Reply to the Referee

We would like to thank the Referee for his/her careful reading of our manuscript, and for finding our results interesting, specially for considering that *"the manuscript is another example how interesting quantum phases can be realized with cold atomic gases"*. Please find here below a detailed answer to the raised comments. Quotes from the Referee are in *italic*, followed by our replies and the associated changes.

(1) There are several short comings in the figures as well as the figures captions:
(i) In Figure 1, there are no axes labels. It is completely unclear from which range J and μ are varied. This is a very poor style and unacceptable for any publication, even if the plot just shows the qualitative phase diagram. The figure has to be significantly improved.
(ii) In Figure 2, it would be important to add the values of the chemical potentials, and the referee was unable the find the value J for the simulation.
(iii) It would help a lot if the two scans along the phase diagram in Fig. 3 are illustrated in Fig.1.
(iv) In figure caption 1, the authors claim that each phase appears with a topological and a trivial sector. This is in contradiction to the text, where the authors state "we find (1) phases with commensurate long-range order that are topologically non-trivial and (2) ..."

Answer: We are grateful to the Referee for pointing out these shortcomings in our manuscript. We have now rectified these issues. Specifically,
(i) We have now added axis labels in parity with with phase diagram presented in Fig. 7.
(ii) We have now mentioned the J values in the figure caption. However, we did not use any chemical potential for these simulations, but symmetric tensor network that conserves particle number to fix the density, which we now mention this in the caption.
(iii) We have added straight lines in Fig.1(b) indicating the scans taken in Fig. 3.
(iv) We have modified the line as "we find (1) phases with commensurate long-range order that have a non-trivial topological sector".

(2) The notion of incommensurability is very unconventional and based on a relation, which is not explained: Below Eq. (6) the authors claim that the appearance of a peak in the spin structure factor is completely determined by m. It might be that for the present parameters this indeed happens, but unfortunately, this statement is not further justified. Especially, the referee is convinced that in general this relation is not correct. Therefore, it is a very weak point, that the manuscript uses a model dependent parameter for the definition of a phase diagram. This in contrast to long standing history in condensed matter physics, where phases are labeled by observable signatures independent on the underlying problem. Especially, the notion of incommensurability is in general understood as compressible phase, where the density varies smoothly and independently on commensurability with the underlying lattice. This is obviously not the case in the present manuscript, as can be seen in Fig. 3a, where the density exhibits clear incompressible plateaux.

The latter is also in contrast to the claim in figure caption 1, where the authors claim that the incommensurable phase is a superfluid: A superfluid is a compressible phase and can not exhibit plateaux as shown in Fig. 3a.

Answer: As the Referee points out, the location of the peak in the structure factor (k_0) is not characterized by m in a general situation. However, this is the case here, since the total magnetization M is a conserved quantity and $m = M/L$ can only take rational values. A more general Peierls relation is established between k_0 and k_F (or more generally ρ), as shown in Eq. 4, which is the standard condition for a Peierls instability and gives rise to a well-defined notion of commensurability. We could have made the whole analysis here using k_0, but we have decided to employ the extra $U(1)$ symmetry that the system possesses and considered m for simplicity. We do not agree with the Referee about this relation being model dependent or valid only for a certain parameter

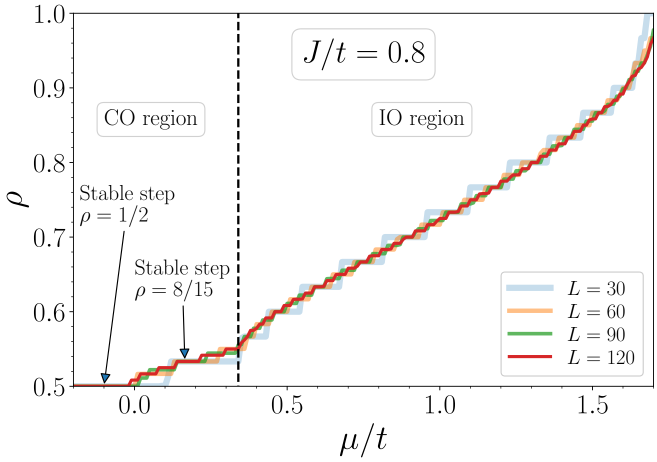

Figure 1: Bosonic density ρ as a function of the chemical potential μ/t for fixed $J/t = 0.8$ and for different system-sizes $L = 30, 60, 90, 120$. The steps in terms of ρ are stable in the commensurate region. As mentioned in the manuscript, some steps (corresponding to more rational values of ρ) are more stable, as seen in the figure for $\rho = 1/2$ and $8/15$. On the contrary, the steps (in terms of ρ) in the incommensurate region are not stable with increasing system-size (and in the thermodynamic limit) showing that the incommensurate region is compressible.

range. It is indeed more general since it depends on the symmetries of the Hamiltonian. We have added some sentences in the text to make these points clearer.

