Charged impurities in a Bose-Einstein condensate: Many-body bound states and induced interactions

Grigory E. Astrakharchik¹,*, Luis A. Peña Ardila²,†, Krzysztof Jachymski³, and Antonio Negreitti⁴

¹Department de Física, Universitat Politècnica de Catalunya, Campus Nord B4-B5, E-08034, Barcelona, Spain
²Institut für Theoretische Physik, Leibniz Universität Hannover, Appelstr. 2, 30167 Hannover, Germany
³Faculty of Physics, University of Warsaw, Pasteur 5, PL-02093 Warsaw, Poland
⁴Zentrum für Optische Quantentechnologien, Fachbereich Physik, Luruper Chaussee 149, D-22761 Hamburg, Germany

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We investigate the static properties of one and two ionic impurities immersed in a bosonic atomic bath at zero temperature using ab initio many-body quantum Monte Carlo methods. We identify three bipolaronic regimes depending on the strength of the atom-ion potential and the number of its two-body bound states: a perturbative regime resembling the situation of a pair of neutral impurities, a non-perturbative regime that loses the quasi-particle character of the former, and a many-body bound state regime. The first two occur in the absence of a bound state that characterizes the two-body atom-ion scattering. The scattering length is varied from small to large values compared to the spatial range of the atom-ion potential. Instead, the latter regime requires the presence of a two-body atom-ion bound state. We study the bipolaron in the three regimes as a function of their spatial separation by inspecting the energy, atom-ion correlation functions and the bath-induced interactions among the two ionic polarons. We show that for strong interactions, large density modulations of the gas induced by the impurities highly affect the form of the induced interaction between them. Our findings show that numerical simulations are indispensable for describing highly correlated impurity models for which the pseudopotential approximation cannot be made. Our study also confirms that atom-ion systems exhibit properties that have no counterparts in neutral atomic mixtures, thus opening exciting perspectives to study mediated interactions with novel features. Finally, our results provide additional insight into quantum information processing protocols based on compound systems with long-range impurity-bath interactions.

I. INTRODUCTION

Compound systems consisting of impurities immersed in a quantum medium are of fundamental importance in quantum many-body physics. A few relevant examples in the solid-state realm are the Kondo effect [1], transport of heavy impurities in a Fermi liquid [2], and pair formation [3, 4]. Dressing the impurity particle with the low-energy excitations of the medium can lead to the emergence of a new quasi-particle called the polaron. Its physical realization in ultracold atomic setups offers a unique opportunity to dynamically control the system’s parameters such as the interaction strength. Atom-ion quantum systems [5–7] hold the promise to study polaron physics in the so-called strong-coupling limit [8], owing to the long-ranged character of the two-body impurity-bath interaction. Furthermore, ionic impurities are an excellent platform for studying transport phenomena, as the charge can be easily detected and dragged with an external electric field [9]. In contrast to the neutral case, novel transport properties due to macroscopic atomic dressing of the ion can be expected [10]. Other quantum ion-atom-based simulation ideas include, e.g., the formation of lattice bipolarons with low effective mass [11] and ion-induced interactions in Tomonaga-Luttinger liquids [12]. A few experimental groups have recently attained the ultracold collisional regime in radio-frequency traps [13, 14]. At the same time, ions are created in an ultracold gas by ionization of selected atoms from the bath [15–17] and their transport properties have been investigated [9].

Since the first observation of a single ion in a radiofrequency trap [18], trapped ions have proven to be an excellent testbed to verify predictions of quantum theory as, e.g., quantum jumps [19, 20] and the Zeno effect [21], but also to trigger various fields of research and technology such as atomic clocks, quantum computation and simulation [22, 23]. Nowadays, tens of ions can be isolated and individually manipulated to implement quantum computing schemes and simulate spin models. Quantum circuits based on one- and two-qubit gates are routinely accomplished in laboratories [24, 25]. Ion logic gates usually require the ions to be sufficiently cold to ensure that the vibrational quantum number $n$ satisfies the condition $\eta \sqrt{n+1} \ll 1$, where $\eta$ is the Lamb-Dicke parameter. With the increasing complexity of the algorithms and thereby with the increasing number of gates, this condition becomes harder to meet as the ions will inevitably be heated by the applied laser pulses. A possible solution to this issue is to use another quantum system as a coolant such that the ions are kept sufficiently cold to ensure fault tolerance. Here, atom-ion quantum mixtures are a prominent candidate since ultracold gases easily reach sub-μK temperatures. Theoretical studies have shown that cooling of ions to the $s$-wave regime in the presence of micromotion can be made efficient by choosing a large ion-to-atom mass
ratio [26–28]. Such studies, however, do not take into account the possibility of the formation of many-body bound states [29–32], whose occurrence substantially affects the properties of the mixture.

