

Gibbs State Simulation with Pauli and Majorana Propagation

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This work is based on Ref. [1].

Thermal state preparation is a critical subroutine in many quantum algorithms, especially in Quantum Machine Learning (QML) [2, 3] and condensed matter physics [4, 5]. Generative modeling tasks, such as training Quantum Boltzmann Machines (QBM), rely heavily on drawing samples from thermal distributions or computing expectation values over Gibbs states to evaluate loss functions and gradients. However, thermal state preparation is generally resource-intensive. Indeed, preparing Gibbs states in quantum computers can be done either via fault-tolerant algorithms that require a fully working quantum computer [6–10], or via variational methods (that suffer from the many different problems found in the literature [11–14]). Classical methods also face several challenges. Conventional finite-temperature Monte Carlo methods [15–20] are frequently hindered by the sign-problem [21]. Furthermore, tensor network methods [22–25] are highly efficient but become increasingly complex to deploy beyond simple one-dimensional topologies.

To address some of these challenges, we introduce a propagation-based approach to thermal state simulation that adapts Pauli [26–40] and Majorana propagation [41–45] to imaginary-time evolution in the Schrödinger picture. Our key observation is that high-temperature states can be sparse in the Pauli or Majorana bases, approaching the identity operator $\mathbb{1}$ at infinite temperature ($\beta = 0$). By formulating imaginary-time evolution directly in these operator bases and evolving from the maximally mixed state, we can access a continuum of temperatures where the state remains efficiently representable.

In this work, we analyze complementary truncation strategies: small coefficient truncation and Pauli-weight (or Majorana-length) truncation. We derive upper bounds on the error depending on the truncation threshold and temperature, and deploy our numerical implementation to study the 1D $J_1 - J_2$ model and the Fermi-Hubbard model on a triangular lattice. Concretely, we study energy estimates across system sizes and temperatures for the former, and demonstrate direct computation of finite-temperature static correlation functions from the propagated thermal state. Beyond that, our algorithm has several natural applications. It provides a route to estimating free energies, combining thermal preparation and time evolution to prove finite temperature corrections to infinite-temperature dynamical correlation functions or perform Gibbs sampling. All our numerical and analytical studies show that simulating high-temperature states is tractable, but low-temperature states remain hard. Our sister submission ¹ explores the potential of using such high-energy thermal states as quantum Boltzmann machines.

Overview of the Propagation Method. Thermal states are simulated by expressing the target state as the normalized action of the imaginary-time propagator on the maximally mixed state:

$$\rho_\beta = \frac{e^{-\beta H}}{\text{Tr}(e^{-\beta H})} = \frac{e^{-\frac{\beta}{2} H} \mathbb{1} e^{-\frac{\beta}{2} H}}{\text{Tr}(e^{-\beta H})}. \quad (1)$$

We use Pauli and Majorana propagation methods to compute the action of this imaginary-time evolution on the identity operator $\mathbb{1}$. The Hamiltonian $H = \sum_m \alpha_m P_m$ is first expanded into local terms in the respective basis (Pauli strings or Majorana monomials). By using qDRIFT [46] (the method can also be naturally used with a standard trotter expansion, but qDRIFT obtains cleaner error bounds), we can approximate the imaginary-time propagator by applying a sequence of randomly chosen gates onto the Paulis (Majoranas) via the propagation rules

$$e^{-\beta H} \approx \prod_{\ell=1}^{L_{\text{qD}}} \exp(-\tau s_{m_\ell} P_{m_\ell}), \quad L_{\text{qD}} := \Lambda\beta/\tau, \quad e^{-\frac{\tau}{2} P} Q e^{-\frac{\tau}{2} P} = \begin{cases} Q, & [P, Q] \neq 0, \\ \cosh(\tau) Q - \sinh(\tau) PQ, & [P, Q] = 0, \end{cases} \quad (2)$$

¹Our submission is strongly aligned with the submission entitled ‘Sampling from Thermal States Via Pauli Propagation’. We think that, together, they represent a notable contribution to QML.

Here each $m_\ell \sim p$ is drawn independently and $s_{m_\ell} := \text{sign}(\lambda_{m_\ell})$, and Λ is a constant related to the commutativity of the terms in H . Crucially, contrary to real-time evolution [31], branching in imaginary-time occurs when the operators *commute*. Iterating this process produces a linear combination of Paulis (or Majoranas) that approximates the propagated identity, that we can use to approximate the thermal state

$$e^{-\frac{\beta}{2}H} \mathbb{1} e^{-\frac{\beta}{2}H} \approx \sum_{P \in \mathcal{P}_n} \alpha_P P \Rightarrow \rho_\beta \approx \frac{\sum_{P \in \mathcal{P}_n} \alpha_P P}{\text{Tr}(\sum_{P \in \mathcal{P}_n} \alpha_P P)} = \frac{\sum_{P \in \mathcal{P}_n} \alpha_P P}{2^n \alpha_{\mathbb{1}}}. \quad (3)$$

Truncation Strategies and Analytic Guarantees. In general, the number of terms generated by repeated application of these branching rules grows exponentially with the number of trotter steps. To ensure the algorithm remains scalable and efficient in practice, we apply two primary truncation strategies: *small-coefficient truncation* and *Pauli-weight* (or *Majorana-length*) *truncation*.