Furthermore, we agree with the Referee that the incommensurate region is indeed compressible. The plateaux of density ρ in Fig. 3(a) appears due to the fact that the system conserves particle number and therefore the density changes in discrete steps in a finite system. In the thermodynamic limit such steps in density ρ in Fig. 3(a) reduces to points and therefore $\frac{\partial \rho}{\partial \mu} \rightarrow \neq 0$ in the incommensurate region (we hereby attach an exemplary Fig. 1 to verify this claim). However, the Devil's staircase structure in the incommensurate phase still persists in terms of other order parameters like m or the structure factor S_σ (see Fig. 7(b)). We have added few sentences regarding the compressibility of the incommensurate region.

(3) There is also a contradiction in the summary of results, where the authors claim that the quasi-superfluid phase extends to the MI at integer fillings. "This occurs for any number of bosons N, which are then in a quasi-superfluid (qSF) phase except at integer fillings, where they form a Mott insulator (MI) (Fig. 1(b))." As it is clearly visible in Fig. 1, the qSF phase does not extend to the MI. This point should clearly be properly explained.

Answer: As the Referee points out, the direct qSF to MI transition is not visible in the current phase diagram. We want to point out this direct transition takes place for $J \ll \alpha$ and at higher values of the chemical potential. In our analysis, we have remained in the $J \sim \alpha$ regime and considered moderate values of the chemical potential. We have now explained such an apparent contradiction in the text.

(4) Furthermore, the referee is extremely puzzled that the notion of Peierls phase: a characteristic property of the Peierls instability is, that it appears for arbitrary weak couplings. This would imply that the system is incompressible for any value of J at half filling. In Figure 1, however, the authors claim that there is always a superfluid phase. At least for $U \to \infty$ this should not be correct due to the famous Peierls instability. The referee would imagine, that a variational approach for the spins with all spins down, but a small additional anti-ferromagnetic modulation allows the hard-core bosons to open a gap and gain energy via the famous Peierls instability. For such a state, the

averaged magnetization would be $m \approx 1$, but the peak in the structure factor appears at 1/2. Such a state would be an example, which violates the above unmotivated definition. The authors should explain in detail and demonstrate, why in the present manuscript there is no such Peierls instability, and why they believe the naming is still meaningful.

Answer: The Peierls instability was first consider in solid-state physics in systems involving the interaction between electrons and phonons, like the SSH or the Holstein model. It is true, as the Referee mentions, that in these systems the Peierls instability, that is the spontaneous breaking of the system's translational invariance, always takes place in a half-filled system at zero temperature. But this is not necessarily the general situation, but rather a specific feature of the mentioned models. In particular, adding extra terms to these Hamiltonians could drive quantum Peierls transitions between gapped ordered and gapless disordered states. Moreover, here we are concentrating on the *bosonic* Peierls mechanism. Bosons possess an affinity to condensate and to form gapless superfluid phases (quasi-superfluid in 1D). In these cases, only a sufficiently strong coupling (i.e., finite value of J in our scenario) can drive the system out of the gapless phase and can result in the Peierls instability in bosons. We have explored such bosonic Peierls transitions in previous works, see for example Phys. Rev. B **99**, 045139 (2019). In that case, the spins can be driven out of the Néel state by adding for example an external magnetic field (σ^z). We have added a few sentence in the manuscript to clarify this point. Finally, as explained in the answer to the second question of the Referee, a Peierls relation depending on m is only possible if the total magnetization is conserved. In that situation, if an antiferromagnetic field is introduced the total magnetization can change. But this will not be a continuous change, rather there will be discrete jumps forming steps with constant magnetization, much like a chemical potential. In particular, the peak in the structure factor will not be the one corresponding to Néel order unless the external field is strong enough. As this field is varied, one would encounter plateaus with different m and therefore different orders characterized by k_0.

