nature portfolio

Peer Review File

Dynamical Aharonov-Bohm cages and tight meson confinement in a Z_2-loop gauge theory

Corresponding Author: Dr Enrico Domanti

This file contains all reviewer reports in order by version, followed by all author rebuttals in order by version.

Version 0:

Reviewer comments:

Reviewer #1

(Remarks to the Author)
I co-reviewed this manuscript with one of the reviewers who provided the listed reports. This is part of the Communications Physics initiative to facilitate training in peer review and to provide appropriate recognition for Early Career Researchers who co-review manuscripts.

Reviewer #2

(Remarks to the Author)
The manuscript “Dynamical Aharonov-Bohm cages and tight meson confinement in a Z2-loop gauge theory” presents a theoretical study of 1+1gauge theory where matter particles are coupled to two distinct Z2 gauge fields which simulate an effective loop term. Here, after a nicely written introduction and the model description the authors use symmetry and gauge constraint arguments to reformulate the original Hamiltonian. This part is followed by an analysis of, basically, the model phase diagram. For a vanishing electric field this latter is derived analytically while DMRG is used when the condition of vanishing electric field is relaxed

I find some aspects of this paper of certain interest and therefore I believe that the manuscript has the potentiality for a future acceptance for publication in Communications Physics. That said, to make this happen, some important aspects need to be elaborated and/or highlighted more carefully.

1) Given that we are in the era of quantum simulation and that this paper has been submitted to a top journal, I believe that the authors can make an effort to derive a concrete experimental scheme paving the way for the implementation of their Z2-loop chain. In my opinion, the 6 last lines in the conclusions do not bring anything really relevant. In this regard, I emphasize that this point would represent an important novel result

2) Keeping the topic on the novelty of this article, I’m a bit skeptical that all the discussion around eq (7) is so necessary, since the properties at density 2/3 have been extensively discussed in [61]. In particular the sentence starting at the end of pp 8 and finishing at the beginning of pp 9 (Therefore, following….limit t<<h) summarizes something already known. Can they convince me that I’m wrong and that here they are presenting something substantially new? Also, I have some further observations on this part:

2a) In case the authors want to keep it, can they at least write down how V_{l_ab} depends on the hopping term and on the electric and (perhaps) magnetic field?

2b) The extracted exponents of the dimer correlator in Figures 9 and 10 seem a little too large compared with [61]. Can the authors explain why? Also, since they correctly refer to eq (7) as an integrable model, can they compare these values with the exact values extracted from the Alcaraz Bariev model [97]?

2c) The definition of \tilde{b}_i comes after the authors say something (not entirely clear to me, since I find this part rather confusing) about the correlator <\tilde{b}_i^\dagger \tilde{b}_i+r>. Probably this ordering is not optimal. Also, if I understand correctly, these operators refer to a different basis than that of b,b^\dagger, is it correct? Is it just the string-length basis already considered in [63]?

3) On pp. 2 the authors very clearly introduce the model in eq. (1). Next, the reader finds two pages in which symmetry arguments and gauge constraints are used to derive eq. (4), which serves as the Hamiltonian employable in the DMRG. I honestly find that, as it is currently presented, this part represents only an academic exercise that makes the text rather heavy and even a bit boring. That said, I am not claiming that all these mappings are not useful, but I would like the authors to demonstrate this qualitatively and quantitatively. In particular, Eq. (1) can be easily studied through DMRG, so what do I gain computationally by using Eq. (2) or Eq. (3) instead? Is it only the fact that I have to enforce “by hand” the Gauss law and that I cannot double the effective system size? Moreover, which bond dimension do I need to get accurate analysis (say truncation error \epsilon<10^-7) of large systems when studying the three equivalent models 1,2,4? I think a figure showing these aspects could be really helpful. In this regard, I would also like to comment that Fig. 3 is completely useless as it presents an analysis for L=9 sites that is trivial. As proof of this, the authors study systems with a number of sites up to L=120

4) Apart from the model introduction, I find the main novel result of this paper to be derivation of the Z3 MI insulator. Although both the Z3 and Z2 MI have been already derived in Z2 LGT, see [63] and M. Kebric et al NJP 25 013035 (2023) (apparently the authors overlooked this last reference despite referring to Z2 MI at the end of sec IIIC), here the authors unveil AB caging as a new mechanism responsible for the appearance of these interesting many-body phases. This is a very interesting result, but I think a more thorough analysis is needed. Specifically, presenting the value of the charge gap, see Fig 11 and 16, for fixed L is not optimal. In this regard, any possible doubt about the existence of this phase would disappear if the same figures showed that the charge gap is finite in the thermodynamic limit, so by performing a finite-size extrapolation (possibly with an inset showing the scaling of the gap as a function of 1/L). Can the authors present this analysis? Moreover, it would be interesting to confirm that the dimer correlation function decays exponentially in the MI phase and as power law elsewhere.

In conclusion, I cannot recommend the current version of the manuscript for publication, but I believe that with a little effort the authors are able to change my mind.

