Reply to the referee 1

We sincerely thank the referee for his excellent work. This report is highly detailed and professional, which is very helpful in improving the quality of our paper. Below, we will elaborate on the revisions and improvements made in the new version of the manuscript and provide a point-by-point response to the referee's questions and comments.

1. *It is not quite clear to me what the physical content of the results (expressions and plots) are. Is the claim that these quantities should be particularly simple to compare to quantities measured in experimental platforms? What about the curves of zeroes; are they measurable? Or do they (or at least: are expected to) separate different phases, like for Lee–Yang? Or do the explicit expressions for low N serve more as a proof of concept, to show that the method gives very explicit results, and is the reader supposed to be able to similarly use the method (if they had the author's software package) to compute quantities that they are actually interested in. Similarly, are the values q=2 etc. meant to be of particular physical relevance, or at least expected to be easily within the experimentally accessible range, or just for illustrative purposes? This should be clarified in the introduction, main text, and conclusion.*

   In this work, we have several physically interesting results, including: 1. The explicit results obtained in this paper are valuable for comparison with quantities measured in quantum circuits, particularly in the context of error mitigation. A significant advantage of our results is that they are both exact and analytical, requiring no approximations, and can, in principle, be evaluated with arbitrary precision. We have computed these results for systems ranging from 8 to 18 qubits, which align with the scales of real-world experiments. The specific values chosen for parameters, such as q=2, are not critical; they were selected for illustrative purposes and can be readily adjusted to other values in the calculations. 2. The method employed in this paper demonstrates that by integrating the rational Q-system approach with computational algebraic geometry, we can compute a range of physically relevant quantities for medium-sized systems, such as the correlation functions examined in this paper. This work extends previous results on the computation of partition functions for the six-vertex model. The method itself holds significant potential and can be applied to compute other quantities of interest for quantum integrable models solvable via the Bethe ansatz. 3. The condensation curves of zeros are indeed a direct analog of Lee-Yang or Fisher zeros. As the referee correctly pointed out, these curves separate different phases of the model. Such zeros can, in principle, be measured and have already been measured in slightly different contexts, as demonstrated in recent experimental works (see [PRL 118, 180601 (2017)] for an example). In our current context, since the zeros emerge in the long-time limit, their observation may exceed the coherence time of existing quantum platforms. This presents an intriguing open question and a significant challenge for measuring Lee-Yang zeros in this setting. Additionally, we would like to emphasize that the correlation function computed in this paper is the lattice analog of the Loschmidt amplitude. This quantity plays a pivotal role in dynamical quantum phase transitions, and the Lee-Yang zeros for the Loschmidt echo are of great interest in characterizing different dynamical quantum phases. From this perspective, our results represent the first step toward modeling dynamical quantum phase transitions on quantum circuits and provide the first theoretical prediction for the Lee-Yang zeros of the Loschmidt echo.

Modifications: 1. We added three paragraphs in the Introduction section to summarize the main physical results and their implications. 2. We also added some discussion on these points in various places in the Conclusion section.

2. *It would be very helpful if the gap between the (somewhat vague or high-level) abstract description of the computational algebraic geometry and the concrete results can be closed by describing the actual computation (e.g. intermediate results) for at least one example to illustrate the theoretical story and give at least a flavour of the actual computations that are done.*

   We have added an explicit example in Section 3.2 to illustrate how the computation works in detail.

   Modifications: An explicit example is added in Section 3.2.

3. *(10) and surrounding text: I believe that $\check{R}$ always has adjacent subscripts, in this case i,i+1 and i+1,i+2 rather than i,j etc.*

   This is correct. The YBE, as it stands, is correct; we can specify to the situation pointed out by the referee. We, therefore, added a sentence around (10).

4. *Remark 1: The phrase 'classical integrable' could be mistaken to mean 'classically integrable'; consider rephrasing to clarify, and perhaps add that these lattice models are 2d.*

   The first sentence is changed to "It first appeared in integrable lattice models, which describe classical 2D lattice systems, by positioning the 6-vertex model on a diagonal lattice" in order to eliminate the potential misunderstanding.

5. *Following (18): clarify that $0 < \gamma \ll 1$.*

   We have changed $\gamma \ll 1$ to $0 < \gamma \ll 1$.

6. *Consider moving footnote 1 to p4 already.*

   It is moved according to the referee's suggestion. Now it is inserted below (3).

