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Review of PhD thesis entitled:
„Simulation of two-dimensional strongly correlated systems via tree-like isometric tensor networks: from physical models to quantum computers”

The subject of this review is a PhD thesis entitled "Simulation of two-dimensional strongly correlated systems via tree-like isometric tensor networks: from physical models to quantum computers", written by Mr. Bartosz Rzepkowski. The thesis has been written at the Faculty of Fundamental Problems of Technology of the Wrocław University of Science and Technology under supervision of prof. Arkadiusz Wójs and Gunnar Möller, PhD.

Quantum description and prediction of properties of the matter unavoidably involves accounting for many-body interactions and correlations of interacting particles. The complexity of the problem grows exponentially with the number of particles. The so-called strongly correlated systems are particularly difficult to simulate since the independent particle approximation, assuming that a particle "lives" in a mean field of other particles - a work horse of many theoretical approaches in quantum chemistry and physics, breaks down. Development of efficient computational techniques for strong correlation is a rapidly developing field with vast applications to simulation of systems of high interest, including biomolecules, low dimensional materials and also quantum computing. The thesis of Mr. Rzepkowski fits this timely topic.

The main subject of the thesis of Mr. Rzepkowski is development of new techniques based on isometric tensor networks for simulating strongly correlated two-dimensional systems. The thesis is written in English. It consists of the introductory chapters 1 and 2, chapters 3-5 presenting main achievements of the Authors and chapter 6, which summarizes the thesis.

I will start by emphasizing that the thesis is exceptionally well written concerning the language. The sentences are concise and logical, there are practically no grammar errors, not even typos. Like other fields, the field of tensor networks developed specific language-code over years, so also the language used by the Author is quite technical and "cryptic". This is not, in general, an obstacle in understanding and appreciating the merit of the thesis, since all phrases and technical terms have been properly introduced and explained. The Author has put a lot of effort in illustrating all concepts and algorithms with tensor network diagrams. They greatly help to grasp the main concepts behind algorithms introduced in the thesis.

Chapter 1 provides an introduction to the content of the thesis and it is followed by Chapter 2 including an extensive presentation of the isometric tensor networks in one dimension. The intention of the Author is to prepare a reader for extending the one-dimension product states and the related computational techniques to higher dimension. This chapter is very pedagogical and starts with the introduction of such elementary concepts as tensor, tensor order, or tensor contractions. The elementary level makes this chapter self-contained. It also explains why Chapter 2 takes almost 50% of the volume of the whole thesis. From Chapter 2 one learns about matrix product state and operators in different representations, including diagrammatic representations, and the compression techniques. Emphasis is put on two key techniques used in the thesis for finding ground state energy of a system whose state is described with matrix product state: time evolving block decimation algorithm (TEBD) for evolution in imaginary time and density matrix renormalization group (DMRG). The latter is presented (and later employed) for finite and infinite variants.

Chapter 3 presents the results of simulating 2D systems using isometric tensor networks. In the first part finite DMRG calculations are carried out for the transverse field Ising model on a square lattice. DMRG calculations were run for different values of the g parameter and bond-size values to investigate the accuracy dependence on the number of parameters in MPS and to generate benchmark values used for comparison with approxi-

mate methods developed specifically for 2D systems. In the second part of Chapter 3, the honeycomb monolayer of CrI_3 is studied assuming the Heisenberg XXZ model Hamiltonian and carrying out DMRG calculations in finite and initiate variants. The focus is on magnetic phases of the studied materials and on comparing quantum simulations with the classical approximations. The valuable finding of this part of the research project was that classical approximation predicts correct magnetic ordering for a wide range of parameter space.

In Chapter 4 the MPS methods have been applied to simulation of quantum circuits. It is demonstrated how quantum random circuits are represented by tensor networks. It is also discussed how the multi-qubit fidelity can be obtained from the products of lower-qubit-fidelity.

