INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS B: ATOMIC, MOLECULAR AND OPTICAL PHYSICS

J. Phys. B: At. Mol. Opt. Phys. **37** (2004) L227–L233 PII: S0953-4075(04)77068-6

**LETTER TO THE EDITOR**

# Universal properties of Bose systems with van der Waals interaction

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Received 2 March 2004
Published 17 May 2004
Online at stacks.iop.org/JPhysB/37/L227
DOI: 10.1088/0953-4075/37/11/L02

**Abstract**

We show that universal properties of a many-atom quantum system exist at a much higher density, or a much shorter length scale, than those implied by traditional theories for a dilute Bose gas. In particular, a universal equation of state at length scale $\beta_6 = (mC_6/\hbar^2)^{1/4}$ (corresponding to the van der Waals interaction) is defined and investigated by combining the concept of effective potential, the constrained variational method and the analytic solution for the van der Waals potential. In one application, we show that a many-atom Bose system with negative scattering length may form a metastable liquid Bose–Einstein condensate (BEC) state with an equilibrium density that is controlled by a scaled scattering length.

The realization of gaseous Bose–Einstein condensate (BEC) [1–3] has brought an explosion of activities in the study of many-atom quantum systems [4, 5]. Considerable advances have been made in using the Gross–Pitevaskii (GP) equation to simulate a vast variety of interesting phenomena that characterize a macroscopic quantum system [4, 5]. In terms of microscopic understanding, however, the rate of advance has been more limited. Much of what we know can still be summarized by the famous equation of state for a quantum gas of hard spheres [6, 7]:

$$E/N = \frac{2\pi\hbar^2 a_0}{m}\rho\left[1 + \frac{128}{15\sqrt{\pi}}\left(\rho a_0^3\right)^{1/2}\right]. \tag{1}$$

Here $\rho = N/V$ is the number density, and $a_0$ is the two-body s-wave scattering length. The first term in this equation represents the mean-field interaction that accounts for much of the GP theory. The second term, often referred as the Lee–Huang–Yang (LHY) correction [6, 7], accounts for quantum fluctuation.

  

While equation (1) represents a universal property of Bose systems with short-range interactions, its range of applicability is very limited. In addition to the well-known restriction of $\rho a_0^3 \ll 1$, equation (1) tells us nothing about how atomic interaction would affect the equation of state for $a_0 = 0$. Is a condensate with zero scattering length stable? For $a_0 < 0$, the LHY correction is not meaningful and all we know is the mean field. It is based on this single term that one has generally believed that a homogeneous condensate with negative scattering length would collapse (see, e.g., [8]). Rigorously speaking, however, all the mean field tells us that the condensate can be expected to contract some to a higher density. Without knowing what happens at higher densities, the fate of a condensate, whether it collapses or not, or the nature of the collapse cannot be understood theoretically. Issues such as these are more than theoretical curiosities, they are of increasing practical importance especially due to experiments in which $a_0$ is adjustable via a magnetic field [9] and can in principle take on any value (see, e.g., [10–12]).

In all cases where equation (1) fails, one has to look at an atomic interaction at a shorter length scale. The key question is then: do universal properties exist at shorter length scales, or equivalently, at higher densities? The underlying physics would be much less attractive if they do not exist. Fortunately, the answer is yes, as we have argued in a recent publication [13]. In particular, at the first length scale beyond the shape-independent approximation, atoms see the van der Waals interaction, $-C_6/r^6$, corresponding to a length scale $\beta_6 = (mC_6/\hbar^2)^{1/4}$. The universal properties at this, and shorter length scales, can be investigated systematically using the concept of effective potential [13].

In this work, we define more explicitly the universal properties at the length scale $\beta_6$ for a many-atom quantum system with the van der Waals interaction. The universal equation of state for a Bose system is investigated by combining the concept of effective potential [13], the constrained variational method [14, 15] and the analytic solution for $-C_6/r^6$ potential [16]. In particular, we show that the energy per particle for a system of negative scattering length does not decrease with density indefinitely as predicted by the mean-field term in equation (1). Instead, it reaches a minimum at an equilibrium density that is determined by a scaled scattering length. One implication of this result is the existence of a liquid BEC state that behaves very much like liquid He II. Its implication on the collapse of a condensate will also be addressed briefly.