7. *p9: mention that the resolution of the identity relies on the completeness of the Bethe ansatz, which will be discussed in Section 3.2.*

   A footnote is added to stress that the resolution of identity relies on the completeness of the Bethe ansatz.

8. *(38): here K is switched to N mid-formula. Pick one symbol and use throughout.*

   This typo is corrected.

9. *p11, before 'Rational Q-system': what does 'medium quantum numbers' mean - M=L, M=L/2, ...?.*

   Here 'medium' means we consider medium system size. To eliminate confusion, the corresponding sentence is now modified to "Our approach nicely covers the range of medium system size with magnon number N ranging in $1, \dots, L$".

10. *Rational Q-system: what does 'more rigorously' mean? which parts are/not rigorous?*

    The corresponding sentence is now changed to "This was first observed in [21] and was proven and generalized in [22, 23, 28]."

11. *Rational Q-system: it should be mentioned that completeness of the (Wronskian BAE =) QQ system has been proven for generic parameters by Mukhin–Tarasov–Varchenko, cf Chernyak–Leurent–Volin; I suppose this includes the case of alternating inhomogeneities* $\theta_j = (-1)^j u/2$ *as here (perhaps with a small twist).*

    We added one sentence at the end of the paragraph "Completeness of the rational Q-system (which is equivalent to the so-called Wronskian Bethe Equations) has been proven in [51], based on earlier works [52, 53]." to mention this point and added three references.

12. *above (53):* $\eta = 0$ *is not the homogeneous case, cf text below (7); but* $\eta \to 0$ *suitably interpreted (by rescaling u) is [to be corrected throughout the paper, e.g. also in footnote 3]*

    This is indeed more accurate. We changed the wording accordingly. Above (53), the sentence in the bracket has been changed to "(see details below (7))" and above (54), the sentence is now changed to "For the XXZ chain, Baxter's polynomial is defined by". Similar modifications are made throughout the paper, including footnote 3.

13. *footnote 5: to clarify the scope of the method used here, it would be good to mention some key applications for which the original BAE have benefits?*

    To clarify the key applications where the original BAE has benefits, we added the following sentence to footnote 5: "In terms of finding *specific* solutions, such as the antiferromagnetic vacuum ground state and the first few excited states, it is more convenient to use the original Bethe ansatz equation (or more precisely, the logarithm of the BAE). For these solutions, the mode number exhibits a clear pattern and the Bethe roots can be found numerically by iteration."

14. *'Symmetrization': what are "all the Q-polynomials"? Isn't there essentially only one? (In App C it becomes clear that there are several, but this is not mentioned in the main text, making the sentence unclear).*

    Indeed by "all the Q-polynomials" we mean all the Q-polynomials of the Q-system. In order to clarify this, we changed the corresponding sentence to "we have all the Q-polynomials of the Q-system (see Appendix C for details)."

15. *it is not explicitly stated what the 'Symmetrization procedure' precisely means. If it is the change of variables from the* u_k *to the* c_k *then I find it a strange name: the functions are symmetric to start with; they are just expressed more compactly in a basis of symmetric polynomials.*

    The meaning of 'symmetrization procedure' indeed means changing variables from u_k to c_k. We change the term 'symmetrization' to 'physical quantities in $\{c_k\}$ both in the main text and Appendix D.

16. *the '(computational) algebraic geometry' used in the paper is really just '(computational) commutative algebra': no geometry is needed or used. I would suggest using the latter term, which sounds less scary, and might help making the paper look more accessible*

The name ‘computational algebraic geometry’ is a standard term in mathematics. The Gröbner basis computation, companion matrix computation used in our paper, are all classified in computational algebraic geometry, according to the standard textbooks “Using algebraic geometry” (Cox, Little & O’Shea, Springer) and ”A First Course in Computational Algebraic Geometry” (Decker and Pfister, Cambridge). In particular, on page 13, the relation between the quotient ring dimension and the number of solutions (variety components) is a typical algebra-geometry dictionary theorem. Therefore we would like to keep the term ‘computational algebraic geometry’.

17. *before (60): ’All polynomials in variables ... form’ is not very clear, -¿ ’The set [or: space] of [all] polynomials in variables ... forms’.*

    The sentence is changed according to the referee’s suggestion.

18. *top of p13: clarify that the coefficients a_i are themselves polynomials and generally not unique*

    The sentence is now changed to “the ideal I consists of all polynomials... where $a_i \in C[x_1, \ldots, x_n]$ are also polynomials.”

