

Nonuniversal Effects in the Homogeneous Bose Gas

Shawn Hermans

Saint John's University, Collegeville, MN 56321

Advisor: Professor Eric Braaten

The Ohio State University, Columbus, OH 43210

Abstract

In 1924 Albert Einstein predicted the existence of a special type of matter now known as Bose-Einstein condensation. However, it was not until 1995 that simple BEC (Bose-Einstein condensation) was observed in a low-density Bosonic gas. This recent experimental breakthrough has led to renewed theoretical interest in BEC. The focus of my research is to more accurately determine basic properties of homogeneous Bose gases. In particular nonuniversal effects of the energy density and condensate fraction will be explored. The validity of the theoretical predictions obtained is verified by comparison to numerical data from the paper *Ground State of a Homogeneous Bose Gas: A Diffusion Monte Carlo Calculation* by Giorgini, Boronat, and Casulleras.

I. INTRODUCTION

The Bose-Einstein condensation of trapped atoms allows the experimental study of Bose gases with high precision. It is well known that the dominant effects of interactions between the atoms can be characterized by a single number a called the S-wave scattering length. This property is known as *universality*. Increasingly accurate measurements will show deviations from universality. These effects are due to sensitivity to aspects of the interatomic interactions other than the scattering length. These effects are known as *nonuniversal* effects. Intensive theoretical investigations into the homogeneous Bose gas revealed that properties could be calculated using a low-density expansion in powers of $\sqrt{na^3}$, where n is the number density. For example the energy density has the expansion

$$\frac{E}{N} = \frac{2\pi na\hbar^2}{m} \left(1 + \frac{128}{15\sqrt{\pi}} \sqrt{na^3} + \frac{8(4\pi - 3\sqrt{3})}{3} na^3 (\ln(na^3) + c) + \dots \right) \quad (1)$$

The first term in this expansion is the mean-field approximation and was calculated by Bogoliubov [2]. The corrections to the mean-field approximation can be calculated using perturbation theory. The coefficient of the $(na^3)^{3/2}$ term was calculated by Lee, Huang, and Yang [3] and the last term was first calculated by Wu [4]. Hugenholtz and Pines [5] have shown that the constant c_1 and the higher-order terms in the expansion are all nonuniversal. Giorgini, Boronat, and Casulleras [1] have studied the ground state of a homogeneous Bose gas by exactly solving the N-bodied Schrödinger (to within statistical error) using a diffusion Monte Carlo method.

In section II of this paper, theoretical background relevant to this problem is presented. Section III is a brief summary of the numerical data from Giorgini, Boronat, and Casulleras. Section IV briefly presents the higher-order approximations and Section V analyzes the higher order approximations by fitting to data from Ref. [1]. Section VI presents conclusions to date and prospects for future analysis.

II. THEORETICAL BACKGROUND

This section discusses the background relevant to understanding the calculations and theory discussed later in the paper.

A. Qualitative Properties of Bose-Einstein Condensation

All elementary particles fall into two exclusive classes, bosons and fermions. The distinction between the two classes is derived from the indistinguishability of particles. To explain what this means take the case of two quantum particles with the same properties¹. If these were classical particles, one could easily distinguish between the two particles by tagging the particles in some way. Number the particles, paint them different colors, but the result is that the particles can be distinguished. This is not possible for quantum particles. After all, how does one paint an electron or a photon? With this option exhausted, an experimenter might suggest simply to follow each of the two particles around. Classically this will work. If I follow two particles around, I would be able to then tell you the difference between them. However, a problem occurs in quantum mechanics. In quantum mechanics the act of observation alters the particle being observed. Therefore the particle cannot be followed because by observing it, the observer cannot be certain that the particle they observed is the particle that was first observed.

With this in mind consider the wavefunction for a multi-bodied quantum mechanical system. For the sake of simplicity, we will only consider the case of a two-body system, but rest assured that the results obtained from this example generalize to N-body system. The wavefunction of this system can be represented as $\Psi(\mathbf{r}_1, \mathbf{r}_2)$ where \mathbf{r}_1 is the coordinate of the first particle and \mathbf{r}_2 is the coordinate of the second particle. Now make the assumption

