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.

I. Report

1. **Reviewer**: I think the calculation of the surface energy and bulk excitations for a Heisenberg spin chain with nearest neighbor, next nearest neighbor, chiral three spins, Dzyloshinsky-Moriya interactions and unparallel boundary magnetic fields (in the thermodynamic limit) is a worthwhile scientific problem.

The treatment of the general case of non-parallel boundary fields would be extremely difficult as it leads to the necessity of emloying the off-diagonal Bethe ansatz. In the thermodynamic limit, however, many problems disappear: the bulk ground state energy does not know about the boundary fields and the surface energies do not know about their mutual orientation, only the 1/N terms do and those are neglected in this work.

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

2. **Reviewer**: Unfortunately, the presentation of the results is truly suboptimal. Although the authors apply a relatively modern approach by avoiding Bethe ansatz like equations and adopting an approach that directly aims at the eigenvalue function of the transfer matrix, it is still unnecessarily cumbersome. The authors consider a functonal equation for the eigenvalue function $\Lambda(u)$ and turn this into an equation for the density function of the zeros of $\Lambda(u)$. This equation is solved and then the function $\Lambda(u)$ is obtained. The short-cut to this is to solve the functional equation for $\Lambda(u)$ directly by use of the Fourier transform.

Under the simplifications that take place in the thermodynamic limit one can apply techniques like in A. Klümper: Europhys. Lett. 9, 815-820 (1989) (for the excitations), F. H. L. Essler, H. Frahm, F. Göhmann, A. Klümper, V. E. Korepin: The One-Dimensional Hubbard Model, Cambridge University Press (2005) (see the derivation of (13.71) from (13.70)) and many other later papers, e.g. a most recent one G A P Ribeiro et al J. Stat. Mech. (2022) 113102 for the bulk properties.

I first show how to shorten the authors calculations for deriving the **surface energy**.

Once (2.22) is written down, in the thermodynamic limit this functional equation means

$$\Lambda(u)\Lambda(u-1) = a(u)d(u-1) = a(u)a(-u), \tag{1}$$

for all u out of the physical strip. Of course this means literally for the bulk and surface terms

$$\Lambda(u) = \Lambda_{bulk}(u) \cdot \Lambda_{sur}(u), \tag{2}$$

$$a(u) = a_{bulk}(u) \cdot a_{sur}(u), \quad a_{sur}(u) := \frac{u+1}{u+\frac{1}{2}}(u+p)(u+\bar{q}), \tag{3}$$

that for instance

$$\Lambda_{sur}(u)\Lambda_{sur}(u-1) = a_{sur}(u)a_{sur}(-u). \tag{4}$$

Now introducing

$$\tilde{\Lambda}(u) := \Lambda_{sur}(-iu) \tag{5}$$

allows for the ansatz of a Fourier transform

$$\frac{d}{du}\log\tilde{\Lambda}(u) = \int_{-\infty}^{\infty} dk L(k) e^{iku} \tag{6}$$

with a yet unknown function $L(k)$. This function can be calculated from (4) by taking the logarithm, the derivative and then the Fourier transform (the RHS gives an explicit function):

$$L(k) \cdot (1+e^k) = -i \cdot sign(k) \cdot (e^{-|pk|} + e^{-|\bar{q}k|} + e^{-|k|} - e^{-|k|/2}). \tag{7}$$

From the last equation one gets $L(k)$ and from this $\frac{d}{du}\log\tilde{\Lambda}(u)$ Fourier transform. The energy is simply obtained by

$$E_{sur} = -\frac{1}{2}(4a^2-1)\Big(i\frac{d}{du}\log\tilde{\Lambda}(u)\Big|_{u=ia} + i\frac{d}{du}\log\tilde{\Lambda}(u)\Big|_{u=-ia}\Big), \tag{8}$$

which straight away gives (4.6-4.8) of the manuscript (where many pages of calculation were not presented).

