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Ion-induced density bubble in a strongly correlated one-dimensional gas

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We consider a harmonically trapped Tonks-Girardeau gas of impenetrable bosons in the presence of a single embedded ion, which is assumed to be tightly confined in an RF trap. In an ultracold ion-atom collision the ion's charge induces an electric dipole moment in the atoms which leads to an attractive r^{-4} potential asymptotically. We treat the ion as a static deformation of the harmonic trap potential and model its short range interaction with the gas in the framework of quantum defect theory. The molecular bound states of the ionic potential are not populated due to the lack of any possible relaxation process in the Tonks-Girardeau regime. Armed with this knowledge we calculate the density profile of the gas in the presence of a central ionic impurity and show that a density *bubble* of the order of 1 μm occurs around the ion for typical experimental parameters. From these exact results we show that an ionic impurity in a Tonks gas can be described using a pseudopotential approximation, allowing for significantly easier treatment.

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Introduction. Since the days of superfluid helium the introduction of charged particles to a superfluid has proven to be a useful tool to explore fundamental physics. Statically they can lead to fundamental structures such as the celebrated ion *snowballs* and electron *bubbles* [1], whereas studying the motion of an immersed ion can be used to characterize the superfluid nature of ^{4}He [2]. Through the advances in the area of atom trapping and laser cooling the number of known superfluids and the environments in which they can be studied has in the past decade vastly increased. Combining these degenerate fermionic and bosonic gases, which come in a wide range of geometries and dimensionalities [3], with cooled and trapped single ions in Paul and Penning traps [4] is therefore currently one of the most exciting and dynamic areas in physics. Such research is motivated by our need to understand the true quantum nature of matter, the quest for scalable quantum information processing, and the possibility of efficient quantum simulation [5]. However, despite the achievements in both the areas of ion and atom physics, currently little is known about the physics of an ion interacting with a many-body atomic system in the ultracold regime [6,7].

By today most studies of atom-ion systems have focused on the scattering properties of single atoms and single ions [8–10]. Controlled collisions of a single atom and a single ion have been studied in Ref. [11] with trap induced resonances predicted. Such resonances along with the strong atom ion interaction have shown to be useful for enhancing the speed and the fidelity of a collisional quantum gate [12]. On the many-body level, it has been proposed to use an ion as a scanning tunneling microscope [13] which can in turn be used to measure the energy distribution of, say, a Fermi gas *in situ* [14]. Despite these promising proposals there is still scarce knowledge of what is to be expected when an ion is introduced to an ultracold many-body system. As the physics of a many-body system is highly nontrivial even without the presence of an ion, such studies are of paramount importance to shed light on the first results of the ongoing experimental progress [15,16]. Two situations have recently been explored. In Ref. [6] the authors consider an ion in a homogeneous condensate and study the capture of atoms into the bound states of the molecular potential. They predict the possibility of observing mesoscopic molecular ions, where hundreds of the atoms can become bound in molecular states of the ion-atom potential. On the other hand, in Ref. [7] the authors consider a situation where the bound states are not accessible. They then estimate by using a thermodynamical as well as a microscopic argument the number of condensate atoms associated with an ion. Both studies suggest strong analogies with the snowball states observed in the case of superfluid helium. In contrast to both of these studies, in this work we demonstrate that in the case of a harmonically trapped and strongly correlated one-dimensional gas, a μm-sized *bubble* in the density may be observed around the ion.

Strongly correlated one-dimensional quantum gases have recently become available in ultracold physics labs worldwide. One of the stand out achievements for cold atoms in low dimensions has been the first observation of the Tonks-Girardeau (TG) regime [17,18]. In this limit the gas is defined to be a one-dimensional, strongly correlated gas [19]. As it is exactly solvable through the Bose-Fermi mapping theorem [19] it is very well suited to study its behavior in the presence of impurities. The physics of impurities interacting with a many-body system is of great importance in understanding many complex condensed matter phenomena and as ultracold systems allow to tailor the interaction they have proven to be versatile model systems for a large number of different areas in physics [20]. In fact, a recent experiment in Cambridge has observed the motion of a spin impurity in a TG gas and reported interesting and complex dynamics [21]. In this work we add to the existing studies [6,7] of ionic impurities interacting with atomic many-body systems by considering an ion embedded

