Reviewers' comments:

Reviewer #1 (Remarks to the Author):

Report on the manuscript "Ionic polaron in a Bose-Einstein condensate" by G. E. Astrakharchik et al.

The authors present a theoretical study of a ionic impurity placed in a gas of bosonic atoms. They show evidence of a rich phase diagram: a standard polaronic regime for weak interactions, and a strongly correlated state with many bosons bound to the ion. The methods and presented results are very rich, and provide a strong ground for a potential realization in future cold atom experiments.

My main concern is the relevance of this work for a practical implementation. The authors consider a model system in which an atom can form at most one bound state with the ion. The authors mention the fact that many deeply bound states actually occur in a real system. The presented study keeps its relevance if the timescale required to see the effects is shorter than the relaxation timescale towards these bound states. The authors discuss this point to some extent, but I would expect a more precise consideration.

For the parameters used in the calculations (atom density n=10-14 cm-3, C4 of Rb atoms, temperature at the threshold of BEC), what is the decay rate gamma, and how does it compare with the typical impurity energy E*? I would expect more precise values for the reader to judge the relevance of this work.

I also have other remarks of less importance:
- in the paragraph dealing with three-body recombination, the formulas do not seem to be consistent, or the definition of polarizability is not the one I am used of. I was not able to find the timescale of 1 second mentionned by the authors.
- The ion residue function g1 is not defined, and I could not understand this paragraph. The authors should maybe remind the definition of the quasi-particle residue, and explain in more detail how to extract it.

Reviewer #2 (Remarks to the Author):

The authors numerically studied an impurity problem which is described by the Hamiltonian (2). In this model, a charged ion with mass M is immersed into a weakly interacting bosonic medium with the particle mass m. The variational and DMC methods were used for performing their numerical study. In fact the model has several interesting regimes like showed in the Fig. 1. However, they only considered the weakly interacting regime and the case M=m. This case much restricts the subtle crossover or phase transition from polaronic physics to a single molecule bound state. Therefore their results so far does not show enough new physics for a warrant of the paper to publish in the journal Communications Physics. The questions are the following:
1) Although the authors introduced a nice scattering potential v_{ai} given by Eq. (3), they failed to discuss the polaronic physics resulted in from different choices of the parameters a and c, as well as the atom-atom scattering. Their assumption of one bound state in their study lacks supporting reasons, see the discussion below Eq. (3). Why did not exist larger bound states? For example, why did not exist a bound state of one ion and 2-atoms?

2) In their study of MBBS, for the N<N_c, the energy of the system is given by Eq. (5), For N>N_c, the energy should be increased when N increases if the interaction between the atoms in the medium is weakly repulsive. The Fig.2 (a) did not show such a increasement. The definition of E_b was not given, see Eq. (5).
3) The polaron energy is given by Eq.(6). Is it a repulsive polaron? It is not clear how to get it. What particular effect from the charged ionic impurity can be seen in comparation with a neutral atomic impurity? The discussion on the unitary limit is not clear, which channel is at unitary?
4) The wave function (4) should be used to understand the discussion of the correlation functions for Figur. 3. But we could not see a connection between the correlation functions and the wave function (4).

The paper is not well written, even the abstract contains too abstract description of their study. They did not clearly explain what is really new to the well-understood neutral atom-atom impurity. I do not recommend this current submission for a publication in Comm. Phys.

Reviewer #3 (Remarks to the Author):

The paper by Astrakharchik et al. investigates a novel mesoscopic quantum state that arises when a ionic impurity is immersed into a Bose-Einstein condensate. The authors show the correlated nature of the state and discuss the differences to usual polaronic states of neutral impurities. The work is of very good scientific quality and describes a qualitatively novel phenomenon. The paper addresses the community of researchers in atomic physics and quantum gases and the style of writing requires and in-depth knowledge of the physics as a prerequisite.

- Figure 1 should represent a "phase diagram". Even though I think I understand the logic behind the representation, I find it not very intuitive. It is clear that for certain interaction strengths one can have several states at different energies (that's already the case for the neutral impurity). Wrapping the state arond the energy axis, however, does not make sense and I have no imagination what the authors intend to label the x and y axes with.

- As compared to the experimental state-of-the-art, the proposal is a few years ahead and hence one should take the numerical values with a grain of salt since - to my knowledge- the atom-ion interaction parameters are not accurately known yet (in particular at short range). A more thorough discussion of the possible ranges would be desireable to understand whether the results are robust with respect to the potential variations of the scattering parameters which still have to be determined. I think Table I falls a bit short of convincing me that the results discussed here will observable in a large enough parameter space.
- In Fig 5 the authors plot the g(1) function over 100 orders of magnitude and find universal scaling from from 20 orders of magnitude below unity. This result is maybe interesting from a theoretical perspective, however, the relevance to experiments is unclear. In detectable range, say between 1 and 0.01 (that's already an optimistic case), the results are indistinguishable. Also, an error budget and error bars would be very much desireable on this plot.

- The authors make reference to atom-ion Feshbach resonances in order to detect the proposed polaronic states. This is highly speculative since (1) these resonances have not yet been observed and (2) reaching the unitary regime with Feshbach resonances in Bose gases is usually accompanied

by strong losses. It would be worthwhile to consider and discuss alternative approaches for detecting the novel many body state.

I think the work is publishable after some revisions/additionas and, maybe, nature communications is a good platform

The authors numerically studied an impurity problem which is described by the Hamiltonian (2). In this model, a charged ion with mass M is immersed into a weakly interacting bosonic medium with the particle mass m. The variational and DMC methods were used for performing their numerical study. In fact the model has several interesting regimes like showed in the Fig. 1. However, they only considered the weakly interacting regime and the case M=m. This case much restricts the subtle crossover or phase transition from polaronic physics to a single molecule bound state. Therefore their results so far does not show enough new physics for a warrant of the paper to publish in the journal Communications Physics. The questions are the following:

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Dear Editor,

please find below a detailed response to all the comments raised by Reviewers. We hope that the article will be suitable for publication in its revised form.

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The authors present a theoretical study of a ionic impurity placed in a gas of bosonic atoms. They show evidence of a rich phase diagram: a standard polaronic regime for weak interactions, and a strongly correlated state with many bosons bound to the ion. The methods and presented results are very rich, and provide a strong ground for a potential realization in future cold atom experiments.

My main concern is the relevance of this work for a practical implementation. The authors consider a model system in which an atom can form at most one bound state with the ion. The authors mention the fact that many deeply bound states actually occur in a real system. The presented study keeps its relevance if the timescale required to see the effects is shorter than the relaxation timescale towards these bound states. The authors discuss this point to some extent, but I would expect a more precise consideration.

Answer: The situation in the current setup is similar to the case of neutral Bose polarons, where finite lifetime is also a limiting factor. However, our estimates show that the losses should not inhibit the prospects for experimental studies. Recent work by Dieterle et al demonstrated that it is indeed feasible to observe the ion dynamics in a dense BEC for at least several milliseconds [19]. Currently, the more challenging problem for an experimental study is reaching sufficiently low ion energies to enable efficient formation of the many-body state. Another important issue consists in designing more efficient Pauli traps and reducing ion micro motion. We also note that apart from three-body recombination, the existence of additional bound states matters only quantitatively for the ground state structure, as their spatial extent is smaller than other length scales. We have slightly expanded the discussion of experimental issues in the main text to account for these remarks.

For the parameters used in the calculations (atom density n=10-14 cm-3, C4 of Rb atoms, temperature at the threshold of BEC), what is the decay rate gamma, and how does it compare with the typical impurity energy E*? I would expect more precise values for the reader to judge the relevance of this work.
I also have other remarks of less importance:

- in the paragraph dealing with three-body recombination, the formulas do not seem to be consistent, or the definition of polarizability is not the one I am used of. I was not able to find the timescale of 1 second mentioned by the authors.