Motivated by experimental progress in the realization and control of atom-ion quantum mixtures as well as their relevance in the context of quantum simulation [11, 33, 34], quantum transport [35–38], as well as applications in quantum information processing [39, 40] and thermometry [41], we investigate here the ground state properties of two ions in a bosonic bath. In Sec. II we outline the most important results of our study and discuss their relevance in connection to the existing literature. In Sec. III we introduce the model that describes our impurity system together with a brief overview of the used simulation methods. In Sec. IV we present our findings, while in Sec. V we discuss their experimental relevance and how our results could be observed in experiments. Finally, in Sec. VI we recap the key aspects of our study and present an outlook for future analyses.

II. MOTIVATION AND SUMMARY OF THE MAIN RESULTS

In our previous study [31], we investigated the polaronic properties of a single ion immersed in a bosonic bath. We found three physically different regimes depending upon the presence of a two-body atom-ion bound state: a polaronic regime when no two-body bound state is present; a many-body bound-state (MBBS) regime when a two-body bound state is supported; and the unitary case at the threshold of the occurrence of a bound state. The first regime concerns many-body dressing where the system is well described by a particle dressed by the low-energy excitations of the gas, similar to the neutral case, yet with a slightly larger effective mass – roughly six times the mass of the bath atom. On the other hand, significant deviations from this behavior are found when approaching the unitary limit. Instead, the MBBS regime is characterized by forming a large cluster – consisting of hundreds of atoms – around the ion with a large effective mass, proportional to the number of bound bosons. This study has shown that atom-ion mixtures exhibit distinct features that have no counterpart in settings with neutral impurities [42–45]. At the same time, it has been shown that the identified polaronic states cannot be described by the conventional Fröhlich paradigm [8, 46, 47] or Bogolyubov theory [48–50], since the system properties rely not only on the scattering length and the effective range of the two-body atom-ion interaction, but also on its long-range tail. The findings presented in Ref. [31] can be considered as the initial step that identifies an exciting research direction: by means of numerical ab-initio many-body simulations, we characterized the key ground state properties of ionic polarons such as their energy, effective mass, and particle residue. Due to the rapid experimental progress, the detection of these quantities is promising in state-of-the-art experiments. We refined the observations based on semi-classical or mean-field models [10, 29], while showing that these methodologies are not sufficient to describe the many-body ground state. For example, renormalization group techniques [51, 52] and diagrammatic methods [53] that fundamentally rely on the Bogolyubov approximation was very successful for neutral impurity systems outside of the strong coupling limit. The formation of an ion MBBS, however, renders the bath density highly inhomogeneous and thus the Bogolyubov approximation has limited applicability. Ab-initio many-body simulations are thus an indispensable tool to account for spatial inhomogeneities as well as strong impurity-bath correlations [54], especially when the polaron residue is far from unity. Because of this and as we demonstrate in this work, the application of field theoretical methods [32, 55] based on ladder approximation is limited to very short times after immersion of the ion in the medium, when the background gas density is constant. On the other hand, approaches based on multi-configurational Hartree methods [56, 57], extensions of Bogolyubov theory and Monte Carlo calculations [58, 59] have been proven to be powerful tools for simulating the static and out-of-equilibrium dynamics of one-dimensional atom-ion systems [30, 60, 61]. However, since the atom-ion polarization potential is intrinsically three-dimensional even for tight axial confinement [62], the extension of those methods to higher spatial dimensions with the large particle numbers and in the presence of multiple energy and length scales – as it is the case for atom-ion systems – is still challenging.

Given this, here we rely on quantum Monte Carlo techniques as in Ref. [31], and we systematically study a model system consisting of one or two ions interacting with a bosonic bath. A timely question is to explore mediated interactions between the impurities and understand to what extent analytical approaches effectively describe them. The interaction between quasi-particles is not only crucial for conventional and high-\(T_c\) superconductivity [3, 63], but it is also instrumental for developing quantum technologies with compound atom-ion systems such as quantum sensors [41, 64, 65] and hybrid interfaces for information processing [39, 40]. Let us consider a concrete and technologically relevant example in this regard. Trapped ions are one of the leading platforms for implementing a quantum computer since they feature high gate fidelities [66, 67]. One of the principal disadvantages of the trapped-ion system is its coupling to flying qubits, which is essential to construct quantum repeaters for entanglement distribution over large distances [68]. Indeed, the cross-section for photon absorption of a two-level atom in free space is proportional to \(\lambda^2\), i.e. is defined by the wavelength \(\lambda\) of the incident light [69]. Since ions in a Paul trap
can be separated from a few to some tens of μm, it is improbable that a single ion can absorb a photonic qubit in the visible range. In order to enhance the probability of absorption, one can either confine ions in an optical cavity or immerse them in a dense medium such as a cold atomic gas. The latter increases the absorption cross-section [70], creating a spin-wave excitation in the medium, which can be transferred from the atomic ensemble to the ion(s) for further processing via a laser-controlled atom-ion coupling [40].

