Dissipation and Thermal States

On a Quantum Computer

Spenser Talkington • University of Pennsylvania • 26 November 2023

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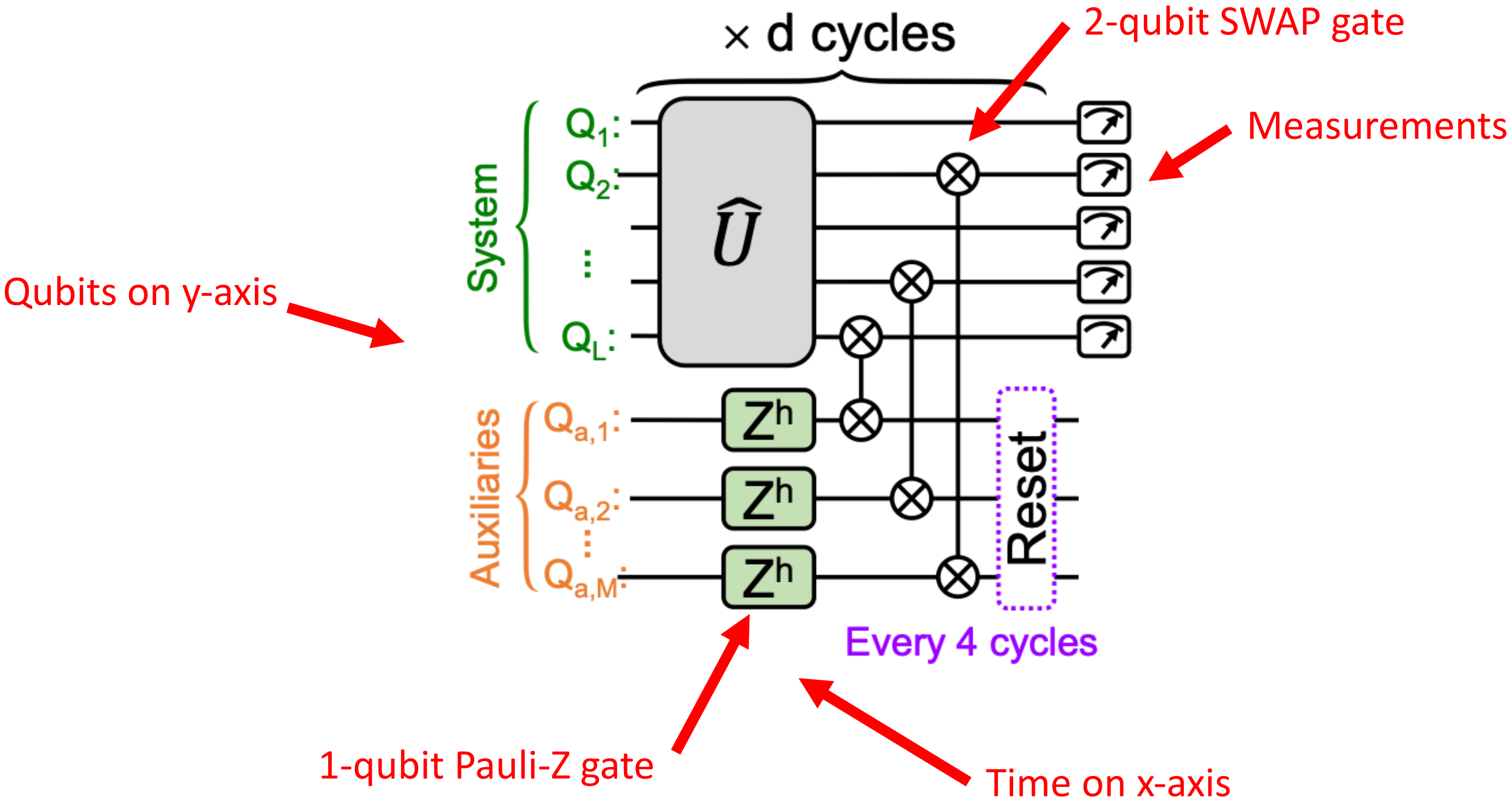
Quantum Computing Notation



