Quantum Impurity in a One-dimensional Trapped Bose Gas

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We present a new theoretical framework for describing an impurity in a trapped Bose system in one spatial dimension. The theory handles any external confinement, arbitrary mass ratios, and a weak interaction may be included between the Bose particles. To demonstrate our technique, we calculate the ground state energy and properties of a sample system with eight bosons and find an excellent agreement with numerically exact results. Our theory can thus provide definite predictions for experiments in cold atomic gases.

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An impurity interacting with a reservoir of quantum particles is an essential problem of fundamental physics. Famous examples include a single charge in a polarizable environment, the Landau-Pekar polaron [1, 2], a neutral particle in superfluid $^4$He [3], and a magnetic impurity in a metal resulting in the Kondo effect [4], and a single scattering potential inside an ideal Fermi gas [5, 6]. The latter system is famous for the Anderson’s orthogonality catastrophe [7]. In these settings the impurity behavior can provide key insights into the many-body physics and guide our understanding of more general setups.

A complicating feature of many impurity problems is the presence of interactions at a level that often precludes the use of perturbative analysis and self-consistent mean-field approximations. This implies that analytical approaches are highly desirable and exact solutions are, when available, coveted tools for benchmarking other techniques. This is particularly true for one-dimensional (1D) homogeneous systems where solutions can often be found based on the Bethe ansatz [8–12]. These solutions are the essential ingredients for our analytical understanding of highly controllable experiments with cold atoms [13–15]. For instance, the exactly soluble problem of the single impurity in a 1D Fermi sea [10] - the Fermi polaron - can be used to study the atom-by-atom formation of a 1D Fermi sea [16].

While Fermi polarons have been studied intensively in recent times using cold atomic setups both experimentally and theoretically [20–24], the physics of impurities in a bosonic environment is only now becoming a frontier in cold atom experiments [25–28]. This pursuit requires theoretical models for describing the Bose polaron [29–40], where, in contrast to the Fermi polaron, an exact solution is not known even for a homogeneous 1D system. Here we provide a new theoretical framework that captures the properties of an impurity in a bosonic bath confined in one spatial dimension. Our (semi)-analytical theory thus provides a state-of-the-art tool for exploring the properties of Bose polarons in 1D.

The proposed framework works with a zero-range potential of any strength and handles any number of majority particles in external confinement of various shapes which is beyond known analytical approaches to this problem. Our method is also applicable to describe experimental setups that have different trapping potentials for the impurity and majority particles and different mass ratios. In addition, weak majority interactions may be included using the well-known Gross-Pitaevskii equation (GPE). While our method is not exact, we have benchmarked the energetics and density profiles against numer-
ical results \[39\] and find agreement for up to ten particles at the level of a few percent. To illustrate the method in this letter, we examine a system of eight bosons and an impurity in a harmonic trap. Fig. (b) shows a sketch of this system with vanishing boson-boson and large boson-impurity interaction. This leads to separation of the two components. Notice that the ground state must retain parity and is thus a linear superposition of the two spatial configurations outlined. Using the pair-correlation function we can clearly see in Fig. (b)-d) how the impurity moves to the edge of the system as a function of the inter-species interaction. Increasing the intra-species interaction we witness the opposite effect as the impurity goes to the center of the system as seen in Fig. (b)-g).

**Formalism** Our two component system consists of one type A (impurity), and \(N_B\) identical type \(B\) bosons (majority) with masses \(m_A\) and \(m_B\) respectively. For the sake of argument, we confine particles in harmonic potentials with trapping frequency \(\omega_B\) for the bosons and \(\omega_A\) for the impurity. In this letter we adopt harmonic oscillator units for the major components, i.e. we measure length in units of \(\sqrt{\hbar/m_{BA}}\) and energy in units of \(\hbar\omega_B\). Accordingly, the Hamiltonians, for the impurity atom with coordinate \(x\) and a majority atom with coordinate \(y\), are expressed as

\[
H_A(x) = \frac{p_A^2 + m_{AB}^2 \omega_{AB}^2 x^2}{2m_{AB}}, \quad H_B(y) = \frac{p_y^2 + y^2}{2}, \tag{1}
\]

where \(m_{AB} = m_A/m_B, \omega_{AB} = \omega_A/\omega_B\), and \(p\) denotes the corresponding momenta. The interaction between \(A\) and \(B\) particles is assumed to be of a short range and hence modeled by the Dirac delta-function with strength \(g\). The boson-boson interaction is also given in the standard pseudopotential interaction model \[38\] with coupling constant \(g_{BB}\). Both interaction strengths are given in units of [\(\hbar\omega_B\)]. The overall Hamiltonian of the system is \(H = H_A(x) + \sum_{i=1}^{N_B} H_B(y_i) + \sum_{i=1}^{N_B} g_B \delta_i(x - y_i) + \sum_{i<k} g_{BB} \delta_i(y_i - y_k)\), where \(y_i\) are the coordinates of the bosons.