To develop such technologies, however, it is of paramount importance to understand the many-body properties of the compound system and our investigations point precisely in this direction. Specifically, we find that the presence of the bosonic bath induces an effective attractive interaction between the ions. By treating the ions statically, we assume that they are either tightly trapped or have a much larger mass than the bosons—a plausible scenario for trapped ions. We analyze the properties of the system as a function of their spatial separation, the magnitude of the atom-ion scattering length and its sign. Depending on the details of the two-body atom-ion interaction and analogously to our single-ion study [31], we identify three regimes:

(i) a perturbative (weak-coupling) regime;
(ii) a non-perturbative (strong-coupling) regime;
(iii) a many-body bound state regime.

These regimes are illustrated pictorially in Fig. 1. The weak-coupling regime, namely Fig. 1(a), corresponds to the scenario in which the ion-induced density perturbation of the bath is small compared to the bath density at large distances from the ions, and therefore it can be treated perturbatively. In the ionic setting, the coupling strength is parametrized by $k_n |a_{ai}|$, where $a_{ai}$ is the three-dimensional atom-ion s-wave scattering length and $k_n = (6\pi^2n)^{1/3}$ is the characteristic momentum related to the bath density $n$. Even though $k_n |a_{ai}| \ll 1$, the impurity-bath interaction cannot be considered as a weak perturbation, akin to the neutral atomic impurities since the long-range part of the potential is always present and makes a crucial difference. Indeed, as we showed in Ref. [31], albeit in that situation the quasi-particle picture for a single ion holds, the effective mass is larger than for a neutral impurity as a consequence that a zero-range potential cannot describe the impurity-bath interaction. In the weak-coupling, we compare our many-body simulations for the induced interactions with the analytical results of Ref. [55], and find qualitatively similar behavior. The analytic theory assumes the validity of the Bogolyubov approximation for the condensate and neglects the contribution of the ion-atom bound states, taking into account only the exchange of phonons, while our theory does not rely on perturbative assumptions.

In the neighbourhood of the ion(s), we find large density modulations, as shown by atom-ion correlation functions [cfr., e.g., panels (b) of Fig. 3 and Fig. 4] and depicted illustratively in Fig. 1(b). We refer to this situation as the non-perturbative regime (ii).

Finally, in the regime (iii) the situation changes drastically because of the appearance of a two-body bound state in the atom-ion polarization potential. Here, a so-called many-body bound state with hundreds of atoms is formed, a peculiarity of the compound atom-ion system. When two of such ionic polarons are present, the nature of their interaction changes substantially. In Fig. 1 (c) we show the situation pictorially. Here, close to
FIG. 2. Atom-ion interaction potentials used in the many-body simulations. Red solid line — weakly-attractive model potential with no hard core; green dashed line — potential with a small negative scattering length leading to the absence of atom-ion bound states ($a_{ai} = -0.01R^*$); blue dash-dotted line — potential with a large negative scattering length ($a_{ai} = -0.1R^*$) leading to the absence of an atom-ion bound state; magenta dash-dot-dot line — potential with a positive scattering length leading to the presence of an atom-ion bound state $a_{ai} = R^*$.

The first term represents the kinetic energy of the bosonic atoms of mass $m$, whereas $V_{aa}(r_n - r_j)$ denotes the repulsive short-range atom-atom potential. The second term in Eq. (1) describes the two-body atom-ion polarization potential, which possesses a long-range tail:

$$\lim_{r \to \infty} V_{ai}(r) \to -\frac{C_4}{r^4}. \quad (2)$$

It is characterised by the length $R^* = (2m_iC_4/\hbar^2)^{1/2}$ and energy scales $E^* = \hbar^2/[2m_i(R^*)^2]$, where $m_i = m_iM/(m + M)$ is the reduced atom-ion mass ($m_i = m$ for infinitely heavy impurities). As an example, for the pair $^{23}$Na/$^{174}$Yb$^+$ we have $R^* \simeq 129.85$ nm and $E^* \simeq k_B \times 0.71 \mu K$ ($k_B$ is the Boltzmann constant). For an atomic density $n = 6 \times 10^{13}$ cm$^{-3}$, the mean interparticle distance scales as $n^{-1/3} \simeq 2R^*$, whereas the gas healing length $\xi = (8\pi n a_{bb})^{-1/2} \simeq 4R^*$ with $a_{ab}$ being the three-dimensional s-wave boson-boson scattering length, set by the gas parameter $n a_{bb}^3 = 10^{-6}$. As these lengths are all comparable, there is no separation of scales, and therefore short-range pseudopotentials cannot be used to replace the polarization potential, thus requiring the theory to take into account the atom-ion interaction potential explicitly, and restricting the predictions of Bogolyubov theory to a limited range, $R^* < r < \xi$. We model this interaction by the regularized potential [27]

$$V_{ai}^r(r) = -C_4 \frac{r^2 - c^2}{r^4 + c^4 \left(\frac{b^2 + r^2}{2}\right)^2}. \quad (3)$$

