Reply to referees for "Out-of-equilibrium full counting statistics in Gaussian theories of quantum magnets"

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We thank the referees for the positive assessment of our work and their useful comments. Below we reply to the points they have raised. We also add at the end of this file a list of additional minor changes we have implemented in the new version of the paper.

1 Reply to the first referee

1. Referee: "*How well the quantum system are described by a Gaussian state basically determines the applicability of the formula proposed by the authors. Indeed, in a few cases, especially in the scenarios of quench dynamics, the authors found large discrepancy between the results calculated with their formula and the strict results. While several of these examples are helpful, it is better if the authors can provide some more general principles and guiding rules for when the formula works the best or fails.*"

The referee is correct in that the key requirement for the application of our FCS formula is proximity of the state of the system to a Gaussian state (in the sense that spatially local properties are well approximated). Unfortunately a precise quantification of the level of proximity is a very non-trivial task for the class of models we consider. The reasons are (i) the lack of exact results and (ii) the unavailability of numerical methods that can tackle this class of problems (for 2D and 3D magnets and large system sizes). Having said that, one general principle for the formula to apply is that there are mean fields (e.g. the ordered magnetic moment) and Gaussian fluctuations only induce a small or at most moderate deviations from their "classical" values. We note that the latter are much easier to evaluate than the FCS itself. Beyond that, as in most of the literature on spin-wave theory, the goodness of our approximations can be only checked a posteriori by comparing our predictions with numerical results, whenever these are available (Figs. 7–11, 14). It is also useful to perform internal consistency checks within the approximate theories, as we do every time we compare the late time dynamics with thermal values or compare different types of Gaussian approximations (Figs. 2, 5, 6, 12, 15, 17, 18).
Regarding the referee's comment "*Indeed, in a few cases, especially in the scenarios of quench dynamics, the authors found large discrepancy between the results calculated with their formula and the strict results*", we would like to stress that the only result on quench dynamics in the paper for which we can compare our FCS formula with exact results is Fig. 9, in which the agreement is excellent (not surprisingly, given that this represents a particularly simple limit and we restrict the comparison to the time regime over which Fig. 8 shows that the SCTDMFT coincides with the exact result). For all the other results on quench dynamics we are limited to internal consistency checks. Furthermore, we already stress at pg. 7 (and again at pg. 29) that it is well known that the SCTDMFT is in many cases not a good approximation for late time dynamics.
The only other case in which we are able to compare our FCS formula with exact (numerical) results is when we compare the equilibrium PDFs from Schwinger boson mean-field theory (SBMFT) with the results obtained by Monte-Carlo sampling in our Reference [20], see Fig. 11. The referee is correct in that the agreement here is found to be poor, especially for the smaller temperature. However, we have traced this problem back to the influence of unphysical states unavoidably introduced by the

mean-field treatment, as shown in Fig.10(a). Thus the disagreement in this case goes even beyond the non-sufficient proximity to a Gaussian state, and implies that this simple mean-field theory is not suitable to quantitatively describe the disordered system we consider (as we explicitly stress at pg. 26). It is important to note this problem equally occurs in the calculation of simpler properties (e.g. the dynamical structure factor). Nevertheless SBMFT continues to be used in the literature to obtain approximate results that show the correct qualitative behaviours. We have been partially able to improve over SBMFT by employing the Takahashi's modified spin-wave theory in Section 3.2. However, as we explain, there we are prevented from applying our FCS formula.
Thanks to the referee's comment we have realized it is better to stress already from the introduction what are the physical systems in which we expect this method to yield a good description of PDFs of observables that can be expressed as quadratic functions of bosons. We have thus inserted at pg. 2 of the introduction the following lines:

"The prototypical example of spin systems where representations in terms of bosons and Gaussian approximations can be successfully employed are those possessing long-range magnetic order. Here Gaussian quantum fluctuations are the dominant contribution beyond the classical mean-field solution. Gaussian approximations can be also employed in absence of long-range order, as we will briefly review later in this work. Beyond spin models, the techniques developed in the following can be straightforwardly applied to any model of bosons in a regime dominated by Gaussian fluctuations."

