

Reply to the Referee's reports

We thank the Editor for sending us the referee reports for our manuscript and two Referees for their comments. Following the suggestions, we have made revisions to improve the paper. For ease of reference, the principal changes in the main text are also typeset green in the resubmitted version.

Sincerely,

Benedikt Bruognolo, Jheng-Wei Li, Jan von Delft and Andreas Weichselbaum

First Referee: Matteo Rizzi The Manuscript offers an ordered review of (i)PEPS techniques, highlighting the most relevant ones for the implementation of an algorithm from scratch, thus sparing considerable efforts to the beginners and newcomers to the field. Particular emphasis is given, in the intentions at least, to the incorporation of fermionic statistics and non-Abelian symmetries, both crucial ingredients when aiming to tackle condensed matter paradigms like the multi-band Hubbard model, where a lot remains to be explored. In this respect, some concrete examples of calculations are provided in the final section, thus motivating the interested reader to struggle with the algorithm implementation to explore new physics.

Certainly, after the first thirty self-contained didactical pages on general aspects of (i)PEPS, the Reader would expect to find the same level of user-friendly description for the ingredients that set the Authors' approach apart from other ones in the literature, namely the QSpace approach to non-Abelian symmetries. Unfortunately, however, apart a short comment about being a fully alternative approach to Ref. [48], not much more is provided to the reader, except for addressing to the extensive Ref. [30]. At least a sketchy recapitulation of the QSpace idea and its implementation details would be highly desirable to keep the review self-contained and homogeneous in style, especially given the promise in the title.

We appreciate the encouragement to include a brief recapitulation of the ideas underlying QSpace. We have accordingly somewhat expanded our discussion of non-abelian symmetries in Section 5.2. Moreover, we added an Appendix A, entitled "Construction of non-abelian symmetric tensors", which provides a sketch of how to introduce non-abelian symmetry in tensor networks. The QSpace tensor library is a code package facilitating such manipulations.

Given the overall spirit of the Manuscript, I would rate it definitely as suitable for the Lecture Notes section of SciPost more than as Regular Article. A few more punctual remarks — anyway not as crucial as the criticism / suggestion above about QSpace — are listed below, with the aim of improving the clarity of the presentation.

1. At page 2, the claim "Computational costs scaling as D^α can thus potentially be reduced by a factor of $(D/D^*)^\alpha$ " should actually be made a bit milder by taking into account the growing number of smaller objects to be contracted, as correctly discussed later in Sec. 6.1.3. E.g., for a matrix-matrix multiplication it should read $(D/D^*)^{\alpha-1}$ since there are order of (D^*/D) small blocks to be multiplied with each other. Anyway, nothing to say about the fact that the gain is going to be quite spectacular :-)

We thank the Referee for careful reading. Indeed, the ideal speedup is difficult to reach due to the growing number of smaller objects to be contracted. *In particular this concerns small D , whereas the overhead becomes smaller with growing D .* Following the suggestion, we adapted our discussion on page 2. However, we disagree with the statement that *there are order of (D^*/D) small blocks to be multiplied.* In particular, note that the argument of small blocks identically also applies to abelian symmetries, yet in which case we have $D^*/D = 1$.

2. At page 4, the statement “In other words, the computational cost to simulate a low-entangled state using a PEPS scales only polynomially with system size.” is misleading at this stage, since it somehow suggests a perfect analogy with the efficiency of MPS algorithms. However, as correctly discussed in Sec. 3.3, the contraction of a PEPS “represents an exponentially hard problem” and one should resort to “a variety of approximate schemes to deal with this issue.”

We agreed with this comment. To avoid the confusion, we remove the statement at p. 4.

3. At the bottom of page 11, more quantitative indications and/or criteria to judge the convergence would be helpful for beginners. In particular, more quantitative substance to expressions like “typically multiple times”, “a few full steps”, “can significantly increase” would be of great help for the beginner trying to assess the performance of its own simulations. Same applies later on in Sec. 3.5.2 when discussing the convergence in terms of the imaginary time steps.

Following the suggestion of the Referee, we modify the sentence accordingly at page 10.

4. At the end of Sec. 3.4, when discussing the convergence in the environment bond dimension χ , I would have expected a small discussion about the extrapolation criteria based on the discarded probability introduced in this specific context by P. Corboz.