This choice of the interaction potential has the benefit of retaining the long-range tail while also having a hardcore part and a simple form convenient for numerical and analytical calculations. As we are aiming for computing the ground state of the system, we choose to work in the range of parameters where the potential supports at most one bound state. This usually requires choosing rather large values of either the $b$ or $c$ parameter as compared to $R^*$. In the following, we assume that the ions are static, i.e., they act as scattering centers for the bosons, and their separation is given by $|\mathbf{R}_1 - \mathbf{R}_2| = R$. Such a scenario is realized when heavy ions confined in a linear Paul trap are in interaction with light atoms. In connection to studies with a similar setup, we note that the one-dimensional band structure of an atom in a potential landscape generated by a chain of equidistant static ions has been studied and solved analytically in Ref. [73], while analytical Green functions for an atom in a potential of static impurities with an arbitrary spatial configuration, whose atom-impurity interaction is described by a regularized pseudopotential, have been obtained in Refs. [74, 75]. The latter can be used to benchmark results based on short-range impurity-bath interactions. Since the ions are static, we omit the direct Coulomb interaction between them as well as their trapping potential. In a radiofrequency trap, the equilibrium positions of the ions along the crystal axis, say the $x$-axis, are approximately given by $\mathbf{R} \simeq \alpha N_i \ell$

III. MODEL SYSTEM AND METHODS

System. The compound atom-ion system consisting of $N$ atoms and $N_I$ pinned impurities is described by the following many-body Hamiltonian [72]:

$$\hat{H} = \sum_{n=1}^{N} \left[ -\frac{\hbar^2 \nabla_{r_n}^2}{2m} + \sum_{j=1}^{N_I} V_{ai}(r_n - r_j) \right] + \sum_{n < j}^{N} V_{aa}(r_n - r_j). \quad (1)$$
with \( \epsilon^3 = e^2/(4\pi \epsilon_0 M \nu^2) \) and \( \alpha_{N_I} \) being a numerical factor that depends on the number of ions \( N_I \) [76]. For large \( N_I \), it can be approximated as \( \alpha_{N_I} = 2.018/N_I^{0.559} \). Specifically, for two ions, we have \( R \approx 1.266 \). For \( R = 1 \) \( \mu \)m and two \(^{174}\)Yb\(^+\) ions a trap frequency of \( \nu = 2\pi \cdot 6 \) MHz is required, while for 20 ions with approximately the same separation \( \nu = 2\pi \cdot 1 \) MHz is needed.

**Numerical method.** We employ the diffusion Monte Carlo method which computes the ground state energy of Hamiltonian (1) by propagating the many-body Schrödinger equation in imaginary time. The boson-boson interaction is modelled by soft-spheres with a diameter \( R_{SS} \) small as compared to the atom-ion range, i.e., \( R_{SS} = 0.1R^* \), whereas the height is adjusted to have a small value of the three-dimensional \( s \)-wave scattering length \( a_{bb} = 0.02R^* \). The guiding wave function is written in a pair product form \( \Psi = \prod_{i<j} f_{BB}(r_{ij}) \prod_{i,a} f_{BI}(r_{ia}) \), similarly to the one used in Ref. [31]. It consists of boson-boson and boson-atom Jastrow pair-product terms, each one constructed in such a way that the two-body scattering at small distances matches the phononic long-range asymptotic [77]. Specifically, calculations are performed for \( N = 200 \) bosons in a box with periodic boundary conditions and with \( N_I = 2, 1, 0 \) ions. We consider dilute densities with the gas parameter equal to \( n a_{bb}^3 = 10^{-6} \). In that case the atomic chemical potential is small as compared to the typical ion energy, \( \mu_{ab} = 4\pi\hbar^2 n a_{bb}^3/m = 0.0314E^* \), and the healing length is larger than the characteristic interaction length, \( \xi = 4R^* \).

The energy shift due to the interaction between two ionic polarons mediated by the bath is computed as
\[
E_{pol-pol} = E(N; 2) - 2E(N; 1) + E(N; 0),
\]
where \( E(N; N_I) \) denotes the ground-state energy of the system containing \( N \) atoms and \( N_I \) ions. In the case of neutral impurities, this value is on the order of the single polaron energy \( E_n = \frac{\pi^2}{2m} (6\pi^2 n)^{2/3} \sim E^* \) for very large values of \( n \) of the neutral impurity-boson scattering length \( a_{ab} \). The induced interaction is attractive regardless the sign of \( a_{ab} \) [32] as well as for the case where a two-body bound-state for \( a_{ab} < 0 \) does not exist. For the atom-ion compound system we consider both two-body bound and scattering states.

**IV. RESULTS**

In this section, we present our findings. We first note that the induced interactions between two ions have been studied in Ref. [55] within the framework of perturbation theory. We compare our numerical simulation results with the aforementioned work’s predictions and discuss the limits of the applicability of both approaches. As outlined in the summary II, we shall analyze each regime separately, while at the end of the section, we shall discuss them in connection to other systems.

