Dilute Bose-Einstein Condensate with Large Scattering Length

Eric Braaten, H.-W. Hammer, and Thomas Mehen
Department of Physics, The Ohio State University, Columbus, Ohio 43210
(Received 24 August 2001; published 8 January 2002)

We study a dilute Bose gas of atoms whose scattering length a is large compared to the range of their interaction. We calculate the energy density $\mathcal{E}$ of a homogeneous Bose-Einstein condensate (BEC) to second order in the low-density expansion, expressing it in terms of a and a second parameter Λ_* that determines the low-energy observables in the three-body sector. The second-order correction to $\mathcal{E}$ has a small imaginary part that reflects the instability due to three-body recombination. In the case of a trapped BEC with large negative a, we calculate the coefficient of the three-body mean-field term in $\mathcal{E}$ in terms of a and Λ_*. It can be very large if there is an Efimov state near threshold.

DOI: 10.1103/PhysRevLett.88.040401 PACS numbers: 03.75.Fi, 03.70.+k, 05.30.Jp

Bose-Einstein condensates of atoms have been extensively studied both experimentally and theoretically for two cases: liquid helium [1] and dilute vapors of alkali atoms [2]. The low-energy length scale $\ell = (mC_6/\hbar^2)^{1/4}$ set by the van der Waals interaction $-C_6/r^6$ is the natural length scale for the S-wave scattering length a and other parameters in the low-energy expansions of scattering amplitudes. In the case of liquid helium, the interparticle spacing $n^{-1/3} = 3.6$ Å is much smaller than $\ell = 37$ Å and $a = 104$ Å [3]. Because the diluteness variable $\sqrt{n\ell^3} \approx 33$ is much greater than 1, the properties of the Bose-Einstein condensate (BEC) in liquid helium depend on the detailed behavior of the interatomic potential. In contrast, BEC's consisting of dilute gases of atoms with $n\ell^3 \ll 1$ have universal properties that depend on the interatomic potential only through the single low-energy parameter a. For example, the first few terms in the low-density expansions for the energy density and the condensate fraction of a homogeneous condensate can be calculated as expansions in powers of $\sqrt{na^3}$.

A fundamental open problem is the behavior of a dilute BEC ($n\ell^3 \ll 1$) with large scattering length ($a \gg \ell$) when na^3 is comparable to or much greater than 1. The diluteness condition $n\ell^3 \ll 1$ excludes the case of liquid helium. The condition $na^3 \gtrsim 1$ implies that the low-density expansion is not applicable, because the expansion parameter $\sqrt{16\pi na^3}$ is not small. The most basic question is whether a BEC even exists as a well-defined quasistable state in this limit. If so, does it have any universal properties that depend on the interatomic potential only through the scattering length a? These questions can be investigated experimentally in vapors of alkali atoms by tuning a background magnetic field to a Feshbach resonance [4]. They can also be studied using numerical methods [5,6].

In this Letter, we take a small step towards addressing this problem by studying the homogeneous BEC with large scattering length ($a \gg \ell$) in the extremely dilute limit $na^3 \ll 1$. We calculate its energy density to second order in $\sqrt{na^3}$, determining the coefficient of na^3 in terms of a low-energy parameter Λ_*. The parameter Λ_* can be determined from any low-energy three-body observable, e.g., the binding energy of the shallowest three-body bound state. We also determine the coefficient of the three-body term in the mean-field contribution to the energy density for $a < 0$. Finally, we comment on the implications of our results for the case of large na^3.

The dilute Bose gas with large scattering length is distinguished from the generic case by having a two-body scattering amplitude $f = -a/(1 + iak)$ that has the scale-invariant form $f \approx i/k$ for wave numbers in the range $1/a \ll k \ll 1/\ell$ [7]. If $a > 0$, it is also characterized by the existence of a two-body bound state with binding energy $B_2 = \hbar^2/ma^2$. As first pointed out by Efimov [8], the three-body sector also exhibits universal properties in the limit of large scattering length, such as the existence of a large number of three-body bound states. The number of these Efimov states is roughly $\ln(|a|/\ell)/\pi$. The Efimov spectrum and other low-energy three-body observables involving wave numbers $k \ll 1/\ell$ are universal in the sense that they depend on the interatomic potential only through a and a single three-body parameter. A convenient choice for this three-body parameter is the low-energy parameter Λ_* introduced in Ref. [9].