We thank the referee for his comment. We added a few sentences at page 17 to address the extrapolation scheme by Corboz, Czarnik, Kapteijns and Tagliacozzo, and by Rader and Läuchli.

5. At the end of Sec. 3.5.3, a sketchy description of the other approaches (e.g., fast-full update, but not only) might be useful, maybe under a further subsection “Alternative Approaches”. One could spare the necessary space, if needed, by dropping some little redundancies in the previous pages (e.g., Fig. 2).

At the end of Sec. 3.5.3, we have a short discussion on the alternative approaches besides full-update. We have now added a subsection heading there, **3.5.4 Alternative approaches**.

6. I am not really sure why Sec. 4 and 5 about fermionic statistics should be two separate ones, and not merged into a single one :-)

We agreed with the Referee’s comment to merge Sec. 5 into Sec. 4.

7. The notation of Eq.(71) is sub-optimal: dropping the dependence of the Clebsch-Gordan coefficients on the symmetry charges (q, q', q'') might implicitly suggest a full decoupling of the factors A and C, which is instead not there.

We thank the Referee for his careful reading. We fixed Eq.(71) and Eq.(72) accordingly at page 33.

8. I was quite surprised not to find any discussion on how the Authors’ approach deals with non-trivial outer multiplicities, being them coming from SU(2) tensors with rank larger than three or form the symmetry group(s) themselves (like for SU(3)). In the end, they understandably claim that this is what “sets our work apart from that of other iPEPS practitioners”, but they do not provide the reader with any detail, even sketchy, about it. Especially for the beginners, who are declared target of the manuscript, that would be of vital importance, without requiring them to dig into the 75 pages of Ref.[30] at first round of reading. Same applies to the compact notation for the SU(N) labels :-)

Outer multiplicity (OM) is systematically taken care of starting with elementary rank-3 tensors as in the A tensor [see Eq. (71)], or also for the elementary irreducible operators as in Eq. (72). We added a brief summary to the paper on its origin and implications. This was described in detail in Ref. 30. Higher-rank tensors then can be built via contraction.

The consistent treatment of OM for these follows Ref. 94. Is this reference correct? I suspect it should be Ref. 33. [AW: nope, it should be Wb20X = 94] We also kindly refer the reader to the detailed discussions there. Now agreed, OM increases with tensor rank. Yet even OM aside, the number of (small) blocks increases exponentially with increasing tensor rank in any case also for abelian symmetries! In either case, this needs to be avoided and can be dealt with efficiently by fusing indices. We describe how to deal with the large number of small objects in Sec. 5.4.3.

9. About the actual data on Hubbard model(s), I wonder whether the extrapolation in $(D^*)^2$ has some deep meaning behind, or is that simply a numerical observation at this stage (I would be perfectly fine with it, if stated). Same applies to the weak (absent?) scaling with χ^* in panel 8(d): by the way, what is the strange bump in the $D^* = 4$ series there? and why is $D^* = 5$ not displayed?

The choice of $(D^*)^2$ in Fig. 8(c) is purely empirical (and we now state so), as well as the choice of χ^* in Fig. 8(d). For Fig. 8(d), we are looking for consistent behaviour at large χ^* limit and we do not think the energy deviation at small χ^* carries significant meaning.

10. Are site occupation and bond energy extrapolated in a similar way before plotting them in Figs. 8-9? If yes, why is then not the same procedure applied to the singlet-pairing amplitudes in Fig. 10?

No. The site occupations and bond energies in Fig. 9 and the singlet-pairing amplitudes in Fig. 10 are plotted without extrapolation. The extrapolation was used only in Fig. 8(a) and Fig. 8(b), because there we were interested in comparing with QMC results. [JvD: The main text should include a phrase somewhere which clarifies this.]

11. How comes that, while the SU(N) symmetries are directly incorporated in the Tensor Network Ansatz, the conservation of total particle number is not included, and the Authors resort to tuning the average filling via a chemical potential? This might be useful to be explained to the Reader.