19. *is a ’basis of the ideal’ just any generating set, or is there some condition that it should be minimal, e.g. one cannot remove any of the generators without changing the ideal*

    Any generating set can be called a ‘basis’; at this point it is not important to impose minimality conditions.

20. *emphasise that the companion matrix P itself no longer depends on the x_i, but does still depend on u (and η for XXZ), as will be discussed below*

    We add a sentence “Note that the companion matrix P no longer depends on the variables $\{x_1, ..., x_n\}$, but it can depend on other parameters such as the spectral parameter u and the anisotropic parameter η (for XXZ case) as discussed below.” at the end of the paragraph below (63).

21. *p13, middle: make explicit which quantum numbers - L, M, Q_0*

    The quantum numbers are added as suggested by the referee.

22. *’Dealing with free parameters’: what is known about the form (or properties) of the resulting functions of u (and possibly η)? try to make this discussion more concrete. it will help understanding the type of interpolation that can be done.*

    We make the discussions more concrete by adding the following sentence at the end of the paragraph: “As will be shown below, the correlation functions are rational functions of u in the XXX case and are rational functions of e^u and e^η in the XXZ case. In both cases, we can factorize out simple common denominators, after which we only need to fit polynomials.”

23. *above and below (68): ’expect’ vs ’find’ - either prove, or make clear throughout that it is an expectation*

    It is rather straightforward to see that the result takes the form of (68) [Eq.(74) in the revised version], so we change ‘expect’ to ‘find’.

24. *(71): perhaps clarify that the polynomials are not necessarily homogeneous (of a fixed total degree) in b, c*

    We add a sentence "Note that the results are not necessarily homogeneous polynomials in b, c." at the end of (71)[Eq.(77) in the revised version] to clarify this point.

25. *:(73) etc: to facilitate comparison, write polynomials in the same order - e.g. in the second line here, c^4 at the end*

    The order of terms has been adjusted according to the referee's suggestions.

26. *above 4.3: clarify in the final sentence that the result is initially independent of L*

    We believe the referee means that the results initially depend on L. To clarify the point, we change the sentence to "If the system is large enough, this spread does not touch the boundary of the system and therefore the result is independent of L, even though the intermediate calculations depend on L."

27. *Fig 2: figure number '2' is missing. Caption: clarify whose zeros are shown*

    The caption is clarified, and the figure number is added.

28. *(81): $\prod(\cdots)^{\otimes}$ is very strange notation.*

    The notation is now changed.

29. *should 'cylinder partition function' be 'torus partition function'? or is it meant to be on an infinite cylinder or with fixed boundaries at the ends?.*

    Here the 'cylinder partition function' means the partition function with a cylinder geometry with fixed boundaries at the two ends. We clarify this in the new version.

30. *clarify that $Z_{L,n}(u)$ is a polynomial only up to an overall factor of u^x (in your normalization of the weights)*

    We changed the sentence to "$Z_{L,n}(u)$ is a polynomial in u for properly chosen normalizations." to clarify this point.

31. *should this be $\widetilde{D}_4(500)$*

    Indeed, it is a typo and is now corrected.

32. *Fig (4,5,)6: pick colours that differ more*

    We don't feel that this is necessary. The current colors are enough to make the point.

33. *in the caption mention which colour is which function (or add a legend)*

    We clarified in the caption which color corresponds to which function.

34. *before Sect 5: clarify whether this argument also explains why the shapes are similar (rather than just the same endpoints for the curves), and whether the curves have a physical meaning - do they also separate different phases?*

    We extended the discussions of the condensation curves before Section 5. The similarity of the shapes of the condensation curves originates from the fact that the two quantities share the same set of eigenvalues of the transfer matrices. However, since the dimer state is an integrable boundary state, its overlap with Bethe states is constrained by selection rules. Therefore, only a subset of the eigenvalues (associated with parity-invariant Bethe roots) contributes to the partition function, whereas in the domain wall state cases all eigenvalues have a non-trivial contribution. This explains the differences between the condensation curves.

35. *I'd say that Q_0, rather than e^{iQ_0}, is the (quasi-)momentum*

    We agree. In the sentence e^{iQ_0} is now changed to Q_0.

36. *the quotient ring is smaller: than what - if we choose another fixed momentum, or when we do not fix the momentum*

    Here we mean the dimension of the quotient ring is smaller than the case without fixing the momentum. The sentence is now changed to "The AG computation procedure is similar, but the dimension of the quotient ring is smaller than the case without constraints on Q_0."

