




Strongly interacting impurities in a dilute Bose condensateNikolay Yegovtsev ¹, Pietro Massignan ², and Victor Gurarie ¹¹*Department of Physics and Center for Theory of Quantum Matter, University of Colorado, Boulder, Colorado 80309, USA*²*Departament de Física, Universitat Politècnica de Catalunya, Campus Nord B4-B5, E-08034 Barcelona, Spain*

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An impurity in a Bose gas is commonly referred to as a Bose polaron. For a dilute Bose gas, its properties are expected to be universal, i.e., dependent only on a few parameters characterizing the boson-impurity interactions. It has been known for some time that when boson-impurity interactions are weak, the properties of the polaron depend only on the scattering length of these interactions. In this paper, which accompanies *Phys. Rev. Lett.* **126**, 123403 (2021) (where some of these results have already been reported), we examine stronger boson-impurity interactions, keeping their range finite. We demonstrate that for attractive interactions between impurity and the bosons up to and including the unitary point, all static properties of a Bose polaron in a dilute Bose gas can be calculated in terms of the scattering length and an additional parameter that characterizes the range of the impurity-boson interactions. Our approach is valid if this parameter does not deviate too much from the scattering length of intraboson interactions, with the precise criterion given in the text. We produce explicit expressions for the energy and other properties of a polaron for the case when the impurity-boson scattering length is tuned to unitarity, and we also provide the first correction away from it.

DOI: [10.1103/PhysRevA.106.033305](https://doi.org/10.1103/PhysRevA.106.033305)**I. INTRODUCTION**

The study of impurities in Bose and Fermi gases has a long history [1–6]. An impurity, i.e., an atom distinguishable from those forming the gas, binds with the atoms of the gas to form a quasiparticle often called a polaron. Polarons in ultracold Fermi gases, both weakly and strongly interacting, have been studied for quite some time [7–16]. Polarons in Bose gases have been getting significant attention over the past decade [17–20]. Somewhat surprisingly, the problem of Bose polarons proved much harder to solve than its fermionic counterpart. The main reason behind the relative simplicity of the Fermi polaron problem is that a Fermi bath is stiff due to the large Pauli repulsion between identical fermions, and a perturbative expansion in particle-hole excitations converges very rapidly to the exact answer. On the other hand, a dilute bosonic bath is highly compressible, and as a consequence even a single impurity can cause major modifications of the surrounding medium. The absence of Pauli pressure in a bosonic bath also leads to much more prominent few-body effects in Bose polarons. For recent developments in the field, we refer the reader to extensive dedicated reviews [21–23].

We would like to apply an expansion in powers of the gas parameter of the Bose gas to the problem of a dilute Bose gas interacting attractively and arbitrarily strongly with a single impurity. We argue that this expansion is valid no matter how strong the boson-impurity interactions are, up to the unitary point, as long as the typical spatial extent of impurity-boson interactions is not too short.

The interactions among the bosons in the gas are taken to be repulsive, with the range roughly of the order of the scattering length of the intraboson interactions, as always the

case for weak repulsive interactions. We further argue that for the purpose of calculations this range can be taken to zero without a qualitative change in the properties of the polaron.

This approach allows us to produce a method to calculate the energy of the Bose polaron at arbitrary negative scattering length characterizing impurity-boson interactions, including when it is infinite. At infinite and close to infinite scattering length, we derive explicit expressions for the energy and other properties of the polaron.

To demonstrate the validity of our approach, we estimate the first subleading term in the expansion in powers of gas parameter. We show that this term is indeed small regardless of the strength of the boson-impurity interactions, under reasonable assumptions on their range. This offers strong support to the claim that the leading term correctly captures the behavior of the impurity when the gas is weakly interacting and the range of the impurity-boson interactions is not too short.

We consider a weakly interacting Bose gas with density n . Suppose a number of impurity atoms are introduced in this gas with density $n_I \ll n$. Let us first briefly consider the thermodynamics of this gas with impurities, following earlier work [24].

The free energy per unit volume of this gas will depend on both densities $F(n, n_I)$. It is advantageous to introduce a “mixed” thermodynamic potential

$$G(\mu, n_I) = F(n, n_I) - \mu n. \quad (1)$$

Here μ is the chemical potential of the gas, $\mu = \partial F / \partial n$. To maintain constant the density of the gas far away from the impurities, we work in the regime where μ is fixed and is independent of n_I .

At small impurity density we expect that $G(\mu, n_I)$ will have a regular Taylor expansion in powers of n_I ,

$$G(\mu, n_I) \approx G(\mu, 0) + E(\mu)n_I + E_2(\mu)n_I^2 + \dots$$

Here $E(\mu)$ is clearly the energy cost of adding a single impurity, while $E_2(\mu)$ and higher-order terms describe interactions among the impurities.

Let us work at a very low density where interactions among the impurities can be neglected. The density of the gas kept at chemical potential μ with the impurity density n_I can now be found according to

$$n = -\frac{\partial G}{\partial \mu} = n_0 - n_I \frac{\partial E}{\partial \mu}, \quad (2)$$

where

$$n_0 = -\frac{\partial G(\mu, 0)}{\partial \mu}$$

is the density of the gas before impurities were introduced.

Multiplying (2) by the volume V on both sides, and noting that Vn_I is the total number of introduced impurities, we find that the number of bosons trapped in the potential created by a single impurity is

$$N(\mu) = -\frac{\partial E}{\partial \mu}. \quad (3)$$

This is a powerful relationship that allows us to concentrate on calculating E while simultaneously also determining the number of trapped bosons N .

The goal of this paper is to calculate $E(\mu)$ and $N(\mu)$. While these quantities can be expected to depend on the details of the interactions among the bosons as well as boson-impurity interactions, and while from the point of view of matching the calculation with experiment it may be important to analyze this problem with the range of parameters relevant for experiment, we expect that the behavior of these functions will be universal to some degree in the limit where the strength of intraboson interactions is taken to zero.

We would like, therefore, to analyze the functions $E(\mu)$ and $N(\mu)$ in the limit of very weak interactions among bosons, while the interaction between the impurity and the bosons remains arbitrary. In particular, the interaction can be allowed to be taken to the unitarity limit where it is effectively the strongest.

As could be expected, we find that in this regime the properties of the polaron do not show any substantial dependence on the range of the boson-boson interactions. However, they do show substantial dependence on the range of the boson-impurity interactions. The results reported here are valid if the range R of the boson-impurity interaction satisfies

$$(n_0 a_B^3)^{1/4} \ll \frac{R}{a_B} \ll \frac{1}{\sqrt{n_0 a_B^3}}. \quad (4)$$

Here a_B is the scattering length of the boson-boson interactions, and n_0 is the density of the Bose gas. Weak interactions among bosons of course imply $n_0 a_B^3 \ll 1$. The first of these two inequalities is obtained by demanding that the gas remains weakly interacting everywhere including at the position of the impurity, while the second of these inequalities asks that the

range of the potential remains smaller than the healing length of the gas.

Note that this excludes the direct comparison of our results to those obtained in the zero range regime where $R \rightarrow 0$ such as Ref. [25]. However, we expect that the conditions (4) are satisfied in experiment, since for realistic interactions $R/a_B \sim 1$.

One of our main results is that in the regime of weak boson-boson interactions, with the range of boson-impurity interaction satisfying the conditions (4), $E(\mu)$ and $N(\mu)$ can be calculated as a function of the boson-impurity scattering length a . In Ref. [26] we showed that in the unitarity limit where a is taken to infinity, they take the analytic form asymptotically valid under the conditions (4),

$$E(\mu) = -\frac{3(\pi n_0)^{2/3}}{2m} \left(\frac{R}{a_B}\right)^{1/3}, \quad (5)$$

$$N(\mu) = \frac{R^{1/3}}{4(\pi n_0 a_B^4)^{1/3}}. \quad (6)$$

Here m is the reduced mass of bosons and impurity defined below in Eq. (9). For the purpose of Eqs. (5) and (6), R needs to be defined quantitatively. A precise definition of R is given below in Eq. (51). We note in passing that our treatment shows that both E and N remain finite even at resonance, due to the presence of repulsion between bath bosons, in agreement with recent work by Schmidt and Enss [27].

Both of these results are asymptotically exact when either a_B or n_0 is taken to zero, as in this limit Eq. (4) is automatically satisfied. The low-density regime is especially interesting, because $E/n_0^{2/3}$ goes to a constant in that limit, a result that may be directly checked in current experiments. In the theory presented in Ref. [25], instead, $E/n_0^{2/3}$ decreased logarithmically at low density.

We also calculate E and N when a deviates from the unitarity limit. While in principle our methods allow us to find these quantities for arbitrary $a < 0$, in practice expressions for those quickly become cumbersome, so we discuss only the expansion of E and N in powers of $1/a$, given in Eq. (57), as well as the behavior of these quantities for small a .

Some of the results reported here already appeared in the earlier work of the authors, Ref. [26]. Specifically, the properties of the polaron at unitarity given by Eqs. (5), (6), as well as the more detailed Eqs. (49) and (50) have already been derived in that work. In the present paper, we go beyond the previously reported results by calculating the properties of the polaron not only exactly at unitarity but also in the vicinity of unitarity as given in Eq. (57), as well as perturbing away from the weak polaron potential limit, as given in Eq. (62). We also discuss the effects of finite-range intraboson interactions, calculate corrections to the results reported here due to quantum fluctuations, and present a number of other results that were not part of the previously reported work.

The rest of this paper is organized as follows. In Sec. II we set up the problem and the techniques we will use to analyze it. Section III describes the solution of the problem both at weak and strong (close to unitarity) impurity-boson attractive interaction, with the simplifying assumption of the intraboson interaction range taken to zero. The first half of this section relies on the results previously reported in Ref. [26]. Section IV

studies fluctuational corrections to the saddle point approximation employed in Sec. III and derives the conditions (4). Section V discusses the implication of finite range intraboson interactions, with the conclusion that the finite range does not strongly affect the behavior of the polaron, unlike the range of the boson-impurity interaction. Section VI discusses a particular technique, expansion about the unperturbed condensate, which, while appealing at first glance, can be shown to fail as one approaches the unitary limit of impurity-boson interactions (see also the discussions in the Appendix, described below). Section VII discusses Bose-impurity interactions that support a bound state, with the conclusion that the polaron behavior in this regime depends on the detailed functional form of these interactions. Section VIII presents our conclusions. Finally, in the Appendix we demonstrate that the technique of Sec. VI, if its range of applicability is ignored, produces the expression (98), which appeared before in the literature [28], but which our analysis indicates is not applicable at strong boson-impurity interactions.

II. SETTING UP THE PROBLEM

We begin with a number of bosons of mass m_b which interact among themselves via a short-range weak interaction V_{bb} , as well as interacting with a single impurity of mass M via another potential U . The problem can be set up according to

$$H = \sum_j \frac{\mathbf{p}_j^2}{2m_b} + \frac{\mathbf{P}^2}{2M} + \sum_{jk} V_{bb}(\mathbf{x}_j - \mathbf{x}_k) + \sum_j U(\mathbf{x}_j - \mathbf{X}).$$

Here \mathbf{x}_j and \mathbf{p}_j are the coordinates and the momenta of the bosons, while \mathbf{X} and \mathbf{P} are the coordinate and the momentum of the impurity.

Before proceeding further, we would like to state explicitly that everywhere in this paper in accordance with conventions common in quantum many-body literature, we set $\hbar = 1$, $k_B = 1$.

