Universal Bose gases near resonance: A rigorous solution

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(Received 28 August 2013; published 11 March 2014)

We obtain a rigorous solution of universal Bose gases near resonance and offer an answer to one of the long-standing challenges of quantum gases at large scattering lengths, where the standard dilute theory breaks down. The solution was obtained by using an $\epsilon$ expansion near four spatial dimensions. In dimension $d = 4 - \epsilon$, the chemical potential of Bose gases near resonance is shown to approach the universal value $\epsilon^2 \epsilon_F \sqrt{\pi} (1 + 0.47\epsilon + \cdots)$, where $\epsilon_F$ is the Fermi energy defined for a Fermi gas of density $n$, and the condensation fraction is equal to $\frac{\epsilon}{\pi} (1 + 0.087\epsilon + \cdots)$. We also discuss the implications on ultracold gases in physical dimensions.

DOI: 10.1103/PhysRevA.89.033614

PACS number(s): 67.85.Jk, 05.30.Jp

I. INTRODUCTION

In recent applications of Feshbach resonances, a few cold-atom laboratories have explored quantum gases of scattering atoms at large positive scattering lengths [1–8], a subject that is beyond the known dilute gas theories for weakly scattering atoms and hence extremely poorly understood. This limit of large scattering lengths with almost no formation of dimers has been called the upper branch Feshbach resonance, as opposed to the lower branch that is best known for its intimate connection to the BCS-BEC crossover physics [9–12]. The upper branch physics is an excellent example of the unique complexities of resonant cold gases. It puts one of the challenges in quantum many-body physics, that is, quantum gases at large scattering lengths, under the spotlight.

Although the physics of lower branch unitary Fermi gases is described by the BCS pairing wave functions and hence has been quite well understood after years of intensive research, the situation for the upper branch resonant gases has been much less encouraging. For Bose gases, the dilute gas theory was developed more than half a century ago [13–18]. The most recent attempt to include higher-order corrections in the dilute limit was made a while ago to address the effect of Efimov trimers [19,20]. However, the existing dilute gas theories are obviously not applicable in the limit of large scattering lengths.

In this article, we take a different approach instead of launching another frontal attack on this puzzling limit of large scattering lengths. It is based on the $\epsilon$ expansion near four spatial dimensions (4D) and it provides a rigorous solution to Bose gases near resonance. A few years ago, Yang had discussed possible extensions of the pseudopotential in dimensions higher than three and illustrated that the pseudopotential further depends on the details of interactions at short distances and becomes ill defined in high dimensions [21]. The peculiar feature of resonance scattering in 4D, on the other hand, was first noticed by Nussinov and Nussinov, who found that the wave function of two scattering atoms is concentrated at a short distance [22]. Later, Nishida and Son had constructed a successful renormalization scheme to evaluate the effective potential or the energy density for the paired fermions in $4 - \epsilon$ dimensions [23] (see other schemes in Refs. [24,25]).

The main motivations of our studies here are at least twofold. Since Feshbach resonances were applied to study many-body physics in laboratories, there have been a few attempts of developing nonperturbative approaches to near-resonance physics. One of the exciting directions is to utilize the ultraviolet properties of the momentum distribution function to establish an exact relation for the energy [26–28]. However, unlike in Fermi gases where a universal contact parameter can be introduced [26], for Bose gases additional nonuniversal regularization had to be carried out [29,30]; its implications need to be examined further. The other direction that has been quite intensively pursued for bosons is to directly evaluate the effective potential for the condensed atomic field [31–33]. This approach is equivalent to applying scale-dependent interaction constants in energy calculations with an emphasis on the infrared physics. It takes into account the varying magnitudes and signs of the running coupling constants over low-energy scales. Although the self-consistent framework in these attempts is exact, in the absence of a controllable expansion parameter, the self-consistency was practically implemented by including correlations in up to three-body channels. Quantitatively, these theories are approximate and $a$ posteriori. They should be tested in either experiments or more sophisticated Monte Carlo simulations, both of which are in infancy as far as the upper branch resonant Bose gases are concerned [34].