37. *below (87): can we easily see why here we need ξ rather than $x = \xi^2$ like before?*

    A function of $x = \xi^2$ can always be written as a function of ξ itself in an obvious way.

38. *above (91): to clarify the scope of the method used here, explain that $\xi = 9$ and $q = 2$ (integers) is much faster than [rational numbers? Or only compared to real/complex numbers?]*

    We add the following sentence and a footnote to clarify the point : "We would like to emphasize that the specific values of ξ and q are not crucial, as they can be easily adjusted. In practice, working with rational values (whether real or complex) is more convenient than using irrational ones for technical reasons*."

39. *p22 onwards: explain the meaning of the $\sim$ (range of integers; at the bottom of p25 a dash is used once as well, is there a difference?)*

    The meaning of $\sim$ means range of integers. We change the dash to $\sim$ since they have the same meaning.

40. *Sect 6: compute the correlation -¿ compute certain correlation; or is the claim that from these special correlation functions one can obtain all others?*

    We change the words in the sentence to "a class of correlation functions".

41. *recall that $\xi = e^u$ and $q = e^\eta$ to help remind the reader*

    It is recalled according to the referee's suggestion.

42. *before (99): clarify what 'symmetric property' here means - does one take the complex conjugate of the scalar product under the assumption that it is real (and using =)?*

    This is a known result for the scalar product using the Slavnov determinant; we cite a reference (Kostov, Matsuo JHEP 10 (2012) 168) where the derivation is given.

*For rational parameter values, the final results depend only on rational numbers, which simplifies the fitting process.

43. *before (107): clarify that this computation depends on a (Gröbner basis and thus) choice of generators and order*

    Below (107), it is explicitly mentioned that the polynomial reduction is done with respect to Gröbner basis. Therefore, we think it should already be clear.

44. *App B.4: which algebraic extension - of scalars?*

    We delete the part 'with algebraic extension' because it is very relevant here.

45. *Does this mean that $q = 11/10$ would take rather longer than $q = 2$? If so, mention this in the main text?*

    No, this is not necessarily true.

46. *Before App C: explain whether this interpolation relies on some knowledge about the form or properties of the coefficient functions*

    We add a sentence: "In general, the efficiency of such interpolation depends on our knowledge about the structure of the final result." In App B.4 to explain this point.

47. *Young diagram: $(M, L-M)$ should be $(L-M, M)$ to be a partition. add a figure to show which alignment of the boxes you have in mind and explain terms such as 'lower left'*

    A figure (Figure 16 in the new version) is added and $(M, L-M)$ is changed to $(L-M, M)$.

48. *recall that $q = e^\eta$*

    It is recalled below (113) (Eq.(119) in the new version).

49. *below (113): clarify what 'up to proportionality' means - by a constant? what can it depend on? Surely the degrees on the two sides of (112) must match, so one cannot just freely rescale the different Q-functions separately*

    Yes, it means a constant that is independent of the spectral parameter. We clarify this point by adding "up to proportionality that is independent of the spectral parameter."

50. *Zero remainder condition: what does 'the upper conditions' mean?*

    We change the sentence to " By fixing the boundary conditions $Q_{2,0} = 1$ and (120) "

51. *before (118): introduce both a new variable w and an equation for that variable*

    The sentence is changed to " We then introduce a new variable w and an equation"

52. The typos and grammar mistakes pointed out by the referee have been corrected.

Reply to the referee 2

1. *After (34), instead of saying that the one-site shift operator is "not compatible" with most Bethe states, I think that the authors should rather say that it does not commute with the evolution operator (1), and go on to explain under which circumstances some Bethe states might still provide eigenvectors for it.*

   The sentence below (34) is now changed to: "Due to our choice of inhomogeneities (24) which is alternating, the one-site shift operator V does not commute with the evolution operator $\mathcal{U}$ defined in (1) and hence is not diagonalized by a generic Bethe state. In our context, it is more natural to define the two-site shift operator $\mathcal{V} = V^2$, which commutes with $\mathcal{U}$. Therefore the Bethe states are also eigenstates of V"

2. *In the beginning of the section, the authors state that results for (48) and (51) cannot be obtained by direct numerical solution. Typical concrete results are given in section 4.1 and are polynomials in the six-vertex weights with integer coefficients. Once this polynomial property is known or assumed, why would it not be possible to obtain such results quite forwardly by computing (66) directly, using no knowledge of integrability whatsoever, but simply keeping track of the coefficients of the polynomials? This kind of question is all the more urgent since, at the end of section 3, the authors themselves admit using Lagrange interpolation to produce certain results. A similar claim is made again at the beginning of section 4.3.*

   Indeed a direct computation using (66) is possible to yield analytical results for small quantum numbers. However, for large n (the discrete 'time') this direct computation becomes very slow and it is much more efficient to apply the computational algebraic geometry method. We thus delete the sentence "Numerical solution cannot achieve this goal" at the beginning of section 3.2. At the beginning of section 4.3, we changed the sentence to "The result can be computed by the AG method, which is much more efficient than a brute force calculation."