Consider a class of $N$-atom quantum systems described by a Hamiltonian

$$H = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\nabla_i^2 + \sum_{i<j=1}^{N} v(r_{ij}), \tag{2}$$

where $v(r) \to -C_n/r^n$ $(n > 2)$ for $r \to \infty$. The universal properties at length scale $\beta_n = (mC_n/\hbar^2)^{1/(n-2)}$ are defined by the corresponding properties of an effective Hamiltonian, $H_{\rm eff}$, in a limit that eliminates all length scales in $H_{\rm eff}$ that are shorter than $\beta_n$ [13].

The effective Hamiltonian, $H_{\rm eff}$, is the same as $H$ with $v(r)$ replaced by an effective potential $v_{\rm eff}(r)$. There is a considerable freedom in the choice of $v_{\rm eff}(r)$, provided that (a) it has the same long-range behaviour as $v(r)$, (b) it yields the same short-range parameter $K^c$ [17, 13] and (c) it is repulsive at short distances and rises faster than $1/r^2$. To be specific, we choose here the effective potential to be a hard-sphere with an attractive tail (HST) [13]:

$$v_{\rm eff}(r) = v_{\rm HST}(r) = \begin{cases} \infty, & r \leqslant r_0 \\ -C_n/r^n, & r > r_0. \end{cases} \tag{3}$$

With this choice, the limit that eliminates short-length scales in $H_{\rm eff}$ will be formally denoted by $r_0 \to 0+$. It has to be understood, however, that this limit is taken in such a way that $K^c$ is kept a constant. For the HST effective potential, this means that $r_0$ takes on a *discrete set* of

successively smaller, but never zero, values. The corresponding effective potentials all have the same $K^c$, with the only difference being that the ones with smaller $r_0$ support a greater number of bound states [13].

The physical properties of $H$ around the $N$-atom threshold are well described by universal properties defined through $H_{\rm eff}$ because their corresponding two-body problems have, to a very good approximation, the same bound spectra, the same scattering properties and the same wavefunctions (where it matters) over a wide range of energies around the threshold [17, 13]. An $N$-body state, be it much more complex, can in principle be constructed by successive coupling of $i$-body states around the threshold to form $(i+1)$-body states around the threshold, starting from $i = 2$ [13]. We emphasize that embedded in this argument is the important concept of angular-momentum-insensitive quantum-defect theory (AQDT) [17], namely two-atom states of different angular momenta can be described by the same short-range parameter $K^c$ around the threshold. If this were not the case, the effective potential would just be another pseudopotential, and would not be able to describe states for which the coupling of difference angular momenta is important.

This method of investigating universal properties of an $N$-atom quantum system is a powerful one. It is applicable to any $N \geqslant 2$, and can be generalized to shorter length scales. The investigation can be either analytical or purely numerical. We focus here on a single property of a single state (the BEC state), namely the equation of state (energy per particle versus density) for a homogeneous system of a large number of bosons. By scaling all energies in $H_{\rm eff}$ by $s_E = (\hbar^2/m)(1/\beta_n)^2$ and all lengths by $\beta_n$, it is clear that the result, in the limit of $r_0 \to 0+$, can be written as

$$E_s/N = \bar{\Omega}^{(n)}(\rho_s, K^c), \tag{4}$$

where $\rho_s = \rho\beta_n^3$ is a scaled density, $E_s = E/s_E$ is a scaled energy and $\bar{\Omega}^{(n)}$ is a universal function that is uniquely determined by the exponent of the long-range interaction, namely the $n$ in $-C_n/r^n$. For $n > 3$, $K^c$ can be related to a scaled s-wave scattering length, $a_{0s} = a_0/\beta_n$, by [13]

$$a_{0s} = \left[b^{2b}\frac{\Gamma(1-b)}{\Gamma(1+b)}\right]\frac{K^c + \tan(\pi b/2)}{K^c - \tan(\pi b/2)}, \tag{5}$$

where $b = 1/(n-2)$. We can therefore write

$$E_s/N = \Omega^{(n)}(\rho_s, a_{0s}). \tag{6}$$

Equation (4) or (6) is what we call the universal equation of state at length scale $\beta_n$.

