Variational Gibbs State Preparation on NISQ devices

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Abstract

The preparation of an equilibrium thermal state of a quantum many-body system on noisy intermediate-scale quantum (NISQ) devices is an important task in order to extend the range of applications of quantum computation. Faithful Gibbs state preparation would pave the way to investigate protocols such as thermalisation and out-of-equilibrium thermodynamics, as well as providing useful resources for quantum algorithms, where sampling from Gibbs states constitutes a key subroutine. The novelty of the variational quantum algorithm (VQA) consists in implementing a parameterized quantum circuit (PQC) acting on two distinct, yet connected, quantum registers. The VQA evaluates the Helmholtz free energy, where the von Neumann entropy is obtained via post-processing of computational basis measurements on one register, while the Gibbs state is prepared on the other register, via a unitary rotation in the energy basis. Finally, the VQA is benchmarked by preparing Gibbs states of several spin-1/2 models and achieving remarkably high fidelities across a broad range of temperatures in statevector simulations. The performance of the VQA was assessed on IBM quantum computers, showcasing its feasibility on current NISQ devices. [1, 2].

Variational Gibbs State Preparation

Gibbs state at inverse temperature β for a Hamiltonian $\mathcal{H}$

$$\rho(\beta,\mathcal{H}) = \frac{e^{-\beta\mathcal{H}}}{\mathcal{Z}(\beta,\mathcal{H})},\ \mathcal{Z}(\beta,\mathcal{H}) = \mathrm{Tr}\{e^{-\beta\mathcal{H}}\} = \sum_{i=0}^{d-1} e^{-\beta E_i} \quad (1)$$

Generalized Helmholtz free energy

$$\mathcal{F}(\rho) = \mathrm{Tr}\{\mathcal{H}\rho\} - \beta^{-1}\mathcal{S}(\rho),\ \mathcal{S}(\rho) = -\sum_{i=0}^{d-1} p_i \ln p_i \quad (2)$$

The Gibbs state is the unique state that minimizes the free energy, we define our cost function as

$$\rho(\beta,\mathcal{H}) = \arg\min_{\rho} \mathcal{F}(\rho). \quad (3)$$

Framework and Structure of the Algorithm

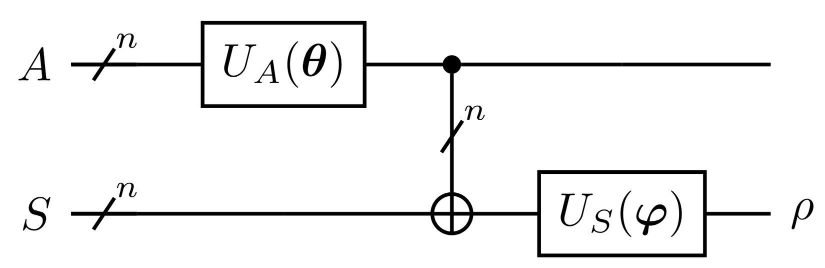

Figure 1. PQC for Gibbs state preparation, with systems A and S each carrying n qubits. CNOT gates act between each qubit A_i and corresponding S_i.

Applying U_A to the ancillary qubits A, followed by the intermediary CNOT gates and then tracing out the ancillary qubits, results in a diagonal mixed state on the system

$$\mathrm{Tr}_A\left\{\mathrm{CNOT}_{AS}(U_A\otimes \mathbb{1}_S)\,|0\rangle_{AS}^{\otimes 2n}\right\} = \sum_{i,j=0}^{d-1}(U_A)_{i,0}(U_A)^*_{j,0}\,\langle i|j\rangle\,|i\rangle\langle j|_S = \sum_{i=0}^{d-1}|(U_A)_{i,0}|^2\,|i\rangle\langle i|_S \quad (4)$$

Tracing out the system qubits we end up with the same diagonal mixed state, but on the ancillary qubit register.

$$\mathrm{Tr}_S\left\{\mathrm{CNOT}_{AS}(U_A\otimes \mathbb{1}_S)\,|0\rangle_{AS}^{\otimes 2n}\right\} = \sum_{i,j=0}^{d-1}(U_A)_{i,0}(U_A)^*_{j,0}\,\langle i|j\rangle\,|i\rangle\langle j|_A = \sum_{i=0}^{d-1}|(U_A)_{i,0}|^2\,|i\rangle\langle i|_A \quad (5)$$

Measuring in the computational basis of the ancillary qubits determines the probabilities p_i, which determines the von Neumann entropy $\mathcal{S}(\rho)$.

