I. REPLY TO REPORT 3

The referee writes:

Strengths

1. *Clear description of a very wide collection of phenomena.*

2. *Simple models are presented which capture the relevant physics.*

3. *Powerful numerical methods which help ellucidate relevant physics and sustain the simple models.*

Weaknesses

1. *Too much topics addressed, which makes difficult the revision of corresponding previous literature, which also is extensive; some from the same group.*

2. *The different topics can be addressed with more detail and focus, and I hope it could be done in the future in other papers.*

Report

The authors study a system of two distinguishable particles interacting with a small number of bosons of a third distinguishable type, with contact interactions in the ultracold regime, in one dimension, in the presence of a harmonic trap. Particularly, they consider NA=15 atoms in the largest component. Their main tool, but not the only one, is the numerical method coined as ML-MCTDHX. Their study focuses on the ground state, which they find via imaginary time evolution method. They study both attractive and repulsive intracomponent and various intercomponent interactions. Their findings reveal a collection of effects, from Bipolaron, bunching or antibunching, trimer state, etc. The paper deals with a lot of different aspects, which one may think that should deserve a bit more attention. Nevertheless, the basic aspects are well captured by numerics and with simple models. So I think the paper should be accepted in Scipost.

Our answer is:

We thank the referee for appreciating our work and providing constructive criticism and further suggestions which helped us to improve the presentation of our results. Below, we provide a detailed response to all questions raised and append a list of changes at the end of the reply letter.

Requested changes

The referee writes:

1. The main comment arises from the fact that the paper tackles so many aspects. I think they miss the context of previous research as a direct consequence. The most prominent lack I think is that classical papers from the open quantum system community should be cited

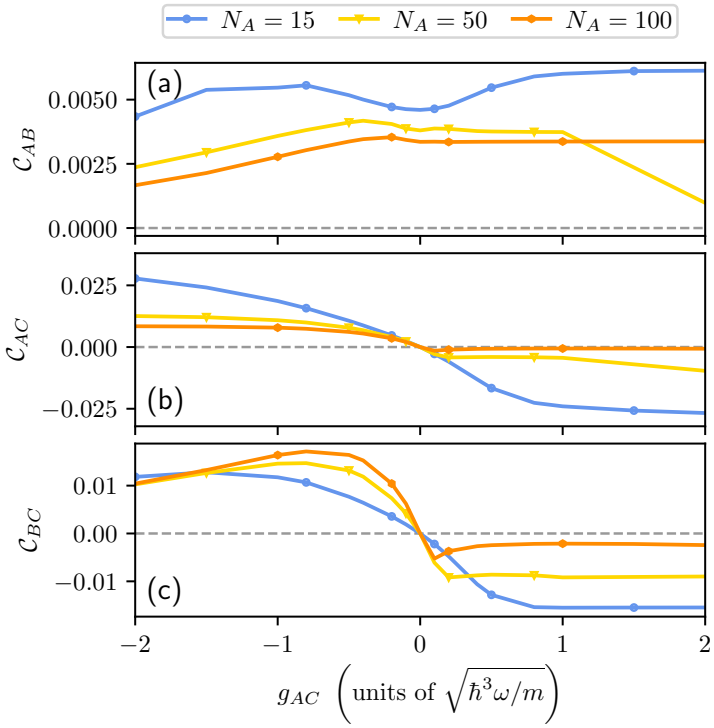

FIG. 1. Integrated intercomponent two-body correlation functions as defined in Eq. (9) of the manuscript as a function of the intercomponent interaction strength g_{AC} and for different number of bath particles (see legend). The overall behavior of the correlation functions is maintained for increasing atom number in the bath.

and commented (such as PRL 97, 25060, PRA 80, 032110, PRA 77, 042305) and others maybe PRL 102, 160501 or JPHYSA 45 065301 - this is not a comprehensive list, it should be researchd).

Our answer is:

We thank the referee for drawing our attention to these works investigating open quantum systems. As suggested, we have commented on them in the introduction of the revised manuscript and also included some relevant references in Appendix A (see also the list of changes).

The referee writes:

2. The second comment is that I find it a bit too much to call $N_A = 15$ atoms a bath, though for most of the physics discussed here it has little practical implication. I leave on

authors hands a comment on this, if they will.

