Editors' Suggestion

Universal Aspects of a Strongly Interacting Impurity in a Dilute Bose Condensate

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We study the properties of an impurity immersed in a weakly interacting Bose gas, i.e., of a Bose polaron. In the perturbatively tractable limit of weak impurity-boson interactions many of its properties are known to depend only on the scattering length. Here we demonstrate that for strong (unitary) impurity-boson interactions all quasiparticle properties of a heavy Bose polaron, such as its energy, its residue, its Tan's contact, and the number of bosons trapped nearby the impurity, depend on the impurity-boson potential via a single parameter characterizing its range.

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The study of impurities in Bose and Fermi gases is an old and important subject [1–6]. When a distinguishable atom is added to the gas, the impurity gets dressed by excitations in the bath and forms a quasiparticle often referred to as a polaron. Polarons in ultracold Fermi gases, both weakly and strongly interacting, have been studied for over a decade and a half [7–16]. The study of polarons in Bose gases picked up relatively recently, with the cases of neutral [17–35], Rydberg [36–39], and charged impurities [40–45] studied in the literature. Effects of finite temperature have also been carefully examined [32,46–52]. Here we point out that an impurity added to a weakly interacting three-dimensional Bose gas at zero temperature exhibits universal features which depend very weakly on the details of the interaction potential (see Fig. 1). Quite remarkably, we prove that the main features of Bose polaron can be calculated analytically even when the impurity interacts strongly, in the so-called unitary limit, with an otherwise weakly interacting Bose gas.

We consider a weakly interacting Bose gas made of atoms of mass m with density n_0. Trading the density n_0 for the chemical potential μ, we denote by $E(\mu)$ the energy cost of introducing a single impurity to the gas kept at this chemical potential. An impurity traps or repels extra bosons in its vicinity. It is possible to show that the number of trapped bosons is [41]

$$N = -\partial E/\partial \mu. \tag{1}$$

Our main goal is to calculate E, thus also determining the number of trapped bosons according to Eq. (1). In this work we limit ourselves to zero temperature.

To describe a single heavy impurity, we can think of it as a radially symmetric potential $U(r)$ it induces on the gas. The Hamiltonian $\mathcal{H}$ of the gas with an infinitely massive impurity is given by (throughout we set $\hbar = 1$)

$$\mathcal{H} = \int d^3x \left[\frac{\nabla\bar{\psi}\nabla\psi}{2m} + [U(r) - \mu]\bar{\psi}\psi + \frac{\lambda}{2}(\bar{\psi}\psi)^2\right], \tag{2}$$

where m is the mass of the bosons. For mobile impurities with mass M, in the latter equation we could replace m with the reduced mass $m_r = mM/(m+M)$ [4,33,34]. However, to simplify equations, we will limit ourselves to the case $M \gg m$, so that $m_r = m$. The coupling constant λ is related to the scattering length $a_B > 0$ characterizing interactions among bosons by $\lambda = 4\pi a_B/m$. The gas we consider here is weakly interacting, which is well known to imply that

$$n_0 a_B^3 \ll 1. \tag{3}$$

The chemical potential μ can be used to define the healing length ξ of the gas according to

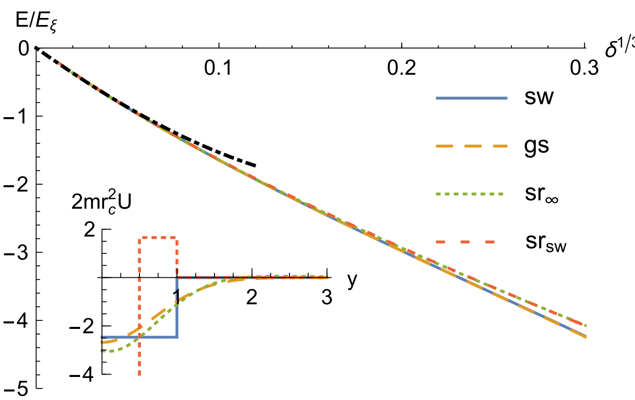

FIG. 1. Polaron energy E at unitarity obtained numerically from various impurity-bath potentials tuned to their first unitary point: square well (sw), Gaussian (gs), and shape resonant (sr_∞ and sr_{sw}, which are, respectively, infinite and finite ranged; both have $r_e = 0$) [53]. Plot as a function of $\delta^{1/3} = (R/\xi)^{1/3}$ in units of $E_\xi = \xi n_0/(2m)$. The dot-dashed black line is our analytic result, Eq. (18). The inset presents a sketch of the potentials $U(y)$.