**A. Analytical expressions**

In Ref. [55], the regularized potential (3) has been utilized to predict induced ion-ion interactions. There, the impurity-bath interaction in second quantization is described by
\[
V_{ib}(\mathbf{R}) = \sum_{k,q} V_q \hat{c}^\dagger_k \hat{c}^\dagger_{k+q} \hat{c}_k (1 + e^{-i\mathbf{q} \cdot \mathbf{R}}),
\]
where \( \mathbf{R} \) denotes the separation among the two ions, \( V_q \) is the Fourier transform of the atom-ion potential, \( \hat{c}^\dagger_k \) \( (\hat{c}_k) \) denotes the creation (annihilation) operator of a boson with momentum \( \mathbf{k} \). The theory implicitly assumes that the boson-boson interaction is sufficiently weak to make the Bogolyubov theory applicable, i.e., \( n a_{bb}^3 \ll 1 \) everywhere with \( n \) being the local gas density. The induced interaction between ions is obtained by calculating the energy shift due to their presence in the bath. In second-order, it is given by
\[
E_2 = \tilde{E}_2 + V_{ind}(R)
\]
with \( \tilde{E}_2 \) a constant energy shift due to each ion separately and \( V_{ind}(R) \) being the bath-induced interaction. For large distances, i.e., \( R \gg b, c, \xi \), it can be shown that
\[
V_{ind}(R) = \frac{V_q=0}{2\pi \hbar^2 a_{bb}} \frac{m}{R^3} C_4
\]
with \( \xi = (8\pi n a_{bb})^{-1/2} \) the healing length, and
\[
V_{q=0} = -\pi^2 \left( \frac{R^*}{b} \right) \left( \frac{b^2 + 2bc - c^2}{(b + c)^2} \right) E^*(R^*)^3.
\]
By substituting (8) into Eq. (7) we obtain
\[
V_{ind}(R) = -\frac{\pi}{4} \left( \frac{R^*}{a_{bb}b} \right) \left( \frac{b^2 + 2bc - c^2}{(b + c)^2} \right) \left( \frac{R^*}{R} \right)^4 E^*.
\]
The interaction (7) has the same dependence on the distance as the atom-ion polarization potential (2), but with varying sign which can be tuned by choosing proper combinations of the parameters \( b \) and \( c \). Due to its long-range power-law decay, we will refer to it as Casimir interaction. Instead, in the short distance limit, namely when \( b, c \ll R \leq \xi \), the bath-induced interaction becomes
\[
V_{ind}(R) = -\frac{\pi^3}{2} n(R^*)^3 \left( \frac{R^*}{b} \right)^2 \left( \frac{b^2 + c^2}{(b^2 - c^2)^2} \right) \times \exp \left\{ -4\sqrt{\pi} n(R^*)^3 a_{bb}/R^* \right\} E^*,
\]

where \( n \) is the local gas density, \( n \equiv \langle n \rangle \).
which has the form of a Yukawa interaction that is also obtained for neutral impurities in a condensate [53, 78]. In addition to this, Ref. [55] shows that for strong atom-ion interactions, e.g., close to a Feshbach resonance, the induced interaction retains the form of Eq. (7) with \( V_{ij} \) replaced by the atom-ion scattering \( T \)-matrix at zero momentum and energy.

**B. Weak-coupling regime**

The weak coupling regime is commonly associated with small values of the scattering length as compared to the inter-particle distance. This typically corresponds to a situation in which the energy shifts are small and the impurities only slightly distort the shape of the host gas.

An important feature of our treatment of the ion impurity is that even for small values of the scattering length, \( a \) polaron-polaron induced interaction obtained for a small value of the atom-ion scattering length, \( a_{ai}/R^* = -0.01 \).

In order to test the correctness of the analytic expressions for induced polaron-polaron interactions in the perturbative regime such that assumptions of both methods match each other, we perform calculations for the following parameter of the model atom-ion potential (3), \( C_4 = E^* \alpha R^4 \), \( b = R^* \), \( c = 1.115R^* \). While such a choice of parameters leads to no hard-core part of the interaction, the resulting potential (shown with a red line in Fig. 2) is not perturbing the bath of atoms too strongly, and therefore the weakly-interacting polaron regime is realized. Figure 4 shows the induced polaron-polaron interactions in the perturbative regime and the polaron density profile. A reasonable agreement with the analytical predictions is found for the induced interactions.

In order to test the correctness of the analytic expression for the induced polaron-polaron interaction between two polarons.