2. Referee: "*Another related point is that the authors mainly focus on the examples when the quantum systems can thermalize or is already at thermal equilibrium. Recently, full counting statistics in integrable systems also receive quite a lot of interest. I also recommend the authors to comment and discuss the validity of their results in those integrable systems which do not fully thermalize to a Gibbs ensemble.*"

We thank the referee for this comment. First, we would like to emphasize that there is a significant difference between the quantities we consider, namely PDFs of order parameters (which are the most interesting ones from a physics point of view), and those considered in most recent works in the context of integrable models, where the focus is on PDFs of subsystem observables which are conserved globally. Physically one expects the latter to behave in a special way, as the subsystem fluctuations of observables that are conserved globally are intuitively expected to be smaller. This expectation is borne out e.g. in the ground state of the spin-1/2 XXZ chain, where PDFs of a variety of subsystem observables have been analyzed (Ref. [17]). Second, there is a more fundamental constraint for applying our results to 1D integrable models: our approach is premised on the applicability of a bosonic (time dependent) mean field theory plus Gaussian fluctuations, whereas the excitations in interacting 1D integrable models are typically better described in terms of interacting fermions (this is certainly the case at low temperatures/energy densities). Put differently, while bosonic spin-wave theories have been applied very successfully in $D = 2, 3$, we would not a priori expect them to apply quantitatively to most 1D interacting integrable models. A possible exception are ferromagnetic spin chains at low energy densities (e.g. after small quenches). In one of the original papers by Takahashi (our reference [91]), he argues that in the 1D integrable XXX Heisenberg ferromagnet his modified spin-wave theory yields an expansion of the free energy with temperature that coincides very well with the results of the Bethe-ansatz integral equations. Thus employing the modified spin-wave theory in this integrable model may indeed provide reasonable results for the first few moments of the PDFs of subsystem observables, both in equilibrium and after quantum quenches. However, we think that this is beyond the scope of the present (already quite long) paper.
We now discuss this interesting direction for further research in the conclusions of our paper.

2 Reply to the second referee

1. Referee: "*The paper lacks a bit of structure as derivations and results as well as equilibrium and non-equilibrium results are mixed.*"

Regarding the equilibrium/non-equilibrium part of the comment: this choice was made intentionally in order to stress how the application of our FCS formula doesn't present conceptual differences in the case of equilibrium or out-of-equilibrium settings, once the reduced Gaussian density matrix of the system is known in either cases.
Regarding derivations vs results: we are not quite sure what the referee refers to here. Throughout the paper we always present mathematical derivations first, and then show in a different subsection the results for PDFs and/or expectation values. For example, within Section 2.1 we explain in subsections 2.1.1 and 2.1.2 how to obtain the Gaussian density matrix in- and out-of-equilibrium (respectively), and then present the corresponding results for the PDFs in sections 2.1.3 and 2.1.4. Similarly, within Section 2.3, we derive the formalism and main formulas in subsections 2.3.1-2.3.5 and then show results in 2.3.6. Sections 3.1 and 3.2 also follow an identical structure, with a clear distinction between mathematical derivations and results.
We have added a table of contents in the hope of making the structure of the paper clearer.

2. Referee "*Extreme value statistics of staggered magnetization in 2d/3d Heisenberg model lacks explanation. This could be an artifact.*"
Also: "*The phenomenological fit of the PDF for the 2d and 3d Heisenberg model to an extreme-value distribution is an interesting observation, which calls for an explanation. The fact that for both 2d and 3d Heisenberg model the PDF of the staggered magnetization follows a Gumbel distribution is rather suspicious, since the former model has no long-range order at finite temperature while the latter has.* "

We thank the referee for these comments. As we already mentioned in the text, the Gumbel fit is purely phenomenological in nature. We have tried, but failed, to a find a justification why extreme value statistics should arise here.
To address the referee's comment we have updated the text at pg. 9 with the following:

- Added the sentence "Indeed, while in [25] the appearance of EVS functions can be analytically understood as arising in the standard way from the distribution of the maximum among a large number of independent variables, we are unable in our context to interpret the appearance of the Gumbel distribution from similar arguments. Furthermore, a proper identification of P_A as a Gumbel distribution would require an analysis of the extreme tails of the curve, which is not possible due to the finite range of values of the staggered magnetization associated with each ℓ."