Given the current status of theories and experiments, a rigorous solution, even though in higher spatial dimensions, can provide enormous insight and even constraints on correct theories of quantum gases in physical dimensions. It can serve as an important benchmark for future theoretical attempts to understand resonant gases of scattering atoms [35]. Furthermore, there has been evidence that three-dimensional (3D) Bose gases are not universally characterized by two-body scattering parameters because of the ultraviolet physics related to Efimov states [19,20,29,31]. One might ask whether there exist universal Bose gases in other spatial dimensions or other universalities of Bose gases. The $\epsilon$ expansion near
4D in this paper provides an answer to this question of universality. Recall that in 3D Bose gases, the Lee-Huang-Yang (LHY) correction is purely a collective effect [14] and gets contributions from all N-body effects with $N = 3, 4, 5, \ldots$; this is one of the main reasons why higher-order effects are very difficult to thoroughly examine. $\epsilon$ expansion provides an effective way to systematically study N-body contributions near resonance. This can be understood by considering the Born-Oppenheimer potential of two noninteracting heavy bosons resonantly scattered by a light one [36,37]. Near 4D, the ground-state energy of the three bosons with two heavy ones fixed at distance $|R|$ apart can be easily estimated. One can then show that the Born-Oppenheimer potential between two heavy bosons mediated by a light one scales as $1/\Omega^1$, and is suppressed by an extra $\epsilon$ factor in $d = 4 - \epsilon$. For the quantum gas under consideration, this implies the contribution from N-body forces with $N > 2$ should be systematically expandable in terms of $\epsilon$. This insight is particularly useful for our analysis.

We shall apply the $\epsilon$ expansion near 4D to the upper branch bosons. We will implement it with two important elements. First, since we are dealing with an upper branch, in principle, the energy density has an imaginary part, indicating a coupling to the lower branch. This shows up as a higher-order effect in the dilute gas theories while, in the $\epsilon$ expansion, it appears as a leading-order correction to the energy density near resonance and it therefore must be included in our discussion. Second, the noninteracting Bose gases are infinitely compressible and therefore, even in the dilute limit, the energy density as a function of scattering length contains terms with fractional powers of the scattering length. This issue can be effectively dealt with by further combining the method of $\epsilon$ expansion with self-consistent equations.

II. MODEL AND METHOD

A condensate with a contact interaction can be described by

$$H = -\mu \sum_k b_k^\dagger b_k + \sum_k (\epsilon_k - \mu) b_k^\dagger b_k + \frac{1}{2} U_0 n_0 \sum_k b_k^\dagger b_k b_k^\dagger b_k - \frac{1}{4} U_0 \sum_{k'k} b_{k'}^\dagger b_k b_{-k}^\dagger b_{-k} + \frac{1}{2} U_0 \sum_{k'k} b_{k'}^\dagger b_k b_{-k}^\dagger b_{-k} + \text{H.c.}$$

(1)

where $\epsilon_k = \hbar^2 k^2/(2m)$; $\hbar$ is the reduced Planck constant and $m$ is the mass of a single atom. We will set $\hbar$ and $m$ to be unity from here on. The sum is over nonzero momentum states. $U_0$ is the strength of the contact interaction related to the renormalized two-body coupling constant $g_2$ via $U_0 = g_2^{-1} - \frac{1}{2} \sum_k (2\epsilon_k)^{-1}$, $\Omega$ is the volume, and $g_2$ is determined by the size of the two-body bound state $\lambda_B$.

$$g_2 = \frac{-4\pi^2}{\Gamma \left(\frac{3}{2} - 1\right)} \lambda_B^{\frac{3}{2} - 1} - \frac{1}{2} \sum_k (2\epsilon_k)^{-1}.$$  

(2)

in $4 - \epsilon$ dimensions, where $\Gamma$ is the gamma function. $n_0$ is the number density of condensed atoms and $\mu$ is the chemical potential of noncondensed particles, both of which are functions of $\lambda_B$ and $\epsilon$ and are to be determined self-consistently.