¹The subsequent explanation is largely based on *Introduction to Quantum Mechanics* by David J. Griffiths

that the wavefunction can be written as a product of the wavefunctions of each particle, $\Psi(\mathbf{r}_1, \mathbf{r}_2) = \psi_a(\mathbf{r}_1)\psi_b(\mathbf{r}_2)$, where ψ_a is the wavefunction of the first particle and ψ_b is the wavefunction of the second particle. However it has been shown that there is no way to distinguish between the two particles so how can particle 1 and particle 2 have different wavefunctions? Because they cannot have distinguishable wavefunctions this means the coordinates \mathbf{r}_1 and \mathbf{r}_2 can be interchanged without effecting the answer. Thus a generalized wavefunction would look like, $\Psi(\mathbf{r}_1, \mathbf{r}_2) = A[\psi_a(\mathbf{r}_1)\psi_b(\mathbf{r}_2) \pm \psi_b(\mathbf{r}_1)\psi_a(\mathbf{r}_2)]$. The case with the plus sign corresponds to bosons and the minus sign corresponds to fermions. In general this result can be stated as $\Psi(\mathbf{r}_1, \mathbf{r}_2) = \pm\Psi(\mathbf{r}_2, \mathbf{r}_1)$. Notice that for fermions if $\psi_a = \psi_b$ then $\Psi(\mathbf{r}_1, \mathbf{r}_2) = 0$. This result is what gives rise to the Pauli exclusion principle: two fermions cannot inhabit the same state. This property also is responsible for the Fermi-Dirac distribution:

$$n(\epsilon) = \frac{1}{e^{(\epsilon-\mu)/K_bT} + 1}. \quad (2)$$

In equation (2) $n(\epsilon)$ is the number-density (the number particles at a particular energy), ϵ is the energy, μ is the chemical potential, T is temperature, and K_b is Boltzmann's constant. As a side note, all fermions have intrinsic angular momentum, or spin, of $\frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \dots$ in units of \hbar . The connection between spin and statistics is a direct result of combining relativity with quantum mechanics.

Bosons are different creatures entirely. Instead of fractional spin, bosons possess integer spin. Also bosons do not obey the exclusion principle. The fact that bosons can share states with other bosons gives rise to Bose-Einstein statistics:

$$n(\epsilon) = \frac{1}{e^{(\epsilon-\mu)/K_bT} - 1}. \quad (3)$$

With equations (2) and (3) many properties of fermions and bosons can be explored. However these statistics are limited in their use. Particularly the Bose-Einstein distribution experiences difficulties when large numbers of particles all condense to the same state. This crisis is called Bose-Einstein condensation. Quantum mechanically what this means is that

a large number of particles exist with the exact same wavefunction. This phenomenon is what is responsible for coherent light in lasers and it is also responsible for superfluidity in liquid helium. However, certain complications such as particle interactions make theoretical descriptions of these states difficult. To verify the simplest properties of BEC, one ideally wants very little interatomic interactions. It was not until 1995 that such a state was created experimentally in a low-density gas of rubidium-87 atoms [9]. This experimental breakthrough created a renewed experimental and theoretical interest into BEC.

B. Formulation of Problem in Ordinary Quantum Mechanics

The problem of Bose-Einstein condensation in ordinary quantum mechanics is best described by the Hamiltonian

$$\hat{H} = \sum_{i=1}^N \left[-\frac{\hbar^2}{2m} \nabla_i^2 + V(\mathbf{r}_i) \right] + \frac{4\pi\hbar^2 a}{m} \sum_{i < j} \delta(|\mathbf{r}_i - \mathbf{r}_j|). \quad (4)$$

From this point forward the bosons involved in BEC will be referred to as atoms. In this situation, a represents the S-wave scattering length of the atoms in question, the delta function represents point-like interactions between the atoms, and the other terms are the normal kinetic energy and potential energy terms of the Hamiltonian. Using this formulation of the problem the first term in the series expansion of (1) can be found. This first term is known as the mean-field approximation and is derived below. The first stage in the mean-field approximation involves minimizing the expectation value of the Hamiltonian. Before this can be done, an assumption needs to be made. The wavefunction for many particles can be written as $\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)$. Since the particles are bosons this wavefunction is the same if two coordinates are interchanged. This property of bosons will come into play later. Now make the assumption that in the ground state all the atoms are in the same state so that the wavefunction can be written as $\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) = \psi(\mathbf{r}_1)\psi(\mathbf{r}_2)\dots\psi(\mathbf{r}_N)$. We want to find the wavefunction $\psi(\mathbf{r})$ that minimizes the expectation value of the Hamiltonian subject to the constraint that the state is properly normalized. In mathematical terms this means

$$\langle \psi | \psi \rangle = \int d^3 r \psi^*(\mathbf{r}) \psi(\mathbf{r}) = 1. \quad (5)$$

