Low-temperature Gibbs state representation by matrix product states

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Studying finite-temperature properties with tensor networks is notoriously difficult, especially at low temperatures, due to the rapid growth of entanglement and the complexity of thermal states. Existing methods like purification and minimally entangled typical thermal states offer partial solutions but struggle with scalability and accuracy in low-temperature regime. To overcome these limitations, we propose a new approach based on generating-function matrix product states (GFMPS) [1]. By directly computing a large set of Bloch-type excited states, we construct Gibbs states that go beyond the area-law constraint, enabling accurate and efficient approximation of low-temperature thermal behavior. Our benchmark results show magnificent agreement with both exact diagonalization and experimental observations, validating the accuracy of our approach. This method offers a promising new direction for overcoming the longstanding challenges of studying low-temperature properties within the tensor network framework. We also expect that our method will facilitate the numerical simulation of quantum materials in comparison with experimental observations.

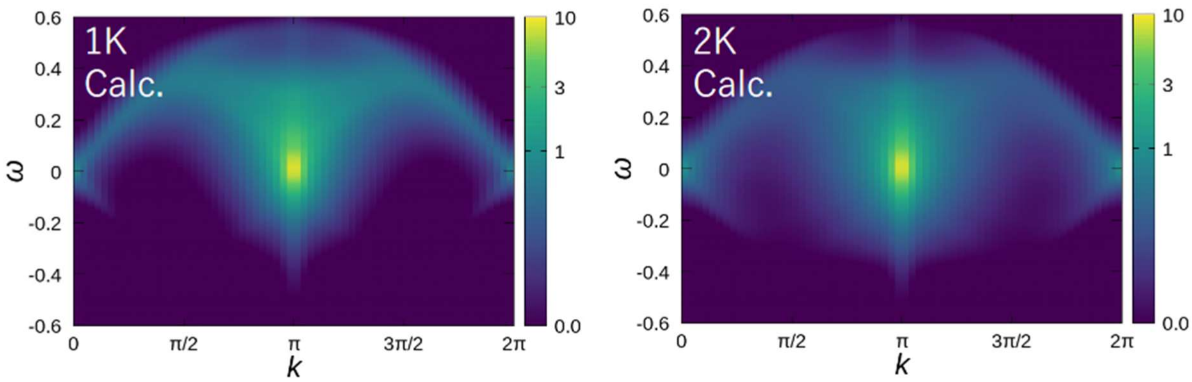

Figure 1: The finite-temperature dynamical structure factor for the Heisenberg model.

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