$$\mu = 1/(2m\xi^2). \tag{4}$$

In a weakly interacting Bose gas $\mu = \lambda n_0$, and the condition for weak interactions can be rewritten as

$$\xi \gg n_0^{-1/3} \gg a_B, \tag{5}$$

where $n_0^{-1/3}$ is the mean interparticle spacing in the gas.

Suppose the impurity-bath potential $U(r)$ is characterized by a scattering length a. It has been known for quite some time that, for small enough $|a|$, the polaron energy and the number of trapped bosons are given by

$$E = 2\pi n_0 a/m, \qquad N = -a/(2a_B). \tag{6}$$

For an attractive potential $E < 0$ and $N > 0$, since $a < 0$.

The results in Eq. (6) are well known, yet it has not been known how small $|a|$ should be in order for it to hold, nor has it been known what it gets replaced by as the potential is made progressively more attractive toward the unitary point $1/a = 0$. Here we show that the appropriate conditions, as well as all polaron quasiparticles at unitarity, can be stated in terms of the range of the potential R. While it might be intuitively clear what the range of the potential represents, we need to define R precisely. In our context, this will be done using the following construction. Consider the zero energy Schrödinger equation,

$$-\frac{\Delta\psi_0}{2m} + U\psi_0 = 0, \tag{7}$$

with the potential U tuned to unitarity (for example, by varying its amplitude). Its solution ψ_0 must go as $1/r$ at large distances, at least for potentials which vanish faster than $1/r^2$. Let us normalize the solution by demanding that $r\psi_0 \to 1$ as r goes to infinity. We now define R as

$$R \equiv \left[\int \frac{d^3x}{4\pi}|\psi_0|^4\right]^{-1}. \tag{8}$$

For potentials with a finite extent, R can be shown to be close to their physical range. Often R is also not far from the usual "effective range" r_e characterizing low-energy two-body scattering. For example, for a unitary square well of width r_c one has $r_e = r_c$ and $R/r_c = 4/[2\pi\mathrm{Si}(\pi) - \pi\mathrm{Si}(2\pi)] \approx 0.557$, where $\mathrm{Si}(x)$ is the "sine integral." We will return to this important point below.

It turns out, as we will show, that for the purpose of solving the polaron problem the potentials can be split into those which satisfy the following condition,

$$R \gg a_B(n_0 a_B^3)^{1/4}, \tag{9}$$

and those which do not. In a weakly interacting bath a_B is of the order of the range of the interaction potential among bath particles, and the latter is expected to be comparable to the range of the interactions with the impurity, so that $R \sim a_B$. Taking into account the condition (3), Eq. (9) is generally comfortably fulfilled in the atomic gases of interest here [54,55]. Note that this still implies $R \ll \xi$ thanks to Eq. (5).

With this setup in place, we now present our results for interacting impurities satisfying Eq. (9). The expression (6) is only valid if

$$|a|^3 \ll \xi^2 R. \tag{10}$$

As the potential U grows more attractive, $|a|$ grows. When the condition (10) is violated, Eq. (6) breaks down. Exactly at unitarity where $a = \infty$, and in the limit $R \ll \xi$, the energy of the polaron and the number of bath bosons in its dressing cloud can be found analytically and are given by

$$E = -\frac{3\pi n_0 \xi}{m}(R/\xi)^{1/3}, \qquad N = 4\pi n_0 \xi^3 (R/\xi)^{1/3}. \tag{11}$$

These constitute the most important results of this Letter. N follows from E in accordance with Eq. (1), where ξ and n_0 have to be traded for μ before differentiating. These results constitute the leading asymptotics of the solution when $R/\xi \ll 1$. Systematic higher order corrections to Eq. (11) are discussed below.

