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Review of Ph.D. thesis entitled
„Simulation of two-dimensional strongly correlated systems via tree-like isometric networks: from physical models to quantum computers."

The Ph.D. thesis I received to review has been composed by Mr. Bartosz Rzepkowski. The thesis is written in English and entitled „Simulation of two-dimensional strongly correlated systems via tree-like isometric networks: from physical models to quantum computers." The Ph.D. project was performed under the supervision of Professor Arkadiusz Wójs and the co-supervision of dr Gunnar Möller.

The thesis topic is computer simulations exploiting tensor-network-states-based algorithms that utilize the isometry condition, which efficiently evaluates expectation values and optimizes tensors—the mathematical building blocks of the wave functions investigated in this work. The computational study focuses on modeling the properties of the ground states of 2-dimensional (2D) systems that are strongly correlated. Such systems are remarkably difficult to model efficiently with satisfying accuracy using conventional quantum many-body methods due to exponentially increasing resources required in classical simulations. Mr. Rzepkowski proposes to tackle this extraordinarily difficult task using isometric tensor-network-states (isoTNS) for which the ground states were optimized employing imaginary time evolution. The critical aspect of his thesis consists of two modifications of the traditional optimization schemes of isoTNSs, which allows him to (1) reduce the bond sizes in calculations, which are directly related to the dimensionality of the problem, and (2) efficiently sweep through the lattice, optimizing the underlying tensors using a clever sequence of contractions, merges, splits, reshapes, and shifts of tensors/centers. Specifically, the first goal is achieved by moving the orthogonality center to the center of the bulk. The second goal is realized by initially rewriting the isoTNS into a tree-like structure and then performing a specific recipe of tensor contractions and singular value decompositions (SVD) to move through the lattice efficiently.

The Ph.D. thesis is divided into six main chapters, a Polish and an English version of the abstract, and a bibliography, in total, comprising 102 pages. The first chapter includes a concise introduction to the problems dealt with in this thesis, namely strongly-correlated systems, noisy simulations in quantum computing, and TNSs, focusing on matrix product states (MPS) and projected entangled pair states (PEPS). Finally, an outline of the thesis is given.

The second chapter briefly reviews the current state of the literature, including tensors, tensor networks, their notation, graphical representation, mathematical operations on them, and the diagrammatic representation of operators. Furthermore, chapter 2 sets the stage for subsequent

chapters: it provides a brief summary of TN compressions using SVD and a variational procedure, real and imaginary time evolution using the time evolution block decimation algorithm, the finite and infinite version of the density matrix renormalization group (DMRG) algorithm, a short remark on charge conversation, and a quick note how a one-dimensional (1D) MPS representation can be used to model 2D problems, exploiting a „snake" MPS (which is the most straightforward extension of a 1D MPS to a 2D problem).

Chapter 3 presents the numerical results of simulations on two strongly-correlated benchmark systems: (1) the transverse field Ising (TFI) model and (2) the spin 3/2 Heisenberg XXZ model on a honeycomb lattice that serves as a model for a monolayer of CrI_3. Both models were studied using the DMRG algorithm. Mr. Rzepkowski searched for the critical g_c points dependent on the lattice length in the former system. These points were identified based on the maximum values of the block entropy (also called block entanglement) for each lattice length. Mr. Rzepkowski performed (finite and infinite) DMRG calculations to scrutinize the ground and lowest-lying excited states of a monolayer of CrI_3 for the latter model system. Specifically, he investigated magnetic phases, average (projected) spin values, energy gaps between the ground and the lowest-lying excited state, and entanglement entropies. The results of this chapter have been published in a peer-reviewed journal.

