Ref.:

Response to points raised by Reviewer

Thank you very much for your many helpful points raised about our paper and we really appreciate your supports. We believe that these comments and suggestions have significantly improved our manuscript. To these comments we respond as follows. The page numbers and equation numbers refer to revised version, unless specify.

1. **Reviewer**: The authors apply the Bethe ansatz scheme introduced in Refs. [22,23] to study bulk and boundary properties of the Heisenberg spin chain with competing interactions constructed from an inhomogeneous six vertex model with open boundary conditions. The scheme is based on the discrete set of discrete inversion relations (2.17). In this formulation boundary conditions breaking the $U(1)$ symmetry of the bulk system appear not to lead to the complications when dealing with unparallel boundary fields in the conventional TBA approach.

Authors: Thank you very much for your comments. It is clear that you have caught the ideas of this paper.

2. **Reviewer**: For the derivation of the integral form (4.2) of the Bethe equations, however, the authors have implicitely assumed that the inversion relations hold for a continuous variable u not just at the special points $u = \theta_j$. This is not correct: for example, in this approach the spectrum would depend only on the effective parameters p and $\bar{q}$ appearing in the eigenvalues of the boundary matrices (which determine the absolute value of the boundary fields) but not on the relative orientation of the boundary fields leading to the breaking of the $U(1)$ symmetry! In fact, it is well known that equations (2.17) only hold up to terms vanishing as powers of $(u - \theta_j)$.

Ignoring this fact (2.17) turns into a functional equation for the transfer matrix eigenvalues. Imposing constraints on their analytical properties (e.g. by considering a particular root pattern $\{z_j\}$) one selects an eigenstate and the functional equation can be solved directly by Fourier methods. As has been observed in previous works this yields the correct results for the bulk and boundary contributions to the corresponding energy in the thermodynamic limit (i.e. with boundaries being infinitely separated). Corrections of order $1/L$ can not be obtained in this way.

Therefore the results obtained in Section 4 based on the configurations of roots of the transfer matrix eigenvalues are correct although straightforward generalizations of what is known for the homogeneous Heisenberg model ($a = 0$), see e.g. Grisaru et al., J. Phys. A28 (1995) 1027-1046 and Kapustin & Skorik, J. Phys. A29 (1996) 1629-1638. Similarly, the spectrum of bulk elementary excitations (Sect. 5) has been studied for the periodic staggered ($a \neq 0$) spin chain before in Frahm & Rodenbeck, Europhys. Lett. 33 (1996) 47-52.

Authors: As you pointed out, the operator product identities (2.17) is valid for $\{u = \theta_j\}$.

In the thermodynamic limit, the zero roots and the inhomogeneities have continuum densities

$$\rho(\tilde{z}) = \frac{1}{2N(\tilde{z}_{j+1} - \tilde{z}_j)}, \quad \sigma(\bar{\theta}) = \frac{1}{2N(\bar{\theta}_{j+1} - \bar{\theta}_j)},$$

where $\{\theta_j \equiv i\bar{\theta}_j\}$ and $\{\bar{z}_j \equiv -iz_j\}$. Taking the continuum limit of Eq.(4.1) and replacing $\bar{\theta}_j$ with u, we obtain Eq.(4.2). Thus the u in Eq.(4.2) is not the spectral parameter. In order to avoid confusion, we have changed the u by the λ in Eqs.(4.2) and (4.10).

By solving the Bethe ansatz equations satisfied by $\rho(\tilde{z})$ and $\sigma(\bar{\theta})$, we obtain the density of zero roots. Then we can calculate the physical quantities such as surface energy and bulk excitations. We find that the spectrum of present isotropic model is indeed determined by the absolute value of the boundary fields. The contribution of relative orientation of the boundary fields leads to the high-order effect in the model. We shall note that the relative orientation of the boundary fields could have contribution to the surface energy in some models such as the XXZ Heisenberg model with unparallel boundary fields [23]

$$\begin{aligned} e_b(\alpha, \beta) = -2\sinh\eta \sum_{k=1}^{\infty} \tanh(k\eta)\{(-1)^k e^{-2k\eta} \\ + e^{-2k|\alpha|} + (-1)^k e^{-2k|\beta|}\} - \tanh\eta \sinh\eta, \end{aligned} \tag{1}$$

where the parameters α, β represent the orientations of the boundary fields. Thus the method distinctly can be used to study the spectrum problems with unparallel boundary fields. It is the symmetry of the present model induces the relative orientation contributes to energy corrections of order $1/L$ or higher order.