Pauli Representation

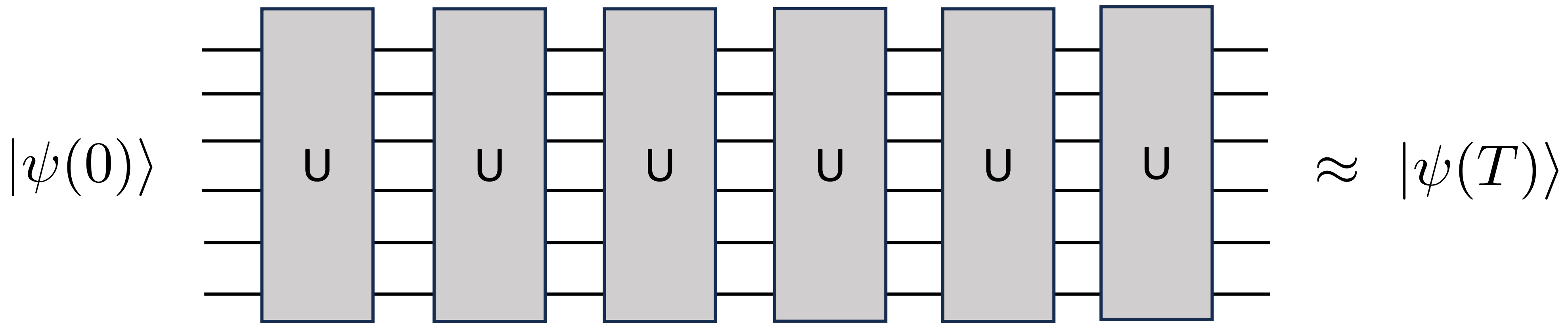
- Pauli operators are natural operations on a quantum computer
- (Tensor products of) Pauli matrices form a complete basis for Hermitian matrices
- We can represent Hamiltonians in terms of these operators and such a representation is feasible provided there aren't too many terms (sub-exponential scaling of number of operators)
  - Ex. Coulomb interaction scales polynomially with system size
    - This goes as the triangular numbers ~ N^2
    - We don't care that much how big the matrix representation of the Pauli operators are
      - No explicit representation of these matrices: a literal action of the operator on a state
- Solovay-Kitaev Thm: for precision eps need at most c $\log^4(1/\text{eps})$ terms

Trotterization

- Suzuki-Trotter expansion—separate terms in the expansion of H

$$e^{A+B} = \lim_{n\to\infty} \prod_i^n e^{A/n} e^{B/n}$$

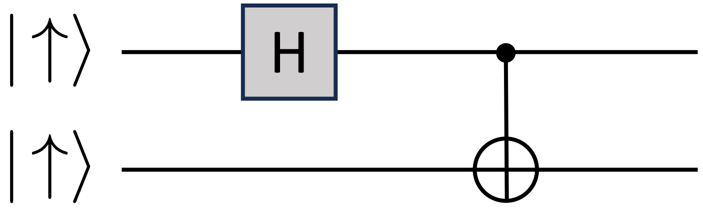
- Ex. Simulate time evolution stroboscopically