In the dilute limit $na^3 \ll 1$, the properties of the Bose gas can be calculated using the low-density expansion. The first few terms in the low-density expansion of the energy density of a homogeneous BEC are

$$\mathcal{E} = 2\pi\hbar^2 an^2/m\{1 + 128/(15\sqrt{\pi})\sqrt{na^3} + 8(4\pi - 3\sqrt{3})/3 \times [\ln(na^3) + 4.72 + 2B]na^3 + \ldots\}. \quad (1)$$

The $\sqrt{na^3}$ correction was first calculated by Lee and Yang in 1957 [10]. The coefficient of the logarithm in the na^3 correction was calculated in 1959 [11]. The constant under the logarithm was calculated by Braaten and Nieto in 1999 [12]. It was expressed in terms of an effective three-body coupling constant $g_3(\kappa)$ that can be determined by

measuring the low-energy behavior of the three-atom elastic scattering rate. This "running coupling constant" depends on an arbitrary wave number κ:

$$g_3(\kappa) = 384\pi(4\pi - 3\sqrt{3})[\ln(\kappa a) + B]\hbar^2 a^4/m, \quad (2)$$

where B is the same constant as in (1). The na^3 correction in (1) is the sum of a mean-field contribution $g_3(\kappa)n^3/36$ coming from the effective three-body contact interaction and a two-loop contribution from quantum fluctuations around the mean field, which also depends on κ. The dependence on κ cancels in (1), reflecting the arbitrariness in the separation of the energy density into mean-field and quantum-fluctuation contributions. The next nonuniversal term in the low-density expansion is determined by the effective range for two-body scattering [13]. It is suppressed by $(na^3)^{3/2}\ell/a$, and is therefore completely negligible in the limit of large scattering length.

To determine the constant B in the expression (1) for the energy density for an extremely dilute Bose gas with large scattering length, we need to calculate $g_3(\kappa)$ as a function of a and the low-energy three-body parameter Λ_* introduced in Ref. [9]. This can be accomplished by calculating the T-matrix element for three-atom elastic scattering in the low-energy limit. As the total energy E of the three atoms goes to 0, the T-matrix element is the sum of divergent terms proportional to $1/E$, $1/\sqrt{E}$, and $\ln E$ [14] and a remainder. The dependence of the T-matrix element on Λ_* enters only through the remainder, which includes a term $-g_3(\kappa)$. For the case $a < 0$, Efimov used simple probability arguments to deduce the dependence of the remainder on Λ_* [8]. These arguments imply

$$B = b_1 + b_2 \tan[s_0 \ln(|a|\Lambda_*) + \beta] \qquad (a < 0), \quad (3)$$

where $s_0 = 1.0064$. Efimov did not determine the functional form of B for $a > 0$. However, unitarity requires that it have an imaginary part that is related to the three-body recombination rate into the shallow two-body bound state [15,16]:

$$\mathrm{Im}B = 0.022 \cos^2[s_0 \ln(a\Lambda_*) + 1.76] \qquad (a > 0). \quad (4)$$

The three-body recombination rate has zeroes at values of $a\Lambda_*$ that differ by multiplicative factors of 22.7, and, consequently, ImB also vanishes at those points.