3. *After (57) the lack of an analytical formula for the Gaudin-like determinants in terms of is mentioned. I think this point is sufficiently important to be recalled in the conclusion section.*

   We added the following sentences in the conclusion: "To address this, it is essential to derive an analytical expression for the overlap between the Bethe state and the state generated by acting string operators on the pseudo-vacuum. A closely related challenge, which is important for enhancing the efficiency of analytical computations, involves reformulating various physical quantities—such as overlaps and the Gaudin norm—in terms of the variables $\{c_k\}$ defined in (57), which are elementary symmetric polynomials of the Bethe roots $\{u_k\}$. The process of achieving this reformulation is notably intricate and computationally demanding. However, despite their fundamental nature, simple analytical expressions for the Gaudin norm in terms of $\{c_k\}$ remain elusive, which is an interesting question to investigate."

4. *The light-cone effect mentioned after (78) should be called by its proper name (as in the conclusion) and a more precise argument provided.*

   We added the following sentence in the paragraph above section 4.3 "This observation is consistent with the general fact that under short-range interactions, the propagation of information is limited in a light-cone structure governed by the Lieb-Robinson bound. ”

5. *In section 4.3 and 4.4 results are presented in the form of Lee-Yang zeros. Here the notion of condensation (accumulation point) should be precisely defined. Is the spread of zeros close to the real axis in figures 3 and 4 a real effect or an imperfection originating from the root solver?*

   We define the notion of condensation following reference [56] above Figure 4 in the revised version. We believe the spread of zeros close to the real axis is a real effect (since n is finite) instead of an imperfection of the root solver.

6. *Finding roots of high-degree polynomials is a numerically challenging problem, so the authors should state which software is being used here. The notation in the first part of (81) should use the index j.*

   We exploit the software MPSolve to find the polynomial zeros, which is a multiprecision implementation of the Aberth method. We have stated this in the revised version. The notation in (81) (Eq(87) in the revised version) has been changed.

7. *Figure 6 shows that the condensation curves of and almost coincide in the lower-half plane, but differ substantially in the upper-half plane. The authors mention how these curves can be obtained (numerically) exactly by studying the equimodularity of eigenvalues, but seemingly only obtain approximations thereof by displaying the roots of high-degree polynomials. Are some of the eigenvalues of the two quantities* exactly *the same, or only approximately? If so, can the notable differences in the upper-half plane be explained by some of the eigenvalues incurring a vanishing prefactor, maybe by some symmetry argument?*

   Indeed in the current work we only obtained the condensation curves approximately by finding roots of high-degree polynomials. Finding the exact curve numerically by studying the equimodularity of eigenstates is an interesting question which requires additional numerical techniques and we leave it for future works. The similarity of the shapes of the condensation curves originates from the fact that the two quantities share the same set of eigenvalues of the transfer matrices. However, since the dimer state is an integrable boundary state, its overlap with Bethe states is constrained by selection rules. Therefore only a subset of the eigenvalues (associated with parity-invariant Bethe roots) contributes to the partition function, whereas in the domain wall state case all eigenvalues have non-trivial contributions. This explains the differences between the condensation curves.

8. *Results in Fourier space are given in section 5. The choice of parameter values should be better explained (unless they just provide an arbitrary example), and if possible, this section would benefit from more effort in making a physical interpretation. For instance, are the spikes in figure 13 relevant for actual physical phenomena, and why do some of them converge but others seemingly not? Is the color coding of figure 13 the same as in figure 12?*

   The choice of parameters only provides an arbitrary example and does not have specific physical meanings. We added extended discussions on the physical interpretations of the results in section 5.1 and 5.2 in the revised version. The qualitatively different behavior is due to the fact that eigenvalues of the transfer matrix in the two regimes have very different behaviors. In the massive regime, we have $|\tau| > 1$ while in the massless regime $|\tau| = 1$. The position of the spikes in the massless regime is associated with the eigenvalues of the transfer matrix. The color coding of figure 13 is the same as in figure 12.