As was already exploited in the literature in this context [29,30], it is convenient to get rid of the impurity coordinate by performing the Lee-Low-Pines unitary transformation [31] of the Hamiltonian. Define

$$W = \mathbf{X} \cdot \sum_j \mathbf{p}_j.$$

Straightforward algebra shows that

$$e^{iW} H e^{-iW} = \sum_j \frac{\mathbf{p}_j^2}{2m_b} + \frac{(\mathbf{p}_0 - \sum_j \mathbf{p}_j)^2}{2M} + \sum_{jk} V_{bb}(\mathbf{x}_j - \mathbf{x}_k) + \sum_j U(\mathbf{x}_j).$$

Here \mathbf{p}_0 is the conserved total momentum of the system. In this representation, the position of the impurity has effectively been set at the origin of the reference frame.

We are now going to choose the interactions among bosons to be zero-ranged,

$$V_{bb}(\mathbf{x}) = \lambda \delta(\mathbf{x}). \tag{7}$$

This is a largely technical step that will simplify further analysis of this problem. A very natural question then is whether a similar simplification can be used with the boson-impurity interaction potential U . We will see later that shrinking the range of U to zero is a singular limit as the properties of the boson-impurity cloud crucially depend on the range of the potential U . At the same time, the dependence on the range of V_{bb} is weak and can be neglected. Below we will also explore how the finite range of V_{bb} modifies our conclusions to confirm that the dependence on this range is indeed weak.

We are now in a good position to rewrite the Hamiltonian in the second quantized notation. It is natural to choose U to depend on the distance r to the impurity only, to find

$$\mathcal{H} = \int d^3x \left(\frac{\nabla \bar{\psi} \nabla \psi}{2m} [U(r) - \mu] \bar{\psi} \psi + \frac{\lambda}{2} (\bar{\psi} \psi)^2 \right) + \frac{(\mathbf{p}_0 + i \int d^3x \bar{\psi} \nabla \psi)^2}{2M}. \tag{8}$$

Here μ is the chemical potential of the gas, and m is the reduced mass of the boson and impurity,

$$m = \frac{m_b M}{m_b + M}. \tag{9}$$

The coupling constant λ is related to the scattering length $a_B > 0$ characterizing interactions among bosons by

$$\lambda = \frac{4\pi a_B}{m}.$$

Throughout this paper, we concentrate on the very heavy impurity where M is very large. In this limit, the term on the second line of Eq. (8) can be entirely neglected. We also note that in this limit $m_b = m$. We plan to discuss the effects of the finite impurity mass in a different publication.

We arrive at a very concrete formulation of the problem we would like to solve. A single heavy impurity can be effectively represented by a potential $U(r)$ it induces on the gas, which can be thought of as centered in the origin of the reference frame. Thus Hamiltonian \mathcal{H} of the gas with an infinitely heavy impurity is simply given by Eq. (8) with M taken to infinity, or

$$\mathcal{H} = \int d^3x \left(\frac{\nabla \bar{\psi} \nabla \psi}{2m} + [U(r) - \mu] \bar{\psi} \psi + \frac{\lambda}{2} (\bar{\psi} \psi)^2 \right). \tag{10}$$

To study the problem given by Eq. (10), we rely on the functional integration formalism. To set up the functional integral, we construct the coherent state imaginary time action

$$S = \int_0^{1/T} d\tau \left(\int d^3x \bar{\psi} \frac{\partial \psi}{\partial \tau} + \mathcal{H} \right), \tag{11}$$

where T is temperature. We will eventually take it to zero in most of the calculations, but it is convenient to keep it finite in some of the intermediate steps. With the help of this action we write down the functional integral, which allows us to calculate G defined in Eq. (1),

$$e^{-\frac{VG}{T}} = \int \mathcal{D}\psi e^{-S}. \tag{12}$$

Here V is the volume of the system. The gas we consider here is weakly interacting, which is well known to imply that

$$n_0^{-1/3} \gg a_B. \quad (13)$$

Note that $n_0^{-1/3}$ is the mean interparticle spacing in the gas. The chemical potential μ can be used to define the healing length ξ of the gas according to

$$\mu = 1/(2m\xi^2). \quad (14)$$

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

$$\xi \gg n_0^{-1/3}. \quad (15)$$

III. SOLUTION VIA SADDLE POINT APPROXIMATION

Starting with the functional integral defined by Eqs. (10), (11), and (12), we apply the saddle point approximation to find the Gross-Pitaevskii (GP) equation describing this Bose condensate, which reads

$$-\frac{\Delta\psi}{2m} + U\psi + \lambda|\psi|^2\psi = \mu\psi. \quad (16)$$

Given the solution of this equation ψ , the energy of the polaron can be deduced by the substitution of it into Eq. (10) and subtracting the energy of the condensate without impurity, to give

$$E = -\frac{\lambda}{2} \int d^3x (|\psi|^4 - n_0^2). \quad (17)$$

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

$$N = \int d^3x [|\psi|^2 - n_0]. \quad (18)$$

We note that if the potential does not vary much on the scale of ξ , then the GP equation can be solved using the local density approximation, as is often done in the case in which 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 .

It is natural to ask whether fluctuations about the GP equation are needed to study the polaron. We will argue in Sec. IV that as long as the gas is weakly interacting and the range of the impurity-boson potential satisfies the conditions (4), the GP equation gives a good approximation to the behavior of the polaron.

Equation (16) is nonlinear and at a first glance looks intractable. Nevertheless, we now demonstrate that its analytic solution is possible as long as $R \ll \xi$.

A. Analytic solution to the Gross-Pitaevskii equation in an external potential

We would first like to work with a potential that is strictly zero beyond some length r_c , $U(r) = 0$ for $r > r_c$ (we will later be able to also consider potentials extending all the way to infinity). We introduce

$$\phi = \frac{\psi}{\sqrt{n_0}}.$$

In terms of this dimensionless condensate density function, the GP equation becomes

$$-\frac{\Delta\phi}{2m} + U\phi = \mu\phi(1 - |\phi|^2). \quad (19)$$

Since we are looking for the lowest energy solution, those will be real-valued and spherically symmetric.

We analyze Eq. (19) by introducing a small parameter

$$\epsilon = \frac{r_c}{\xi} \quad (20)$$

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 $0 \leq r \leq r_c$ and $r_c \leq r < \infty$. In the first interval, we introduce

$$y = \frac{r}{r_c}, \quad \phi = \frac{\chi(y)}{y}.$$

$\chi(y)$ satisfies

$$-\frac{d^2\chi}{dy^2} + 2mr_c^2U\chi = \epsilon^2 \left(\chi - \frac{\chi^3}{y^2} \right) \quad (21)$$

on the interval $y \in [0, 1]$, as well as $\chi(0) = 0$. In the second interval, we introduce

$$z = \frac{r}{\xi}, \quad \phi = 1 + \frac{u(z)}{z},$$

to find

$$\frac{d^2u}{dz^2} - 2u = 3\frac{u^2}{z} + \frac{u^3}{z^2} \quad (22)$$

on the interval $z \in [\epsilon, \infty]$, where $u \rightarrow 0$ when $z \rightarrow \infty$. We need to solve Eqs. (21) and (22), matching the behavior of their solutions at the boundary $r = r_c$.

1. Weak potential

Let us first examine the case of a weak attractive potential with a small scattering length $a < 0$. We solve Eq. (21) in the interval $0 \leq y \leq 1$ neglecting its right-hand side as it contains a small parameter ϵ . Then Eq. (21) reduces to a Schrödinger equation in the potential U at zero energy,

$$-\frac{d^2\chi}{dy^2} + 2mr_c^2U\chi = 0, \quad (23)$$

whose solution χ_0 must satisfy $\chi_0(0) = 0$. At $y > 1$ the potential U is zero, so χ must be a linear function. Bethe-Peierls boundary conditions fix the form of this function to be

$$\chi_0(y) = \frac{\alpha}{1 - \frac{r_c}{a}} \left(1 - \frac{r_c}{a} y \right), \quad y > 1, \quad (24)$$

where a is the scattering length in the potential U , and α is the normalization of the solution chosen in such a way that

$$\chi_0(1) = \alpha. \quad (25)$$

We can rewrite Bethe-Peierls boundary conditions in a convenient way by observing that they are equivalent to

$$\chi'_0(1) = \frac{\alpha}{1 - \frac{a}{r_c}}. \quad (26)$$

Now we solve Eq. (22) neglecting its right-hand side to find

$$u = Ae^{-\sqrt{2}z}. \tag{27}$$

We can construct corrections to it by means of successive approximations. Those will be small as long as A is small, and as will be shown below, this is the case here. So for now we neglect those corrections. Matching amplitudes and derivatives of $\chi(y)$ and $u(z)$ at $z = \epsilon$, or correspondingly $y = 1$, produces

$$A = \epsilon(\alpha - 1), \quad -\sqrt{2}A = \frac{\alpha}{1 - \frac{a}{r_c}} - 1. \tag{28}$$

Taking into account that $\epsilon \ll 1$, we find

$$A = -\frac{a}{\xi}, \quad \alpha = 1 - \frac{a}{r_c}. \tag{29}$$

Let us now examine if the terms neglected to arrive at this solution are indeed small. We solve (21) by successive approximations, plugging χ_0 into the right-hand side of Eq. (21) and producing a correction χ_1 . This correction satisfies

$$-\frac{d^2\chi_1}{dy^2} + 2mr_c^2U\chi_1 = \epsilon^2\left(\chi_0 - \frac{\chi_0^3}{y^2}\right). \tag{30}$$

χ_1 could be a small correction to χ_0 since $\epsilon \ll 1$. Looking at it more carefully, we see that if $|a| < r_c$, 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 $\chi_0(1) = \alpha \sim a/r_c$, 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 $\epsilon^2|a|^3/r_c^3 \ll 1$, or equivalently

$$|a|^3 \ll \xi^2 r_c. \tag{31}$$

This is the condition to neglect the right-hand side of Eq. (21) or equivalently to neglect χ_1 relative to χ_0 . We will see later that this condition signifies the transition from the weak impurity potential, where Eq. (31) holds true, to the strong potential including the unitary point $a \rightarrow \infty$, where it is violated.

Under the condition (31) $A \ll 1$, so obviously we can indeed neglect the right-hand side of (22) as we did above.

To compute the energy of the polaron, we can now plug our solution into Eq. (17). The integral in this formula needs to be split into two parts, $0 < r < r_c$ and $r_c < r$. It is easy to see that the contribution of the interval $0 < r < r_c$, under the condition (31), is negligible, so we only need to integrate over $r > r_c$ with $u = A \exp(-\sqrt{2}z)$. Performing the integration and again taking into account Eq. (31) to get rid of some terms suppressed relative to the main contribution, we find

$$E = \frac{2\pi n_0 a}{m}. \tag{32}$$

This is the well known result for the energy of the polaron at weak scattering length $|a| \ll \xi$. We now see that the validity condition for this to hold true is Eq. (31).

We can now take advantage of the relationship (3) to find

$$N = -\frac{\partial E}{\partial \mu} = -\frac{2\pi a}{m} \frac{\partial n_0}{\partial \mu} = -\frac{a}{2a_B}, \tag{33}$$

where $n_0 = \mu m / (4\pi a_B)$ was used. Alternatively, we could substitute our solution into Eq. (18) to find the same result

for the number of trapped particles N . This analysis also tells us that only the negligible number of bosons trapped in the polaron reside within the potential radius r_c . Most of the bosons reside within the cloud whose size is the coherence length $r \lesssim \xi$.

2. Strong potential

Suppose now that the potential U is made more attractive so that its scattering length increases, violating the condition (31) 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. (21) perturbatively, using its right-hand side as a perturbation, to find nonzero $\chi_1'(1)$ contributing to $\chi'(1)$. The same is true for Eq. (22).