A convenient way to calculate $g_3(\kappa)$, both for $a > 0$ and $a < 0$, is to use the effective field theory method developed by Bedaque, Hammer, and van Kolck in Ref. [9]. The effective theory is defined by the Lagrangian density

$$\mathcal{L} = i\psi^* \frac{\partial}{\partial t}\psi + \frac{1}{2m}\psi^*\nabla^2\psi - \frac{2\pi a}{m}|\psi|^4 + \frac{2\pi a}{m}|d - \psi^2|^2 - \frac{g_3}{36}|d|^2|\psi|^2, \quad (5)$$

where we have set $\hbar = 1$. The auxiliary field d, which annihilates a pair of atoms at a point, can be eliminated using the equation of motion $d = \psi^2[1 + mg_3/(72\pi a)|\psi|^2 + \ldots]$. However, it is more convenient to keep it, because three-body observables can be conveniently calculated in terms of four-point Green functions of ψ, d, $\psi^\dagger$, and $d^\dagger$. For example, the T-matrix element for three-atom elastic scattering can be expressed as a sum of nine connected four-point Green functions. If the incoming atoms have momenta $\mathbf{k}_1$, $\mathbf{k}_2$, and $\mathbf{k}_3$ with $\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3 = 0$, the external energies and momenta of ψ and d are set to $(k_1^2/2m, \mathbf{k}_1)$ and $((k_2^2 + k_3^2)/2m, \mathbf{k}_2 + \mathbf{k}_3)$, respectively, and similarly for the outgoing atoms. The Green function is then summed over the three cyclic permutations of $\mathbf{k}_1$, $\mathbf{k}_2$, and $\mathbf{k}_3$, and over the three cyclic permutations of the final momenta to get the T-matrix element. The Green functions can be calculated nonperturbatively by solving the integral equations shown in Fig. 1a. The single lines are propagators for ψ and the double lines are exact propagators for d. An ultraviolet cutoff Λ must be imposed on the loop momentum in the integral equation. The three-body coupling constant g_3 in (5) is tuned as a function of Λ so that the low-energy three-body observables depend only on a and the low-energy parameter Λ_*.

It is not necessary to calculate a physical observable to determine $g_3(\kappa)$. For small external energies and momenta $(\omega, \mathbf{k})$ with $m|\omega|a^2 \ll 1$ and $|\mathbf{k}| \ll 1$, a Green function associated with the Lagrangian (5) can also be calculated perturbatively in a and g_3 using the methods of Ref. [12]. By computing the same Green function using the nonperturbative method of Ref. [9], we can determine g_3 as a function of a and Λ_*. We choose the two particle-irreducible connected Green function $T(p)$ with external energies and momenta $(0, \mathbf{0})$ for ψ and d, $(p^2/2m, \mathbf{p})$ for $\psi^\dagger$, and $(-p^2/2m, -\mathbf{p})$ for $d^\dagger$. As $p \to 0$, $T(p)$ has divergent terms proportional to $1/p^2$, $1/p$, and $\ln(p)$ that come from the diagrams in brackets in Fig. 1b. The coupling constant $g_3(\kappa)$ in Ref. [12] was defined using dimensional regularization in $3 - 2\epsilon$ dimensions to regularize the ultraviolet divergences and minimal subtraction with renormalization scale κ to remove the poles in ϵ. Calculating the diagrams that contribute to $T(p)$ in the limit $p \to 0$ using perturbation theory to first order g_3 and fourth order in a, we obtain

$$T(p) \longrightarrow -g_3(\kappa)/36 + 16\pi^2 a^4/m \times \{1/(p^2a^2) - 2\pi/(3pa) - 2(4\pi - 3\sqrt{3})/(3\pi) \times [\ln(p/\kappa) + A_{\mathrm{MS}}]\}, \quad (6)$$

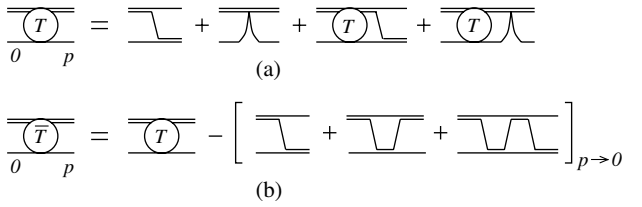

FIG. 1. (a) Integral equation satisfied by the off-shell amplitude $T(p)$. (b) Definition of the subtracted amplitude $\overline{T}(p)$.