To obtain these results we treat the Hamiltonian (2) classically and solve the mean-field time-independent Gross-Pitaevskii (GP) equation instead of working with the fully quantum problem. One might worry that the GP equation is applicable only far away from the impurity where the condition (3) holds, but not nearby an attractively interacting impurity, where the local density of the gas n_l is substantially higher than n_0. We will see later, however, that at unitarity $n_l = n_0(\xi/R)^{4/3}$; thus the condition $n_l a_B^3 \ll 1$ is equivalent to Eq. (9) which, as we already discussed, we expect to hold true.

The GP equation reads

$$-\frac{\Delta\psi}{2m} + U\psi + \lambda|\psi|^2\psi = \mu\psi. \tag{12}$$

Given the solution of this equation ψ, the energy of the polaron can be deduced by the substitution of it into Eq. (2) and subtracting the energy of the condensate without impurity, to give

$$E = -\frac{\lambda}{2}\int d^3x(|\psi|^4 - n_0^2). \tag{13}$$

At the same time, the number of particles trapped in the polaron can be found by evaluating

$$N = \int d^3x(|\psi|^2 - n_0). \tag{14}$$

We note that if the potential does not vary much on the scale of ξ, then the GP equation can be solved using local density approximation, as is often done in the case when U represents the smooth potential of a trap holding the condensate. However, we are interested in the opposite limit where the range of the potential is much smaller than ξ. Equation (12) is nonlinear and at a first glance looks intractable. We now demonstrate that nevertheless its analytic solution is possible as long as $R \ll \xi$.

We would first like to work with a potential which is strictly zero beyond some length r_c, $U(r) = 0$ for $r > r_c$. Later we will show that it is also possible to consider potentials extending all the way to infinity. R introduced above is of the order of r_c but is not necessarily equal to it. We introduce $\phi = \psi/\sqrt{n_0}$. Since we are looking for the lowest energy solution, this will be real valued and spherically symmetric.

We analyze the Eq. (12) by introducing a small parameter $\epsilon = r_c/\xi$ and constructing its solution as an expansion in powers of this parameter. As a first step, it is convenient to split the range of r into $0 \le r \le r_c$ and $r_c \le r < \infty$. In the first interval we introduce $y = r/r_c$ and $\phi = \chi(y)/y$. $\chi(y)$ satisfies

$$-\frac{d^2\chi}{dy^2} + 2mr_c^2 U\chi = \epsilon^2\left(\chi - \frac{\chi^3}{y^2}\right). \tag{15}$$

In the second interval we introduce $z = r/\xi$ and $\phi = 1 + u(z)/z$, to find

$$-\frac{d^2u}{dz^2} - 2u = 3\frac{u^2}{z} + \frac{u^3}{z^2}, \tag{16}$$

where $u \to 0$ when $z \to \infty$. We need to solve Eqs. (15) and (16), matching the solutions at the boundary $r = r_c$.

Now we will sketch the steps needed to follow through with this strategy, leaving details for Supplemental Material [56]. Let us first examine the case of weakly attractive potential with a small scattering length $a < 0$. We solve Eq. (15) in the interval $0 \le y \le 1$ neglecting its right-hand side as it contains a small parameter ϵ. Then Eq. (15) reduces to a Schrödinger equation in the potential U at zero energy, whose solution χ_0 must satisfy $\chi_0(0) = 0$. We normalize the solution so that $\chi_0(1) = \alpha$, then $\chi_0'(1)$ satisfies Bethe-Peierls boundary conditions $\chi_0'(1) = \alpha/(1 - a/r_c)$.

Now we solve Eq. (16) neglecting its right-hand side to find $u = Ae^{-\sqrt{2}z}$. This would be valid as long as A is small. Matching amplitudes and derivatives of $\chi(y)$ and $u(z)$ at $z = \epsilon$, or correspondingly $y = 1$, produces $A = \epsilon(\alpha - 1), -\sqrt{2}A = \alpha/(1 - a/r_c) - 1$. Taking into account that $\epsilon \ll 1$, this gives $A = -a/\xi$, and $\alpha = 1 - a/r_c$. We can now plug our solution into Eq. (13) and recover the answer (6) under the condition (10).

