Reply to Referee 2 questions and comments:

R_2.(1) *"The authors focus on thermal properties of one-dimensional quantum spin chains that admit a free-fermion representation via the Jordan-Wigner transformation. Explicitly, they consider a finite-size quantum XY spin chain under periodic boundary conditions. The resulting even and odd fermion parity sectors are carefully treated to obtain explicit expression of the exact partition function, which is compared with the one in the even parity sector only for different temperatures and transverse fields. The discrepancy between the two in the low-temperature regime is explained by a two-level approximation. In addition, the full counting statistic of observables that preserves the fermion parity (such as the transverse magnetization and the number of kinks) is provided.*

Investigation of finite-temperature and non-equilibrium properties of finite-size integrable spin chains in a mathematically rigorous way is important to the understanding of various concepts in statistical mechanics and mathematical physics. The manuscript is clearly written and the results are reliable. I believe the paper is worth being published in SciPost Physics, though have several comments the authors may wish to address."

<u>Answer:</u>

We thank the referee for the concise summary of our work and recognizing the timeliness of our contribution, as well as for the recommendation to publish the manuscript in SciPost Physics.

R_2.(2) *"The derived exact partition function for the spin-1/2 XY chain given by Eq. (46) seems quite similar to Eq. (1.46) in Minoru Takahashi's book [M. Takahashi, Thermodynamics of one-dimensional solvable models (Cambridge University Press, Cambridge, 1999)]. The authors my wish to point out the connection/difference between the two results."*

<u>Answer:</u>

We are very grateful to the referee for pointing out this reference.

In the new version of manuscript, we cite Takahashi's book, and comment on this limit after deriving the general expression. In the isotropic case the expressions we provide and those in Takahashi book agree. Unfortunately, in the anisotropic case, we find a serious flaws in the notation and the treatment of the Bogoliubov modes π and 0 in Takahashi's book. The presnetation is very terse and the information provided does not suffice to reproduce the correct results. Let us ellaborate on this in the next points:

(a) As a convention we used Eq.T# and Eq.B# to indicate the numbering equation in Takahashi's book and Białończyk et a.l's work (the current manuscript).

(b) Following the logic line of Takahashi's book, he introduces for the first time a Fourier transforms in Eq.T(1.9), using the notation q to indicate the modes with values $q = 2\pi n/N$, where n is an integer (half-odd integer) for odd (even) M, with M the total number of down-spins and the system size N. Then, he writes down the complete partition function for the Isotropic Heisenberg model:

$$Z = z^{-N/2}\left(\frac{1}{2}\left[\prod_{l=1}^{N}\left(1+z\exp\left[\frac{J\cos(2\pi l/N)}{T}\right]\right)-\prod_{l=1}^{N}\left(1-z\exp\left[\frac{J\cos(2\pi l/N)}{T}\right]\right)\right]\right. \quad \text{(Eq.T(1.17))}$$
$$\left.+\frac{1}{2}\left[\prod_{l=1}^{N}\left(1+z\exp\left[\frac{J\cos(\pi(2l-1)/N)}{T}\right]\right)+\prod_{l=1}^{N}\left(1-z\exp\left[\frac{J\cos(\pi(2l-1)/N)}{T}\right]\right)\right]\right)$$

where $z = \exp[-2h/T]$, J is the hopping parameter and h the transversal magnetic field.

On the other hand, in the **Summary 3.1: Exact partition function for spin$-\frac{1}{2}$ XY model**, we wrote exact partition function (see Eq.B(47)) and the elementary excitation energy per mode (see Eq.B(47)). The wave-vector k takes values in the positive ($\mathbf{K}^+$) and negative ($\mathbf{K}^-$) parity sectors given by Eq.B(10) and Eq.B(11). By direct substitution and using $\gamma = 0$ (isotropic case), we show the numerical agreement between Eq.T(1.17) and Eq.B(47) in Figure 1, for different temperatures and systems sizes.