In Chapter 4, the complexity of the problem is further increased by going from the moderately to the highly-entangled regime. The aforementioned numerical study is extended to simulations of random quantum circuits as they allow us to generate much entanglement with only a few operations. In contrast, conventional 1D algorithms can be easily extended to the 2D case, avoiding the well-known convergence problems that plague 1D methods when applied to 2D problems. Thus, they represent ideal systems for benchmark purposes. Most importantly, Chapter 4 comprises issues that were designed to be difficult so that they serve as a suitable testing ground in the following chapter. The simulations of quantum circuits presented in this Chapter are divided into two parts: studies on a 1D and 2D quantum computer. Both are performed using a 1D MPS representation and a specific computational setup. Specifically, Mr. Rzepkowski restricts his analysis to three kinds of gates only (CNOT, CZ, and ISWAP). By doing so, he can optimize the simulations as such a quantum circuit can be directly translated to a 1D MPS, facilitating its optimization. Finally, he introduces two fidelity measures to assess the accuracy and performance of simulations: the multi-qubit fidelity and the average two-qubit fidelity. These measures are obtained using a recurrence relation. He approximates the multi-qubit fidelity as a product of, essentially, singular values. Overall, his computational results are satisfying in terms of accuracy. To simulate the 2D problem, he generalizes the approach of Zhou and co-workers to the 2D case. Specifically, he translates the 1D MPS representation to the 2D case, as discussed in the previous Chapter. Since applying a 1D MPS to a 2D problem is numerically problematic, his numerical results are as expected and indicate a faster drop in the multi-qubit and averaged two-qubit fidelity.

Chapter 5 finally focuses on 2D isometric tensor networks—the main objective of this thesis. First, Mr. Rzepkowski briefly summarizes current approaches suitable for 2D problems, like PEPS, tree TN (TTN), and isoTNS. In the first half of Chapter 5 (up to including Chapter 5.6), he discusses and follows the methodology presented by Zaletel and Pollmann and Lin and co-workers, who classify a canonized PEPS as an isoTNS. Specifically, Chapters 5.1 to 5.5 exemplify

in greater detail the initialization of an isoTNS, how to compute observables, how to optimize an isoTNS using the Moses Move procedure, a variational procedure, and the imaginary time evolution extended to two dimensions. In section 5.6, he extends his previous numerical study of Chapter 3.1 (using a 1D MPS) and assesses whether a 2D isoTNS provides meaningful numerical results for the TFI model's ground state. Mr. Rzepkowski points out the weaknesses of the time evolving block decimation (TEBD) algorithm generalized to a 2D lattice, where the Moses Move introduces numerical inaccuracies, destroying a smooth convergence of ground-state energies. Up to this point, the Ph.D. thesis dealt with conventional methods and applied literature procedures to strongly-correlated 1D and 2D problems. From Chapter 5.7 onwards (or starting from page 74), Mr. Rzepkowski introduces his modifications to isoTNS to improve simulations on 2D systems. The following two sections describe their proposed modifications' main idea, validation, and numerical procedure. The idea of moving the orthogonality center to the center of the bulk might appear trivial and obvious, especially considering that the pruning of variational parameters performed with an SVD step—an essential part in most TN optimizations—should favor such an arrangement in terms of computational cost and efficiency. However, the benefits of moving the orthogonality center to the center of the bulk unfold not before the optimization of the TN is modified. To arrive at an improved and more efficient 2D TN-based model, Mr. Rzepkowski proposes a second modification, where the isoTNS is transformed into a tree-like structure with L-shaped connections and presents an optimization scheme of such a tree-like isoTNS, which includes the traditional Moses Move procedure but eliminates its limitation. In short, the Ph.D. candidate imposes an elegant structure on the computationally complex starting isoTNS model, reducing selected bond dimensions, and suggests a modified optimization scheme to arrive at a computationally more robust 2D optimization algorithm.
Most importantly, this novel tensor network structure and optimization scheme do not suffer from the original limitations that plague traditional isoTNS optimizations. For instance, the arbitrariness in choosing variational parameters is eliminated (there is only one to choose), Moses Move does not introduce numerical problems, and disentanglers represent a redundant operation and become nonessential. At the same time, the predicted fidelities are by construction well behaved (no loss in precision or error accumulation appears due to the setup of the TN structure). Last but not least, Mr. Rzepkowski applies this novel TNS representation to benchmark its performance and accuracy for the model systems mentioned in the previous Chapters, namely, the simulation of the ground state of the TFI model and 2D quantum computers. For both test systems, he chose the 1D MPS results as reference data, while for the former, he additionally compared them to the traditional TEBD^2 algorithm. Most importantly, the proposed methodology features much more stable convergence, where the ground state energy smoothly and systematically converges toward the exact result, while multi-qubit and averaged two-qubit fidelities feature a similar behavior and can be well approximated using the recurrence relation discussed in Chapter 4. Chapter 5 concludes with a short outlook of further possible improvements to their algorithm and methodology. The results of this Chapter have yet to be published (as of the day of submitting this thesis).

