Response to the first Report by Reviewer 2

Reviewer:

Strengths

1) Clearly written.
2) Extensive review of current picture.
3) Methodology explained in details.

Weaknesses

1) Explicit application limited to a simple case.
2) Importance of the findings somehow overstated.

The paper describes a possibly novel variational technique capable to treat non-linearities arising in the formation of Feshbach molecules and the occurrence of many-body bound states at intermediate energies between the attractive and repulsive polaron branches.

The paper is nicely written and interesting. I particularly appreciated the extensive review of the literature made by the authors.

Our reply:
We thank the referee for their time and effort in reviewing our work. We are delighted to read that they found the work interesting.
As outlined in our response to the following point, we strongly disagree with the two main weaknesses highlighted by the referee.

Reviewer:
However, I found somehow a mismatch between the very general picture delineated in the introduction and the results section where the only case treated is the one of an impurity in a Bose gas.

Our reply:
As clearly laid out in every section of our work starting in the introduction, our goal is to study a single mobile impurity in a Bose gas. We believe the title "A unified theory of strong coupling Bose polarons:.." leaves no doubt that we study a Bose polaron problem, i.e. a problem of a single impurity interacting with a surrounding Bose gas. In the ultracold atom community that we address, the term 'Bose polaron' refers to precisely the problem of a mobile quantum impurity interacting with a surrounding Bose-Einstein condensate. Given the overall length of our article, 14 pages without references or appendices, we found it appropriate to provide an introduction that is sufficiently broad and puts the problem into context (that the referee appears to appreciate according to their previous comment).

Given the lack of a more specific description of the "mismatch between the very general picture delineated in the introduction and the results section" we could not identify how to best adapt our work in order to take this comment by the referee into account. However, we feel this could be a good place to emphasize that a main achievement of our work is constituted by the results in Section II "Theoretical Formalism", i.e. the title "results" of Sec. III of our work truly refers to "quantitative numerical results" discussed in that section, whereas key new conceptional developments and insights are presented in Section II. This includes for example Figure 2, which summarizes the major conceptual advances of our work.

Reviewer:
For example the authors clearly state that the many-body bound states they discuss have already been studied in the literature and that their scope is to include effects of inter-boson repulsion. However, these effects seem to give no relevant physical effects. The physics discussed is rather straightforward and I could

not find any reason why these effects are expected to be important.

Our reply:
First, we would like to mention that we are unsure about the logical connection of this 'example' to the previous comment by the referee concerning a mismatch of the introduction and the results.

That said, we would like to address the point raised here by the referee. Let us start by providing some context: The referee refers to earlier discussion of the many-body bound states in the literature, which we describe in our work on top of page 3 as follow:
"*Such many-body bound states were studied before in the context of Rydberg [71] and ionic [72] impurities immersed in bosonic quantum gases, and for neutral impurities in two dimensions [73]. While for Bose polarons, such metastable bound states have been predicted before [49], the crucial effects of inter-boson repulsion have not been included so far.*"
The first part here, citing Refs. [71-73] refers to broadly related many-body bound states in similar single-impurity settings. The second part, citing Ref. [49], then refers to the Bose polaron problem at hand: As clearly stated here, meta-stable bound states have been predicted before but the key effects of inter-boson interactions have not been properly treated. Here Ref. [49] is [Shchadilova et al., Phys. Rev. Lett. 117, 113002 (2016)].

Now the referee in their report claims that boson-boson interactions "seem to give no relevant physical effects". This is wrong and points to a deep conceptual misunderstanding of the referee that we regret. Let us try to clarify the situation as best as we can (beyond the discussion found above the above-cited section from our manuscript starting from § 5 of Sec. I of our work, where the intuitive reason for strong effects of boson-boson interactions is explained):

