Two-Body and Three-Body Contacts for Identical Bosons near Unitarity

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In a recent experiment with ultracold trapped ^{85}Rb atoms, Makotyn *et al.* studied a quantum-degenerate Bose gas in the unitary limit where its scattering length is infinitely large. We show that the observed momentum distributions are compatible with a universal relation that expresses the high-momentum tail in terms of the two-body contact C_2 and the three-body contact C_3. We determine the contact densities for the unitary Bose gas with number density n to be $\mathcal{C}_2 \approx 20 n^{4/3}$ and $\mathcal{C}_3 \approx 2 n^{5/3}$. We also show that the observed atom loss rate is compatible with that from 3-atom inelastic collisions, which gives a contribution proportional to C_3, but the loss rate is not compatible with that from 2-atom inelastic collisions, which gives a contribution proportional to C_2. We point out that the contacts C_2 and C_3 could be measured independently by using the virial theorem near and at unitarity, respectively.

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Introduction.—Ultracold atoms allow the study of many-body systems with simple zero-range interactions whose strength, which is given by the S-wave scattering length a, can be controlled experimentally. These studies are directly relevant to problems in other areas of physics in which an accidental fine-tuning makes a much larger than the range of interactions. In particular, it is relevant to nuclear physics, because nucleons have relatively large scattering lengths and because the parameters of QCD are near critical values for which those scattering lengths are infinite [1]. In the unitary limit where a is infinitely large, it no longer provides a length scale. One might therefore expect the interactions to be scale invariant, so that the only length scales are provided by environmental parameters, such as the temperature T and the number density n. This expectation is realized in the simplest Fermi gas, which consists of fermions with two spin states. There have been extensive studies, both experimental and theoretical, of the unitary Fermi gas [2].

The simplest Bose gas consists of identical bosons. The unitary Bose gas is qualitatively different from the simplest unitary Fermi gas in two important ways. The obvious difference comes from the statistics of the particles. The other important qualitative difference is that scale invariance in the unitary Bose gas is broken by the Efimov effect, which is the existence of infinitely many three-body bound states (Efimov trimers) whose binding energies differ by powers of $e^{2\pi/s_0} \approx 515$, where $s_0 \approx 1.00624$ [3]. This difference is shared with more complicated Fermi gases, including fermions with three spin states and nucleons near the QCD critical point for infinite nucleon scattering lengths. The breaking of scale invariance by Efimov physics introduces a length scale $1/\kappa_*$, where κ_* is the binding momentum of one of the Efimov trimers at unitarity, but physical observables can only depend log-periodically on κ_* [4]. This anomalous symmetry breaking can give rise to logarithmic scaling violations at unitarity.

Experimental studies of the unitary Bose gas using ultracold atoms have been hindered by atom losses from inelastic collisions. In the low-density limit, the rate of decrease in the number density n from three-body recombination into a deeply bound diatomic molecule (deep dimer) is proportional to $a^4 n^3$, so it grows dramatically as a is increased. If there was a well-defined unitary limit in which n provided the only length scale, dn/dt would be proportional to $n^{5/3}$. The plausibility of a well-defined unitary limit was increased by experimental studies of dilute thermal gases of ^{7}Li atoms [5] and of ^{39}K atoms [6] and by exact theoretical calculations of the loss rate for a dilute thermal Bose gas [5], all of which showed that dn/dt at unitarity is proportional to n^3/T^2. Recently, Makotyn *et al.* carried out the first studies of a quantum-degenerate Bose gas at unitarity using ^{85}Rb atoms [7]. They found that, after a quick ramp of a Bose-Einstein condensate (BEC) to unitarity, the time scale for the saturation of the momentum distribution was significantly shorter than the time scale for atom loss.

Theoretical studies of the unitary Bose gas have been hindered by the absence of rigorous theoretical methods that can be used to calculate its properties with controlled errors. Theoretical studies of the unitary Fermi gas have faced similar problems, but the absolute stability of the system allows the use of Monte Carlo methods that have controlled errors. In the case of the unitary Bose gas, the possibility of recombination into deeply bound Efimov trimers guarantees that, even in the absence of inelastic collisions, the system can be at best metastable.

An alternative to directly calculating the properties of a many-body system is to use exact solutions to few-body problems to derive universal relations between various properties of the system that hold for all possible states. Universal relations for fermions with two spin states were first derived by Tan [8–10]. They all involve the two-body contact C_2. It is an extensive quantity that can be expressed as the integral over space of the two-body contact density $\mathcal{C}_2$, which has dimensions $(\text{length})^{-4}$ and can be interpreted as the number of pairs per $(\text{volume})^{4/3}$. The two-body contact plays an important role in many of the most important probes of ultracold fermionic atoms [11]. Universal relations for identical bosons were first derived by Braaten, Kang, and Platter [15]. They involve not only C_2 but also the three-body contact C_3. It is an extensive quantity that can be expressed as the integral over space of the three-body contact density $\mathcal{C}_3$, which has dimensions $(\text{length})^{-5}$ and can be interpreted as the number of triples per $(\text{volume})^{5/3}$.