![Diagram showing induced polaron-polaron interaction and single polaron density profile](image)

FIG. 3. Induced polaron-polaron interaction and single polaron density profile (for a static ion directly reflected by the ion-atom correlation function) as a function of their separation for a small value of the atom-ion scattering length, \( a_{ai}/R^* = -0.01 \).
weakly interacting polaron regime: \( C_i = E_i^* R_i^* \), \( b = R_i^* \), \( c = 0 \)

FIG. 4. (a) Induced polaron-polaron interaction and single polaron density profile for the case of a perturbative potential \( b = 1 \), \( c = 0 \). Symbols: results of QMC calculation, black dash-dotted line: polaron chemical potential, black dash-dot-dotted lines: two polaron chemical potentials, blue long-dashed line, Yukawa potential (10) applicable at intermediate distances; green short-dashed line, Casimir potential (9) applicable at large distances. (b) Polaron density profile as obtained from QMC calculations.

\[ C_i = E_i^* R_i^* \], \( b = R_i^* \), \( c = 0 \)

FIG. 5. Density profiles projected onto a line denoted by the \( x \)-axis connecting two impurities in the regime of weak interactions (arbitrary units). Symbols: Blue squares denote the results of QMC calculations, while the solid line is a fit to the defect in the projected atom density \( n_{\text{atoms}}(x) = 1 + f_{\text{pol}}(x) \) with \( f_{\text{pol}}(x) = \Delta n + A \exp[-(r/\sigma)^p] \), where \( \Delta n, A, \sigma, p \) are fitting parameters. Panel (a): Single ion (polaron) density profile used to obtain the fit \( f_{\text{pol}}(x) \). Panels (b,c,d): Two ions (bipolaron) density profile for distances between them equal to 0, \( 2R_i^* \), \( 5R_i^* \) as compared to the prediction for two non-interacting polarons located at the same ion positions.
results in the density profiles $n_{\text{atom}}(x)$, which depend on one coordinate (denoted by $x$) as shown in Fig. 5 for characteristic distances between the two ion impurities. While the actual amplitude of $n_{\text{atom}}(x)$ depends on the integration volume and hence arbitrary units are used on the vertical axis, still for a fixed volume size, it is instructive to compare the shape and the height of the projected density for different atom-ion interactions.

In the case of a single impurity, shown in Fig. 5(a), there is a mild density increase around the vicinity of the polaron. Its shape can be well fitted with a Gaussian-like profile. Panels Fig. 5(a,b,c) report the bipolaron density profile for three different separations between the impurities: $r = 0, 2R^*, 5R^*$, and show the density profile of two non-interacting polarons separated by $r$. The bipolaron density profile recovers the density of two non-interacting polarons placed at large separation. This conclusion agrees with Bogolyubov’s theory in which the induced interaction is small for distances large compared to the healing length, $r \gg \xi$. On the other hand, an enhancement in the density is visible for smaller and comparable distances, elucidating the attractive character of the induced interactions between polarons. For $r = 0$ the density profile is a single pinned impurity having twice a stronger interaction strength.

**C. Hard-sphere impurity**

In order to investigate further the role of the excluded region in the atom-ion interaction potential, i.e., in the region of the barrier, we perform simulations by considering a hard-sphere potential defined as $V_{\text{HS}}(r) = +\infty$ for $|r| < a_{ai}$ and zero otherwise. The atom-ion $s$-wave scattering length $a_{ai}$ is given by the diameter of the hard-sphere. The QMC results are shown in Fig. 6. The polaron density depicted in Fig. 6(b) is completely depleted for distances $r < R^*$. This fact has several important consequences: first, for zero separation between two hard spheres, the excluded volume remains exactly the same as for a single impurity and two overlapping hard spheres, and the system energy matches with $E(N,2) = E(N,1)$. This allows to find the value of the induced interactions within the Born-Oppenheimer approximation for zero separation as $V_{\text{ind}}(r = 0) = E(N,2) - E(N,0) - 2\mu = -\mu$. Second, the amplitude of the induced polaron-polaron interaction is known exactly and it is given by the polaron chemical potential in that case. Third, the situation is clearly non-perturbative, as zero separation between two pinned impurities is equivalent to having a single impurity of double strength, $2V_{\text{ind}}(r)$. Within perturbation theory, the bipolaron shift energy is equal to two polaron shift energies, while for hard spheres, both shift energies are equal. Fourth, the Fourier transform of a hard-sphere potential is not well defined. Therefore, applying the standard Bogolyubov theory as typically used in impurity physics is not plausible. Finally, the bipolaron energy $E(N,2) - E(N,0)$ is a continuous function, which goes from $\mu$ at $r = 0$ to $2\mu$ at $r \gg \xi$, as shown in Fig. 6(a).

Typical bipolaron density profiles are presented in Fig. 7. The repulsive hard-sphere potential leads to a depletion of the density around the impurity. Let us note that for the hard-core potential, it holds $2V_{\text{HS}}(r) = V_{\text{HS}}(r)$, that is, the potential experienced by the bath is the same for both a single impurity and two impurities separated by zero distance. As a consequence, the polaron density profile [Fig. 7(a)] is exactly the same as the bipolaron density profile for $r = 0$ [Fig. 7(b)]. To a certain extent, this is the least perturbative case since the atom density is totally voided around the impurities. Notwithstanding, for a large separation $r$ between the impurities, the atom density is roughly equal to the densities of two independent polarons, signaling that the induced interactions are weak for such values of $r$.