Reviewer #3

(Remarks to the Author)
The authors of this manuscript investigate the intricate quantum phase diagram of the Ising lattice gauge theory coupled to dynamical quantum matter in a one-dimensional chain. A key novelty of the study is the introduction of a chain composed of interconnected loops, allowing for the inclusion of a magnetic Wilson plaquette term. The authors identify the emergence of Aharonov-Bohm cages, separated by visons, which significantly influence matter tunneling along the chain.

By employing a combination of analytical and numerical techniques, the authors comprehensively map out the quantum phase diagram, revealing a rich landscape of both gapped and gapless phases. On the numerical front, they introduce an innovative approach to the DMRG encoding, setting their work apart from previous studies.

This paper represents a significant advancement in the quantum simulation of lattice gauge theories, and its findings hold promise for experimental validation in near-term trapped-ion platforms.

We will recommend publication after the following points are addressed by the authors:

\begin{itemize}

\item In the paper the quantum phase diagram is determined by minimizing the triplet Hamiltonian (2). Given, however, that the original problem is governed by the Hamiltonian (1), is it clear that the phase diagrams of the two models coincide? In other words, is it clear that singlet configurations do not contribute to the total energy?

\item Fig. 1 is confusing on page 1. In its current form, it is not suitable as the first figure in the paper. It provides little intuition about the system under investigation and relies on a detailed reading of Section IIB to be understood. We suggest moving it closer to section IIB, and referencing explicitly the sections of the main text where the Bell states are defined.

\item The model is originally defined in terms of $\mathbb{Z}_2$-charged hardcore bosons, and a Jordan-Wigner mapping to $\mathbb{Z}_2$-charged fermions is subsequently used. In turn, following ideas from previous literature, in supplemental material the fermionic system is mapped to a spin 1 model. Although the latter mapping is eventually not used for the numerics, it is worth pointing out that going through the Jordan-Wigner transformation is not necessary, and new gauge-invariant spins X, Y and Z can be defined in terms of the original hardcore bosons and S-spins.

\item It would be beneficial to schematically depict some of the cage patterns in Fig. 4, at least for the largest regions with $l_{AB}=1,2,3$. In Fig. 5 the cages are shown, but it is confusing that the cages are centered where $\bar W$ jumps. We would also suggest including two extra red dots to delimit the AB-trimers, to make the periodicity of the pattern more clear.

\item In Fig. 4 several phases with different l_{AB} are illustrated. Do phases with periodicity $l_{AB}>5$ exist in this model?

\item In Fig. 9, the authors show a correlator starting from site one of the chain. To mitigate finite size effects, we would

suggest starting from the middle of the chain and going to the right. In this way the first $40-50$ points, which provide the algebraic decay, are less affected by boundary effects.

\item Would it be possible to compare the numerical results in Fig. 9 with the analytical values for exponent (slope of the algebraically decaying part of the curve) originating from the effective perturbative Hamiltonian which is the Alcaraz-Bariev integrable model?
\end{itemize}

Version 1:

Reviewer comments:

Reviewer #1

(Remarks to the Author)
I co-reviewed this manuscript with one of the reviewers who provided the listed reports. This is part of the Communications Physics initiative to facilitate training in peer review and to provide appropriate recognition for Early Career Researchers who co-review manuscripts.

Reviewer #2

(Remarks to the Author)
I thank the authors for their efforts in trying to clarify some points I raised in my previous report.

Honestly, I am not impressed by the new part concerning a possible experimental implementation of the model, but I understand that this is probably beyond the authors' reach. Based on the new arguments provided, this seems justified as many subtle points, especially of experimental expertise, seem rather complicated. Therefore, I do not want to insist more in this direction.

I thank the authors for clarifying some aspects of eq 6 (I believe it was eq 7 in the previous version of the article), and I am pleased with this clarification.

I know quite well that boundary effects can make it difficult to extract the expected critical exponents but fixing the first index at site at L/2 and let the last index run till the end of the chain is certainly not optimal as in this way the size of the fit is more limited and boundary effects are still detrimental. The technique usually employed to mitigate this issue is based on considering large chains (it seems that for the authors L=120 is a kind of critical value, but this L can be at least doubled) and removing at least 20-30 sites from both edges. Also, I certainly believe the authors when they say that the extracted value of the exponent is compatible with that obtained from the integrable model, but how do I see it in Fig. 19? In particular, the usual way of showing finite size extrapolations is to report on the x-axis 1/L (not L) so that the point where the fitting equation crosses the y-axis is exactly the thermodynamically extrapolated value of a generic quantity. Note that this argument applies also to the gap discussion in Figs 12 and 18. I firmly believe that this analysis would make the author's claims more reliable.

As I have employed DMRG in different versions of Z_2 LGT, I disagree with the authors comment on the apparent difficulty in simulating eq.1. First, increasing the number of sweeps obviously increases the computation time, but this latter certainly remains affordable. Second, as long as the penalties for enforcing the Gauss's law are sufficiently strong, no fine-tuning is necessary, since nonphysical states are automatically “removed” or, at least, are so irrelevant that no extracted physical property can be altered. And third, based on the latter argument, post-selection procedures are usually unnecessary. Moreover, the authors do not need to remark that ED analysis is limited in size, as this is obviously known, just as it should be known that for a large bond dimension (not specified in Fig 3) and a small enough L (like L=9) even DMRG becomes essentially exact so Fig 3 does not prove much. Overall, I can only stand firm with my observations and suggestions about the usefulness of comparing the different models.