where $A_{\rm MS} = -0.772\,68$ and the subscript MS stands for "minimal subtraction." The nonperturbative calculation of the Green function $T(p)$ using the method of Ref. [9] requires solving the integral equation in Fig. 1a. It is convenient to define a subtracted Green function $\overline{T}(p)$ that has a finite limit as $p \to 0$ using the subtraction shown in Fig. 1b. We solve the integral equation for $\overline{T}(p)$ as a function of p, a, and Λ_* and then set $p = 0$. The resulting expression for $T(p)$ in the limit $p \to 0$ is

$$T(p) \longrightarrow 16\pi^2 a^4/m \times \{1/(p^2a^2) - 2\pi/(3pa) - 2(4\pi - 3\sqrt{3})/(3\pi) \times [\ln(pa) + A(a\Lambda_*)]\}, \quad (7)$$

where $A(a\Lambda_*)$ is a function of $a\Lambda_*$ that is determined numerically. Matching the expressions (6) and (7), we find that the constant B in (2) is given by $B = -A_{\rm MS} + A(a\Lambda_*)$.

We first consider the case of large positive scattering length. For $a > 0$, our result for B is complex. Its imaginary part is equal to (4), as required by unitarity. For the real part, we obtain a good fit with the empirical formula

$$\mathrm{Re}B = 1.22 + 0.021\cos^2[s_0\ln(a\Lambda_*) + 1.0] \quad (a > 0). \quad (8)$$

The real part is much larger than the imaginary part given in (4). The oscillatory term in the real part has almost the same amplitude as the imaginary part, but a different phase.

In the coefficient of na^3 in the expression (1) for the energy density, the real part of the factor in brackets can be separated into two terms: $2\ln(\kappa a) + 2\,\mathrm{Re}B$, which comes from the mean-field contribution to the energy density, and $\ln(na/\kappa^2) + 4.72$, which comes from quantum field fluctuations. Although κ is arbitrary, we can by a suitable choice of κ arrange for most of the na^3 correction to come from the mean-field contribution. The smallest value of κ that is physically reasonable is of order $\sqrt{16\pi na}$, which is the inverse of the coherence length. Below this scale, the dispersion relation for the atoms is modified by collective effects, and three-atom scattering is therefore no longer described accurately by the vacuum T-matrix. If we choose $\kappa = 1.5\sqrt{16\pi na}$, the entire na^3 correction in (1) is taken into account by the mean-field contribution $g_3(\kappa)n^3/36$.

The na^3 correction to the energy density has an imaginary part that comes from the imaginary part of B given in (4). This imaginary part reflects the fact that the BEC is only a quasistable state. Atoms will be continually lost from the condensate by three-body recombination into the shallow two-body bound state and a recoiling atom. In the mean-field approximation, the rate of decrease of the number density is $(\partial/\partial t)n = -(\mathrm{Im}g_3/6\hbar)n^3$. Note that $\mathrm{Im}g_3$ is independent of κ. The energy loss rate is given by $\partial\mathcal{E}/\partial t = (\partial\mathcal{E}/\partial n)\partial n/\partial t$. The condensate is particularly stable at values of a that correspond to $\ln(a\Lambda_*) = 2.93 \bmod \pi/s_0$. At these discrete values of a that differ by multiplicative factors of 22.7, there is an interference effect that causes the three-body recombination rate to vanish [15,16]. The recombination process that gives the energy density an imaginary part produces atoms and bound states with wave number $k = 2/\sqrt{3}a$. These high energy atoms and bound states can subsequently thermalize and cool by elastic scattering with atoms in the condensate. The cross section for elastic scattering of the atoms and bound states can be calculated as a function of a and Λ_*. For example, the scattering length was calculated in Ref. [9] and the effective range in Ref. [17].

