Resubmission:
A unified theory of strong coupling Bose polarons: From repulsive polarons to non-Gaussian many-body bound states

Referee Reply

June 13, 2024

Report

Reviewer #1: "*The manuscript suggests a novel variational ansatz to tackle the Bose polaron problem in ultracold gases with positive scattering lengths. Using this ansatz, the paper studies attractive and repulsive quasiparticle branches. The focus is in particular on what happens to the Bose polaron spectrum across an impurity-boson Feshbach resonance, see Fig. 1 for an illustration.*
I read the work with great interest. The manuscript is somewhat technical and sometimes hard to follow but overall it is written well, and will definitely be useful for researchers working on Bose polarons.
The main weakness of the paper is that it does not provide a mathematical or numerical proof of the proposed variational ansatz. This ansatz seems definitely reasonable for a bound state with (approximately) one boson bound to an impurity, but I am not sure that I understand why it should work for N-boson-plus-impurity bound states, here N is (approximately) the number of bound bosons.
Looking at the acceptance criteria of SciPost Physics, the manuscript might "Open a new pathway in an existing or a new research direction, with clear potential for multi pronged follow-up work". However, in my opinion, to meet this criteria, some further work is needed to validate the ansatz.

We thank the esteemed referee very much for their time and accepting to review our manuscript, and we are delighted to hear that they found our work interesting. We also thank them for their thoughtful and precise comments on various aspects of our work, which definitely helps to improve the strength and clarity of the arguments. We believe that our work has offered a novel framework to formulate strong coupling Bose polaron problem, by a sequence of arguments which we now try to elaborate more on in our revised manuscript.

Requested changes

Major:

1. The manuscript should provide a stronger justification for the use of the variational ansatz. Is it possible to estimate the effect of the neglected piece of the Hilbert space in the spirit of the mentioned in the manuscript Born-Oppenheimer approximation? Alternatively, are there any numerical results in the literature for few- or many-body systems that can be used for benchmarking?

We thank the referee very much for their request regarding a stronger justification for the variational ansatz. In the revised manuscript, we give a rigorous justification of the variational principle in the added Appendix B entitled "Justification of the effective model and the variational principle". To justify the use of the variational ansatz, we present a formulation of the initial impurity-boson problem in which the many-body bound states emerge as an effective impurity with multiple internal states coupled to a bath of weakly interacting, renormalized phonons. The coupling causes transitions between different impurity internal states (i.e., many-body bound states) via phonon scattering. Due to the large separation of energy scales between the different impurity internal states compared to the strength of transitions, one can treat the impurity-bath coupling within perturbation theory. Crucially, the relevant eigenstates of the unperturbed Hamiltonian corresponding to different metastable branches have the same product state form of the variational state $|\psi_{(\mathrm{var})}\rangle$ in Eq. [10] of the main text. Since the variational manifold includes the leading order term of the true eigenstates, optimizing the variational parameters enables to partially capture perturbative corrections to the eigenstates. We hope that the added appendix and further explanations in the text adequately address the referee's concerns.

Note that our main purpose in this work is to present a framework for modelling 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 extends to generic impurity-boson problems. However, we expect, based on arguments detailed in the manuscript, that it provides a plausible description of the problem when N (the approximate number of bound bosons) is of the order of a few (and not tens or hundreds of) particles. Of course, application of this framework to problems such as ionic or Rydberg impurities in BECs where many-body bound states consisting of hundreds of bosons bound to the impurity can exist is an intriguing future research direction which deserves to be addressed in further publications. This type of problems, however, is beyond the scope of the present work.

Regarding benchmarks with the existing literature, we note that the lowest-energy (attractive polaron) state closely follows GPE predictions, see e.g. Fig. [4] in our manuscript. GPE has been shown to provide very accurate description of both experiments and numerically exact QMC calculations, see e.g. *Physical Review A, 103(1), p.013317*, *Physical review letters, 126(12), p.123403* and *arXiv:2311.14313 (2023)*.

Minor:

A. Annals of Physics 19, 234 (1962) and J. Phys. B: At. Mol. Opt. Phys. 53 205302 (2020) are relevant references that might be considered together with the mentioned mean-field studies of the Bose polaron, e.g., [61-63].

We thank the referee for bringing these works to our attention. We have added these works to the references of our manuscript. In the revised manuscript, these are references [64] and [65].

B. The manuscript states that "the repuslive [typo!] polaron cannot exist without its attractive counterpart." This statement should probably be clarified, as the repulsive polaron is expected to be a stable ground state for purely repulsive interactions, see for example Fig. 7 of Atoms 10, 55 (2022).

We thank the referee for raising this important point. Indeed, this is one of the intriguing differences of the repulsive polaron between the attractive versus repulsive impurity-boson interactions. For repulsive impurity-boson interactions, repulsive polaron is the stable ground state of repulsively interacting bosons, thus no attractive polaron exists. The point we were trying to emphasize is, for attractive impurity-boson interactions, whenever the repulsive polaron branch exists, other lower energy resonances such as the attractive polaron branch and/or, depending on the setting, further few- and many-body states such as clusters or many-body bound states necessarily have to exist. This is because the repulsive polaron is not anymore a stable lowest energy state. Thus, novel experimental schemes for detecting the low-lying states and characterizing their properties is worthy of more research efforts, although detection of these states is difficult with the conventional impurity spectroscopy techniques.