Answer: We thank the referee for noticing that this paragraph requires clarification. We have rewritten the formulas in more appropriate units consistent with the rest of the manuscript, along with a few realistic examples. As now mentioned in the text, for the dense BEC at 10^14 cm^-3 the decay rate gamma exceeds 100kHz, but our numerics is performed at the gas parameter 10^-6 which can be translated to the gas density of about 6.6*10^12 cm^-3 which gives gamma of roughly 600Hz, while E* for this system is 1646Hz.

- The ion residue function g1 is not defined, and I could not understand this paragraph. The authors should maybe remind the definition of the quasi-particle residue, and explain in more detail how to extract it.

Answer: We have added in the new version the definition of the residue function $g_1(r)$, i.e., one-body correlation function, and the residue Z as its limiting value for $r\to\infty$.

Reviewer #2 (Remarks to the Author):

The authors numerically studied an impurity problem which is described by the Hamiltonian (2). In this model, a charged ion with mass M is immersed into a weakly interacting bosonic medium with the particle mass m. The variational and DMC methods were used for performing their numerical study. In fact the model has several interesting regimes like showed in the Fig. 1. However, they only considered the weakly interacting regime and the case M=m. This case much restricts the subtle crossover or phase transition from polaronic physics to a single molecule bound state. Therefore their results so far does not show enough new physics for a warrant of the paper to publish in the journal Communications Physics. The questions are the following:

Answer: We stuck to the particular case $m=M$ as this is an experimentally realistic situation (see, e.g., [19]), but we have verified that the transition from the polaronic to the many-body bound state regime holds for different ion mass as well. Regarding the coupling strengths, from Fig. 2 one can observe that we consider a large difference in coupling strengths, hence one scans both the weak and strong coupling regime (lower part of the helix plotted in Fig.1).

Note that, within our state-of-the-art method, we do not distinguish between weak or strong coupling as the technique does not rely on the Bogoliubov approximation.

1) Although the authors introduced a nice scattering potential v_{ai} given by Eq. (3), they failed to discuss the polaronic physics resulted in from different choices of the parameters a and c, as well as the atom-atom scattering. Their assumption of one bound state in their study lacks supporting reasons, see the discussion below Eq. (3). Why did not exist larger bound states? For example, why did not exist a bound state of one ion and 2-atoms?

Answer: We have verified that for different choices of the parameters b (a is the scattering length in the manuscript) and c we obtain a qualitatively similar behavior. That is, the main claim of our paper on the existence of the many-body bound state remains valid.

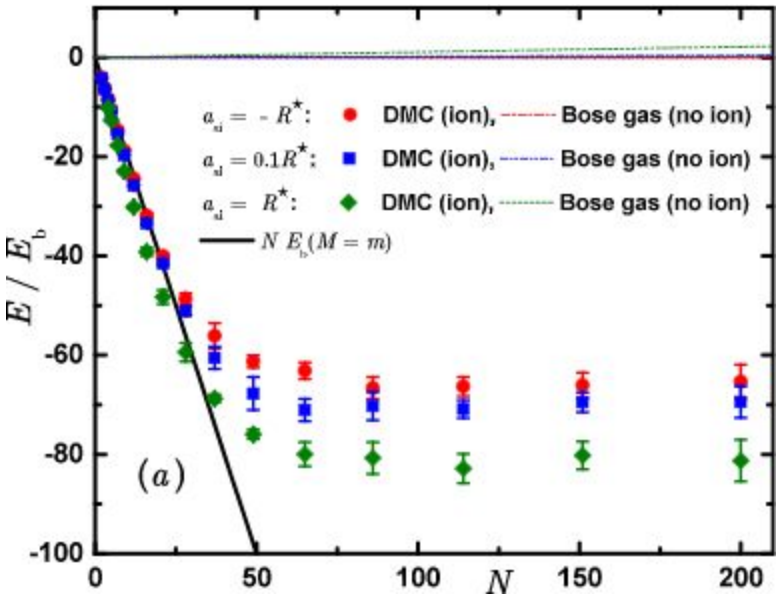
The choice of one bound state seems natural to us, as the most interesting physics usually happens when a new bound state appears. With the present choice of the interaction potential we are able to reproduce such a situation. An additional justification comes from the field of dilute alkali atoms where in many cases it is enough to consider the *s*-wave scattering length associated with the less bound energy state and ignore presence of deeply bound states. Adding more deeply bound two-body states does not affect the physics qualitatively, as the ground state is still a many-body bound state composed of a large number of atoms bound to the charge.

We would like to clarify that while the two-body problem supports only a single bound state, still the bound state of one ion and 2 atoms, i.e. a trimer state, does exist. That is, the energy with one ion and N=2 atoms is lower compared to the energy with one ion and N=1 atom, see Fig. 2a. Furthermore, bound states with one ion and 3 atoms (tetramer), 4 atoms (pentamer), *etc* as well exist. We find that the maximal number of atoms which can be bound to a single ion for considered conditions is N_c ~ 140.

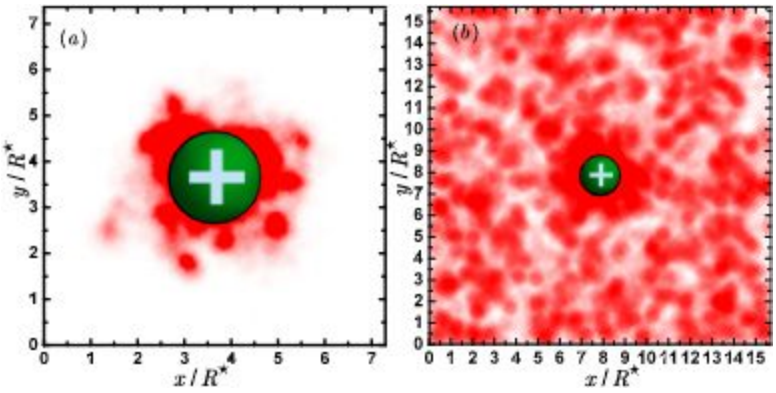
Finally, we note that we have studied a wide range of interactions from weak to the unitary case, not only the weakly interacting regime. Furthermore, the interaction energy scale and the resulting binding energy of the many-body bound state are much larger than the chemical potential of the BEC even in the case of the regularized potential studied here.

2) In their study of MBBS, for the N<N_c, the energy of the system is given by Eq. (5), For N>N_c, the energy should be increased when N increases if the interaction between the atoms in the medium is weakly repulsive. The Fig.2 (a) did not show such a increasement. The definition of E_b was not given, see Eq. (5).

Answer: The expected increase in the energy is associated with the increase in the density of the weakly interacting gas, $E \sim Ng\, n/2$. The expected increase in the energy is shown by the red, blue and green dashed lines close to the zero energy axis.



As it can be appreciated from the figure, such an increase is smaller compared to the binding energy E_b. The dependence of the Monte Carlo energy on the number of particles for $N>N_c$~140 is consistent with the expected slow increase. Partially, this effect is masked by the error-bars. On the other hand, the evolution of the snapshots of the particle coordinates suggests that the physics is correctly understood.



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Answer: Equation (6) is an approximate variational formula from Ref. [53] (we moved the respective citation to make it more clear), which describes both the repulsive and attractive cases. For the polaronic branch (Fig. 2b) the formula (6) captures the energy dependence relatively well, so in this regime the physics is similar to the neutral impurity case, as written in the discussion below Eq. (6). The unitarity limit is defined with the sentence "The unitary regime is reached when the atom-ion scattering length significantly exceeds the mean interparticle distance." in the

next paragraph. We have modified the following sentence to clarify that the continuous quantity we refer to is the ground state energy.

4) The wave function (4) should be used to understand the discussion of the correlation functions for Figur. 3. But we could not see a connection between the correlation functions and the wave function (4).

Answer: The wave function (4) is chosen in a generic Bijl-Jastrow form and it depends on the positions of all particles and the impurity. The correlation functions are obtained by integrating out all degrees of freedom except one. Generally, there is no simple connection between the correlation functions and the many-body wave function. This is the case for the two-body correlation function shown in Fig. 4.