The energy density for a fixed $n_0$ and $\mu$ can be obtained as $E(n_0, \mu)$; then the following set of self-consistent equations can be applied to study the chemical potential for a gas with total number density $n$,

$$\mu_c(n_0, \mu) = \frac{\partial E(n_0, \mu)}{\partial n_0},$$

$$n = n_0 - \frac{\partial E(n_0, \mu)}{\partial \mu},$$

(3)

where $\mu_c$ is the chemical potential for the condensed atoms. In equilibrium, $\mu_c$ has to be equal to $\mu$, the chemical potential of noncondensed atoms, as indicated in Eq. (3). Calculations of $E(n_0, \mu)$ are carried out diagrammatically using the standard effective field theory method [15,38]. This quantity in 2D and 3D was studied in Refs. [31,33]. The general structure of $E(n_0, \mu)$ is given below. Its $\epsilon$ dependence is shown explicitly,

$$E(n_0, \mu) = \frac{g_2 n_0^2}{2} \sum_{N \geq 2} (2g_2 n_0 \lambda_B)^N A^{(N)}(k_B \lambda_B, \epsilon).$$

(4)

where $A^{(N)}(k_B \lambda_B, \epsilon)$ represent the contributions from the renormalized N-body forces, and $k_B = \sqrt{2} \mu$. From the point of view of running coupling constants [32], the healing length $\xi = 1/k_B$ is a crucial length scale which separates the short-distance few-body physics controlled by the renormalization flow of coupling constants from the long-wavelength hydrodynamic regime of cold gases where collective effects dominate. At the healing length, the usual renormalization flow generated under scale transformation is subject to a boundary condition due to a thermodynamic constraint. Alternatively, one states that the chemical potential is dictated by the running coupling constants at the scale of healing length, which leads to a self-consistent equation. This is also fully reflected in Eqs. (3) and (4), where the running coupling constants $A^{(N)}(k_B \lambda_B, \epsilon)$, $N = 2, 3, \ldots$, defined at a presumed healing length $\xi = 1/k_B$, are further applied to evaluate the chemical potential.

III. RESULTS

We have carried out a thorough study on these renormalized forces and shall report our results here. Detailed derivations will be published in a followup technical article. The energy density (in units of the Hartree-Fock energy $g_2 n_0^2/2 \approx 4\pi^2 \epsilon \lambda_B^{3-2\epsilon} n_0^2$) turns out to be a function of two dimensionless parameters, $\epsilon$ and $n_0 \lambda_B^{1-\epsilon}$. The contribution to $A^{(N)}$ is further specified by coefficients $a^{(N)}_k$, $b^{(N)}_k$, and $c^{(N)}_k$ (see Ref. [39] and below), with $L$ standing for the number of loops in the diagrams involved, as illustrated in Fig. 1. The asymptotic
behaviors of $A^{(2)}(k_{\mu}A,\epsilon)$ when $\epsilon$ becomes zero very much depend on the self-consistent parameter $k_{\mu}A$, which we now turn to. In 3D, the dilute limit is defined as the limit where the number of atoms within the volume defined by the size of dimers $A$ (or scattering length $a = A$) is much less than one, i.e., $nA^3 < 1$. Therefore, we define the gas parameter in 4-\(n\lambda^{-1}\) dimensions simply to be $nA^4$, and the dilute limit is $n\lambda^{-1} < 1$. We shall discuss this limit first. There, the dominating contribution to the energy density in this limit is the Hartree-Fock energy $g_2n_0^2/2$ and the corresponding chemical potential is $g_2n_0$. The self-energy in this limit is $\Sigma = 2g_2n_0 = 2\mu$, and the relevant momentum scale is $k_{\mu} = \sqrt{2\mu}$. The leading correction is purely from irreducible two-body contributions which are of a form

$$A^{(2)} = 1 + (k_{\mu}A)^{2-\epsilon} + \cdots.$$  

(5)

In the dilute limit, the second term in Eq. (5) scales as $(n\lambda^{3}n_0)^{1-\epsilon}/2$ and yields the most dominating correction to the Hartree-Fock energy (first term), which is an analog of the LHY effect in 3D; the other terms that are not shown explicitly in Eq. (5) are further suppressed by higher powers of $(n\lambda^{3}n_0)^{1-\epsilon}/2$. The next order correction contains an additional power of $\epsilon$ and has both real and imaginary parts. The real part is from the leading-order $N = 4,6, \ldots$ terms, and the imaginary part from the leading-order terms with $N = 3$.