The many-body problem with $v_{\rm HST}(r)$ is, of course, still nontrivial. But like the many-body of hard spheres, it is easier than the original problem because two-body solutions for the van der Waals potential are known analytically [16]. We investigate $\Omega^{(6)}$ here using the lowest order constrained variational method (LOCV) [14, 15]. Not only has it been shown to give excellent results for hard spheres over a wide range of densities [15], but also one approach in which the limit of $r_0 \to 0+$ can be taken analytically. The method is based on the Jastrow wavefunction [18] for a many-body Bose system:

$$\Psi = \prod_{i<j} F(\mathbf{r}_i - \mathbf{r}_j). \tag{7}$$

Defining $u(r) = rF(r)$, a variational procedure leads to [14, 15]

$$\left[-\frac{\hbar^2}{2\mu}\frac{{\rm d}^2}{{\rm d}r^2} + v(r) - \lambda\right]u_\lambda(r) = 0, \tag{8}$$

to be solved with boundary conditions $u_\lambda(r=d)=d$ and $u'_\lambda(r=d)=1$, and a normalization condition

$$4\pi\rho\int_0^d u_\lambda^2\,\mathrm{d}r=1. \tag{9}$$

Here $\mu=m/2$ is the two-body reduced mass, and $d$ is a healing distance beyond which $F=1$. To the lowest order, the energy per particle is given through $\lambda$ by

$$E/N=\lambda/2-\frac{1}{2}\frac{C_6}{d^3}\left(\frac{4\pi}{3}\rho\right), \tag{10}$$

where the second term arises from contributions beyond the healing distance $d$, due to the long-range nature of the van der Waals interaction.

Replacing $v(r)$ by $v_{\mathrm{HST}}(r)$, the solution of equation (8) is simply [16, 17]

$$u_\lambda(r)=A_\lambda\big[f^c_{\lambda_s l=0}(r_s)-K^c g^c_{\lambda_s l=0}(r_s)\big]. \tag{11}$$

Here $A_\lambda$ is a normalization constant. $f^c_{\lambda_s l}$ and $g^c_{\lambda_s l}$ are the analytic solutions for the $-C_6/r^6$ potential [16, 13] that depend on $r$ only through a scaled radius $r_s=r/\beta_6$, and on energy only through a scaled energy $\lambda_s=\lambda/s_E$. Specifically,

$$\begin{pmatrix}f^c\\ g^c\end{pmatrix}=B\begin{pmatrix}\sin\left(\frac{1}{2}\pi\nu-\theta\right) & \sin\left(\frac{1}{2}\pi\nu+\theta\right)\\ -\cos\left(\frac{1}{2}\pi\nu-\theta\right) & \cos\left(\frac{1}{2}\pi\nu+\theta\right)\end{pmatrix}\begin{pmatrix}\xi\\ \eta\end{pmatrix}, \tag{12}$$

where

$$B_{\lambda_s l}=\left\{\left[2\big(X^2_{\lambda_s l}+Y^2_{\lambda_s l}\big)\right]^{1/2}\sin(\pi\nu)\right\}^{-1}, \tag{13}$$

$$\xi_{\lambda_s l}(r)=\sum_{j=-\infty}^{\infty} b_j r_s^{1/2}J_{\nu+j}(y), \tag{14}$$

$$\eta_{\lambda_s l}(r)=\sum_{j=-\infty}^{\infty}(-1)^j b_j r_s^{1/2}J_{-\nu-j}(y), \tag{15}$$

$y=(1/2)r_s^{-2}$, and $\tan\theta=Y_{\lambda_s l}/X_{\lambda_s l}$. Here the order $\nu$, the coefficients $b_j$, and $X_{\lambda_s l}$ and $Y_{\lambda_s l}$ are those defined in [16].