Instead, for the residue function shown in Fig. 5, we are able to extract the shape of the leading decay from the wave function, according to Eq. (7). This is possible because of the fast exponential decay.

As well, it is important to notice that the diffusion Monte Carlo method corrects wave function (4) and the obtained DMC energy and correlation functions are exact.

Reviewer #3 (Remarks to the Author):

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Answer: Here, the intention was to picture the periodic changes of the scattering length as new two-body bound states appear at threshold; one should picture the Figure in cylindrical rather than cartesian coordinates. Specifically, our intention is to illustrate that the same values of the scattering length might correspond to very different physical states, depending on the number of bound states in the ion-atom problem. Importantly, the energy, as a function of the scattering length, is a continuous function, as indicated by the spiral. One should picture the Figure in cylindrical rather than cartesian coordinates, i.e. the reader should think about it in terms of the

energy E, as a function of atom-ion scattering length a_{ai} and an angle, rather than as a function of (x, y).

- As compared to the experimental state-of-the-art, the proposal is a few years ahead and hence one should take the numerical values with a grain of salt since - to my knowledge- the atom-ion interaction parameters are not accurately known yet (in particular at short range). A more thorough discussion of the possible ranges would be desireable to understand whether the results are robust with respect to the potential variations of the scattering parameters which still have to be determined. I think Table I falls a bit short of convincing me that the results discussed here will be observable in a large enough parameter space.

Answer: Indeed, in this work we are using a model potential, which is parametrized in a rather simple form. However, we checked that the observed effects are generic and do not require specific choice of the potential. Of course, a quantitative comparison with experimental data would require a more accurate choice of the potential parameters.

- In Fig 5 the authors plot the g(1) function over 100 orders of magnitude and find universal scaling from from 20 orders of magnitude below unity. This result is maybe interesting from a theoretical perspective, however, the relevance to experiments is unclear. In detectable range, say between 1 and 0.01 (that's already an optimistic case), the results are indistinguishable. Also, an error budget and error bars would be very much desireable on this plot.

Answer: We totally agree that from an experimental point of view, exponentially small values are irrelevant as being indistinguishable from zero. Still, conceptually, it is important to distinguish between a finite, but small residue, and a zero one.

We added error bars in the new version of the figure.

- The authors make reference to atom-ion Feshbach resonances in order to detect the proposed polaronic states. This is highly speculative since (1) these resonances have not yet been observed and (2) reaching the unitary regime with Feshbach resonances in Bose gases is usually accompanied by strong losses. It would be worthwhile to consider and discuss alternative approaches for detecting the novel many body state.

Answer: As mentioned in the response to Referee A, we estimate that the losses should not inhibit a successful experimental study, although directly at unitarity the ion lifetime will indeed be limited. The existence of ion-atom Feshbach resonances is certain from the theoretical point of view and already several groups are approaching the energies at which it will be possible to observe them. Furthermore, while access to Feshbach resonances would be highly appreciated, the basic effects that we predict (existence and structure of the many-body state) do not require changing the scattering length, but only reaching sufficiently low energies which seems to be within reach as well [17-19].

I think the work is publishable after some revisions/additionas and, maybe, nature communications is a good platform

We hope that in the new version, the article is suitable for the publication.

Sincerely yours,
G. E. Astrakharchik
L. A. Peña Ardila
R. Schmidt
K. Jachymski
A. Negretti

REVIEWERS' COMMENTS:

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I am satisfied by the answers to my concerns and the modifications to the manuscript. I have no objection for publication.

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The authors have addressed all questions raised up in my reports and other reports. The revised version look satisfactory. It would be useful for readers if the authors could address little more on the experimental proposal for testing such novel ionic polaron through the hybrid atom-ion setups. Anyhow, in view of their rich discussions on the iconic polaronic behaviour, I would like to recommend this submission for a publication in Communications Physics.

Response to Reviewers

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We thank the Reviewer 1 for a positive judgement of our work.

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We have reworked and expanded the discussion of a possible experimentation observation. The “diff” version of the Manuscript follows below.

Ionic polaron in a Bose-Einstein condensate

~~G.~~ Grigory E. Astrakharchik[1,1*], ~~L.~~ Luis A. Peña Ardila[2], ~~R.~~ Richard Schmidt[3,4], ~~K.~~ Krzysztof Jachymski[5,6], ~~A.~~ Antonio Negretti[7]

[1] *Department de Física, Universitat Politécnica de Catalunya, Campus Nord B4-B5, E-08034, Barcelona, Spain*
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[5] *Forschungszentrum Jülich Gmbh, Institute of Quantum Control (PGI-8), D-52425 Jülich, Germany*
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(Dated: March 18, 2021)

Abstract The presence of strong interactions in a many-body quantum system can lead to a variety of exotic effects. Here we show that even in a comparatively simple setup consisting of a charged impurity in a weakly interacting bosonic medium the competition of length scales gives rise to a highly correlated mesoscopic state. Using quantum Monte Carlo simulations, we unravel its vastly different polaronic properties compared to neutral quantum impurities. Moreover, we identify a transition between the regime amenable to conventional perturbative treatment in the limit of weak atom-ion interactions and a many-body bound state with vanishing quasi-particle residue composed of hundreds of atoms. In order to analyze the structure of the corresponding states we examine the atom-ion and atom-atom correlation functions which both show nontrivial properties. Our findings are directly relevant to experiments using hybrid atom-ion setups that have recently attained the ultracold regime.

Introduction

An impurity immersed in a many-body quantum system constitutes a fundamental building block in condensed-matter physics, particularly with regards to transport properties of materials [1, 2]. In order to investigate this paradigmatic problem, ultracold atoms are especially suited as they allow for experimental control of multiple parameters such as the shape of the confinement and the form of interparticle interactions [3]. Over the last decade atomic systems have proven to be capable to observe the formation of quasi-particles such as the celebrated polaron in bosonic [4–6] and fermionic [7–12] quantum gases as well as in a Rydberg system [13], with the possibility of exploring impurity physics also in the presence of dipolar interactions [14].

Within the plethora of compound atomic quantum systems available, atom-ion systems provide a ~~new~~ unique arena for investigating many-body quantum physics in the strongly interacting regime. Indeed, the interaction between the charge and the induced dipole of the neutral particle results in the asymptotic form

$$V_{\rm ai}(\mathbf{r}) \overset{r\to\infty}{\longrightarrow} -\frac{C_4}{r^4}\,. \tag{1}$$

Importantly, this polarization potential has a characteristic length scale that is about an order of magnitude larger than in the case of van der Waals interactions typical for neutral atoms and it can become comparable to the mean interparticle distance. Moreover, the characteristic interaction energy is typically in the microkelvin range and thus comparable to experimentally achievable collision energies [15]. Hence, although the polarization potential has in principle short-ranged nature one cannot replace it with a pseudopotential due to the lack of separation of length and energy scales between the two-body and the many-body systems. While this lack of scale separation gives rise to a striking competition of few- and many-body processes, it poses a theoretical challenge due to the necessity to account for details of the potential that severely inhibits the possibility of using analytical methods to describe the properties of an ionic impurity such as its effective mass.

Recently, it has been demonstrated that for certain atom-ion combinations the ultracold regime is within experimental reach [16–18]. Exploiting the charge of the impurity, one appealing possibility is to study transport properties by dragging the ion by means of electric fields and detect it with high spatial and temporal resolution [19]. The long range of the atom-ion potential, on the other hand, allows to investigate the formation of mesoscopic bound states [20–22] that would have dramatic impact on the ion transport dynamics.