When implementing symmetries in PEPS, one needs to bear in mind that the tensor network itself must adhere to translational invariance. Therefore symmetries cannot pick up a ‘drift’ in the average value of the symmetry labels as one moves through the system. For SU(2), for example, clearly for every multiplet with spin S , S_z varies from $-S$ to $+S$ in a completely symmetric way if SU(2) is preserved. Hence the average value for S_z does not drift away. The argument generalizes to SU(N), since all generators are traceless. In the case of particle-hole symmetry, with charge labels taken relative to half-filling, this also generalizes to particle number. The constraint on half-filling is important here, because otherwise one accumulates particles or holes as one increases block sizes when moving through the tensor network. Conversely, if one enforces translational invariance with charge labels defined relative to half-filling, this would always simulate half-filling, irrespective of the chemical potential chosen in the Hamiltonian. One could play trickery with the U(1) charge labels. Here, however, in order to tune the average particle filling smoothly, we simply relax charge symmetry labels to the minimum requirement, namely tracking charge parity. We added a brief remark in this regard after discussing the symmetries with the Hamiltonian in Eq. (76). On the upside, this automatically also permits superconducting correlations.

12. In Fig. 9, orienting the μ and δ axis the same way (i.e., so that left-to-right the population grows / decreases) would probably help the reader a bit.

We thank the referee for his suggestion, We modify the Fig. 9 at page 42 accordingly, so that δ and μ axes are aligned now in the same way.

Second Referee This review provides a detailed introduction to infinite projected entangled-pair states (iPEPS) for fermionic systems with a non-abelian symmetry. It is explained in detail how the symmetry and fermions can be implemented on the level of the PEPS tensors. The involved technical frameworks are not new and have been previously discussed in other papers, however, here they are presented in a unified way. The most important ingredients of the iPEPS algorithms based on imaginary time evolution are also discussed. As example applications, the authors present initial results for two different multi-band Hubbard models.

The paper is clearly structured and written in a pedagogical way, making it a valuable reference especially for non-experts. The example applications are interesting (although a full study will require more calculations as the authors point out), providing evidence of the validity of the approach and showing the impressive bond dimensions that can be reached by exploiting the non-abelian symmetry.

Thus, I can recommend this paper to be published in SciPost Physics. I only have minor comments, listed below, which the authors may want to address when revising their paper.

List of comments

1. Eq.6: is there a particular motivation to use a ket notation ($|\sigma_x^y\rangle$) on the physical leg, rather than just putting a physical index? After Eq (4) the physical index σ_y^x is introduced, thus why not using the physical index instead, which is more common, rather than a ket? That notation may be confusing (also calling the tensor in Eq.6 a rank-4 tensor, rather than a rank-5 tensor may be confusing). The same comment holds also for other figures with labels on the physical leg (Eq(7), Eq(11), ...)

We agree with the referee's suggestion. We fixed Eq. 5, Eq. 6, Eq. 7, Eq. 11 and Eq. 12 accordingly.

2. In Sec 3.5 it would be good to also mention the latest developments in using automatic differentiation to perform a gradient-based energy optimization, see H.-J. Liao, J.-G. Liu, L. Wang, and T. Xiang, Phys. Rev. X 9, 031041 (2019).

We agree with the referee's suggestion. For that, we added a small paragraph at page 25.

3. In the study of the spinful two-band Hubbard model, it would indeed be interesting to study larger unit cell sizes (as the authors point out). But I agree that this is probably beyond the scope of the present work.

We agree with the referee that this would be interesting, indeed, yet is left for the future.

4. Figure 11(a) and (c): on this scale it is difficult to see which energy is lower. Maybe it would be better to show the difference between the two (or subtracting the mean value), in order to better see which of the two states is lower in energy and by how much.

The simple update method used here gives roughly the same ground state energy for 2×2 and 3×3 clusters. As the simple update is too crude to resolve the small energy difference, it may be misleading to investigate the energy difference in more detail, hence we refrain from doing so.

5. Minor typos: - on page 40, 2nd line: a verb is missing after "10⁹ individual contractions" - page 41, line 4: "But whom" -> "But when" - page 42, in the middle: "(a) Either" -> "(a) either" - page 46, second paragraph, after Qspace [30]: "fter" -> "After"

We thank the referee for spotting the typos and letting us know. They are fixed now.