> To start with, we strongly disagree with the referee's view on the significance of the many-body resonances, and the current status of their understanding. First, we draw the referee's attention to the fact that the study of the Bose polaron on the repulsive side of a Feshbach resonance is a topic of **high recent interest in the current research on Bose polarons**, and not much work has been done to characterize the — as of today not experimentally observed — many-body resonances, their interplay with cluster formation and polaronic effects such as phonon dressing. In fact, different theoretical models predict drastically different characteristics for these states, as we will review in detail in this reply. Altogether, the properties of these resonances are not settled by now, by any means. As such, the many-body bound states associated with strong-coupling Bose polarons constitute a long-standing open problem that we address in our manuscript.
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> The referee states that "*However, these effects [meaning inter-boson repulsion] seem to give no relevant physical effects*". We draw the referees attention to the following points, stated multiple times throughout our manuscript:
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> 1. The mean-field models including only the quadratic terms **do not describe any attractive polaron when the impurity-boson scattering length $a_{\rm IB} > 0$**. Instead, they predict resonances corresponding to multiple occupation of the impurity-boson dimer with energies $E_{\rm B} = -n\varepsilon_{\rm B}, n = 1,2,\cdots$. While for Rydberg impurities (where the impurity-boson potential range $r_{\rm IB}$ is much larger than the inter-boson scattering length $a_{\rm BB}$) such resonances have been experimentally observed, for neutral atomic impurities (where $r_{\rm IB} \sim a_{\rm BB}$), it is strongly believed in the community **that this prediction is unphysical and is a mere artifact of the model.** In this case, there is still a **dispute even over the existence of these resonances**, let alone their quasiparticle properties and their appropriate theoretical description. Thus, studies which shed light on their existence and characteristics cannot be simply dismissed as "insignificant" or "irrelevant" without ignoring an entire contemporary research field.
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> 2. For the case of narrow Feshbach resonances described by two-channel models, it was shown that even in the extreme case of non-interacting bosons and static impurity (which is the most unstable case imaginable), transitions to the closed channel induce an effective inter-boson repulsion. The

number of resonances close to the impurity-boson and boson-dimer scattering resonances, are still infinite, and their binding energy increases with increasing particle number, while their energy remains finite in the thermodynamic limit. See e.g. Refs. [Shi et al., Phys. Rev. Lett. 121, 243401 (2018)] or [Yoshida et al., Phys. Rev. A 98, 062705 (2018)]. It is also conjectured in these references that $(N+1)$-body bound states can exist for $0 < 1/a < 1/a*$ ($a*$ being a critical scattering length), while it is only shown for trimers and tetramers. While two-channel models are better understood compared to other models, this conjecture highlights that the precise number of many-body bound states remains an open question.

In our manuscript, we consider a single channel potential which is suitable to model broad Feshbach resonances. In contrast to the two-channel model, this model remains unstable at positive $a_{\mathrm{IB}} > 0$ for non-interacting bosons **unless explicit inter-boson repulsion is included in the model,** again signifying the non-trivial physics of many-body resonances that can completely change depending on the setting. Indeed, our predictions — which would not be possible without inclusion of inter-boson interaction via H_{3} and H_{4} — reveal completely different characteristics of the resonances:

(a) The number of resonances is finite, is not fixed and depends particularly on the strength of inter-boson repulsion relative to the impurity-boson attraction. Our calculations make quantitative predictions for the number of resonances and their dependence on the involved interaction strengths. **These findings go significantly beyond what has so far been known/proposed about the new many-body resonances, qualitatively as well as quantitatively.** For a comparison with the current state-of-the-art, see [Shchadilova et al., Phys. Rev. Lett. 117, 113002 (2016)].

(b) Contrary to the monotonous dependence of binding energy on the particle number expected from a linear model [Shchadilova et al., Phys. Rev. Lett. 117, 113002 (2016)], we find this behavior to be non-monotonous: many-body states with more particle number can have higher energy. This leads to the following effects:

(i) Level crossings: contrary to the wisdom gained from the previous studies on many-body resonances (non-interacting boson models, with either Rydberg impurities, neutral short-range impurities or two-channel models), the many-body resonances that we discovered do not possess a well-defined particle number close to the level crossings and for inter-boson interactions comparable to the impurity-boson interaction; we attribute this to a mixing resulting from low-energy processes such as particle exchange with the condensate. This information is clearly conceivable from Figs. [4 -7] in the manuscript by inspecting the behavior close to the level crossings.

(ii) Again, contrary to the previously studied non-interacting settings, we predict the resonances to occur between the attractive and repulsive polaron, thus they are **different from any possible tightly bound few- and many-body cluster states that lie below the attractive polaron**. The many-body resonances studied here are thus metastable and are intermediate states, located energetically between the repulsive and attractive polaron states / resonances.

(c) The many-body resonances we propose and analyze **do not exist in a model that includes boson repulsion within a Gaussian state variational ansatz**. Note that using a Gaussian state variational ansatz includes the mean-field treatment as a special case, and thus is more general in treating the deformation of the BEC background; nevertheless Gaussian states are insufficient to treat the strong interactions that give rise to multi-boson bound states to the impurity. The only recent Gaussian state theory that includes inter-boson repulsion explicitly is SciPost Physics, 16(3), p.067, where at most two saddle point states where observed: for light impurities in the polaronic instability regime where a notable trimer state exists, one connected to the dimer, and the other to a trimer. The other mean-field theories, such as Gross-Pitaevskii theory, only predict a single branch with negative energy, that is the attractive polaron. **Thus, our scheme goes beyond these Gaussian theories: We predict further resonances in addition to the attractive and repulsive polaron branches.**

3. The above are all "physical effects" whose prediction relies not only on "the inclusion of H_{3} and H_{4} terms", but also on the particular "non-Gaussian form of the variational ansatz".