$$U = e^{iHT/n} \approx 1 + iHT/n$$

State Preparation

- Ex. Bell state



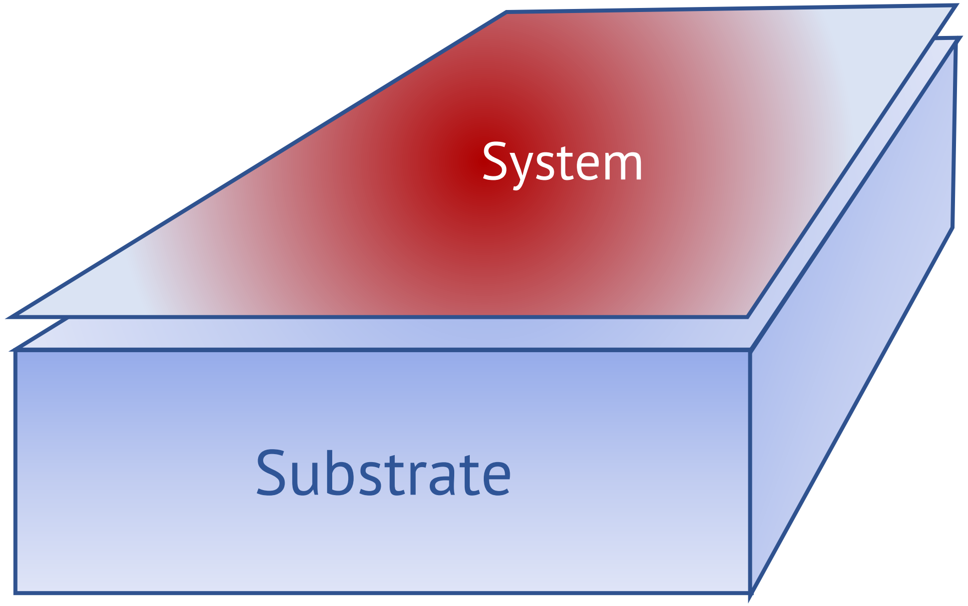
$$\frac{|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle}{\sqrt{2}} = CX(H \otimes I)|\uparrow\uparrow\rangle$$

$$H = \frac{X+Z}{\sqrt{2}} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \qquad CX = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

- Can use unitaries or measurements to prepare states

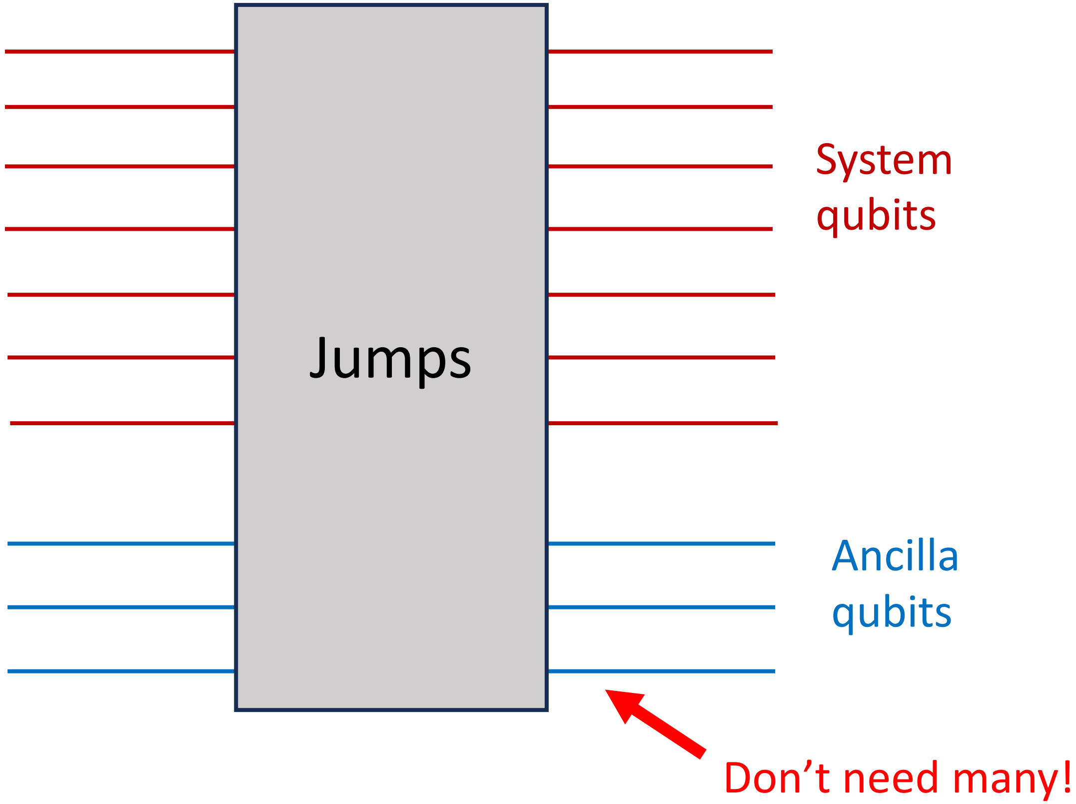
Dissipation

- Couple to a reservoir



$$\dot{\rho} = -i[H,\rho] + \sum_{j=1}^{m}\left(L_j \rho L_j^\dagger - \frac{1}{2}L_j^\dagger L_j \rho - \frac{1}{2}\rho L_j^\dagger L_j\right)$$