Studies of the mobility of an ion moving in a bosonic medium date back to the early sixties with the aim of explaining the small ion mobility in liquid helium [23–27]. Later, mean-field approaches were used to predict the formation of mesoscopic molecular ions [20], to estimate the number of excess atoms around an ion in a homogeneous Bose-Einstein condensate (BEC) [28], and path integral methods to determine the ion polaron properties in the strong-coupling regime [29]. While such approaches allow one to obtain a qualitative picture of

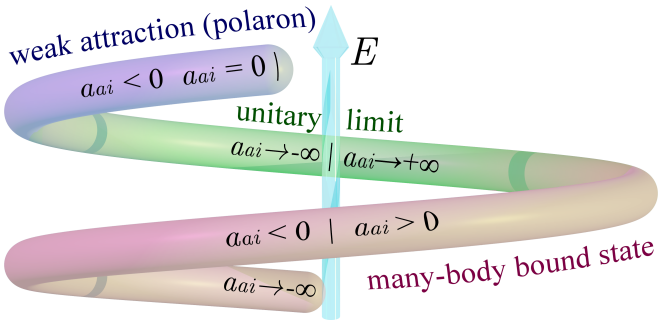

FIG. 1. A schematic phase diagram showing various regimes ~~found~~ for a single ion immersed in ~~the system~~ a dilute Bose gas upon changing the atom-ion scattering length and the number of the two-body bound states. The vertical axis indicates the change of the ion energy E as the value of atom-ion s-wave scattering length a_{ai} is varied. The spiral refers to a continuous change of the energy leading to realization of different physical regimes as the value of a_{ai} is cyclically changed from minus to plus infinity. Departing from the non-interacting case $a_{ai} = 0$, with zero ion energy, $E = 0$, and by making the ion attraction stronger the following regimes are observed. A weak attraction leads to the polaronic regime where the ion can be described in terms of a quasiparticle. Such a description is no longer possible in the unitary regime marked by a diverging s-wave scattering length. The unitary point, $|a_{ai}| = \infty$, is the threshold value for the formation of an ion-atom two-body bound state. For stronger atom-ion attraction many-body bound state is formed in which a large number of atoms is effectively trapped by the ion.

the underlying phenomenology, the interplay between the long-ranged potential and strong interactions not only leads to substantial shifts to the relevant observables such as the energy of the system, but also has drastic consequences for the structural properties of the ground state. In line with the recent experiments with ion-atom mixtures [16, 30–38], in this letter we study the many-body ground state properties of an ion immersed in a three-dimensional (3D) bosonic gas. To this end, we employ quantum Monte Carlo techniques that have been successful in the context of the 3D Bose polaron [39–41], bipolarons [42], as well as in two-dimensional (2D ~~[?] and~~) [43] and one-dimensional (1D) polarons [44–46]. The method allows us to fully take into account the quantum many-body correlations that turn out to be ~~crucial to predict~~ important for predicting how the competition between the few- and many-body length scales gives rise to a striking impurity physics that is governed by a transition from a polaron to a many-body polaron bound state. The resulting states cannot be captured by conventional tools such as the Frölich model or Bogolyubov theory. The system properties depend not only on the scattering length and effective range of the two-body potential, but rely on the presence of the long-range tail of the interaction, indicating the failure of the pseudopotential approximation.

Results

System. We consider an ion of mass M immersed into a gas consisting of N bosonic atoms of mass m at average density $n = N/L^3$. For simplicity we focus here on the mass-balanced case (i.e. $M = m$). We consider periodic boundary conditions in a box of size L chosen large compared to the healing length $\xi = (8\pi n a_{\rm aa})^{-1/2}$, where $a_{\rm aa}$ is the boson-boson s-wave scattering length.

The microscopic many-body Hamiltonian is given by -[47]

$$\hat{H} = -\frac{\hbar^2\nabla^2_{\mathbf{R}}}{2M} - \sum_{n=1}^{N}\frac{\hbar^2\nabla^2_{\mathbf{r}_n}}{2m} - V_{\rm ai}(\mathbf{r}_n - \mathbf{R}) + \sum_{n<j}^{N} V_{\rm aa}(\mathbf{r}_n - \mathbf{r}_j). \tag{2}$$

Hereafter, we denote the ion's characteristics such as position and mass with capital Latin letters, while for atom ones we use small Latin letters. Furthermore, bold symbols refer to three-dimensional vectors and cursive ones the respective norms. The first two terms in Eq. (2) represent the kinetic energy of the ion and of the atoms, respectively, and $V_{\rm aa}(\mathbf{r}_n - \mathbf{r}_j)$ is a repulsive short-range potential with coupling constant $g = 4\pi\hbar^2 a_{\rm aa}/m$. The potential $V_{\rm ai}$ describes the atom-ion interaction, for which it is essential to retain the long-range tail (1). It is further characterised by the length $R^\star = (2m_{\rm r}C_4/\hbar^2)^{1/2}$ and energy scales $E^\star = \hbar^2/[2m_{\rm r}(R^\star)^2]$, where $m_{\rm r} = mM/(m+M)$ is the reduced mass. For the ^{87}Rb/^{87}Rb$^+$ system one has $R^\star \simeq 265.81$ nm and $E^\star \simeq k_{\rm B} \times 79$ nK ($k_{\rm B}$ is the Boltzmann constant). ~~Crucially~~Importantly, the separation of length scales is lacking as for typical atom density $n = 10^{14}{\rm cm}^{-3}$ the mean interparticle distance $n^{-1/3} \simeq 0.8\, R^\star$ is of the same order as the interaction range as well as the healing length ($\xi \simeq R^\star$).

At short range, the real interaction potential will deviate from the asymptotic formula (1). Here, we model the short-range details by the regularization [48]:

$$V^r_{\rm ai}(\mathbf{r}) = -C_4\frac{r^2 - c^2}{r^2 + c^2}\frac{1}{(b^2 + r^2)^2}. \tag{3}$$

Here, the b and c parameters have units of length and control the properties of the potential such as the number of bound states and their energies as well as the scattering length, while the long-range effects of the tail (1) remain accounted for. Crucially, the properties of the system depend not only on the energies, but also on the number of the available two-body bound states, as it will be demonstrated below. In most of the calculations we tune the potential in such a way that it has only one two-body bound state. Under this assumption, there is a unique connection between the b, c parameters and the s-wave scattering length $a_{\rm ai}$ of the resulting potential.

The simulations are performed by using variational (VMC) and diffusion Monte Carlo (DMC) methods. The

VMC method samples the square of the trial wavefunction that we choose in the Bijl-Jastrow [49, 50] form

$$\Psi_{\rm T}(\mathbf{R};\mathbf{r}_1,\ldots,\mathbf{r}_N)=\prod_{j<n} f_{\rm B}(|\mathbf{r}_n-\mathbf{r}_j|)\prod_{j<n} f_{\rm I}(|\mathbf{r}_n-\mathbf{R}|). \tag{4}$$

Here, $f_{\rm B}$ and $f_{\rm I}$ account for two-particle intra- and inter-species correlations, respectively. These functions are constructed by matching the solution of the two-body scattering problem at short distances to an appropriate tail (see Methods), i.e. phononic decay in $f_{\rm B}$ and mean-field prediction for a heavy ion in $f_{\rm I}$. Both functions contain variational parameters that are optimized by minimizing the expectation value of the Hamiltonian (2). VMC calculations provide the upper bound to the ground-state energy. In contrast the DMC approach aims to obtain the exact ground state energy of the system by solving the Schrödinger equation in imaginary time. We are interested in the regime of weak atom-atom interactions and fix the gas parameter to $na_{\rm aa}^3 = 10^{-6}$ with $a_{\rm aa} = 0.02\,R^\star$.