In the case when a was small, we found earlier that the amplitude $\chi_0(1) = \alpha$, $\alpha = 1 - a/r_c$. This is of the order of 1 when a is very small, but it starts growing as $|a|$ is increased. When $|a|^3 \sim \xi^2 r_c^2$, $\alpha \sim \epsilon^{-2/3}$. We will see that $\chi(1)$ remains of the order of $\epsilon^{-2/3}$ even as a is taken all the way to infinity, so it is convenient to introduce the notation

$$\beta = \alpha \epsilon^{2/3},$$

so that

$$\chi_0(y) = \frac{\beta}{\epsilon^{2/3}} v(y). \tag{34}$$

Here v is the solution of the Schrödinger equation

$$-\frac{d^2v}{dy^2} + 2mr_c^2Uv = 0 \tag{35}$$

normalized so that $v(1) = 1$. $v'(1) = 0$ since U is tuned to unitarity. β is thus a yet unknown ϵ -independent normalization coefficient.

We will need a correction to this that satisfies

$$-\frac{d^2\chi_1}{dy^2} + 2mr_c^2U\chi_1 = -\epsilon^2 \frac{\chi_0^3}{y^2}. \tag{36}$$

The term $\epsilon^2\chi_0$ from the right-hand side of Eq. (30) goes as $\epsilon^{4/3}$ and can be neglected. At the same time, we see that χ_1 is of the order of ϵ^0 . Solving Eq. (36) gives

$$\chi_1 = \beta^3 v(y) \int_0^y \frac{ds}{v^2(s)} \int_0^s \frac{dt v^4(t)}{t^2}.$$

Putting it together produces

$$\chi = \frac{\beta}{\epsilon^{2/3}} v(y) + \beta^3 v(y) \int_0^y \frac{ds}{v^2(s)} \int_0^s \frac{dt v^4(t)}{t^2} + \dots \tag{37}$$

The next term χ_2 which can be obtained by continuing successive approximations goes as $\epsilon^{2/3}$. We will not need it here, but note that it will have an even more complicated dependence on v and by extension on features of the potential $U(r)$ than the already obtained term χ_1 .

From this solution, we find that

$$\chi(1) = \frac{\beta}{\epsilon^{2/3}} + O(1), \quad \chi'(1) = \beta^3 c + O(\epsilon^{2/3}), \tag{38}$$

where the dimensionless coefficient c is defined via

$$c = \int_0^1 \frac{dy v^4(y)}{y^2}. \quad (39)$$

Now we turn our attention to Eq. (22). Its solution $u(z)$ needs to be matched with the boundary conditions (38). It is easy to verify that these boundary conditions imply

$$u(\epsilon) = \beta\epsilon^{1/3} + O(\epsilon), \quad u'(\epsilon) = -1 + \beta^3 c + O(\epsilon^{2/3}). \quad (40)$$

Equation (22) differs from Eq. (21) in that its nonlinear terms do not have an explicit factor of ϵ in front of them. We will nonetheless solve Eq. (22) by means of successive approximations, and verify later that this is a legitimate approach. Without its right-hand side, the solution to Eq. (22) reads as before,

$$u_0(z) = A e^{-\sqrt{2}z}. \quad (41)$$

We can plug it into the right-hand side of Eq. (22), however we will follow a slightly different procedure. We use Eq. (41) to rewrite Eq. (22) as an integral equation via a standard procedure. This involves solving the auxiliary equation

$$\frac{d^2 u}{dz^2} - 2u = g(z)$$

with arbitrary given $g(z)$, then substituting the actual right-hand side of Eq. (22). We find

$$u(z) = A e^{-\sqrt{2}z} + \frac{e^{-\sqrt{2}z}}{2\sqrt{2}} \int_z^\infty \frac{ds e^{\sqrt{2}s}}{s} (3u^2(1+u') + \sqrt{2}u^3) - \frac{e^{\sqrt{2}z}}{2\sqrt{2}} \int_z^\infty \frac{ds e^{-\sqrt{2}s}}{s} (3u^2(1+u') - \sqrt{2}u^3). \quad (42)$$

We now use this equation to calculate $u(\epsilon)$ and $u'(\epsilon)$ in perturbative expansion in powers of ϵ . Anticipating that the leading behavior $A \sim \epsilon^{1/3}$, as should be clear from comparing Eqs. (41) and (40), we iterate Eq. (42) by plugging $u_0(z)$ into the right-hand side of Eq. (42). The resulting integrals can be computed in terms of Γ functions and expanded in powers of ϵ . We omit rather lengthy algebra involved, and just state that this allows us to evaluate $u(\epsilon)$ to find

$$u(\epsilon) = A + \frac{3 \ln 3}{2\sqrt{2}} A^2 - A^3 \ln \epsilon + O(\epsilon). \quad (43)$$

We also evaluate $u'(\epsilon)$. Differentiating Eq. (42) gives

$$u'(z) = -\sqrt{2}A e^{-\sqrt{2}z} - \frac{u^3}{z} - \frac{e^{-\sqrt{2}z}}{2} \int_z^\infty \frac{ds e^{\sqrt{2}s}}{s} (3u^2(1+u') + \sqrt{2}u^3) - \frac{e^{\sqrt{2}z}}{2} \int_z^\infty \frac{ds e^{-\sqrt{2}s}}{s} (3u^2(1+u') - \sqrt{2}u^3). \quad (44)$$

We can again substitute $u_0(z)$ into the integrals on the right-hand side of Eq. (44) to find

$$u'(\epsilon) = -\sqrt{2}A - \beta^3 + 3A^2 \ln \epsilon + O(\epsilon^{2/3}). \quad (45)$$

Here we took advantage of the boundary conditions (40), which tell us that $u(\epsilon) = \beta\epsilon^{1/3}$ within the accuracy with which we work.

Combining Eqs. (43) and (45) with Eq. (40) gives

$$A + \frac{3 \ln 3}{2\sqrt{2}} A^2 - A^3 \ln \epsilon = \beta\epsilon^{1/3}, \quad (46)$$

$$-\sqrt{2}A - \beta^3 + 3A^2 \ln \epsilon = -1 + \beta^3 c.$$

We now need to solve these equations for A and β perturbatively, in powers of ϵ . Introduce

$$\delta = \frac{\epsilon}{1+c}.$$

The solution to Eq. (46) reads

$$A = \delta^{1/3} - \left(\frac{3 \ln 3}{2\sqrt{2}} + \frac{\sqrt{2}}{3} \right) \delta^{2/3} + 2\delta \ln \delta + O(\delta),$$

$$\beta\epsilon^{1/3} = \delta^{1/3} - \frac{\sqrt{2}}{3} \delta^{2/3} + \delta \ln \delta + O(\delta). \quad (47)$$

We can now use the parameters we obtained in this way to calculate the energy and the particle number of the polaron. It turns out to be technically easier to calculate the particle number first and then use Eq. (3) to find the energy, which is the strategy we will follow here.

The excess number of particles due to the polaron is given by Eq. (18) or

$$N = \int d^3x [|\psi|^2 - n_0] = 4\pi n_0 \xi^3 \int_0^\infty z^2 dz [\phi^2 - 1].$$

It is natural to split the integral over z into two intervals, from 0 to ϵ and from ϵ to infinity. Now the contribution of the first interval can be safely neglected. Indeed, it gives

$$\int_0^\epsilon z^2 dz [\phi^2 - 1] = \epsilon^3 \int_0^1 dy \left(\frac{\chi^2}{y^2} - 1 \right) \sim \epsilon^{5/3}.$$

Here we used that $\chi(y) \sim 1/\epsilon^{2/3}$. This contribution is very small and exceeds the accuracy in ϵ with which we were doing our calculations. This also indicates that the bulk of the particles bound by the impurity are located farther than distance r_c away from the impurity. The contribution of the second interval gives

$$\int_\epsilon^\infty z^2 dz \left(\left(1 + \frac{u}{z} \right)^2 - 1 \right). \quad (48)$$

To evaluate this integral, we again iterate Eq. (42) once to find u up to the terms of the order of A^2 , and we substitute that into Eq. (48). The result of this evaluation is

$$N = 4\pi n_0 \xi^3 \left(\delta^{1/3} - \frac{5}{3\sqrt{2}} \delta^{2/3} + 2\delta \ln \delta + \dots \right). \quad (49)$$

It should be clear that all these excess particles reside roughly within the cloud whose size is given by the coherence length of the condensate ξ , similarly to the polaron at weak impurity potential, Eq. (33). Only a negligible number of bosons reside within the impurity potential at distances $r \lesssim r_c$.

Thus we evaluated the number of particles trapped in the polaron up to terms of the order of $\delta \ln \delta$. To go beyond this order, starting from terms of the order of δ and beyond represented by the dots above, we would need to go beyond the terms presented in Eq. (37). We expect that this will produce

terms that depend on the features of the potential other than the coefficient c .

To construct the energy of the polaron, it is easiest at this stage to take advantage of Eq. (3). The subtlety in evaluating the derivative there is that the particle number n_0 as well as ξ have to be traded for μ before differentiating. Doing the algebra, we arrive at

$$E = -\frac{\pi n_0 \xi}{m} (3\delta^{\frac{1}{3}} - 2\sqrt{2}\delta^{\frac{2}{3}} + 4\delta \ln \delta + \dots). \quad (50)$$

This constitutes the answer that we seek, namely the energy of the polaron at unitarity as an expansion in powers of $\delta \sim r_c/\xi$. Finally, let us examine $\delta = \epsilon/(1+c)$ in a little more detail. From the definition of c given in Eq. (39), we can write

$$1+c = 1 + r_c \int_0^{r_0} \frac{dr v^4}{r^2} = r_c \left(\int_{r_c}^{\infty} \frac{dr}{r^2} + \int_0^{r_c} \frac{dr v^4}{r^2} \right).$$

v is the solution of the Schrödinger equation with the potential tuned to unitarity, so that $v'(r_c) = 0$. Since it is normalized such that $v(r_c) = 1$, it will naturally satisfy $v(r) = 1$ for all $r \geq r_c$.

Therefore, we can rewrite this as

$$1+c = r_c \int_0^{\infty} \frac{dr v^4}{r^2}.$$

Now

$$\delta = \frac{\epsilon}{1+c} = \frac{1}{\xi \int_0^{\infty} \frac{dr v^4}{r^2}}.$$

It is now convenient to define

$$R^{-1} = \int_0^{\infty} \frac{dr v^4}{r^2} = \int \frac{d^3x}{4\pi} |\psi_0|^4, \quad (51)$$

where $\psi_0 = v/r$ is the solution of the Schrödinger equation

$$-\frac{\Delta}{2m} \psi_0 + U \psi_0 = 0.$$

R constitutes a properly defined range of the potential, finite even for potentials that extend all the way to infinity, which correctly captures its extent for the purposes of solving the polaron problem.

This gives us a definition

$$\delta = \frac{R}{\xi}. \quad (52)$$

At this stage, r_c drops from the equations and no longer needs to be finite. It can be taken to infinity if desired, with the answer for the energy of the polaron (50) as well as the number of particles trapped in the polaron (49) expressed entirely in terms of $\delta = R/\xi$.

Finally, we remark that for small δ , only the first terms in the expressions (49) and (50) should be retained. Then these two expressions can be rewritten in the form (6) and (5) given earlier by expressing ξ in terms of a_B .

