Nonuniversal Effects in the Homogeneous Bose Gas

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Abstract

Effective field theory predicts that the leading nonuniversal effects in the homogeneous Bose gas arise from the effective range for S-wave scattering and from an effective three-body contact interaction. We calculate the leading nonuniversal contributions to the energy density and condensate fraction and compare the predictions with results from diffusion Monte Carlo calculations by Giorgini, Boronat, and Casulleras. We give a crude determination of the strength of the three-body contact interaction for various model potentials. Accurate determinations could be obtained from diffusion Monte Carlo calculations of the energy density with higher statistics.

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I. INTRODUCTION

The Bose-Einstein condensation of trapped atoms allows the experimental study of cold Bose gases with high precision. It is well-known that the dominant effect of the interactions between the atoms can be captured by a single constant $a$ called the S-wave scattering length. This property is often called universality. However, sufficiently accurate measurements will reveal the sensitivity to aspects of the interatomic interactions other than the scattering length. These are called nonuniversal effects.

Theoretical investigations of the homogeneous Bose gas in the 1950’s showed that its 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 per particle has the expansion

$$
\frac{E}{N} = \frac{2\pi \hbar^2}{m} an \left\{ 1 + \frac{32}{15\pi} \sqrt{16\pi na^3} + \left[ \frac{4\pi - 3\sqrt{3}}{6\pi} \log(na^3) + c' \right] (16\pi na^3) + \ldots \right\}.
$$

The leading term is the universal mean-field contribution first determined by Bogoliubov [1]. The $\sqrt{na^3}$ correction was first calculated by Lee, Huang, and Yang for bosons interacting through a hard-sphere potential [2]. In the $na^3$ correction, the coefficient of $\log(na^3)$ was first calculated by Wu for a hard-sphere potential [3]. These leading terms in the expansion were shown to be universal [4], applying to bosons interacting through any short-range potential with scattering length $a$. On the other hand, Hugenholtz and Pines showed that the constant $c'$ in (1) as well as higher-order corrections are not universal [5]. They depend on properties of the interactions between the bosons other than the S-wave scattering length, although the specific properties were not identified.

Giorgini, Boronat, and Casulleras have studied the properties of the ground state of homogeneous Bose gases numerically using a diffusion Monte Carlo method [6]. They considered 4 different two-body potentials as models for the interaction between the bosons, and calculated the energy per particle and condensate fraction for the homogeneous gas. In the case of the energy per particle, the universal $\sqrt{na^3}$ correction in (1) accounts for most of the deviations from the universal mean-field prediction at the densities studied, which ranged from $na^3 = 10^{-6}$ to $na^3 = 0.244$. However, they also observed small differences between the model potentials, i.e. nonuniversal effects.

Effective field theory provides a powerful method for analyzing the nonuniversal effects in the homogeneous Bose gas. It identifies precisely which aspects of the interactions between low-energy bosons enter at each order in the expansion in $\sqrt{na^3}$. For example, the coefficient $c'$ in the $na^3$ correction in (1) is determined by an effective three-body contact interaction between low-energy bosons [7]. The $(na^3)^{3/2}$ correction is completely determined by $c'$ and by the effective range for S-wave scattering.

The nonuniversal corrections in the low-density expansion of the Fermi gas at zero temperature have been studied previously [8 11]. The low-density expansion can be expressed as an expansion in $k_F$, where $k_F$ is the Fermi wavenumber. For fermions with a single spin state, the leading correction to the energy of an ideal Fermi gas is proportional to $k_F^3 a_p^3$, where $a_p$ is the P-wave scattering length [8]. For fermions with $g > 1$ degenerate spin states, the universal corrections to the energy can be expanded in powers of $k_F a$, where $a$ is the S-wave scattering length [8]. The leading nonuniversal corrections are the $k_F^3 a_p^3$ term and a...
In this paper, we use effective field theory to calculate the leading and next-to-leading nonuniversal corrections to the energy density and condensate fraction for a homogeneous Bose gas. We compare the calculations with the diffusion Monte Carlo data from Ref. [6] and attempt to determine the coefficient of the three-body contact interaction for each of the interaction potentials that were considered.

In Section II, we describe the general philosophy of effective theories for dealing with the low-energy behavior of physical systems. We use an effective quantum field theory to identify those parameters that give the leading nonuniversal contributions to the properties of a homogeneous Bose gas. The calculations of the leading and next-to-leading nonuniversal contributions to the energy density and the condensate fraction are presented in Section III. In Section IV, we describe the model interaction potentials used by Giorgini, Boronat, and Casulleras [6] and review their diffusion Monte Carlo results. In Section V, we analyze the diffusion Monte Carlo results of Ref. [6] and give a crude determination of the three-body contact parameter for each of the potentials that was considered. A summary and our conclusions are presented in Section VI.

II. EFFECTIVE FIELD THEORY

Effective theory is a general approach to understanding the low energy behavior of a physical system that has deep roots in several branches of physics. Some of these roots are described in Ken Wilson’s Nobel lecture on the Renormalization Group [12]. In elementary particle physics, the roots have two main branches. One branch evolved from efforts to make intuitive sense of renormalization in quantum electrodynamics (QED) [13]. In perturbative calculations in QED, intermediate steps are plagued by “ultraviolet divergences” that indicate strong sensitivity to physics at extremely short distances. The renormalization procedure eliminates the ultraviolet divergences and allows extremely accurate predictions of the properties of electrons and their bound states in terms of two fundamental parameters: the electron mass and the fine structure constant. The other main branch evolved from efforts to understand the low-energy behavior of pions and nucleons. The fundamental description of these strongly interacting particles is provided by quantum chromodynamics (QCD). However, an effective theory can be used to describe the low-energy behavior of these particles accurately without using any information about QCD other than its global symmetries and measurements of a few low-energy observables [14]. Starting from these two main roots, effective field theory has developed into a universal language for modern elementary particle physics [15]. It is used to develop low-energy approximations to the Standard Model of elementary particle physics and also to quantify corrections to the Standard Model arising from a more fundamental theory, such as a unified field theory or string theory.
potential \( U(r) \). Suppose we are interested only in the low-energy observables of the system, where “low-energy” refers to energy \( E \) close to the threshold \( E = 0 \). These observables include bound-state energy levels close to threshold and the low-energy scattering amplitudes. Suppose also that we know the potential \( U(r) \) accurately at long distances \( r > R \), but that its behavior at short distances \( r < R \) is not known accurately. (If it is a short-range potential with range smaller than \( R \), then \( U(r) = 0 \) for \( r > R \). If the particles are real atoms interacting at long distances through a van der Waals potential, then \( U(r) = -C_6/r^6 \) for \( r > R \).) Given sufficiently precise information about some low energy observables, effective theories allow other low-energy observables to be calculated with arbitrarily high accuracy without having any information about the short-distance potential.