We now turn to the case of large negative scattering length. If $a < 0$, the expression (1) for the energy density does not apply, because the homogeneous condensate is unstable to collapse. However, a condensate with $a < 0$ can be stabilized by a trapping potential as long as the number of atoms is below some critical value $N_{\rm max}$ [18]. An effective three-body contact interaction $-g_3$ gives a mean-field contribution $g_3n^3/36$ to the energy density. The effect of such a term on the stability of a trapped condensate has been studied by adding a three-body term to the Gross-Pitaevski equation [19]. Even a small positive value of g_3 can considerably increase the critical number $N_{\rm max}$.

In the case of large negative scattering length, the three-body coupling constant $g_3(\kappa)$ is given by (2). The dependence of our result for B on $a\Lambda_*$ has the functional form (3) predicted by Efimov. The values of the constants are $b_1 = 1.23$, $b_2 = -3.16$, and $\beta = 0.19$. The appropriate choice for κ in this case is the lowest wave number above which three-body scattering can be described by the T-matrix for scattering in the vacuum. The vacuum T-matrix becomes inaccurate not only because of the nontrivial quasiparticle dispersion relation but also because of the inhomogeneities of the trapping potential $V(r)$. The minimum value of κ set by the coherence length is $\kappa^2 > 4m[\mu - V(r)]$, where μ is the chemical potential. For a harmonic potential with frequency ω, the minimum set by the inhomogeneity of the potential is $\kappa^2 > m\omega/\hbar$. In previous studies of the mean-field effects of the three-body term [19], the coefficient g_3 was assumed to be a constant. If the large scattering length is obtained by tuning the magnetic field to a Feshbach resonance, g_3 is given by the expression (2), which scales roughly similar to a^4. Note that the constant B given in (3) diverges at values of a that correspond to $\ln(a\Lambda_*) = 1.37 \bmod \pi/s_0$. At these discrete values of a, there is an Efimov state at the three-atom threshold. Near these values of a, the three-body term in the Gross-Pitaevski equation becomes particularly important. However, if the Efimov state is too close to threshold, the mean-field approximation breaks down because the energy dependence of the three-body elastic scattering amplitude from terms proportional to $1/(E + B_3)$ is not properly taken into account.

We turn finally to the problem of a homogeneous BEC with a large scattering length ($a \gg \ell$) that is dilute enough so that $n\ell^3 \ll 1$ but dense enough so that $na^3 \gg 1$. Our results for the extremely dilute limit provide a reference point for discussing this problem. The fact that our energy density has an imaginary part serves to emphasize that such a state will at best be quasistable. Monte Carlo methods that search for the absolute ground state [5] will therefore be of limited utility. In the extremely dilute limit, the condensate is quasistable because the imaginary part of the energy density is suppressed by na^3. Is there any mechanism that can provide quasistability at large na^3? If a quasistable Bose-Einstein condensate does exist, there are some other obvious questions. At what rate does the number density in the condensate decay, and what is the fate of the atoms that disappear from the condensate? We have answered these questions for the extremely dilute limit.

Assuming that a quasistable BEC exists in the limit $na^3 \to \infty$, does it have universal properties that depend only on a? If so, dimensional analysis implies that the energy density must have the form $\mathcal{E} = C\hbar^2 n^{5/3}/m$, where C is a constant. In the extremely dilute limit, we found that $\mathcal{E}$ depends on Λ_* at second order in $\sqrt{na^3}$. Does $\mathcal{E}$ depend on Λ_* in the limit $na^3 \to \infty$? If so, the coefficient C in the energy density is not a constant, but depends on n in a peculiar way. It must be a periodic function of $\ln(n^{-1/3}\Lambda_*)$ that returns to the same value when n is increased by a factor of about 11 700. This follows from the discrete scaling symmetry of low-energy three-body observables discovered by Efimov [8,17], which implies that $C(n^{-1/3}\Lambda_*) = C(22.7n^{-1/3}\Lambda_*)$. This discrete scaling symmetry is related to the fact that there are Efimov states with sizes differing by factors of 22.7 and ranging all the way from order ℓ to order a. The question of whether C depends on Λ_* is not addressed by the constrained variational calculations of Ref. [6]. Their variational ansatz excludes states with three-body configurations that are sensitive to Λ_*. For example, in the three-body sector, it would exclude the Efimov states.