In conclusion, because some of my comments and suggestions were not sufficiently clarified or considered, I cannot convincingly recommend the manuscript for publication. In particular, I still have doubts about the clarity and completeness of the numerical analysis supporting important claims. That said, I recognize the potential of this manuscript, so if a rapid publication is necessary for editorial timing reasons, I prefer to defer the final decision on the acceptance of this manuscript to the editor.

Reviewer #3

(Remarks to the Author)
The authors addressed properly the comments of all referees and improved the paper substantially. We are happy to recommend publication.

Answer to Reviewer 2(1).

We would like to thank the Reviewer for the assessment of our work and for recognizing the interest of some of our findings. Hereafter, we shall comment on the questions raised in the report, clarifying various points and providing further arguments to support the value of our manuscript as a regular article in Communications Physics.

R: "Given that we are in the era of quantum simulation and that this paper has been submitted to a top journal, I believe that the authors can make an effort to derive a concrete experimental scheme paving the way for the implementation of their Z2-loop chain. In my opinion, the 6 last lines in the conclusions do not bring anything really relevant. In this regard, I emphasize that this point would represent an important novel result."

A: We understand that the derivation of a concrete experimental scheme would be an important result, grounding for possible future observations of the physical phenomena presented in our manuscript. In this direction, in the conclusions, we have provided some more details on the recent (yet unpublished) trapped-ion experiment that has been employed to realize a single Z2 gauge-loop and the building blocks to investigate the interplay between Aharonov-Bohm interference and the particle's gauge-invariant dynamics. In particular, we have expanded on a possible strategy to extend this scheme to a full chain of loops, and to account for the required Ising couplings generating the magnetic plaquette terms. We believe that a more detailed analysis to devise a realistic experimental scheme goes beyond the scope of the present paper, and we leave a more detailed exploration discussing realistic parameters and possible sources of noise for a future work. We hope that this new paragraph, which points at the key additions that would need to be developed with respect to already-published schemes for implementing a Z2 chain, meets some balance and suffices to address the Reviewer's suggestion.

R: "Keeping the topic on the novelty of this article, I'm a bit skeptical that all the discussion around eq (7) is so necessary, since the properties at density 2/3 have been extensively discussed in [61]. In particular the sentence starting at the end of pp 8 and finishing at the beginning of pp 9 (Therefore, following. . . .limit $t \ll h$) summarizes something already known. Can they convince me that I'm wrong and that here they are presenting something substantially new?"

A: We thank the Reviewer for raising this point. We would like to emphasize that Eq.(7) is indeed a novel result, specific of the small electric field regime of the loop chain and has no equivalent in the $\mathbb{Z}_2$ chain investigated in [61]. Indeed, while the strong electric field limit of the $\mathbb{Z}_2$ chain provides an effective description in terms of the Alcaraz-Bariev model with a two-site constraint, the chain fragmentation resulting from our caging phenomenon determines different possible constraints that depend on the size of the Aharonov-Bohm cages and, importantly, occurs in a parameter regime that is completely unrelated to the

tight confinement by a strong electric field of the Z2 chain. In particular, we show that the formation of the cages and their sizes depend on the interplay between the Hamiltonian parameters and the filling fraction ν, so that different values of ν correspond to clusters of different size $\ell_{\rm AB}$ and nothing is really special about $\nu = 2/3$, as similar observations hold, for instance, at $\nu = 1/2$, as explained in the main text and in the Appendices. The discussion revolving around the properties of the effective Alcaraz-Bariev model is thus needed, in our opinion, also to account for the various possible constrained regimes. Let us emphasise that the fact that we find a mapping to the same family of effective models in a weak electric field does not mean that these properties have already been covered in the strong-field limit of the standard Z2 chain [61]. It should actually be seen as the opposite: it is quite remarkable that, due to AB interference, we can find a mapping to the same model but for weak electric fields, and that this mapping depends on the different geometric caging.

Concerning the large electric field regime of the loop model, when $h \gg t$ and $h \gg J$, pairs of Z2 charges get connected by short electric field lines carrying one unit of electric field, while all the other bonds in the chain are eigenstates of the electric field operator with zero eigenvalues. In this case, we refer to the equivalent behaviour of the $\mathbb{Z}_2$ chain in the same limit, as described in [61]. While the analogy strictly holds for $h \gg t, J$, the validity of the effective description in terms of dimers extends to any value of the magnetic coupling, even up to $J \approx h$, for which, in the manifold of lowest-energy states, not all bonds are found in eigenstates of the electric field operator. This is also an important difference with respect to the standard Z2 chain, and the fact that we demonstrate that the charges still form dimers separated by short electric field lines in this regime is also not straightforward.

