Response to the Second Report by Reviewer 1

Reviewer:
I thank the authors for addressing the comments in my first report. All in all, the manuscript has been substantially improved.

Our reply:
We appreciate the reviewer's careful consideration of our revised manuscript and are pleased to hear that our revisions have been well received.

Reviewer:
Now, it became clear to me that the "main purpose in this work is to present a framework for modelling impurity-boson problems" with "a heavy (or static) impurity". This assumption appears in multiple places in the text; it is open to question which of the results hold also for a mobile impurity, arguably, the main motivation of this work. Based on this, I conclude that the manuscript does not meet the acceptance criteria of SciPost Physics. My recommendation is to resubmit to SciPost Physics Core, where this work can be published as is.

Our reply:
We acknowledge that certain statements in our referee reply and in Appendix B of the revised manuscript may have inadvertently led to a misunderstanding. This misunderstanding seems to have led the reviewer to conclude that our results are limited to the case of an "immobile impurity," thus deeming our findings as irrelevant to the study of mobile impurities—a central topic in ongoing ultracold atom experiments. This interpretation also led the reviewer to assert that our work does not meet the acceptance criteria of SciPost Physics. We regret any confusion caused and would like to clarify our position.

Nevertheless, strongly disagree with the reviewer's assessment. Throughout the manuscript and our previous response, we did not intend to suggest that our approach is limited to static or immobile impurities. In fact, our Hamiltonian fully incorporates the finite impurity mass (using the Lee-Low-Pines transformation), as well as in both our theoretical analysis and numerical results. Furthermore, the effect of the finite impurity mass is also evident in the renormalization of the boson-boson correlation length, referred to as the "reduced healing length." As we will explain further, our predictions are indeed applicable to mobile impurities unless the impurity is so light that phenomena like polaronic instability arise, leading to the formation of large correlated clusters (as discussed in Christian et al. PRA, 105(5), 053302, and Christian et al. PRL, 128(18), 183401).

To avoid complications that arise in the case of light impurities—where Efimov physics can become significant and cause qualitative changes in both the few-body spectrum and many-body effects such as polaronic instability—we emphasized heavy impurities (i.e., mobile impurities with a heavier mass than the bosons) in our text. However, this does not imply that our framework is inapplicable to mobile impurities. The literature shows that even for equal mass ratios, the heteronuclear Efimov scaling factor can be as large as 1986.12 (Naidon et al. RPP, 80(5), 056001). Moreover, experimental results for K-Rb mixtures with mass ratios less than one are in excellent agreement with the Gross-Pitaevskii theory, which does not account for three-body physics, thereby questioning the relevance of three-body physics in the many-body limit for such mass ratios. Only recently, a study demonstrated that genuine three-body physics due to the light mass of the impurity can lead to observable effects such as polaronic instability for mass ratios as small as 6/133, corresponding to Li-Cs mixtures.

We believe that our framework not only applies to mobile impurities but also a wide range of experimentally relevant ultracold atomic mixtures currently under investigation, such as K-Rb (JILA), K-K (Aarhus, Cambridge), and K-Na (MIT, Munich), have the impurity-boson mass ratio in this range.

Below, we will further elaborate on the origins of this misunderstanding, clarify our statements, and explain why we believe our work meets the acceptance criteria of SciPost Physics.

The reviewer refers to this statement in our reply:

"Note that our main purpose in this work is to present a framework for modeling impurity-boson problems where a heavy (or static) impurity forms a single-particle bound state with a boson whose energy is much higher than any other energy scales in the problem. As such, the scope of the problem is quite restricted, and while it is interesting to apply this framework to various settings to evaluate its performance, we do not claim that its assumptions and applicability extend to generic impurity-boson problems."

As stated earlier, our work does not assume an immobile impurity in either our numerical results or the theoretical analysis. The core assumption in our work is clearly stated multiple times: the boson-impurity binding energy is much larger than other energy scales in the problem, not that the impurity has infinite mass.

Regarding the purpose of our work, one of our primary goals is to introduce and establish this framework within the polaron research community as an effective tool for studying many-body bound states at strong couplings in ultracold gases, along with the associated polaronic effects. Our formalism has uncovered significant properties of these states, including inter-particle correlations, quantum state structure, and polaronic dressing with phonon modes. We aimed to demonstrate that this framework offers comprehensive insights into many-body bound states, whether the impurity is mobile or immobile.