Imposing boundary conditions and taking the limit of $r_0\to 0+$, we arrive at the following two equations for two unknowns $\lambda_s$ and $d_s=d/\beta_6$:

$$\frac{f^c_{\lambda_s l}(d_s)-d_s f^{c\,\prime}_{\lambda_s l}(d_s)}{g^c_{\lambda_s l}(d_s)-d_s g^{c\,\prime}_{\lambda_s l}(d_s)}=K^c, \tag{16}$$

$$4\pi d_s^2\big[f^c_{\lambda_s l}(d_s)-K^c g^c_{\lambda_s l}(d_s)\big]^{-2}\int_0^{d_s}\big[f^c_{\lambda_s l}(r_s)-K^c g^c_{\lambda_s l}(r_s)\big]^2\,\mathrm{d}r_s=1/\rho_s, \tag{17}$$

in which $l=0$. The only system-specific parameters in equations (16) and (17) are, as expected, $\rho_s$ and $K^c$. Their solution gives us the universal $\Omega^{(6)}$ function in LOCV approximation:

$$E_s/N=\Omega^{(6)}(\rho_s,a_{0s})\approx\lambda_s/2-\frac{1}{2d_s^3 r_{\rho s}^3}, \tag{18}$$

where $r_{\rho s}=r_\rho/\beta_6=(4\pi\rho/3)^{-1/3}/\beta_6$ is the scaled average separation between atoms at density $\rho$.

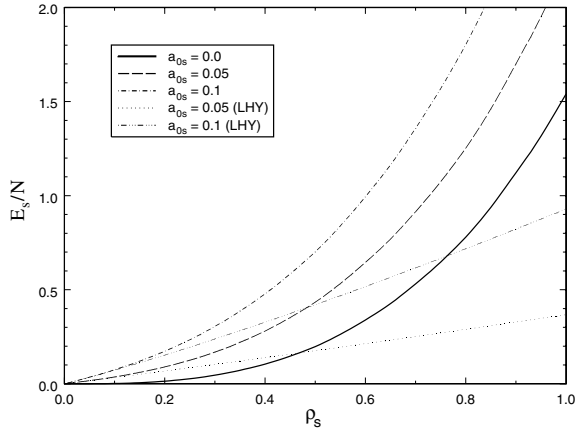


**Figure 1.** The universal equations of state at length scale $\beta_6$ for many-atom Bose systems with zero and positive scattering lengths, in LOCV approximation. The LHY results, as given by equation (1), are also shown for comparison. The LHY results for zero scattering length are identically zero and are not shown.

This formulation has been tested for both low and high densities (more details will be presented elsewhere). For low densities ($\rho_s \ll 1$), the length scale $\beta_6$ disappears and the results are in excellent agreement with the LHY results of equation (1). For high densities, the theory has been tested with liquid He II using $C_6 = 1.461$ au and $a_0 = 172$ au, obtained from the HFD-B(HE) potential of Aziz *et al* [19], the theory predicts an equilibrium density of $1.80 \times 10^{22}\,\mathrm{cm}^{-3}$, and an equilibrium energy per particle of $-6.53$ K, in good agreement with experimental values of $2.18 \times 10^{22}\,\mathrm{cm}^{-3}$ and $-7.17$ K, respectively [20]. Because $^4$He has the weakest van der Waals interaction among all atoms, this comparison gives us a worst-case scenario test of both our theoretical formulation and the concept of universal equation of state at length scale $\beta_6$. When combined, these results show that the present theory provides a unified understanding of Bose systems over a very wide range of densities. The theory is also applicable to an arbitrary scattering length as the representation of $u_\lambda(r)$ is well defined in all cases. For alkali atoms, the equations of state are expected to follow universal properties up to $\rho_s \sim 10$, since the two-body wavefunction is accurately represented by equation (11) for $r_s > 0.5$ [13]. Beyond this density, interactions of shorter range are expected to come into play.