Ground state energy. In Fig. 1 we illustrate the 'phase diagram' of the system that is characterized by two distinct sets of ground states: many-body bound state (MBBS) and a polaronic one. ~~As the "helix" structure indicates, for negative atom-ion scattering lengths both solutions are possible, while positive scattering lengths always lead to a MBBS. Indeed, while~~ A spiral is used to illustrate that the energy E depends monotonously on the s-wave scattering length $a_{\rm ai}$, although different energies correspond to the same value of $a_{\rm ai}$ depending on the number of bound states. While for $a_{\rm ai} > 0$ the potential (3) always has a bound state, for negative scattering lengths the atom-ion interaction can be tuned such that either a bound state is supported (left-bottom part of the helix, MBBS), or no bound state is present (left-upper part, polaronic). The 'attractive' polaron is typically encountered in ultracold quantum gases with neutral atomic impurities [4, 5, 39, 40, 51]. On the other hand, in the MBBS regime many bosons can be bound to the ion with a large binding energy. Importantly, the spatial range of the atom-ion interaction plays a crucial role in the formation of the MBBS, while for neutral impurities physics can typically be well described by assuming an effective short-range interaction.

Figure 2 provides characteristic examples of the dependence of the system's total energy on the number of bosons in the MBBS (a) and polaronic (b) regime. In the MBBS case, we find that the absolute value of the energy grows almost linearly for a sufficiently small number of bosons. The dependence can be roughly approximated by the energy of N non-interacting particles bound to the ion,

$$E(N) \simeq N E_{\rm b}(M=m)\,, \tag{5}$$

as shown with a solid black line in Fig. 2 (a). We also have verified that the effective impurity mass approaches the total mass of the MBBS, $M^\star \approx Nm$. As the number of bosons is increased further, the energy starts to significantly deviate from the behavior (5) and it reaches a minimum at a critical number $N_{\rm c}$, which can be estimated from the extremum condition $\partial E/\partial N = 0$ [47]. The value $N_{\rm c}$ can be interpreted as the maximal number of bosons bound to the impurity, similarly to the analysis of the 1D case [22]. We note that $N_{\rm c}$ could be defined in different ways, e.g. from the form of the atom-ion correlation function, $g_2^{\rm ai}(r)$, as $N_{\rm c} = n\int[g_2^{\rm ai}(r)-1+N_{\rm c}/N]4\pi r^2 dr$, or from the atom density far from the ion, i.e. $n(1-N_{\rm c}/N)$. For the chosen parameters we obtain $N_{\rm c} \simeq 140$ almost irrespective of the exact value of the atom-ion scattering length, contrarily to the mean-field prediction of Ref. [20]. This indicates that while the scattering physics of quasi-free bosons is determined by the scattering length, it is the large range of the potential that determines the number of bound particles. Note that our result is significantly larger as compared to the many-body bound states for the case of a neutral impurity, for which ~~MC calculation predicts~~ Monte Carlo calculations predict only few atoms to be bound [39]. At the same time $N_{\rm c}$ is much smaller than the number of bound atoms predicted by a mean-field-based estimate, suggesting that the effective gas parameter is significantly increased in the vicinity of the ion. For $N > N_{\rm c}$ the energy increases, meaning that no more bosons are able to bind to the ion and the excess atoms start to form an almost uniform gas. This view is further corroborated by the snapshots of the system taken in Fig. 3 for different system sizes, where the green sphere of radius $R^\star$ depicts the position of the ion (red symbols for bosons). Figure 3(a) shows the snapshot of the system in the case when the number of bosons is smaller than the critical one, $N < N_{\rm c}$, and therefore all bosons are close to the ion forming a spatially localised MBBS. Contrarily, ~~panel~~ Fig. 3(b) depicts the case with $N > N_{\rm c}$. In this scenario, the boson density around the ion is still higher than the average one and the excess bosons form a background gas.

Figure 2(b) shows the energy dependence on N following the "polaronic" branch where no two-body bound states are present, for three characteristic values of the atom-ion scattering lengths: $a_{\rm ai} = -0.1R^\star$, $a_{\rm ai} = -R^\star$, and the unitary case $a_{\rm ai} \to \pm\infty$. For large system sizes it is expected that the total energy can be decomposed into two contributions, the chemical potential $\mu_{\rm pol}$ of the ion and the energy of a homogenous gas, $E = \mu_{\rm pol} + Ngn/2$. For sufficiently small $|a_{\rm ai}|$, the polaron energy can be calculated variationally [52]

$$\mu_{\rm pol} = 4\pi(n\,a_{\rm aa}^3)\left(\frac{R^\star}{a_{\rm aa}}\right)^2\left(\frac{a_{\rm aa}}{a_{\rm ai}}-\frac{a_{\rm aa}}{a_0}\right)^{-1}E^\star\,, \tag{6}$$

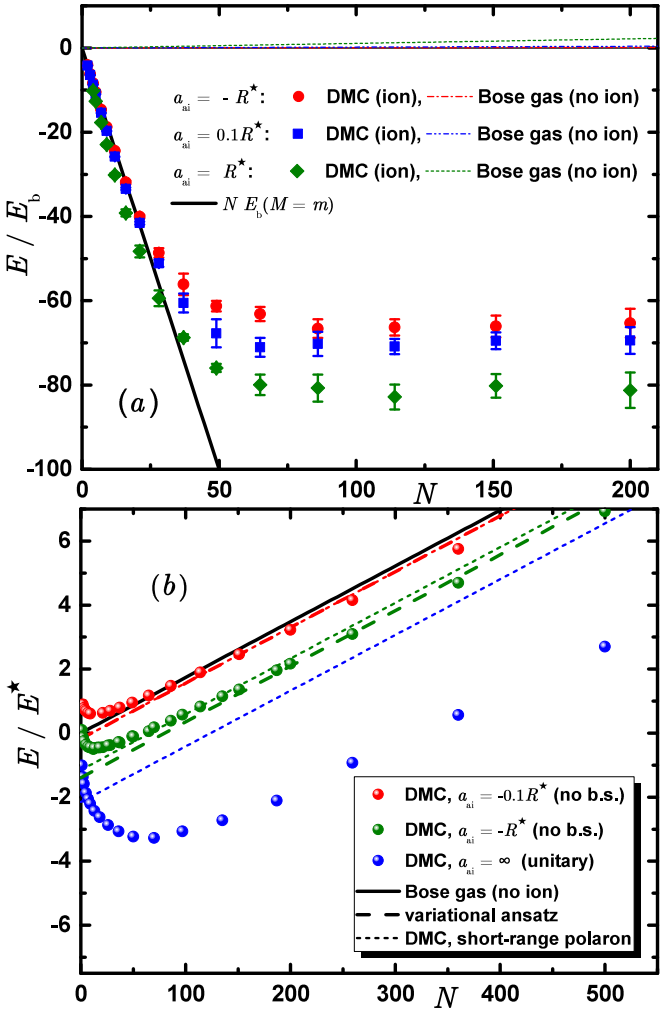

FIG. 2. Ground-state energy of the many-body system. (a) Total energy obtained as the expectation value of the Hamiltonian (2) in units of the binding energy of the ion-atom molecule E_b as a function of the number of bosons N. The symbols represent the energy obtained ~~via DMC~~ in diffusion Monte Carlo simulations, while the black solid line shows the energy (5). Error bars show the standard deviation of Monte Carlo simulations. (b) Total energy in units of $E^\star$. For the lines, the mean-field Gross-Pitaevskii energy is shifted by the polaron energy, i.e. $E(N) = \mu_{pol} + gnN/2$; solid line, no ion, $\mu_{pol} = 0$; long-dashed line, variational ansatz [52], μ_{pol} is given by Eq. (6); short-dashed line, ~~DMC~~ diffusion Monte Carlo calculation for short-ranged impurity-boson interactions from Ref. [39].