In order to find the eigenspectrum of the Hamiltonian for arbitrary \(g\) we introduce a new (semi)-analytical approach. More specifically, we consider the impurity as the ‘slow’ variable and introduce the adiabatic decomposition of the total wave function

\[
\Psi(x,y_1,\ldots,y_{N_B}) = \sum_{j=1}^{N_B} \phi_j(x) \Phi_j(y_1,\ldots,y_{N_B}|x), \tag{2}
\]

where \(\Phi_j\) is the \(j\)th normalized eigenstate of the eigenvalue problem \(\sum_{i=1}^{N_B} H_B(y_i) \Phi_j = \varepsilon_j(x) \Phi_j\) which we solve assuming that the impurity gives rise to a zero-range potential at a fixed position \(x\) (see Supplemental Material \[49\]). First we consider an ideal Bose gas, i.e. \(g_{BB} = 0\), and write \(\Phi_j(y_1,\ldots,y_{N_B}|x) = S \prod_{i=1}^{N_B} f_k^j(y_i|x)\) with a symmetrization operator \(S\) (acting on the \(y_i\) coordinates) and \(f_k^j(y_i|x)\) being the \(k_i\)th normalized eigenstate of \(H_B(y_i)\) for a given \(x\). Notice that every function \(f_k^j(y_i|x)\) has a discontinuous derivative at \(y_i = x\) due to the zero-range interaction. This is quantified with the standard delta function boundary condition which dictates that the difference in the slopes of the wave function, from the left and right sides of \(x\), times a \(1/(2g)\) factor must be equal to the value of the wave function taken at \(y_i = x\). As \(1/g \to \infty\) the wave function must therefore vanish at \(y_i = x\).

We can include interactions among the majority particles under the assumption that these may be described by the 1D GPE (see Supplemental Material \[47\]). In this case we need to use a dressed single-particle wave function \(\tilde{f}_{k_i}^j\) instead of \(f_{k_i}^j(y_i|x)\). The function \(\tilde{f}_{k_i}^j\) satisfies the 1D GPE complemented with the boundary condition at \(y_i = x\),

\[
\mu(x) \tilde{f}_{k_i}^j = \left( -\frac{1}{2} \frac{\partial^2}{\partial y_i^2} + \frac{1}{2} y_i^2 + N_B \cdot g_{BB} |f_{k_i}^j|^2 \right) \tilde{f}_{k_i}^j, \tag{3}
\]

where \(\mu(x)\) is a chemical potential, \(g_{BB}\) is determined through the three-dimensional boson-boson scattering length, \(a_s\), as \(g_{BB} = \frac{\sqrt{a_s}}{\sqrt{2\pi \omega_B}}\), where \(\omega_{B_1}\) and \(\omega_{B_2}\) are the two frequencies in the directions of strong confinement \[49\]. The boson-impurity coupling constant can be also related to the corresponding scattering length \[51\].

After determining the function \(f_{k_i}^j\) we obtain a coupled system of equations for \(\phi_j(x)\) (see Supplemental Material...
The coupling terms in this system correspond to the transition of a majority particle from $f_k$ to $f_j$. For bosons, this is a coherent process which contributes significantly if the impurity is placed in a region with high density of majority particles. Physical intuition, however, tells us that in the ground and low-lying excited states the impurity is pushed to the edge of the trap if $g_{BB} \ll g$ and $N_B \gg 1$. Otherwise, the impurity would deplete the majority particles notably from the ground state of the one-body harmonic oscillator which is very expensive energywise for $N_B \gg 1$. Hence, for large $N_B$ we neglect the coupling terms between different $\phi_j(x)$, which rigorously gives us an upper bound for the exact energy of the ground state \([51]\). However, we expect this approximation to be very accurate also for low-lying excited states. We can therefore obtain $\phi_j(x)$ by solving numerically a single differential equation. From the mathematical point of view the presented approach is similar to the Born-Oppenheimer approximation or the hyperspherical adiabatic method \([52]\). The physics is, however, different. Indeed, we develop our method for a many-body system where we expect that for the same computational time the relative precision is increasing with the number of particles. Clearly, the discussion above applies to a Bose polaron problem in arbitrary confinement. Moreover the trapping potentials as well as the masses can be different for the $A$ and $B$ particles.

To conclude the presentation of our method we compare its predictions with the exact results obtained using the numerical approach developed in Refs. \([49, 53]\) for $g_{BB} = 0, m_{AB} = \omega_{AB} = 1$. We find that the relative precision of the method increases with $N_B$ and we pick a sample system with $N_B = 8$. We start by analyzing the energies in Fig. 2. Our model yields results that are slightly above the numerically exact values with a maximum deviation of a few percent. Next we check that the model reproduces the derivative of the ground state energy with respect to the coupling constant, $\partial E/\partial (1/g)/N_B$, vs. $N_B$, see the inset in Fig. 2. This derivative for fixed $g$ determines the probability for a given boson to be close to the impurity \([52, 55]\). We see that for a large number of bosons this probability becomes smaller, manifesting that the impurity is pushed far from the center of the trap. It is also interesting to note that for large $N_B$ we find numerically that $\partial E/\partial (1/g)$ is almost independent of $N_B$.