In figure 1, we show equations of state for zero and positive scattering lengths. In particular, it shows that a condensate with zero scattering length has energy per particle that increases with density, and is therefore stable energetically. Experimentally, this state has been used regularly as the initial state for collapse [10, 11].

Figure 2 illustrates equations of state for a set of negative scattering lengths. It shows that energy per particle does not decrease monotonically with increasing density. Instead, it reaches a minimum and rises again and eventually becomes positive. This behaviour has a number of important implications. In particular, it means that a many-atom Bose system with negative scattering length does not have to collapse. It may form a liquid BEC state with a scaled equilibrium density, $\rho_{0s}$, corresponding to the minima in figure 2. A system in such a state behaves very much like liquid helium II, with the following characteristics. (a) It obviously has negative energy per particle. This means that unlike a gaseous BEC state that requires a trap to keep it together, a system in a liquid BEC state, once created, stays together

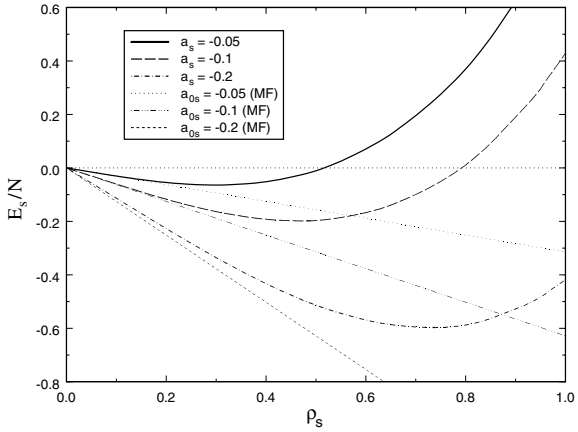


**Figure 2.** Universal equations of state at length scale $\beta_6$ for many-atom Bose systems with negative scattering lengths, in LOCV approximation. The mean-field (MF) results, as given by the first term in equation (1), are also shown for comparison.

when released from a trap. (b) It has positive compressibility, meaning that it supports phonons and is a superfluid. For most atoms, the liquid BEC state is metastable just like the gaseous BEC, with stability determined by the rate of molecular formation (see, e.g., [21]).

The example of $^{85}$Rb, which is of special interest in collapse experiments [11], gives a feel for orders of magnitudes involved. Using $C_6 = 4700$ au [22], which corresponds to a $\beta_6 = 164$ au, the following results are obtained. For $a_0 = -1$ au, corresponding to $a_{0s} = -6.09 \times 10^{-3}$, an equilibrium density of $8.78 \times 10^{-2}\left(1/\beta_6^3\right) = 1.34 \times 10^{17}\,\mathrm{cm}^{-3}$ and an equilibrium energy per particle of $-174$ nK are predicted. For $a_0 = -10$ au, corresponding to $a_{0s} = -0.0609$, an equilibrium density of $0.332(1/\beta_6^3) = 5.05 \times 10^{17}\,\mathrm{cm}^{-3}$ and an equilibrium energy per particle of $-6.65\ \mu$K are predicted. For $a_0 = -30$ au, corresponding to $a_{0s} = -0.183$, an equilibrium density of $0.685\left(1/\beta_6^3\right) = 1.04 \times 10^{18}\,\mathrm{cm}^{-3}$ and an equilibrium energy per particle of $-39.1\ \mu$K are predicted. Thus for alkali atoms, which have $\beta_6 \gg 1$ au, the densities of liquid BEC states are generally much smaller than those of normal liquids. They are also much softer and have much smaller (absolute) energies per particle.

The equations of state presented here also suggest a different mechanism, or picture, for the collapse of a condensate [11], in addition to the possibility of collapsing via three-body recombination [8, 23]. Some ingredients of this picture are as follows. (a) A many-atom system with negative scattering length is unstable at $\rho_s < \rho_{0s}$ not because an equilibrium state does not exist for negative scattering lengths, but because it is away from the equilibrium. The collapse is thus a relaxation process towards equilibrium. (b) Collapsing may occur collectively through condensation into the metastable liquid state, even in the absence of three-body recombination. A more careful quantitative analysis of this picture is still in progress. But it seems likely that the liquid BEC state has already shown itself in the collapse experiment as a part of the 'missing' atoms [11].