Let us now examine if the terms neglected to arrive at this solution are indeed small. We solve Eq. (15) by successive approximations, plugging χ_0 into the right-hand side of Eq. (15) and producing a correction χ_1. If $|a| < r_0$, then both $\chi_0(1)$ and $\chi_0'(1)$ are of the order of 1 while χ_1 will be of the order of $\epsilon^2 \ll 1$ and can be neglected. It gets more interesting if $|a| > r_c$. Then $\chi_0(1) = \alpha \sim a/r_0$, while $\chi_0'(1) \sim 1$. At the same time, $\chi_1 \sim \epsilon^2(a/r_c)^3$. The magnitude of this had better be smaller than 1, so that the contribution of $\chi_1'(1)$ to the derivative of χ could be neglected. This condition gives $\epsilon^2|a|^3/r_c^3 \ll 1$. We thus recover the condition (10) for the scattering length a to be small enough so that the weak coupling solution is valid. Note that $A \ll 1$ and the right-hand side of Eq. (16) could indeed be neglected.

Suppose now that the potential U is made more attractive so that its scattering length increases, violating the condition (10) and eventually reaching infinity at the unitary point. We can follow the same strategy to obtain the solution in this case. The new element is that Bethe-Peierls boundary conditions now imply $\chi_0'(1) = 0$, so we need to solve Eq. (15) perturbatively, using its right-hand side as a perturbation, to find nonzero $\chi_0'(1)$. The same goes for Eq. (16). Leaving the details of the calculation for Supplemental Material [56], we find $\alpha = A/\epsilon$ with

$$A^3 = \epsilon\left(1 + \int_0^1 dy v^4/y^2\right)^{-1}. \tag{17}$$

Here $\psi_0 = v(y)/y$ is the solution of the Schrödinger equation at unitarity, Eq. (7), normalized so that $v(1) = 1$ ($y = 1$ corresponds to $r = r_c$).

Note that $\alpha \approx 1/\epsilon^{2/3}$ controls the amplitude of the solution to the Gross-Pitaevskii equation at $r < r_0$. It follows that the density of the gas at $r < r_0$ is roughly $n_l \sim n_0\alpha^2 = n_0/\epsilon^{4/3}$. This was used earlier to argue that $n_l a_B^3 \ll 1$ [or in other words, $n(r)a_B^3 \ll 1$ for every r] implies Eq. (9).

We can further observe that $v(y > 1) = 1$, so that A can be conveniently rewritten as $A = (R/\xi)^{1/3}$, where R was defined in Eq. (8). Note that R can be computed even when the potential extends to infinity, so at this point we can safely take the limit $r_c \to \infty$ if desired. The algebra leading to this result is also presented in the Supplemental Material [56]. Wave functions obtained numerically for two different $U(r)$ are shown in Fig. 2. Even though the potentials have very different features (sw is finite ranged with effective range $r_e = r_c$, while sr$_\infty$ is infinite ranged with $r_e = 0$), the wave functions obtained at equal values of $\delta = R/\xi$ are remarkably similar.

We can now plug the solution thus computed into Eq. (13) to find the expression for the energy, which is Eq. (11). The procedure outlined here can actually be further used to construct a perturbative expansion in powers of ϵ or, more precisely, $\delta = R/\xi$, which gives

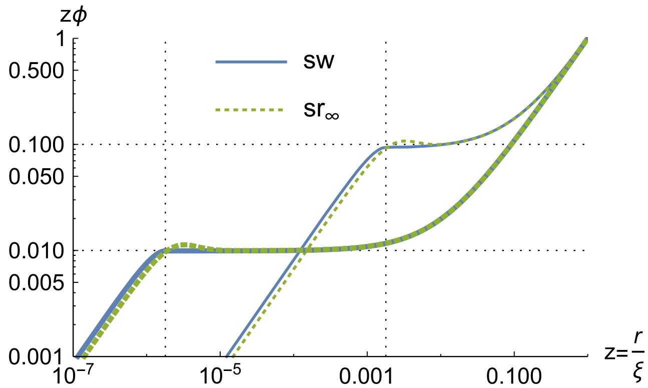

FIG. 2. Short-distance behavior. Wave function $z\phi$ obtained from two unitary potentials (sw and sr_∞) at $\delta = 10^{-3}$ (thin line) and $\delta = 10^{-6}$ (thick line). The horizontal and vertical dotted lines denote, respectively, the radii r_c of the square well potentials and the corresponding predictions $z\phi|_{r=r_c} \approx \delta^{1/3}$.