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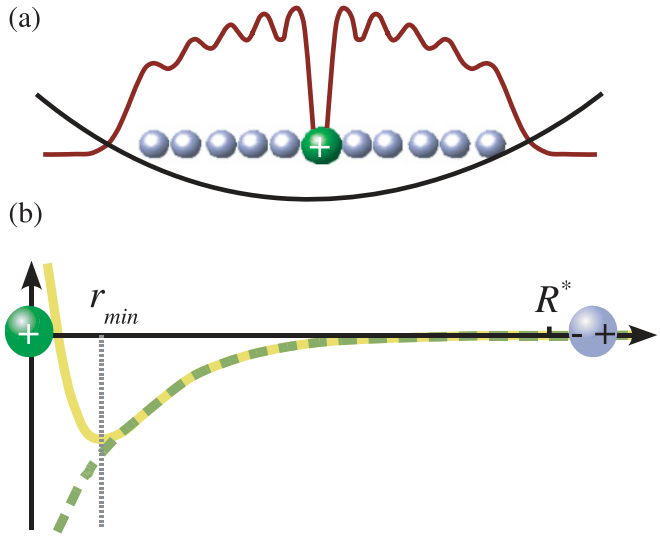

FIG. 1. (Color online) Schematic showing (a) an positively charged ion embedded in a harmonically trapped Tonks-Girardeau gas and (b) the interaction potential for the ion-atom interaction under the Born-Oppenheimer approximation (dashed). The potential minimum is at $r_{\min}$ and the polarization length of the ion is indicated by R^*. The potential curve goes as r^{-4} at large distances.

in a TG gas [see Fig. 1(a)]. Utilizing the Fermi-Bose mapping theorem [19] we calculate the single-particle density of a TG gas in the presence of an ion. We treat the ion's presence as a perturbation on the harmonic trap and model its short-range interaction in the framework of quantum defect theory.

Ultracold atom-ion interactions. Under the Born-Oppenheimer approximation, the interaction between an atom and a positively charged ion, at large distance r and low energies, is given by the potential $V(r) = -\alpha e^2/2r^4$. Here α is the dipolar polarizability of the atomic species and e is the charge on the electron. This approximation is valid only if the atom is in an atomic s state as for higher electronic states the Born-Oppenheimer potential significantly changes shape. A characteristic length scale of this interaction can be found by equating the interaction energy and the relative kinetic energy of an atom-ion pair. This gives the so-called polarization length $R^* = \sqrt{2\mu\alpha e^2/\hbar^2}$, where μ is the reduced mass and which allows to define the interaction energy of a typical atom ion collision as $E^* = \hbar^2/2\mu(R^*)^2$.

The Hamiltonian for the axial dynamics of an atom and an ion in *separate* one-dimensional harmonic traps maybe written as [11],

$$\mathcal{H}_{1D} = \sum_{\nu=i,a}\left(-\frac{\hbar^2}{2m_\nu}\frac{\partial^2}{\partial x_\nu^2} + \frac{1}{2}m_\nu\omega_\nu^2 x_\nu^2\right) + V_{\rm int}(|x_i - x_a|), \tag{1}$$

where $V_{\rm int}$ is the full one-dimensional interaction potential, which at large distances has the same power law as in three dimensions, i.e., $V(|x|) = -\alpha e^2/2x^4$. In many realistic experimental scenarios the frequency of the ion trap will be many orders of magnitude greater than that of the atom trap and it is reasonable to approximate the ion to be located quasistatically at the center of the atom trap. In this approximation one may neglect the kinetic and potential energy of the ion in (1). This allows us to write a single-particle Hamiltonian which describes an atom in a harmonic trap which is deformed at the trap center by the ionic interaction potential,

$$\mathcal{H} = -\frac{\hbar^2}{2m_a}\frac{\partial^2}{\partial x_a^2} + \frac{1}{2}m\omega_a^2 x_a^2 + V_{\rm int}(x_a). \tag{2}$$