Chapter 6 briefly summarizes all aspects of the thesis, including theory, methodology, numerical results, and an outlook on future work.

In general, the thesis is well written. The language is clear and understandable. Sentences are coherent and concise. There are some minor grammar mistakes due to missing articles. However,

these are minor problems and do not impede the understanding of the thesis. Most importantly, scientific terms are correctly used. The list of references is acceptable. However, I expect a more complete bibliography list, especially considering the significance of the field.

The vital parts of the thesis include the following:

- Although most of the thesis is dedicated to a review and summary of the literature, it provides the fundamental basics of tensor notation and operations, which are required to understand the remainder of the thesis, namely the proposed modifications to isoTNS presented in Chapter 5. Furthermore, this thesis can be read as a textbook as it provides the most essential and fundamental knowledge, know-how, and toolset to introduce (young) researchers to the field of tensor network states and their optimization. This is an excellent advantage of the presented work.
- Almost all tensor operations are explained using Penrose graphical notation (as they should be). This visualization is essential to follow and understand all algorithms and their individual optimization steps. Thus, the Ph.D. candidate put much effort into composing this manuscript.
- All essential graphs, figures, and tables are included in the thesis, and numerical data properly support the discussion.

Despite the aforementioned positive aspects of this thesis, I have some general remarks considering its weak parts and questions that have not been addressed:

- In Chapter 1, the author states that *DMRG allows us to obtain ground states of 1D physical systems*. DMRG can also describe excited states and (ground and excited states of) more compact („3D") quantum systems. Obviously, it will come with a cost. However, the author never mentions this, which does not do justice to DMRG.
- Considering the DMRG algorithm in Chapter 2.7, I have some general remarks as this section is missing some state-of-the-art procedures.
  - The two-site DMRG protocol has, in general, a better convergence behavior as it allows to avoid local minima efficiently and can be used with various acceleration techniques like the dynamic block state selection protocol. Is there a reason why a greater emphasis is put on the one-site version?
  - Another diagonalization algorithm is the Davidson procedure. Why is the Lanczos diagonalizer the preferred method here?
  - Targeting excited states in DMRG can also be simpler by optimizing several roots during the diagonalization process of the Hamiltonian. The Lanczos diagonalizer performs better than the Davidson algorithm for such problems.
- What is the reason for drawing the „snake" MPS in the proposed way (see Figure 2.42) instead of using „S-snake" paths? For inhomogeneous systems, the snake's path will matter in terms of convergence.
- The DMRG optimization protocol the author chose is unconventional. Increasing the number of block states or bond size during the sweeping procedure does not help avoid local minima, as states lost during the DMRG optimization procedure cannot be picked up again. To ensure that local minima are avoided, and essential states are not lost, one typically starts with a large bond size and systematically decreases it after some initial algorithm sweeps have been performed. Does the computational setup used in this thesis guarantee that local minima are avoided?