Although our manuscript deals only with even system sizes, we would like to observe, that formula given by Takahashi (Eq.T(1.17)) is wrong for odd system sizes. For odd N it should have the following form:

$$Z = z^{-N/2}\left(\frac{1}{2}\left[\prod_{l=1}^{N}\left(1+z\exp\left[\frac{J\cos(2\pi l/N)}{T}\right]\right)+\prod_{l=1}^{N}\left(1-z\exp\left[\frac{J\cos(2\pi l/N)}{T}\right]\right)\right]\right. \quad \text{(Eq.T(1.17)')}$$
$$\left.+\frac{1}{2}\left[\prod_{l=1}^{N}\left(1+z\exp\left[\frac{J\cos(\pi(2l-1)/N)}{T}\right]\right)-\prod_{l=1}^{N}\left(1-z\exp\left[\frac{J\cos(\pi(2l-1)/N)}{T}\right]\right)\right]\right)$$

(c) In section 1.2 of Takahashi's book, the anisotropic XY model is introduced in Eq.T(1.35). In the next step, the author uses a Jordan-Wigner transformation, obtaining a fermionic hamiltonian given by Eq.T(1.37), and he defines the Fourier transform in Eq.T(1.38). The wave-vector q takes values $q = 2\pi n/N$, where n is integer (half-odd integer) for parities $\alpha = -1\,(+1)$, respectively. By direct substitution, the author obtains the hamiltonian Eq.T(1.39) in the momentum space. Following this equation the author states:

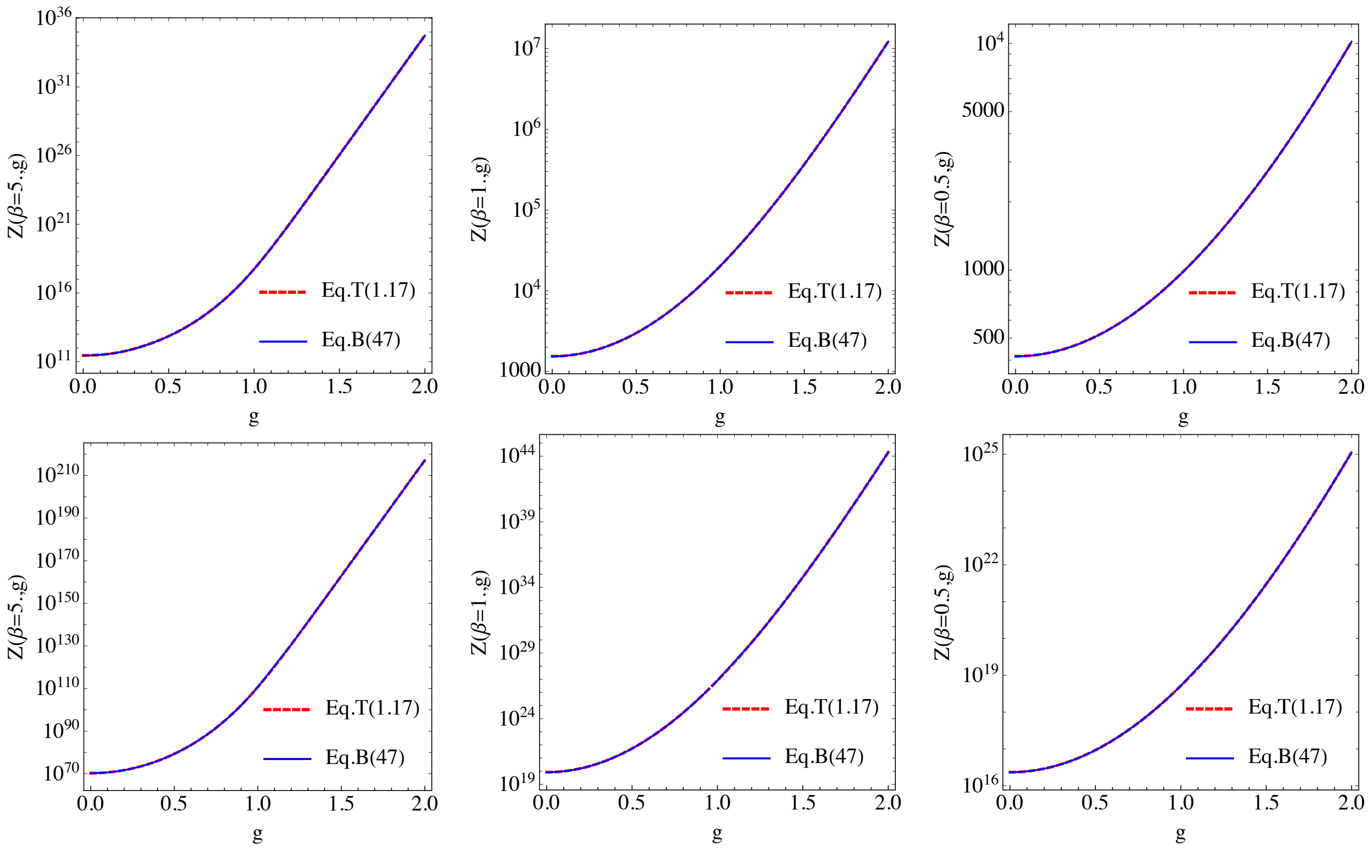

Figure 1: **Agreement between Eq.T(1.17) and Eq.B(47) in the isotropic case**. We show the numerical agreement for the partition function. The system sizes are 8 and 50 for the up and down panel. The inverse of temperature is change from left to right by $\beta = 5$, $\beta = 1$, and $\beta = 0.5$.