When we stated that our approach does not extend to 'generic impurity-boson problems,' we referred to a broader class of problems, such as those involving neutral, ionic, or Rydberg impurities in BECs, exciton/polariton impurities in exciton/polariton BECs, impurities in dipolar quantum gases, or impurity-BEC systems in optical lattices in the context of Bose-Hubbard model, among others. One might think that our framework has such a generality that it can be applied to all these settings when a deeply bound impurity-boson bound state, and consequently, several many-body bound states exist — as indeed, the steps including the mode decomposition, derivation of the effective Hamiltonian can be applied to all such situations, and the variational ansatz can be straightforwardly be generalised to the form

$$|\Psi_{(\mathrm{var})}\rangle = \sum_{n} |\psi_n\rangle \otimes |\underline{\theta}_n\rangle ,$$

Where $|\psi_n\rangle$ is the n'th many-body bound state (the derivation of which is extensively discussed in the manuscript), and $|\underline{\theta}_n\rangle$ is a (generally un-normalized) variational state with parameters $\underline{\theta}_n = (\theta_{n,1}, \theta_{n,2}, \cdots)$ (a coherent state in our manuscript) whose choice depends on the particular setting under study. What we tried to point out is, since all those settings have extremely different length and energy scales and encompass drastically different physics, one should be conservative and might not expect that the particular coherent state form of the ansatz be applicable to each and every setting. This is a natural expectation, as no single theoretical method is universally applicable to all settings. However, it is important to note that the standard coherent state ansatz is frequently used for mobile impurities and its predictions are reliable when "the impurity-phonon coupling is weak." This crucial point is derived and stated in Appendix B of our revised manuscript, where we reduce the "strong-coupling" impurity-boson problem to the "weak-coupling" problem of phonons interacting with "many-body bound states" emerging as an effective multi-state impurity.

A potentially misleading statement we made in Appendix B was: *"In the rest of this appendix, to avoid complications in the arguments arising from finiteness of the impurity mass, we assume an infinitely heavy impurity (M → ∞), while for the sake of completeness, we keep the impurity mass M formally in all the expressions."* This may have led the reviewer to conclude that our arguments only apply to infinite mass impurities. We emphasize that all the arguments in this section are independent of the impurity mass.

By "complications in the arguments arising from finiteness of the impurity mass," we referred to scenarios where the decay of many-body bound states leads to the creation of multiple phonons. When the impurity is light, the LLP term in $\hat{H}_4$ may lead to the presence of Efimov-type trimers tied to the many-body bound state. Whether this type of situations arises depends on the sign and strength of the residual interaction between the phonons and the impurity. This potential arises in the $\delta\hat{\phi}^{(B)}$-dependent terms on the right-hand-side of Eq. (B6), and its sign and strength depends on many factors, including the bound mode field operator expected values over the particular many-body bound state, the bound state wave function and the repulsive polaron coherent state, and whether there exist any Efimov state tied to a many-body bound state and whether its physics is relevant depends very much on the particular case at hand. To avoid such complications and maintain a general framework, we focused on heavy (but still mobile) impurities where the Efimov effect is strongly suppressed. Given the meaning stated above, the phrase “complications in the arguments arising from finiteness of the impurity mass” is clearly misleading, as it implies that such complications arise because the impurity mass is “finite” and not “light”. We apologize for the misunderstanding and and try to clearly state what we meant in the manuscript.

Point regarding the acceptance criteria:

Our work paves the way for several distinct research directions in the study of few- and many-body physics of many-body bound states at strong coupling, and the interplay of interactions, finite mass effects, few-body correlations, and phonon dressing on their properties. In this regard, clearly there are several distinct aspects and directions that our work motivates:

1. Applying our framework to various settings, such as ionic, Rydberg, and dipolar impurities, benchmarking against existing methods, and exploring its applicability across different regimes. Particularly, since many-body bound state formation is observed in Monte-Carlo simulations for ionic impurities, it is interesting to see what our scheme predicts for the metastable many-body bound state resonances in these settings.

2. Investigating the potential formation of few-body states of two phonons bound to many-body bound states in light impurities, akin to tetramers and higher-body states tied to Efimov trimers. Possibility of formation of such states needs to be investigated. To this end, one can apply our scheme to study the interplay of many-body bound state formation and Efimov effect by extending the phonon part of the variational ansatz $|\underline{\theta}_n\rangle$ from a coherent state to other types of ansatzes like Gaussian state or truncated basis ansatz. This also shows the flexibility of our framework.

3. In Appendix B of the revised manuscript, we showed that the problem can be transformed to the problem of an emergent multi-state impurity weakly interacting with phonons. As such, the machinery of perturbation theory can be applied to find the spectral function of the many-body bound states and to study the phonon dressing of the many-body bound states, that are polaronic states of a many-body bound state. Such “many-body bound state polarons” can be thought of as boson analogs of “molarons” in the context of impurities coupled to a Fermi sea. Such a perturbation theory can give access to the spectral function and lifetime of these impurities.

4. Mapping the phase diagram of the strong coupling polaron, exploring the impact of various parameters such as the impurity-boson mass ratio, inter-particle interactions, and BEC density on the number of many-body bound states, their level crossing, and their phonon dressing. It is especially interesting to investigate the implication of phonon dressing on the spectral function at the level crossings, since the crossing many-body bound states can strongly mix.

5. Motivating experimental upgrades for molecular spectroscopy to observe many-body bound states with significant spectral weight.

All the above points firmly supports that our work “opens a new pathway” (that is the study of the spectra of intermediate many-body bound state resonances, their polaronic dressing and their interplay with few-body physics) “in an existing or a new research direction” (that is strong coupling Bose polaron on the repulsive side of the Feshbach resonance), “with clear potential for multi-pronged follow-up work” (states in the points above).