Simulation of two-dimensional strongly correlated systems via tree-like isometric tensor networks: from physical models to quantum computers

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Abstract

The analysis of two-dimensional (2D) strongly correlated systems poses a significant challenge due to the exponentially increasing amount of computational resources required by an exact simulation. However, tensor network methods have arisen as potent approximation techniques that enable the resolution of this issue in certain cases. In this thesis, we conduct an extensive investigation of the application of these methods for the analysis of strongly correlated systems, emphasizing the study of the monolayer of CrI_3 and the simulation of random unitary (quantum) circuits.

We begin by applying the Matrix Product State (MPS) based techniques to analyze the magnetic ordering in the spin-3/2 XXZ Hamiltonian on a honeycomb lattice, being an effective model of the monolayer of CrI_3. We demonstrate that magnetic phases emerging in the system can be predicted with high precision by the classical approximation of the model, in a wide range of the parameter space. We find the correlation energy to be the greatest in magnitude for the in-plane ferromagnetic and antiferromagnetic phases, while being equal to zero in the case of the off-plane ferromagnetic one.

Next, we give a pedagogical introduction to two-dimensional Isometric Tensor Networks (isoTNS) and discuss the Moses Move and 2D version of Time Evolving Block Decimation ($TEBD^2$) algorithms that operate on them. We then present modifications to the basic isoTNS framework, which allow for the entire orthogonality surface to be moved into the bulk of the lattice, resulting in a reduced bond-size required when performing calculations. Additionally, we rearrange the entanglement flow in the network to create a tree-like structure, and provide a technique allowing for application of two-site operators on nodes lying on different branches. We compare the two methods on the task of finding the ground state of the transverse field Ising model on a square lattice, by means of imaginary time evolution.

Finally, we show how the modified $TEBD^2$ algorithm can be used to emulate the execution of random quantum circuits, with simultaneous estimation of both the two-qubit and the multi-qubit fidelities, which we compare with the ones obtained by an existing MPS-based technique. For the two demonstrated methods we note very high average fidelity, with respect to the number of parameters used, which is inversely proportional to the amount of entanglement being present in the system. We analyze the bottleneck of the altered $TEBD^2$ algorithm and suggest alternative approaches allowing for its circumvention.