Authors comments upon resubmission

Nitya Cuzzuol, Luca Barbiero and Arianna Montorsi

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1 Report1

We thank the referee for the very positive comments evaluation of our paper and for recommending it for publication.

2 Report2

This is my second reviewer's report on this manuscript. I stand by the conclusion of my previous report: In its present form, the considered manuscript does not seem suitable for publication in SciPost. A substantial revision may change this.The following three comments, all present in my previous report, still apply to the revised version:
We thank the referee for her/his second report. Here we clarify, once more, the comments raised by the referee:

- 1) *The 'odd parity' order parameter, which the Authors put forward as their key contribution in this paper, should be defined more carefully, including an explicit discussion of the mechanism whereby either 'parity' or 'odd parity' may be finite while the other is not.*
  First, let us stress that our definition of odd parity is careful and consistent, as explicitly in the opinion of referee 3 as well. As discussed in the previous authors' reply letter, and at the end of section 2.1 of the previously emended version of the manuscript, parity and odd parity are related by

$$O_P(j) = (-1)^{j-1} O_P^{(o)}(j) \quad . \tag{1}$$

  As for the underlying mechanism, we repeat below the main ingredients in the definition of odd parity to end with the explicit discussion of the physical mechanism underlying its finiteness in the PSF phase.
  As also explained in Ref.[11] for the very same relation holding between charge and spin parity in fermionic case, eq. (1) implies the finiteness of the expectation value of the uniform part of at most one of the two parities. In particular, O_P turns out to have a finite uniform part $(O_P(j)+O_P(j+1))/2$ in the MI phase, in which the uniform part of $O_P^{(o)}$ is vanishing. Instead the latter becomes finite in the PSF phase, in which the uniform part of O_P goes to zero. This property can be easily understood looking at the argument of the exponential in the definition of the two parities. When the density distribution over the chain is uniformly one (MI phase), the argument of the exponential of parity is identically vanishing and the parity is one; the argument of the exponential in the odd parity oscillate between $i\pi$ and zero, so that the expectation value of the uniform part of odd parity is identically vanishing. Analogously, when the interaction is such that bosons just form pairs (PSF phase), the argument of the exponential of odd parity is identically vanishing, while that of parity oscillates. In our paper we show that in the latter case, consistently with predictions of bosonization, odd parity behaves as an order parameter for the paired superfluid phase also when some pairs of bosons in the PSF phase break into correlated pairs of single bosons, as shown in the cartoon of fig. 1 in 2D. In order to further encounter this referee comment, we modified lines 139-143 in the paper.

- 2) *The Authors' claim that 'odd parity' is the "unique order parameter" for pair superfluids (abstract, l. 7; page 2, 3 lines from end) should be justified, by comparing it to previously proposed order parameters for pair superfluids, and explicitly giving the assumptions which make them inapplicable in the case considered by the Authors.*
  We understand that the concern of the referee is due to a misunderstanding: we stress once more that in the present context the total number of particles is conserved, thus $\langle b_i^2 \rangle$ is vanishing by definition also in PSF phase. As a consequence $\langle b_i^2 \rangle$ cannot be considered as its order parameter at fixed number of particles. Notably, it is worth to underline that configurations with conserved number of particles are the typical regimes explored in ultracold atomic systems. More importantly, in such regimes (as now specified in the paper at line 8 in the abstract and line 63 in section 1) our derived parity operator results to be the unique order parameter. While we certainly agree with the referee that $\langle b_i^2 \rangle$ is an additional order parameter of PSF (as now specified in the text at line 161) when the particle number conservation is not enforced.

- 3) *The Authors' presentation is quite technical. Including an overview of the roles of the employed approaches would make it more accessible.*
  As discussed in the previous authors' reply letter, both Bosonization [8, 57] and DMRG [69, 71, Catarina2023[1]] are standard methods for strongly correlated low dimensional quantum systems, with a huge dedicated literature. This holds also for the specific case treated here of the constrained Bose Hubbard model [10, 41, 48, 65, 82] (but also for different models [11, 12, 17, 55, 67]). For the latter, also nonlocal order parameters have been largely exploited in both the theoretical [10, 13–17, 68] and experimental [25–30] characterization of quantum phases.
  While for this reason we don't feel appropriate to enter the technical details of the above methods, we have rephrased the last sentence at the end of the introduction section to make clearer which is the role of these methods along the paper.