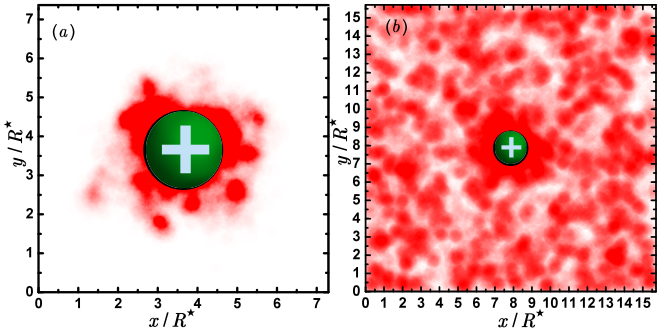

FIG. 3. Snapshots of the calculated particle coordinates. Particle coordinates are represented for two characteristic numbers of bosons: ~~Left panel~~ (a) $N = 50$ ~~, right panel~~ particles (b) $N = 500$ particles. Note that in the critical number of atoms which can be trapped by the ion, $N_c = 140$ ~~and~~ , is (a) larger (b) smaller than the number of particles N, correspondingly. Parameters of the interaction are chosen such that the value of the atom-ion s-wave scattering length equals to the characteristic length-scale $R^\star$ of the C_4 decay (1), $a_{ai} = R^\star$. The red areas denote instantaneous positions of the bosons in the box potential. Coordinates are shifted so that the ion appears in the center.

where $a_0 = \frac{32}{3\sqrt{\pi}}\sqrt{na_{aa}^3}$ is the shift of the scattering resonance due to the bosonic ensemble ~~[52]~~. Therefore, in the regime of sufficiently weak interactions the energy is universal as it depends only on a_{ai} and no finite range corrections are required.

It is important to notice that the Fröhlich model [29] alone is not sufficient to describe the ion quantitatively, predicting $\mu_{pol} = -0.096E^\star$ for $a_{ai} = R^\star$. Instead, beyond-Fröhlich perturbation theory correctly describes the polaron energy both in the weakly-interacting regime [$a_{ai} = -0.1\,R^\star$ data in Fig. 2(a)] and remarkably even for strongly interacting polarons ($a_{ai} = -R^\star$). In the regime of weak interactions, the ion behaves similarly to a neutral impurity with short-range interactions, for which the VMC energy is shown with short-dashed lines. The unitary regime is reached when the atom-ion scattering length significantly exceeds the mean interparticle distance. An important feature of the ion impurity is that the ~~unitary limit is continuous~~ energy of the many-body ground state is continuous when crossing the $a_{ai} \to \infty$ point and connects the polaron and MBBS which are both stable branches. We note that directly at unitarity the prediction (6), which is derived within Bogolyubov approximation, is beyond its validity and thus it is not shown in Fig. 2(b). In particular, the Bogolyubov approximation becomes questionable close to unitarity, where the correlation functions shown in Fig. 4 indicate a varying local gas parameter similar to the discussion of beyond Bogolyubov corrections in Ref. [53]. For the same reason, the Bogolyubov-Fröhlich description of the ion polaron [29] has to be significantly revisited.

Correlation functions. In order to analyse the spatial structure of the many-body bound state we further turn our attention to the atom-atom and atom-ion correlation functions. Typical examples are displayed in Fig. 4. As it can be seen, the atom-ion correlation features a pronounced peak indicating a strong bunching effect at distances where the atom-ion interaction potential is strongly attractive. Moreover, for $N < N_c$ (see red lines) the atom-atom correlation function does not ap-

proach a constant at long distances, but instead it decays exponentially, supporting the interpretation that essentially all bosons are bound to the ion and are localized at distances of the order of a few $R^\star$. The width of $g_2^{\rm ai}$ can be used as the definition of the size of the MBBS that can be interpreted as a mesoscopic molecular ion. For $N > N_{\rm c}$ (see blue lines) the position of the peak does not change; the atom-atom correlation function, however, converges to a constant value which is slightly below unity. This demonstrates that the excess atoms are not bound to the ion and indeed form a bosonic background for the MBBS. The atom-atom correlation functions in the presence of the ion (dashed lines) also indicate the bunching behaviour close to the ion. The effect is the strongest for small systems, $N < N_{\rm c}$, where the bosons tend to stay close to each other as they are a part of the MBBS [see also Fig. 3(a)]. This can be interpreted as an effective interaction within the medium induced by the impurity. As the system size is increased, $g_2^{\rm aa}(r)$ starts to approach a constant value at large distances, i.e. the whole volume is filled with the gas [see also Fig. 3(b)], and the peak at short distances is correspondingly lowered. The asymptotic value $g_2^{\rm aa}(r) \to 1 - N_{\rm c}/N$ reflects a smaller effective density, as $N_{\rm c}$ atoms are bound to the ion. Eventually, in the thermodynamic limit atom-atom correlations will coincide with those of a homogeneous Bose gas without an ion (green line in Fig. 4).

We have also found that for $a_{\rm ai} < 0$ the two branches have very different behaviors in terms of coherence, which is quantified by the quasiparticle residue ~~Z~~ $Z = \lim_{r\to\infty} g_1(r)$ corresponding to the long-range asymptotic of the residue function $g_1(|\mathbf{r}-\mathbf{r}'|) = \langle \Psi^\dagger(\mathbf{r})\Psi(\mathbf{r}')\rangle$ where the field operator $\Psi^\dagger(\mathbf{r})$ creates an ion at position $\mathbf{r}$ and $\langle\rangle$ denotes the ground-state average. Indeed, the residue is finite in the polaron branch and approaches unity (full coherence) in the limit of weak attraction, $a_{\rm ai} \to 0^-$. Instead, in the MBBS branch the residue vanishes exponentially fast. Figure 5 shows typical examples of the decay of the ion residue function, $g_1(r)$, for a fixed number of particles for several choices of the atom-ion s-wave scattering length. We observe an exponential decay, which on the semi-logarithmic scale of Fig. 5 is seen as a linear dependence. This can be understood using a simple model. As discussed in the context of Fig. 2(a), the energy of small clusters of bosons in the MBBS branch can be reasonably well interpreted in terms of N non-interacting atoms bound to the ion. The two-body scattering solution (8) for each atom-ion pair scales as $f(r) = \exp(-r/a_{\rm ai})/r$ with $r = |\mathbf{R} - \mathbf{r}_i|$ for $r \gg R^\star$. By assuming a product over $\mathbf{r}_i$, $i = 1, \cdots, N$ we arrive at the following approximate form for the residue function at large distances

$$g_1(r) \propto \exp\left(-\frac{N_{\rm c} r}{a_{\rm ai}}\right) . \qquad (7)$$

For deeply bound states, $a_{\rm ai} \to 0$, all N particles are bound and participate in the MBBS. In turn, for weaker interactions or larger ~~number~~ numbers of particles, the ion is able to capture only $N_{\rm c}$ atoms. We take this effect into account by substituting N by $N_{\rm c}$ in Eq. (7). As it can be seen in Fig. 5, the asymptotic expression (7) captures correctly the exponential loss of coherence.

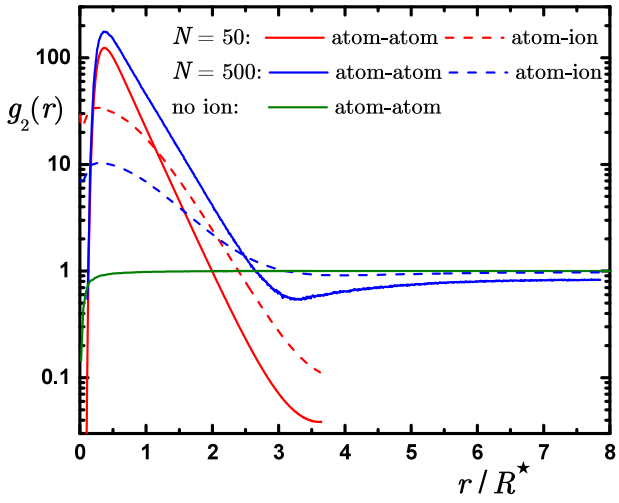

FIG. 4. Two-body correlation functions. Atom-atom (solid line) and atom-ion (dashed line) two-body correlation function $g_2(r)$ obtained from ~~VMC~~ variational Monte Carlo calculation for $N = 500$ atoms (upper curves) and $N = 50$ atom (lower curves) for $a_{\rm ai} = R^\star$; $g_2(r)$ in a weakly interacting Bose gas in absence of the ion is shown with a green line. The critical number of atoms $N_{\rm c}$ which can be trapped by an ion is larger than the number of particles for $N = 50$, which explains the pronounced maximum observed in the red lines at distances of the order of the ion potential range, $r \approx R^\star$. The data is shown up to the half-size of the simulation box $L/2$ and as a result the data with $N = 50$ abruptly stops without yet reaching a plateau. Instead, for $N = 500$ particles, the number of atoms is larger than the critical number $N_{\rm c}$ and the half-size of the simulation box $L/2$ is larger than the size of the many-body bound state. As a result the long-range plateau observed for $N = 500$ atoms signals presence of a homogeneous gas of atoms.