The method is very simple. Simply replace \( U(r) \) by an effective potential \( U_{\text{eff}}(r) \) that is identical for \( r > R \) and whose form for \( r < R \) involves an adjustable parameter \( c_1 \). For \( r < R \), the effective potential need not bear any resemblance to the original potential \( U(r) \) as long as it has an adjustable parameter. A sufficient condition on the short-distance potential is that by varying \( c_1 \), one should be able to change the number of bound states by \( \pm 1 \). This guarantees that the scattering length \( a \) can be tuned to any value from \(-\infty \) to \(+\infty \). A simple example is a constant potential with adjustable depth \( V_1 \). Tune the value of this parameter \( c_1 \) so that the scattering amplitude at threshold is reproduced exactly. Then the Schrödinger equation with \( U_{\text{eff}}(r) \) will reproduce all other low-energy observables with errors that scale linearly with \( E \). To achieve higher accuracy, use an effective potential \( U_{\text{eff}}(r) \) with two independent adjustable parameters \( c_1 \) and \( c_2 \). A simple example is a 2-step potential with adjustable depths \( V_1 \) and \( V_2 \). The equality of \( U_{\text{eff}}(r) \) and \( U(r) \) guarantees that the difference between their scattering amplitudes is an analytic function of the wavevector \( k \). If we tune \( c_1 \) and \( c_2 \) so that the S-wave scattering amplitudes agree to second order in \( k = |k| \), then \( U_{\text{eff}}(r) \) will reproduce all low-energy S-wave observables with errors that scale like \( E^2 \). By tuning a third parameter \( c_3 \), we can guarantee that P-wave observables also have errors that scale like \( E^2 \). If we add more adjustable parameters and tune the scattering amplitude to higher order in \( E \), the errors will scale as higher powers of \( E \). Low-energy observables at energies within the appropriate radius of convergence can therefore be calculated to any specified accuracy by adjusting a finite number of parameters in the effective potential.

The problem of a Bose gas at zero temperature is an ideal application of effective field theory. Suppose we have a gas with number density \( \rho \) consisting of identical bosons of mass \( m \) interacting through a short-range two-body potential \( U(\mathbf{r}) \). (For convenience, we will refer to these particles as “atoms.”) Using the method of second quantization, this system can be described by a quantum field theory. The quantum field operator \( \psi(\mathbf{r},t) \) annihilates an atom at the point \( \mathbf{r} \), and \( \psi^\dagger \psi \) is the number density operator. The dynamics of this quantum field theory can be summarized by a nonlocal Lagrangian density:

\[
\mathcal{L} = \frac{1}{2i\hbar} \left[ \psi^\dagger \psi - \psi^\dagger \psi^* \right] - \frac{\hbar^2}{2m} \nabla \psi^* \cdot \nabla \psi + \mu \psi^* \psi - \frac{1}{2} \int d^3 r' \psi^* \psi(\mathbf{r}) U(\mathbf{r} - \mathbf{r}') \psi^* \psi(\mathbf{r}'). \tag{2}
\]

The parameter \( \mu \) is the chemical potential. If we wish to describe a system consisting of a small number of atoms, such as a two-body or three-body system, then the \( \mu \psi^* \psi \) term can be ignored. To describe a homogeneous gas of number density \( \rho \), \( \mu \) must be tuned so that the expectation value of \( \psi^\dagger \psi \) in the ground state of the quantum field theory is equal to \( \rho \).
Now suppose we are interested only in low-energy observables, such as the properties of the ground state. The principles of effective theory tell us that the short-range potential $U(r)$ can be replaced by any other set of effective short-range interactions, so long as they have adjustable parameters that can be tuned to reproduce a set of low-energy measurements. 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. A simpler example is the coefficients in the low-momentum expansions for the scattering amplitudes of atoms in the two-body sector, three-body sector, etc..

If we wish to carry out analytic calculations, one particularly convenient choice for the effective short-range interactions is to take them all to be purely local. The dynamics of the resulting quantum field theory is then described by a local Lagrangian density:

\[
L_{\text{eff}} = \frac{1}{2} i \hbar \left[ \bar{\psi} \dot{\psi} - \dot{\bar{\psi}} \psi \right] - \frac{\hbar^2}{2m} \nabla \bar{\psi} \cdot \nabla \psi + \mu \bar{\psi} \psi \\
- \frac{A_0}{4} (\bar{\psi} \psi)^2 - \frac{A_2}{4} \nabla (\bar{\psi} \psi) \cdot \nabla (\bar{\psi} \psi) - \frac{B_0}{36} (\bar{\psi} \psi)^3 + \ldots
\]

The terms in the Lagrangian are constrained by the symmetries of the original Lagrangian: Galilean invariance, parity, and time reversal. We have included explicitly those terms that contribute the leading nonuniversal corrections to the properties of the homogeneous gas. All other terms are either higher order in $\psi$ or in $\nabla$. The $[\nabla (\bar{\psi} \psi)]^2$ term is the only possible term that is fourth order in $\psi$ and second order in $\nabla$. Up to total divergences, the only other independent term is $(\bar{\psi} \nabla \psi - \bar{\psi} \nabla \psi)^2$, but it is forbidden by Galilean invariance. Note that while the original Lagrangian (2) included only terms of 2nd and 4th order in $\psi$, the effective Lagrangian (3) includes terms of 6th order and higher. The 6th order terms are necessary, because a local Lagrangian without such terms could not reproduce the low-energy behavior of scattering amplitudes in the three-body sector. It would also be unable to reproduce the $na^3$ correction term in the low-density expansion (1) for the energy density of the homogeneous gas.

The coefficients $A_0$ and $A_2$ in (3) can be determined by demanding that the effective theory reproduces the amplitude for low-energy atom-atom scattering up to errors that scale like the square of the energy. The T-matrix element at tree-level for two atoms with wavenumbers $k_1, k_2$ to scatter into atoms with wavenumbers $k'_1, k'_2$ can be deduced from the interaction terms in (3):

\[
(T_2)_{\text{tree}} = -A_0 + \frac{1}{2} A_2 \left[ (k_1 - k'_1) \cdot (k_2 - k'_2) + (k_1 - k'_2) \cdot (k_2 - k'_1) \right].
\]

Going to the center of momentum frame with $k_1 = -k_2 = k$ and $k'_1 = -k'_2 = k'$ and using the energy conservation condition $k^2 = k'^2$, this reduces to

\[
(T_2)_{\text{tree}} = -A_0 - 2A_2 k^2.
\]

The corrections from loop diagrams depend on the regularization and renormalization prescriptions, but they form a geometric series that can be summed analytically. If we impose an ultraviolet cutoff $\Lambda$ on the wavenumber, the exact T-matrix element can be determined analytically by solving a simple integral equation and has the form
\[ T_2 = -\left[ \frac{1}{\mathcal{A}_0 + 2\mathcal{A}_2 k^2} + \frac{m}{4\pi\hbar^2} \left( \Lambda + \frac{\pi}{2} k \right) \right]^{-1}, \]  

(6)

where \( \mathcal{A}_0 \) and \( \mathcal{A}_2 \) are complicated functions of \( \mathcal{A}_0, A_2, \) and \( \Lambda \). The absence of any angular dependence indicates that there is S-wave scattering only. We get a much simpler expression if we use dimensional regularization, which automatically subtracts ultraviolet divergences that grow like a power of \( \Lambda \). In this case the exact T-matrix element is

\[ T_2 = -\left[ \frac{1}{\mathcal{A}_0^{(dr)} + 2\mathcal{A}_2^{(dr)} k^2} + \frac{m k}{8\pi\hbar^2} \right]^{-1}. \]  

(7)

The expressions (6) and (7) for \( T_2 \) do not have precisely the same functional dependence on \( k \). However, if we make the identifications \( 1/\mathcal{A}_0^{(dr)} = 1/\mathcal{A}_0 + m\Lambda/(4\pi\hbar^2) \) and \( \mathcal{A}_2^{(dr)}/(\mathcal{A}_0^{(dr)})^2 = \mathcal{A}_2/(\mathcal{A}_0)^2 \), the expansions of (6) and (7) for small \( k \) are identical through order \( k^3 \). The difference scales like \( E^2 \), where \( E = \hbar^2 k^2/m \) is the total energy. From the effective theory point of view, including the \( \mathcal{A}_2 \) term in the effective Lagrangian (3) allows low-energy observables in the two-body sector to be reproduced up to errors that scale like \( E^2 \). Different regularizations require different values of \( \mathcal{A}_0 \) and \( \mathcal{A}_2 \), but they give the same low-energy observables up to errors that scale like \( E^2 \).