One can compute the energy density and then solve Eq. (3) for the chemical potential perturbatively in the low-density limit. The result is

$$\text{Im} \mu = -\frac{(4\pi)^{2-\frac{\epsilon}{2}}}{\Gamma\left(\frac{\epsilon}{2} - 1\right)} \frac{\lambda^{3-\epsilon}}{\lambda} n_0 \left\{ \frac{-2(4\pi)^{2-\frac{\epsilon}{2}}}{\Gamma\left(\frac{\epsilon}{2} - 1\right)} \frac{\lambda^{4-\epsilon}}{\lambda} n_0 \right\} \frac{3\pi}{2} + \cdots,$$

$$\text{Re} \mu = -\frac{(4\pi)^{2-\frac{\epsilon}{2}}}{\Gamma\left(\frac{\epsilon}{2} - 1\right)} \frac{\lambda^{3-\epsilon}}{\lambda} n_0 \left\{ 1 + \frac{-2(4\pi)^{2-\frac{\epsilon}{2}}}{\Gamma\left(\frac{\epsilon}{2} - 1\right)} \frac{\lambda^{4-\epsilon}}{\lambda} n_0 \right\}^{1-\frac{\epsilon}{2}} \times \left[ 2 + \epsilon \left( \frac{1}{2} \ln 4 - \frac{5}{4} \right) + \cdots \right].$$  

(6)

The dimensionless parameter $\eta = 2g_2n_0A^2 \approx 16\pi^2\epsilon^{2-\epsilon}n_0$ appears naturally in our result because it defines the ratio between the Hartree-Fock chemical potential $g_2n_0 \sim \epsilon^{2-\epsilon}n_0$ and the molecular binding energy $1/A^4$, which is a measure of the effective interaction strength. When extrapolated to the limit $\epsilon = 1$, the leading correction scales as $\sqrt{nA^4}$, resembling the LHY result in 3D.

Now we turn to the most interesting limit where $\eta$ is of order of unity or even larger. When $k_{\mu}A \gg 1$, one can easily show that $A^{(N)}$ is still an analytical function of $\epsilon$ and contains no singular terms (see Fig. 1). For instance, for $N > 2$,

$$A^{(N)}(k_{\mu}A,\epsilon) \to \infty, \epsilon = \sum_{L=1}^{\infty} b_L^N(\epsilon^2(k_{\mu}A)^{-2N+6+\epsilon(N-1)}).$$  

(7)

Since $L = 2, 3, 4, \ldots$-loop diagrams contain higher powers of $\epsilon$ and become negligible when approaching 4D, the dominating contributions are simply $L = 1$-loop, $N = 3, 4, 5, \ldots$-body diagrams that contain both real and imaginary parts; the imaginary parts represent the $N$-body recombination processes. This aspect is unique near four spatial dimensions and provides a systematic way to sum up contributions even though the quantum gas is near resonance or $n\lambda^{-1}n_0 \gg 1$. In the linear order of $\epsilon$, the self-consistent equations in Eqs. (3) and (4) can be cast in a simple form [40]

$$\frac{n}{n_0} = 1 + \text{Re} \left[ \frac{\eta(-iZ)^{\epsilon}}{2[1+(-iZ)^{2-\epsilon}]^2} - \frac{2-\epsilon}{2} + \epsilon d\left( \frac{Z^2}{\eta}, \frac{1}{\sqrt{\eta}} \right) \right] + \cdots,$$

$$Z^2 = \frac{1}{1-(-iZ)^{2-\epsilon}} + \epsilon \frac{d^2}{\eta \frac{1}{\sqrt{\eta}}} f\left( \frac{Z^2}{\eta}, \frac{1}{\sqrt{\eta}} \right) + \cdots,$$

where $Z = k_{\mu}A, d(x,y)$ and $f(x,y)$ are two dimensionless functions defined as.

