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Targeting the most typical state among the thermal pure quantum states

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We propose a new class of typical quantum states, called Markov-shielded typical (MST) states, for one-dimensional quantum systems with open boundary conditions. Unlike conventional typicality arguments based on random sampling[1], MST states are derived from a variational principle that naturally connects to the variational formulation of ground states. This connection enables a numerical scheme in which thermal states can be efficiently and stably constructed by gradually increasing the temperature, starting from the ground state.

Our formulation builds on the generalized Markov free energy, introduced in Ref.[2] as a variational lower bound on the thermodynamic free energy. For a density operator ρ, it is defined as $F_M(\rho;T) = \mathrm{Tr}[\rho H] - TS_M(\rho)$, where $S_M(\rho)$ is the Markov entropy computed from local reduced density matrices. The approximate quantum Markov property of Gibbs states[3] ensures that the generalized Markov free energy $F_M(\rho;T)$ closely approximates the thermodynamic free energy when evaluated on states within local regions. This insight justifies restricting the minimization of F_M to the set of pure states $\rho = |\psi\rangle\langle\psi|$, leading to the definition of MST states as those pure states that variationally minimize $F_M(|\psi\rangle\langle\psi|;T)$.

We implement this scheme using matrix product states (MPS) as a variational ansatz. Numerical results for the transverse-field Ising model show that the MST-MPS method achieves high accuracy for local observables, even at low temperatures and with small bond dimensions. These results highlight the practical significance of MST as an efficient and scalable numerical method for simulating finite-temperature quantum systems.

References

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