(5) The referee is very confused by the notion that, the authors observe a symmetry protected topological phases. The only signature are what they call edge states, which are protected by inversion symmetry. According the seminal work by F. Pollmann [PRB, 064439 (2010)] it is clearly stated that edge states are not a signature of a topological phase protected by inversion symmetry for bosons in one-dimension. This is also nicely confirmed by Ref. [68], where the edge states continuously disappear onto change of the parameters. Furthermore, the general classification of symmetry protected topological phases based on the seminal work above requires a fourfold ground state degeneracy in the thermodynamic limit. This property is not demonstrated in the present manuscript. The referee expects, that the authors rather find some phases which are characterized by some hidden string order as in Ref. [21] or a finite polarization is in Ref. [68]. In the referees opinion it is very important that the authors properly explain their results in the well established context of topological states of matter, and explain which topological signature is a true characteristic property of their system. If the authors are convinced that they observe a symmetry protected topological phase, they should clearly demonstrate the robust fourfold ground state degeneracy and explain the projective symmetry realized on the edge and easy accessible within matrix product states. At the moment, they only demonstrate a two-fold degeneracy, which would be fully consistent with the observations in Ref [21] and [68].

Answer: First, we would like to point out that the seminal paper by F. Pollmann et. al. [PRB, 064439 (2010)] does not consider four-fold degeneracy of the ground state, but Phys. Rev. B **85**, 075125 (2012) from the same group (also, Ref. [21]) does. But that four-fold degeneracy comes from spontaneous breaking of $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry in spin-1 Haldane insulators. Moreover, we should stress that not all type of degeneracies would signal a topological character, but only those where the energy gap closes exponentially with increasing system size, commonly referred to as the *topological* *degeneracy*. In this respect, we point out that for $U \to \infty$, $J \gg \alpha$ and at half-filling, our system boils down to topological SSH model, which shows such two-fold topological degeneracy in the non-trivial phase.

Nevertheless, to firmly establish the topological character of the present system, we now also consider topological invariant in terms of local many-body Berry phases, proposed by Hatsugai [Journal of the Physical Society of Japan **75**, 123601 (2006)]. However, such calculations of local many-body Berry phases are tricky, and requires that the gap does not close under introduction of local twist needed for such calculations (see Phys. Rev. B **99**, 045139 (2019)). That is why, we now consider more stable steps in the CO region, namely $\rho = 1/2$ and $2/3$, where the gap is large enough to perform such calculations using MPS with finite bond dimensions (as opposed by less stable step of $\rho = 8/15$ in the earlier version). In the updated Fig. 4, we now plot the pattern of these local many-body Berry phases. For $\rho = 1/2$, these Berry phases are quantized to either 0 or to π for weak and strong bonds respectively in the bulk. For $\rho = 2/3$, the Berry phases are again quantized to π for the bonds (in the bulk) that respect the inversion symmetry. Such a quantization of Berry phases provides the convincing proof the phases studied here are of topological in nature.

(6) The authors fail completely to provide any evidence of fractional excitations. Especially, the the extreme limit with J ggt and half filling, the spin pattern just provides a static back ground, and the model smoothly connects to the famous SSH model for $U \to \infty$ via a Jordan-Wigner string. It is well established that the SSH model does not give rise to fractional excitations. Therefore, the present model can also not give rise to fractional excitations. Furthermore, the explained signatures are fully consistent with an integer charge at the edge. A clear signature of fractionalization would be that the system exhibits two degenerate quantum many-body ground state, which differ by one particle, and the density between the two states exhibits a difference by 1/2 at each edge. However, such a signature is completely missing in the present manuscript, and therefore the referee is convinced that the notion of fractionalization is incorrect.

Answer: We are grateful to the Referee for pointing out this shortcoming in the earlier version of the manuscript. To mitigate this shortcoming, we now consider the site-resolved density deviation, $\delta \langle \hat{n}_j \rangle = \langle \hat{n}_j \rangle - \rho$ and the corresponding integrated density deviation (IDD) $\delta N_j = \sum_{i \leq j} \delta \langle \hat{n}_j \rangle$. In the updated Fig. 4, we show the profile of IDD δN_j for $\rho = 1/2$ and $2/3$, where it becomes $1/2$ as soon as left edge is crossed (corresponding to $1/2$ particle excitation), and remains fixed at $1/2$ in the bulk (modulo the deviation coming from density pattern in case of $\rho = 2/3$). On the other hand, it suddenly goes to zero in the right edge signaling a $1/2$ hole excitation.

In summary, in the present form the manuscript can not be accepted for publication and significant improvement and clarifications are required before a final decision can be made.

We thank again the Referee for the effort of critically reviewing our manuscript. Her/his concerns have given us the opportunity to substantially improve our work in those aspects that were unclear in the first version. We hope that with our revised version and the above explanations she/he will agree that our manuscript can be considered to be published in SciPost Physics.