The solution of the Schrödinger equation for the single-particle states is complicated by the fact that the real interaction potential $V_{\rm int}$ begins to deviate from the long-range asymptotic law and begins to quickly diverge toward $+\infty$ [see Fig. 1(b)]. However, at this distance the effect of the harmonic trapping potential can safely be neglected and at short range we may approximate the scattering behavior to be equivalent to a free atom-ion scattering event. The Schrödinger equation, in this region, maybe written as

$$\left(-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial x^2} - \frac{\alpha e^2}{2x^4}\right)\psi_n(x) = \epsilon_n\psi_n(x), \tag{3}$$

where μ is the reduced mass and ϕ_e and ϕ_o are the unknown scattering phases to be determined [see Eqs. (4) and (5) below]. In one dimension the solutions for Eq. (3) have even and odd parity. The asymptotic solutions, $|x| \to 0$, to Eq. (3) are given in Ref. [11]

$$\psi^e \sim |x|\sin\left(\frac{R^*}{|x|} + \phi_e\right) \tag{4}$$

$$\psi^o \sim x\ \sin\left(\frac{R^*}{|x|} + \phi_o\right). \tag{5}$$

The principal idea of the quantum defect theory is to replace the real interaction potential in Eq. (2), $V_{\rm int}$, with the asymptotic potential and use Eqs. (4) and (5) as boundary condition for the numerical solution of the Schrödinger equation for Hamiltonian Eq. (2). In analogy to the three-dimensional case the short-range phase may be related to the one-dimensional even (s wave) and odd (p wave) scattering lengths of an ultracold atom-ion collision via $a_{1D}^{e,o} = \lim_{k\to 0}[\tan(\phi_{e,o}(k))/k] = -\cot(\phi_{e,o})$. Unfortunately, the exact values for the scattering lengths of current experimental systems are not yet known and we therefore take $\phi_{e,o}$ to be adjustable parameters for now. The set of single-particle states obtained using this approach are the ones which are used to calculate the groundstate of a Tonks-Girardeau gas in the presence of a centrally embedded ion.

The Tonks-Girardeau gas. The effective one-dimensional Hamiltonian of a gas of N bosons in trapping potential $V(x)$ can be written as $\mathcal{H} = \sum_{n=1}^{N}[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_n^2} + V(x_n)] + \sum_{i<j}V(|x_i - x_j|)$, where m is the mass of a single atom. For low densities two-body collisions dominate the dynamics, and for low temperature we can approximate these by employing a pointlike potential of the form $V(|x_i - x_j|) = g_{1D}\delta(|x_i - x_j|)$. Here g_{1D} is the one-dimensional coupling constant, which is related to the three-dimensional scattering length, a_{3D}, via $g_{1D} = \frac{4\hbar^2 a_{3D}}{ml_\perp}(l_\perp - Ca_{3D})^{-1}$, where C is a constant of value $C = 1.4603\cdots$ [22] and $l_\perp$ is the transverse trapping length. In the Tonks-Girardeau limit of infinitely strong repulsion ($g_{1D} \to \infty$), the problem may be mapped to the problem of noninteracting spinless fermions, which is the so-called Fermi Bose mapping theorem [19]. The main idea of the mapping is that one can treat the atom-atom interaction

term by replacing it with the following boundary condition on the allowed bosonic wave function, $\Psi_B(x_1 \cdots x_N) = 0$, if $|x_i - x_j| = 0$ for $i \neq j$ and $1 \leqslant i \leqslant j \leqslant N$. As this is formally equivalent to the Pauli exclusion principle, one can solve for the associated ideal fermionic wave function $\Psi_F(x_1, \ldots, x_N) = \frac{1}{\sqrt{N!}} \det_{n,j=1}^{N}[\psi_n(x_j)]$ and calculate the bosonic solution from this by appropriate symmetrization, $\Psi_B = A(x_1, \ldots, x_N)\Psi_F(x_1, x_2, \ldots, x_N)$, where the unit antisymmetric function is given by $A = \prod_{1 \leqslant i < j \leqslant N} \mathrm{sgn}(x_i - x_j)$ [19]. As a consequence of this mapping the single-particle density of a TG gas has the particularly simple form

$$\rho(x) = \sum_{n=0}^{N-1} |\psi_n(x)|^2 \tag{6}$$

and thus all one needs to know to solve the many-particle problem are the eigenstates of the single-particle problem.

