The Dilute Bose-Einstein Condensate with Large Scattering Length

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(March 22, 2022)

Abstract

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 \( \Lambda_* \) that determines the low-energy observables in the 3-body sector. The second-order correction to \( \mathcal{E} \) has a small imaginary part that reflects the instability due to 3-body recombination. In the case of a trapped BEC with large negative \( a \), we calculate the coefficient of the 3-body mean-field term in \( \mathcal{E} \) in terms of \( a \) and \( \Lambda_* \). It can be very large if there is an Efimov state near threshold.
Bose-Einstein condensates of atoms have been extensively studied both experimentally and theoretically for 2 cases: liquid helium \[1\] and dilute vapors of alkali atoms \[2\]. The low-energy length scale \(\ell = (mC_6/h^2)^{1/4}\) 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 \(n^{-1/3} = 3.6\ \text{Å}\) is much smaller than \(\ell = 37\ \text{Å}\) and \(a = 104\ \text{Å}\) \[3\]. 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 \(na^3 \approx 1\) excludes the case of liquid helium. The condition \(na^3 \gg 1\) 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 \(a^2\)? These questions can be investigated experimentally in vapors of alkali atoms by tuning a background magnetic field to a Feshbach resonance \[1\]. They can also be studied using numerical methods \[4,5\].

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 \(\Lambda^*\). The parameter \(\Lambda^*\) can be determined from any low-energy 3-body observable, e.g. the binding energy of the shallowest 3-body bound state. We also determine the coefficient of the 3-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 2-body scattering amplitude \(f = -a/(1 + iak)\) that has the scale-invariant form \(f \approx i/k\) for wavenumbers in the range \(1/a \ll k \ll 1/\ell\) \[7\]. If \(a > 0\), it is also characterized by the existence of a 2-body bound state with binding energy \(B_2 = \hbar^2/ma^2\). As first pointed out by Efimov \[8\], the 3-body sector also exhibits universal properties in the limit of large scattering length, such as the existence of a large number of 3-body bound states. The number of these Efimov states is roughly \(\ln(|a|/\ell)/\pi\). The Efimov spectrum and other low-energy 3-body observables involving wavenumbers \(k \ll 1/\ell\) are universal in the sense that they depend on the interatomic potential only through \(a\) and a single 3-body parameter. A convenient choice for this 3-body parameter is the low-energy parameter \(\Lambda^*_s\) 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
\[ E = 2\pi \hbar^2 an^2/m \left\{ 1 + 128/(15\sqrt{\pi})\sqrt{na^3} \right. \\
+ 8(4\pi - 3\sqrt{3})/3 \left[ \ln(na^3) + 4.72 + 2B \right] na^3 + \ldots \}. \] (1)

The \( \sqrt{na^3} \) correction was first calculated by Lee and Yang in 1957 [1]. 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 3-body coupling constant \( g_3(\kappa) \) that can be determined by measuring the low-energy behavior of the 3-atom elastic scattering rate. This “running coupling constant” depends on an arbitrary wavenumber \( \kappa \):

\[ g_3(\kappa) = 384\pi(4\pi - 3\sqrt{3})[\ln(\kappa a) + 2.72 + 2B] \bar{\hbar}^2 a^4/m, \] (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 3-body contact interaction and a 2-loop contribution from quantum fluctuations around the mean field, which also depends on \( \kappa \). The dependence on \( \kappa \) 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 2-body scattering [13]. It is suppressed by \( (na^3)^{3/2}/a \), 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 3-body parameter \( \Lambda_* \) introduced in Ref. [3]. This can be accomplished by calculating the T-matrix element for 3-atom elastic scattering in the low-energy limit. As the total energy \( E \) of the 3 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 \( \Lambda_* \) 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 \( \Lambda_* \) [8]. These arguments imply

\[ B = b_1 + b_2 \tan(s_0 \ln(|a|\Lambda_*) + \beta) \quad (a < 0), \] (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 3-body recombination rate into the shallow 2-body bound state [15],[16]:

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

The 3-body recombination rate has zeroes at values of \( a\Lambda_* \) that differ by multiplicative factors of 22.7, and consequently \( \text{Im} B \) 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

\[ \mathcal{L} = i\psi^* \frac{\partial}{\partial t} \psi + \frac{1}{2m} \psi^* \nabla^2 \psi - \frac{2\pi a}{m} |\psi|^4 \\
+ \frac{2\pi a}{m} |d - \psi|^2 - \frac{g_3}{36} |d||\psi|^2, \] (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 $d = \psi^2(1 + mg_3/(72\pi a)|\psi|^2 + ...)$.

However, it is more convenient to keep it, because 3-body observables can be conveniently calculated in terms of 4-point Green’s functions of $\psi$, $d$, $\psi^\dagger$ and $d^\dagger$. For example, the T-matrix element for 3-atom elastic scattering can be expressed as a sum of 9 connected 4-point Green’s functions. If the incoming atoms have momenta $k_1$, $k_2$, and $k_3$ with $k_1 + k_2 + k_3 = 0$, the external energies and momenta of $\psi$ and $d$ are set to $(k_1^2/2m, k_1)$ and $((k_2^2 + k_3^2)/2m, k_2 + k_3)$, respectively, and similarly for the outgoing atoms. The Green’s function is then summed over the 3 cyclic permutations of $k_1$, $k_2$, and $k_3$, and over the 3 cyclic permutations of the final momenta to get the T-matrix element. The Green’s functions can be calculated nonperturbatively by solving the integral equations shown in Fig. 1a. The single lines are propagators for $\psi$ and the double lines are exact propagators for $d$. An ultraviolet cutoff $\Lambda$ must be imposed on the loop momentum in the integral equation.

The coupling constant $g_3$ in (5) is tuned as a function of $\Lambda$ so that the low-energy 3-body observables depend only on $a$ and the low-energy parameter $\Lambda_*$. For small external energies and momenta $(\omega, k)$ with $m|\omega|a^2 \ll 1$ and $|k| \ll 1$, a Green’s 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’s function using the nonperturbative method of Ref. [9], we can determine $g_3$ as a function of $a$ and $\Lambda_*$. We choose the two particle-irreducible connected Green’s function $T(p)$ with external energies and momenta $(0, 0)$ for $\psi$ and $d$, $(p^2/2m, p)$ for $\psi^\dagger$, and $(-p^2/2m, -p)$ 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 $\kappa$ to remove the poles in $\epsilon$. Calculating the diagrams that contribute to $T(p)$ in the limit $p \to 0$ using perturbation theory to first order $g_3$ and 4th order in $a$, we obtain

$$T(p) \to -g_3(\kappa)/36 + 16\pi^2 a^4/m\left\{1/(p^2 a^2) - 2\pi/(3pa) -2(4\pi - 3\sqrt{3})/(3\pi) [\ln(p/\kappa) + A_{\text{MS}}]\right\},$$

(6)
where \( A_{MS} = -0.77268 \) and the subscript MS stands for “minimal subtraction.” The non-perturbative calculation of the Green’s function \( T(p) \) using the method of Ref. requires solving the integral equation in Fig. 1a. It is convenient to define a subtracted Green function \( \mathcal{T}(p) \) that has a finite limit as \( p \to 0 \) using the subtraction shown in Fig. 1b. We solve the integral equation for \( \mathcal{T}(p) \) as a function of \( p, a, \) and \( \Lambda_* \) and then set \( p = 0 \). The resulting expression for \( \mathcal{T}(p) \) in the limit \( p \to 0 \) is

\[
\mathcal{T}(p) \rightarrow 16\pi^2 a^4/m \left\{ 1/(p^2 a^2) - 2\pi/(3pa) \right. \\
\left. -2(4\pi - 3\sqrt{3})/(3\pi) \right\} \ln(pa) + A(a\Lambda_*) \},
\]