"Here $\sum_q'$ means the sum over $0 < q < \pi$". **Therefore this condition eliminates the modes** 0 **and** π. At this level, we could conclude that the partition function for the anisotropic model given by Eq.T(1.46) is incorrect.

(d) Without lost of generalization, we consider the limit Ising $\gamma = 1$ for all analysis exposed in the following items.

(e) To prevent any misunderstanding due to what appears to be a lack of complete information in Takahashi's book, we carried out a detailed analysis. Takahashi's writes the

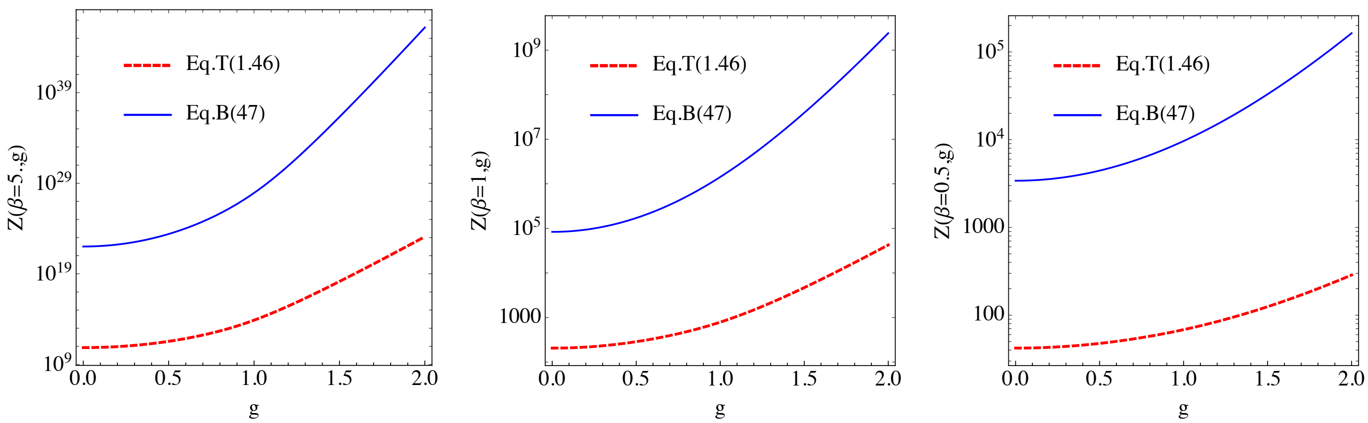

Figure 2: **TEST #1: Comparison between Eq.T(1.46) and Eq.B(47)**. We show the numerical comparison for the total partition function in the anisotropic model. The system size is $N = 8$; Therefore $q = \left\{\frac{\pi}{10}, \frac{3\pi}{10}, \frac{\pi}{2}, \frac{7\pi}{10}, \frac{9\pi}{10}\right\}$ and $q' = \left\{\frac{\pi}{5}, \frac{2\pi}{5}, \frac{3\pi}{5}, \frac{4\pi}{5}\right\}$. The inverse of temperature is change from left to right by $\beta = 5$, $\beta = 1$, and $\beta = 0.5$. Only blue curves match the exact diagonalization results.

total partition for the anisotropic XY model in the following form:

$$Z = \exp\left[\frac{\sum_q \epsilon(q)}{2T}\right] \frac{1}{2}\left[\prod_q \left(1 + \exp\left[-\frac{\epsilon(q)}{T}\right]\right) + \prod_q \left(1 - \exp\left[-\frac{\epsilon(q)}{T}\right]\right)\right] \tag{Eq.T(1.46)}$$

$$\exp\left[\frac{\sum_{q'} \epsilon(q')}{2T}\right] \frac{1}{2}\left[\prod_{q'} \left(1 + \exp\left[-\frac{\epsilon(q')}{T}\right]\right) - \prod_{q'} \left(1 - \exp\left[-\frac{\epsilon(q')}{T}\right]\right)\right]$$