Let us finally briefly discuss the dynamic properties of the system. In the polaronic case, the ion effective mass approaches its bare value $M^\star \approx m$ in the limit of weak attractions, whereas for stronger ones it gradually increases for the given boson-boson scattering length to the value at unitarity $M^\star \approx 6m$, which is substantially larger than the neutral impurity result $M^\star \approx 1.65m$ [39]. In the MBBS regime, $M^\star$ becomes exceedingly large. In particular, for large $E_{\rm b}$ and small N we find that $M^\star \approx N_{\rm c} m$ and the total energy is given by Eq. (5). We could not verify whether the relation $M^\star \approx N_{\rm c} m$ holds in the thermodynamic limit due to computational limitations.

Discussion

Our calculations are focused on the ground state properties of the system. Furthermore, we have assumed that the two-body ion-atom potential only supports one or

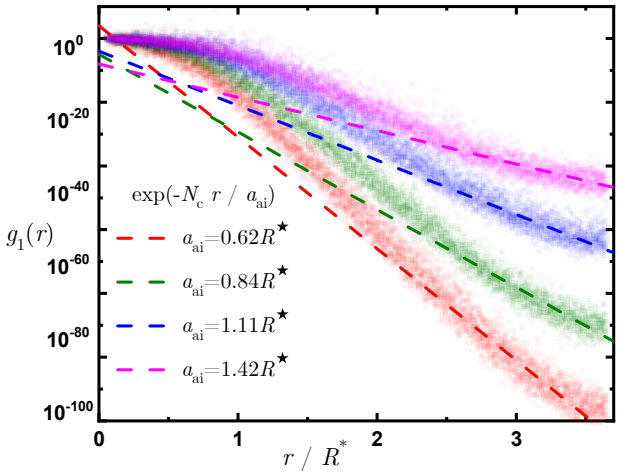

FIG. 5. Residue function of the ion impurity showing an exponential decay in the ~~MBBS for $N = 50$ atoms~~many-body bound state. The symbols show the extrapolated ~~value from VMC and DMC calculations~~values of the residue $g_1(r)$; the lines show the analytical approximation in terms of a decaying exponent, Eq. (7). Different values of the atom-ion s-wave scattering length are obtained by fixing $b = 0.0023R^\star$ and by changing c in the ion-atom interaction potential. Simulation is done for $N = 50$ atoms. Extrapolation procedure based on combining variational and diffusion Monte Carlo data is used to minimize bias on the choice of the trial wave function.

zero bound states, while a realistic interatomic potential typically features hundreds of vibrational levels, similar to the potentials with van der Waals tails describing the interactions between neutral atoms. For the latter, however, the occupation of bound states of the interatomic potential is less likely for typical quantum gas densities, unless the system is tuned close to a Feshbach resonance, since the spatial range of the potential is on the order of a few nms, and therefore it can be well described by a pseudopotential. This is not the case for the atom-ion system, whose spatial range of the polarisation potential is tens of times larger. A natural question is then the experimental relevance and the prospects for observing the phenomena we have described.

The main process stemming from the existence of deeply bound states is the three-body recombination, which will inevitably lead to losses, as it also does for neutral Bose polarons. The timescale for such losses can be estimated with the classical trajectory result for the three-body recombination rate constant ~~$K_3 \simeq 2.51[\alpha^5/m^2/(k_B T)^3]^{1/4}$~~, which can be expressed as $K_3 \simeq 12.52\frac{\hbar}{m}(R^\star)^4(E/E^\star)^{-3/4}$ and the decay rate given by $\gamma = K_3 n^2$ [54, 55]. ~~Here, the static polarizability of the atom, α, is connected to the dispersion coefficient as $C_4 = \frac{\alpha e^2}{2}\frac{1}{4\pi\epsilon_0}$ with e being the electron charge and ϵ_0 the vacuum permittivity. While for thermal gases~~ While for a thermal gas with density $n = 10^{12}\text{cm}^{-3}$ and collision energies of the order of a milikelvin this gives lifetimes of the order of a second (with $\gamma \approx 2.4\,\text{Hz}$), an ion in a high density BEC is subject to much stronger losses ~~. We~~ (for $n = 10^{14}\text{cm}^{-3}$ at 1μK $\gamma \approx 140\,\text{kHz}$). This leads to submilisecond time scales, which nevertheless are sufficient to observe ion dynamics in experiments [19]. For our gas parameter $\gamma \approx 600\,\text{Hz}$ while the characteristic energy $E^\star/\hbar = 1646\,\text{Hz}$. We further note that the quantum three-body recombination involving an ion is still not fully understood and may deviate from the classical result, e.g. it may feature minima for certain parameters (similar to loss recombination minima found for neutral atoms [56]). In particular, the dependence on the binding energy of the weakly bound state should be similar to the case of van der Waals interactions for which $K_3 \propto a_{ai}^4$.

For sufficiently small loss rates~~the signature of the formation of the polaron and~~, experimental detection of the signatures of the many-body bound state ~~can be observed in experiment in which the ion is slowly dragged through the gas due to~~ formation can be realized e.g. by injecting the ion into a cold gas and dragging it slowly using an external electric field, as has been done in [19]. The response of the impurity and the measured time of arrival at the detector will then be mainly determined by the dramatically increased effective mass of the impurity. ~~High~~ Moreover, one can use precise *in situ* imaging techniques with high spatio-temporal resolution ~~enabling these measurements, as well as the observation of the~~ such as the setup based on charged particle optics [57] to study the increase in the gas correlation functions due to the presence of the ion which would provide further information about MBBS formation dynamics~~can be provided~~. Radiofrequency and microwave spectroscopy developed for neutral gases can be used here as well, in particular to investigate the polaronic branch. Finally, quenching protocols in which one makes use of the ion hyperfine structure can be implemented. Taking advantage of the existence of Feshbach resonances, one can transfer an initially noninteracting ion to a superposition state with vastly different scattering lengths and perform Ramsey spectroscopy [58, 59] to determine e.g. ~~by means of recently developed charged-particle optics setup [?]~~ the quasiparticle weight. We note that most of these techniques still require some experimental progress in reaching sufficiently low temperatures to increase the interaction times and the number of partial waves involved.

In conclusion, we have investigated the ground-state properties of an ion immersed in a dilute Bose gas by means of Quantum Monte Carlo and Bogolyubov techniques. We identify three physically different regimes in the many-body system depending on the presence of the bound state in the atom-ion scattering problem: (i) polaronic branch, two-body bound state is absent;

(ii) many-body bound-state (MBBS) branch, two-body bound state is present; (iii) unitarity, at the threshold of the appearance of the bound state. In the polaronic branch, many-body dressing leads to formation of a quasiparticle (ionic polaron). In the limit of weak interactions, variational methods developed for neutral atomic polarons accurately predict the energy of the system. Close to the unitarity limit the calculations unveil strong deviations from the approximate results. Finally, the MBBS branch is characterized by the formation of a large cluster (consisting of hundreds of atoms) around the ion, which in this case possesses a large effective mass, thus providing a strong analogy between the MBBS and a localized state. These quite distinct regimes should give rise to different timescales in the impurity dynamics observed in experiment, especially when combined with Feshbach resonances that allow for tuning the position of the last bound state [60]. Our results highlight the ~~crucial~~ important role of the interatomic interactions which are strongly enhanced in the proximity of the ion, driving the system away from the weakly interacting regime to a non-trivial state characterized by the interplay of long-range interaction and high local density. Apart from the atomic gases, these findings can be relevant to condensed matter systems such as electron-doped exciton gases in heterostructures of two-dimensional semiconductors, where the long-range electron-exciton interaction also has long-range character which cannot be neglected for typical experimental parameters [61].