**D. Strong-coupling regime**

A characteristic feature of ion impurities is the possibility of being realized in a strongly-interacting regime. Here, we consider a large value of the atom-ion scattering length as well as a situation in which the atom-ion interaction does not support a bound state so that the scattering length is negative. A characteristic example of the (induced) polaron-polaron interaction potential in this regime is displayed in Fig. 8. A qualitative difference with respect to the previous two regimes (i.e., weak interaction and hard-spheres) is that the polaron density profile is no longer monotonous as it acquires a peak at a distance set by the potential range $R^*$, see Fig. 8(b). Unlike the neutral polarons, the induced interaction potential also displays a non-monotonous behavior. Notably, the position of the peak in $V_{\text{ind}}(r)$ coincides with the position of the peak in the density profile. We elaborate on this effect in the following paragraphs, where it is much more evident. Note that the strong-coupling regime differs from the previous two scenarios by a larger energy shift.

**E. Unitary limit**

The most strongly interacting regime associated with $s$-wave scattering is the unitary limit in which the atom-ion scattering length diverges, $a_{ai} \to \infty$. Analytically, such a regime is challenging due to the absence of a small parameter. Thus, it is instructive to study the ion bipolaron at unitarity. Figure 9 shows the results obtained for unitary interactions. Already at the level of the single polaron case, atoms create a many-body
hard sphere interaction: $a_{\text{si}} = R^*$

FIG. 6. Panel (a): Induced polaron-polaron interaction. Panel (b): Single polaron density profile for hard-sphere interactions.

hard sphere interaction: $a_{\text{si}} = R^*$

FIG. 7. Density profiles projected onto a line denoted by $x$-axis connecting two impurities for hard spheres (arbitrary units). Symbols: Blue squares denote the results of QMC calculations, while the solid line is a fit to the defect in the projected atom density $n_{\text{atoms}}(x) = 1 + f_{\text{pol}}(x)$ with $f_{\text{pol}}(x) = \Delta n + A \exp[-(r/\sigma)^2]$, where $\Delta n$, $A$, and $\sigma$ are fitting parameters. The dashed lines represent the estimation of the density of non-interacting polarons, $1 + f_{\text{pol}}(x + r/2) + f_{\text{pol}}(x - r/2)$. Panel (a): Single ion (polaron) density profile used to obtain the fit $f_{\text{pol}}(x)$. Panels (b,c,d): Two ion (bipolaron) density profile for distance between ions equal to 0, $2R^*$, $5R^*$ as compared to the prediction for two non-interacting polarons located at the ion positions.

bound state around the impurity as signaled by the presence of a very high peak in the density profile, see Fig. 9(b). The characteristic length at which the maximum appears in the polaron density profile is set by $R^*$, and the induced ion-ion interactions have a spatial feature at that point, see Fig. 9(a). The bipolaron energy becomes an order of magnitude larger manifesting the formation of a deeply bound state which can be already understood at the single-atom level. Moreover, for large distances between the impurities resonantly interacting
with the host bath, a bound state has vanishing energy. For short separations, the potential landscape drawn by the two ions has an amplitude that is twice larger, leading to a formation of an atom-ion-ion bound state. Adding other atoms populates this bound state further, lowering the energy.

**F. Many-body bound state regime**

The situation in which an ion impurity differs the most from neutral polarons is characterized by the formation of many-body bound states. Such a regime is reached when the two-body atom-ion problem supports a bound state. The properties of the system are dominated by the presence of a many-body bound state which acquires a large population (hundreds of atoms). On the single impurity level, this is manifested by the correlation function reaching higher values than the equilibrium gas density [see Fig. 10(b)].

The effect gets weaker at larger separations as the correlation function for a single impurity drops back to lower values, and thereby the mutual response between the impurities in attracting the bosons is inhibited.

The projected density profiles in the MBBS regime are reported in Fig. 11. The polaron density becomes large, differently from the weakly interacting regime presented in Fig. 5. Even though the Bogolyubov theory no longer describes the induced interaction potential, the bipolaron density corresponds to the one of non-interacting impurities when the distance between them is large compared to the healing length, similarly to the weakly interacting regime. Instead, for small separations, the role of the induced interaction becomes crucial, as it is manifested by significant differences in the density profile between interacting and non-interacting cases.

Summarizing the results, we notice that in all the cases we studied, regardless of the scattering length value, the induced interaction turns out to be attractive. We found that the induced interactions are consistent with a power-law Casimir decay and the magnitude of interactions strongly depends on the presence of the two-body bound state.

