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Report on the doctoral thesis by Aritra Sinha “Time Evolution of Quantum Many-body Systems using Tensor Network States”

The doctoral thesis by Aritra Sinha studies various strongly interacting quantum systems using a tensor network approach. In general the thesis consists of two parts. The first one concerns the (real) time evolution of an interacting system driven across a quantum phase transition. The second part *a priori* also discusses the time evolution of a many-body system – albeit driven in the imaginary time and hence this part basically discusses the thermal properties of the interacting system in equilibrium. Let me note at this point that, in my opinion, the fact that these two part of the thesis are somewhat distinct does not constitute a drawback of the dissertation.

Before diving into the physics discussed by the thesis, let me quickly discuss the general impact of the results of this thesis as well as his role in obtaining them. In my view the former exceeds the average level of a PhD dissertation in this country: not only all of the results are published as three Physical Review B articles and have gathered a few citations, but also the paper on the bubble nucleation in the first order transitions appeared in the letter sections of Physical Review and has (since 2021) gathered 14 citations (according to google scholar). These are very good results in this subfield of theoretical condensed matter. Besides, Aritra Sinha was the first author of all three papers and none of the papers had more than four authors. Therefore, I judge that Aritra Sinha played a key role in obtaining the results presented in this thesis.

Let me now (critically) discuss the three physical problems presented in the thesis:

The first one (published as Phys. Rev B **102**, 214203) concerns the question whether a particular quantum continuous phase transition can solely be driven adiabatically – or rather the non-adiabatic, so-called Kibble-Zurek, regime may appear around the critical point. While such a question has been extensively discussed for cases with short-range interactions, the longer-range case seems more intriguing. This is because in the latter case the information could in principle travel instantaneously through the system leading to the adiabatic regime and no Kibble-Zurek-like freezing. Nevertheless, together with the other co-authors, Aritra Sinha has shown that in the case of the longer-range Ising model in external field, the adiabaticity is not guaranteed once the critical front speed exceeds a threshold given

by a particular Kibble-Zurek mechanism. What I like about this result is that it was obtained both for the nonintegrable model (using MPS and supposedly by Aritra Sinha) as well as for its integrable “cousin” model (analytically, probably by the other co-authors). This makes the presented results both physically relevant and “convincing”.

The second problem (published as Phys. Rev B **103**, L220302) is related to the adiabatic quenches across the first order quantum phase transition. In contrast to the continuous phase transition and the associated Kibble-Zurek mechanism discussed above, this case in general far less studied and hence it is even more interesting. In principle what is relatively well-known is the fact that during such a drive the system may become stuck in the local minima (fake vacuum) – from which it can escape e.g. by the creation of bubbles of the true vacuum driven by quantum fluctuations of the fake vacuum. Interestingly, in the study co-authored by Aritra Sinha it is shown that such a process can be achieved by the nucleation of bubbles of specific size once the quantum Ising model with transversal field and longitudinal field is subject to a quench in the latter field. What is really nice is about this result is that, as shown by Aritra Sinha *et al.*, it can basically be understood using the simple Landau-Zener picture.

Finally in the last part of the thesis (published as Phys. Rev B **106**, 195105) Aritra Sinha *et al.* apply a specific iPEPS algorithm, exploiting the Abelian symmetries, to uncover spin and charge correlations in the 2D doped Hubbard model at finite temperature. As it is well-known the properties of the latter problem are not really well-understood – not least because of the lack of the reliable numerical techniques. In fact, the obtained results are quite impressive: (i) on one hand, they are far more reasonable than e.g. the other widely used tensor network approach – the DMRG which typically is performed on a cylinder geometry, (ii) on the other hand, the lowest calculated temperature is relatively low, as e.g. compared to the typical quantum Monte Carlo approaches (which suffer from the sign problem).

If I may, I would have here a few comments and questions concerning the obtained 2D Hubbard results. *First*, I would appreciate a more detailed discussion of the physical picture which better explains the charge correlators dependence on the doping, as plotted in Fig. 5. Maybe it is written in the paper but I could not find a more detailed discussion of e.g. the origin of the “dip” in some of these correlators at around ~ 0.18 doping. *Second*, I was also thinking that it might be interesting to look at the dependence of the number of double occupied sites (doublons) on doping and temperature. Is there a “peculiar” behavior (such e.g. change in the curvature) associated with the density of the on-site doublons as a function of doping or temperature? *Third*, I would appreciate if we could discuss during the defence what could be the limits in going down in temperature in the employed iPEPS (for the 2D Hubbard model) and to what extent the technique can be used to study properties of the doped frustrated systems (e.g. doped Hubbard on Kagome)? Last but not least, I suggest that one could in the future calculate and study the three-point spin-charge correlation function [as defined by T. A Hilker *et al.* in Science **357**, 484-487 (2017)] as well as the static spin and charge structure factors in momentum space. These could even more insight into the intriguing physics of the doped Hubbard model.

Finally, let me comment on the style of the presentation. In general I must admit that I am very satisfied by the fact that the main part of the thesis consists of a preface, three rather short introductory chapters, and a very short overview of the presented results. On top of that the three published articles, which present the main results of the dissertation, are attached in the end of the thesis. Altogether, I find this structure ideal as this way the reader can understand the thesis content in the quickest manner possible – and this is irrespective

of the reader's familiarity with the subject. Besides, the PhD student does not have to spend too much of precious time while writing the thesis. I also like the language of the thesis and the way the key physical concepts are introduced. My only critical comment concerns a few typos and a bit too sketchy drafting of the thesis.

In conclusion, I am certain that the PhD dissertation by Aritra Sinha fullfills all formal and customary requirements of a PhD thesis. Therefore I request the admission of Aritra Sinha to further stages of the doctoral dissertation procedure. Besides, I propose to consider the recognition of this PhD thesis. In my opinion the very high quality of the results obtained (and published) by Aritra Sinha during his PhD studies, fully justifies awarding the *cum laude* title to this thesis.

Sincerely

Krzysztof Wohlfeld