Ion in a Tonks-Girardeau gas. By combining the ideas of the previous two sections we are now in a position to calculate the effect of a centrally embedded ion on the ground state of a harmonically trapped TG gas. The Hamiltonian of the combined system can be written as

$$\mathcal{H} = \sum_{n=1}^{N} \left[-\frac{\hbar^2}{2m_a} \frac{\partial^2}{\partial x_n^2} + \frac{1}{2} m_a \omega_a^2 x_n^2 + V_{\mathrm{int}}(x_n) \right] + g_{1D} \sum_{i<j}^{N} \delta(x_i - x_j) \, . \tag{7}$$

We now focus on obtaining the eigenstates of the single-particle part of the Hamiltonian, i.e., Eq. (2). Using the prescription of the Fermi-Bose mapping we neglect the interaction part of the Hamiltonian and numerically solve the single-particle Schrödinger equation to find the eigenstates ψ_n and eigenvalues ϵ_n. For this we use the iterative Numerov method [23] and impose the Eqs. (4) and (5) as short range boundary conditions.

Due to the infinitely diverging nature of the ionic potential, there exists a spectrum of bound molecular states between the ion and the atoms [6]. In order for these to be populated, however, a relaxation process must be present that allows to take away the excess energy of the binding process. In an ultracold gases this process would be equivalent to a three body recombination. However, for the TG gas the density-density correlation function becomes suppressed on the length scale of the interparticle distance [24]—and thus no relaxation process for capture is available. We therefore do not need to consider the bound-state spectrum in the following.

Our calculations are carried out for the experimentally relevant systems of ^{135}Ba$^+$-^{87}Rb and ^{174}Yb$^+$-^{87}Rb. We assume a typical axial trap frequency of $\omega = 70Hz$ for a one dimensional gas of ^{87}Rb. The ^{135}Ba$^+$ and ^{174}Yb$^+$ ions have typical polarization lengths of $R^* = 5544a_0$ and $6294a_0$, respectively, where a_0 is the Bohr radius. For the ^{135}Ba$^+$-^{87}Rb system we show the first two single-particle eigenstates in Fig. 2. One can see that the center of the eigenstates is perturbed by the presence of the ion and a close up of this central region is shown in the inset for the $n = 0$ state. One can also see that in this region the wave function is rapidly oscillating, with the exact details of the oscillations depending on the short-range

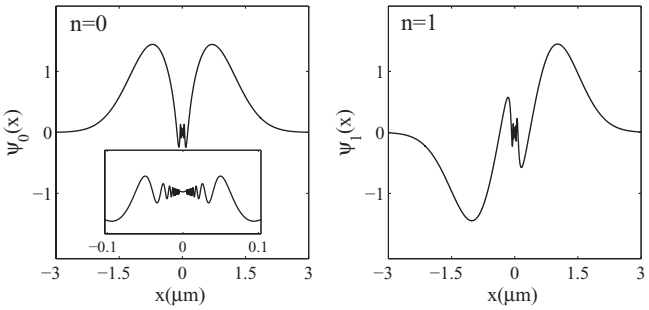

FIG. 2. The first two trap states of a harmonic trap with a centrally embedded ion for a ^{135}Ba$^+$-^{87}Rb system for axial trapping frequency, $\omega = 70$ Hz. The inset for the $n = 0$ state shows a zoom in of the region around zero where the wave function is rapidly oscillating. The short-range phases are chosen to be $\phi_e = \frac{\pi}{4}$ and $\phi_o = -\frac{\pi}{4}$.

