Response to the first Report by Reviewer 2

Reviewer:

Strengths

1) Nicely written, with an extensive review of Bose polarons
2) Promising variational approach

Weaknesses

1) The calculations use an unphysical (zero range) boson-boson repulsion
2) The results are not consistent with the few-body limit

This work theoretically investigates the problem of a mobile impurity in a Bose Einstein condensate — the so-called Bose polaron problem. A variational framework is developed, which extends Gaussian-state approaches to include non-Gaussian correlations. Using this approach, the authors find a series of “many-body bound states” that exist in the energy spectrum between the attractive and repulsive polaron branches for positive scattering lengths.

Overall, I think this provides a worthwhile contribution to the study of the Bose polaron, and I would be interested to see the variational framework applied to the case of a more physical boson-boson repulsion (i.e., not zero range like in this work). However, as it currently stands, I am not convinced this provides a “unified theory” of the strong coupling Bose polaron.

The fundamental issue with theories that only treat the boson-boson repulsion as a low-energy zero-range interaction is that the energy is unbounded from below when the scattering length is positive, and there is nothing to restrict multiple bosons from binding to the impurity. It does not account for the short-range repulsion and the resulting correlations that are necessary to correctly describe bound states. Thus, one ends up with pathologies in the spectrum like the multiple many-body bound states of Ref [49], which also only treats the boson repulsion at the low-energy level.

In particular, I find the many-body bound states observed in this work very puzzling, since they do not agree with the expected behavior in the few-body limit. Note that, while the Bose polaron problem is many body, it should recover the few-body bound states in the limit of low density, i.e., large E/E_n and $1/k_n a$, which is accessed in this work.

For small positive impurity-boson scattering lengths and realistic boson-boson repulsion, one expects the ground state to correspond to a tightly bound dimer that cannot bind any more bosons and is weakly interacting with the surrounding Bose gas, i.e., similar to the regime where the scattering length is small and negative. This is the behavior that was obtained for the case of an infinitely heavy impurity using QMC and other exact methods (e.g., Ref [69,70]). One can also arrive at this conclusion by estimating the energy to bind a second boson: $\Delta E \approx -1/ma^2 + U_0/a^3$, where U_0 is the repulsion. Thus, we require the impurity-boson scattering length $a \gtrsim U_0 m$ for the boson to bind (i.e., $\Delta E<0$).

Furthermore, according to the few-body spectra for both mobile and infinitely heavy impurities, I would expect the higher body bound states to lie below the two-body bound state in the region near unitarity, rather than above like in Fig 1 and 2.

To conclude, I think this work should certainly be published in some form (e.g., in SciPost Core), but I am not convinced it satisfies the criteria for SciPost Physics given my reservations above.

Reviewer:

This work theoretically investigates the problem of a mobile impurity in a Bose Einstein condensate — the so-called Bose polaron problem. A variational framework is developed, which extends Gaussian-state approaches to include non-Gaussian correlations. Using this approach, the authors find a series of "many-body bound states" that exist in the energy spectrum between the attractive and repulsive polaron branches for positive scattering lengths.

Overall, I think this provides a worthwhile contribution to the study of the Bose polaron, and I would be interested to see the variational framework applied to the case of a more physical boson-boson repulsion (i.e., not zero range like in this work).

Our reply:

We thank the referee for their time and their acceptance to review our work, and we are delighted to know that they found our work a worthwhile contribution to the study of the Bose polaron problem.

Reviewer:

However, as it currently stands, I am not convinced this provides a "unified theory" of the strong coupling Bose polaron.

Our reply:

Calling a theory "unified" is a subjective matter, and the meaning and scope of any unification has to be clarified. This is what we do, as we explain in the introduction what we mean by a "unified theory".

Reviewer:

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Our reply:

The referee here refers to the phenomenon of "Thomas collapse", which occurs in systems exhibiting Efimov effect with zero-ranged, attractive, resonant potentials at fixed inter-particle scattering lengths, where the ground state three-body bound state energy is unbounded from below. This effect can also arise in systems consisting of an impurity (X) and two bosons (A), known as AAX systems, where the impurity-boson and boson-boson potentials are resonant, attractive and zero-ranged. However, there is a fundamental difference from this setting, and the setting we consider in this work: although the boson-boson interaction in our study is zero-range, the impurity-boson potential has finite range. This finite range is enough to introduce a natural short-range scale on the effective hyper-radial potential for the three-body problem, making the ground state three-body bound state energy finite and preventing the Thomas collapse to occur in our case.

There are several comments in order regarding the zero-range boson-boson interaction with positive scattering length:

1. It is true that a boson-boson interaction with positive scattering length comes from an underlying attractive potential, and as a result, the whole system of impurity-boson-boson is unstable toward forming tightly bound three-body states. However, this effect is acknowledged by now in many studies of the Bose polaron to introduce no conceptual problem in the study of Bose polarons, since the polaron state is a metastable state itself and is prone to decay into the tightly bound clusters, see for ***Physical Review Letters, 127(3), p.033401 (page 3 § 1)***. Due to this fact, the polaron calculations are always done numerically with an explicitly repulsive boson-boson potential (not an attractive potential with positive scattering length).