- Added the word "phenomenological" to the description of the Gumbel fit in the caption of Figs. 1-2.

3. Referee: "*Why is the PDF in Fig. 1 at zero temperature not a semicircular distribution like in Fig. 3 of the supplemental material of Ref. [20] ? Is this an artifact of the spin-wave expansion around an ordered state with well-defined orientation of the spins ? The PDF for the 2d Heisenberg antiferromagnet in section 3 appears to have the correct Gaussian shape, but this is the same model as in Fig. 1, only the mathematical treatment is different.*

Fig. 3 of the supplemental material of our Ref. [20] shows the PDFs of the staggered magnetization Σ in the 2D repulsive Hubbard model for $U/t = 7.2$ at a few *non-zero* temperatures. A few remarks are important

- The PDFs shown there are all symmetric around $\Sigma = 0$, yielding a zero average staggered magnetization as expected in such a disordered system (temperature is non-zero). On the other hand, in our Fig. 1 we consider the 2D Heisenberg antiferromagnet at *zero temperature* (ordered phase), for which long-range order is present and thus the *exact* PDF cannot be symmetric around $\Sigma = 0$. Note that our Gumbel-like PDFs from Fig. 1 yield an average Σ that exactly coincides with the standard result from spin-wave theory, which is known to be extremely close to the exact value. We therefore expect the PDFs shown in Fig. 1 to be quite close to the exact PDFs of 2D Heinseberg antiferromagnet at zero temperature.

- The results from our Section 3 regard the 2D Heisenberg model at *non-zero temperatures* (disordered phase), and thus we obtain approximate PDFs that are correctly symmetric around $\Sigma = 0$. We note that in comparing our approximate PDFs from this Section 3 with the data from [20], we use the Monte-Carlo results for the Heisenberg antiferromagnet ($U/t \to \infty$) rather than the Hubbard model data at $U/t = 7.2$.

4. Referee: "*The long-range transverse-field Ising chain has a finite-temperature Kosterlitz-Thouless floating phase at alpha=2 (See e.g. PRB 64, 184106 (2001); Journal of Computational Physics, vol. 228, 7 (2009) and J. Stat. Mech. (2020) 063105). Here, indeed one might expect non-Gaussian magnetization fluctuations inside a relatively narrow temperature window. This is definitely the case for the related 2d XY model, see Bramwell et al. Nature 396, 552 (1998). An interesting question is whether the authors' spin-wave approximation can reproduce this regime.*"

We thank the referee for this comment. For the long-range transverse-field Ising chain we have restricted our study to quench dynamics and we haven't addressed the equilibrium physics of the model. Out-of-equilibrium, as we state at pg. 23, our approach is expected to be accurate for short and intermediate time scales only for $0 < \alpha < 1$. The equilibrium phase diagram at $\alpha = 2$ is indeed quite rich, and we fully agree with the referee that it would be interesting to investigate PDFs of subsystem magnetizations in particular in the KT phase with power-law correlations. However, this requires a fundamentally different Gaussian approximation from the one we employed (which is based on the presence of long-range magnetic order), and is therefore beyond the scope of our work. We have added a comment in our conclusion section that mentions the study of the equilibrium PDFs in the long-range TFIC as a direction for future work.

5. Referee: "*In the section on quantum quenches (before Eq. 32) it is not stated what the Hamiltonian after the quench is.*"

We thank the referee for spotting this. We have now added the following sentence after Eq. (33) of the new draft:

"and then quenching to the XXX Hamiltonian (15) corresponding to $\eta = 1$".

3 Additional minor changes

- At pg. 10 we have removed the remark "$\eta = 1$ being the Heisenberg model", as we now say it before.
- Inserted current Equation (10), because that particular choice is used throughout the entire work and it is then better to stress it from the beginning.
- Added a few relevant references in the introduction and conclusion, and changed the citations of arXiv preprints to citations of journal articles.