Thanks to the Reviewer's comment, we have reflected that the novelty of our findings might not have been emphasized enough in the previous version of the manuscript. Therefore, in the discussion of Sec.IIIB we have clarified both differences and analogies to the known case of the Z2 chain, highlighting the novelty of our results. We thank the Reviewer for his comment, which has induced us to improve the clarity of the presentation.

R: "In case the authors want to keep it, can they at least write down how $V_{\ell_{\rm AB}}$ depends on the hopping term and on the electric and (perhaps) magnetic field?"

A: We thank the Reviewer for raising this suggestion. In the $h \ll t, J$ limit, an analytical expression for the parameters of the effective Hamiltonian can be obtained only for $\ell_{\rm AB} = 2$ and is reported in the text. For $\ell_{\rm AB} > 2$, the parameters are evaluated from lengthy analytical expressions derived from perturbation theory in the Appendix: the dependence on h is always given by h^2/t, due to the second order perturbative approach for small h, while the dependence on the magnetic coupling J has to be analyzed numerically. In the case $\nu = 1/2$, the ratio $\delta_{\ell_{\rm AB}=3} = V_{\ell_{\rm AB}=3}/2t_{\ell_{\rm AB}=3}$ is reported as a function of J/t in Fig.(16) of the Appendix.

The parameters of the Alcaraz-Bariev model in the dimerized regime at $h \gg t$ are also reported in the Appendix (where we have corrected a typo) and we have added the expression for the effective hopping to the main text, for completeness.

R: "The extracted exponents of the dimer correlator in Figures 9 and 10 seem a little too large compared with [61]. Can the authors explain why? Also, since they correctly refer to eq (7) as an integrable model, can they compare these values with the exact values extracted from the Alcaraz Bariev model [97]?"

A: We thank the Reviewer for raising this point, and for suggesting a more detailed comparison. This apparent discrepancy with the exact values reported in [97] is due to finite-size effects. While in [97] these exponents are obtained with iDMRG, our chain is limited to 120 sites and finite-size effects are still important for these sizes. Indeed, the analysis of the correlator sensibly depends on the initial point at which it is evaluated. In the previous version of the manuscript, we had used $g(r) = \langle b_1^\dagger b_{1+r} \rangle$. To minimize boundary effects, we have now adopted a prescription that starts from the bulk of the chain $g(r) = \langle b_{L/2}^\dagger b_{L/2+r} \rangle$, which reduces the value of the fitted exponent. Moreover, we have performed a more careful finite-size analysis that allows us to extrapolate an approximate value for the exponents in the thermodynamic limit, which is now reported in the newly added Appendix G. As suggested by the Reviewer, we can compare these values quantitatively to the exact results of the Alcaraz-Bariev model, and we find that they are both compatible. We note that we have restricted our analysis to lengths that allow for an even number of dimers, as an even/odd parity effect exists at finite-size, which produces a larger value of the correlator $g(r)$ at $r = 1$ for an odd number of dimers. Working with an odd number of dimers would lead to an overestimation of the exponents.

We thank the Reviewer for this suggestion, which has helped us improving the quality of our manuscript and the presentation of our results.

R: " The definition of $\tilde{b}_i$ comes after the authors say something (not entirely clear to me, since I find this part rather confusing) about the correlator $\langle \tilde{b}_i^\dagger \tilde{b}_{i+r} \rangle$. Probably this ordering is not optimal. Also, if I understand correctly, these operators refer to a different basis than that of b,$b^\dagger$, is it correct? Is it just the string-length basis already considered in [63]?"

A: We thank the Reviewer for raising this point. Let us try to explain in more detail the differences of these meson-type operators. The discussion preceding the definition of the operators $\tilde{b}_i$ concerns the behaviour of the dimer-correlator in the low electric field regime of the model, in terms of the operators $b_i = a_i |\Psi_{i\ell}^+\rangle\langle\Phi_{i\ell}^-| a_{i+1}$: in this case, the local Hilbert space of each bond in the chain effectively involves only two Bell states $\{|\Phi^-\rangle, |\Psi^+\rangle\}$, as the two particles in a dimer are separated by a 0-flux eigenstate of $(S^z)^2$, namely $|\Phi^-\rangle$ and are bordered by the π-flux states $|\Psi^+\rangle$. It is afterwards emphasized that an equivalent dimerized regime is realized for $h/t, h/J \gg 1$, as particles are now connected by short electric field lines, being located at nearest neighboring po-

sitions and enclosing a link in an eigenstate of the electric field operator. When the requirement $h/J \gg 1$ is relaxed and the magnetic coupling is allowed to reach values $J \approx h$, dimers are still formed, where two particles are still separated by a link eigenstate of the electric field operator, while all other links are not. Working in a basis of the local Hamiltonian of each bond, which accounts for both the electric and magnetic terms, the local Hilbert space of each link is spanned by three states, that we have denoted as $|\epsilon_{\Uparrow}\rangle, |\epsilon_0\rangle, |\epsilon_{\Downarrow}\rangle$ of which $|\epsilon_{\Uparrow}\rangle$ lies at a much higher energy and thus effectively decouples. In this case, a dimer would appear as a charged excitation on top of a polarized vacuum state in which all the links are in the $|\epsilon_{\Downarrow}\rangle$ state and thus corresponds to the operators $\tilde{b}_i, \tilde{b}_i^\dagger$, where $\tilde{b}_i = a_i|\epsilon_{\Downarrow}\rangle\langle\epsilon_0|a_{i+1}$. Hence, the redefinition of the dimer operators reflects the most appropriate choice of the basis states spanning the local Hilbert space of each bond of the chain, in the studied regime.