2. It is also quite customary in many studies of boson-boson interactions in the Bose polaron problem to assume zero-range delta like potentials (see for instance ***SciPost Physics* 13, no. 3 (2022): 054, *Physical review letters* 126, no. 12 (2021): 123403, *Physical Review A, 106(3), p.033305, Physical Review A, 103(1), p.013317)*** Especially, in ***Physical Review A, 106(3), p.033305*** a systematic study for the attractive polaron was done, and it was found that a finite boson-boson range only introduces minimal quantitative changes in the energy and the density profile of the attractive polaron. Note that a finite range boson-boson interaction makes the repulsion softer (as the wave function of one boson can penetrate the barrier made by the other boson), thus, the delta boson-boson potential overestimates the repulsive interaction.

3. The thing that restricts the build up of bosons around the impurity is repulsive potential. Even a delta potential can do that by introducing nodes in the wave function whenever two bosons meet, which increases the kinetic energy and stabilized the system.

4. The pathologies in the spectrum of Ref [49] has a completely different origin. This is due to the Bogoliubov approximation and neglecting H_3 and H_4, and only retaining H_2, using the formalism from our paper. Even in a theory that models boson-boson interaction with a finite range potential, if one neglects H_3 and H_4 in the many-body limit, this pathologies happen.

In conclusion, this concern by the referee does not apply.

Reviewer:
In particular, I find the many-body bound states observed in this work very puzzling, since they do not agree with the expected behavior in the few-body limit. Note that, while the Bose polaron problem is many body, it should recover the few-body bound states in the limit of low density, i.e., large E/E_n and $1/k_na$, which is accessed in this work.

Our reply:
We respectfully disagree with the referee that the behaviour of the many-body bound states predicted in this work does not agree with the few-body limit. As we discuss below, the condensate density of $n_0 \simeq 180\,\mu m^{-3}$ fixed throughout our study keeps the physics far away from the few-body limit and deep into the intermediate density limit (for the impurity-boson system, not the boson system), although the gas parameter $\lambda_B \simeq 0.03$ is still in the dilute limit for the Bose gases only. Although in the first sight, it might be tempting to draw conclusions for the few-body limit from large E/E_n and $1/k_na$, as we make clear below this is not the case due to the involvement of the effective range r_0 .

A necessary condition to compare the few-body spectra across different settings is a demonstration of **universality** in the corresponding regime. This fact is also well acknowledged in the literature, as it is only in the limit where the inter-boson distance, the three-body parameter, and the scattering lengths far exceed the short range details that one can expect the Bose polaron physics to be universal and simple model potentials (such as Gaussian) can provide reliable results. In the non-universal regime, the quantitative physics depends on all the details of the interaction potentials among all particles (or at least several length scales beyond only the scattering length and effective range). Especially, in the physics of Bose polarons in the strong coupling regime, the relevant length scales are comparable, which makes the physics non-universal by nature. To see this, note that for $1/k_na \simeq 4$— deep in the strong coupling regime — the relevant length scales are: effective range $r_0 \simeq 7.3\,nm$, boson-boson scattering length $a_{BB} \simeq 5.29\,nm$, impurity-boson scattering length $a \simeq 11.36\,nm$, and for the JILA experiment with $n_0 \simeq 180\,\mu m^{-3}$, the inter-particle distance $n_0^{-1/3} \simeq 177.11\,nm$ (thus $r_0 n_0^{1/3} \simeq$ 0.0412). To have an order-of-magnitude estimate, this value corresponds to $n_0^{1/3}|a_-| \simeq 101.64$ in ***Physical Review X 8, no. 1 (2018): 011024***, which is far away from the few-body limit (which occurs for $n_0^{1/3}|a_-| \sim 1$) and deep into the intermediate density limit, see Fig. 2 of ***Physical Review X 8, no. 1 (2018): 011024.***

In this sense, one can only obtain representative results using simple potentials, since unless the exact multi-channel potentials among particles are not taken into account, taking any other potentials and changing them leads to changing the quantitative results, thus being equally quantitatively inconclusive. Nevertheless, we make clear in our work that the physical conclusions that we draw are qualitative but we expect them to occur if all the realistic setting is taken into account in an ab initio treatment, since the conclusions are based on very general arguments and effects. The study of scattering within realistic multi-channel potentials, although a very interesting question, lies far beyond the scope and purpose of the current work and deserves to be addressed in a separate publication.

As a last remark, we emphasise that in our framework, there is a systematic approach conceptually separate from treating the Gaussian correlation matrix as variational parameters (similar to *SciPost Physics, 16(3), p.067).* This approach is able to systematically include exact few-body correlations to not only obtain the excited state but also the correlations leading to deeply bound state. We do not do it in this work as we aim to present it independently in a follow-up publication.