In conclusion, we have shown that universal properties of many-atom quantum systems exist at length the scale $\beta_6$. The behaviour of a BEC at this length scale exhibits many interesting features, including a liquid BEC state for systems with negative scattering lengths. A generalization to inhomogeneous systems (to take into account the trap) is straightforward, especially in local density approximation. The results point to new challenges ahead for both theory and experiment. What is the best way to achieve a liquid BEC state? Can it be created

directly, instead going through a gaseous BEC state? What is the stability or the lifetime of a liquid BEC state, especially for relatively large equilibrium densities? As stated earlier, the stability is determined by the rate of molecular formation. This process is poorly understood even in the gas phase [21], and no theory seems to exist at higher densities. As a rough guide to future investigations, we point out that molecular formation will ultimately be quenched at sufficiently high densities, with helium being an example. Let $r_{\rho 0}$ be the average separation between atoms at an equilibrium density. Molecular formation can only happen if there exist molecular states that have sizes smaller than $r_{\rho 0}$. As density increases from zero, the rate of molecular formation first increases with density, then decreases and reaches a local minimum at a density where the molecular state that is closest to the (two-body) threshold effectively merges into the many-atom continuum. The rate will oscillate around a decreasing background as the same happens to more tightly bound molecular states, until it eventually becomes zero for sufficiently high densities. This qualitative picture gives hope that there may exist other high density, robust superfluids other than liquid helium II that are sufficiently stable to be of practical interest. Even for short lifetimes, the liquid BEC state can be expected to manifest itself in the dynamical evolution of a condensate, such as collapse.

## Acknowledgment

This work was supported by NSF under the grant number PHY-0140295.

## References

[1] Anderson M H *et al* 1995 *Science* **269** 198
[2] Davis K B *et al* 1995 *Phys. Rev. Lett.* **75** 3969
[3] Bradley C C *et al* 1995 *Phys. Rev. Lett.* **75** 1687
[4] Dalfovo F *et al* 1999 *Rev. Mod. Phys.* **71** 463
[5] Leggett A J 2001 *Rev. Mod. Phys.* **73** 307
[6] Lee T D and Yang C N 1957 *Phys. Rev.* **105** 1119
[7] Lee T D, Huang K and Yang C N 1957 *Phys. Rev.* **106** 1135
[8] Kagan Y, Muryshev A E and Shlyapnikov G V 1998 *Phys. Rev. Lett.* **81** 933
[9] Tiesinga E *et al* 1992 *Phys. Rev.* A **46** R1167
[10] Roberts J L *et al* 2001 *Phys. Rev. Lett.* **86** 4211
[11] Donley E A *et al* 2001 *Nature* **412** 295
[12] Claussen N R *et al* 2002 *Phys. Rev. Lett.* **89** 010401
[13] Gao B 2003 *J. Phys. B: At. Mol. Opt. Phys.* **36** 2111
[14] Pandharipande V R and Bethe H A 1973 *Phys. Rev.* C **7** 1312
[15] Cowell S *et al* 2002 *Phys. Rev. Lett.* **88** 210403
[16] Gao B 1998 *Phys. Rev.* A **58** 1728
[17] Gao B 2001 *Phys. Rev.* A **64** 010701(R)
[18] Jastrow R 1955 *Phys. Rev.* **98** 1479
[19] Aziz R A, McCourt F R W and Wong C C K 1987 *Mol. Phys.* **61** 1487
[20] Ouboter R D B and Yang C N 1987 *Physica* B **44** 127
[21] Suno H *et al* 2002 *Phys. Rev.* A **65** 042725
[22] Roberts J L *et al* 1998 *Phys. Rev. Lett.* **81** 5109
[23] Savage C M, Robins N P and Hope J J 2003 *Phys. Rev.* A **67** 014304