R: "On pp. 2 the authors very clearly introduce the model in eq. (1). Next, the reader finds two pages in which symmetry arguments and gauge constraints are used to derive eq. (4), which serves as the Hamiltonian employable in the DMRG. I honestly find that, as it is currently presented, this part represents only an academic exercise that makes the text rather heavy and even a bit boring. That said, I am not claiming that all these mappings are not useful, but I would like the authors to demonstrate this qualitatively and quantitatively. In particular, Eq. (1) can be easily studied through DMRG, so what do I gain computationally by using Eq. (2) or Eq. (3) instead? Is it only the fact that I have to enforce "by hand" the Gauss law and that I cannot double the effective system size? Moreover, which bond dimension do I need to get accurate analysis (say truncation error $\epsilon < 10^-7$) of large systems when studying the three equivalent models 1,2,4? I think a figure showing these aspects could be really helpful. In this regard, I would also like to comment that Fig. 3 is completely useless as it presents an analysis for L=9 sites that is trivial. As proof of this, the authors study systems with a number of sites up to L=120."

A: We agree with the Reviewer that the section about our encoding for DMRG was breaking the flow of the paper towards the main physical results. Therefore, we have kept only the main points of our approach in the main text, moving the rest for the Appendix. Let us extend on some of the points raised, and explain why the presented approach is crucial for accurate and efficient calculations. To the best of our knowledge, trying to enforce all the symmetries of the model as other approaches aim, does not allow to simultaneously enforce both particle-number and Gauss' law conservations. First, we would like to highlight that, while it is true that DMRG could be applied directly to Eq.(1), in passing from equation (1) to (2) we make use of the local conservation of the total spin angular momentum to get rid of all the zero-energy dark-states corresponding to the $s = 0$ representation of the algebra. Note that, as discussed in the paper, these dark states decouple from the dynamics and lead to a fragmentation of the chain that may lead to a high number of almost-degenerate states depending on the fragmentation point, making the DMRG convergence very slow and requiring

a huge number of sweeps. Therefore, we do not want to perform a DMRG approach directly based on Eq.(1), as we are eventually interested only in the physics within the $S = 1$ triplet sector of each link, and we want to avoid that an initial random MPS has any overlap with configurations containing any number of $s = 0$ states. On the other hand, when applying DMRG to Eq.(2), we would now need to ensure that our state lies in the chosen gauge sector, by enforcing an extensive number of local conservation laws that extend over three neighboring sites of the MPS (two for gauge and one for matter degrees of freedom). In order to do this, the typical approach is to add artifical penalty terms in the Hamiltonian that push unphysical configurations that do not belong to the neutral gauge sector to higher energies. Finding the correct strength of these penalty terms, such that it does not interfere with the physics we aim at studying, can be non-trivial and very problem-dependent.

Instead, the method that we propose in which each bond is divided into two half-links leading to Eq.(4), is partially inspired by the rishon approach for studying quantum-link models in two dimensions, demonstrated in Phys. Rev. X 10, 041040. In that case, as in ours, doubling the number of links comes with the advantage of a Gauss' law having support on single "supersites" of the newly defined system, but requires additional local conditions for the states on neighbouring half-links, which the authors of the PRX enforce through a penalty term, that again needs to be carefully tuned at each DMRG iteration. Dealing with these kind of penalties also requires post-selection of the results, to ensure that DMRG converges to a state that has vanishing overlap to the unwanted configurations. With our method, we identify a global symmetry that has support on single sites of the MPS and can thus be easily imposed numerically without the need of any penalty term: in a specific symmetry sector, all the necessary constraints are automatically enforced, as is demonstrated in the Appendix. For these reasons, we do not think that a comparison of different DMRG approaches based on Eq.(1), (2) or (4) is actually necessary, as the main advantages coming from Eq.(4) are that we can significantly reduce the size of the computational basis for the MPS algorithm, by removing all the states not belonging to the studied symmetry sectors, and that we do not need either to control Hamiltonian penalties to enforce these symmetries or any post-selection of the results to check that they are fulfilled.

Concerning Fig.3, we would like to point out that it is meant to provide a simple benchmark that our DMRG strategy is correctly enforcing all symmetries of the model (especially in the absence of the more formal details contained in the Appendix), by direct comparison to exact diagonalization which limits the maximum system size to those reported. We also note that the size of the physical Hilbert space for L sites grows as 3^{L-1} and hence quickly becomes out of the reach of exact diagonalization methods. In the exact diagonalization, these symmetries are enforced by explicitly working with the reduction of the model's Hamiltonian to the correct symmetry sectors, and the quantitative comparison thus provides a consistent validation of our MPS approach, which can then be

extended to larger sizes.