**V. EXPERIMENTAL IMPLICATIONS**

Our results are directly connected with the physical system consisting of a chain of trapped ions immersed in a bosonic gas. The energy spectrum of such a chain, described by phonon modes, depends on the relation between the ion separation and the Coulomb interaction. The precise knowledge of phonon frequencies is crucial for implementing quantum gates. When the size of the quantum circuit grows, even small shifts such as the ones discussed here can lead to sizable errors.
We now estimate the typical phonon frequency shift from the induced interaction expected for an experimentally relevant situation. For ion separations of $\sim 1 \mu m$ ($R \approx 13 R^*$ assuming Yb$^+$-Li) the Coulomb repulsion is $E_C \approx k_B \times 16.73$ K, or $2.3 \times 10^6 E^*$, while the induced interaction is typically of the order of $1 E^*$ at such a large distance. For the case of two ions, the lowest oscillation frequency mode corresponds to the center of mass motion and is unaffected by the interaction, but the second one can be tuned [76]. One can easily calculate the shift to this mode resulting from the interaction with the bath, with the result being typically a fraction of a percent. Naturally, their equilibrium separation decreases for tight ion traps and the average induced interaction becomes stronger. Note that the apparent giant enhancement of the shift close to unitarity predicted in Ref. [55] is not reproduced in our treatment as we find for this case that the presence of the bound state near the threshold dominates the physics. Nevertheless, the effect can be measurable for long-time dynamics.

Furthermore, the presence of ionic polarons can be detected by in situ imaging of the gas. Finding a significant increase in ion-atom correlation functions as well as in the atomic density indicates the buildup of the many-body bound state. The quest for observing the induced interactions is more subtle, as typically the direct Coulomb repulsion would be too strong to allow for the formation of bipolaronic bound states or scattering resonances. However, in this case, the study of atomic density looks promising. One could measure e.g. the deviation of the density profile from the double Gaussian peak describing separated noninteracting ionic polarons.

Finally, we note that our results are also relevant for other systems with long-ranged interactions competing with the length scales of the medium where the direct interaction potential may not be dominating, such as Rydberg-dressed mixtures.
$a_i = R^*; \; C_4 = E^* R^*^4, \; b = 0.02 R^*, \; c = 0.225 R^*$

**FIG. 11.** Density profiles projected onto a line denoted by $x$-axis connecting two impurities in the MBBS regime (arbitrary units). Symbols: Blue squares denote the results of QMC calculations, while the solid line is a fit to the defect in the projected atom density $n_{\text{atoms}}(x) = 1 + f_{\text{pol}}(x)$ with $f_{\text{pol}}(x) = \Delta n + A/(1 + Br^C)$ with $\Delta n, A, B, C$ being fitting parameters. Panel (a): Single ion (polaron) density profile used to obtain the fit $f_{\text{pol}}(x)$. Panels (b,c,d): Two ion (bipolaron) density profile for distances between ions equal to 0, $2R^*$, $5R^*$ as compared to the prediction for two non-interacting polarons located at the ion positions.

**VI. CONCLUSIONS**

We have demonstrated that impurities strongly interacting with the host medium not only experience an effective interaction that can lead to the formation of bipolaronic states, but also dramatically modify the gas properties. Because of the strong modification of the gas density profile around the ion(s), perturbative methods based on dressing the cloud with Bogolyubov excitations and neglecting the bound state occupation do not fully capture the description of the induced potential which features a kink close to the local density maximum. This indicates that ab-initio many-body simulations are of paramount importance for studying long-ranged impurity-bath interactions.

While the magnitude of the effective potential is vast compared to the gas energy scales, it is still much smaller than the Coulomb repulsion between the ions. Notwithstanding, it leads to shifts in the phonon mode energies of an ionic chain compared to the vacuum case that can be experimentally observed. This fact might be relevant for quantum technologies based on trapped ions, where the phonon modes are exploited as a “quantum bus” to mediate interactions between spatially separated quantum bits. As we discussed in the introduction, a cold atomic ensemble could be exploited to keep the ions cold to aim at fault-tolerance quantum computation for long times. Our investigations show that the phonon modes can be affected by the presence of the gas. At the same time, however, our findings prove that the phononic shift can be controlled by tuning both the number of two-body atom-ion bound states and the ion-atom scattering length, providing thus, an additional tool for tuning the phonon modes of an ion crystal.

In the future, it will be interesting to investigate the impact of the ion motion degrees of freedom both on the ground state and transport properties, especially in the many-body bound state regime. Furthermore, the role of larger ionic chains and the possibility of multipolarons states [79] in hybrid atom-ion systems may also be an interesting path to explore. Finally, an important issue is finite temperature effects and how thermal fluctuations affect our findings. In this regard, we note that Monte Carlo techniques can be used as well, as has been shown in a recent study on the neutral Bose polaron [80].
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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, the bold symbol refers to three-dimensional vectors and cursive ones to their respective norms.