The expectation value for the Hamiltonian can be computed with little trouble. First compute

$$\langle \Psi | [-\frac{\hbar^2}{2m} \nabla_i^2 + V(\mathbf{r}_i)] | \Psi \rangle = - \int d^3 r_i \psi^*(\mathbf{r}_i) [-\frac{\hbar^2}{2m} \nabla_i^2 + V(\mathbf{r}_i)] \psi(\mathbf{r}_i) \quad (6)$$

A few things need to be noted at this point. First note that the expectation value for one particle is being computed. This is okay since all of the particles are identical, so by finding the expectation value for one, all the expectation values have been found. Next note that ∇_i^2 is only applied to the i th wavefunction. This means that $N - 1$ factors of $[\int d^3 r \psi^*(\mathbf{r}) \psi(\mathbf{r})]$ can be factored out in all values of i . Since the wavefunctions are normalized, this term is 1. Also note that from this point forward the subscripts are dropped from the \mathbf{r} . This is acceptable since all the wavefunctions are identical under interchanges of coordinates. Next the $\langle \Psi | 4\pi\hbar^2 a/m \delta(\mathbf{r}_1 - \mathbf{r}_2) | \Psi \rangle$ term needs to be dealt with. In this case $N - 2$ factors of $[\int d^3 r \psi^*(\mathbf{r}) \psi(\mathbf{r})]$ can be factored out. This leaves

$$\langle \Psi | \frac{4\pi\hbar^2 a}{m} \delta(\mathbf{r}_1 - \mathbf{r}_2) | \Psi \rangle = \int d^3 r_1 \int d^3 r_2 \psi^*(\mathbf{r}_1) \psi^*(\mathbf{r}_2) \frac{4\pi\hbar^2 a}{m} \delta(\mathbf{r}_1 - \mathbf{r}_2) \psi(\mathbf{r}_1) \psi(\mathbf{r}_2). \quad (7)$$

This is easy to integrate and gives a final result of

$$\langle \Psi | \frac{4\pi\hbar^2 a}{m} \delta(\mathbf{r}_1 - \mathbf{r}_2) | \Psi \rangle = \int d^3 r \frac{4\pi\hbar^2 a}{m} (\psi^* \psi)^2. \quad (8)$$

This term should be multiplied by $(N - 1)N/2$ since the delta function potential acts on N choose 2 pairs of particles. Notice that when dealing with large amounts of particles it is safe to assume that $(N - 1)N/2$ is close to $N^2/2$. Combining (6) and (8), the expectation value of the Hamiltonian is

$$\langle \Psi | \hat{H} | \Psi \rangle = N \int d^3 r \psi^* [-\frac{\hbar^2}{2m} \nabla^2 + V] \psi + \frac{N^2}{2} \frac{4\pi\hbar^2 a}{m} \int d^3 r (\psi^* \psi)^2 \quad (9)$$

To minimize $\langle \Psi | H | \Psi \rangle$ subject to the constraint that $|\Psi\rangle$ is normalized we use the Lagrange multiplier method. Add a term consisting of the constraint $\int d^3 r \psi^*(\mathbf{r}) \psi(\mathbf{r}) = 1$ times a Lagrange multiplier.

$$\langle \Psi | H | \Psi \rangle - \mu \left[\int d^3 r \psi^* \psi - 1 \right] \quad (10)$$

Next variations are made in μ , ψ^* , and ψ . One will notice that the variation $\delta\mu$ gives

$$\int d^3 \psi^* \psi = 1. \quad (11)$$

This result is simply reasserting the fact that the wavefunction is normalized. Next a small variation of the form $\psi^* \rightarrow \psi^* + \delta\psi^*$ is made where ψ is held constant. A similar variation can be made in ψ , however a variation of this form will simply give an equation that is the complex conjugate of one given by making variations in ψ^* with ψ held constant. First compute the variation of the quantity $(\psi^* \psi)^2$. Making this variation yields

$$[(\psi^* + \delta\psi^*)\psi]^2 = [(\psi^*)^2 + 2\delta\psi^* \psi^* + (\delta\psi^*)^2] \psi^2. \quad (12)$$

The variation made in equation (12) can be truncated to the linear term to give the variation to be $2\delta\psi^*(\psi^* \psi)\psi$. Inserting this result into equation (10) and making variations with respect to ψ^* yields

$$N \int d^3 r \delta\psi^* \left[-\frac{\hbar^2}{2m} \nabla^2 + V \right] \psi + \frac{N^2}{2} \int d^3 r \frac{4\pi\hbar^2 a}{m} 2\delta\psi^*(\psi^* \psi)\psi - N\mu \left[\int d^3 r \delta\psi^* \psi \right] = 0. \quad (13)$$