R: "Apart from the model introduction, I find the main novel result of this paper to be derivation of the Z3 MI insulator. Although both the Z3 and Z2 MI have been already derived in Z2 LGT, see [63] and M. Kebric et al NJP 25 013035 (2023) (apparently the authors overlooked this last reference despite referring to Z2 MI at the end of sec IIIC), here the authors unveil AB caging as a new mechanism responsible for the appearance of these interesting many-body phases. This is a very interesting result, but I think a more thorough analysis is needed. Specifically, presenting the value of the charge gap, see Fig 11 and 16, for fixed L is not optimal. In this regard, any possible doubt about the existence of this phase would disappear if the same figures showed that the charge gap is finite in the thermodynamic limit, so by performing a finite-size extrapolation (possibly with an inset showing the scaling of the gap as a function of 1/L). Can the authors present this analysis? Moreover, it would be interesting to confirm that the dimer correlation function decays exponentially in the MI phase and as power law elsewhere."

We thank the Reviewer for the interest in our derivation of the Mott insulating phases generated by the dynamical Aharonov-Bohm caging phenomenon. We take the opportunity to remark that we believe that, in addition to these results on ZN Mott insulators, the main result of our paper is the fact that destructive Aharonov-Bohm interference provides a novel mechanism of strong particle confinement, and that this tight confinement can be found in spite of having a vanishingly small electric-field strength h. Due to the interplay of the magnetic coupling and the particle filling, visons (π-flux configurations) proliferate along the chain and can break it in caged structures in which particles are strongly confined in pairs, which can have different sizes and move or be packed in the chain depending on the filling, either behaving as a Luttinger liquid or as a Mott insulator.

As suggested by the Reviewer, to confirm the stability of the Mott phases in the thermodynamic limit, we now provide additional figures that show how the charge gaps scale to non-zero values in the limit $L \to \infty$ (Fig.12 in the main text for $\nu = 2/3$ and Fig.18 in the Appendix for $\nu = 1/2$). At the same time, in Fig.12, we have also shown that the dimer correlation function decays exponentially only in the Mott insulating phase.

Answer to Reviewer 3.
We would like to thank the Reviewer for deeming our paper as "a significant advancement in the quantum simulation of lattice gauge theories" and for recognizing the interest about our findings. In the following, we address the comments and suggestions.

R: "In the paper the quantum phase diagram is determined by minimizing the triplet Hamiltonian (2). Given, however, that the original problem is governed by the Hamiltonian (1), is it clear that the phase diagrams of the two models coincide? In other words, is it clear that singlet configurations do not contribute

to the total energy?"

A: We point out that our decision of choosing $s = 1$ for each link is equivalent to fixing a "gauge-sector" for the local symmetry corresponding to the local conservation of $S^2_{i_\ell} = \sum_\alpha (S^\alpha_{i_\ell})^2$, as in the case of the $\mathbb{Z}_2$ gauge symmetry, for which we work in the neutral gauge sector. The phase diagrams of the two models thus strictly coincide in the selected symmetry-sector. Singlet states are π-flux dark-states that completely decouple from the dynamics, and lead to an effective fragmentation of the chain that remains fixed and has no dynamics. Indeed, all terms of the Hamiltonian vanish at an $s = 0$ state, which thus does not contribute to the energy of the system. Doping the lattice with a certain number M of $s = 0$ states will reduce to studying independent triplet Hamiltonians describing chains of smaller lengths L_i, $i \in \{1, \dots, M + 1\}$. Therefore, addressing the triplet case is the most natural choice, as the ground state of the total system in the presence of $s = 0$ states will be given by a product state of the ground states of each independent sub-chain. However, if one is interested in which symmetry sector has the lowest energy, a similar analysis to the one of Sec.IIIA of the paper would be needed, to find the number and distribution of $s = 0$ states corresponding to the lowest energy, accounting for all possible ways of arranging particles in each independent subchain. However, while the discussion of Sec.IIIA analogously relies on the local conservation of $(S^z_{i_\ell})^2$ at $h = 0$, with the different caged configurations corresponding to different symmetry sectors, the analysis is justified by the explicit breaking of the local symmetry when $h \neq 0$.

R:"Fig. 1 is confusing on page 1. In its current form, it is not suitable as the first figure in the paper. It provides little intuition about the system under investigation and relies on a detailed reading of Section IIB to be understood. We suggest moving it closer to section IIB, and referencing explicitly the sections of the main text where the Bell states are defined."

A: We thank the Reviewer for raising this point. We have moved Fig.1 to Sec.IIB, with reference to the parts of the main text where the Bell states are defined later on in the text.

R:"The model is originally defined in terms of $\mathbb{Z}_2$-charged hardcore bosons, and a Jordan-Wigner mapping to $\mathbb{Z}_2$-charged fermions is subsequently used. In turn, following ideas from previous literature, in supplemental material the fermionic system is mapped to a spin 1 model. Although the latter mapping is eventually not used for the numerics, it is worth pointing out that going through the Jordan-Wigner transformation is not necessary, and new gauge-invariant spins X, Y and Z can be defined in terms of the original hardcore bosons and S-spins."

