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## Report

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In this paper, the authors present a new analysis to the isotropic Heisenberg chain with arbitrary boundary fields, explicitly retaining terms that depend on the angle between the boundary field. I believe it deserves to be published in Scipost after the following comments have been appropriately addressed:

1. **Reviewer:** Above Eq(5)-(7), the authors state: "In analogy to [26, 27], we find that the following functions are useful"

It would be helpful to further clarify the physical motivation for adopting these particular functional forms. For example, do they offer specific advantages in numerical implementations? Moreover, are there alternative formulations that might also be viable?

2. **Reviewer:** Below Eq(10), the authors state: "We want to 'solve' these functional equations of multiplicative type with constant shifts in the arguments. The first step is the application of the logarithm, turning the product form into additive form. In the second step, we apply the Fourier transform, which turns functions with shifts in the arguments into transforms with simple factors, eventually leading to a set of linear equations. Care has to be taken that the Fourier transform exists and that the region of convergence of the inverse transform—the Fourier representation—is wide enough for our purposes."

It would be helpful if the authors could elaborate on the role and necessity of the Fourier transform in this formulation. In particular, what are the specific advantages it offers in the numerical iteration?

3. **Reviewer:** In Figure 1, the authors state: "Depiction of Bethe roots and zeros of the eigenvalue function for the ground-state and parameters  $\{p, q, \xi\} = \{-0.6, -0.3, 1.2\}$ "

Could the authors clarify whether the zero root distribution presented in this work is valid across the full range of boundary parameter values? If not, it would be helpful to provide a comprehensive list or classification of the distinct root distributions associated with different boundary parameters. Additionally, above the Eq.(11), the authors state "In case of the largest eigenvalue...". A clarification is needed as to whether this particular distribution of zero roots corresponds to the ground state or to the state associated with the largest eigenvalue.

4. **Reviewer:** Above the Eq. (18), the authors state: "In any case, for large system size, the bulk of the zeros of  $D(x)$ , respectively  $\bar{D}(x)$ , is close to  $\text{Im}(x) = +2$ , respectively  $\text{Im}(x) = -2$ ."

It would be helpful if the authors could clarify, from a numerical perspective, the minimal system size required for the stated distribution of zeros of  $D(x)$  to manifest. Furthermore, does this imply that equations (35)-(37) are only valid in the large-system-size limit?

5. **Reviewer:** Above the Eq. (23), the authors state: "We will factor out of  $a(x)$  and  $\bar{a}(x)$  an explicit function yielding the zero of high order. It will appear that, in some of the formulas below, the shift  $x \rightarrow x \pm i$  should be understood as  $x \rightarrow x \pm (1 - \varepsilon)i$  with small positive  $\varepsilon$ ."

Could the authors provide a detailed explanation of how to factor out of  $a(x)$  and  $\bar{a}(x)$  an explicit function yielding the zero of high order? Additionally, is the introduction of the small positive parameter  $\varepsilon$  intended to numerically regularize potential divergences? In equations (35)-(37), this small parameter appears only in  $K_{12}$  and  $K_{21}$ . Could the authors clarify why the regularization is required exclusively for these two terms? Finally, with regard to Figure 2, what specific value of  $\varepsilon$  was used during the numerical iteration? It would be helpful if the authors could provide comparative plots for different values of  $\varepsilon$  to numerically demonstrate that the results are indeed insensitive to its precise value.

6. **Reviewer:** Above the Eq. (38) in Section 3, the authors state: "where the convolutions in (37) are done with  $\log A$  and  $\log \bar{A}$  evaluated on symmetric intervals  $[-R, +R]$  with  $R \rightarrow \infty$ ." Could the authors clarify how the expression  $\log(\infty)$  should be interpreted in this context?

7. **Reviewer:** About the Eq. (39) in Section 4, the authors state: "After formulating the NLIEs for the derivatives  $(\log a(x))', \dots, (\log A(x))', \dots$ , the NLIEs are integrated with respect to the argument  $x$ , and the integration constants are fixed by considering the limit  $x \rightarrow \infty$ . The result is...". It would be helpful if the authors could elaborate on the derivation of equation (39) in more detail.

8. **Reviewer:** Could the authors provide more details on how equation (43) is obtained or why you choose these numbers? Furthermore, in the numerical implementation, what specific value is chosen for the parameter  $\delta$ , and does this choice affect the outcome of the iterative solution? It would be helpful to clarify whether the results are robust with respect to variations in  $\delta$ .

9. **Reviewer:** Below Eq(43) in section 4, the authors state: "By use of qualitatively similar initial data for the iterative treatment of the NLIEs, we found convergence for much larger system

sizes, like that shown in Fig. 2 for  $N = 10^3$ . However, increasing the system size further will ultimately, and independently of the chosen boundary parameters, lead to the loss of convergence.”

It would be helpful if the authors could elaborate on how the initial data are distributed in the iterative approach. Additionally, is it feasible to reproduce similar structures to those in Fig. 2 for smaller system sizes such as  $N = 6, 8, 10$ ?

10. **Reviewer:** Above the Eq. (44) in Section 4, the authors state: ”Under this condition, the above-described winding happens so fast that the convolution integrals produce contributions that cancel the leading  $(2N + 1) \log \tanh(\frac{\pi}{4}x)$ . On the basis of this reasoning, we found solutions of the NLIEs with much larger system sizes, like those illustrated in Fig. 3.”

Is Figure 3 obtained by performing the numerical iteration based on equations (35)-(37) after omitting the leading term  $(2N + 1) \log \tanh(\frac{\pi}{4}x)$ , or does it result from using equation (39), after omitting the leading term  $(2N + 1) \log \tanh(\frac{\pi}{4}x)$ ? A clarification on this point would be appreciated.

11. **Reviewer:** Is there any difference in the numerical results obtained by iterating equations (35)-(37) as opposed to equation (39)? Should the outcomes be identical in principle? If so, it would be helpful if the authors could provide a comparative plot to demonstrate the agreement between the two approaches.

12. **Reviewer:** In conclusion, the authors state: ”The large  $N$  results allow for future analytical study of the finite size properties of the system with non-parallel boundary fields. The next step will be the derivation of a suitable scaling limit of the NLIEs.”

This part of the analysis may be difficult to follow, but in this context, it seems insufficient to limit the numerical results to the distribution of the  $A$  function. A direct comparison of the ground state energy with independent DMRG data at fixed, finite system sizes but not in the thermodynamic limit would be essential to substantiate the correctness of the result. Could the authors comment on this and possibly include such a comparison?