3. Perturbing away from unitary point

We can go further and generalize the above analysis to account for the small deviations away from unitarity using a $1/a$

expansion. To accomplish this, it is convenient to parametrize a by a new variable η according to

$$\eta = \frac{r_c^{1/3} \xi^{2/3}}{a}. \quad (53)$$

Declaring $\eta \ll 1$ is equivalent to saying that we are in the strongly interacting regime [compare with the condition (31), which is violated once we cross over from weak to strong potentials, as explained earlier]. We then proceed to work out the expansion in powers of η . The advantage of this reparametrization is due to the form that Bethe-Peierls boundary conditions take. Indeed, Eq. (26) at large a , where close to unitarity we should write $\alpha = \beta/\epsilon^{2/3}$, implies

$$\frac{\beta}{\epsilon^{2/3}(1-\frac{a}{r_c})} \approx -\frac{\beta r_c}{\epsilon^{2/3}a} = -\beta\eta. \quad (54)$$

Because $r_c/a \sim \epsilon^{2/3}$, the correction to the nonlinear term and that to the right-hand side of the top equation in (46), which arise from the correction to $v(y)$ in Eq. (37), are of higher order in powers of ϵ and thus can be neglected. Thus slightly away from unitarity, the only modification to the formalism presented in the previous section is the addition of the $-\beta\eta$ term to the right-hand side of the second equation in (46):

$$\begin{aligned} A + \frac{3 \ln 3}{2\sqrt{2}} A^2 - A^3 \ln \epsilon &= \beta \epsilon^{1/3}, \\ -\sqrt{2}A - \beta^3 + 3A^2 \ln \epsilon &= -1 - \beta\eta + \beta^3 c. \end{aligned} \quad (55)$$

Notice that now in order to find the leading term in the expansion of β in powers of ϵ , we have to solve the cubic equation:

$$\beta_0^3(1+c) - \beta_0\eta - 1 = 0.$$

The number of real roots of this equation depends on the value of the discriminant $\Delta = 4(\frac{\eta}{1+c})^3 - \frac{27}{(1+c)^2}$. If $\Delta > 0$, there are three real roots, and if $\Delta < 0$, there is only a single real root. The critical value of η is obtained by setting $\Delta = 0$, and it gives $\eta_c = (\frac{27(1+c)}{4})^{1/3} > 0$. A positive value of η corresponds to a positive value of the scattering length, which means that we are in the regime where the potential has a single bound state. It is known that when a potential admits ν number of bound states, then the GP equation can have up to $2\nu + 1$ solutions [24]. This means that the approach outlined above can in principle be used to construct other solutions for the GP equation, but since we are interested only in the ground-state physics, we do not consider them here. Instead, just as already elaborated on earlier, we are going to assume that $|\eta| \ll 1$, so that we are in the regime where there is only a single solution and we can do an expansion in η on top of the expansion in ϵ . The first-order correction in $1/a$ corresponds to the first-order correction in η . Note that the case of a large and positive scattering length corresponds to the presence of the bound state with energy $E_{\text{binding}} = -\frac{1}{2ma^2}$. Since $r_c/a = \eta\epsilon^{2/3}$, in order to capture $1/a^2$ effects we would need to construct further corrections to the matching equations that would include higher powers of ϵ and therefore depend on other details of the potential. Therefore, in the lowest-order approximation

in η that we are going to employ, we are not sensitive to the presence of the bound state even if a is positive.

Section VII further elaborates on what we expect to happen in the regime where $a > 0$ and a bound state is present once we move away from the unitary point. In particular, we

expect that in this regime the behavior of the polaron strongly depends on the details of the impurity-boson potential U .

Let us go back to staying in the vicinity of the unitary point by demanding $|\eta| \ll 1$. Since $\frac{\eta}{(1+c)^{1/3}} = \frac{\delta^{1/3}\xi}{a}$, the solution to the system (55) reads

$$A = \delta^{1/3} \left(1 + \frac{\delta^{1/3}\xi}{3a} \right) - \left(\frac{3 \ln 3}{2\sqrt{2}} + \frac{\sqrt{2}}{3} \right) \delta^{2/3} - \frac{\xi\delta}{\sqrt{2}a} \ln 3 + 2 \left(1 + \frac{2\delta^{1/3}\xi}{3a} \right) \delta \ln \delta + O(\delta),$$

$$\beta\epsilon^{1/3} = \delta^{1/3} \left(1 + \frac{\delta^{1/3}\xi}{3a} \right) - \frac{\sqrt{2}}{3} \delta^{2/3} + \left(1 + \frac{\delta^{1/3}\xi}{3a} \right) \delta \ln \delta + O(\delta). \quad (56)$$

Note that at this step r_c dropped out just like it did in the previous subsection of this paper, getting replaced by R via the definition (52). R is defined even with potentials that extend all the way to infinity, so the results obtained here, just as elsewhere in this paper, are valid as long as R can be defined via Eq. (51) and is finite.

Repeating the same steps that lead to (49) and (50), we finally obtain the expression for the number of trapped bosons and the energy of the polaron:

$$N = 4\pi n_0 \xi^3 \left[\delta^{1/3} - \frac{5}{3\sqrt{2}} \delta^{2/3} + 2\delta \ln \delta + \dots + \frac{\xi\delta^{1/3}}{3a} (\delta^{1/3} - \sqrt{2}\delta^{2/3} + 4\delta \ln \delta + \dots) \right],$$

$$E = -\frac{\pi n_0 \xi}{m} \left[3\delta^{1/3} - 2\sqrt{2}\delta^{2/3} + 4\delta \ln \delta + \dots + \frac{\xi\delta^{1/3}}{a} \left(2\delta^{1/3} - \frac{4\sqrt{2}}{3}\delta^{2/3} + 4\delta \ln \delta + \dots \right) \right]. \quad (57)$$

We verify the above expressions by numerically solving the GP equation (16), where we choose U to be the square-well potential. The analytic expression for the scattering length in this potential is well known, so it is easy to tune the strength of the potential to get the desired value of a . Far away from impurity, one can use the asymptotic solution $\phi = 1 + \frac{u}{z}$, where u is given by Eq. (27). With two values of parameter A , namely A_{\min} and A_{\max} , our algorithm performs the Newton bisection until we find the value of A such that the derivative of the solution at the origin is zero. The graphs of the polaron energy and the number of trapped bosons slightly away from unitarity are presented in Figs. 1 and 2.

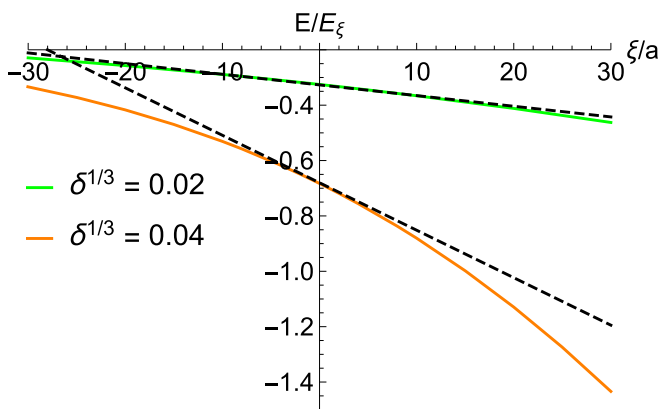


FIG. 1. Polaron energy E away from unitarity for the square-well impurity-bath potential computed at two different values of δ . The two solid lines correspond, from top to bottom, to $\delta^{1/3} = 0.02$ and 0.04 . The dashed black lines correspond to the analytical expression given by Eq. (57). The energy is plotted in units of $E_\xi = \xi n_0 / (2m)$.

4. a/ξ corrections for weak potentials

Now that we have established the machinery for solving the GP equation in both regions, let us revisit the case of the weak potential and find the next-order correction to the energy (32) in powers of the scattering length a . Note that the contribution to the energy from the first interval goes in powers of a/r_c , while in the second interval it is in powers of $a/\xi = a\epsilon/r_c$, so in principle the energy expansion should be in powers of $(\frac{a}{r_c})^i \epsilon^j$. Moreover, from the equation one can show that the contribution of the region $z \in [0, \epsilon]$ to the energy goes as $\sim \frac{n_0 a}{m} (\epsilon + \frac{a}{\xi} \epsilon)$, while the region $z \in [\epsilon, \infty]$

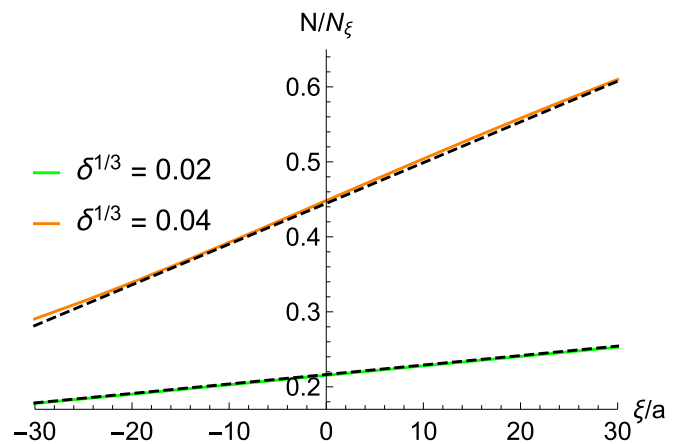


FIG. 2. Number of trapped bosons N (in units of $N_\xi = \xi^3 n_0$) away from unitarity for the square-well impurity-bath potential computed at two different values of δ . The two solid lines correspond, from bottom to top, to $\delta^{1/3} = 0.02$ and 0.04 . The dashed black lines correspond to the analytical expression given by Eq. (57).

contributes $\sim \frac{n_0 a}{m} (1 + \frac{a}{\xi})$, so in the limit $\epsilon \rightarrow 0$, only the second region is important. The $\sim a^2$ contribution to the energy comes from the $\frac{a^2}{r_c^2} \epsilon^2$ term, so in order to find the energy up to order a^2 , one needs to find the expression for the amplitude A in the second region up to order ϵ^2 . The structure of equations in (28) tells us that the matching of amplitudes determines A , while the matching of derivatives determines α . Since we need to know only A up to order ϵ^2 , we need to correct the first equation by the terms of order ϵ^2 , while the second only by the terms of order ϵ . Notice that iteration of the right-hand side of Eq. (22) will produce terms of higher order than we need, so this tells us that the result should be independent of the further details of the potential. Having in mind that $A \sim \epsilon$, in the second interval we expand Eq. (42) up to ϵ^2 terms to produce

$$A + \frac{3 \ln 3}{2\sqrt{2}} A^2 - \sqrt{2} \epsilon A = \epsilon(\alpha - 1),$$

$$-\sqrt{2} A = \frac{\alpha}{1 - \frac{a}{r_c}} - 1. \tag{58}$$

Looking for the solution of this system in the form $\alpha = \alpha_0 + \epsilon \alpha_1$ and $A = \epsilon A_0 + \epsilon^2 A_1$, we get

$$\alpha = 1 - \frac{a}{r_c} + \sqrt{2} \frac{a}{r_c} \left(1 - \frac{a}{r_c}\right) + O(\epsilon^3 \ln \epsilon),$$

$$A = -\frac{a}{r_c} \epsilon - \frac{(4 + 3 \ln 3)}{2\sqrt{2}} \left(\frac{a}{r_c} \epsilon\right)^2 + O(\epsilon^3 \ln \epsilon). \tag{59}$$

The energy of the polaron is given by

$$E = -\frac{\lambda}{2} \int d^3x (|\psi|^4 - n_0^2) = -2\pi \lambda n_0^2 \xi^3 \int_0^\infty dz z^2 (\phi^4 - 1). \tag{60}$$

The region from 0 to ϵ does not contribute, while the second interval produces

$$\int_\epsilon^\infty dz z^2 \left(\left(1 + \frac{u}{z}\right)^4 - 1 \right). \tag{61}$$

Once again, we use Eq. (42) with A given by Eq. (59) to compute the integral in Eq. (61) and expand the result up to ϵ^2 terms. Plugging this into Eq. (60), we finally produce

$$E = \frac{2\pi n_0 a}{m} \left(1 + \frac{\sqrt{2} a}{\xi} + \dots \right). \tag{62}$$

The second term in the parentheses was obtained before in Ref. [32]. This shows that the GP approach discussed above is well suited for studying both weak potentials and potentials tuned to unitarity.