C. What is meant by "the third solution" on page 5 (at the very top of the right column)?

It is shown in *Physical Review A, 71(2), 023606*, and *Physical Review A 106, no. 3 (2022): 033305* (Refs. [74] and [61]) that the Gross-Pitaevskii equation (GPE) for an attractive impurity having ν bound states has $2\nu + 1$ solutions. Indeed, in our numerics we find a third solution to the GPE other than the attractive and repulsive polaron. This solution to the coherent state has an absolute value very similar to the attractive polaron, but with a negative sign. Its energy is positive and lies above both the attractive and repulsive polarons. Thus, it is not relevant for our current study.

D. The manuscript uses a delta function to model boson-boson interactions. It is unclear if this is justified for the present beyond-mean-field study, i.e., when H_3 and H_4 are included. The manuscript should clarify this issue.

We thank the referee for bringing this great point up. Indeed, for a generic beyond mean-field treatment, the use of a delta potential is questionable. However, a crucial property of the particular class of problems in this work is the large binding energy of the impurity-boson bound state, such that the impurity-boson scattering length a is much smaller than the BEC length scales (interparticle spacing and the healing length). To be more concrete, let $\eta_{\mathbf{x}}$ be the impurity-boson bound state wavefunction (as argued in Appendix C of the revised manuscript, the Bogoliubov mixing is unimportant for the bound state), and $U_{\mathrm{BB}}(\mathbf{x}-\mathbf{x}')$ the boson-boson potential. The finite range of interactions definitely affect the interaction of bosons bound to the impurity. The effect of finite range is thus more pronounced for the following terms in the $\hat{H}_{\mathrm{eff,B}}$ of the bound-boson Hamiltonian (see Eq. [11] page 7 in the main text),

$$\hat{H}_{4,\mathrm{B}} = \frac{1}{2}\left(\int_{\mathbf{x},\mathbf{x}'} |\eta_{\mathbf{x}}|^2 U_{\mathrm{BB}}(\mathbf{x}-\mathbf{x}')|\eta_{\mathbf{x}'}|^2\right)\hat{b}^{\dagger 2}\hat{b}^2\,, \tag{1}$$

$$\hat{H}_{3,\mathrm{B}} = \left(\int_{\mathbf{x},\mathbf{x}'} \eta^*_{\mathbf{x}}\eta^*_{\mathbf{x}'} U_{\mathrm{BB}}(\mathbf{x}-\mathbf{x}')\varphi_{\mathbf{x}}\eta_{\mathbf{x}'}\right)\hat{b}^{\dagger 2}\hat{b} + h.c.\,, \tag{2}$$

describing the interaction of two bosons bound to the impurity. Since in the regime of interest, a is of the order of the ranges of the impurity-boson and boson-boson potentials, the value in the parantheses in Eqs. 1 and 2 is nonuniversal and strongly depends on the shape of interparticle potentials. In our manuscript, changing the potential from delta function to any other (for instance a Gaussian potential) will affect the corresponding term in $\hat{H}_{\mathrm{eff,B}}$ and consequently, the position of many-body bound states in Figs. [2], [4] and [5] in the main text. However, the coupling constants of the bound mode to the scattering modes are affected much less, since the scattering modes are extended and delocalized over the system volume, while the bound mode is strongly localized, thus the transition matrix elements between these modes, as well as the interaction between scattering modes obtain insignificant corrections due to the finite range of U_{BB}. Especially, the $\hat{H}_3$ and $\hat{H}_4$ terms in the interaction Hamiltonian of the scattering modes have the same effect of phonon interaction terms in the standard Bogoliubov treatment of the weakly interacting Bose gas. Indeed, the scattering modes here are very similarly to phonons of the textbook weakly interactig Bose gas in several respects:

- They have positive energy.
- The condensate profile corresponds to the repulsive polaron, which is quite close to a uniform condensate for $1/k_n a \gg 1$.
- The mode profile of the scattering modes differ from plane waves only by a weakly-momentum-dependent phase shift $\delta_0(k) \sim \pi - k\,a$ for $1/k_n a \gg 1$. The difference in the scattering mode wavefunctions and plane waves is thus only in a region of the size of the impurity potential range, and a small phase shift outside.
- Regarding the above point, the momentum-dependent interaction coefficients in the $\hat{H}_4$ term for the scattering modes are the same as those for the phonon modes of a uniform BEC up to corrections due to the nonvanishing size of the impurity.
- Similarly, the $\hat{H}_3$ term for the scattering modes resembles closely the $\hat{H}_3$ term in the BEC phonon Hamiltonian.

Adding to the above points, we mention again the finding in our numerics that the required coherent state displacement of the scattering modes (as a result of coupling to the bound bosons) is so small that the state of the scattering modes is close to a vacuum state (an average occupation number $\ll 1$ for scattering states with momenta $\sim 1/\xi$, see Fig. [5] in the main text). For such small number of long wavelength excitations, the kinetic energy of the scattering modes dominates, and due to the long wavelength nature of the excited scattering modes, the effect of finite boson-boson interaction range becomes insubstantial.