- Considering the CrI_3 model, what kind of spin-orbit interactions are modeled/included in the model Hamiltonian of eq. (3.2)? As iodine is rather heavy, while chromium can be considered a „light" element, spin-orbit coupling is significant and will affect the electronic structure of the whole system. Furthermore, what is the rationale for changing the parameters in the Hamiltonian? Does it guarantee that, for instance, spin-orbit coupling is adequately described? Or in other words, how does changing the parameters affect the physics of the system?
- Throughout the thesis, the entanglement entropy (also known as block entropy in a DMRG optimization) is taken to assess the simulations' quality or better understand the quantum states under study. However, there are more correlation functions that the candidate could have investigated. Examples are one-site entropies, two-site entropies, or two-site correlators like the correlation index. These measures are typically used in the DMRG community and are directly transferable to more general TNS.
- The Penrose graphical representations generally display all crucial TNS optimization steps. However, there are some Figures where this representation could have been improved by showing some additional intermediates, which would have made the thesis more complete, especially for those new to the field. For instance, Figures 5.4, 5.6, and 5.9 are harder to follow, which is most concerning since the latter diagrams form the centerpiece of the thesis. Specifically, Figure 5.6 is ambiguous concerning the rotation procedure, while Figure 5.9 would be easier to follow if selected intermediate steps of the $TEBD^2$ algorithm were mentioned. These additional clarifications would have been helpful for a quicker/ more profound understanding of the proposed methodology.
- My main concern and criticism are related to the actual work that the Ph.D. candidate has performed. It is unclear whether he has derived, implemented, and tested the novel isoTNS models and/or done the numerical simulations. Based on the written thesis, I assume no derivations and implementational work have been performed. This issue does not reduce the merit of the thesis as it still contains significant contributions to the field of condensed matter physics, particularly strongly-correlated 2D problems. It is an ambiguity that requires clarification.

In addition, there are some minor typos and inconsistencies, which the author might wish to correct:

- In Figure 2.1, according to the notation used in the thesis, the row and column indices (i,j) of matrix $M_i{}^j$ must be exchanged.
- Without any cutoffs, an SVD should be exact. Thus, to my understanding, the „≈" sign should be replaced by an equal sign („="), for instance, in Figure 2.9.
- In Figure 2.24, the letter „**F**" is missing in subfigure (b).
- The Pauli spin matrices are not introduced after their first appearance in eq. (2.38).
- The equation after eq. (4.6), the equation is missing a „**\rangle**."
- On page 42, most likely, there is a type: „**(i+)**" instead of „(i+1)".
- On page 68: „it can **be also be**."
- On page 68: „tensor to **by** factorized" (by -> be)
- In Figure 5.11: if I am correct, the circle on the right-bottom edge should be red, not blue.

I definitely confirm that this thesis meets the statutory demand for an original solution to a scientific problem. Indeed, no satisfactory TNS algorithm is currently able to model strongly-

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correlated 2D problems with very high numerical precision efficiently. To tackle this problem, one requires fundamental knowledge of the mathematical aspects of tensor optimization, the skill to reformulate expensive physical problems into cheaper „solutions," and the ability to perform scientifically sound numerical simulations. Obviously, it is also impossible to apply any written program without understanding the physics behind the problem or the details of the optimization algorithms. In this work, the Ph.D. candidate embarked on a complex problem encountered in condensed-matter physics and performed excellently. The material presented in Chapter 5 represents an important step toward more efficient TN representations and their optimization schemes for 2D problems—a hot topic that is still insufficiently solved. The good performance in terms of accuracy, efficiency, and numerical stability surpasses traditional formulations, which is supported by the numerical data presented in this thesis. Although the proposed methodology could benefit from additional improvements to obviate drawbacks—a crucial point also addressed by the Ph.D. candidate—it is an undoubtfully substantial contribution to the field.

To sum up, I rate the work highly, and hence, by *article 190 sec. 2 of the Act of July 20, 2018 — Law on Higher Education and Science (i.e., Journal of Laws of 2020, item 574, as amended) and § 1 para. 11, § 19 para. 5 in connection with § 7 para. 1 Regulations for conferring academic degrees*, **apply for admission to further procedural stages of the dissertation**.

Sincerely,

Katharina Boguslawski

Signature Not Verified
Digitally signed by Katharina Boguslawski; UMK
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Dr hab. Katharina Boguslawski, prof. UMK