5. Quasiparticle properties of the Bose polaron

Having established the expressions for the solution of the GP equation, now we can compute other key quasiparticle properties such as quasiparticle residue Z and Tan’s contact C . This was already reported in Ref. [26]. Let us reproduce it here for completeness.

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 [33]

$$\ln Z = - \int d^3x |\psi(x) - \sqrt{n_0}|^2.$$

At unitarity, the above analysis shows that to leading order,

$$\ln Z = -\sqrt{2} \pi n_0 \xi^3 \delta^{2/3} + \dots$$

Another key quasiparticle property is the impurity-bath Tan contact, which quantifies the change in the polaron energy in response to a small change of the inverse scattering length,

$$C = -8\pi m \frac{\partial E}{\partial (a^{-1})}.$$

Using the expression (57) for energy of the polaron slightly away from unitarity, we obtain

$$C = 16\pi^2 n_0 \xi^2 \left(\delta^{2/3} - \frac{2\sqrt{2}}{3} \delta + 2\delta^{4/3} \ln \delta + \dots \right). \tag{63}$$

We note that an alternative definition of the contact is based on the impurity-bath density-density correlator evaluated at the core radius, $\tilde{C} = 16\pi^2 r_c^2 |\psi(r_c)|^2$. Using the expression (47) for the amplitude β of the GP equation at the core radius, it is easy to show that both expressions for contact agree in the universal regime, where the effects of impurity-boson potentials are captured by a single parameter δ .

B. Summary: The solution of the Gross-Pitaevskii equation

We collect here the main features of the solutions worked out above. In the previous subsection, we obtained the solution to the GP equation (16) both when the scattering length in the potential U was small and when the potential U was tuned to unitarity. In the latter case, we could obtain the analytic solution when the range of the potential R was much smaller than the scattering length ξ , as an expansion in powers of R/ξ which corresponded to the asymptotic behavior of the polaron in a very weakly interacting condensate.

The method discussed above allows us in principle to find the solution for any negative scattering length, from small a to infinite a . However, the general expression is cumbersome. Here we only give the answer in the limiting cases of small a and large a .

Let us summarize how the solution looks. In all cases, the normalized solution $\phi = \psi/\sqrt{n_0}$ to the GP equation

$$-\frac{\Delta \phi}{2m} + U\phi = \mu\phi(1 - |\phi|^2)$$

is constructed out of a reference function $v(y)$, which is the solution of the zero-energy Schrödinger equation

$$-\frac{d^2 v}{dy^2} + 2mr_c^2 U(y) v = 0. \tag{64}$$

Here $y = r/r_c$, where r_c is the radius of the potential, so that $U(r) = 0$ for all $r > r_c$ or $y > 1$. $v(0) = 0$, while $v(1) = 1$.

When a is small so that

$$|a|^3 \ll \xi^2 r_c, \tag{65}$$

the solution is

$$\phi(r) \approx \begin{cases} \frac{r_c}{r} \left(1 - \frac{a}{r_c}\right) v\left(\frac{r}{r_c}\right), & r < r_c, \\ 1 - \frac{a}{r} e^{-\frac{\sqrt{2}r}{\xi}}, & r > r_c. \end{cases} \quad (66)$$

This can be extracted from Eqs. (24), (27), and (29). Note that Eq. (66) is valid even if $a/r_c > 1$, as long as Eq. (65) is valid.

On the other hand, if

$$|a|^3 \gg \xi^2 r_c, \quad (67)$$

then the solution is

$$\phi(r) \approx \begin{cases} \frac{\xi^{2/3} R^{1/3}}{r} v\left(\frac{r}{r_c}\right), & r < r_c, \\ 1 + \frac{\xi^{2/3} R^{1/3}}{r} e^{-\frac{\sqrt{2}r}{\xi}}, & r > r_c. \end{cases} \quad (68)$$

This in turn can be extracted from Eqs. (34), (41), and (47).

Clearly the solution behaves as if when $|a|$ is increased past $\xi^{2/3} R^{1/3}$, a needs to be simply replaced by $-\xi^{2/3} R^{1/3}$ in the solution.

The energy and the particle number corresponding to this solution have been worked out above in Eqs. (49) and (50), and summarized in Eqs. (5) and (6). We also worked out perturbative corrections to the solution for small a and for large a in Secs. III A 4 and III A 3, respectively, with the results for the energy in particular summarized in Eqs. (62) and (57).

IV. FLUCTUATIONAL CORRECTIONS TO THE GROSS-PITAEVSKII EQUATION

Let us look at the condensate density at and nearby the point where impurity is located. This can be extracted from the solution of the GP equation found above. The density grows as one approaches the center of the polaron. At $r < r_c$, the solution is given by Eq. (34). Here v is the solution of the Schrödinger equation (35), so it takes values of the order of 1 for all $0 < r < r_c$. The magnitude of the solution is controlled by the coefficient in front of $v(y)$, which is of the order of $1/\epsilon^{2/3}$. Therefore, the density of the condensate at the origin is roughly

$$n(0) \sim \frac{n_0}{\epsilon^{4/3}}.$$

We can now estimate the gas parameter at the position of the impurity,

$$n(0)a_B^3 = \frac{n_0 \xi^{4/3} a_B^3}{R^{4/3}} \sim n(0)^{1/3} \frac{a_B^{7/3}}{R^{4/3}}.$$

The condition that this parameter is small, or

$$\frac{n_0}{\epsilon^{4/3}} a_B^3 \ll 1, \quad (69)$$

is equivalent, upon expressing ϵ in terms of n_0 , a_B , and R , to

$$R \gg a_B (n_0 a_B^3)^{1/4}. \quad (70)$$

Under this condition, the gas remains weakly interacting everywhere, including at the position of the impurity. We expect that the fluctuational corrections remain small under these conditions, and the results obtained from GP equation remain valid.

Let us briefly note that the criterion (70) puts a lower bound on R . But at the same time, our solution of the GP

equation relied on R being much smaller than ξ . This criterion can be rewritten as

$$\delta = \frac{R}{\xi} \sim \frac{R}{a_B} \sqrt{n_0 a_B^3} \ll 1.$$

Combining this with Eq. (70), we find the window of R where our approach works, given by

$$(n_0 a_B^3)^{1/4} \ll \frac{R}{a_B} \ll \frac{1}{\sqrt{n_0 a_B^3}},$$

as was advertised earlier in Eq. (4). Let us now present the formalism where we formally derive this criterion. We follow the standard approach to fluctuations in a weakly interacting Bose gas. Denote the solution to the GP equation (16) as ψ_0 and write

$$\psi = \psi_0 + \varphi. \quad (71)$$

We now substitute this into the action (11) and expand the action up to the quadratic terms in φ . These steps are standard in the theory of weakly interacting Bose gas. The only new aspect of this problem here is the impurity potential U present in our theory. The result of the expansion reads

$$S_q = \int d^3x d\tau \left[\bar{\varphi} \left(\partial_\tau - \mu - \frac{\Delta}{2m} + U + 2\lambda \psi_0^2 \right) \varphi + \frac{\lambda}{2} \psi_0^2 (\varphi^2 + \bar{\varphi}^2) \right]. \quad (72)$$

Here S_q denotes the part of the action quadratic in the field φ .

This action can now be used to calculate the density of particles that are expelled from the condensate by interactions and are not contained within the solution to the GP equation. This density must be much smaller than the density contained within the solution to the GP equation in order for the mean-field approximation which led to the GP equation to remain valid. In the absence of the potential U , this calculation is standard and the answer is given in textbooks, leading to the criterion $n_0 a_B^3 \ll 1$ as the condition for the applicability of the GP equation. Our aim is to repeat this calculation in the presence of the impurity potential U .

The density of particles can be accessed via calculating the Green's functions of the field φ . As is standard in this approach, we define the matrix of Green's functions \mathcal{G} which include both normal and anomalous Green's functions, according to

$$\mathcal{G}(x_1, x_2, \tau) = - \begin{pmatrix} \langle \varphi(x_1, \tau) \bar{\varphi}(x_2, 0) \rangle \langle \varphi(x_1, \tau) \varphi(x_2, 0) \rangle \\ \langle \bar{\varphi}(x_1, \tau) \bar{\varphi}(x_2, 0) \rangle \langle \bar{\varphi}(x_1, \tau) \varphi(x_2, 0) \rangle \end{pmatrix}.$$

It is convenient to work with \mathcal{G} in the frequency domain, by Fourier transforming it over τ resulting in $\mathcal{G}(x_1, x_2, \omega)$. Note that it is not as straightforward to Fourier transform \mathcal{G} in space, because the presence of the impurity makes \mathcal{G} dependent on both x_1 and x_2 and not just on their difference, as would have been the case in the Bose-Einstein condensate without the external potential U .

\mathcal{G} satisfies the following matrix equation:

$$\mathcal{X}(x_1) \mathcal{G}(x_1, x_2, \omega) = -\delta(x_1 - x_2), \quad (73)$$

where \mathcal{X} is the operator-valued matrix

$$\mathcal{X} = \begin{pmatrix} -i\omega - \frac{\Delta}{2m} - \mu + U + 2\lambda\psi_0^2 & \lambda\psi_0^2 \\ \lambda\psi_0^2 & i\omega - \frac{\Delta}{2m} - \mu + U + 2\lambda\psi_0^2 \end{pmatrix}. \quad (74)$$

In the definition of \mathcal{X} , the Laplacian Δ implies differentiation over x_1 , while ψ_0 and U depend on x_1 . These equations are difficult to solve exactly given this explicit x_1 dependence.

Instead of trying to solve these exactly, we employ the local density approximation. That includes working with a Wigner transform of \mathcal{G} defined as

$$\mathcal{G}(x, p, \omega) = \int d^3y \mathcal{G}(x + y/2, x - y/2, \omega) e^{-iy \cdot p}.$$

This object can be calculated approximately by replacing Δ [Eq. (74)] by $-p^2$ and working with it as if V and ψ_0 are constants, despite their explicit dependence on x_1 . Within this approximation, $\mathcal{G}(x, p, \omega)$ is given simply by the inverse of this matrix derived from \mathcal{X} ,

$$\begin{pmatrix} -i\omega + \frac{p^2}{2m} - \mu + U + 2\lambda\psi_0^2 & \lambda\psi_0^2 \\ \lambda\psi_0^2 & i\omega + \frac{p^2}{2m} - \mu + U + 2\lambda\psi_0^2 \end{pmatrix}.$$

In particular, the upper left corner of that inverse defines the usual normal Green's function and gives

$$G(x, p, \omega) = -\frac{i\omega + \frac{p^2}{2m} - \mu + U(x) + 2\lambda\psi_0^2(x)}{\omega^2 + \left(\frac{p^2}{2m} + U(x) + \lambda\psi_0^2(x)\right)^2 - \lambda^2\psi_0^4(x)}. \quad (75)$$

Equation (75) is by no means exact. It is the result of the local density approximation, which relies on $\psi_0(x)$ and $U(x)$ being slowly varying on the scale of the coherence length ξ , which itself defines the values of the typical momenta p . Because of this, it is sometimes also referred to as the gradient expansion, with Eq. (75) being the first term in it. An explicit procedure allowing to compute further terms in this expansion is available, but it will not be needed here.

Now in practice $\psi_0(x)$ varies roughly on the scale of ξ , so it is at the limit of the applicability of the local density approximation. $U(x)$ varies on the scale of $r_0 \ll \xi$ so it definitely breaks the conditions of applicability of Eq. (75). Nonetheless, in the absence of a better and equally accessible technique, and mindful that our goal is not to calculate the fluctuational particle density but just to estimate it, we will continue the calculation using Eq. (75).

