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Review of Ph.D. thesis by Aritra Sinha

Time Evolution of Quantum Many-body Systems using Tensor Network States

written under the supervision of
Prof. Jacek Dziarmaga and Prof. Marek Rams
in the Institute of Theoretical Physics, Jagiellonian University

The reviewed Ph.D. thesis is based on three research papers, all published in one of the leading journals in the field – Physical Review B, in three successive years from 2020 to 2022. Mr. Sinha is the first author in all three publications and all three are written in collaboration with one or both Supervisors and one additional co-author. Already the fact of publication in Physical Review B is strongly indicative of the very good level of the Ph.D. student's work and the importance of the research topic. It is worth to note also that Mr. Sinha is a co-author of three additional papers, published in Physical Review B as well.

The articles are accompanied by an introduction and three chapters discussing the physics of quantum phase transitions and the methodology of numerical investigation employing 1D and 2D tensor network methods – matrix product states (MPS) and projected entangled pair states (PEPS), respectively. Motivation for each of three thesis papers is also included.

There are two physically rather distinct threads in the Ph.D. thesis, with a common denominator of time evolution investigated by tensor networks. The first thread concerns evolution in real time, but the second one deals with thermal properties, formally described by evolution in imaginary time and thus accessed numerically. The methodological difficulty increases significantly in the second thread along with the increase of dimensionality from one to two. I will now move on to the characterization of the papers that constitute the dissertation.

In the first paper (Phys. Rev. B102 (2020) 214203), the authors study a one-dimensional transverse-field Ising model with long-range interactions decaying according to a power-law as $r^{-\alpha}$. This model has a solvable version when a string operator is inserted between the interacting spins and it amounts then to a long-range Kitaev chain. In turn, the version without the string operator can only be studied numerically (apart from some limits) and the authors undertake such an investigation with MPS and time-dependent variational principle (TDVP). The model becomes particularly interesting in an intermediate regime of $5/3 < \alpha < 3$, situated between the small-α regime in the mean-field universality class and large-α one belonging to the Ising universality class. In the intermediate regime, the critical exponents are not known analytically and evolve smoothly between the mean-field and Ising values. The authors concentrate on $\alpha = 2$ and employ tensor networks to determine the critical exponents and use them to analyze quench dynamics across the paramagnetic-ferromagnetic quantum phase transition (QPT) driven by the transverse field. First, a homogeneous quench is analyzed and three regimes are found in the residual energy (with respect to the ground state energy of the final-state Hamiltonian): size-independent regime (fast quenches), quantum Kibble-Zurek (intermediate) and Landau-Zener exponential decay (slow quenches). The analysis leads to a conclusion of a crossover between the Kibble-Zurek and adiabatic regimes. Second, a spatially inhomogeneous quench is considered, shown before to bring about a "shortcut to adiabacity" in some models, allowing to achieve adiabacity with a fast process instead of the trivial way of very slow parameter changes. The inhomogeneity opens an energy gap in the quasiparticle spectrum and leads to the existence of a characteristic crossover velocity of the inhomogeneous front. This dynamically generated scale is shown to indeed lead to an advantage of the optimal inhomogeneous quench with respect to the homogeneous one. The methodology of the paper is relatively simple, with the TDVP for MPS as the main tool, but this tool is simply optimal for the physical question. The paper is insightful, among other things in showing that a seemingly simple model can offer very interesting physical features. Obviously, the non-trivial key to such success is the identification of the proper parameter regimes, based on physical reasoning and knowledge.

In the second paper (Phys. Rev. B103 (2021) L220302), published as a letter, attention is switched from second-order to the comparatively less explored area of first-order QPTs. In this case, interesting phenomena can occur due to the presence of metastabilities, i.e. local minima of the free energy. A system can relax to the global minimum by dynamical instability or by quantum fluctuations driving nucleating bubbles of the true vacuum. The authors undertake the task of understanding in detail the dynamics across a first-order QPT without employing approximations such as the time-dependent Gutzwiller method that could obscure the true physical picture. They consider again the Ising model, this time only with nearest-neighbor coupling, but with both transverse and longitudinal fields. As far as I understand from the accompanying material, the motivation came from initial exact-diagonalization studies of small systems, already wherein non-trivial energetic features were revealed. Employing TDVP based on MPS, much larger system sizes could obviously be reached. The model posesses a first-order QPT between two ferromagnetic phases, driven by the longitudinal field. The main finding of the study is the existence of several regions where the bubble nucleation becomes energetically favorable and the discovery that only specific bubble sizes are possible, i.e. they are quantized. A simple intuitive relation is found between the value of the instantaneous longitudinal field and the bubble size n, which is n-th order perturbative in the transverse field. Importantly, the discovered behavior can be interpreted and understood in terms of the classic Landau-Zener theory, with two-level transitions enough for low-density nucleations and higher-level ones needed in general. Overall the results of this paper are novel and important theoretically, as well as experimentally, since such phenomena are within reach of the current technology, e.g. with Rydberg atoms.

