Dear Editor,

We thank the second referee for the report on our manuscript *Bethe Ansatz, Quantum Circuits, and the F-basis*, with pre-pint link scipost_202411_00037v1. Below, we address each of the referee's remarks in detail, indicating the corresponding change made to the manuscript.

As also noted in our response to the first referee, we have corrected various typographical errors, removed redundancies, updated the bibliography, and improved the clarity and readability of the text. A summary of the most substantial changes introduced in the revised version is provided at the end of the response to the first referee. The relocation of equation (3.23) to equation (3.31), accounted among the changes, has shifted the numbering of equations on pages 15–17. To avoid confusion, we refer to the labels of equations in the new version in this response, unless otherwise stated.

Response to the referee

1. **Reviewer**: 'To my understanding, the Bethe states discussed in this work are the off-shell Bethe states, which are not yet eigenstates of the transfer matrices. There is no discussion of the Bethe ansatz equations, which is another crucial ingredient of the Bethe ansatz. It would therefore be helpful to clarify the distinction between on-shell and off-shell Bethe states and to emphasize that the states considered here are of the latter type.'

   We agree with the referee in that we had not adequately emphasised that neither the representation of Bethe states as matrix-product states (MPSs) nor the unitarisation of these MPS into quantum circuits by the canonical form requires the Bethe states to be on-shell. The referee correctly notes that Bethe states of the inhomogeneous XXZ model, whether in the formulation of the algebraic Bethe Ansatz (ABA) (3.2) or the coordinate Bethe Ansatz (CBA) (3.24), are eigenstates of the transfer matrix only when the Bethe equations are satisfied.

   To clarify on this point, we have introduced the following changes in the manuscript. In the third paragraph of page 2, we improved the paragraph with the following sentences.

   - The computation of the unitaries of ABCs does not require Bethe states to be eigenstates of the Hamiltonian; that is, the Bethe equations need not hold.

   The first paragraph below (3.14) in page 15 ends with the following sentence.

   - We stress that neither the MPS of the ABA (3.2) nor its reformulation as an MPS of the CBA (3.10) requires u_a to satisfy the Bethe equations. Therefore, the Bethe states under consideration are not necessarily eigenstates of the Hamiltonian of the homogeneous XXZ model (2.3).

   The paragraph below (3.25) (equation (3.26) of the previous version) in page 16 now begins with the following sentence.

   - We assume that u_a, and consequently $p_{a,j}$, do not necessarily satisfy the Bethe equations. This means that the Bethe state (3.24) is not an eigenstate of the transfer matrix that defines the inhomogeneous spin chain in general.

2. **Reviewer**: 'A point that warrants further explanation is the difference between the two MPS representations of the Bethe states introduced in the authors' previous works. The introduction highlights that one is "numerical" while the other is "analytical." Since the algebraic Bethe ansatz (ABA) is an analytical method for constructing eigenstates (assuming we are dealing with off-shell states), why does the corresponding MPS become "numerical"? Clarifying this distinction would help readers better appreciate the significance of the alternative MPS and the current work.'

5. **Reviewer**: 'The authors should elaborate on why the key property of the F-basis —— namely, its invariance under the exchange of auxiliary states—— is useful in transforming the numerical MPS into the analytical MPS. What specific advantage does this property provide?'

   We agree with the referee that we should have been clearer in stressing the distinction between the two MPS representations of Bethe states. The explanation also highlights the importance of the F-basis in the MPS representation of Bethe states. Let us briefly summarise the key features of each representation.

   First and foremost, we stress that the MPS representations arising from the ABA and the CBA are both exact. The MPS of the ABA is constructed from the R-matrix and the associated monodromy matrices, according to which the Bethe states are given by equation (3.1). Due to the absence of apparent structural properties that would allow for an analytic computation of the canonical form of this MPS, the authors of [19], who focused on the homogeneous XXZ model, employed a QR-factorisation to unitarise the dual monodromy matrices (2.31) and to eliminate the post-selected qubits, thereby obtaining the quantum circuits. However, the QR-factorisation yields the unitaries through recurrence relations that cannot, in general, be solved analytically. Thus, while the MPS derived from the ABA is exact, the associated unitaries must be constructed numerically.

   In contrast, the MPS representation based on the CBA is defined using the tensor in equation (3.8) for the homogeneous spin chain, and the tensor in equation (3.9) for the inhomogeneous case. In addition to satisfying the appropriate normalisation, these tensors are characterised by their invariance with respect to the exchange of qubits. This symmetry, inherited from the property of the F-basis (2.34), is essential to define the one-to-one mapping (3.48) between the initialisation of the auxiliary space and Bethe states on a non-maximal number of sites $1 \leqslant k \leqslant N$ and with a non-maximal number of magnons $1 \leqslant r \leqslant N$.