The amplitude for atom-atom scattering in the original theory described by the Lagrangian (2) can be determined by solving the Schrödinger equation with the appropriate interatomic potential \( U(r - r') \). The contribution from S-wave scattering can be expressed in a manifestly unitary form in terms of the S-wave phase shift \( \delta_0(k) \):

\[ T_2 = \frac{8\pi\hbar^2}{mk} e^{i\delta_0(k)} \sin[\delta_0(k)]. \]  

(8)

The scattering length \( a \) and the effective range \( r_s \) for S-wave scattering are defined by the low-momentum expansion of the phase shift. Because of the identity \( e^{i\delta} \sin \delta = 1/(\cot \delta - i) \), the low-momentum expansion is conveniently written in the form

\[ k \cot[\delta_0(k)] = \frac{1}{a} + \frac{1}{2} r_s k^2 + \ldots, \]  

(9)

which defines the effective range \( r_s \). After inserting this into (8), the T-matrix element can be expanded in powers of \( k \). The expansions of (7) and (8) match through third order in \( k \) if the coefficients \( \mathcal{A}_0^{(dr)} \) and \( \mathcal{A}_2^{(dr)} \) have the values

\[ A_0^{(dr)} = \frac{8\pi\hbar^2 a}{m}, \]  

(10)

\[ A_2^{(dr)} = \frac{8\pi\hbar^2 a}{m} \times \frac{a r_s}{4}. \]  

(11)

These are the coefficients if we use dimensional regularization to remove ultraviolet divergences. If we used a wavenumber cutoff as in (6), the coefficients \( \mathcal{A}_0 \) and \( \mathcal{A}_2 \) in the Lagrangian would depend on \( \Lambda \) in a very complicated way. However, their values are uniquely determined by the dimensional regularization coefficients (10) and (11).
The \((\psi^*\psi)^3\) term in the Lagrangian (3) is necessary in order for the effective theory to reproduce the amplitude for the low-energy scattering of three atoms with errors that scale linearly in the energy \(E\). At tree level, this term gives a momentum independent contribution \(-B_0\) to the T-matrix element \(T_3\) for \(3 \rightarrow 3\) scattering. One can see the necessity for such a term by considering the perturbative expansion for \(T_3\) in powers of \(A_0\), or equivalently \(a\). At 4th order in \(a\), there are 2-loop Feynman diagrams that depend logarithmically on the ultraviolet cutoff \(\Lambda\) for the wavenumber of atoms in intermediate states \([7]\). They give an additional momentum-independent contribution to \(T_3\) that is universal. The T-matrix element therefore includes the terms

\[
T_3 = -B_0 + \frac{3(4\pi - 3\sqrt{3})}{32\pi^3} m^3 A_0^4 \frac{32}{\hbar^6} \log \frac{\Lambda}{\kappa} + \ldots,
\]

(12)

where \(\kappa\) is a wavenumber set by the energies of the scattering particles. In the original theory, the ultraviolet cutoff is provided by the interaction potential \(U(r)\). The ultraviolet divergence in (12) therefore indicates that there is a momentum-independent contribution to \(3 \rightarrow 3\) scattering that depends on the interaction potential. The T-matrix element (12) can be made independent of the cutoff \(\Lambda\) if the coefficient \(B_0\) depends on \(\Lambda\) as specified by the following renormalization group equation:

\[
\Lambda \frac{d}{d\Lambda} B_0 = \frac{3(4\pi - 3\sqrt{3})}{32\pi^3} m^3 A_0^4 \frac{32}{\hbar^6}.
\]

(13)

The parameter \(B_0\) could in principle be determined from the numerical solution to the three-body problem for the scattering of three atoms interacting pairwise through the potential \(U(r)\). However, it can equally well be determined from calculations of the ground state energy for a large number of atoms interacting through the potential \(U(r)\). This is the strategy we will follow in this paper.

Using dimensional analysis, the coefficient of the three-body contact interaction term in (3) can be written as

\[
B_0 = \frac{8\pi \hbar^2 a^4}{m} \times (144\pi c),
\]

(14)

with \(c\) a dimensionless constant. The factor of 144\(\pi\) has been chosen for later convenience. We will refer to \(c\) as the three-body contact parameter.

III. NONUNIVERSAL CORRECTIONS

In this section, we calculate the leading and next-to-leading nonuniversal corrections to the energy density of a homogeneous Bose gas. We also calculate the leading nonuniversal corrections to the condensate fraction.

A. Mean-field corrections to the energy density

The leading nonuniversal correction to the energy density \(\mathcal{E}\) can be obtained by applying the mean-field approximation to the Lagrangian \(\mathcal{L}_{\text{eff}}\) in (3), including the \((\psi^*\psi)^3\) term. In
the mean-field approximation, $\psi$ is replaced by its ground-state expectation value $v$, which can be taken real-valued. The condensate number density is $n_0 = v^2$. The free energy density $F$ in the mean-field approximation is simply $-\mathcal{L}_{\text{eff}}$, with $\psi$ replaced by $v$:

$$F_{\text{mf}} = -\mu v^2 + \frac{1}{4} A_0 v^4 + \frac{1}{36} B_0 v^6.$$ (15)

Setting $v^2 = n_0$ in the energy density $E = F + \mu n$, it becomes

$$E_{\text{mf}} = \frac{1}{4} A_0 n_0^2 + \frac{1}{36} B_0 n_0^3 + \mu (n - n_0).$$ (16)

The chemical potential is obtained from the condition $\partial F / \partial v = 0$, which guarantees that $v$ minimizes the free energy:

$$\mu_{\text{mf}} = \frac{1}{2} A_0 n_0 + \frac{1}{12} B_0 n_0^2.$$ (17)

Substituting the expressions (10) and (14) for the coefficients into (16), we have

$$E_{\text{mf}} = \frac{2\pi \hbar^2}{m} a n_0^2 \left[ 1 + c(16\pi n_0 a^3) \right] + \mu (n - n_0).$$ (18)

In the mean-field approximation, the number density $n = \psi^* \psi$ reduces to $n = v^2$. Setting $n = n_0$ in (18), the first term gives the familiar universal mean-field energy density:

$$E_{\text{umf}} = \frac{2\pi \hbar^2}{m} a n_0^2.$$ (19)

The constant $c$ in (18) corresponds to a nonuniversal contribution to the constant $c'$ under the logarithm in the coefficient of $na^3$ in (1).

The universal $\log(na^3)$ term in the coefficient of $na^3$ in (1) can be obtained through complicated two-loop calculations in many-body quantum field theory. However, as pointed out by Braaten and Nieto [7], it follows from the term in (18) proportional to $c$ by a simple renormalization group argument. If $3 \to 3$ scattering amplitudes are to be independent of the ultraviolet cutoff $\Lambda$ on the wavenumber of atoms in the intermediate states, the coefficient $c$ defined by (14) must depend logarithmically on the ultraviolet cutoff $\Lambda$ in the way prescribed by the renormalization group equation (13). The mean-field contribution (16) to the energy density depends on the ultraviolet cutoff through the coefficient $c(\Lambda)$. The total energy density after renormalization must be independent of $\Lambda$. Therefore, there must be loop diagrams in many-body perturbation theory that have logarithmic ultraviolet divergences that precisely cancel the $\Lambda$-dependence of $c(\Lambda)$. The only momentum scale in these diagrams is the inverse of the coherence length $\xi = (16\pi n_0 a)^{-1/2}$, which appears in the quasiparticle dispersion relation. Thus the logarithmic divergences are of the form $\log(\Lambda \xi)$. The energy density can be independent of $\Lambda$ only if the explicit logarithmic divergences and the coefficient $c(\Lambda)$ appear in the combination