The unitary gate U_S transforms the computational basis states of the system qubits to the eigenstates of the Gibbs state

$$\rho = U_S\left(\sum_{i=0}^{d-1}|u_{i,0}|^2\,|i\rangle\langle i|_S\right)U_S^\dagger = \sum_{i=0}^{d-1} p_i\,|\psi_i\rangle\langle\psi_i| \quad (6)$$

where the expectation value $\mathrm{Tr}\{\mathcal{H}\rho\}$ of the Hamiltonian can be measured. At the end of the optimization procedure (ideally)

$$\rho(\beta,\mathcal{H}) = \sum_{i=0}^{d-1}\frac{e^{-\beta E_i}}{\mathcal{Z}(\beta,\mathcal{H})}\,|E_i\rangle\langle E_i| \quad (7)$$

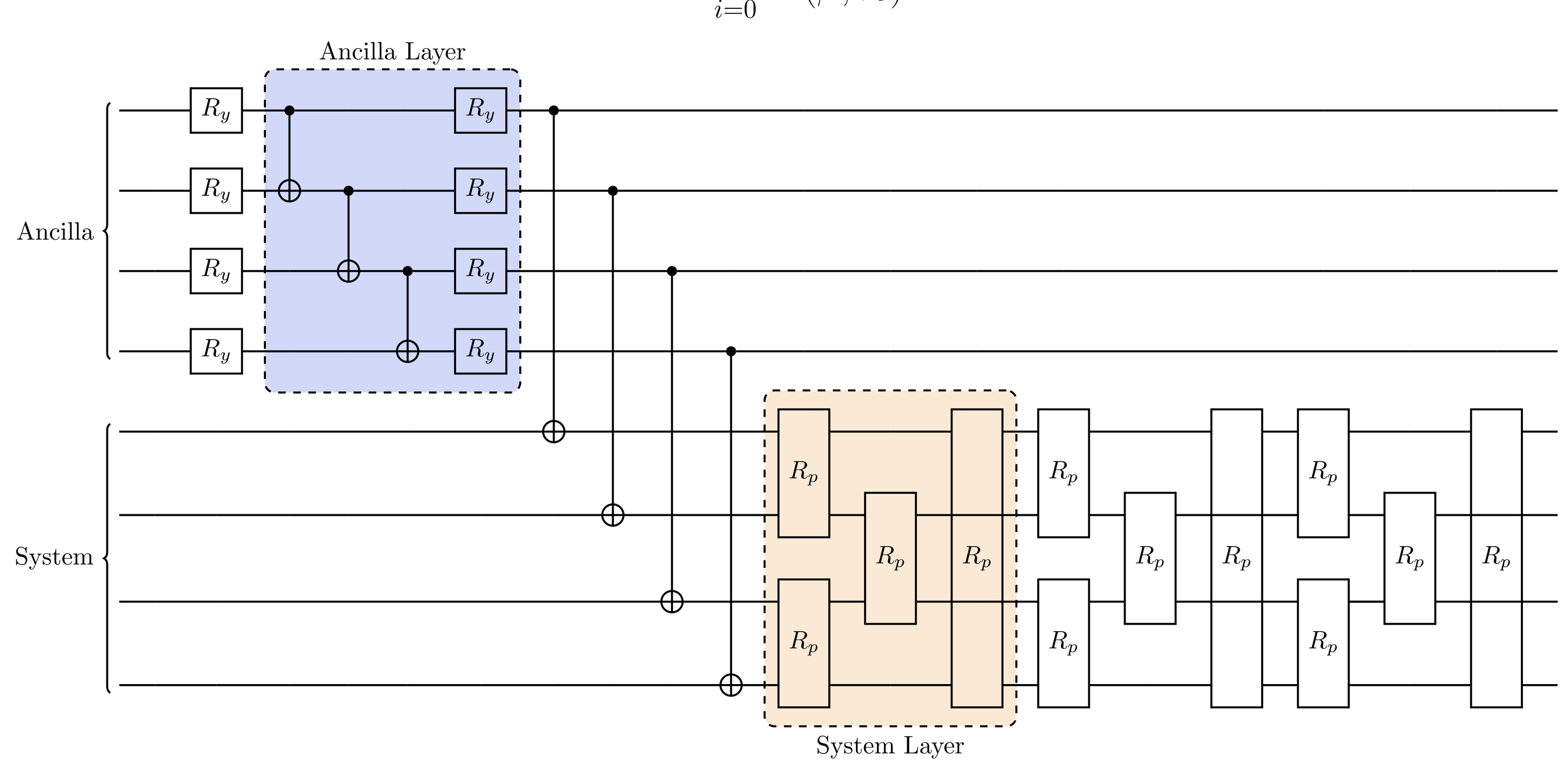

Figure 2. Example of an eight-qubit PQC, consisting of one ancilla layer acting on a four-qubit register, and three $(n-1)$ system layers acting on another four-qubit register. Each R_y gate is parameterized with one parameter θ_i, while each R_p gate has two parameters φ_i and φ_j. U_A must be an entangling unitary, while U_S is parity-preserving.

References