Next I derive the **bulk excitations**. In fact I like to start with a remark: The authors' result (5.2) can be presented in a simplified, explicit form, by doing the Fourier integral resulting in:

$$\delta_{e_1}(\bar{z}) = -(4a^2-1)\cdot\Big(\frac{\pi}{\cosh\pi(\bar{z}+ia)}+\frac{\pi}{\cosh\pi(\bar{z}-ia)}\Big). \tag{9}$$

How to derive this in a most transparent manner? Define for an arbitrary excited state, actually for an eigenvalue $\Lambda_x(u)$ the ratio to the leading eigenvalue $\Lambda(u)$ of the transfer matrix:

$$l(u) := \frac{\Lambda_x(u)}{\Lambda(u)}. \tag{10}$$

In the thermodynamic limit this function satisfies the functional equation (derived from two times (1) for $\Lambda(u)$ and for $\Lambda_x(u)$)

$$l(u)l(u-1) = 1. \tag{11}$$

This is solved uniquely for a given set of zeros z_m in the physical strip by tanh resp. tan function (for any distribution of inhomogeneity parameters θ_j). Let us assume there are only two such zeros z_1 and z_2 , then

$$l(u) = \tan\Big(\frac{\pi}{2}(u-z_1)+\frac{1}{2}\Big)\Big(\frac{\pi}{2}(u-z_2)+\frac{1}{2}\Big). \tag{12}$$

The shift $+\frac{1}{2}$ is due to the authors' own convention (2.23). The logarithmic derivative and then inserting $u=\pm a$ and $z_m = i\bar{z}_m$ gives directly (5.2).

I am not sure if a referee is authorized to prescribe a specific set of tools for achieving the goal. However, the reader of this manuscript has the right to be informed about the most elegant way of deriving the goals. I really fear that "young people" will continue to believe that integrable systems means Bethe ansatz and Bethe ansatz means density functions and complicated calculations.

Authors: Thank you very much! Very clear and simple method!

Here, we note that this method requires that there do not exist the zero roots between the lines $\mathrm{Re}(z) = 0$ and $\mathrm{Re}(z) = -1$ at the ground state. Otherwise, the Fourier transform (A.7) would have problem. In ferromagnetic regime of present model, some zero roots at the ground state are located in line $\mathrm{Re}(z) = -\frac{1}{2}$. Please see the section 7. (According to the convention (2.23), the zero roots shift $+\frac{1}{2}$ and are located in real axis in Fig.8(a)).

Therefore, we prefer to keep using our approach in the main text. In order to introduce readers to the concise method you mentioned, we present the simple method in Appendix A.

II. Requested changes

1. **Reviewer**: In (2.5) the coupling constant J_1 seems to depend on an index j. How can that be?

Authors: You are right. The NN coupling J_1 depends on the site index j,

$$J_1 = \begin{cases} 1 + c_1, & j = 1, \\ 1, & j = 2, \cdots, 2N-2, \\ 1 + c_{2N-1}, & j = 2N-1. \end{cases} \tag{13}$$

Thus the couplings in the bulk are the same except the two boundary bonds, because the boundary bonds can be polarized by the boundary fields.

2. **Reviewer**: In (2.15) the $c_2^{-1} t(a) t(-a)$ simplifies enourmously, but this is not further explained. So maybe the authors could simply replace that term by let us say $-\frac{1}{2}(4a^2 - 1)$ or similar?

Authors: Very good suggestion! According to your suggestion, we have replaced the term $c_2^{-1} t(a) t(-a)$ by the factor $-\frac{1}{2}(4a^2 - 1)$ and corrected the typo in Eq.(2.15). The detailed calculation of the factor is as follows. From the operator identities (2.17) and the crossing symmetry (2.19), we obtain

$$t(\theta_j + a) t(-\theta_j - a) = a(\theta_j + a) d(\theta_j + a - 1), \quad j = 1, \cdots, 2N. \tag{14}$$

At the points of $\{\theta_j = 0\}$, we have

$$\begin{aligned} t(a)t(-a) &= a(a)d(a-1) \\ &= \frac{(2a+2)(2a-2)}{(2a+1)(2a-1)}(a+p)(a-p)[(1+\xi^2)^{\frac{1}{2}} a + q][(1+\xi^2)^{\frac{1}{2}} a - q][(2a+1)(2a-1)]^{2N} \\ &= -\frac{1}{2}(4a^2 - 1) c_2. \end{aligned}$$

3. **Reviewer**: The authors write after (4.3) “In the derivation, we have used the relation $\sigma(\theta) = \delta(\theta)$.” It would be more appropriate to write “From now on, we use $\sigma(\theta) = \delta(\theta)$”.

Authors: Thank you for your kind advice. 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**: Instead of chiral three spin interaction the authors refer to “charity interaction”. This is a severe misprint.

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