One can then factor out $\delta\psi^*$ term from equation (13) to give

$$N \int d^3 r \delta\psi^* \left(\left[-\frac{\hbar^2}{2m} \nabla^2 + V \right] \psi + \frac{N}{2} \frac{4\pi\hbar^2 a}{m} 2(\psi^* \psi)\psi - \mu\psi \right) = 0. \quad (14)$$

Equation (14) implies that the term $-\hbar^2/2m\nabla^2 + V\psi + N/24\pi\hbar^2 a/m2(\psi^* \psi)\psi - \mu\psi$ is equal to zero. The result of this is the Gross-Pitaeskii equation:

$$-\frac{\hbar^2}{2m} \nabla^2 \psi(\mathbf{r}) + [V(\mathbf{r}) + N \frac{4\pi\hbar^2 a}{m} |\psi(\mathbf{r})|^2] \psi(\mathbf{r}) = \mu\psi(\mathbf{r}). \quad (15)$$

The mean-field approximation can be derived by going back a few steps to equation (8). The expectation value of the delta function potential term can be thought of as the mean-field energy of the Bose gas. Evaluating equation (8) yields

$$E_{mf} = \frac{2\pi\hbar^2 a}{m} N^2 \int d^3 r (\psi^* \psi)^2. \quad (16)$$

Which can be rewritten as

$$E_{mf} = \frac{2\pi\hbar^2 a}{m} N^2 \int d^3r n^2(r). \quad (17)$$

It can then be shown that

$$E_{mf} = \frac{2\pi\hbar^2 a}{m} N \langle n(r) \rangle. \quad (18)$$

Since we are dealing with a homogeneous gas, $n(r)$ is independent of r and therefore $\langle n(r) \rangle = n$.

$$\frac{E_{mf}}{N} = \frac{2\pi\hbar^2 na}{m} \quad (19)$$

C. Effective Field Theory

Effective field theory is a general approach used to understand the low energy behavior of physical systems.

To date, most applications of effective field theories have been in the context of quantum field theory. Some roots of effective theory are described in Ken Wilson's Nobel lecture on the Renormalization Group [6]. In elementary particle physics, effective theory is used to make sense of the process of renormalization. Currently, effective theory has developed into a universal language for modern elementary particle physics. Despite the complex uses of effective theories, the philosophy behind effective theories is rather simple and can be elucidated by using ordinary, non-relativistic quantum mechanics [8]. Consider a two particle system interacting through a potential $U(\mathbf{r})$. Next make the assumption that the only quantities of interest are low-energy observables. These observables include bound-state energy levels close to threshold and the low-energy scattering amplitudes. Next assume that the potential is known accurately at long distances $r > R$, but unknown at short-distances for $r < R$. Given information about some of the low energy observables, effective theories allow all other low-energy observables to be calculated with arbitrarily high accuracy without having any information about the short-term potential.

The method used is fairly simple. Replace the actual potential, $U(\mathbf{r})$, with some effective potential, $U_{eff}(\mathbf{r})$. This effective potential should reproduce the long-range at $r > R$, but need not reproduce the short-term potential accurately. There should be an adjustable parameter in the potential for $r > R$ that should be adjusted to fit the low-energy data. Adding one adjustable parameter gives error that scales linearly in $|E|$. Adding another adjustable parameter gives error that scales like $|E|^2$. In general, n adjustable parameters gives error that scales like $|E|^n$.

A few things need to be noted about effective field theory. First, the results of effective field theory cannot be applied accurately to high-energy/short distance interactions. These processes require knowledge of the real potential. Second, while adding adjustable parameters to the effective potential does give better results, it does not mean that the effective potential will converge to the real potential. In fact, the effective potential only needs to coincide with the real potential at distances beyond the cutoff.

D. Field Theory Formulation of Problem

This section is a brief introduction to the workings of many-bodied quantum mechanics also known as field theory. The method of moving from ordinary quantum mechanics to the field theory formulation of quantum mechanics is known as second quantization. In this formulation of quantum mechanics the wavefunction is replaced by operators. First consider the state $|\emptyset\rangle$ which is used to represent the vacuum state (i.e. no particles present). Application of operator $\psi^\dagger(\mathbf{r}, t)$ to the vacuum state adds a particle of wavefunction $\psi(\mathbf{r}, t)$ at the point \mathbf{r} and at time t . In this formulation of quantum mechanics all the ordinary operators can be written. For example the number density operator is given by $\rho(\mathbf{r}) = \psi^\dagger(\mathbf{r})\psi(\mathbf{r})$. Similarly the kinetic energy operator is given by $T = 1/2m \int d^3r \nabla\psi^\dagger(\mathbf{r}) \cdot \nabla\psi(\mathbf{r})$. In ordinary quantum mechanics a system is fully described by its Hamiltonian. In quantum field theory the Lagrangian density describes the state of a system. The dynamics of the system in question can be summarized by a nonlocal Lagrangian Density:

$$\mathcal{L} = \frac{1}{2}i\hbar \left[\psi^\dagger \left(\frac{\partial}{\partial t} \psi \right) - \left(\frac{\partial}{\partial t} \psi \right)^\dagger \right] - \frac{\hbar^2}{2m} \nabla \psi^\dagger \cdot \nabla \psi + \mu \psi^\dagger \psi - \int d^3 r' \psi^\dagger \psi(\mathbf{r}) U(\mathbf{r} - \mathbf{r}') \psi^\dagger \psi. \quad (20)$$

The chemical potential, μ , must be tuned so that the expectation value of $\psi^\dagger \psi$ in the ground state is equal to the specified number density, n . If the system being described contains only 2 or 3 particles, then the chemical potential can be ignored. Next the principles of effective field theory are introduced to this system. Effective field theory tells us that if we are only interested in the low-energy observables of the system, then the real short-range potential can be replaced by any other set of effective short-range potentials as long as those potentials contain adjustable parameters that can be fit to low-energy data. An example of such a set of low-energy measurements is the coefficients of the expansions in $\sqrt{na^3}$ for the energy density and other properties of the many-body system.

$$\begin{aligned} \mathcal{L}_{eff} = \frac{1}{2}i\hbar \left[\psi^\dagger \left(\frac{\partial}{\partial t} \psi \right) - \left(\frac{\partial}{\partial t} \psi \right)^\dagger \right] - \frac{\hbar^2}{2m} \nabla \psi^\dagger \cdot \nabla \psi + \mu \psi^\dagger \psi - \frac{A_0}{4} (\psi^\dagger \psi)^2 \\ - \frac{A_2}{4} \psi^\dagger \psi [\psi^\dagger (\nabla^2 \psi) + (\nabla^2 \psi)^\dagger \psi] - \frac{B_0}{36} (\psi^\dagger \psi)^3 + \dots \end{aligned} \quad (21)$$

The terms in this Lagrangian are constrained by the symmetries of the original Lagrangian. These symmetries are Galilean invariance, parity, and time reversal. The terms included are those that contribute to the leading nonuniversal corrections to the properties of the homogeneous gas. By computing Feynman diagrams for this system it can be concluded that,

$$A_0 = \frac{8\pi\hbar^2 a}{m} \quad (22)$$

$$A_2 = \frac{8\pi\hbar^2 a}{m} \frac{ar_e}{4} \quad (23)$$

$$B_0 = \frac{8\pi\hbar^2 a}{m} ca^3 \quad (24)$$

In this case c is a dimensionless constant that will be determined later.

III. DIFFUSION MONTE CARLO RESULTS

In this section, the diffusion Monte Carlo results of Giorgini, Boronat, and Casulleras are presented [1]. We compute the effective ranges for each of the model potentials they considered. Also their results for the energy and condensate fraction of the homogenous gas are presented.

A. Model Potential

In the low-density limit, only universal terms are relevant in explaining the nature of the Bose gas. At non-zero densities, aspects of the interatomic potential other than the S-wave scattering length will play an important role. These nonuniversal effects scale as higher powers of n and become negligible in the low-density limit. In Ref. [1] they considered the Hamiltonian $\hat{H} = -(\hbar^2/2m) \sum_{i=1}^N \nabla_i^2 + \sum_{i<j} V(|\mathbf{r}_i - \mathbf{r}_j|)$ where $V(r)$ is the two-body, spherical, interatomic potential. In their paper, Giorgini, Boronat, and Casulleras considered three types of interatomic potentials each with scattering length a :

1) Hard-sphere (HS) potential defined by

$$V(r) = \begin{cases} +\infty & (r < a) \\ 0 & (r > a) \end{cases} \quad (25)$$

where the diameter a of the hard sphere corresponds to the scattering length.

2) Soft-sphere (SS) potential defined by

$$V(r) = \begin{cases} V_0 & (r < R) \\ 0 & (r > R) \end{cases} \quad (26)$$

The scattering length, a , for the soft-sphere is $a = R[1 - \tanh(K_0 R)/K_0 R]$ where $K_0^2 = V_0 m/\hbar^2$ and $V_0 > 0$. Two sets of calculations of the energy density were done with the soft-sphere potential. The first calculation was done with $R = 5a$. This gives a value for $V_0 = 0.03154\hbar^2/(a^2 m)$ The second calculation was done with $R = 10a$, giving a value of $V_0 = .003408\hbar^2/(a^2 m)$.