According to your suggestions, we have added the discussions of previous results [30, 31] obtained by using the conventional Bethe ansatz method. We also explained that the spectrum of bulk elementary excitation covers the previous result for the periodic staggered ($a \neq 0$) spin chain [32] after Eq.(5.2). We have added the related references:

[30] M. T. Grisaru, L. Mezincescu and R. I. Nepomechie, *J. Phys. A: Math. Gen.* **28**, 1027 (1995).

[31] A. Kapustin and S. Skorik, *J. Phys. A: Math. Gen.* **29**, 1629 (1996).

[32] H. Frahm and C. Rödenbeck, *Europhys. Lett.* **33**, 47 (1996).

3. **Reviewer**: In Sect. 6 the authors study the boundary excitations and observe a different behaviour of their energy around $p = 0$ for the homogeneous ($a = 0$) and the staggered ($a \neq 0$) spin chains. Given the p-dependence of the boundary term (2.3) this not really surprising.

Authors: As you pointed out, the results given in section 6 are consistent with the physical picture and are reasonable. The boundary excited energies for different values of boundary parameter p are different, including the homogeneous ($a = 0$) and the staggered ($a \neq 0$) cases.

4. **Reviewer**: In summary, most of the physical quantities considered in the manuscript are either known or straightforward extensions of known results which could have been obtained without using the 'novel Bethe ansatz scheme'. Moreover, the tacit assumption underlying the integral Eqs. (4.2) rules out an application of the proposed scheme to studies of the finite size spectrum. This would be necessary to address the particularly interesting case of unparallel fields advertised in the abstract and the introduction. Given these limitations I see little potential for the proposed scheme beyond what has already been done using established Bethe ansatz methods.

Authors: In fact, the inhomogeneous parameters are not necessary. In the homogeneous limit $\{\theta_j = 0 | j = 1, \cdots, 2N\}$, the operator identities (2.17) can be replaced by

$$[t(u+a)t(u+a-1)]^{(n)}|_{u=0} = [a(u+a)d(u+a-1)]^{(n)}|_{u=0}, \quad n = 0, 1, \cdots, 2N-1, \tag{2}$$

$$t(0) = 2\,p\,q\,(1-a^2)^{2N}, \tag{3}$$

where the superscript (n) indicates the n-th order derivative. Then the functional relations (2.22) reads

$$[\Lambda(u+a)\Lambda(u+a-1)]^{(n)}|_{u=0} = [a(u+a)d(u+a-1)]^{(n)}|_{u=0}, \quad n = 0, 1, \cdots, 2N-1, \tag{4}$$

$$\Lambda(0) = 2\,p\,q\,(1-a^2)^{2N}, \tag{5}$$

Eqs. (5) and (4) can determine the $2N+1$ zeros roots $\{z_j\}$ in the homogeneous limit in finite system size. We have added these arguments in the paper. However, the finite size effect is not the main focus of our research. Our method proposed in [23] is primarily employed for the investigation of the energy spectrum in the thermodynamic limit. It is of importance to study the zero roots of the transfer matrix for the present model with NNN interactions and generalize the Bethe ansatz method introduced in [22,23] to these models.

In conclusion, the method can be used to study the unparallel boundary fields and our research of present model makes certain contributions to the direction of exact solutions in the field of integrable systems. Our results cover the previous ones and are important. We think this paper meets the requirement of SciPost Phys..

Requested changes

1. **Reviewer**: The authors should extend their discussion the effect of the inhomogeneities θ_j at the end of Section 2. Also, only in Fig.2 their choice underlying the numerical data is stated. I assume that $\theta_j \equiv 0$ in Figs. 3, 6 and 7 (i.e. alternating inhomogeneities $\pm a$) but that should be clearly stated in the figure captions.