Reviewer:

For small positive impurity-boson scattering lengths and realistic boson-boson repulsion, one expects the ground state to correspond to a tightly bound dimer that cannot bind any more bosons and is weakly interacting with the surrounding Bose gas, i.e., similar to the regime where the scattering length is small and negative. This is the behavior that was obtained for the case of an infinitely heavy impurity using QMC and other exact methods (e.g., Ref [69,70]). One can also arrive at this conclusion by estimating the energy to bind a second boson: $\Delta E \approx -1/ma^2 + U_0/a^3$, where U_0 is the repulsion. Thus, we require the impurity-boson scattering length $a \gtrsim U_0 m$ for the boson to bind (i.e., $\Delta E<0$).

Our reply:

The setting in Ref. [69] is fundamentally different from the setting we consider. In Ref [69] the authors take a two channel model suitable for narrow resonances together with non-interacting bosons, but here we take a single channel potential suitable for broad resonances together with boson-boson interaction. Furthermore, the two-channel model of Ref [69] enables the authors to draw conclusions also for the universal regime (given that the relevant length scales far exceeds the short range details, see ***Physical Review X 8, no. 1 (2018): 011024***). However, our model is less universal, by the arguments made above. Thus, a direct comparison with the results of Ref [69] is not straightforward.

In Ref [70], in their Quantum Monte Carlo (QMC) calculations the authors take a similar model to us (square well single channel impurity-boson potential and boson-boson repulsion), but QMC is only suitable for ground state. The ground state of the Bose polaron for the range of $1/k_n a$ values considered in Ref [70] ($-2.566 \leq 1/k_n a \leq 0.513$) is known to agree well with the results of the GPE theory, so it agrees with the results of our work. For $0.513 \leq 1/k_n a$ we could not find data in Ref [70] to compare.

In Ref [70], for a few-body system (i. e., in the presence of no condensate) the authors make the crucial observation that when $a \gg a_{BB}$ ($a/a_{BB} = 75$ in Fig. 2) and the boson-dimer binding energy ε_T is much smaller than the impurity-boson binding energy ε_B ($\varepsilon_T \ll \varepsilon_B$), then the ground state few-body energy follows closely the Eq. [2]. The many-body version of this situation is when a single boson resonantly scatters off a many-body bound state. However, we explicitly state in the arguments around Eq. [18] in our work that this lies outside the validity condition of the results presented in this work, as it leads to significant mixing with the scattering states. In short, the validity condition in Eq [18] makes sure that adding the other boson gives a significant contribution to the change in energy, while the energy of the resulting state is still far below the threshold. According to this criteria, the theory presented in our work is valid for all scattering lengths except a narrow range of scattering lengths close to the level crossings or when new branches are entering the negative energy region. In these situations, as discussed in the Appendix B of our work, the systematic perturbation theory is able to account the excitations in the scattering states. We do not do this calculations, however, in the present work.

Note also that the focus of this work is the metastable many-body bound states. These states are actually excited states of a few-body system and lie in the continuum of scattering states. However, as we argued in detail in appendix B, when they form, they have a long lifetime since the decay processes outlined there are argued to be very slow.

We also totally agree with the intuitive boson-counting argument put forward by the referee, and in fact we carry out a similar calculation in our work (in the introduction) to motivate multiple bosons binding to the impurity. However, contrary to the expectation of the referee, we found that this number can not only be one, but many.

Reviewer:

Furthermore, according to the few-body spectra for both mobile and infinitely heavy impurities, I would expect the higher body bound states to lie below the two-body bound state in the region near unitarity, rather than above like in Fig 1 and 2.

Our reply:

As stated above, and also in the manuscript, those states are ground states or few excited states of few-body clusters. Those ground states lie way lower than the attractive polaron state, which is already itself a metastable state and decays to those large clusters. To describe those lower lying states, one has to include few-body correlations (three and even higher) exactly into the scheme. For three-body correlations, as stated above, our method introduces a systematic way to include them, which we aim to address in a separate publication.

The states that we discuss here, however, are those metastable states that lie in a continuum. To make any conclusion about these states by numerics, one has to obtain the position of these resonances not by normal exact diagonalization but by complex scaling methods as done for the Bose polaron in ***Physical Review A, 99(1), p.013613*** based on the complex scaling method (***Physics reports***, ***302***(**5-6), pp.212-293,** ***International Journal of Quantum Chemistry 14, no. 4 (1978): 529-542***) since these states are resonances lying in a continuum of scattering states. To the best of our knowledge, there has not been any work to find all such resonances at negative energies for particle numbers up to 6 (note that ***Physical Review A, 99(1), p.013613*** considers the complementary regime of light impurities and for particle numbers more than 4, only obtains ground and very first excited states). In this view, we believe that there is still a long way until our results can be compared with few-body calculations inspired from quantum chemistry for the number of particles and regimes that we consider here.

Reviewer:

To conclude, I think this work should certainly be published in some form (e.g., in SciPost Core), but I am not convinced it satisfies the criteria for SciPost Physics given my reservations above.

Our reply:

We respectfully disagree with the referee's assessment, since the objections of the referee are again subjective. From their report, we could not understand in what way the referee believes that the results of our paper do not meet the scipost criteria that we argued for, namely "Open a new pathway in an existing or a new research direction, with clear potential for multi-pronged follow-up work" and "Present a breakthrough on a previously-identified and long-standing research stumbling block".