In light of this, we do not agree with the referee's view, according to which points (a)-(c) would constitute "no relevant physical effects", and their doubt that "these effects are expected to be important". To place this into context, let us elaborate on our results in relation to Bose polaron research in general. One of the main goals of this field is to characterize the spectral features of the interacting impurity in different parameter regimes, and for a long time the focus of the theoretical research in this field has been to obtain more accurate predictions of energy, lifetime, and residue of the already known repulsive and attractive polaron branches. By predicting that the number of resonances, their position, their mixing and other characteristics are different from the established expectations based on Bose polaron models without boson-boson interaction, our work takes a very significant step. Furthermore, we elaborate on the origin of this difference.

We were also startled by the fact that the Referee found the physics discussed in our manuscript "rather straightforward". We would like to kindly invite the Referee to draw our attention to any existing literature or method that would be able to produce the locations of the multi-body resonances that we have calculated, e.g. in Figs. 2(a) or Fig. 4. We are not aware of any existing literature or trial states that would be able to solve this task, but would be interested to learn what the Referee has in mind when they dismiss our results as "rather straightforward".

Reviewer:
In this perspective the authors state:

"It is crucial to retain the higher order terms H_{3} and H_{4} to describe essential strong coupling effects such as non-Gaussian correlations of Bose polaron…"

This sentence appears to be overly grandiose , but it is kind of a tautology. Including H_{3} and H_{4}, which are non-quadratic terms in the effective Hamiltonian expansion, leads to non-Gaussian correlations (it is obvious and, almost, tautological)

Our reply:
It is true, of course, that including H_{3} and H_{4} terms, which are non-quadratic terms in the effective Hamiltonian expansion, leads to non-Gaussian correlations in the actual eigenstates of the model. However, the importance of those non-Gaussian correlations in the physics of a certain problem depends on the particularities of the system under study.

For instance, it is obvious that the true ground state of the textbook weakly interacting Bose gas is a highly correlated non-Gaussian state, due to the inter-boson interactions, but addition of H_{3} and H_{4} for such a standard setting leads only to perturbative contributions to the physical quantities of the gas in the weakly interacting limit, and therefore, depending on the context, they might be irrelevant for understanding the key physics. In stark contrast, inter-boson repulsion leads to dramatic non-perturbative effects in other settings. A prominent example is constituted by the Mott insulator in a Bose-Hubbard model, with integer boson number occupancies per site.

In the present context of Bose polarons, the referee appears to underestimate the complexity of the problem at hand. Different from e.g. typical quantum optical problems, there are infinitely many bosonic modes. In most of these modes, interactions and non-Gaussian corrections are expected to merely lead to small quantitative modifications. However, for the mode bound to the impurity identified at the beginning of Sec. II.C, the situation is entirely different: Here, non-Gaussian correlations play an essential role and the state is affected non-perturbatively by the strong inter-boson repulsion. A key insight of our work is to single out this mode, derive the form of the relevant non-linear effective Hamiltonian and characterize the resulting many-body states.

Reviewer:

Including H_{3} and H_{4}, which are non-quadratic terms in the effective Hamiltonian expansion, leads to non-Gaussian correlations (it is obvious and, almost, tautological) but why are these ESSENTIAL?

Our reply:

As we discussed in detail on pages 2-4 above, inter-boson interaction effects included in the H_{3} and H_{4} terms in the bound mode are absolutely essential for understanding the properties of the multi-body bound states we predict. For example, the positions of the resonances in Figs. 2a and Fig. 4 of our manuscript, as well as the existence of non-trivial level crossings in these spectra, are dictated in an essential way by the inter-boson repulsion. These constitute key new results of our work that go significantly beyond the state-of-the-art in the field of Bose polarons.

Reviewer:

What physical phenomenon is enabled by non-quadratic terms and could not be captured by the standard mean field?

Which experimental observation NEEDS non gaussian correlations to be justified and why is this relevant to the field?