Methods.

Values of the parameters of the regularized potential. For the sake of numerical convenience we employed in our Monte Carlo simulations the regularized atom-ion potential (3) of the main text. We only considered a few specific values of the pair (b, c) that are characteristic of the three regimes outlined in the diagram of Fig. 1 of the main text: weak-coupling Bose polaron (WCP), many-body bound state (MBBS), and strong-coupling Bose polaron (SCP). In table I we list those values in units of $R^\star$ and $E^\star$.

Trial wave functions for the Monte Carlo simulations. The trial wave functions are written as a pair product of Jastrow functions for both atom-atom and atom-ion correlations, featuring appropriate short and long-range asymptotic behavior [see Eq. (4) of the main text].

The short-range part of both the atom-atom and atom-ion Jastrow function is taken from the lowest energy solution of the two-body scattering problem

$$-\frac{\hbar^2}{2m_{\rm r}}\nabla^2\psi(\mathbf{r}) + V^r_{\rm ai}(r)\psi(\mathbf{r}) = E\psi(\mathbf{r}), \tag{8}$$

where $V^r_{\rm ai}(r)$ is the corresponding interaction potential of Eq. (3) of the main text and $m_{\rm r}$ is the reduced mass. For the atom-atom wave function we choose scattering states with energy $E = 0$, whereas for the atom-ion wave function we use the exact two-body bound state with energy $E_{\rm b}$ when a bound state is present.

$a_{\rm ai}$ $[R^\star]$	b $[R^\star]$	c $[R^\star]$	$E_{\rm b}$ $(m = M)$ $[E^\star]$	Regime
-1.0	0.0023	0.1511	-35	MBBS
0.1	0.0033	0.1847	-9.0	MBBS
0.9	0.0200	0.2256	-1.6	MBBS
10	0.0858	0.2910	0.0	MBBS
97	0.0846	0.3034	0.0	SCP
1086	0.0903	0.3044	0.0	SCP
-1.1	0.0023	0.4738	NBS	SCP
-0.2	0.0023	0.9070	NBS	WCP

TABLE I. Parameters of the regularized atom-ion interaction potential. Parameters b and c of the regularized atom-ion interaction with corresponding ~~3D~~ three-dimensional s-wave atom-ion scattering length, $a_{\rm ai}$, at zero-energy and energy of ~~the uppermost energy level $E_{\rm b}$, i.e. the most loosely~~ bound state. NBS means no bound state is supported. The acronyms in the last column refer to: many-body bound state (MBBS); strong-coupling polaron (SCP); weak-coupling polaron (WCP). Close to unitarity the sensitivity of the b and c parameters is higher and therefore more digits are provided. The length and energy scales $R^\star \equiv \sqrt{mC_4/\hbar^2}$ and $E^\star \equiv \hbar^4/(m^2C_4)$, respectively, are defined with respect to $m_{\rm r} = m/2$, i.e. equal atom and ion masses.

The long-range (large distance) part of the Jastrow term is taken from hydrodynamic theory. As shown by Reatto and Chester in Ref. [62], if phonons are the lowest-energy excitations in the system, the long-range behavior of the many-body wave function can be factorized as a pair-product of Jastrow functions.

The atom-atom potential $V_{\rm aa}$ in Eq. (2) of the main text is modelled by a repulsive soft-sphere potential: $V_{\rm aa}(r) = V_0 > 0$, for $r < R_{ss}$ with $R_{ss} = 0.1R^\star$ and zero elsewhere. The height V_0 is chosen to reproduce the desired value of the s-wave atom-atom scattering length $a_{\rm aa} = 0.02R^\star \ll R^\star$. We further choose the density $n(R^\star)^3 = 0.1288$, resulting in gas parameter $n(a_{\rm aa})^3 = 10^{-6}$.

Mean-field estimate of the effective mass and critical number. In order to formulate a self-consistent mean-field theory in the ion's frame of reference, the following wave function can be used [27]

$$\Psi_{\rm G}(\mathbf{R}, \mathbf{k}; \mathbf{r}_1, \ldots, r_N) \propto e^{i\mathbf{k}\cdot\mathbf{R}} \prod_{n=1}^{N} f(\mathbf{r}_n - \mathbf{R}) e^{is(r_n - R)}. \tag{9}$$

Here, $\mathbf{k}$ is the ion momentum, f^2 the relative probability distribution of the position of the ion and the bosons, while $\nabla_{\mathbf{r}} s(\mathbf{r} - \mathbf{R})$ indicates the fluid velocity relative to the ion. Performing functional variation of the expectation value of the Hamiltonian (2) of the main text, one obtains the ion effective mass [27, 63]:

$$\frac{M^\star}{m_{\rm r}} = 1 + \frac{M}{M + m_{\rm r}} \frac{R_\mu}{R_0} 4\pi R_\mu^3 n. \tag{10}$$

Here, R_0 is a hard-core radius physically meaning the distance at which the atom-ion interaction starts to deviate from its long-range $\frac{C_4}{r^4}$ asymptote. Typically $R_0 \sim 10\,a_0$ with $a_0 \simeq 53$ pm being the Bohr radius. Furthermore, the distance R_μ is defined as $|V_{\rm ai}(R_\mu)| = \mu$ with $\mu = gn$ the chemical potential of the bosons, from which we get

$$R_\mu = R^\star \left(\frac{E^\star}{\mu}\right)^{1/4}. \tag{11}$$

For the pair ^{87}Rb/^{87}Rb$^+$ with an atomic density $n = 10^{14}$ cm^{-3} we obtain $R_\mu \simeq 1.2R^\star \simeq 6061a_0$. Given this, the formula (10) predicts an effective mass $M^\star \simeq 8.4 \times 10^3\, M$. Thus, the critical number of bosons bound to the ion can be estimated as: $N_{\rm c} = M^\star/m - 1$ with $M^\star$ given by Eq. (10) and $M = m$.

Another estimate of $N_{\rm c}$ can be attained via rate and Gross-Pitaevskii equations [20]. Denoting the binding energy of the two-body bound state as $E_{\rm b} = -\hbar^2/(2m_{\rm r}a_{\rm ai}^2)$, it can be shown that in the presence of many weakly interacting bosons $E_{\rm b}(N_{\rm b}) = E_{\rm b}[ma_{\rm ai}/(6m_{\rm r}a_{\rm aa}N_{\rm b})]^{2/3}$. At thermal equilibrium one would expect that

$$|E_{\rm b}(N_{\rm c})| = k_{\rm B}T \;\;\Rightarrow\;\; N_{\rm c} = \frac{1}{6}\frac{m}{m_{\rm r}}\frac{a_{\rm ai}}{a_{\rm aa}}\left(\frac{E_{\rm b}}{k_{\rm B}T}\right)^{3/2}. \tag{12}$$

For the pair ^{87}Rb/^{87}Rb$^+$ with $a_{\rm ai} = R^\star$ (i.e. $E_{\rm b} \equiv E^\star$), $a_{\rm aa} = 100\,a_0$, and $T = 10\,$nK ($\ll E^\star/k_{\rm B}$), we obtain a critical number of $N_{\rm c} \simeq 372$. This number is much smaller than the previous estimate (10), but also does not agree with our numerical simulations. Moreover, our study predicts that $N_{\rm c}$ emerges already at zero temperature. Thus, it is not only determined by charge hopping and thermal fluctuations, but also by interaction-induced correlations. Finally, the formula (12) predicts a reliance on the atom-ion scattering length as $a_{\rm ai}^4$, while our many-body analysis [see Fig. 2(a)] shows that there is almost no dependence on that length parameter. This finding highlights once more how semi-classical estimates can be quantitatively erroneous.

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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