phase. In the limit of such large trap lengths the effects of the oscillations on the physics are only marginal and only in the opposite limit to ours, if the traps were tight, do the oscillations and hence the exact short-range phase become important. The fact that the antisymmetric states are affected means that a certain amount of p-wave scattering is to be expected; however, it will be very small in our wide trap. With the single-particle wave functions at hand, we can now calculate the density distribution of a many-particle gas using Eq. (6). In Fig. 3 we show the density for the two separate systems of ^{135}Ba$^+$-^{87}Rb and ^{174}Yb$^+$-^{87}Rb. The thick black line shows the results using the quantum defect theory and the Numerov method including the full atom-ion polarization potential. It can be seen that the ion's presence drastically perturbs the density distribution of the gas by causing a bubble in the density around its position at $x = 0$. The size of this bubble is of the order of 1 μm. At first this may seem counterintuitive for an attractive impurity but one should recall that scattering is repulsive at short distances [see Fig. 1(b)] and with the lack of access to the bound states of the molecular potential in the TG regime—we see no buildup of atomic density around the ion.

Let us finally note the possibility of treating atom-ion systems in the Tonks limit with a simpler approach, by

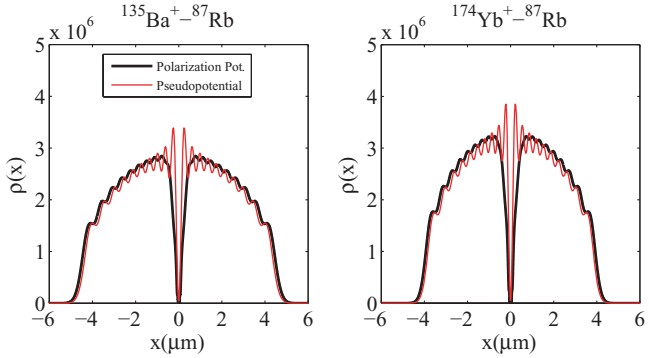

FIG. 3. (Color online) The single-particle densities of a TG gas of 20 particles in the presence of a central ion for ^{135}Ba$^+$-^{87}Rb and ^{174}Yb$^+$-^{87}Rb systems with a typical trapping frequency, $\omega = 70$ Hz (thick black line). The short range phases in each case are chosen to be $\phi_e = \frac{\pi}{4}$ and $\phi_o = -\frac{\pi}{4}$. The thin red line in the plots represents the result of a pseudopotential approximation for the ion, using a large value for the scattering length.

approximating the exact interaction with a pointlike potential [25]. The polarization lengths for both $^{135}Ba^{+}$ and $^{174}Yb^{+}$ are, 0.29 and 0.33 μm, and therefore smaller than trap lengths for one-dimensional systems, which for the traps considered here are $\sim$1.3 μm. This suggests that a localized pseudopotential approximation can be used. In Fig. 3 the pseudopotential approximation is shown by the thin red line and one can see that the two descriptions are in good agreement despite the fact that the scattering length in this case is not much smaller than the trap length. Therefore one can expect that the pseudopotential approximation will encapsulate much of the essential physics on the many-body level. In particular, the analytic accessibility of the pseudopotential model allows one to easily calculate the correlation functions and momentum distribution [26] of a TG gas in the presence of a localized impurity [25]. The pseudopotential model accurately describes the localized nature of the disturbance but due to its zero width nature it underestimates the size of the bubble. It is also important to mention, where densities are concerned, that these results are also true for spin-polarized samples of noninteracting fermions in one dimension.

Conclusions. In this work we have shown that the presence of a single ion in a TG gas leads to the formation of a density bubble around the impurity. Using quantum defect theory we have calculated the exact eigenstates of an atom-ion system in one dimension and then applied the Bose-Fermi mapping theorem to calculate the many-particle density. The bubble was found to be of the order of a μm and should therefore be observable in typical experiments. We also outlined that the density can be very well approximated using a pseudopotential model under typical experimental constraints, which will allow to connect the atom-ion systems in the Tonks limit to a large number of results already existing in the literature.

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