Our answer is:

We remark that already the case of $N_A = 15$ bath atoms, used in the manuscript, shows the main effects of the dressing of the two indistinguishable impurities. To address the comment of the referee, in the revised manuscript, we comment that according to our analysis it is expected that the main features of the impurities dressing, e.g. the crossover from attractive to repulsive induced interactions, are retained for larger number of bath atoms. Nevertheless, a finite size scaling analysis would be desirable (see also the list of changes).

In order to argue about the robustness of our main results in larger settings let us consider below a bath consisting of $N_A = 50$ and 100 atoms. Figure 1 presents the respective integrated correlation functions while keeping fixed the mean-field interactions of the bath, i.e. $g_{AA}N_A = 3$. The main objective here is to show that a qualitative similar behavior of observables used for our analysis, e.g. the interspecies correlation, is maintained for mesoscopic particle numbers in the bath. Indeed, important features of the results of this work which are, for instance, the crossing from positive to negative values of $\mathcal{C}_{AC}$ and $\mathcal{C}_{BC}$ for varying g_{AC} from attractive to repulsive values persist even though deviations of the correlation values from the scenario with $N_A = 15$ are evident. Moreover, the overall behavior of the distinct correlation functions with respect to g_{AC} for different N_A is maintained (see also the corresponding discussion in Appendix D). Similar conclusions can also be drawn for other observables e.g. the densities of the components and the impurities relative distance. Let us also note at this point that the simulations with larger number of bath particles, namely $N_A = 50$ and 100, have been performed using $d_A = 2$ orbitals for the bath in order to be accelerated and testify the main behavior of the observables. Certainly, in order to strictly reach numerical convergence one needs to employ also a different number of orbitals. We expect that by doing so there will be no qualitative change on the behavior of the correlation function (and in general other used observables in the main text) which would contradict our findings.

The referee writes:

3. This is a technical comment about convergence: at the end of section 3. More details on this may be helpful for anyone to reproduce results.

Our answer is:

We thank the referee for their suggestion. In the revised manuscript we provide more details on the size of the used basis for obtaining our results and the reasoning behind this choice (see also the list of changes).

In order to clarify any possible confusion, in order to judge the quality of the results we perform extensive convergence studies for the observables used by varying the underlying orbital configuration space. The latter consists of the species function of number D_A, D_B and D_c as well as the amount of orbitals for each component denoted by d_A, d_B and d_C. Specifically, numerical convergence is achieved when the observables of interest remain essentially unchanged when increasing the orbital configuration space. Such an analysis is provided here

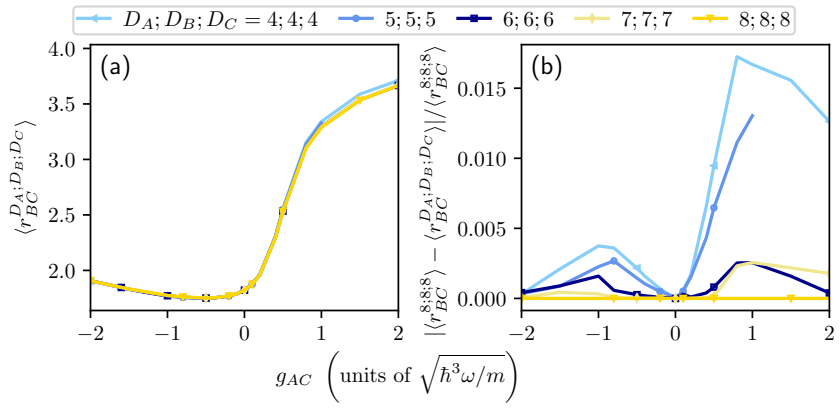

FIG. 2. (a) Two-body relative distance between the impurities with respect to g_{AC} for different numbers of species functions D_σ (see legend), where $\sigma \in [A, B, C]$ and fixed $g_{AB} = 0.2$. Note here that the number of orbitals for the impurities is the same with the species functions, i.e. $D_{B,C} = d_{B,C}$. (b) Relative deviation between the respective relative distances obtained for different values of D_σ (see legend). The relatively small deviations testify numerical convergence on the two-body level. Similar results occur for varying single-particle functions of the bath, d_A (not shown for brevity).

in Figure 2(a) where the relative two-body distance among the impurities is depicted for different number of species functions. For instance, it can be readily seen that the relative deviation between relative distances calculated with $D_A = D_B = D_C = 6$ and $D_A = D_B = D_C = 8$ are below 5% thus testifying numerical convergence. Finally, notice that the relative distance is a two-body observable and thus lower order ones such as densities or energies exhibit even smaller deviations.