It is said further, that "$qN/2\pi$ is a half-odd integer and $q'N/2\pi$ is an integer and here $\epsilon(q) = \sqrt{(J\cos q - 2h)^2 + (J'\sin q)^2}$". The parameters J and J' are defined in Eq.T(1.36). **A natural and open question for the reader is: Is this q's values independent of the systems size (even/odd)?** The author never defined it; However we concluded that it could work if the system size is even. We chosen a system size $L = 10$ (Remembering that we tested the expression for the total partition function by exact diagonalization) and we choose the q and q' values according the condition expressed in the previous numeral (c) ($0 < q < \pi$ and $0 < q' < \pi$). In Figure 2 we show the a first comparison between Eq.T(1.46) and Eq.B(47).

(f) Now, we go back to do a similar previous analysis, but now we include the modes 0 and π in the q' values as a Test #2. We presented the numerical contrast in Figure 3.

(g) We did a Test #3, in the which, we now **ignored the condition expressing by book's author signalized in the numeral (c)**. We consider that the modes q and q' can take positivs and negative values, including 0 and π. We present the qualitative and quantitative agreement for $g > 1$ in Figure 4.

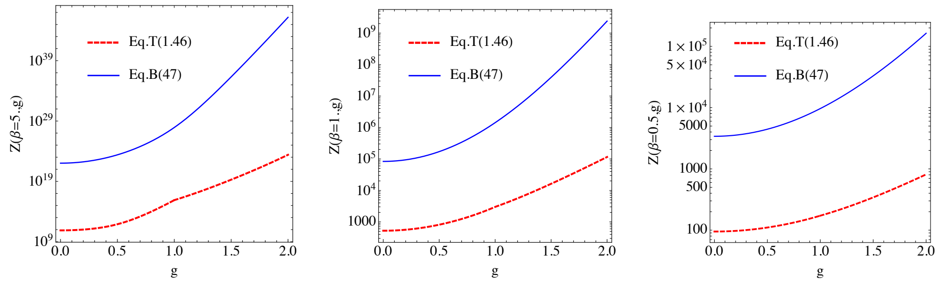

Figure 3: **TEST #2: Comparison between Eq.T(1.46) and Eq.B(47)**. We show the numerical comparison for the total partition function in the anisotropic model. The system size is $N = 8$. In this test #2, we used $q = \left\{\frac{\pi}{10}, \frac{3\pi}{10}, \frac{\pi}{2}, \frac{7\pi}{10}, \frac{9\pi}{10}\right\}$ and $q' = \left\{0, \frac{\pi}{5}, \frac{2\pi}{5}, \frac{3\pi}{5}, \frac{4\pi}{5}, \pi\right\}$. The inverse of temperature is change from left to right by $\beta = 5$, $\beta = 1$, and $\beta = 0.5$.

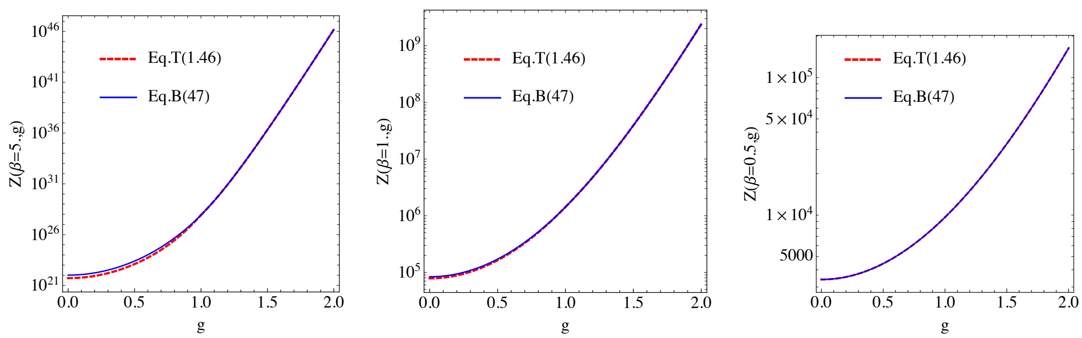

Figure 4: **TEST #3: Comparison between Eq.T(1.46) and Eq.B(47)**. We show the numerical comparison for the total partition function in the anisotropic model. The system size is $N = 8$. In this test #3, we used $q = \left\{-\frac{9\pi}{10}, -\frac{7\pi}{10}, -\frac{\pi}{2}, -\frac{3\pi}{10}, -\frac{\pi}{10}, \frac{\pi}{10}, \frac{3\pi}{10}, \frac{\pi}{2}, \frac{7\pi}{10}, \frac{9\pi}{10}\right\}$ and $q' = \left\{-\frac{4\pi}{5}, \frac{3\pi}{5}, -\frac{2\pi}{5}, -\frac{1\pi}{5}, 0, \frac{\pi}{5}, \frac{2\pi}{5}, \frac{3\pi}{5}, \frac{4\pi}{5}, \pi\right\}$. The inverse of temperature is change from left to right by $\beta = 5$, $\beta = 1$, and $\beta = 0.5$.