3) Hard-core square-well (HCSW) potential defined by

$$V(r) = \begin{cases} +\infty & (r < R_c) \\ -V_0 & (R_c < r < R) \\ 0 & (r > R) \end{cases} \quad (27)$$

For the hard-core square-well the scattering length is given by: $a = R_c + (R - R_c)\{1 - \tan[K_0(R - R_c)]/K_0(R - R_c)\}$. For the hard-core square-well calculations were done for values with $R = 5R_c$ and $a = 10R$ which gives $V_0 = 412.815\hbar^2/(a^2m)$

However, nonuniversal effects in the Bose gas depend on aspects of the interatomic interactions other than the S-wave scattering length. One of the most important effect is the effective range for the S-wave scattering, r_e . It is defined in terms of the expansion of the S-wave atom-to-atom scattering amplitude $f(k)$ in powers of the wavenumber k :

$$f(k) = -a + ia^2k + (a^3 - \frac{a^2r_e}{2})k^2 + \dots \quad (28)$$

The effective range for the hard-sphere potential is

$$r_e = \frac{2a}{3} \quad (29)$$

The effective range for the soft-sphere potential is

$$r_e = 4a - R + \frac{R^3}{3a^2} - \frac{1}{aK_0^2} \quad (30)$$

For the model potentials SS-5 and SS-10, the effective ranges are $r_e = 8.9609a$ and $r_e = 33.9061a$, respectively. For the hard-core square-well potential the effective range is

$$r_e = R - \frac{R^3}{3a^2} - \frac{1}{aK_0^2} + \frac{R_c \sec^2[K_0(R - R_c)]}{a^2K_0^2} \quad (31)$$

Substituting $R_c = a/50$, $R = a/10$, and $V_0 = 412.815\hbar^2/(a^2m)$ yields the result

$$r_e = .0970398a \quad (32)$$

na^3	HS	SS-5	SS-10	HCSW
	SS ($R = 5a$)	SS ($R = 10a$)	HCSW	
1×10^{-6}	1.00427(80)	1.00427(80)	1.00427(80)	1.00427(80)
5×10^{-6}	1.00952(16)			
1×10^{-5}	1.01382(80)	1.01382(80)	1.01302(80)	1.0162(16)
5×10^{-5}	1.02957(48)			
1×10^{-4}	1.04326(80)	1.04167(80)	1.03689(80)	1.04565(80)
5×10^{-4}	1.09499(64)			
1×10^{-3}	1.13318(16)	1.11011(80)	1.07907(80)	1.1380(40)
5×10^{-3}	1.29775(95)			
1×10^{-2}	1.42921(80)			
5×10^{-2}	2.1295(16)			
1×10^{-1}	2.8855(56)			
0.166	3.9597(96)			
0.244	5.446(33)			

TABLE I. Energy per particle for the HS,SS, and HCSW potentials (in units of $2\pi na\hbar^2/m$)

B. Energy Density and Condensate Fraction

Using these potentials, they calculated 13 data points for the energy density using the hard-sphere potential. They calculated energy per particle, E/N , and the condensate fraction $\nu = N_0/N$, as a function of na^3 . These data points were calculated for values of na^3 as low as 1E-6 to values as high as .244. Because of the complexity of the calculations involved, only four data points each were computed for the soft-sphere and hard-core square-well potentials. These points ranged from values of na^3 as low as 1E-5 to as high as 1E-3. The results of their calculations can be found in Table I.

For convenience E/N is normalized to the universal mean-field energy per particle $E/E_0 = (2\pi\hbar^2/m)an^2$. The errors in parentheses are the statistical errors from the dif-

na^3	HS	SS-5	SS-10
1×10^{-6}	0.998(1)	0.997(1)	0.997(2)
5×10^{-6}	0.997(1)		
1×10^{-5}	0.996(2)	0.997(2)	0.996(1)
5×10^{-5}	0.991(2)		
1×10^{-4}	0.987(3)	0.989(2)	0.992(1)
5×10^{-4}	0.967(3)		
1×10^{-3}	0.948(5)	0.971(3)	0.986(1)
5×10^{-3}	0.876(6)		
1×10^{-2}	0.803(3)		
5×10^{-2}	0.501(5)		
1×10^{-1}	0.277(3)		
0.166	0.109(4)		
0.244	0.031(4)		

TABLE II. Condensate Fraction for HS and SS potentials

fusion Monte Carlo. The number of particles in the simulation box was large enough so that finite-size effects were small as compared to statistical errors. In Ref. [1] the results for the condensate fraction were only presented in a graph. The authors of Ref. [1] graciously provided us with their original results for their calculations of the condensate fraction as well. All the potentials are the same, except they did not calculate any data for the hard-core square-well potential. The calculations for the condensate fraction can be found in Table II.

