Ref.:

Response to points raised by Reviewer

Thank you very much for your supports. To these comments we respond as follows. The page numbers and equation numbers refer to revised version, unless specify.

1. **Reviewer**: I am convinced that (7.4) must simplify considerably to something like N times $(J_1 + J_2)$.

Authors: Thank you for your kind advice! We have simplified the expression of (7.4) in the new version.

$$\begin{aligned} E_g^{ferr} &= N(4a^2-1)\int_{-\infty}^{\infty}\tilde{a}_1(k)\cos(\bar{a}k)\tilde{\rho}(k)dk + c_0 \\ &= (2N+1)(2a^2-1) - \frac{2a^4-6a^2+1}{a^2-1} + E_b^{ferr}. \end{aligned} \tag{1}$$

2. **Reviewer**: Also, the explicit result in (7.5) resembles the terms in (2.3) and (2.4), but there are differences. At this point the physical intuition tells us that the bulk interactions favour a highly degenerate ground state of fully polarized spins (in arbitrary direction). The calculations become simple and can be done by elementary means. However, a fully polarized state will "see" the differently oriented boundary fields and the result of the boundary energy should depend non-trivially on the parameter ξ. However ξ dropped out in the authors' calculation or has been set to 0 from the beginning.

Authors: To clarify this issue, let us consider the following open XXX Heisenberg spin chain for simplicity

$$H_{XXX} = -\sum_{j=1}^{N-1}\vec{\sigma}_j\cdot\vec{\sigma}_{j+1} - \frac{1}{p}\sigma_1^z - \frac{1}{q}\sigma_N^z, \tag{2}$$

As you point out, the bulk interactions favour a highly degenerate ground state of fully polarized spins (in arbitrary direction)

$$|\Psi_n\rangle = (J^-)^n|\uparrow,\uparrow,\cdots,\uparrow\rangle, \quad n = 0,\cdots,N. \tag{3}$$

where $J^- = \frac{1}{2}\sum_{j=1}^{2N}(\sigma_j^x - i\sigma_j^y)$ is the spin-flipping operators. To give a physical picture of the boundary fields can not "see" each other, we consider 2 cases: the first one $p, q > 0$, which represent the orientations of boundary fields are same; The second one $p \cdot q < 0$, which represent the angle between 2 boundary fields is 180°.

In the first case, the ground state is fully polarized state $|\Psi_0\rangle$ in (3), and the ground state energy given by exact diagonalization is

$$E_g^p = -14, \qquad \text{with} \quad p = 0.5, q = 1, N = 12. \tag{4}$$

In the second case, the expected value of H_{XXX} at fully polarized state $|\Psi_0\rangle$ is

$$E^{ap} = \langle \Psi_0 | H_{XXX} | \Psi_0 \rangle = -12, \qquad \text{with} \quad p = 0.5, q = -1, N = 12. \tag{5}$$

The result shows that the contribution of the angle between 2 boundary fields to energy belongs to $O(1)$ terms for the fully polarized state, and thus the fully polarized state can "see" the differently oriented boundary fields. **However, the fully polarized state $|\Psi_0\rangle$ is not the ground state**

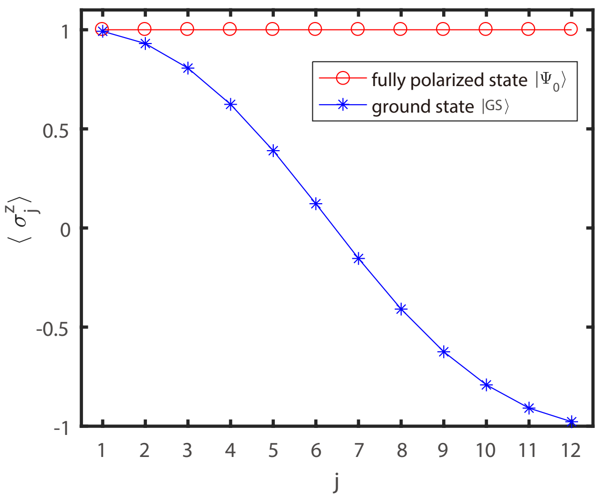

FIG. 1: The expected value $\{\langle \sigma_j^z \rangle | j = 1, \cdots, N\}$ at the fully polarized spins state $|\Psi_0\rangle$ and at the ground state in the second case $|GS\rangle$ with $p = 0.5, q = -1, N = 12$.

in the second case. The ground state energy in the second case with exact diagonalization is

$$E_g^{ap} = -13.6383, \qquad \text{with} \quad p = 0.5, q = -1, N = 12, \tag{6}$$

which is lower than the energy of the fully polarized state E^{ap}. Comparing E_g^{ap} with E_g^p, we can find the contribution of the angle between 2 boundary fields to energy belongs to $O(1/N)$ terms at the ground state. To show the ground state clearly, we plot the expected values $\langle GS|\sigma_j^z|GS\rangle$

and $\langle\Psi_0|\sigma_j^z|\Psi_0\rangle$ in Fig.1, where $|GS\rangle$ is the ground state in the second case and $j = 1, \cdots, N$. From this figure, we can find that the ground state in the second case is obviously not the fully polarized state. The expected value of σ_j^z for the fully polarized states $|\Psi_n\rangle$ is a line parallel to the x-axis. In conclusion, if the orientations of boundary fields are different, the ground state is not fully polarized state, and it can not "see" the differently oriented boundary fields. Thus the result of the boundary energy depends trivially on the parameter ξ.