Authors: Thank you for your kind advice! According to your suggestion, we have added the discussion of inhomogeneities $\{\theta_j\}$ at the end of section 3. Please see them as follows. *We also find that the choice of pure imaginary inhomogeneities $\{\bar{\theta}_j\}$ does not change the patterns of zero roots $\{\bar{z}_j\}$ but the roots density, as shown in Fig.2. This result allows us to calculate the physical quantities such as the surface energy and the elementary excitations of the system in the thermodynamic limit with the help of suitable $\{\bar{\theta}_j\}$ [23]*".

We also added the explanation "for $\{\bar{\theta}_j = 0|j = 1, \cdots, 2N\}$" in the captions of Figs. 3, 5, 6 and 7.

2. **Reviewer**: Summation indices in (4.1) should be l and k, not j.

Authors: Thank you for your careful reading. We have corrected the typo.

3. **Reviewer**: Where in the derivation of (4.3) has $\sigma(\theta) = \delta(\theta)$ been used?

Authors: We use $\sigma(\theta) = \delta(\theta)$ after Eq.(4.3) to derive the density of zero roots in the thermodynamic limit. We have replaced "In the derivation, we have used the relation $\sigma(\theta) = \delta(\theta)$" with "From now on, we use $\sigma(\theta) = \delta(\theta)$" after Eq.(4.3).

4. **Reviewer**: The boundary elementary excitation (Sect. 6) should described more clearly: it is unclear how the root configuration of the excitation displayed in Fig. 7(a) for parameters from regime III can be obtained from the ground state one similar to that in Fig. 3(a) by just changing the boundary string (i.e. what happens to the roots at $\pm\alpha$ and $\pm\beta$)?

Authors: Thank you for your kind advice! From the expression (2.23) of $\Lambda(u)$, we find that if

z_k is a zero root of $\Lambda(u)$, then $-z_k$ must be the root. We can also prove that

$$[t(u)]^{\dagger} = t(u^*), \quad [\Lambda(u)]^* = \Lambda(u^*). \tag{6}$$

Substituting Eq.(2.23) in the paper into (6), we obtain

$$\prod_{k=1}^{2N+2}\left(u^* - z_k^* + \frac{1}{2}\right)\left(u^* + z_k^* + \frac{1}{2}\right) = \prod_{k=1}^{2N+2}\left(u^* - z_k + \frac{1}{2}\right)\left(u^* + z_k + \frac{1}{2}\right), \tag{7}$$

which means that if z_k is a zero root of $\Lambda(u)$, then $-z_k$, z_k^* and $-z_k^*$ must be the roots. Thus, four zero roots form the bulk string at the $\pm i$ axes.

In the regime III, the boundary elementary excitation is the 2 roots at the real axis $\pm\alpha$ and 2 roots at the imaginary axis $\pm i\beta$ at the ground state form the bulk strings at the $\pm i$ axes, which can be seen more clearly from the redrawn Fig.7(a). In Fig.7(a), the blue asterisks represent the pattern of zero roots at the ground state and the red circles denote those at the excited state with boundary string $i(\frac{1}{2} - |p|)$. According to your suggestion, we have redrawn the Fig.7(a) and added the corresponding descriptions.

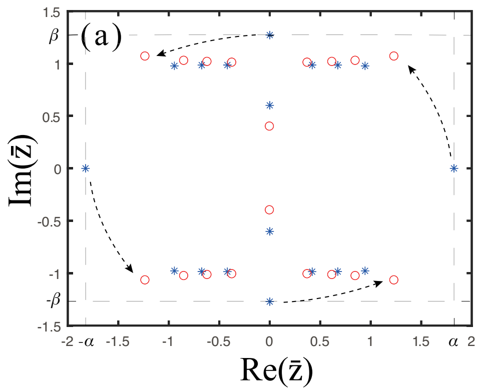

FIG. 7: (a) The distribution of $\bar{z}$-roots for $\{\bar{\theta}_j = 0|j = 1, \cdots, 2N\}$ with $2N = 8$, $a = 0.66i$, $p = 0.1$, $\bar{q} = 1.2$ and $\xi = 1.2$. Here the blue asterisks represent the pattern of zero roots at the ground state and the red circles denote those at the excited state with boundary string $i(\frac{1}{2} - |p|)$.