A: We have added a comment in the section of the Appendix about the derivation of the spin-1 model, remarking that the Jordan-Wigner transformation is not essential, but rather a way to make contact with the previous literature. We thank the Reviewer for pointing this out.

R:" It would be beneficial to schematically depict some of the cage patterns in Fig. 4, at least for the largest regions with $l_{AB} = 1, 2, 3$. In Fig. 5 the cages are shown, but it is confusing that the cages are centered where $\bar{W}$ jumps. We would also suggest including two extra red dots to delimit the AB-trimers, to make the periodicity of the pattern more clear.

A: We thank the Reviewer for this suggetsion. We have modified Fig.4 to show the periodic flux configurations in the fully-connected and in the caged regimes at $\ell_{\rm AB} = 1, 2, 3$. In Fig.5, we have preferred to remove the schematic representation of the configurations, writing explicit labels to describe the different regimes qualitatively. This is to avoid confusion with the new version of Fig.4, in the case $\ell_{\rm AB} = 2$. While in Fig.4 we show the region of parameter space in which $\ell_{\rm AB} = 2$ dimers completely cover the chain, in Fig.5 we study the filling $\nu = 2/3$ at which dimers can no longer fully cover the chain, but instead arrange in several degenerate configurations, as specified in the caption. In this case, the distribution of fluxes is, in general, not periodic.

R:"In Fig. 4 several phases with different l_{AB} are illustrated. Do phases with periodicity $l_{AB} > 5$ exist in this model?"

A: We haven't found any phase with $\ell_{\rm AB} > 5$ in the ground-state of the system. Configurations with $\ell_{\rm AB} > 5$ certainly exist, but we believe they are higher in energy.

R:" In Fig. 9, the authors show a correlator starting from site one of the chain. To mitigate finite size effects, we would suggest starting from the middle of the chain and going to the right. In this way the first $40 - 50$ points, which provide the algebraic decay, are less affected by boundary effects."

A: We thank the Reviewer for the suggestion, and we agree that evaluating the correlator away from the boundaries mitigates finite-size effects. Therefore, we have replaced our figures with equivalent ones in which the dimer correlator is evaluated starting from the middle point of the chain, reporting the modified values of the exponent for the algebraic decay.

R:"Would it be possible to compare the numerical results in Fig. 9 with the analytical values for exponent (slope of the algebraically decaying part of the curve) originating from the effective perturbative Hamiltonian which is the Alcaraz-Bariev integrable model?"

A: The numerical results of Fig.9 and 10 are affected by finite-size effects. To estimate the exponents in the thermodynamic limit, we have performed a more careful finite-size analysis that is presented in the new Appendix G. Calculating the exponents for different values of the system size L, we managed to extrapolate their value in the limit $L \to \infty$, which are perfectly compatible with the analytical results of the Alcaraz-Bariev model. The analysis requires that only lengths L allowing for an even number of dimers are explored. Indeed, a finite-size effect, determining a larger peak of the dimer correlator $g(r)$ for $r = 1$, exists

when the number of dimers in the chain is odd, producing an over-estimation of the decay's exponent.

Best regards,

The authors.

Answer to Reviewer 2(1).

We would like to thank the Reviewer for the assessment of our work and for recognizing "the potential of this manuscript". We are glad that we managed to clarify some aspects of our work that were highlighted in the previous report. In the following, we shall provide further arguments to elucidate the points that the Reviewer still considers to be unsatisfactory.

R: Honestly, I am not impressed by the new part concerning a possible experimental implementation of the model, but I understand that this is probably beyond the authors' reach. Based on the new arguments provided, this seems justified as many subtle points, especially of experimental expertise, seem rather complicated. Therefore, I do not want to insist more in this direction.

A: Devising a detailed experimental scheme and discussing specific parameters and sources of noise and gauge-violation, requires a very careful analysis that would deviate us from the current scope of the present work. It is certainly not "beyond authors' reach" (we find such wording very unfortunate), but simply beyond the scope of the present work. We will provide a more in depth analysis in a future paper.

R: I know quite well that boundary effects can make it difficult to extract the expected critical exponents but fixing the first index at site at L/2 and let the last index run till the end of the chain is certainly not optimal as in this way the size of the fit is more limited and boundary effects are still detrimental. The technique usually employed to mitigate this issue is based on considering large chains (it seems that for the authors L=120 is a kind of critical value, but this L can be at least doubled) and removing at least 20-30 sites from both edges. Also, I certainly believe the authors when they say that the extracted value of the exponent is compatible with that obtained from the integrable model, but how do I see it in Fig. 19? In particular, the usual way of showing finite size extrapolations is to report on the x-axis 1/L (not L) so that the point where the fitting equation crosses the y-axis is exactly the thermodynamically extrapolated value of a generic quantity. Note that this argument applies also to the gap discussion in Figs 12 and 18. I firmly believe that this analysis would make the author's claims more reliable.