The referee writes:

4. The last paragraph of section 6.1. about larger number of atoms, referring to appendix D is an example of the paper tackling too many aspects: there, some results with a few more atoms are found, but just some; I don't know if everything what happens with more particles can be deduced from here as the paragraph seems to indicate.

Our answer is:

We thank the referee for their comment. As stated above, see also our response to question 2 of the referee, we find indications that our main conclusions e.g. the overall shape of the integrated intercomponent correlation function persists also for a larger number of bath particles. However, we agree with the referee that a more systematic finite size scaling analysis regarding the number of bath atoms is required. For this reason we added a respective comment in the conclusions of the manuscript and in Appendix D (see also the list of changes).

The referee writes:

5. I find the simple model in 6.2 very nice and appealing, catching the relevant physics in a simple way. No change is required here, of course.

Our answer is:

We thank the referee for their appreciation regarding the effective description of the impurities. It is indeed our aim to provide an intuitive simple understanding by constructing this model.

The referee writes:

6. Section 8 stands out over the rest of the paper for being confusing, as compared to the rest of the paper which is very clear. I assume they have calculated with 17 atoms, and traced out to obtain three particle correlations. This is what indicates Eq. 15 and caption of fig. 6. But I find that there is confusion introduced with sentences like "The three particles are correlated" before eq. 15; "demonstrating a bunching behavior of the three particles. "; or in the very abstract "trimer state in the strongly attractive regime, where the latter consists of two impurities and a medium atom". Also, the Jacobi coordinates, if one has 15 A atoms, should go over all centers of mass. That is the distance of the third particle to COM of 1 and 2; then distance of 4th to COM of 1,2,3, etc, I believe. So I misunderstand probably eqs. 16 and following, being possible that there is some assumption or evident fact that I miss here.

Our answer is:

The comment of the referee is correct regarding the assumption that the calculation has been performed for 17 atoms (i.e., 15 bath particles and 2 impurities) and that for the analysis of the three particle distance the three-body density (extracted by tracing out all bath atoms except one) was used. Experimentally, the three-body density can be measured by detecting simultaneously the positions of three particles, i.e., the two impurities and one bath atom, and then averaging over many experimental realizations. Thereby, it does not matter which bath atom is detected since we consider them to be indistinguishable. The resulting three-body density is then a reduced quantity to describe the conditional spatial distribution of a representative atom of each species. We note that three- and higher-body densities have been experimentally measured e.g. in Ref. [1]. Moreover, the definitions of the three-body Jacobi coordinates and the hyperspherical radius given by Eqs. (16) and (17) in the manuscript follow the same scheme used for the impurities relative distance where the two-body density was required (Eq. (10) in the manuscript). An alternative representation of Eq. (17) in the manuscript can be obtained by constructing the respective Jacobi operator, e.g. $\hat{r}_{BC-A} = |\hat{x}^A - \frac{1}{2}(\hat{x}^B + \hat{x}^C)|$, and calculating the expectation value as $\langle \Psi^{\mathrm{MB}} | \hat{r}_{BC-A} | \Psi^{\mathrm{MB}} \rangle$.

On the other hand, the scheme suggested by the referee to measure the Jacobi coordinates would imply the usage of a 17-body operator, i.e., an operator which acts simultaneously on all particles of the system. In principle our method allows to calculate such an object, but it will be naturally quite computationally demanding and certainly not within the scope of this work. To clarify the issues raised, we have rewritten parts of Section 8 in the manuscript

and the abstract where we explain better what is meant by the three-body density and the respective trimer state (see also the list of changes).

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[1] T. Schweigler, V. Kasper, S. Erne, I. Mazets, B. Rauer, F. Cataldini, T. Langen, T. Gasenzer, J. Berges, and J. Schmiedmayer, Nature **545**, 323 (2017).