- Couple to “ancilla” qubits



Simulating Lindbladians on a Quantum Computer

- Repeated unitary evolution of system qubits and ancillas followed by resetting the ancillas (for Markovianity)
  - This mid-circuit reset functionality is now possible on Google and IBM hardware

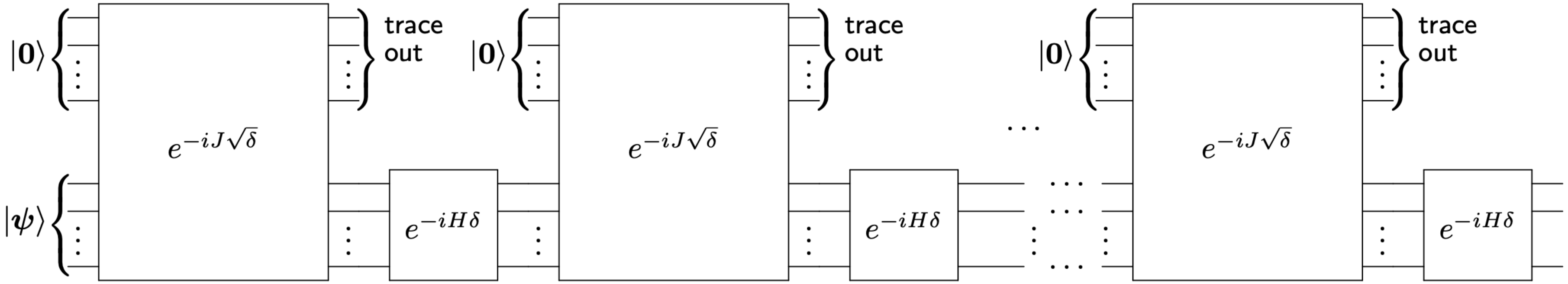


Figure 1: Lindblad evolution for time t approximated by unitary operations. There are N iterations and $\delta = t/N$. This converges to Lindblad evolution as $N \to \infty$.

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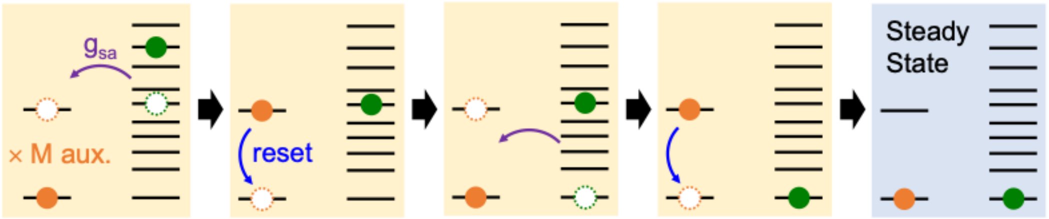
$$J = \begin{pmatrix} 0 & L_1^\dagger & \cdots & L_m^\dagger \\ L_1 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ L_m & 0 & \cdots & 0 \end{pmatrix}$$