A: We thank the Reviewer for their comments. However, such technical comments on numerics are of marginal importance in our discussion, which is focused on the novelties inherent in our new Z_2 loop model. Specifically:

- the present finite-size analysis of the charge gap already demonstrates that it does not tend to zero as the system's size grows, which supports one of our main claims that the Mott phases are stable in the thermodynamic limit. A more computationally-demanding study could achieve a more accurate estimate of its value as $L \to \infty$, but we certainly believe that this is not the main point of our work.

- Concerning the dimer correlators, we agree that much larger sizes or iDMRG would be required to achieve a reliable estimate of the decay's exponents in the thermodynamic limit, and we have remarked this point in the Appendix. However, we note that, strictly speaking, Fig.20 is not the right place to look at to track the exponent. Our approach, instead, is based on the analytical derivation of the Alcaraz-Bariev model, for which the exponents are known exactly, as an effective description of our system in two different parameters regimes. Therefore, it should be clear that further computationally-exhaustive analysis are not worth in this case.

For the avoidance of doubt, we have replaced our figures with equivalent ones in linear scale, in which the data is plot against $1/L$ and the extracted values of both the charge gaps and the correlators' exponents can be read on the y-axis.

R: As I have employed DMRG in different versions of Z_2 LGT, I disagree with the authors comment on the apparent difficulty in simulating eq.1. First, increasing the number of sweeps obviously increases the computation time, but this latter certainly remains affordable. Second, as long as the penalties for enforcing the Gauss's law are sufficiently strong, no fine-tuning is necessary, since nonphysical states are automatically "removed" or, at least, are so irrelevant that no extracted physical property can be altered. And third, based on the latter argument, post-selection procedures are usually unnecessary. Moreover, the authors do not need to remark that ED analysis is limited in size, as this is obviously known, just as it should be known that for a large bond dimension (not specified in Fig 3) and a small enough L (like $L = 9$) even DMRG becomes essentially exact so Fig 3 does not prove much. Overall, I can only stand firm with my observations and suggestions about the usefulness of comparing the different models.

A: The purpose of our approach is to avoid using penalties by fixing *a priori* all the symmetry sectors, demonstrating that working with a larger computational basis, as would be required by simulating directly Eq.(1), is not needed. Primarily, in our study we only focus on the $s = 1$ representation of the spin matrices at each link of the chain: simulating Eq.(1) would imply keeping all the $s = 0$ states, which would greatly increase the size of the computational basis. Moreover, these states are energetically decoupled and might result in many degenerate configurations that would need to be penalized artificially by the addition of suitable Hamiltonian terms. In the same way, as remarked by the Reviewer, energetic penalties would be required to fix the neutral gauge sector. In our experience with this study (and as reported in other independent studies - see e.g. Phys. Rev. X 10, 041040), such penalties are generally non-trivial to control, and we believe that this can be model dependent. In our particular case, we have indeed experienced the problem that penalty-guided DMRG methods end up converging to wrong minima of the energy for some parameter regimes of our model, and this was the motivation to put forth the alternative method. While we acknowledge that other authors, such as the Re-

viewer, might have found better routes to successfully deal with this issue in other models, it is difficult for us to understand the position of the Reviewer at this point. Regardless of being able to do more sweeps or finding appropriate ways to add penalties without changing the physics, our method is simply more straightforward and computationally less demanding, as it provides an alternative to fix the gauge sectors without using penalties. We take the opportunity to remark that the purpose of our work is not to benchmark our method against alternative DMRG approaches in terms of performance, even though there is a clear and objective advantage of working with a reduced computational basis. Our aim instead is to propose another way to correctly enforce all the symmetries of the problem without the need of tuning penalty terms. The comparison with exact diagonalization, for which all symmetries can be manually imposed, has to be understood in this context: the agreement simply shows that we are indeed working in the correct symmetry sectors, as nothing is really special, in this sense, about any value of L. We note that the fact that DMRG is quasi-exact upon increasing the bond dimension, particularly for gapped models, is also common knowledge. What is not straightforward, and thus benefits from a direct benchmark against exact diagonalization, is that our new DMRG strategy deals with the gauge symmetry correctly.

Still, in order to address the concerns of the Reviewer on the quantitative reliability of simulations based on the new devised approach at large system sizes, we compare the ground state energies obtained with our method at $L = 120$, with the values extracted by applying DMRG to the spin-1 model that describes the system in the neutral gauge sector (see Appendix B of the manuscript). In this case, the correct particle sector has to be fixed by a fine-tuning of a chemical potential term. We notice that a similar mapping has been used in previous works on the standard $\mathbb{Z}_2$ chain and that the resulting spin-1/2 Hamiltonian has been employed to perform DMRG for certain aspects of these studies - see Phys. Rev. Lett. 124, 120503. The newly added comparison is presented at the end of Appendix C, in Fig.(14) and shows a perfect quantitative agreement.

Answer to Reviewer 3.
We thank the Reviewer for assessing our work and we hope that, with our answer, we can move to the next step of the publication process in Communications Physics.

Best Regards,

The authors.