$$c(\Lambda) = \frac{4\pi - 3\sqrt{3}}{3\pi} \log(\Lambda / \sqrt{16\pi n_0 a})$$

$$= c(\Lambda) - \frac{4\pi - 3\sqrt{3}}{3\pi} \log(\Lambda a) + \frac{4\pi - 3\sqrt{3}}{6\pi} \log(16\pi n_0 a^3).$$ (20)
The three-body contact parameter $c$ need not be defined by a wavenumber cutoff $\Lambda$. For example, one can define a $\Lambda$-independent parameter $c$ by absorbing the logarithm of $\Lambda a$ in (20) into $c(\Lambda)$. Alternatively, one can use dimensional regularization and minimal subtraction to define a parameter $c(\kappa)$ that depends on an adjustable renormalization scale $\kappa$. One could even define $c$ by making a specific choice for the universal constant under the logarithm in the low-density expansion for the energy per particle in (1). We will adopt such a definition later in this paper. Regardless of the definition, any dependence of a many-body observable on $c$ must be accompanied by a logarithm of $n_0 a^3$ in the combination

$$c + \frac{4\pi - 3\sqrt{3}}{6\pi} \log(16\pi n_0 a^3).$$

Replacing $c$ in (18) by this combination and setting $n_0 = n$, we reproduce the universal logarithmic $n a^3$ correction in (1).

**B. Semiclassical corrections to the energy density**

The next-to-leading order nonuniversal corrections to the energy density can be obtained by computing the semiclassical (one-loop) correction to $\mathcal{E}$, including the effects of the effective range term and the three-body contact interaction in $\mathcal{L}_{\text{eff}}$. The semiclassical correction before renormalization is simply the sum of the zero-point energies of the quasiparticles:

$$\mathcal{E}_{\text{sc}} = \int \frac{d^3k}{(2\pi)^3} \frac{1}{2} \epsilon(k),$$

where $\epsilon(k)$ is the quasiparticle dispersion relation. This expression is ultraviolet divergent, and renormalization is necessary to obtain a finite result. If we insert the Bogoliubov dispersion relation

$$\epsilon_{\text{Bog}}(k) = \frac{\hbar^2}{2m} k \sqrt{k^2 + 16\pi a n_0},$$

renormalization can be accomplished by subtracting powers of $k$ from the integrand to make it convergent:

$$\mathcal{E}_{\text{LHY}} = \frac{\hbar^2}{8\pi^2 m} \int_0^\infty dk k^3 \left[ \sqrt{k^2 + 16\pi a n_0} - k - 8\pi n_0 a^2 \frac{1}{k} + 32\pi^2 n_0^2 a^2 \frac{1}{k^3} \right].$$

The three subtractions can be identified with renormalizations of the vacuum energy, the chemical potential, and the scattering length, respectively. If we imposed a cutoff $\Lambda$ on the wavenumber, the three subtractions would be proportional to $\Lambda^5$, $\Lambda^3$, and $\Lambda$, respectively. The result of evaluating the convergent integral in (24) is

$$\mathcal{E}_{\text{LHY}} = \frac{\hbar^2}{60\pi^2 m} (16\pi n_0 a)^{5/2}.$$

Setting $n_0 = n$, this reproduces the $\sqrt{n a^3}$ correction in (1) first calculated by Lee, Huang, and Yang [2].
The result (25) can also be obtained by using dimensional regularization. The integral is generalized from 3 dimensions to $3 - 2\epsilon$ dimensions, evaluated for a value of $\epsilon$ for which it converges, and then analytically continued to $\epsilon = 0$:

$$E_{\text{LHY}} = \frac{\hbar^2}{8\pi^2 m} \int_{0}^{\infty} dk \, k^{3-2\epsilon} \sqrt{k^2 + 16\pi an_0} \bigg|_{\epsilon \to 0}. \tag{26}$$

To be more specific, the integral is separated into two regions: $k < k^*$ and $k > k^*$, where $k^*$ is an arbitrary wavenumber. The contribution from $k < k^*$ is evaluated for complex values of $\epsilon$ satisfying $\text{Re} \, \epsilon < 2$. The contribution from $k > k^*$ is evaluated for complex values of $\epsilon$ satisfying $\text{Re} \, \epsilon > \frac{5}{2}$. The sum of the two contributions is

$$E_{\text{LHY}} = \frac{\hbar^2}{8\pi^2 m} \Gamma(2 - \epsilon) \Gamma\left(-\frac{5}{2} + \epsilon\right) \frac{1}{2\Gamma\left(-\frac{\epsilon}{2}\right)} (16\pi an_0)^{\frac{3}{2} - \epsilon}. \tag{27}$$

Setting $\epsilon = 0$, we recover (25).

The effective range and three-body contact terms in (3) change the quasiparticle dispersion relation $\epsilon(k)$. To determine $\epsilon(k)$, we substitute $\psi(\mathbf{r}, t) = v + \phi(\mathbf{r}, t)$ into (3). The quasiparticle Lagrangian $L_2$ consists of the terms that are second order in $\phi$. Using the mean-field expression (17) for the chemical potential and setting $v^2 = n_0$, the quasiparticle Lagrangian reduces to

$$L_2 = \frac{1}{2} i\hbar \left[ \phi^* \dot{\phi} - \dot{\phi}^* \phi \right] - \frac{\hbar^2}{2m} \left[ \nabla \phi^* \cdot \nabla \phi + 4\pi n_0 a^2 r_s \nabla (\text{Re} \phi) \cdot \nabla (\text{Re} \phi) \right]$$

$$- \frac{\hbar^2}{2m} (16\pi n_0 a)[1 + 3c(16\pi n_0 a^3)] (\text{Re} \phi)^2. \tag{28}$$

The quasiparticle dispersion relation $\epsilon(k)$ can be determined by Fourier transforming the fields $\text{Re} \phi$ and $\text{Im} \phi$ and finding the eigenvalues of the resulting $2 \times 2$ matrix. The result is

$$\epsilon(k) = \frac{\hbar^2}{2m} k \sqrt{(1 + 4\pi n_0 a^2 r_s)k^2 + 16\pi an_0[1 + 3c(16\pi n_0 a^3)]}. \tag{29}$$

Setting $r_s = c = 0$, we recover the Bogoliubov dispersion relation in (23).

Since the dispersion relation (29) has the same functional form as the Bogoliubov dispersion relation (23), we can compute the semiclassical energy simply by rescaling the integrand and the integration variable $k$ in the dimensionally regularized expression (26):

$$E_{\text{sc}} = \frac{\hbar^2}{60\pi^2 m} (1 + 4\pi n_0 a^2 r_s)^{-2} \left\{ 16\pi n_0 a[1 + 3c(16\pi n_0 a^3)] \right\}^{5/2}. \tag{30}$$

Expanding to first order in $r_s$ and $c$, this reduces to

$$E_{\text{sc}} = \frac{2\pi \hbar^2}{m} an_0^2 \left\{ \frac{32}{15\pi} \sqrt{16\pi n_0 a^3} + \left[ \frac{16}{\pi} c - \frac{16}{15\pi} \frac{r_s}{a} \right] (16\pi n_0 a^3)^{3/2} \right\}. \tag{31}$$
C. Semiclassical corrections to the number density

The total number density is \( n = \langle \psi^\dagger \psi \rangle \), while the number density of atoms in the condensate is \( n_0 = |\langle \psi \rangle|^2 \). In the mean-field approximation, the operator \( \psi \) is replaced by its ground-state expectation value \( v \), in which case \( n = n_0 \). In the semiclassical approximation, we have

\[
\begin{aligned}
n_{sc} &= n_0 + \frac{1}{4} \int \frac{d^3k}{(2\pi)^3} \left[ \frac{\hbar^2 k^2/(2m)}{\epsilon(k)} + \frac{\epsilon(k)}{\hbar^2 k^2/(2m)} \right]. \quad (32)
\end{aligned}
\]