Finally, we again emphasize that the whole physics discussed in our work is strongly non-universal, and unless accurate models of interparticle collisions are taken, one should not expect the quantitative results of this work to directly match experimental measurements or ab initio calculations. However, we believe that our quantitative results provide qualitative and general insights about the physics of many-body bound states, and are representative of what might actually be observed in the future experiments.

E. The manuscript states that "it is essential to include the effects of quantum fluctuations through Γ" for low spatial dimensions. It is worth clarifying this point. Naively, one would assume that quantum fluctuations become important only when one considers long-range physics, but it might be that I am missing something.

We thank the referee for bringing up this subtle point. We added an explanation to the main text, which we hope clarifies this point. Indeed, this is completely correct that the effect of quantum fluctuations is important for long range physics, and a more detailed treatment has to account for such effects. However, in our context, the excitations are either highly localized around the impurity (the bound mode), that the effect of Bogoliubov transformation becomes insignificant, or the number of excitations is so small that the scattering modes are almost in their vacuum state. In both cases, Bogoliubov transformation does not add much information to the conclusions about the physics of the problem. It is also argued in the text that, since the fluctuation terms scale as $\mathcal{O}(\lambda^{3/2})$, in the extreme dilute regime $\lambda \ll 1$, their effect is minor quantitative corrections. Note also that, by virtue of the similarity between the scattering modes and a uniform BEC phonon modes discussed above, when considering the repulsive polaron saddle point, terms containing Γ has similar effects in the mean-field energy as they do in a weakly interacting Bose gas, which for instance lead to the LHY correction. The LHY correction is not significant in conventional BEC settings. However, inclusion of quantum fluctuations through Γ terms is essential when considering light impurities and studying impurity-induced instabilities, as studied for instance in Christianen et al. *Physical Review A 105, no. 5 (2022): 053302*, *Physical Review Letters, 128(18), p.183401* and *SciPost Physics, 16(3), p.067.* This regime, although very interesting, is not a subject of study in our current work.

Regarding our comments about lower dimensions, what we had in mind was mostly related to polariton condensates in two dimensional semiconductor heterostructures, where due to the effect of reduced dimensionality and strong polariton interactions, it is essential to account for fluctuations. It is also the case that in two dimensions, the effect of quantum fluctuations is fundamentally different, and great care must be taken in application of standard methods for weakly interacting Bose gases, as discussed for instance in *Stoof, H. T. C., and M. Bijlsma."Kosterlitz-Thouless transition in a dilute Bose gas." Physical Review E 47, no. 2 (1993): 939.* We clarify this point accordingly in the main text, and thank the referee again for their precise reading of our work.

F. Related to E. Note that a low dimensional geometry might provide a testbed for the employed variational approach – there are a number of various numerical techniques that can provide accurate results. Therefore, it might make sense to motivate further studies of low-dimensional Bose polarons using the proposed variational ansatz.

We thank the referee very much for suggesting this interesting point. We added a comment in the conclusions section as a perspective to motivate future studies of Bose polarons in lower dimensions using the proposed variational ansatz and comparing to the results of already existing methods.

G. The manuscript introduces r_0 to model the range of the boson-impurity interaction. Unfortunately, the reader is left wondering what is the role of r_0 on the reported results. What will happen if r_0 is changed?

Changing r_0 has a number of effects on the quantitative results. First, it is noted in the studies of Bose polarons within Gross-Pitaevskii theory such as *Physical Review A, 103(1), p.013317* and *Physical review letters, 126(12), p.123403* that the predictions of the GP theory match excellently to the experimental data and Monte Carlo simulations, if the effective range of the impurity-boson pseudopotential (here the squarewell) matches the effective range of the actual potential. Accordingly, we tune r_0 in the same manner to get the same effective range as the one for the realistic interaction potentials between species. However, since the problem by nature is non-universal and is sensitive to the details of the interparticle interactions, changing r_0 will change the quantitative predictions presented in the main text.

H. The manuscript states "it takes into account the quantum correlations of bound Bogoliubov excitations exactly, without restricting the number of excitations." It is worth clarifying what is meant by 'exactly' here.

We thank the referee for mentioning this point. Here, by exact we mean that the Hamiltonian governing the dynamics of the bound mode includes all the interaction terms involving the interaction of the bound mode with itself, as well as the interaction of the bound mode with the condensate. This Hamiltonian is very easy to treat numerically since it is the Hamiltonian of a single mode. Thus, one can use exact diagonalization to find the eigenstates and eigenenergies of this Hamiltonian. For the treatment of the coupling of the bound mode to the scattering modes, and the interactions among the scattering modes, approximations are inevitable. We have added an explanation in the main text following the referee's suggestions.

Finally, we would like to express our gratitude to the referee again for their valuable time a careful consideration of our work. We believe that their comments have had a direcet impact on improving the strength of our work, and we hope that their concerns are properly addressed by our response.