The deviations of the results of Ref. [1] from the universal mean-field predictions $E/E_0 = 1$ and $\nu = 1$ vary over several orders of magnitude. A convenient way to present their results is in terms of an effective coefficient of the na^3 term in the expansion around the universal mean field prediction. The effective coefficients $c_{eff}(na^3)$ and $d_{eff}(na^3)$ are defined as follows:

$$\frac{E}{N} = \frac{2\pi\hbar^2}{m}an \left[1 + \frac{128}{15\sqrt{\pi}}\sqrt{na^3} + c_{eff}(na^3)na^3 \right] \quad (33)$$

$$\frac{N_0}{N} = 1 - \frac{8}{3\sqrt{\pi}}\sqrt{na^3} + d_{eff}(na^3)na^3 \quad (34)$$

IV. LOW-DENSITY EXPANSIONS

In this section, the nonuniversal corrections to the energy density and condensate fraction of a homogeneous Bose gas are presented. The calculations used to derive these results involve quantum field theory and are beyond the scope of this paper. The derivations of these equations will be in a paper by E. Braaten, H.-W. Hammer, and S. Hermans [12]. The second-order corrections to the energy-density can be computed applying the mean-field approximation to the Lagrangian \mathcal{L}_{eff} in (21). In the mean-field approximation, ψ is replaced by its ground-state expectation value ν which can be taken to be real-valued and independent of \mathbf{r} . Letting $\psi = \nu$ and identifying $n = |\nu|$, we find

$$\frac{E_{mf}}{N} = \frac{2\pi\hbar^2}{m}an^2 \left[1 + \frac{c}{9}na^3 \right]. \quad (35)$$

The third-order corrections to the energy-density involve much more complicated calculations than the mean-field term and therefore the third-order corrections are given without proof in equation (36).

$$\mathcal{E} = \frac{2\pi\hbar^2}{m}na^2 \left\{ 1 + \frac{128}{15\sqrt{\pi}}\sqrt{na^3} - \left[\frac{1024\sqrt{\pi}r_e}{15} \frac{r_e}{a} - \frac{64}{9\sqrt{\pi}}(c + \log(na^3))na^3 \right] (na^3)^{3/2} \right\} \quad (36)$$

Similarly the second-order corrections to the condensate fraction are presented without proof.

$$\frac{N}{N_0} = 1 - \frac{8}{3\sqrt{\pi}}\sqrt{na^3} + 32\sqrt{\pi}(na^3)^{3/2}\frac{r_e}{a} - \frac{4}{3\sqrt{\pi}}c(na^3)^{3/2} \quad (37)$$

V. ANALYSIS

In this section the constants in equations (1), (36), and (37) are calculated by least-squares fitting the equations to the numerical calculations from Ref. [1]. The χ^2 per degree

n	c	δc	χ^2 p.d.f	n	c	δc	χ^2 p.d.f
3	.176424	1.06257	.672279	9	4.42674	.00263542	466.243
4	4.86488	0.326901	4.03225	10	3.26836	0.00105033	13174.4
5	5.91788	0.215378	5.31602	11	3.10005	0.00093031	17814.9
6	6.29478	0.0448063	4.5729	12	2.93336	0.000849099	24935.6
7	6.15924	0.0352871	5.81885	13	2.90036	0.000836165	24939.1
8	4.91131	.00674459	97.7099				

TABLE III. Fits to n data points with only statistical error taken into account.

of freedom is calculated for the mean-field and higher order approximations to verify that the higher-order approximations are improvements upon the lower-order approximations.