We have also compared density profiles and pair-correlation functions for the ground state and again find only minute differences, see Fig. 3a) and b). Note that the impurity density splits for large $g$. On the other hand, the majority particles are almost unperturbed by the interaction. This means that an adiabatically slow increase of $g$ moves the impurity to the edge of the system, as also shown in Fig. 3b)-d). As the number of bosons increases the impurity gets pushed further towards the edge of the trap, and $\partial E/\partial (1/g)/N_B$ decreases. In the energy domain it leads to a doubly degenerate ground state at $1/g = 0$ since the impurity can be pushed to either the left or the right edges of the trap, see Fig. 2 and Fig. 1b). This should be contrasted with the Fermi polaron system where for large interaction the ground state is $N_B + 1$ times degenerate and the impurity is localized in the middle of the trap \([52, 56, 57]\).

**Results** To further illustrate the model we continue our discussion of an impurity interacting with eight bosons. However now we allow weak interaction between the bosons as well as different mass (or frequency) ratios. For large interactions this setup is already beyond current numerical approaches. We stress once again that in our method the numerical complexity does not increase with $N_B$, and $N_B = 8$ is chosen as a particular example.

First we fix $g = 1, m_{AB} = 1, \omega_{AB} = 1$ and change the intra-species interaction strength, $g_{BB}$. In Fig. 3c)-d) we show the density for the impurity and majority atoms in the ground state. In this case the energy is minimized if the impurity is pushed towards the middle of the trap. This is readily understood for the case $g = g_{BB}$ where the impurity particle should have the same density distribution due to the boson-impurity exchange symmetry of the Hamiltonian. In our case the difference in the densities of majority and impurity for
The impurity density in the middle of the trap compared to mapping \([58]\), where one also expects enhancement of the purity with different values of \(m_{AB}\) and \(\omega_{AB} = 1\). For \(\omega_{AB} = 0\) case. Next we compute the pair-correlation function which again demonstrates that the impurity is situated close to the origin, see Fig. 3(b)-g). Consider now different masses for \(A\) and \(B\) particles for \(g_{BB} = 0\), \(g = 1\) and \(\omega_{AB} = 1\) \([59]\). As shown in Fig. 3(e)-f), when \(m_{AB}\) becomes larger the external potential localizes the impurity in the middle of the system. For \(m_{AB} \rightarrow \infty\) the impurity constitutes a delta-function barrier in the middle of the harmonic trap, the solution to which can be found in Ref. \([60]\). From this picture it is apparent that the density of the majority particles should be suppressed at the origin, see Fig. 3(f).

Next we consider the momentum distribution which is an observable to gain information about cold atomic gas systems. The momentum distributions of the impurity for \(g_{BB} = 0\) and \(\omega_{AB} = 1\) is shown in Fig. 4 for different mass ratios and interaction strengths. These distributions can be understood from the discussions above. When the mass ratio increases the impurity wave function is almost a Gaussian function, and therefore the momentum distribution will also assume a Gaussian form. Notice the characteristic oscillations in the wings of the distributions which could be very helpful for the experimental detection of the Bose polaron. The momentum distribution for majority particles is not plotted because there is no noticeable change in the distribution as we change \(g\) and/or \(m_{AB}\).

As a final characteristic of the Bose polaron, we consider the overlap between the non-interacting and strongly interacting states for different values of \(g_{BB}\) and mass ratios as function of \(N_B\). This quantity is related to the orthogonality catastrophe \([3]\) and has generated recent interest as a probe of many-body physics with cold atoms \([57, 58, 61]\). In Fig. 5 we see a power-law behavior, but more interestingly, the exponent changes with both \(g_{BB}\) and mass ratio. The original work of Anderson \([2]\) uses a potential to model the impurity which corresponds to the limit \(m_{AB} \rightarrow \infty\). Consistent with Anderson, this limit shows very fast decay (high negative power dependence on \(N_B\)) but already for mass ratio \(m_{AB} = 3\) the suppression is considerable as seen in Fig. 5. On the contrary, in the opposite limit of equal masses we see much longer tails. Experiments using equal mass two-component setups and two atomic species with different masses could therefore complement each other perfectly when studying the orthogonality catastrophe for Bose polarons.

Experiments. Our predictions should be addressable using current experimental setups. In particular, effective 1D systems have been produced that exhibit behavior consistent with zero-temperature predictions for both bosonic \([13, 16]\) and fermionic atoms \([17, 19]\). Two-component bosonic systems in 1D \([28, 62, 63]\) can be used to explore the equal mass Bose polarons. Mass-imbalanced Bose-Bose mixtures in 1D have been explored with \(^{87}\text{Rb}\) and \(^{41}\text{K}\) \((m_{AB} < 1)\) \([25]\) and new experiments with \(^{87}\text{Rb}\) and \(^{133}\text{Cs}\) \((m_{AB} > 1)\) appear promising if an effective 1D geometry can be reached \([26]\). Our theory provides predictions for experiments in the 1D regime taking into account any experimental features such as different trap frequencies for different atoms, relative displacement of the trap, and mass imbalance.

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