Because $\sinh(\tau) \approx \tau$ for small time steps, paths that branch frequently accumulate many $\sinh(\tau)$ factors and thus exponentially decaying coefficients. Small-coefficient truncation simply discards terms whose amplitudes fall below a defined threshold. We rigorously bound the error of this strategy by analyzing paths that accumulate more than k non-identity updates (branches).

Theorem 1 (Small-angle truncation error, Informal). *Let $\tilde{\rho}$ be the approximate thermal state obtained by truncating any path that accumulates more than k factors of $\sinh(\tau)$. Let Λ be the 1-norm of the Hamiltonian coefficients. The trace distance (1-norm) between the exact and approximate states is bounded by:*

$$\|\rho - \tilde{\rho}\|_1 \in \mathcal{O}\left(e^{\beta\Lambda/2} \left(\frac{e\beta\Lambda}{2k}\right)^k\right), \quad (4)$$

This theorem mathematically guarantees that in the high-temperature regime (where $\beta\Lambda = \mathcal{O}(1)$), the truncation error is suppressed super-exponentially in the truncation order k , ensuring that one can compute this efficiently without the need to store the exponential number of terms that may appear. Because this bounds the trace distance, the approximated state is particularly well-suited for sampling-based applications¹. Alternatively, one can truncate based on the spatial support of the operators (weight or length truncation). Compared to coefficient truncation, the runtime of weight truncation improves in practice; however, it only applies to expectation values as shown in the following theorem.

Theorem 2 (Weight truncation Backflow Error, Informal). *Consider the qDRIFT simulation of a thermal state starting from the identity $\mathbb{1}$ and let O be a constant weight observable, where $\|O\|_1$ is the 1-norm of its Pauli coefficients of O . Let $\tilde{\rho}$ be the state obtained by truncating any Pauli string with weight exceeding k . For sufficiently large $k \in \mathcal{O}(1)$, the error in the expectation value is bounded by:*

$$|\text{Tr}[O(\rho - \tilde{\rho})]| \in \mathcal{O}\left(\|O\|_1 e^{\beta\Lambda/2} \left(\frac{e\beta\Lambda q_{\text{bf}}(k)}{2k}\right)^k\right), \quad (5)$$

For approximately uniform all-to-all Hamiltonians the backflow probability is quadratically suppressed $q_{\text{bf}}(k) \in \mathcal{O}(k^2/n^2)$, whereas for 1D Hamiltonians it is linearly suppressed $q_{\text{bf}}(k) \in \mathcal{O}(k/n)$.

Large-scale Numerical Implementations. To demonstrate the practical utility of our algorithm, we perform large-scale numerical simulations using the open-source packages [PauliPropagation.jl](#) [39] and [MajoranaPropagation.jl](#). Figure 1 displays the imaginary-time evolution of the 1D J_1 - J_2 Heisenberg model on up to 40 qubits, a frustrated model. We observe that high-temperature energy densities can be effectively and accurately tracked. The complexity (number of Pauli strings generated) remains manageable at high temperatures, and the exponential growth only manifests as an issue at lower temperatures. Furthermore, we extend our analysis to a 74 mode Fermi-Hubbard model on a triangular lattice in Figure 2. Operating in the strong coupling regime ($U = 8, t = 1$) at half-filling ($\mu = U/2$), our algorithm directly evaluates finite-temperature static spin-spin correlations from the propagated state. These results demonstrate that Pauli/Majorana propagation effectively simulate high-temperature thermal states.