Inserting the Bogoliubov dispersion relation (23) and using dimensional regularization to remove the power ultraviolet divergences, this can be written

\[
\begin{aligned}
n_{Bog} &= n_0 + \frac{1}{8\pi^2} \int_0^\infty dk k^{2-2\epsilon} \left[ \frac{k}{\sqrt{k^2 + 16\pi n_0 a}} + \frac{\sqrt{k^2 + 16\pi n_0 a}}{k} \right] \left. \right|_{\epsilon \to 0}. \quad (33)
\end{aligned}
\]

Evaluating the integrals and analytically continuing to \( \epsilon = 0 \), we obtain the classic result of Bogoliubov [1]:

\[
\begin{aligned}
n_{Bog} &= n_0 + \frac{1}{24\pi^2} (16\pi n_0 a)^{3/2}. \quad (34)
\end{aligned}
\]

In order to compute the complete semiclassical correction to the condensate density, including the effects of the effective range and the three-body contact coefficient, we must insert the quasiparticle dispersion relation (29) into the integral (32). Since (29) has the same functional form as the Bogoliubov dispersion relation (23), we can evaluate the integral simply by rescaling the integrand and the integration variable \( k \) in the expression (33):

\[
\begin{aligned}
n_{sc} &= n_0 + \frac{1}{24\pi^2} \left[ 2(1 + 4\pi n_0 a^2 r_s)^{-2} - (1 + 4\pi n_0 a^2 r_s)^{-1} \right] \times \left\{ 16\pi n_0 a[1 + 3c(16\pi n_0 a^3)] \right\}^{3/2}. \quad (35)
\end{aligned}
\]

Expanding to first order in \( r_s \) and \( c \), this reduces to

\[
\begin{aligned}
n_{sc} &= n_0 \left( 1 + \frac{2}{3\pi} \sqrt{16\pi n_0 a^3} \left[ \frac{3}{\pi} c - \frac{1}{2\pi a} r_s \right] \right) (16\pi n_0 a^3)^{3/2}. \quad (36)
\end{aligned}
\]

D. Low-density expansion for the condensate fraction

The semiclassical expression (36) for the number density includes both the leading universal corrections and the leading nonuniversal corrections to the mean-field result \( n = n_0 \). The coefficient \( c \) in the \((n_0 a^3)^{3/2}\) correction must be accompanied by a universal logarithmic correction in the combination (27). There are universal corrections proportional to \((n_0 a^3)\) and \((n_0 a^3)^{3/2}\) whose coefficients are as yet unknown. Including all corrections through order \((n_0 a^3)^{3/2}\), the expression for the number density is
\[ n = n_0 \left\{ 1 + \frac{2}{3\pi} \sqrt{16\pi n_0 a^3} + d(16\pi n_0 a^3) \right. \]
\[ + \left( \frac{3}{\pi} \left[ c_E + \frac{4\pi - 3\sqrt{3}}{6\pi} \log(16\pi n_0 a^3) \right] - \frac{1}{2\pi} \frac{r_s}{a} + e \right) (16\pi n_0 a^3)^{3/2} \left\} \right. . \] (37)

The parameters \( c_E \) and \( r_s \) depend on the interaction potential, while \( d \) and \( e \) are universal coefficients. The subscript on \( c \) is a reminder that we will define this parameter by the form of the low-density expansion for the energy of the homogeneous gas.

The low-density expansion for the condensate fraction \( n_0/n \) can be obtained by inverting (37) to obtain \( n_0 \) as a function of \( n \). Including all terms through order \((na^3)^{3/2}\), the expression for the condensate fraction is

\[ \frac{n_0}{n} = 1 - \frac{2}{3\pi} \sqrt{16\pi na^3} - d'(16\pi na^3) \]
\[ - \left( \frac{3}{\pi} \left[ c_E + \frac{4\pi - 3\sqrt{3}}{6\pi} \log(16\pi na^3) \right] - \frac{1}{2\pi} \frac{r_s}{a} + e' \right) (16\pi na^3)^{3/2}, \] (38)

where \( d' = d - \frac{2}{3\pi^2} \) and \( e' = e - \frac{7}{3\pi} d + \frac{7}{9\pi^2} \).

E. Low-density expansion for the energy density

The mean-field contribution to the energy density in (18) includes the leading nonuniversal correction to the universal mean-field energy density. The semiclassical contribution in (31) includes the leading universal correction and the next-to-leading nonuniversal corrections. The coefficient \( c \) in the nonuniversal correction must be accompanied by a universal logarithmic correction in the combination (21). There is a universal correction proportional to \( n_0 a^3 \) that was calculated by Braaten and Nieto [17]. There is also a universal correction proportional to \((n_0 a^3)^{3/2}\) that has not been calculated. Including all corrections through order \((n_0 a^3)^{3/2}\), the expression for the energy density is

\[ \mathcal{E} = \frac{2\pi \hbar^2}{m} a n_0^2 \left\{ 1 + \frac{32}{15\pi} \sqrt{16\pi n_0 a^3} + \left[ c_E + \frac{4\pi - 3\sqrt{3}}{6\pi} \log(16\pi n_0 a^3) + \frac{4}{9\pi^2} \right] (16\pi n_0 a^3) \right. \]
\[ + \left. \left( \frac{16}{\pi} \left[ c_E + \frac{4\pi - 3\sqrt{3}}{6\pi} \log(16\pi n_0 a^3) \right] - \frac{16}{15\pi} \frac{r_s}{a} + b \right) (16\pi n_0 a^3)^{3/2} \right\} \]
\[ + \mu (n - n_0). \] (39)

The parameters \( c_E \) and \( r_s \) depend on the interaction potential, while \( b \) is a universal coefficient. The chemical potential \( \mu \) is determined by the condition \( \partial \mathcal{F} / \partial v = 0 \), which is equivalent to

\[ \frac{\partial}{\partial n_0} (\mathcal{E} - \mu n) = 0. \] (40)

The constant \( 4/(9\pi^2) \) in the coefficient of the \( n_0 a^3 \) correction in (39) is part of the universal coefficient. The rest of that coefficient has been absorbed into the nonuniversal coefficient \( c_E \).
This represents a specific definition of the three-body contact parameter \( c \) whose motivation will become evident below in Eq. (41).

The low-density expansion for the energy density can be obtained by using (38) to eliminate \( n_0 \) from (39) in favor of \( n \). Including all terms through order \( (na^3)^{3/2} \), the expression for the energy density is

\[
\frac{\mathcal{E}}{\mathcal{E}_{\text{umf}}} = 1 + \frac{32}{15\pi}\sqrt{16\pi na^3} + \left[ c_E + \frac{4\pi - 3\sqrt{3}}{6\pi}\log(16\pi na^3) \right] (16\pi na^3)^{3/2} + \left( \frac{16}{\pi} \left[ c_E + \frac{4\pi - 3\sqrt{3}}{6\pi}\log(16\pi na^3) \right] - \frac{16r_s}{15\pi a} + b' \right) (16\pi na^3)^{3/2},
\]

(41)

where \( b' = b - \frac{4}{3\pi^2}d - \frac{8}{9\pi^4} \).