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

\[
B = -A_{MS} + A(a\Lambda_*).
\]

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

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

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 (4) for the energy density, the real part of the factor in brackets can be separated into 2 terms: \( 2\ln(\kappa a) + 2\text{Re}B \), 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 \( \kappa \) is arbitrary, we can by a suitable choice of \( \kappa \) arrange for most of the \( na^3 \) correction to come from the mean-field contribution. The smallest value of \( \kappa \) 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 3-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 (4) 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 3-body recombination into the shallow 2-body bound state and a recoiling atom. In the mean field approximation, the rate of decrease of the number density is \( (\partial n/\partial t) = -(\text{Im}g_3/6\hbar)n^3 \). Note that \( \text{Im}g_3 \) is independent of \( \kappa \). The energy loss rate is given by \( \partial E/\partial t = (\partial E/\partial n)\partial n/\partial t \). The condensate is particularly stable at values of \( a \) that correspond to \( \ln(a\Lambda_*) = 2.93 \mod \pi/s_0 \). At these discrete values of \( a \) that differ by multiplicative factors of 22.7, there is an interference effect that causes the 3-body recombination rate to vanish \([15][16]\). The recombination process that gives the energy density an imaginary part produces atoms and bound states with wavenumber \( k = 2/(\sqrt{3}a) \). 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 \( \Lambda_* \). For example, the scattering length was calculated in Ref. [4] 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 \( N_{\text{max}} \) [18]. An effective 3-body contact interaction \(-g_3\) gives a mean-field contribution \( g_3 n^3/36 \) to the energy density. The effect of such a term on the stability of a trapped condensate has been studied by adding a 3-body term to the Gross-Pitaevski equation [19]. Even a small positive value of \( g_3 \) can considerably increase the critical number \( N_{\text{max}} \).

In the case of large negative scattering length, the 3-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 \( \kappa \) in this case is the lowest wavenumber above which 3-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 \( \kappa \) set by the coherence length is \( \kappa^2 > 4m(\mu - V(r)) \), where \( \mu \) is the chemical potential.

For a harmonic potential with frequency \( \omega \), 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 3-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 like \( a^4 \). Note that the constant \( B \) given in (3) diverges at values of \( a \) that correspond to \( \ln(a \Lambda_*) \) = 1.37 mod \( \pi/s_0 \). At these discrete values of \( a \), there is an Efimov state at the 3-atom threshold. Near these values of \( a \), the 3-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 3-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 [2] 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 \( E = C\hbar^2 n^{5/3}/m \), where \( C \) is a constant. In the extremely dilute limit, we found that \( \mathcal{E} \) depends on \( \Lambda_* \) at second order in \( \sqrt{na^3} \). Does \( \mathcal{E} \) depend on \( \Lambda_* \) 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 3-body observables discovered by Efimov \cite{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 \( \ell \) to order \( a \). The question of whether \( C \) depends on \( \Lambda_* \) is not addressed by the
constrained variational calculations of Ref. \cite{6}. Their variational ansatz excludes states with
3-body configurations that are sensitive to \( \Lambda_* \). For example, in the 3-body sector, it would
exclude the Efimov states.

If the coefficient \( C \) in the energy density depends on the 3-body parameter \( \Lambda_* \), one might
worry that it may also depend on infinitely many other low-energy parameters associated
with 4-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
4-body and higher \( n \)-body sectors are all calculable to leading order in \( \ell/a \) in terms of \( a \) and
\( \Lambda_* \) 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 \( \Lambda_* \) only.

This research was supported in part by DOE grant DE-FG02-91-ER4069 and by NSF
grant PHY-9800964.

Note added.—After this work was submitted for publication, we became aware of a
related study by Bulgac \cite{20}. 

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