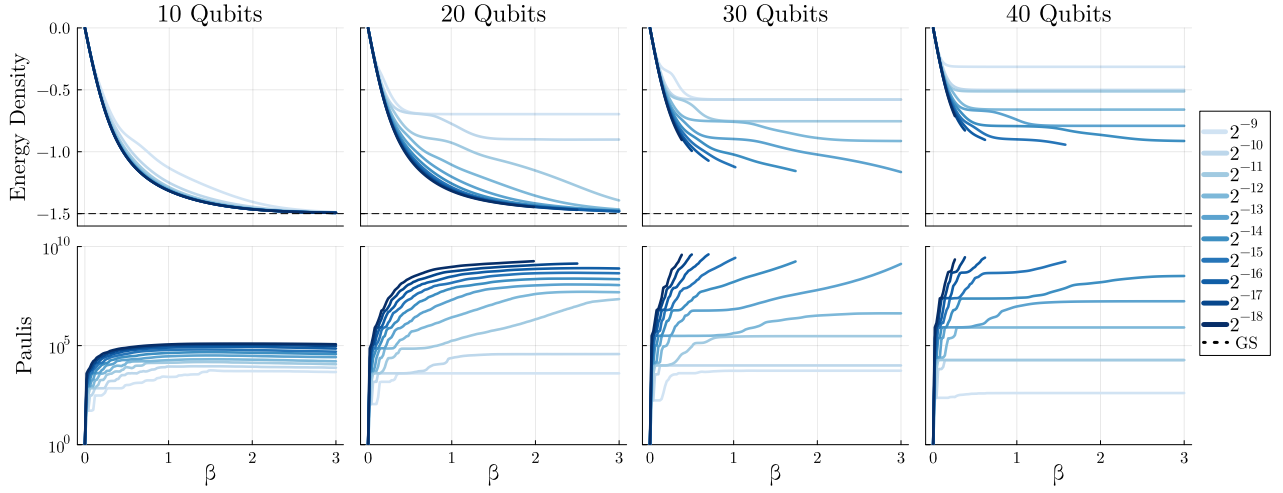


Figure 1: **Imaginary time evolution under the J1-J2 Heisenberg model.** We present numerical results across system sizes, from 10 to 40 qubits. The top row shows the estimated energy density $\langle H \rangle / n$ converging toward the ground state (dashed line) as the inverse temperature β increases. The bottom row tracks the number of Pauli strings generated. The divergence of lines (corresponding to different coefficient truncation thresholds) indicates the breakdown of the approximation.

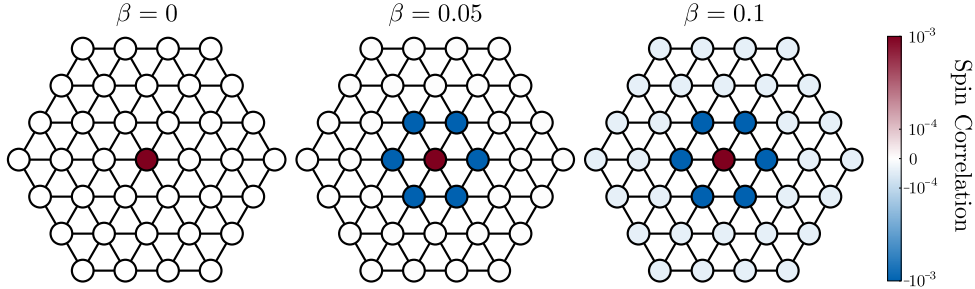


Figure 2: **Spin correlation in the Fermi-Hubbard model on a triangular lattice.** Snapshots of spin-spin correlations (C_{ZZ}) emerging in a Fermi-Hubbard model on a 37 site triangular lattice (corresponding to 74 Majorana modes). As we lower the temperature from $\beta = 0$ to $\beta = 0.1$, we can observe magnetic order and correlations beginning to form around the central site (red). While reaching the deep frustration patterns of lower temperatures ($\beta \sim 2$ to $\beta \sim 3$) remains challenging for current propagation techniques, this demonstrates the ability to compute static correlations for complex geometries directly from the propagated state.

Applications to QML. The preparation, measurement, and sampling of Gibbs states are fundamental tasks in quantum machine learning. For instance, quantum Boltzmann machines (QBMs) [47] leverage Gibbs states for quantum generative modeling. Training a QBM typically involves minimizing the quantum relative entropy, $S(\eta || \rho_\theta)$, between a target state η and the model’s Gibbs state ρ_θ . This optimization reduces to matching the expectation values of the model’s observables to those of the target state (a procedure that can be executed efficiently within this framework). This approach can be applied in three ways. 1) For sufficiently high-temperature models, one can train and deploy the QBM classically, as the combination of our guarantees in Ref. [1] and ¹) allow for polynomial-time classical sampling. 2) Our method could be used to classically train a QBM, before deploying it quantumly and sampling the trained model on quantum hardware (with polynomial speed ups over ¹). 3) Our method could be used to classically pre-train a QBM before finishing the training (and the sampling) at lower temperatures on a quantum computer.

Conclusions. We have extended propagation methods to simulate imaginary-time evolution. By providing rigorous error bounds and demonstrating scalability on frustrated systems like the 1D J_1 - J_2 and triangular Fermi-Hubbard models, we show that the high-to-moderate temperature regimes are classically simulable. This framework provides a robust, topology-agnostic method for finite-temperature Gibbs state simulation. This opens new directions train QBMs and for studying finite-temperature quantum physics.

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