We have chosen to define the three-body contact parameter \( c_E \) so that it includes all the universal terms under the logarithm \( \log(16\pi na^3) \) in the \( na^3 \) term in (41). This is a perfectly acceptable definition of the three-body contact parameter, because it can be related to any other definition by a well-defined calculation. For example, dimensional regularization and minimal subtraction can be used to define a three-body coefficient \( c_{MS}(\kappa) \) that depends on an arbitrary renormalization scale \( \kappa \). The two-body and three-body coupling constants \( g \) and \( g_3(\kappa) \) in Ref. [17] are equal to \( A_0 \) and \( B_0 \) up to factors of \( \hbar \). The energy density was calculated to order \( na^3 \) using dimensional regularization and minimal subtraction in Ref. [17]. By equating the coefficient of the \( (16\pi na^3) \) term in the expression (41) with the corresponding coefficient in Ref. [17], we find

\[
c_E + \frac{4\pi - 3\sqrt{3}}{6\pi}\log(16\pi na^3) = c_{MS}(\kappa) + \frac{4\pi - 3\sqrt{3}}{6\pi}\left[ \log \frac{16\pi na^3}{\kappa^2} + 0.80 \right].
\]

(42)

Thus the parameter \( c_E \) defined by the expression (41) is equal to the running parameter \( c_{MS}(\kappa) \) at a scale of order \( 1/a \):

\[
c_E = c_{MS}(\kappa = 1.5/a).
\]

(43)

IV. DIFFUSION MONTE CARLO RESULTS

In this section, we present the diffusion Monte Carlo results of Giorgini, Boronat, and Casulleras [1] for the energy and the condensate fraction of the homogeneous Bose gas. We also compute the effective ranges for each of the model potentials they considered.

A. Model potentials

In the low-density limit, a homogeneous Bose gas exhibits universal behavior that is determined completely by the S-wave scattering length \( a \). However, at any nonzero density, its properties will also depend at some level on aspects of the interactions between atoms other than the scattering length. These nonuniversal effects scale as higher powers of \( n \) and become negligible in the low-density limit.
If Ref. [6], the authors considered 4 different two-body potentials as models for the interactions between the bosons. These potentials all have the same scattering length $a$.

The potentials are

- the hard-sphere potential (HS):
  \[ V^{(\text{HS})}(r) = \begin{cases} \infty, & r < a, \\ 0, & r > a. \end{cases} \]  
  (44)

- two soft-sphere potentials (SS-5 and SS-10):
  \[ V^{(\text{SS})}(r) = \begin{cases} V_0, & r < R, \\ 0, & r > R. \end{cases} \]  
  (45)

The radii are $R = 5a$ for SS-5 and $R = 10a$ for SS-10. The heights of the two potentials are $V_0 = 0.031543 \frac{\hbar^2}{(ma^2)}$ for SS-5 and $V_0 = 0.0034084 \frac{\hbar^2}{(ma^2)}$ for SS-10.

- a hard-core square-well potential (HCSW):
  \[ V^{(\text{HCSW})}(r) = \begin{cases} +\infty, & r < R_c, \\ -V_0, & R_c < r < R, \\ 0, & r > R. \end{cases} \]  
  (46)

The outer radii of the hard core and the square well are $R_c = a/50$ and $R = a/10$, respectively. The depth of the square well is $V_0 = 412.815 \frac{\hbar^2}{(ma^2)}$. The potential supports a single two-body bound state with energy $-1.13249 \frac{\hbar^2}{(ma^2)}$.

Nonuniversal effects in the Bose gas depend on aspects of the interactions between the bosons other than the S-wave scattering length. One of the most important is the effective range for S-wave scattering $r_s$, which is defined by the low-momentum expansion (9) of the phase shift for atom-atom scattering. The effective range for the hard-sphere potential is $r_s = 2a/3$. For the soft-sphere potentials, the S-wave scattering length is

\[ a = R - \frac{\tanh(k_0 R)}{k_0}, \]  
(47)

where $k_0 = \sqrt{mV_0/\hbar^2}$. The effective range is

\[ r_s = R - \frac{R^3}{3a^2} + \frac{1}{k_0 a}. \]  
(48)

Its numerical value is $r_s = -4.96372a$ for SS-5 and $r_s = -29.936a$ for SS-10. For the HCSW potential, the S-wave scattering length is

\[ a = R - \frac{\tan[k_0(R - R_c)]}{k_0}. \]  
(49)

The effective range is

\[ r_s = R - \frac{R^3}{3a^2} + \frac{R_c(R - a)^2}{a^2} + \frac{R_c - a}{k_0^2 a^2}. \]  
(50)

Its numerical value is $r_s = 0.113493a$. 

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| \( na^3 \)   | HS          | SS-5        | SS-10       | HCSW        |
|------------|-------------|-------------|-------------|-------------|
| 1 \times 10^{-6} | 1.00427(80) | 1.00427(80) | 1.00427(80) | 1.00427(80) |
| 5 \times 10^{-6} | 1.00952(16) |             |             |             |
| 8 \times 10^{-6} | 1.01262(99) | 1.01163(99) |             |             |
| 1 \times 10^{-5} | 1.01382(80) | 1.01302(80) | 1.0162(16)  |             |
| 1.2 \times 10^{-5} | 1.01528(66) | 1.01395(66) |             |             |
| 5 \times 10^{-5} | 1.02957(48) |             |             |             |
| 1 \times 10^{-4} | 1.04326(80) | 1.04167(80) | 1.04565(80) |             |
| 5 \times 10^{-4} | 1.09499(64) |             |             |             |
| 1 \times 10^{-3} | 1.1332(16)  | 1.11011(80) | 1.1380(40)  | 1.1380(40)  |
| 5 \times 10^{-3} | 1.29775(95) |             |             |             |
| 1 \times 10^{-2} | 1.42921(80) |             |             |             |
| 5 \times 10^{-2} | 2.1295(16)  |             |             |             |
| 1 \times 10^{-1} | 2.8855(56)  |             |             |             |
| 0.166       | 3.9597(96)  |             |             |             |
| 0.244       | 5.446(33)   |             |             |             |

TABLE I. Energy normalized to the universal mean-field energy for the HS, SS-5, SS-10, and HCSW potentials from the diffusion Monte Carlo calculations of Ref. [6]. The statistical errors are given in parentheses.

B. Energy and Condensate Fraction

In Ref. [6], the authors used the diffusion Monte Carlo method to calculate the properties of a homogeneous gas of bosons interacting through each of the four model potentials. In the case of the potentials HS, SS-5, and SS-10, the homogeneous gas is the ground state of the system. In the case of the potential HCSW, the homogeneous gas is a metastable state in which there are no two-body bound states.

They calculated the energy per particle \( E/N \) and the condensate fraction \( N_0/N \) as functions of \( na^3 \), with \( na^3 \) ranging over several orders of magnitude from \( 10^{-6} \) to 0.244. Their results are reproduced in Tables II and III. The condensate fraction was not calculated for the HCSW potential. Most of the values in Table II were given in a table in Ref. [6]. The energy values for \( na^3 = 8 \times 10^{-6} \) and \( na^3 = 1.2 \times 10^{-5} \) and all the condensate values in Table III were provided to us by the authors. For convenience, we have normalized \( E/N \) to the universal mean-field result \( E_{\text{umf}}/N = (2\pi\hbar^2/m)n \). The errors in parentheses are the statistical errors from the diffusion Monte Carlo. The number of particles in the simulation box was \( N = 500 \), which the authors claimed is large enough that finite-size effects are well below the statistical errors.

V. ANALYSIS

In this section, we obtain crude determinations of the three-body contact parameter \( c_E \) defined by (41) for each of the interaction potentials by analyzing the diffusion Monte Carlo data for the energy. We also use the diffusion Monte Carlo data for the HS potential to
TABLE II. Condensate fractions for the HS, SS-5, and SS-10 potentials from the diffusion Monte Carlo calculations of Ref. [6]. The statistical errors are given in parentheses.