3 Report3

I presume that the odd parity is numerically estimated from an extrapolation of finite-size numerical data to infinity, but the details are lacking in the paper. It looks rather strange that the authors show the size dependence explicitly for the gap in Figure 3 but not for the odd parity, which is the main subject of the paper. There is a brief cryptic remark just before Section 3.1 – "the nonlocal order parameter $O_P^{(o)}$ has been extracted from $O_P^{(o)}(j)$ by fixing j to a sufficiently large value.... (i.e. not close to the transition)", but this description is not sufficient. First, the authors should demonstrate the point explicitly since this is the central point of the paper. Furthermore, it seems like the authors actually study the parameter U/t quite close to the critical point in Fig. 2(c). Are they still "not close to the transition" concerning the odd parity?? (It would be rather surprising if that is the case.) In any case, the authors should show the size dependence of the odd parity explicitly for Fig. 2(c), Fig. 4(c), Fig. 5, and Fig. 6.
We thank the referee for the thorough reading of the new version of the paper.

- In order to clarify this point, we want to remark here that the numerical method we exploited to obtain the odd parity (as specified in section 3) is the infinite-size variant of the DMRG (iDMRG) algorithm [69], that leads to obtain a fixed-point translationally invariant matrix product wavefunction. When the algorithm is converged, the resulting quantum state approximates the 1D thermodynamic limit. In this way we are able to perform our simulations directly for an approximated infinite chain, avoiding the necessity of an infinite size extrapolation typical of the finite size DMRG results. However, in practice, the simulated chain is not infinite and we are forced to select a finite maximum j in accordance with the algorithm, when computing the expectation of the odd parity operator (as in eq.(8)). Not too close to the transition, $O_P^{(o)}$ quickly converges to zero or a constant, and thus a small value of j is sufficient to have a perfectly converged $O_P^{(o)}$.

[1] Catarina G and Murta B 2023 The European Physical Journal B 96 ISSN 1434-6036 URL http://dx.doi.org/10.1140/epjb/s10051-023-00575-2

Contrary to the calculation of $O_P^{(o)}$, extracting the gaps requires a finite chain and so finite size simulations. Indeed the iDMRG method doesn't support the calculation of excitations and one has to extrapolate the thermodynamic limit of the systems from a set of finite sizes.
To assess the consistency between the two procedures, as required by the reviewer, we can compare the results from both algorithm for $O_P^{(o)}$ of the 1D Bose-Hubbard model (eq.(1) of the paper). This is shown in figure 1. The light blue crosses are the iDMRG results (the same as in figure 2.c of the paper), while the red diamonds are the extrapolated results from finite size DMRG. Both methods distinguish between a region of zero $O_P^{(o)}$ (the atomic SF) and one where the same quantity is finite (PSF): the estimated transition point by iDMRG is in accordance with the extrapolated TDL data. This comparison shows that, by exploiting the iDMRG method, we are obtaining an accurate approximation of the TDL, avoiding the extrapolation procedure. Moreover the match between iDMRG and finite size results is supported by the agreement with the opening of the single particle gap Δ_1 in figure 3 of the paper.

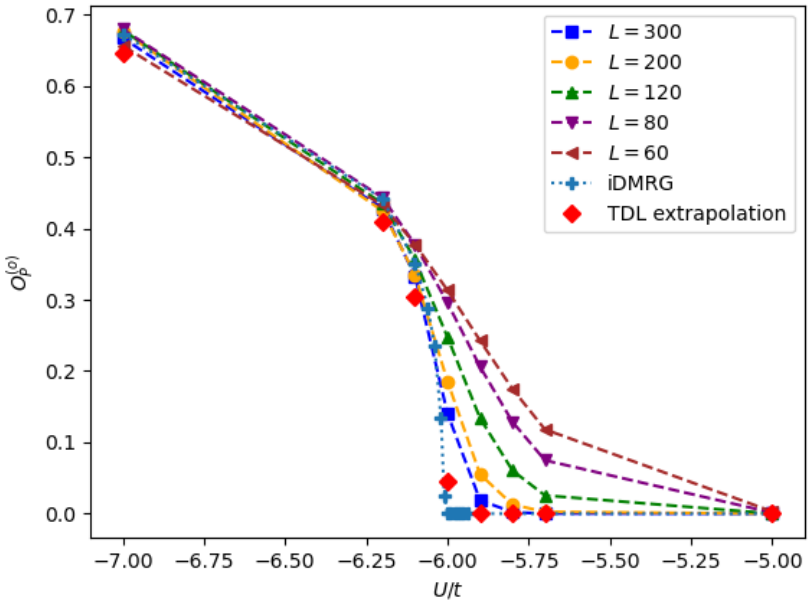

Figure 1: The figure shows the $O_P^{(o)}$ results for: different sizes of a finite chain by DMRG, the thermodynamic limit extrapolation obtained by these sizes, and the same quantity obtained by the iDMRG method.