(h) Finally, we complete our analysis by correct the expression for the eigenenergy for the modes $q = 0, \pi$, where it is given by:

$$\epsilon\,(q = 0) = 2\,(h - 1)\,, \quad \epsilon\,(q = \pi) = 2(h + 1).$$

we show the complete agreement between Eq.T(1.46) and Eq.B(47), after several notation corrections in Figure 5. We emphasize, that according to Takahashi's expression $\epsilon\,(q) = \sqrt{(J\cos q - 2h)^2 + (J'\sin q)^2}$ these eigenenergies are equal $2|h-1|$ and $2|h+1|$, respectively. Therefore, main source of mistake in Takahashi's book lies in applying formula for $\epsilon(q)$ directly to modes 0 and π instead of correctly treating them separately, as in our manuscript.

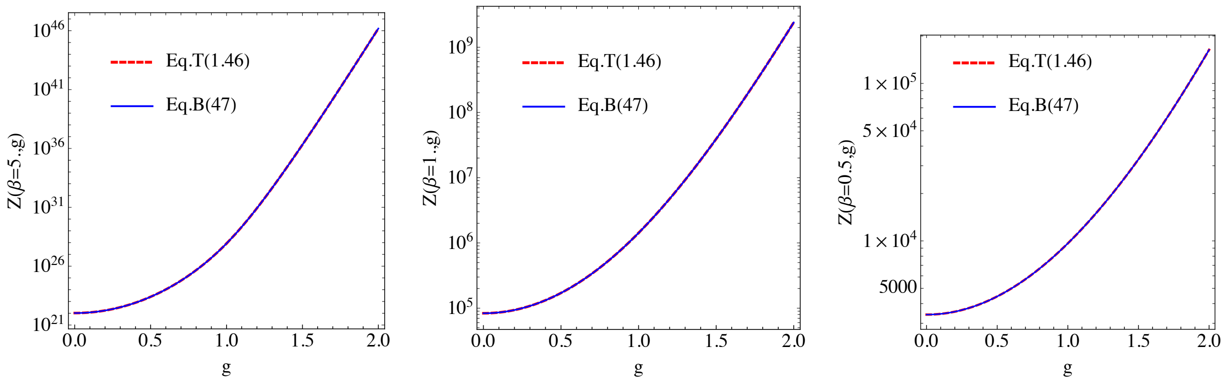

Figure 5: **TEST #4: Comparison between Eq.T(1.46) and Eq.B(47)**. We show the numerical comparison for the total partition function in the anisotropic model. The system size is $N = 8$. In test #4, we used $q = \left\{-\frac{9\pi}{10}, -\frac{7\pi}{10}, -\frac{\pi}{2}, -\frac{3\pi}{10}, -\frac{\pi}{10}, \frac{\pi}{10}, \frac{3\pi}{10}, \frac{\pi}{2}, \frac{7\pi}{10}, \frac{9\pi}{10}\right\}$ and $q' = \left\{-\frac{4\pi}{5}, \frac{3\pi}{5}, -\frac{2\pi}{5}, -\frac{1\pi}{5}, 0, \frac{\pi}{5}, \frac{2\pi}{5}, \frac{3\pi}{5}, \frac{4\pi}{5}, \pi\right\}$. Additionally, we use the correct eigen-energies for the mode $k = 0$. The inverse of temperature is change from left to right by $\beta = 5$, $\beta = 1$, and $\beta = 0.5$.

R_2.(3) *"On page 15 it is mentioned that the treatment of observables having components linear in fermion operators is beyond the scope of the present paper. The authors should comment further on the possible difficulties in obtaining the full counting statistics of such kind of operators."*

We thank the referee for this remark. We expanded the first paragraph on the page 15. We included the description of the possible procedure one could apply, however, without going into mathematical details. Moreover, we described more precisely results in the literature on this topic.