   Identifying the mapping (3.48) enables one to recognise that the gauge-transformation matrix in the auxiliary space, which brings the MPS into canonical form, coincides with the change-of-basis matrix that orthonormalises the non-orthogonal basis of Bethe states in equation (3.51). Moreover, this identification clarifies that replacing the original tensor with the second short tensor (3.58), as illustrated in Figure 17, preserves the bijectivity of the mapping (3.63) and permits the simultaneous analytic determination of both the gauge-transformation matrix and a consistent and rigorous elimination of post-selected qubits.

   We have implemented the following changes in the introduction to the manuscript to clarify ambiguity highlighted by the referee. In the third paragraph of page 2, we improved the paragraph with the following sentences.

- In [19], the unitaries of ABCs were extracted from the exact tensors of the ABA by numerically solving a set of intricate recurrence relations arising from a unitarization procedure. Closed formulae for the unitaries of ABCs were later obtained in [20] by a complementary approach. The key step in [20] was the derivation of an exact representation of the linear superpositions of plane waves of the CBA as an MPS. The tensors of this MPS, unlike those of the ABA, directly provide analytical expressions for the unitaries of ABCs, as unitarization in this case can be identified with the orthonormalization of a basis of Bethe states.

In the first paragraph of page 3, we have added the following sentence.

- The crucial property of the F-basis is its invariance under exchange of qubits, which characterizes the MPS of the CBA.

Finally, we have added the following sentence below equation (3.51) in page 21.

- We note that the identification of X_j with the change-of-basis matrix relies on the existence of the mapping (3.48), which, as showed at the end of Subsection 3.1, follows from the invariance of the F-basis with respect to the exchange of qubits.

3. **Reviewer**: '3. In ABA, the choice of auxiliary space is arbitrary. For the XXZ spin chain, for instance, the auxiliary space can be in either the fundamental representation or a higher-spin representation. Is a specific choice of auxiliary space required, or is any choice permissible? Addressing this point would be useful, particularly for future applications in constructing spin-s XXZ chains'.

   The possibility of representing Bethe states as quantum circuits analytically relies on the existence of F-basis in the auxiliary space. The spin-s XXZ model posseses an F-basis in the auxiliary space, as demonstrated in [26]. However, the Bethe states are usually created with the auxiliary space being still of spin-1/2. This might cause some difficulties in applying our method, because of the mixed dimensionality of the auxiliary and physical spaces. We believe that sorting this problem out could be a topic for further research.

   This is fact is stressed in the end of the third paragraph of page Section 5, between pages 36–27.

   - Another generalization of our circuits involves the preparation of Bethe states in spin-s XXZ models [4,6], which possess an F-basis in both the quantum and auxiliary spaces [26]. The main distinction in these models is that the spins are spin-s qudits, while the ancillae remain qubits. Although the corresponding MPS tensor of the CBA is available and retains symmetry under the exchange of ancillae, care must be taken in constructing a quantum circuit, particularly in determining the change-of-basis matrices of the gauge transformation, since the tensors act on spin-1/2 qubits but realize Bethe wave functions for spin-s qudits. This mismatch, in particular, could obstruct the elimination of post-selected qubits in the final circuit.

4. **Reviewer**: '4. Equation (3.2) would benefit from additional explanation—either via an instructive figure or a few more lines of derivation—as it serves as the starting point for the

subsequent MPS derivation. The equivalence between (3.1) and (3.2) is not immediately obvious, at least to me (and possibly to other readers as well). Similarly, more clarification on the transition between the second and third equalities in (3.10) would be helpful.'

We agree with the referee that the equivalence between equations (3.1) and (3.2) is not immediately obvious. To clarify the equivalence, we have promoted equation (3.1) in page 11 to

$$B(u_1)\dots B(u_M)\,|0\rangle^{\otimes N} = \prod_{a=1}^{M}\left[\langle 0|_a\, T_a\, |1\rangle_a\right]|0\rangle^{\otimes N} = \prod_{a=1}^{M}\left[\langle 0|_a \prod_{j=0}^{N-1} R_{aN-j}\,|1\rangle_a\right]|1\rangle_a\,|0\rangle^{\otimes N} \quad .$$

In addition, to make contact with the graphical derivation, we have a added a sentence to the first paragraph of page 12.

- It is worth noting that Figure 10, corresponding to (3.2), can be obtained graphically from Figures 7–9 by taking into account the relation (3.4).

On the other hand, to clarify the transition between the second and third equalities in (3.10), iwe have added a comment to the last paragraph of page 13.

- The proof of the equivalence between the first and second lines of (3.10) appears in Appendix B of [20]. (We provide an analogous proof for the Bethe wave function of the inhomogeneous spin chain in Appendix A.)

6. **Reviewer**: ' In the second paragraph of the conclusion, the first two sentences ("A key property of...exchange of the ancilliae") and the following two sentences ("The key property of...exchange of the ancilliae") are nearly identical in meaning. One of these pairs should be removed to avoid redundancy.'

   We have removed the redundancy of the paragraph following the suggestion of the referee.

We hope that the paper is suitable for publication with the aforementioned changes.

Kind regards,

Roberto Ruiz, Alejandro Sopena, Esperanza López, Germán Sierra, and Balázs Pozsgay