\begin{align*}
    d(x,y) &\equiv \frac{8\pi^2}{4(x+y)^2} \left\{ i \int \frac{dv}{2\pi} \frac{d^2q}{(2\pi)^2} h_+(x,y)h_-(x,y) \left[ \frac{d}{4(x+y)^2} + h_+(x,y) + h_-(x,y) + 2l_2(x,y)h_+(x,y) + 2l_2(x,y)h_-(x,y) \right] \right. \\
    &\left. - \frac{4}{x+y} \int \frac{d^2q}{(2\pi)^2} \frac{1}{x-q^2+i\delta} - \int \frac{d^2q}{(2\pi)^2} \frac{2}{x-q^2+i\delta} \right\},
\\
    f(x,y) &\equiv \frac{8\pi^2}{(x+y)^2} \left\{ i \int \frac{dv}{2\pi} \frac{d^2q}{(2\pi)^2} h_+(x,y)h_-(x,y) \left[ 1 + \frac{d}{4(x+y)^2} h_+(x,y)h_+(x,y) + \frac{d}{4(x+y)^2} h_-(x,y)h_-(x,y) \right] \right. \\
    &\left. - \int \frac{d^2q}{(2\pi)^2} \frac{1}{x-q^2+i\delta} \right\}.
\end{align*}
where \( l(v, q; x, y) = (v - \frac{q^2}{4} + x + y + i\delta)^{-1} \), \( h(v, q; x, y) = [v - \frac{q^2}{4} + \frac{1}{2} - l(v, q; x, y) + i\delta]^{-1} \), \( h_{\pm}(x, y) = h(\pm v, q; x, y) \), and \( l_{\pm}(x, y) = l(\pm v, q; x, y) \).

It is important to note that the right-hand side of Eq. (8) is a function of the self-consistent variable \( Z \) and two dimensionless parameters, \( \eta \) and \( \epsilon \). When \( \eta \) is small, the solution reproduces the dilute limit result. Near resonance when \( \eta \to \infty \), Eq. (8) yields a solution that is universal, independent of ultraviolet physics,

\[
\mu = \epsilon \sqrt{\frac{2}{3}} \sqrt{1 + 0.474 \epsilon - i 1.217 \epsilon + \cdots},
\]

\[
n_0 = \frac{2}{3} n(1 + 0.0877 \epsilon + \cdots).
\]  

(9)

Here one can see that indeed \( k_B T_R \sim \eta^{1/4} \gg 1 \). The leading terms in Eq. (9) are fully dictated by the renormalized two-body interactions, \( N \)-body interactions with \( N > 2 \) only contribute to the corrections proportional to \( \epsilon \). Equation (9) also indicates that the chemical potential of a unitary Bose gas is proportional to \( \epsilon^{1/2} \) near 4D and its lifetime which is inversely proportional to the imaginary part of the chemical potential scales as \( \epsilon^{-3/2} \). Although \( \mu \) vanishes as \( \epsilon \) goes to zero, it scales as \( \epsilon^{1/2} \) instead of \( \epsilon \) as in the dilute limit, indicating a strongly interacting regime. The corresponding condensation fraction near 4D appears to approach the value of 2/3. By contrast, in 3D, the chemical potential further depends on a nonuniversal three-body ultraviolet momentum scale \([19, 31]\).

IV. DISCUSSIONS

Very recently, a few theoretical attempts have been made to understand upper branch Bose gases in two dimensions (2D) and 3D by applying a single-parameter scaling approach to the running coupling constants \([31–33]\). The main intention there was to provide a simple theoretical framework on upper branch Bose gases, analogous to the BCS-BEC crossover theory of unitary Fermi gases. It was illustrated that the chemical potential reaches a maximum at a critical scattering length or density and Bose gases are nearly fermionized before an onset of many-body instability sets in and the compressibility becomes negative \([41, 42]\). The predicted correlation between the instability and occurrence of fermionization near the maximum still needs vindication in experiments. In 4D, the Bose gases are more stable and even when the system is very close to resonance, the lifetime (scales as \( \epsilon^{-3/2} \)) is much longer than the many-body time scale defined by the chemical potential (scales as \( \epsilon^{-1/2} \)). The main reason for this difference between 4D and 3D or 2D is that three-, four-body processes, etc., become strongly suppressed as \( \epsilon \) approaches zero. Consequently, the mean-field shift of the dimer binding energy which results in instabilities at finite scattering lengths in 2D and 3D \([32]\) is expected to be vanishingly small near 4D.

Despite this difference in the lifetime, Eq. (9) still offers unique and valuable implications about Bose gases in physical dimensions. For instance, when extrapolated to the limit of \( \epsilon = 1 \) or 3D, Eq. (9) does imply that the chemical potential is of the order of the Fermi energy \( \epsilon_F \) and so Bose gases are nearly fermionized. This is in agreement with the previous numerical evidence in 3D \([43–45]\) as well as the lower bound of chemical potentials measured in experiments \([4]\).