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Performance of the Algorithm

The Ising model is defined as

$$\mathcal{H} = -\sum_{i=1}^{n}\sigma_i^x\sigma_{i+1}^x - h\sum_{i=1}^{n}\sigma_i^z \quad (8)$$

- U_A is a simple, linearly entangled PQC using $R_y(\theta_i)$ and CNOT gates.
- U_S is a parity-preserving PQC using $R_p(\varphi_i,\varphi_j) \equiv R_{yx}(\varphi_j)R_{xy}(\varphi_i)$ gates.

We calculate the fidelity (effective measure of the closeness or overlap of two quantum states) of the prepared Gibbs state with the Gibbs state obtained via exact diagonalization.

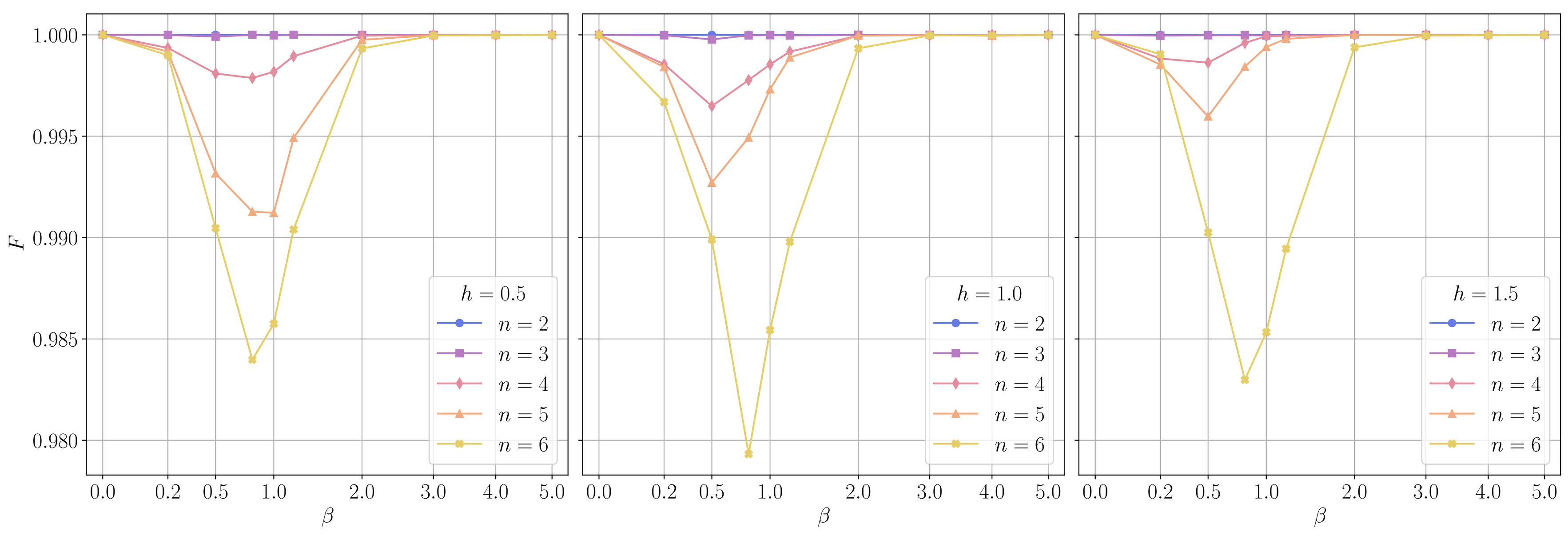

Figure 3. Fidelity F, of the obtained state via statevector simulations with the exact Gibbs state, vs inverse temperature β, for two to six qubits of the Ising model with $h = 0.5, 1.0, 1.5$. A total of 100 runs are made for each point, with the optimal state taken to be the one that maximizes the fidelity. We used one layer for the ancilla ansatz, and $n-1$ layers for the system ansatz.