If the coefficient C in the energy density depends on the three-body parameter Λ_*, one might worry that it may also depend on infinitely many other low-energy parameters associated with four-body and higher n-body observables. If this is the case, the dilute BEC with large scattering length would have no universal properties at large na^3. The most favorable possibility is that, in the limit of large scattering length, the low-energy observables in the four-body and higher n-body sectors are all calculable to leading order in ℓ/a in terms of a and Λ_* only. If this is the case, then a dilute BEC with large na^3 may have properties that are universal in the sense that they are determined by a and Λ_* only.

This research was supported in part by DOE Grant No. DE-FG02-91-ER4069 and by NSF Grant No. PHY-9800964.

Note added.—After this work was submitted for publication, we became aware of a related study by Bulgac [20].

[1] See, for example, *Bose-Einstein Condensation,* edited by A. Griffin, D. W. Snoke, and A. Stringari (Cambridge University Press, Cambridge, England, 1995).
[2] See, for example, A. J. Leggett, Rev. Mod. Phys. **73**, 307 (2001).
[3] R. E. Grisenti *et al.,* Phys. Rev. Lett. **85**, 2284 (2000).
[4] J. Söding *et al.,* Appl. Phys. B **69**, 257 (1999); J. Stenger *et al.,* Phys. Rev. Lett. **82**, 2422 (1999); S. L. Cornish *et al.,* Phys. Rev. Lett. **85**, 1795 (2000).
[5] M. H. Kalos, D. Levesque, and L. Verlet, Phys. Rev. A **9**, 2178 (1974); S. Giorgini, J. Boronat, and J. Casulleras, Phys. Rev. A **60**, 5129 (1999).
[6] S. Cowell *et al.,* cond-mat/0106628.
[7] T. Mehen, I. W. Stewart, and M. B. Wise, Phys. Lett. B **474**, 145 (2000).
[8] V. Efimov, Sov. J. Nucl. Phys. **12**, 589 (1971); **29**, 546 (1979).
[9] P. F. Bedaque, H.-W. Hammer, and U. van Kolck, Nucl. Phys. **A646**, 444 (1999); Phys. Rev. Lett. **82**, 463 (1999).
[10] T. D. Lee and C. N. Yang, Phys. Rev. **105**, 1119 (1957); T. D. Lee, K. Huang, and C. N. Yang, Phys. Rev. **106**, 1135 (1957).
[11] T. T. Wu, Phys. Rev. **115**, 1390 (1959); K. Sawada, Phys. Rev. **116**, 1344 (1959); N. M. Hugenholtz and D. Pines, Phys. Rev. **116**, 489 (1959).
[12] E. Braaten and A. Nieto, Eur. Phys. J. B **11**, 143 (1999).
[13] E. Braaten, H.-W. Hammer, and S. Hermans, Phys. Rev. A **63**, 063609 (2001).
[14] R. D. Amado and M. H. Rubin, Phys. Rev. Lett. **25**, 194 (1970).
[15] E. Nielsen and J. H. Macek, Phys. Rev. Lett. **83**, 1566 (1999); B. D. Esry, C. H. Greene, and J. P. Burke, Phys. Rev. Lett. **83**, 1751 (1999).
[16] P. F. Bedaque, E. Braaten, and H.-W. Hammer, Phys. Rev. Lett. **85**, 908 (2000).
[17] H.-W. Hammer and T. Mehen, Nucl. Phys. **A690**, 535 (2001).
[18] P. A. Ruprecht, M. J. Holland, K. Burnett, and M. Edwards, Phys. Rev. A **51**, 4704 (1995).
[19] N. Akhmediev, M. P. Das, and A. V. Vagov, Int. J. Mod. Phys. B **13**, 625 (1999); A. Gammal, T. Frederico, L. Tomio, and Ph. Chomaz, J. Phys. B **33**, 4053 (2000).
[20] A. Bulgac, cond-mat/9902131.