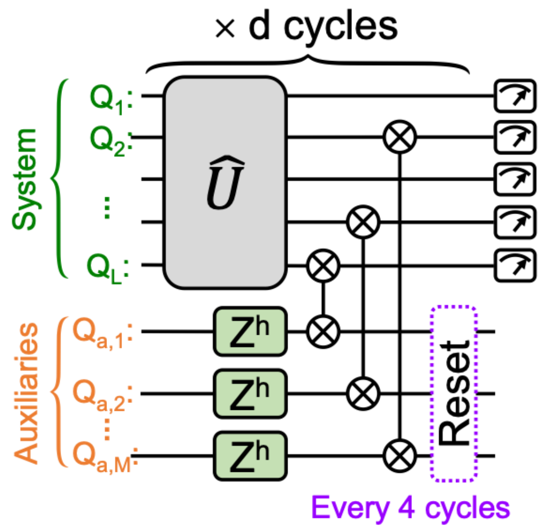
Example: dissipative cooling

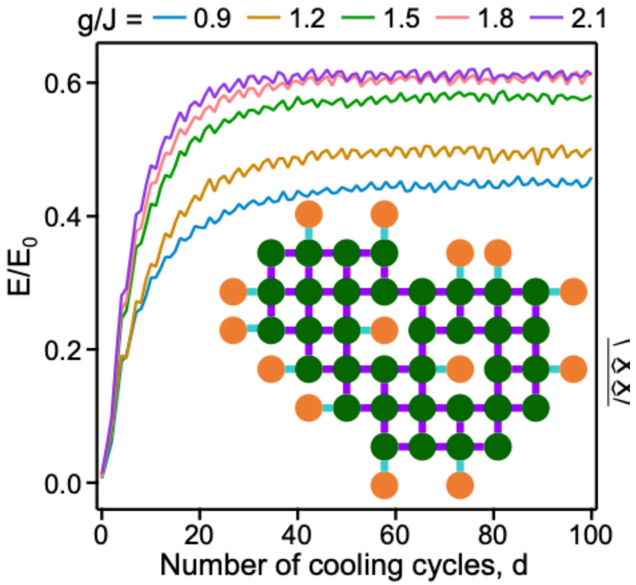
- Repeatedly reset ancillas to "cold" ferromagnetic alignment
- Stroboscopic time evolution
  - Trotterized Hamiltonian
  - Partial SWAP gates between system and ancilla

$$iSWAP(\theta) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(\theta) & i\sin(\theta) & 0 \\ 0 & i\sin(\theta) & \cos(\theta) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

- Get to 60-80% of the (negative) ground state energy







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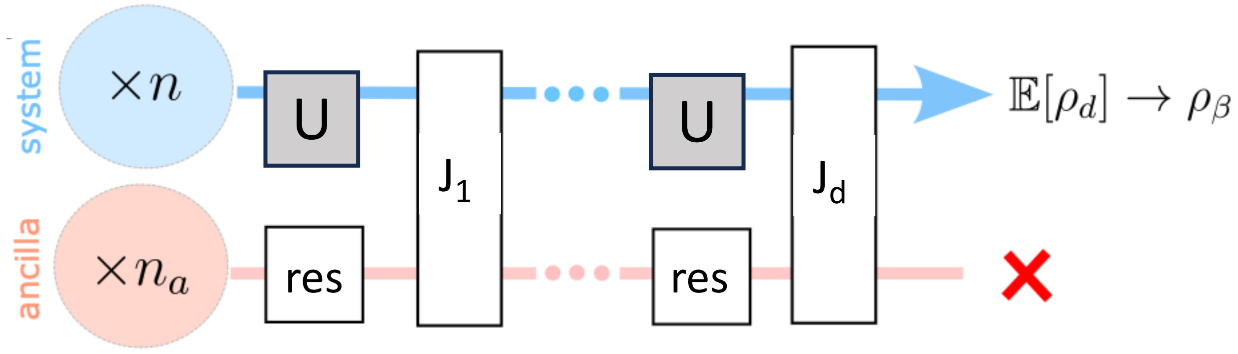
Thermal States

- Gibbs-type states $|\psi\rangle \in \rho = e^{\beta H}$
  - Finite temperature states are mixed, so sample over them
- (Re)Set ancillas to one-qubit thermal state
- Unitary evolution of the system
- Random coupling to system
  - Each ancilla couples to the system with n-local random Paulis



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- Thermalizes over time (assuming ETH of system)
  - To precision eps in time c n^3/eps^2; faster methods exist, e.g. 2303.18224
- Can sample over multiple final states if desired