The third paper (Phys. Rev. B106 (2022) 195105) moves to another thread, where the time evolution proceeds in imaginary time, i.e. in temperature. The investigated model is the fermionic Hubbard model, the simplest model of interacting fermions on a lattice, but with a wealth of physical properties relevant to several physical mechanisms. Despite this simplicity, several parameter regimes are very difficult to study, leading to the fermionic sign problem in Monte Carlo simulations. This motivates tensor network studies, which are, however, technically complicated in two or more dimensions, due to the fact that the MPS ansatz is proper only for one-dimensional systems with its built-in entanglement scaling. Thus, the Ph.D. student's task was ambitious to switch to two-dimensional tensor networks, projected entangled pair states (PEPS) in its infinite-volume variant (iPEPS). Obviously, the ealier experience with MPS was a good build-up for this challenge. The authors concentrated on a specific choice of parameters, with one value of the on-site repulsion and average fermion concentrations of 0.875 and 1, in a parameter regime relevant for e.g. high-T_c superconductivity. They use the fermionic version of the neighborhood tensor update (NTU) algorithm recently proposed by Prof. Dziarmaga, one of the Ph.D. advisors. This algorithm is argued to be a good compromise between the standard simple/full update choices. The Abelian symmetries are implemented in the tensors and fermionic statistics is enforced according to the proposal of Corboz and

Vidal. Thus, the methodological side of the work can be considered state-of-the-art, with novel elements. The main observables studied in the paper are two-point spin and charge correlation functions, evaluated over a broad range of temperatures. The obtained results are complementary to arguably the most important zero-temperature results of Corboz et al., as well as to other finite-temperature results in the literature.

Summarizing, the thesis comprises three papers, with physically interesting and non-trivial problems solved in each of them, based on most likely the best numerical technologies to address them. Each paper encompasses novel physical aspects, which is particularly worth emphasizing for the real-time evolution papers, where a big part of the success is already the formulation of the non-trivial problem. In the imaginary-time evolution thread, the physical problem is comparatively more obvious in terms of the motivation and thus, I see more merit in the novel methodological side. This does not detract anything from my evaluation of the methodological side of the first two papers or the problem addressed in the third one. Even if the methodology is pretty standard for one-dimensional real-time dynamics, it is all that is needed to efficiently address such problems. In turn, even if the motivation for the third paper was very clear, attacking such a problem needed improved tools and technical proficiency. This brings me to a very high opinion about the thesis. Apart from the papers, the introductory material is also well-presented. I have noticed a couple of flaws in it – some statements are not precise (e.g. that second-order QPTs do not have any abrupt changes or discontinuities – taking the ferromagnetic transition as an example, the first derivative (magnetization) is indeed continuous, but the second derivative (magnetic susceptibility) is not), there is quite a lot of inconsistent punctuation (e.g. in including equations) and several typos. However, these are minor details, while, in general, the introductory material reads well and contains a lot of useful material that explains some aspects of the papers and their motivation.

At this point, I would like to ask some questions to the Ph.D. candidate.

1. What is the robustness of the obtained numerical results of the first two papers in terms of the standard tensor-network convergence criteria? For example, what bond dimensions are needed for the studied models? It is well known that entanglement increases quickly during real-time evolution. Was this observed and has it been checked that the results at later real times are not affected?

2. Standard equilibrium phase transitions, like the paramagnetic-ferromagnetic one in the Ising model, are characterized by a non-analytic structure of the free energy. In real-time dynamics, a natural generalization of the partition function can be defined, the Loschmidt amplitude, and one can consider dynamical quantum phase

transitions (DQPTs) manifested by a non-analytic structure of such Loschmidt amplitude. Could the Ph.D. candidate comment whether an analysis in terms of the DQPT language could make sense for the models of the first two papers? Could it consitute a potentially interesting thread of follow-up work? Perhaps some results are already available in the literature (definitely for several other variants of Ising-like models).

3. I would like to ask about the Ph.D. candidate's opinion on the future prospects for PEPS simulations of fermionic systems. What are the biggest challenges and is it likely that next years will bring efficient simulations of three-dimensional models? How do the prospects for PEPS compare to alternative tensor-network methods like (augmented) tree tensor networks or tensor renormalization group approaches?

Overall, in my opinion, the thesis clearly satisfies all formal and customary requirements for Ph.D. dissertations. Thus, I conclude that the Ph.D. candidate should be admitted to the next stages of the doctoral procedure.

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