto e^{-\beta(H+\epsilon h)}$, we want the sequence:

$$\rho^{(0)} \to \rho^{(\epsilon)} \to \rho^{(2\epsilon)} \to \cdots \to \rho^{(1)}$$

- Each step is correct up to an error of $\mathcal{O}(\epsilon^2)$, resulting an overall error of $\mathcal{O}(\epsilon)$.

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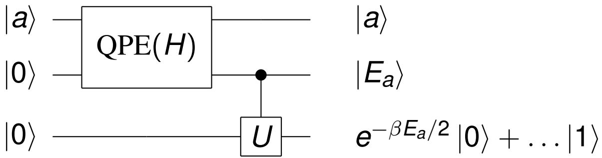
- Update the eigenvalues using QPE:



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- This procedure updates all the eigenvalues of ρ correctly to the leading order in ϵ.

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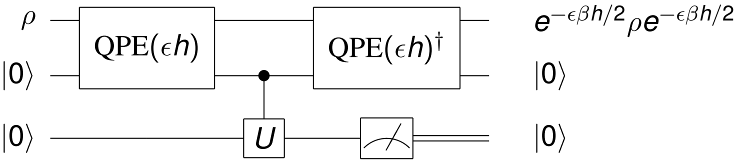

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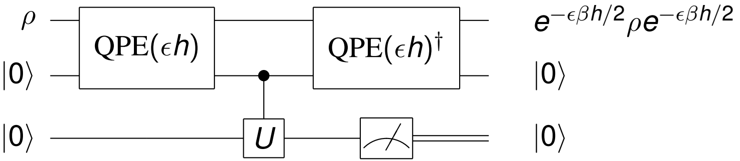

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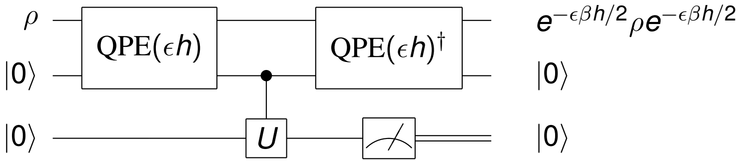

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- We dephase in the eigenbasis of the new Hamiltonian, $H + \epsilon h$.
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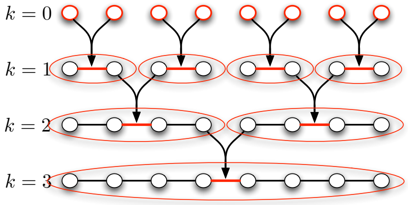
- To thermalize a chain of $N = 2^k$ qubits, we use the recursive merging procedure from earlier:



$$\tau(k) = \alpha\, 2\, \tau(k-1) + m$$

- For an error $\bar{\epsilon}$, running time for 1D: $\tau \sim \beta N^{\beta \|h\|} / \bar{\epsilon}^2$
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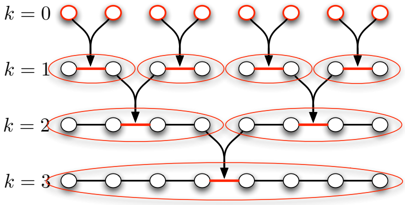

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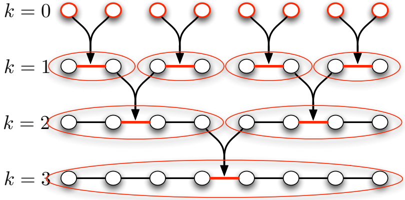

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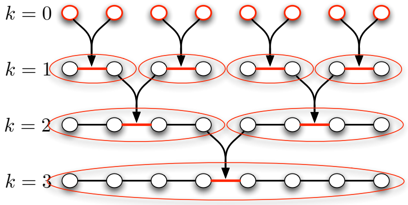

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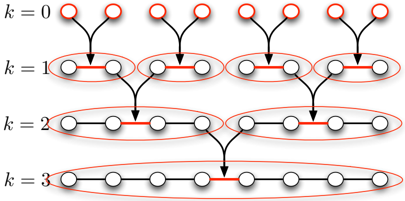
- Made possible by recursively merging smaller regions using QPE and dephasing



arXiv:1008.4162; Phys. Rev. Lett. 105, 170405 (2010)