Our reply:

As discussed above, the standard mean-field approach with non-interacting bosons (phonons) predicts multi-boson bound states with any number of occupations, and equal spacings in energy [Shchadilova et al., Phys. Rev. Lett. 117, 113002 (2016)]. This is believed to be unphysical for neutral short-range impurities, and has led many in the community to the conclusion that the multi-boson bound states cannot be observed in polaron spectra, not even as meta-stable resonances. Therefore standard mean-field theory including weak inter-boson repulsion (i.e. the Gross-Pitaevskii theory) captures only one single saddle point solution with negative energy when a single impurity-boson bound state exists: i.e., it only describes the attractive polaron. A time-dependent version of a non-local extension of the Gross-Pitaevskii theory (which is an improvement to a standard mean-field theory) also predicts a single renormalized resonance, see for instance *Physical Review Research, 2(3), p.032011.*

In our manuscript, we show that — owing to the strong inter-boson repulsion of the beyond-quadratic terms in the Hamiltonian — metastable multi-body bound states can exist as long-lived resonances in the Bose polaron spectrum. Due to the strongly correlated, molecular character of these states, clear signatures of these resonances should be observable by extending the current experimental settings to give access to molecular spectra, as we also discuss in our manuscript.

Reviewer:

None of these questions are discussed.

Our reply:

We do not share this opinion by the referee. In the introduction to our work where we describe the state-of-the-art, we discuss the problems encountered when describing multi-body bound states using mean-field theory, and we use this to motivate a way out: This leads us to the new variational state proposed in our manuscript.

In order to take into account the feedback by the reviewer, we have revised our manuscript. Now we highlight the relevance of non-Gaussian correlations and their non-perturbative origin more clearly in the introduction and conclusion sections of our work. We thank the referee for highlighting these points.

Reviewer:

As it stands the paper is just a methodological development, which although interesting, leads to no real finding. The fact that the methodology can IN PRINCIPLE be extended to include further effects or to describe Efimov states is not enough for me to believe that the paper will "open a new pathway in an existing or a new research direction", because all mean-field approaches can be generalized to include multi-body correlations expanding around a saddle point solution. The problem is that these methods are numerically very challenging and the actual solutions of the equations beyond the quadratic order is often not possible.

In conclusion, the physical picture is rather straightforward and the many-body states described do not present particular surprises when beyond quadratic terms are included. The appearance of non-Gaussian correlation is obvious beyond quadratic order and does not bear "per se" any physical significance.

Our reply:

With all due respect, we strongly disagree with the referee's assessment that the physics of the many-body resonances discussed in our work constitute "no real findings". As explained just above, these cannot be captured by mean-field approaches, or simple perturbative extensions thereof. The referee correctly notes that "all mean-field approaches can be generalized to include multi-body correlations expanding around a saddle point solution. The problem is that these methods are numerically very challenging and the actual solutions of the equations beyond the quadratic order is often not possible." However, this is exactly where the achievement in the present work lies: We have singled out and identified in which mode the strong inter-boson repulsion needs to be fully included to all orders, non-perturbatively, which is precisely what makes the complicated non-linear equations underlying our variational ansatz numerically tractable; i.e. owing to the very choice of our ansatz wavefunction, we can capture the essential interaction effects!

The physics we discuss in our work has not been discussed in previous publications on the topic, simply because state-of-the-art methods are either suitable for non-interacting bosons, or they give access only to the properties of the attractive polaron resonance as the ground state (for instance, Quantum Monte Carlo methods, and other existing Gaussian state theories and mean-field theories).

The potential extensions we outlined in response to the first referee, including the incorporation of the Efimov effect, clearly shows that the second part of the SciPost acceptance criterion is met, namely the "clear potential for multi-pronged follow-up work". Regarding the first part "opening of a new pathway in an existing or a new research direction", as we already mentioned in our response to the first referee, the new research direction our work points to is not to extend the approach to include higher-body correlations, but to further motivate the experimental and theoretical research on "the intermediate many-body resonances", "the more accurate characterisation of their behaviour" such as lifetime, mixing, appearance and disappearance by tuning interaction strengths, etc., and experimentally search for their signatures by going beyond current spectroscopic techniques.

These all constitute very promising next steps for the field, both theoretically and experimentally, on the way towards observing a lot more intriguing effects in Bose polarons. As we point out several times here and in the manuscript, the current framework predicts clear qualitative changes in the properties of the many-body resonances when strong inter-boson repulsion is included non-perturbatively in the model, we strongly believe that characterizing such many-body resonances is indeed "physically significant" and constitutes an exciting and fruitful research direction.

Reviewer:

I share the 1st Referee opinion that the paper shall be published on SciPost core.

Our reply:

We strongly object to this conclusion. We kindly ask the Referee to clarify the acceptance criteria which, in their opinion, would justify a rejection from this journal.

As outlined above we firmly believe that our work has brought major advances to the field of Bose polarons and squarely fulfills the acceptance criteria of SciPost Phys.

We sincerely hope that our reply along with our clarifications in the manuscript have clarified the concerns of the Referee, and that they will support publication of our work in SciPost Phys. We thank them for reviewing our work.