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

obtain a crude determination of the universal coefficient $d'$ in the low-density expansion (38) for the condensate fraction.

A. Three-body contact parameters

In Section IV, we have calculated the effective range $r_{s}^{\text{pot}}$ for each of the four model potentials used in Ref. [6]. As a consequence, the only unknowns in the expression (41) for the energy density are the three-body coefficient $c_E^{\text{pot}}$, which depends on the interaction potential, and the universal coefficient $b'$. At small densities, the contribution of $b'$ is suppressed by a power of $\sqrt{na^3}$ compared to the contribution of $c_E^{\text{pot}}$. We define a function $C^{\text{pot}}(na^3)$ that in the limit $na^3 \to 0$ approaches $c_E^{\text{pot}}$ via

$$C^{\text{pot}}(na^3) = \frac{1}{16\pi na^3} \left[ \frac{c_E^{\text{pot}}}{E_{\text{umf}}} - 1 - \frac{32}{15\pi} \sqrt{16\pi na^3} - \frac{4\pi - 3\sqrt{3}}{6\pi} (16\pi na^3) \log(16\pi na^3) \right]. \quad (51)$$

The approach to the limiting value $c_E^{\text{pot}}$ as $na^3 \to 0$ is given by

$$C^{\text{pot}} \to c_E^{\text{pot}} + \left( \frac{16}{\pi} \left[ c_E^{\text{pot}} + \frac{4\pi - 3\sqrt{3}}{6\pi} \log(16\pi na^3) \right] - \frac{16}{15\pi} \frac{r_{s}^{\text{pot}}}{a} + b' \right) (16\pi na^3)^{1/2}. \quad (52)$$

For sufficiently small values of $na^3$, the approach of the function $C^{\text{pot}}$ to the constant value $c_E^{\text{pot}}$ should be dominated by the logarithmic term in (52).

We first consider the HS potential. In Fig. [1], we show the values of $C^{\text{HS}}$ calculated from the diffusion Monte Carlo data in Table II. The curves give some idea of the expected size of the corrections from next order in $\sqrt{na^3}$. The dashed and dot-dashed curves show the corrections from the logarithmic term and the effective range term, respectively. The
FIG. 1. The value of $C^{(HS)}$ for the data points from Table I. The dot-dashed curve shows the corrections from the effective range term. The dashed curve shows the corrections from the logarithmic term at the next order.

correction from the $b'$ term in (52) has the same density dependence as the effective range term, but its normalization in unknown. The logarithmic correction will be the largest in the region $na^3 \leq 1.2 \times 10^{-5}$ unless $|b'| > 14.8$ or $|c^{(HS)}_E| > 2.9$. For $na^3 \leq 1.2 \times 10^{-5}$, the statistical errors in the data are larger than the expected size of the corrections from higher orders. We can therefore obtain a rough determination of $c^{(HS)}_E$ by averaging $C^{(HS)}$ at the 5 density values $na^3 \leq 1.2 \times 10^{-5}$ weighted by the inverse-squares of the statistical errors. The lowest data point could equally well be omitted because of its large error bar. The resulting value is

$$c^{(HS)}_E = -0.9 \pm 0.5.$$  (53)

The error was estimated by adding the inverses of the statistical errors in quadrature and then taking the reciprocal. The value $c^{(HS)}_E$ is dominated by the data point at $na^3 = 5 \times 10^{-6}$, because it has such a small statistical error. The systematic error from the $\sqrt{na^3}$ corrections in (52) is expected to be smaller than the magnitude of the logarithmic correction in (52), which is 0.26 at $na^3 = 5 \times 10^{-6}$.

We also performed a global $\chi^2$-fit of the data using (41) through order $na^3$. We assigned a theoretical error $\pm (16 \pi na^3)^{3/2}$ to quantify the error from leaving out the unknown higher order terms in the expansion. We computed the $\chi^2$ for the difference between the data in Table I and the theoretical expression (41) through order $na^3$ using the error obtained by adding the theoretical error and the statistical error from Table I in quadrature. The preferred value is $c^{(HS)}_E = 0.8$. In this case, the data points at higher density favor a positive value for $c^{(HS)}_E$ in spite of their larger theoretical error.
We next consider the SS-10 potential, for which there are six data points in Table I. In Fig. 2, we show the values of $C^{(SS-10)}$ calculated from the diffusion Monte Carlo data for the SS-10 potential in Table I. The curves are the same as in Fig. 1 except that the effective range correction is much larger, because $r_s^{(SS-10)}$ is larger than $r_s^{(HS)}$ by about a factor of 45. For $na^3 \leq 1.2 \times 10^{-5}$, the statistical errors in the data are larger than the expected size of the corrections from higher orders. We can therefore obtain a rough determination of $c^{(SS-10)}$ by averaging $C^{(SS-10)}$ at the 4 density values $na^3 \leq 1.2 \times 10^{-5}$ weighted by the inverse-squares of the statistical errors. The resulting value is

$$c_E^{(SS-10)} = -1.6 \pm 0.8 .$$

For both the SS-5 and HCSW potential, there are only four data points in Table I. In Fig. 3 we show the corresponding values of $C^{(SS-5)}$ and $C^{(HCSW)}$. The expected error from higher orders is smaller than the statistical error for the 2 data points with $na^3 \leq 10^{-5}$. If we use the value of $C^{(pot)}$ at $na^3 = 10^{-5}$ as an estimate for $c_E^{(pot)}$, we obtain $c_E^{(SS-5)} = 0.2 \pm 1.6$ and $c_E^{(HCSW)} = 4.9 \pm 3.2$.

We have given a rough determinations of the three-body contact parameter $c_E^{(pot)}$ for each of the potentials HS, SS-10, SS-5, and HCSW. The error bars are large enough that we cannot identify a deviation from universality in the three-body coefficients. More accurate determinations would require higher statistics in the diffusion Monte Carlo calculations. It might also require increasing the number of particles in the simulation box in order to keep finite-size effects smaller than the statistical errors. Ideally, one would like to have high enough statistics at several values of $na^3$ between $10^{-4}$ and $10^{-6}$ so that the rate of
FIG. 3. The values of $C^{(SS-5)}$ (left plot) and $C^{(HCSW)}$ (right plot) for the data points from Table I. The curves are as in Fig. I.

approach of $C^{(pot)}(na^3)$ to the constant value $c^{(pot)}_E$ could also be used to determine the universal coefficient $b'$ in (52).

B. Universal 2nd-order correction to the condensate fraction

In the expression (52) for the condensate fraction, the only unknowns are the three-body coefficient $c^{(pot)}_E$ and the universal coefficients $d'$ and $e'$. We define a function $D^{(pot)}(na^3)$ that approaches the universal coefficient $d'$ as the density approaches zero by

$$D^{(pot)}(na^3) = -\frac{1}{16\pi na^3} \left[ \left( \frac{n_0}{n} \right)^{(pot)} - 1 + \frac{2}{3\pi} \sqrt{\frac{\pi}{16\pi na^3}} \right].$$ (55)

The approach to the limiting value $d'$ as $na^3 \to 0$ is given by

$$D^{(pot)} \to d' + \left( \frac{3}{\pi} \right) \left[ c_E^{(pot)} + \frac{4\pi - 3\sqrt{3}}{6\pi} \log(16\pi na^3) \right] - \frac{1}{2\pi} \frac{r_s^{(pot)}}{a} + e' \right) (16\pi na^3)^{1/2}.$$ (56)