To calculate the density of particles due to fluctuations, we need to calculate $\delta n = \langle \bar{\varphi}(x, 0)\varphi(x, 0) \rangle$. This can be found by the following succession of steps. First we evaluate

$$-\lim_{\tau \rightarrow 0^-} \int \frac{d\omega}{2\pi} G(x, p, \omega) e^{-i\omega\tau},$$

with the result

$$\delta n(x, p) = \frac{\frac{p^2}{2m} - \mu + U(x) + 2\lambda\psi_0^2(x) - E(p, x)}{2E(p, x)},$$

where

$$E(p, x) = \sqrt{\left(\frac{p^2}{2m} - \mu + U(x) + 2\lambda\psi_0^2(x)\right)^2 - \lambda^2\psi_0^4(x)} \quad (76)$$

can be interpreted as a local in space dispersion of the Bogoliubov quasiparticles. The density of particles due to fluctuations can be evaluated using

$$\delta n(x) = \int \frac{d^3p}{(2\pi)^3} \delta n(x, p). \quad (77)$$

To evaluate the remaining integral over the momentum, we need the explicit form of ψ_0 . Let us do it at U tuned to unitarity. We can then use Eq. (68) for ψ_0 . In particular, with r representing the distance of the point x to the origin, for $r \gg r_c$ we use that

$$\lambda\psi_0^2 \approx \mu \left(1 + \frac{2\xi^{2/3}R^{1/3}}{r} e^{-\frac{\sqrt{2}r}{\xi}} + \dots \right). \quad (78)$$

At the same time, at these values of r beyond the range of the potential, $U = 0$. This can be substituted into the integral in Eq. (77), and the integral can be evaluated perturbatively in powers of the second term in Eq. (78), which is small when $r \gg r_c$. Denoting this term as

$$\zeta = 2 \frac{\xi^{1/3}R^{2/3}}{r} e^{-\frac{\sqrt{2}r}{\xi}},$$

we find

$$\delta n(x) = \delta n_0 + \frac{(m\mu)^{3/2}}{32} \zeta \ln \zeta.$$

Here $\delta n_0(x)$ is the standard answer for the density of particles expelled from the condensate in the absence of any external potential, given by $\delta n_0 = -4(m\mu)^{3/2}/(3\pi^2)$.

Let us compare the density of particles expelled from the condensate to the excess density of particles in the GP solution compared to the density in the absence of impurity. The latter is extracted from Eq. (78) and is simply $n_0\zeta$. Thus the condition that the density of particles expelled from the condensate is much smaller than the density in the solution to GP solution is

$$(m\mu)^{3/2} \zeta \ln \zeta \ll n_0\zeta. \quad (79)$$

Recalling that $\mu m \sim n_0 a_B$ and neglecting the logarithm in (79), this is equivalent to

$$n_0 a_B^3 \ll 1.$$

Thus we arrive at the conclusion that at $r \gg r_c$ the fluctuational corrections to the solution of the GP equation are small simply if the interactions in the Bose gas are weak.

Now suppose we bring r close to r_c . At this point U is still zero, but the estimate for $\lambda\psi_0$ again taken from Eq. (68) produces

$$\lambda\psi_0^2 \sim \frac{\mu}{\epsilon^{4/3}}.$$

Evaluating Eq. (77) again produces

$$\delta n(x) \sim \frac{(m\mu)^{3/2}}{\epsilon^2}.$$

The condition that this is much smaller than the density from the GP solution gives

$$\frac{(m\mu)^{3/2}}{\epsilon^2} \ll \frac{n_0}{\epsilon^{4/3}}.$$

Again using $m\mu \sim n_0 a_B$, we rewrite this as

$$\frac{n_0 a_B^3}{\epsilon^{4/3}} \ll 1,$$

equivalent to Eq. (69). Note that this is stronger than just requiring the gas to be weakly interacting. Thus we reproduced the condition (70) introduced earlier by qualitative reasoning.

In Ref. [25] it was stated that a GP approach should be valid only when the number of bosons trapped within the radius of the potential is large, i.e., when $n(0)r_c^3 \gg 1$. However, this criterion does not appear within our approach. For the GP approach to be valid, one simply needs to ensure that quantum fluctuations are negligible everywhere, including within the potential range. As demonstrated in detail throughout this section [see the discussion around Eq. (70)], this leads to the first of the two inequalities in Eq. (4).

Finally, we note that if $r < r_c$, the energy spectrum (76) becomes poorly defined for small enough $p \lesssim 1/r_0$ due to $U \sim -1/(mr_0^2)$. This is to be expected as the local density approximation should break down for such small r . One way to get around it is to restrict the momenta in the integral in Eq. (77) to be larger than $1/r_0$. However, this would constitute an uncontrolled approximation and would in any case be beyond what we need to obtain the rough estimate of the fluctuations, the task that we already accomplished by limiting r to $r > r_c$.

V. FINITE-RANGE BOSON-BOSON POTENTIAL

Here we would like to discuss the effects of a finite-ranged V_{bb} on the solution to the GP equation when the impurity potential U is close to the unitary limit. We will see that, as promised earlier, these effects are mild and mostly quantitative, without changing the main qualitative aspects of the solution.

A finite-ranged V_{bb} changes the GP equation (16) to read

$$\left(-\frac{\Delta}{2m} + U(x) - \mu + \int d^3y V_{bb}(x-y)|\psi(y)|^2\right)\psi(x) = 0. \quad (80)$$

We note here that understood literally, this is only true if V_{bb} satisfies the conditions of applicability of the Born approximation. For example, if V represents the scale of this potential, and r_b is its range, we would need to require that $V \ll 1/(mr_b^2)$. Equivalently, we could require that the scattering length a_B in this potential is much shorter than its range, $a_B \ll r_b$. If we would like to work with potentials that do not obey the conditions of applicability of the Born approximation, the potential V_{bb} in Eq. (80) should be replaced by the T -matrix of this potential, as is well known [34]. Conversely, for potentials that do obey Born approximation conditions, the T -matrix reduces back to the potential itself. In what follows, we will assume that the potentials we work with satisfy the Born approximation conditions.

Remember that in the local theory we described above, the expansion was constructed by matching the asymptotic

solution far away from the impurity with the solution in the region $r < r_c$. For the theory at hand, the asymptotic behavior of the solution in the regime $r \gg r_c$ is expected to be roughly the same as in the local case, provided that $\epsilon \ll 1$ and $r_b \lesssim r_c$. The leading-order solution in the region $r < r_c$ is independent of r_b , and since the structure of the higher-order perturbative terms depends on the structure of the solutions discussed above, we expect that the effect of the nonlocal interaction is to modify the perturbative terms without changing the scaling in ϵ . More formally, the structure of the system of Eqs. (46) is such that all numeric coefficients are of the order of unity, and this allows us to solve the system in powers of $\epsilon^{1/3}$. The nonlocal generalization would introduce more terms that should depend on r_b/r_c . Provided that $r_b/r_c \sim 1$, we can still solve the resultant system of equation in powers of $\epsilon^{1/3}$, so the expansion for energy and the number of the trapped bosons would have a similar form to that in the local scenario, but the values of the coefficient cannot be determined analytically. As such, we performed extensive numerical evaluations of this equation.

First, the energy of the polaron is given by

$$E = -\frac{1}{2} \int d^3x d^3y V_{bb}(x-y)[|\psi(x)|^2|\psi(y)|^2 - n_0^2]. \quad (81)$$

Here n_0 is the uniform density of the gas in the absence of the impurity. The number of trapped bosons is given by the same expression as in the local GP theory, Eq. (18), or

$$N = \int d^3x [|\psi|^2 - n_0]. \quad (82)$$

To make contact with our previous discussion of the zero-ranged boson-boson potentials, it is convenient to define V_{bb} in such a way that we formally retrieve the expression given by (7) once the range r_b of the boson-boson interaction is taken to zero. This also implies that $n_0 = \frac{\mu}{\lambda}$ as for the local case. In our numerical study, we will use a purely repulsive Gaussian boson-boson potential of the form

$$V_{bb} = \frac{\lambda}{\pi^{3/2} r_b^3} e^{-\frac{(x-y)^2}{r_b^2}}. \quad (83)$$

An advantage of using this potential is that for spherically symmetric solutions, one can explicitly perform the angular integration on the right-hand side of Eq. (80), so the resultant equation becomes one-dimensional. For the potential given in (83), this gives

$$\int d^3y V_{bb}(x-y)|\psi(y)|^2 \rightarrow \frac{\lambda}{\sqrt{\pi} r_b x} \int_0^\infty y dy e^{-\frac{(x-y)^2}{r_b^2}} \left(1 - e^{-\frac{xy}{r_b^2}}\right) |\psi(y)|^2. \quad (84)$$

Since the GP theory treats the boson-boson potential in the Born approximation, the relation between the coupling constant λ and the boson-boson scattering length a_B is the same as in the local theory: $\lambda = 4\pi a_B/m$.

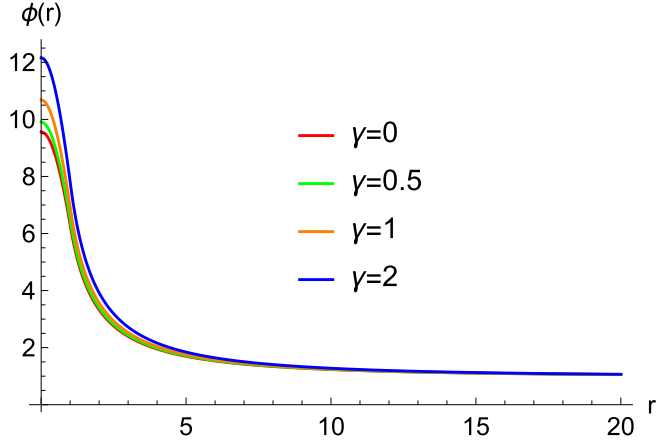


FIG. 3. Solution of the nonlocal GP equation for various values of γ (increasing, from bottom to top) at fixed $\epsilon = 0.05$. Figures 3–6 correspond to the case when boson-impurity potential is tuned to unitarity. The radial coordinate is in units of r_c , and the plot is obtained with radial step size $\Delta r = r_c/25$.

To find the ground state of Eq. (80), we perform evolution in imaginary time τ :

$$\begin{aligned}
 -\partial_\tau \psi = & -\frac{1}{2m} \left(\frac{\partial^2 \psi}{\partial x^2} + \frac{2}{x} \frac{\partial \psi}{\partial x} \right) + [U(x) - \mu] \psi(x) \\
 & + \frac{\lambda \psi(x)}{\sqrt{\pi} r_b x} \int_0^\infty y dy e^{-\frac{(x-y)^2}{r_b^2}} \left(1 - e^{-\frac{4xy}{r_b^2}} \right) |\psi(y)|^2.
 \end{aligned}
 \tag{85}$$

Here the initial state at $\tau = 0$ is taken to be the solution of the GP equation (16) given by Ref. (68). As $\tau \rightarrow \infty$, this produces the solution to Eq. (80). We discretize the spatial part of the above equation, so that (85) becomes a system of coupled nonlinear equations. The continuum limit is retrieved by extrapolating numerical results to zero step-size.

It is convenient to introduce a new dimensionless parameter $\gamma = \frac{r_b}{r_c}$, so that in the limit $\gamma \rightarrow 0$ we retrieve the original GP equation. Carrying out the numerical procedure, we find that for the fixed value of ϵ , as we increase γ from zero to some finite value such that $\gamma \sim 1$, the solutions to Eq. (80) evolve in such a way that the amplitude of the solution at the origin is an increasing function of γ , and all solutions approach the same asymptotic value far away from the impurity as indicated in Fig. 3. Equation (82) tells us that for a fixed r_c and ξ , increasing r_b increases the number of trapped particles, which in turn lowers the energy of the polaron.