$$E = -\frac{\pi n_0 \xi}{m}(3\delta^{1/3} - 2\sqrt{2}\delta^{2/3} + 4\delta \ln \delta + \cdots),$$
$$N = 4\pi n_0 \xi^3 \left(\delta^{1/3} - \frac{5}{3\sqrt{2}}\delta^{2/3} + 2\delta \ln \delta + \cdots\right). \tag{18}$$

Terms beyond those shown here will require constructing further perturbative expansion of Eq. (15), and are expected to be less universal, depending on the features of the potential beyond those controlled by R. In Fig. 1 we show that the numerical solution of the GP equation using various (finite- and infinite-ranged) unitary impurity-bath potentials $U(r)$ [53] yields polaron energies which are remarkably independent of $U(r)$, and are in very good agreement with our analytical result Eq. (18).

The residue Z quantifies the overlap between the solutions in the presence and absence of the impurity. Within the GP treatment, this is given by $\ln Z = -\int d^3x |\psi(x) - \sqrt{n_0}|^2$ [34]. At unitarity, the above analysis shows that to leading order $\ln Z = -\sqrt{2}\pi n_0 \xi^3 \delta^{2/3}$.

Another key quasiparticle property is the impurity-bath Tan's contact, which quantifies the change in the polaron energy in response to a small change of the inverse scattering length, $C = -8\pi m \partial E/\partial a^{-1}$. An alternative definition of the contact is based on the impurity-bath density-density correlator evaluated at the core radius, $\tilde{C} = 16\pi^2 r_c^2 |\psi(r_c)|^2$. Our formalism allows us to compute both quantities, and we have directly verified that at unitarity an identical answer is obtained from both definitions:

$$C = \tilde{C} = 16\pi^2 n_0 \xi^2 \delta^{2/3}(1 - 2\sqrt{2}\delta^{1/3}/3 + \cdots), \tag{19}$$

in the leading approximation in δ. However, we have not established whether C remains to be equal to $\tilde{C}$ in higher order terms in δ, and neither are we aware of a general argument establishing their equality. We also note that the definition $\tilde{C}$ given above stops working when r_c is infinity, as is the case with infinite-range potentials.

To get a grasp on the physical meaning of R for finite-ranged potentials, consider the inequality $\int_0^{r_c} r^2 dr(\gamma + v^2/r^2)^2 \geq 0$, which obviously holds for every γ. Minimizing with respect to γ, and using that the effective range at unitarity is given by $r_e = 2\int_0^{r_c} dr(1 - v^2)$ [57], we find

$$\frac{r_c}{R} \geq \frac{3r_e^2}{4r_c^2} - \frac{3r_e}{r_c} + 4. \tag{20}$$

Quite remarkably, this bound is approximately saturated by many interesting potentials, as we show in Fig. 3. This gives a way to estimate R starting from the knowledge of r_e, which is experimentally of easy access. A direct measurement of R is instead possible, for example, using the single-atom detection scheme developed in Ref. [58].

As the potential U increases in strengths beyond the unitary limit, which implies that it now has a bound state with binding energy $-\nu = -1/(2ma^2)$, a becomes positive. If a becomes sufficiently small so that the relationship (10) holds again, simple arguments give the energy and the number of trapped particles of the polaron as

$$E \sim -mR^3\nu^2/a_B, \qquad N \sim mR^3\nu/a_B, \tag{21}$$

where the precise coefficients now depend on the details of the potential U [59].