Chapter 5 includes the most original contribution of the Author to the methods based on tensor networks for 2D systems. He proposes two improvements to the Time Evolving Block Decimation algorithm $TEBD^2$ with the aim of lowering the computational cost of the method while preserving the accuracy. The modified algorithm has been applied within the tree-like isoTNS to the TFI model. Its performance was benchmarked against the accurate results obtained using the DMRG technique in Chapter 3. It has been observed that the modified $TEBD^2$ exhibits more stable convergence than the original one. Concerning the actual performance in predicting the energy of the TFI model by modified $TEBD^2$ and the energy error as a function of the variational parameters, the results, in my opinion, are not conclusive. The errors were only smaller than those from the DMRG method for unrealistically small number of parameters. The modified $TEBD^2$ algorithm has been also applied to random quantum circuit simulation. For this kind of applications, the modifications proposed for the algorithm have turned out to bring substantial benefits. Namely, it has been shown that thanks to the improvements employed in the algorithm a multiqubit fidelity can be obtained with the higher precision than with the isoTNS with the Moses Move.

Despite my overall positive evaluation of the thesis, I have a few critical remarks and comments, which could be addressed during the thesis defense:

- When presenting a TEDB algorithm in section 2.6, the Author mentions that it enables time evolution of "slightly entangled physical states". Why is it so? Is it because bond Hamiltonians do not commute? The systems investigated in the thesis are in strongly entangled states, how can one be sure that TEDB algorithm with the second-order Trotter-Suzuki decomposition is sufficiently accurate?

- Section 2.9, which is intended to present extension of the 1D tensor network methods to 2D problems is disappointingly sketchy. In particular, one does not find a discussion of the nonuniqueness of mapping of the 2D onto 1D lattices. Long-range interactions between the sites of the chain depend on the site-ordering, which is not unique, and it poses a problem in real calculations. What was the algorithm used to find the optimal ordering of sites?
- Presentation and discussion of the results in Tables 3.1-3.3 could be improved. First of all, when the Authors claims (page 56) that the aim of the presented simulations was to "check the scaling of the properties obtained from finite DMRG ..." it is not clear what kind of scaling was investigated. Second, it is not clear what is the purpose of showing iDMRG energies for different bond-sizes if the energy values are the same (but different from DMRG) for the chosen values of the bond-size. What do we learn from it? Finally, it is not clear to me what the Table 3.3, captioned "Average correlation in the XY plane" shows. Are these correlation energies?
- In section 5.9, page 80, the Author compares errors in the energy for the TFI model obtained using the modified TEBD^2 algorithm and DMRG as a function of bond-size (i.e. the number of parameters). The former method leads to obtaining a smaller error only for low values of bond-sizes. I presume that the energy errors from both methods in this range of bond-size are too large to be acceptable so the advantage of the modified TEBD^2 is only apparent. The valid question is if for the range of bond-size for which the energy error from compressed DMRG is acceptably low, the modified TEBD^2 offers any real advantage over DMRG with compression? Has the Author checked and compared the computational efficiency of the methods?
- In text on p. 80 and in the caption to Fig. 5.14 one finds the phrase "Error density of energy ...". Should it not be "Error of energy density ..."?
- I could not find information about the computer code used by the Author. Has he coded the novel algorithms presented in the thesis himself? I am also wondering about the computer infrastructure he has the access too and how did he test the efficiency of the algorithms (timings). The overall timing of quantum simulations is depending on the level of parallelization of the implementation of the underlying algorithms. Is the implementation of TEBD^2 parallelized? How does it scale with the number of computation cores/nodes?

The comments listed above are of minor nature. I have no doubt that the thesis meets requirements for a PhD degree in physics. Bartosz Rzepkowski presented a significant contribution to the rapidly developing field of isometric tensor networks for strongly correlated systems by (1) extending the existing methods to the 2D systems, exploring their usefulness and limits of applicability to both physical systems and to simulation of random quantum qubits and (2) development of the improved techniques based on the TEBD^2 algorithm and their implementations, showing possible direction of further development of tensor networks methods for strong correlation in two dimensions. All the tasks undertaken by the Author were highly nontrivial and by successfully accomplishing them the PhD candidate proved his skills in numerical mathematics and theoretical physics, as well as the capabilities to turn a complex physical problem into a treatable simplified model.

I conclude that the dissertation presented to me for review meets the requirements set forth in the Art. 190 Act 3 of 20 July 2018 of the Law on Higher Education and Science (Dz. U. z 2021 r. poz. 478 z późn. zm.), and I request that Mr. Bartosz Rzepkowski be admitted to the next stages of the doctoral dissertation.