We test this assertion numerically by studying the scaling of the amplitude at the origin, and we show that it indeed scales as $\sim \epsilon^{-2/3}$, as is shown in Fig. 4.

The discussion above shows that introducing a finite-ranged boson-boson interaction introduces quantitative but nonqualitative changes to the problem. It is interesting now to study what happens if one tries to shrink the other range in the problem, the one between the bosons and the impurity. To do so, we decrease r_c at fixed r_b and ξ . In the language of ϵ and γ , this corresponds to the limit $\epsilon \rightarrow 0$, $\gamma \rightarrow \infty$ with $\epsilon\gamma$ kept fixed, which is the limit of a contact boson-

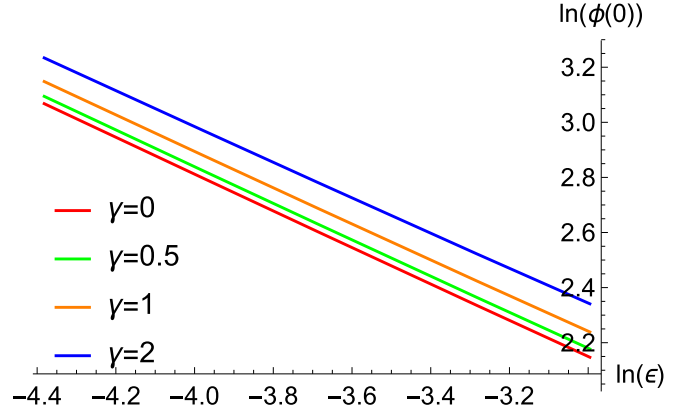


FIG. 4. Scaling of the amplitude of the nonlocal GP equation at the origin for various values of γ (increasing, from bottom to top). Plot obtained extrapolating simulations to zero radial step size Δr . All lines are parallel to the $\gamma = 0$ line, which has $\sim \epsilon^{-2/3}$ scaling predicted by local theory, indicating that this scaling survives when γ is small.

impurity interaction. Figure 5 shows that making the range of the impurity potential smaller, while keeping the range of the boson interaction and the healing length fixed, significantly increases the density at the origin. This is consistent with the expectation that making the potential softer will decrease the effective repulsion between bosons, and as a result more bosons will be attracted to the impurity. We would like to note that, as emphasized earlier in Sec. IV, at a very high density of the condensate at the origin we should treat the solution to the GP equation with care. Indeed, once $n(0)a_B^3 \gtrsim 1$ the entire approach of the GP equation breaks down.

In the intermediate regime, where $r_b \ll r_c$ at fixed r_b/ξ , we studied the scaling of the amplitude at the origin and found that it follows the $\sim \epsilon^{-2/3}$ scaling as is shown in Fig. 6. Thus in the limit $r_b \ll r_c$ and even $r_b \sim r_c$, we expect that solutions to the GP equation will look qualitatively similar to the $r_b = 0$

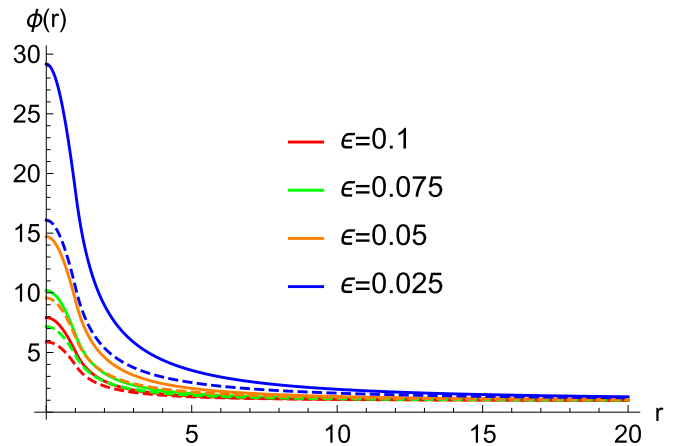


FIG. 5. Amplitude of the wave function close to the impurity for various values of ϵ (increasing, from bottom to top). Solid lines show the result of the nonlocal theory with boson-boson range $r_b = r_c/(4\epsilon)$ (equivalently $\epsilon\gamma = r_b/\xi = 1/4$), while dashed lines are obtained setting $r_b = 0$ (i.e., they are obtained from the usual local GP equation). The radial coordinate is in units of r_c .

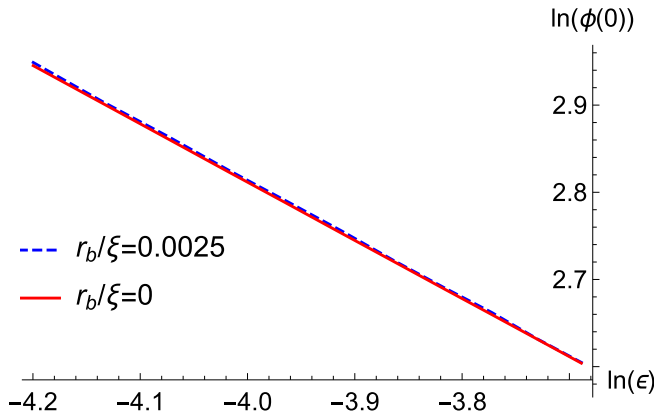


FIG. 6. Amplitude of the wave function obtained in the case $r_b \ll r_c$. The dashed line shows the result for $\gamma = 0.0025/\epsilon$, while the solid line shows the result of the local GP equation ($\gamma = 0$).

case explored analytically. Numerics shows that when $\gamma = 1$, the energy of the polaron is about 10% lower than when γ equals 0.

VI. EXPANDING ABOUT THE UNPERTURBED CONDENSATE

An alternative method of evaluating the functional integral (12) exists. Instead of calculating it by the saddle point approximation, that is, by minimizing the action and expanding it about the minimum, we expand about a flat unperturbed condensate

$$\psi = \sqrt{n_0} = \sqrt{\frac{\mu}{\lambda}}, \quad (86)$$

$$\int \mathcal{D}\varphi \mathcal{D}d \exp \left(- \int d^3x d\tau \left[\bar{\varphi} \left(\frac{\partial}{\partial \tau} - \mu - \frac{\nabla^2}{2m} \right) \varphi + \frac{\mu}{2} (\varphi^2 + \bar{\varphi}^2) + \mu \bar{\varphi} \varphi - \sqrt{n_0} (d + \bar{d}) - \bar{d} \varphi - \bar{\varphi} d - U^{-1} \bar{d} d \right] \right). \quad (89)$$

Crucially, this integral is Gaussian, so it can be calculated exactly. This is what we are going to do now. We first integrate out bosonic fluctuations φ . With the standard definition of the Fourier transform

$$d(\tau, \mathbf{r}) = T \sum_{\mathbf{p}, \omega} d(\omega, \mathbf{p}) e^{-i\omega\tau + i\mathbf{p}\cdot\mathbf{r}}, \quad (90)$$

we work in the frequency-momentum domain and find the effective action

$$\begin{aligned} \frac{S}{V} = & -\sqrt{\rho} (d(0) + \bar{d}(0)) + T \sum_{\omega, \mathbf{p}} G_n \bar{d}(\omega, \mathbf{p}) d(\omega, \mathbf{p}) \\ & + \frac{T}{2} \sum_{\omega, \mathbf{p}} G_a (d(\omega, \mathbf{p}) d(-\omega, -\mathbf{p}) + \bar{d}(\omega, \mathbf{p}) \bar{d}(-\omega, -\mathbf{p})) \\ & + T \sum_{\mathbf{p}, \mathbf{q}} U^{-1} (\mathbf{p} - \mathbf{q}) \bar{d}(\omega, \mathbf{p}) d(\omega, \mathbf{q}). \end{aligned} \quad (91)$$

ignoring at first the polaron potential U . Unlike the approach discussed in the previous section, this method is an uncontrolled approximation. It turns out that it produces the correct answer only if the scattering length a of the potential U describing impurity-boson interactions is sufficiently small. However, in principle this method produces an answer [given below in Eq. (98), first appearing in Ref. [28]] that one could attempt to use for arbitrary values of a . In fact, this expression for the polaron energy already appeared in the literature before, obtained using a variety of different techniques. Here we argue that this answer breaks down as a becomes larger, and is entirely incorrect as the potential is tuned to unitarity where a is infinity, despite some claims in the literature to the contrary.

To apply this method to our problem, it is convenient to begin by introducing a Hubbard-Stratonovich field. To do that consistently, we will focus only on the case when the attractive potential U is negative everywhere, $U(r) < 0$. We can then write

$$e^{\int d\tau d^3x U \bar{\psi} \psi} = \int \mathcal{D}d e^{\int d\tau d^3x (\bar{d} \psi + \bar{\psi} d + U^{-1} \bar{d} d)}. \quad (87)$$

With this done, we apply the expansion about the unperturbed condensate into the functional integral defined in Eq. (12). We write

$$\psi = \sqrt{n_0} + \varphi. \quad (88)$$

Then we expand the action in powers of φ , keeping only quadratic terms, which corresponds to the Bogoliubov approximation to the weakly interacting Bose gas. We emphasize that it is this step that is approximate, and as we will discuss later, this step breaks down if the potential is strongly attractive.

This produces the following functional integral:

Here $\omega = 2\pi nT$ are the usual bosonic Matsubara frequencies, $d(0)$ above implies d calculated at both zero frequency and momentum, and G_n and G_a are normal and anomalous Green's functions of the Bose gas in the Bogoliubov approximation,

$$G_n = -\frac{i\omega + \frac{p^2}{2m} + \mu}{\omega^2 + \left(\frac{p^2}{2m} + \mu\right)^2 - \mu^2}, \quad (92)$$

$$G_a = \frac{\mu}{\omega^2 + \left(\frac{p^2}{2m} + \mu\right)^2 - \mu^2}. \quad (93)$$

We note that at nonzero frequencies, S is quadratic in fields, while at zero frequency it includes a linear term. Therefore, the most important contribution will come from the zero-frequency terms. To integrate over zero-frequency terms, we minimize the action, solve the resulting equation, and substitute back into the action. Minimizing gives the following

equation:

$$-\frac{\sqrt{\rho}}{T} U(\mathbf{p}) + d(\mathbf{p}) + \sum_{\mathbf{q}} U(\mathbf{p} - \mathbf{q}) [G_n(\mathbf{q}) d(\mathbf{q}) + G_a(\mathbf{q}) \bar{d}(-\mathbf{q})] = 0, \quad (94)$$

where everything is now at zero frequency. Look for a solution in terms of a real function $d(\mathbf{r})$, or in other words $d(\mathbf{p}) = \bar{d}(-\mathbf{p})$, and denote

$$f(\mathbf{p}) = T \frac{d(\mathbf{p})}{2\mu + \frac{p^2}{2m}}. \quad (95)$$

Then Eq. (94) can be rewritten in the position space as

$$\sqrt{n_0} U + \left(-\frac{\Delta}{2m} + 2\mu + U \right) f = 0. \quad (96)$$

We now note that this is simply the expansion of the GP equation (16) about the flat solution. In other words, Eq. (96) can be obtained from Eq. (16) by substituting $\psi \approx \sqrt{n_0} + f$ and expanding in powers of f . This should already tell us that the applicability of the method we are using is limited, since f is not always small.

Ignoring this issue for now, we note that once Eq. (96) is solved, the solution needs to be substituted back into Eq. (91) to find the action

$$S = -V \sqrt{n_0} d(0), \quad (97)$$

which constitutes the answer obtained in this calculation.

We now know enough about the solution to the full GP equation to easily solve Eq. (96). For $0 < r < r_c$ we can neglect μ . The solution is then simply

$$\frac{f}{\sqrt{n_0}} = -1 + B \frac{v}{r},$$

where v , as defined earlier, is the solution of the zero-energy Schrödinger equation (64), normalized as explained after Eq. (64), and B is yet some unknown constant.