A. Energy Density

We began by determining the constant, c , in equation (1). The authors in Ref. [1] set this constant equal to zero and discovered a somewhat worse fit for larger values of na^3 . In order to obtain the best fit value for c , the error in each data point had to be accurately determined because the method of minimizing χ^2 tries to fit points with small error better than those points with large error. A prime example of this principle in action is found in the first analysis of the numerical data. During the first trial of fits, only the statistical error in the numerical data was taken into account. Since it is known that equation (1) works well for lower densities the data analysis began by only fitting the first three data points. Next the first four data points were fit, then the fifth, six, seventh...until finally all 13 data points were fit. These results can be found in Table III. As can be seen the reduced chi-squared values (which should ideally be one for a perfect fit) become very large when higher density data points are included in the fits. This can mean one of two things. One, the data has more inaccuracy than is accounted for in the error bars, or the theoretical prediction is not completely accurate. The later option seems to be the more plausible explanation since it

n	C	δC	χ^2 p.d.f	n	C	δC	χ^2 p.d.f
3	0.193109	1.08431	0.661064	9	4.4049	0.550839	1.49931
4	3.39668	0.667869	2.78489	10	4.40422	0.5507	1.33289
5	4.25529	0.575329	2.88964	11	4.40373	0.55063	1.19976
6	4.36266	0.560109	2.37842	12	4.40338	0.550588	1.09081
7	4.40273	0.552937	1.99879	13	4.40312	0.55056	1
8	4.40507	0.551536	1.7135				

TABLE IV. Fits with theoretical error of $4\pi na^3 3109.83(na^3)^{3/2}$

is already known that equation (1) is only the second-order approximation.

In order to accurately determine the value for C , a semi-accurate estimate for the theoretical error needs to be formulated. Looking to the form of equation (1) one can see that the energy-density expansion is expanded around powers of $\sqrt{na^3}$. With this in mind an estimate for the theoretical error is taken to be $4\pi na^3 b(na^3)^{3/2}$. In this case b is a constant that is to be determined by computing the reduced chi-squared for fit with all thirteen data points and setting it equal to one. The results of this calculation gave a value for b of 3109.83. After b has been determined, fits were done in a similar fashion to the preceding fits. The results of these fits can be found in Table IV. This table of results indicates a value for c of $4.40 \pm .55$. Next we examine equation (36) using similar methods. The results of the fits with statistical error are given in Table V. We plot the energy-density data from Ref. [1] in Figure (1) with second-order and third-order correction terms also plotted for various values of c .

B. Condensate Fraction

Analysis of the condensate fraction will be conducted in the paper [12].

n	c	χ^2 p.d.f	δc	n	c	χ^2 p.d.f	δc
3	1.60126 E8	11.2351	1.7393 E7	9	78.0336	241.579	0.726233
4	3.33072 E6	21.0373	249127.	10	1.85952	826.747	0.0262458
5	852280.	29.2238	70414.	11	1.09718	802.426	0.0138158
6	29752.7	37.0273	1050.4	12	0.749107	767.71	0.00684328
7	11446.9	61.1103	424.639	13	0.669956	721.765	0.00568797
8	321.805	101.414	4.9827				

TABLE V. Fits to Third-Order in Energy Density using Statistical Error

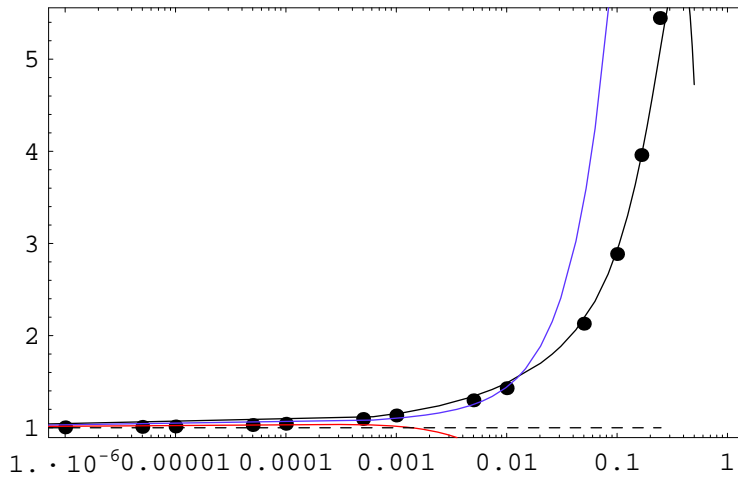


FIG. 1. Plot of Energy-density per mean-field vs. $\log(na^3)$. Dashed Black=Mean-Field;

Blue=2nd-Order with $c = 4.4$; Red=2nd-Order with $c = 0$; Black=3rd-order with $c = .67$

VI. CONCLUSIONS

At the moment, no solid conclusions can be drawn. Preliminary results show that nonuniversal effects can be observed for the hard-sphere potential. As can be seen in Figure (1) the third-order correction improves the fit to the higher density terms. Hopefully a more thorough analysis will show the importance of the nonuniversal terms in predicting high-density properties of the homogenous Bose gas.

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