Indeed, suppose N bosons get trapped in this bound state, then the polaron energy is $E = -N\nu + gN^2/2$, where the self-repulsion constant g can be estimated as $g \sim \lambda/R^3$. Minimizing E with respect to N we find Eq. (21). This solution can also be obtained from the GP equation if one notes that it corresponds to the density of bosons being

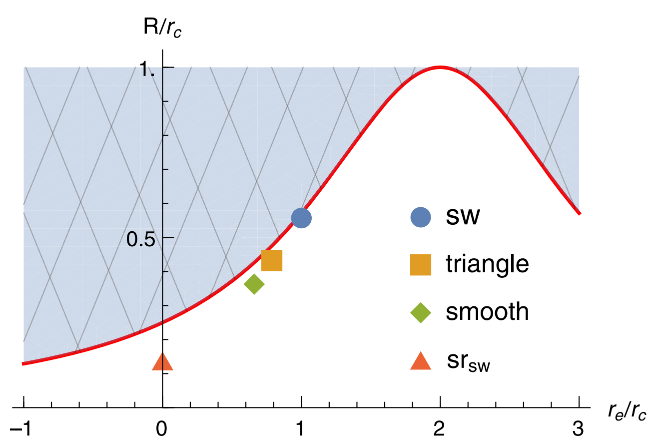

FIG. 3. Upper bound to R. The range R of potentials with a finite range [i.e., such that $U(r > r_c) = 0$] is bound from above by a simple function of the effective range r_e (red line); see Eq. (20). The symbols show the range R/r_c obtained from various finite-ranged potentials [53].

$n_l \sim N/R^3 \sim \nu/\lambda$, and that results in the nonlinear term in the GP equation $\lambda|\psi|^2\psi \sim \nu\psi$, thus turning the GP equation into the Schrödinger equation at energy close to $-\nu$. Such solution of the GP equation, which would fix the coefficients in Eq. (21), can only be found numerically and the answer will depend strongly on details of U. It is easy to see that $n_l a_B^3 \sim (a_B/a)^2 \ll 1$, justifying the use of the GP equation. Detailed studies on Bose polarons beyond unitarity have been performed by complementary approaches in Refs. [27,28,41,44].

In conclusion, we presented here the complete analytic solution of a challenging many-body problem, the one of describing an impurity in strong interaction with a very compressible Bose bath. Our formalism shall hold under typical experimental conditions found in Bose polaron experiments, and it allows us to compute many relevant quasiparticle properties, like the energy, the number of trapped bosons, the residue, and the contact. In agreement with earlier studies, we showed that a strong attractive interaction generates a macroscopic coherent dressing of the impurity, which gives rise to a bosonic version of the orthogonality catastrophe in the limit of an infinitely compressible bath. Interesting open questions concern the determination of the effective mass of the Bose polaron, and of the mutual interaction between these quasiparticles. In the presence of a nonzero range for the interactions between bath particles, the GP equation transforms into the integral equation discussed in Ref. [33]. We speculate that a similar $\delta^{1/3}$ scaling of quasiparticle properties will be found in that case as well (such scaling being mostly determined by the portion of the wave function lying outside of the potential range). On the other hand, we do not expect that the universality discussed above will extend to reduced spatial dimensions, because in one or two dimensions even an infinitesimal attraction leads to the presence of a two-body bound state.

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[53] Throughout this Letter we consider two-body potentials tuned at their first unitary point. Here we provide their precise functional forms $2mr_c^2U(y)$. Some of those are finite ranged; for example, square well, $-(\pi/2)^2\Theta(1-y)$; shape resonant$_{\rm sw}$, $-12.6(y<0.5), 1.66(0.5<y<1), 0(y>1)$; triangle, $-7.84(1-y)\Theta(1-y)$; smooth, $4.51(1-\tanh\{\tan[\pi(2y-1)/2]\})\Theta(1-y)$. The other ones are instead infinite ranged; Gaussian, $-2.68e^{-y^2}$; shape resonant$_\infty$, $-3.73e^{-y^2}+0.71e^{-y}$. The two potentials termed "shape resonant" have a vanishing effective range ($r_e=0$).

[54] In recent experiments, typical values for $(n_0a_B^3)^{1/4}$ were 0.01 [23], 0.03 [32], and 0.07 [22].

[55] Looking at potentials with a very small R violating the condition (9) may still be interesting from a purely theoretical standpoint, but is out of the scope of the present work. We plan to do it elsewhere.

[56] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevLett.126.123403 for a

stand-alone and detailed derivation of the results presented in the main Letter.

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[59] A subtlety in trying to use Eq. (1) in Eq. (21) is that an additional term in E suppressed by a power of a factor of δ compared to what is presented in Eq. (21) is needed to recover the expression for N.