IBM Quantum Device Results

The VQA was carried out on an actual quantum device. Quantum state tomography for two-qubit Gibbs states of the Ising model was carried out on `ibm_nairobi`, with 1024 shots, for the cases of $\beta = 0, 1, 5$, where the fidelities obtained were 0.992, 0.979, and 0.907, respectively.

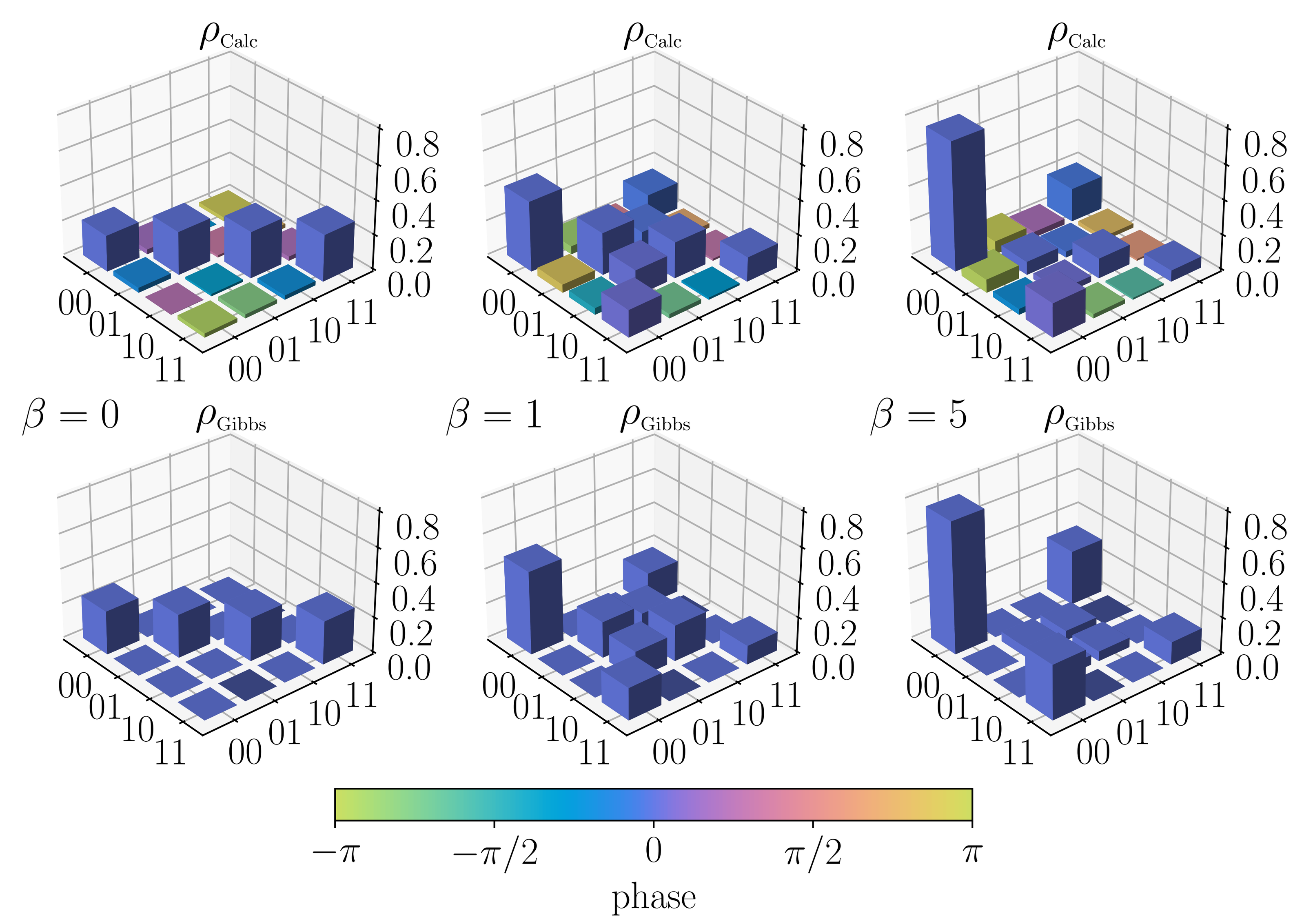

Figure 4. 3D bar plot of the two qubit results from `ibm_nairobi` for $\beta = 0, 1, 5$, of the Ising model with $h = 0.5$. The exact Gibbs states are shown in the bottom row, while the tomographically obtained Gibbs States are shown in the top row.