In Fig. I, we show the values of $D^{(HS)}$ calculated from the diffusion Monte Carlo data for the HS potential in Table I. The curves give some idea of the expected size of the corrections from next order in $\sqrt{na^3}$. The dashed and dot-dashed curves show the corrections from the logarithmic term and the effective range term, respectively. The correction from the $e'$ term in (56) has the same density dependence as the effective range term, but its normalization is unknown. The logarithmic correction should be the largest in the region $na^3 \leq 10^{-4}$, unless $|e'| > 2.0$ or $|c_E^{(HS)}| > 2.1$. For $na^3 \leq 10^{-4}$, the statistical errors in the data are larger than the expected size of the corrections from higher orders. We can therefore obtain a rough determination of $d'$ by averaging $D^{(HS)}$ at the 5 density values $na^3 \leq 10^{-4}$ weighted by the inverse-squares of the statistical errors. The resulting value is...
FIG. 4. The values of \( D^{(\text{HS})} \) calculated from the diffusion Monte Carlo data in Table I. The dashed line shows the corrections from the logarithmic term while the dash-dotted line shows the corrections from the effective range.

\[
d' = -0.5 \pm 0.5. \tag{57}
\]

The systematic error from the \( \sqrt{na^3} \) corrections in (56) is expected to be smaller than the size of the logarithmic correction in (56), which is 0.14. We have also determined \( d' \) by using a global \( \chi^2 \)-fit to the data of Eq. (37) through order \( na^3 \), using a theoretical error of \( \pm (16\pi na^3)^{3/2} \) that is added in quadrature to the statistical error. The preferred value is \( d' = 0 \), which agrees with Eq. (57) to within the error bars.

For both the SS-5 and SS-10 potentials, there are only 4 data points for the condensate fraction in Table I. The condensate fraction was not calculated in Ref. [6] for the HCSW potential. In Fig. 3, we show the values of \( D^{(\text{SS-5})} \) and \( D^{(\text{SS-10})} \) calculated from the diffusion Monte Carlo data in Table I. The curves are the same as in Fig. 2 except for the different value of the effective range. The expected error from higher orders is smaller than the statistical error for the 2 data points with \( na^3 \leq 10^{-5} \). If we use the value of \( D^{(\text{pot})} \) at \( na^3 = 10^{-5} \) as an estimate for \( d' \), we obtain \( d' = -3.5 \pm 4.0 \) from the SS-5 potential and \( d' = -1.5 \pm 2.0 \) from the SS-10 potential. These values are consistent within errors with the value (57) obtained from the condensate fraction for the hard-sphere potential.

VI. SUMMARY

Effective field theory is an ideal tool for the theoretical study of nonuniversal effects in the homogeneous Bose gas. The central idea of effective field theory is to exploit the separation...
of scales in a physical system. In a low-density Bose gas, the important length scales include the interparticle spacing, which is proportional to $n^{-1/3}$, and the coherence length, which is proportional to $(na)^{-1/2}$. These are both much larger than the physical size of the atoms, and in typical experiments they are also much larger than the scattering length $a$. The number of atoms per cubic scattering length $na^3$ is therefore a small parameter, and it allows for a controlled, perturbative expansion of low-density observables in $\sqrt{na^3}$. This systematic expansion is conveniently implemented using effective field theory. In low-energy observables, all the sensitivity to the details of the interactions between atoms at short distances is captured in low-energy constants, such as the scattering length, the effective range, and the effective three-body contact interaction. Universal results that depend only on the scattering length can also be obtained using more traditional many-body methods, but the calculations can be simplified using effective field theory. However, the real power of effective field theory becomes apparent in the systematic calculation of nonuniversal corrections.

Effective field theory can be used to easily determine at what order in the low-density expansion various nonuniversal effects will enter. The scattering length is associated with the $(\psi^*\psi)^2$ term in the local effective Lagrangian (3). The low-energy parameters associated with nonuniversal effects can be identified with terms in the effective Lagrangian that are higher order in $\psi^*\psi$ or in $\nabla$. In general, there are infinitely many such terms, but only a finite number contribute to any observable at a given order in the low-density expansion. The order in $\sqrt{n}$ at which a given term contributes is determined by the powers of $\psi^*\psi$ and $\nabla$ and by the order in the loop expansion at which it first enters. For example, if we consider the energy density, every power of $\psi^*\psi$ contributes a factor of $n$. Every power of $\nabla$ contributes a factor of $\sqrt{na^3}$. Finally there is a quantum suppression factor of $\sqrt{na^3}$ associated with each order in the loop expansion. For example, the three-body contact term $(\psi^*\psi)^3$ gives a mean-field contribution proportional to $n^3$. The effective range term
\[ (\nabla(\psi^*\psi))^2 \] does not contribute in the mean-field approximation, because the gradients vanish for a homogeneous gas. Its first contribution is at the semiclassical (one-loop) order and is proportional to \( \sqrt{n a^3}(\sqrt{n a^3})^2 n^2 \sim n^{7/2} \). Thus the leading nonuniversal contribution comes from the three-body contact interaction. The effective range enters at one order higher in \( \sqrt{n} \). At order \( n^4 \), there is also a nonuniversal contribution to the energy density associated with the \( (\psi^*\psi)^4 \) term in the effective Lagrangian.

We have calculated the leading and next-to-leading nonuniversal corrections to the energy density and the leading nonuniversal corrections to the condensate fraction for a homogeneous Bose gas. These nonuniversal corrections are determined by the effective range \( r_s \) and the three-body contact parameter \( c \). These parameters are in general different for different potentials, even if they have the same scattering length \( a \). For a given potential, the effective range can be extracted from the amplitude for \( 2 \rightarrow 2 \) scattering in the standard way. The parameter \( c \) could in principle be determined from a three-body observable, such as the amplitude for \( 3 \rightarrow 3 \) scattering in the vacuum. However, it can equally well be obtained from a low-density observable. In fact, we chose to define the parameter \( c_E \) using the form of the low-density expansion for the energy density in (41).

We analyzed the nonuniversal effects in the diffusion Monte Carlo results of Giorgini, Boronat, and Casulleras [4] for a homogeneous Bose gas with four different interaction potentials. We attempted to extract the unknown three-body coefficient \( c_E \) from the diffusion Monte Carlo data for the energy density. We found that the statistical errors at small values of \( na^3 \) allowed only a crude determination of this parameter. Our values for the hard-sphere and SS-10 potentials are given in (53) and (54), respectively. Within the error bars, we were unable to see a deviation from universality in the three-body coefficients. To determine \( c_E \) precisely enough to see the nonuniversality, one would need higher statistics at several densities in the range \( 10^{-4} < na^3 < 10^{-6} \).

We also attempted to extract from the diffusion Monte Carlo data the universal coefficient \( d' \) in the low-density expansion (38) for the condensate fraction. The value obtained from the data for the hard-sphere potential is given in (57). Again we found that the statistical errors at small values of \( na^3 \) allowed only a crude determination of this coefficient. In order to get a useful determination of \( d' \), one would need higher statistics at several densities in the range \( 10^{-3} < na^3 < 10^{-5} \). The coefficient \( d' \) can also be calculated from Feynman diagrams using the methods used in Ref. [17] to compute the \( na^3 \) corrections to the energy density. Such a calculation would provide a useful check on the accuracy of diffusion Monte Carlo results.

The achievement of Bose-Einstein condensates in atomic vapors has opened up the possibility for experimental study of Bose gases. As the experiments become more and more precise, it will be important to understand nonuniversal effects. Effective field theory provides a perturbative framework within which nonuniversal effects can be systematically calculated in the low density limit in terms of a few low-energy parameters. These effects can also be calculated nonperturbatively using diffusion Monte Carlo simulations. More extensive diffusion Monte Carlo calculations would be extremely valuable for testing the understanding of nonuniversal effects provided by effective field theory.
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