Furthermore, the extrapolation also indicates that in 3D the quantum depletion fraction or the fraction of noncondensed atoms is 0.275, surprisingly close to the value of 0.27 obtained in Ref. \([31]\). More importantly, it is mainly from the two-body channel (0.333) while the other channels contribute very little (0.058). This is consistent with early experiments which demonstrated that the contribution of nonuniversal three-body contact to the momentum distribution appears to be unmeasurable near resonance \([5, 46]\). In Ref. \([5]\), the authors measured Tan’s contact using rf spectroscopy for \( ^{85}\)Rb atoms. It is demonstrated that when fitted to the frequency dependence of the tail of the rf spectrum, the experiment data exhibit no visible evidence of measurable three-body effects. Equally importantly, Eq. (9) shows that in general the three-body and other higher-order effects (i.e., the terms proportional to \( \epsilon \)) become more important when the dimensionality decreases. This is again fully consistent with the previous renormalization studies which show that the three-body effect increases from a few percent in 3D \([31]\) to around 20%–40% in 2D \([33]\).

In conclusion, we have obtained a rigorous solution to a unitary Bose gas or a quantum gas at infinite scattering length, which offers an answer to one of the long-standing challenges in quantum many-body physics. This solution can further shed light on future studies of other aspects of large-scattering-length physics such as the ultraviolet properties of a Bose gas.

**Note added.** Recently, we noticed an experimental work on universal Bose gases \([47]\), and a subsequent analysis of the data obtained in the above-mentioned experiment \([48]\).

**ACKNOWLEDGMENTS**

This work is supported in part by CIFAR, NSERC (Canada), NKBRDF under Grants No. 2011CB921502 and No. 2012CB821305, and NSFC under Grants No. 11228409, No. 61227902, and No. 61378017. We thank Joseph H. Thywissen, Tao Xiang, Yupeng Wang, and Zhengyu Weng for constructive discussions.

[39] For $N = 4, 6, \ldots$-body forces, they in general read as $A^{(N)} = i c_i^{(N)} e + a_i^{(N)} e(k,\mu,\gamma)^{-2(N)-4} + \ldots$. Contributions from $a_i^{(N)}$ to the energy density simply contain higher powers of $e$ and can be ignored in the $e$ expansion. Meanwhile, the contributions of $A^{(3)}$ are of the form $A^{(3)} = i c_i^{(3)} e + a_i^{(3)} e^2 + \ldots$, where $c_i^{(3)}$ is the imaginary part of the one-loop three-body contribution and gives the most dominating contribution to the imaginary part of the ground-state energy density; the next order terms are from $L = 2$ processes and contain higher powers of $e$. Similarly, $A^{(5,7,\ldots)}$ have the form $A^{(N)} = i c_i^{(N)} e + a_i^{(N)} e^2(2N-4) + \ldots$.
[40] The ground-state energy density up to the one-loop effect can be summed as $E(n_0,\mu) = \frac{\gamma^2 n_0^2}{2} \frac{1}{1-(\xi k^2/2)^{N/2}} + \frac{\gamma^2 n_0^2}{2} \frac{1}{1-(\xi k^2/2)^{N/2}} - \frac{\gamma^2 n_0^2}{2} \frac{1}{1-(\xi k^2/2)^{N/2}} + \frac{\gamma^2 n_0^2}{2} \frac{1}{1-(\xi k^2/2)^{N/2}} = G(\omega,k)G(-\omega,-k) = \frac{\gamma^2 n_0^2}{2} \frac{1}{1-(\xi k^2/2)^{N/2}} - \frac{\gamma^2 n_0^2}{2} \frac{1}{1-(\xi k^2/2)^{N/2}} + \frac{\gamma^2 n_0^2}{2} \frac{1}{1-(\xi k^2/2)^{N/2}} + \frac{\gamma^2 n_0^2}{2} \frac{1}{1-(\xi k^2/2)^{N/2}} = \text{the self-energy}. Taking the derivatives with respect to $n_0$ and $\mu$ and substituting into Eq. (3), we obtain the self-consistent equation below.
[46] Smallness of the three-body contribution also appeared in the self-consistent calculation in Ref. [31].

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