Error Analysis of Entropy Estimation

We compared the additive error (bias) of the von Neumann entropy using the Maximum Likelihood (ML) and Nemenman–Shafee–Bialek (NSB) [3] estimators.

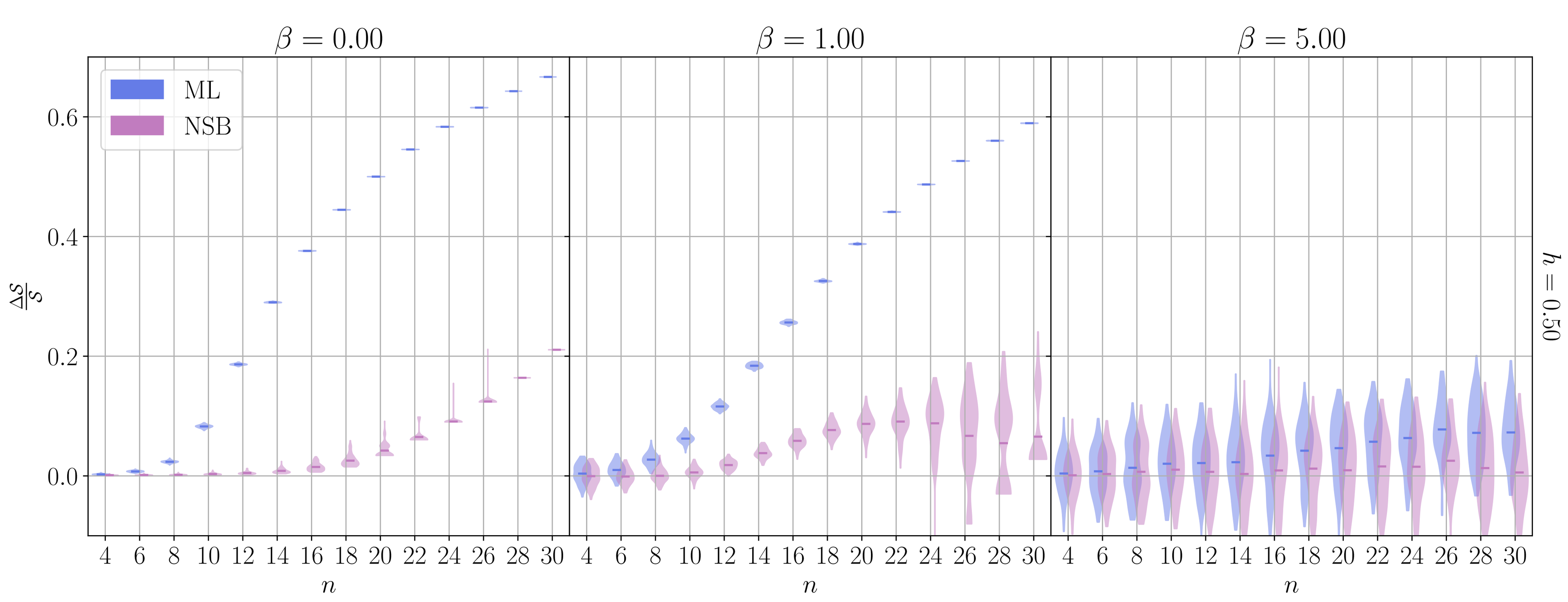

Figure 5. Violin plots for the relative error $\Delta\mathcal{S}/\mathcal{S}$ (bias) in entropy estimation as a function of the number of qubits n. Each violin plot is obtained by calculating the entropy of 100 samples taking 1024 shots.

Conclusion

- The VQA avoids the entire difficulty of measuring the von Neumann entropy of a mixed state on a quantum computer, and instead transfers the task of post-processing measurement results to the classical computer.
- The algorithm has been tested on the Ising, *XY* and *XXZ* models. More complex (chemical, physical, or else) models would be interesting to investigate.
- Algorithm can be possibly extended to carry out Hermitian matrix diagonalization, partition function evaluation, and calculate the probability density function of work in quench dynamics.

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