At $r > r_c$ the potential vanishes and the solution to Eq. (96) reads

$$\frac{f}{\sqrt{n_0}} = \frac{A}{r} e^{-\sqrt{2}r/\xi}.$$

We now match these by taking advantage of the Bethe-Peierls boundary conditions satisfied by v ,

$$-r_c + B = A, \quad -A\sqrt{2}/\xi = -1 + B/(r_c - a).$$

Solving these in the limit $r_c \ll \xi$, we find

$$A = \frac{\xi}{\sqrt{2} - \xi/a}, \quad B = \frac{\xi}{\sqrt{2} - \xi/a}.$$

We now calculate the action according to Eq. (97),

$$S = -\frac{2\mu\sqrt{n_0}}{T} \int d^3x f(x).$$

The leading contribution to the integral produces

$$S = \frac{2\pi a n_0 V}{T m (1 - a\sqrt{2}/\xi)}.$$

From here we finally deduce that, since $S = EV/T$,

$$E = \frac{2\pi a n_0}{m(1 - \sqrt{2}a/\xi)}. \quad (98)$$

This is a very appealing expression, and not surprisingly it appeared previously in the literature [see Ref. [28], in particular their Eq. (4) as well as their supplemental material]. The first two terms of its expansion in powers of a/ξ are given by

$$E \approx \frac{2\pi a n_0}{m} \left(1 + \frac{\sqrt{2}a}{\xi} \right) + \dots \quad (99)$$

The first of these is the standard well-known weak potential answer, which we obtained before in Eq. (32). The second term is the correction to that in the expansion in powers of a/ξ , which we already obtained earlier in Eq. (62) and which goes back to the work in Ref. [32]. Both of these are definitely correct.

It is very tempting to use the expression for the energy (98) at larger $|a|$ as well, all the way to a going to infinity where it produces $E = -\sqrt{2}\pi n_0 \xi / m$. However, there is no reason to expect that this would be correct, despite Eq. (98) featuring in the earlier work such as Ref. [28]. See the Appendix below for a toy problem, which illustrates why only the first two terms of Eq. (98) as given in Eq. (99) can be trusted [see also Ref. [25] for further discussions of Eq. (98)].

VII. IMPURITY-BOSON INTERACTIONS SUPPORTING A BOUND STATE

Let us now briefly explore the regime where the potential U is so strongly attractive that it now supports a bound state, further elaborating on the results reported in our earlier publication [26].

As the potential U increases in strengths beyond the unitary limit, the scattering length a in such a potential is now positive. This implies that it now has a bound state with binding energy

$$E_{\text{binding}} = -v < 0. \quad (100)$$

For a sufficiently bound state [roughly speaking, so that the relationship (31) holds again], we can give simple balance of energy arguments to estimate the energy and the number of particles trapped within the range R of the potential.

Indeed, supposing N bosons get trapped within the range of the potential r_c , then their energy is

$$E = -Nv + g \frac{N^2}{2},$$

where the self-repulsion constant g can be estimated as

$$g \sim \frac{\lambda}{r_c^3}.$$

Minimizing with respect to N and calculating E at this minimum gives the energy and the number of trapped particles within the range of the potential as

$$E \sim -\frac{mr_c^3 v^2}{a_B}, \quad N \sim \frac{mr_c^3 v}{a_B}, \quad (101)$$

where the potential U vanishes for $r > r_c$. Here we used that $\lambda \sim a_B/m$.

This solution can also be obtained from the GP equation (16) if one notes that it corresponds to the density of bosons being $|\psi|^2 = n \sim N/r_c^3 \sim v/\lambda$, and that results in the nonlinear term in the GP equation $\lambda|\psi|^2\psi \sim v\psi$, thus turning the GP equation approximately into the Schrödinger equation at energy $-v$, whose solution will roughly follow the bound state solution of the Schrödinger equation.

It is instructive to understand the behavior of this solution at $r > r_c$, where the potential vanishes. To do that, we rely on the same construction that allowed us to find the solution for the GP equation for the potential close to unitarity. We take Eq. (22) describing the GP equation for $r > r_c$. Note that the function u in that equation is constructed from ϕ , which in turn is $\psi/\sqrt{n_0}$. Since we expect that $\psi(r_c) \sim \sqrt{v/\lambda}$, we find $\phi(r_c) \sim \sqrt{mv/n_0 a_B}$. Yet another convenient relationship $\xi^2 \sim 1/(n_0 a_B)$ allows us to estimate $\phi(r_c) \sim \xi\sqrt{mv}$. Now $u(z)$ is defined via $\phi(z) = 1 + u(z)/z$, where $z = r/\xi$. At the point where $r = r_c$, $z = r_c/\xi$, therefore

$$u(\epsilon) \approx r_c \sqrt{mv}. \quad (102)$$

At $z > \epsilon$, u satisfies Eq. (22). At some large enough z , u becomes smaller than z . At even larger z , u then satisfies $d^2u/dz^2 = 2u$ with the solution

$$u \approx Cr_c \sqrt{mv} e^{-\sqrt{2}z} = Cr_c \sqrt{mv} e^{-\frac{\sqrt{2}r}{\xi}}. \quad (103)$$

Here C is some dimensionless number that can be found if one solves Eq. (22) from $z = \epsilon$ to $z \sim u$. Importantly, it is of the order of 1.

Equation (103) can now be used to estimate the number of particles trapped in the tail of the polaron that extends to $r \sim \xi$, as well as their contribution to the energy, by using Eqs. (18) and (17).

The number of particles can be estimated as

$$N_{\text{tail}} \sim \frac{r_c \sqrt{mv}}{\sqrt{n_0 a_B^3}}, \quad (104)$$

while the energy is

$$E_{\text{tail}} \sim -\frac{r_c \sqrt{n_0 v}}{\sqrt{m a_B}}. \quad (105)$$

Remarkably, while the number of particles in the tail diverges in the limit when the unperturbed density n_0 is very small and thus dominates over N found in Eq. (101), in accordance with the prediction of Ref. [35], their contribution to the polaron energy goes to zero and does not affect the analysis that led to Eq. (101).

Such a solution of the GP equation, described qualitatively above, can only be found numerically, and the answer, which will fix the numerical coefficients in Eq. (101), will be highly dependent on the details of the potential U .

It is straightforward to estimate $na_B^3 \sim mv a_B^2$ for $r < r_c$, justifying the use of the GP equation as long as a_B is sufficiently small.

VIII. CONCLUSIONS

We presented here a theory of impurities in weakly interacting Bose condensates, attractively interacting with bosons that formed the condensate. Our theory is based

on the GP equation in external potential. We demonstrate that the approximation of the GP equation is valid as long as the range of the potential is not too small and not too large, as described by the criteria (4). The theory remains valid for arbitrary impurity-boson scattering length, including in the unitary limit where the scattering length goes to infinity.

We demonstrate that for weakly interacting Bose gases, it is possible to solve the corresponding GP equation (16) analytically. Therefore, the weakness of intraboson interactions plays a dual role in our theory: it allows for the analytic solution of the GP equation, and it suppresses quantum fluctuations about the GP solution, if the properly defined range of the potential is finite and lies within the interval (4). Within this theory, we found the binding energy of the polaron and the number of bosons that become trapped in the vicinity of the impurity. In the regime of impurity-boson interactions at unitarity, they are given by Eqs. (5) and (6). Perturbing away from unitarity slightly, we find Eq. (57). For generic attractive potential with negative scattering length that is neither small nor large, the answer can be found analytically via the formalism developed here, but we found its analytic expression too cumbersome to present here.

We work with intraboson interactions of zero range. We explore the effects of a finite range of intraboson interactions and demonstrate that taking it into account does not appreciably change our results.

The questions that we have not yet addressed include the behavior of the polaron at finite momentum, including the determination of its effective mass. We leave these questions for future work.

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APPENDIX: FAILURE OF THE EXPANSION ABOUT THE UNPERTURBED CONDENSATE: A TOY PROBLEM

To illustrate the method used in this paper, we study the following toy problem. First we would like to evaluate the integral

$$I = \int_0^\infty dx e^{ax^2 - bx^4} \quad (A1)$$

in the case in which b is small and a is positive. We will evaluate it by the saddle point method. The saddle point is

$$x_0 = \sqrt{\frac{a}{2b}}. \quad (A2)$$

Writing $x = x_0 + y$ and $ax^2 - bx^4 = a^2/(4b) - 2a(x - x_0)$, we find

$$I \approx \sqrt{\frac{\pi}{2a}} \exp\left(\frac{a^2}{4b}\right). \quad (\text{A3})$$

This is the standard answer to I , produced as an exponential of the power series in b .

Now suppose we would like to evaluate the following integral ($a > 0$, $c > 0$, b is small):

$$f = \frac{\int_0^\infty dx e^{ax^2 - bx^4} e^{cx^2}}{\int_0^\infty dx e^{ax^2 - bx^4}}. \quad (\text{A4})$$

On the one hand, from Eqs (A1) and (A3), the answer is

$$f \approx e^{\frac{2ac+c^2}{4b}} \sqrt{\frac{a}{a+c}}. \quad (\text{A5})$$

On the other hand, we attempt to evaluate f by taking the following steps, mimicking the approach employed in Sec. VI. We introduce a Hubbard-Stratonovich variable y ,

$$f = \frac{1}{\int_0^\infty dx e^{ax^2 - bx^4}} \int_0^\infty dx \int_{-\infty}^\infty \frac{dy}{\sqrt{4\pi c}} e^{ax^2 - bx^4 + xy - \frac{y^2}{4c}}. \quad (\text{A6})$$

To evaluate the integral over x in the numerator of the expression above, we use

$$x = \sqrt{\frac{a}{2b}} + z, \quad (\text{A7})$$

and we expand in powers of z . Note that this is not a legitimate way to approach this problem; however, this is what was done in Sec. VI when the functional integral was expanded about

an unperturbed condensate. We find

$$\begin{aligned} f &\approx \frac{1}{\int_0^\infty dx e^{ax^2 - bx^4}} \int_{-\infty}^\infty \frac{dz dy}{\sqrt{4\pi c}} e^{\frac{a^2}{4b} - 2az^2 + (\sqrt{\frac{a}{2b}} + z)y - \frac{y^2}{4c}} \\ &= \sqrt{\frac{a}{2\pi^2 c}} \int_{-\infty}^\infty dz dy e^{-2az^2 + (\sqrt{\frac{a}{2b}} + z)y - \frac{y^2}{4c}}. \end{aligned} \quad (\text{A8})$$

Evaluating the integral over z gives

$$\begin{aligned} f &\approx \frac{1}{\sqrt{4\pi c}} \int_{-\infty}^\infty dy e^{\sqrt{\frac{a}{2b}}y + \frac{y^2}{8a} - \frac{y^2}{4c}} \\ &= \sqrt{\frac{2a}{2a-c}} e^{\frac{a^2 c}{b(2a-c)}}. \end{aligned} \quad (\text{A9})$$

Compare this with the correct answer (A5). Expanding the leading asymptotic of the answer in the exponential in powers of c if c is small,

$$\frac{a^2 c}{b(2a-c)} \approx \frac{ac}{2b} + \frac{c^2}{4b} + \frac{c^3}{8ab} + \dots, \quad (\text{A10})$$

so the first two terms do indeed coincide with the correct expression in the exponential

$$\frac{2ac + c^2}{4b}. \quad (\text{A11})$$

However, the rest of the terms have nothing to do with the correct answer.

This is an indication that in Eq. (98) only the first two terms in the expansion in powers of a , as given in Eq. (99), could be trusted.

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