In this Letter, we present universal relations for the loss rate of a Bose gas from inelastic 2-atom and 3-atom collisions. We show that the momentum distributions at unitarity in the JILA experiment of Ref. [7] are consistent with the universal relation for the tail of the momentum distribution in Ref. [15] and can be used to determine $\mathcal{C}_2$ and $\mathcal{C}_3$ for the unitary Bose gas. The result for $\mathcal{C}_3$ is consistent with the atom loss rate in the JILA experiment being dominated by 3-atom inelastic collisions. In our analysis, we assume that the unitary Bose gase in the JILA experiment is in a locally equilibrated metastable state, and we ignore the possibility that transient or turbulent phenomena could produce steady-state momentum distributions.

Contacts for identical bosons.—The two-body contact C_2 and the three-body contact C_3 for a state with energy E can be defined in terms of derivatives of E at fixed entropy [15]:

$$\left(a\frac{\partial E}{\partial a}\right)_{\kappa_*} = \frac{\hbar^2}{8\pi m a}C_2, \tag{1a}$$

$$\left(\kappa_*\frac{\partial E}{\partial \kappa_*}\right)_{a} = -\frac{2\hbar^2}{m}C_3. \tag{1b}$$

Equation (1a) can be used as an operational definition of C_2 if the scattering length a can be controlled experimentally. The normalization of C_2 has been chosen so that the tail of the momentum distribution at large wave number k [given in Eq. (2)] is C_2/k^4. The normalization of C_3 in Eq. (1b) implies that the three-body contact in the unitary limit for an Efimov trimer with binding energy $\hbar^2\kappa_*^2/m$ is κ_*^2. The value of κ_* can be inferred from the scattering length a_- at which that Efimov trimer crosses the 3-atom threshold, producing a resonance in the three-body recombination rate. They are related by a universal constant: $a_-\kappa_* = -1.50763$ [12]. In the case of ^{85}Rb atoms, a three-body recombination resonance was observed by Wild *et al.* at $a_- = -759(6)\ a_0$ with inelasticity parameter $\eta_* = 0.057(2)$ [13].

The contacts C_2 and C_3 determine the high-momentum tail in the momentum distribution $n(k)$. We normalize $n(k)$ so that the total number of atoms is $N = \int d^3k n(k)/(2\pi)^3$. A systematic expansion for $n(k)$ at large wave number k can be derived using the operator product expansion for the quantum field operators ψ and $\psi^\dagger$ [14]. The universal relation for the tail of the momentum distribution for identical bosons was derived in Ref. [15]:

$$k^4 n(k) \to C_2 + \frac{A\sin[2s_0\ln(k/\kappa_*)+\phi]}{k}C_3 + \cdots, \tag{2}$$

where $A = 89.2626$ and $\phi = -1.338\,13$. The additional terms are suppressed by higher powers of $1/k$ that may be noninteger.

Inelastic loss rates.—One complication of ^{85}Rb atoms is that the only hyperfine state with a Feshbach resonance that can be used to control the scattering length has a 2-atom inelastic scattering channel into a pair of atoms in a lower hyperfine state. The scattering length a is therefore complex with a negative imaginary part. The imaginary part of $1/a$ is essentially constant, independent of the magnetic field [16]: $\text{Im}(1/a) = 1/(1.44\times 10^7 a_0)$. The 2-atom inelastic scattering channel gives a contribution to the loss rate of low-energy atoms that is proportional to the two-body contact [17]. This follows from the fact that the effects of two-particle inelastic scattering with large energy release on a system of low-energy particles can be taken into account through an anti-Hermitian term in the Hamiltonian that allows a pair of particles to disappear if they are sufficiently close together. In a quantum field theory framework, the anti-Hermitian term in the Hamiltonian density can be chosen to be the local operator $\psi^\dagger\psi^\dagger\psi\psi$ multiplied by an imaginary coefficient. This same operator multiplied by an appropriate ultraviolet-sensitive coefficient is the two-body contact density operator [14]. The loss rate dN/dt can be expressed as the double integral over space of a correlator of the number density $\psi^\dagger\psi$ and the two-body contact density [17]. Using the commutation relations for ψ, the loss rate can be expressed in the form

$$\frac{dN}{dt} = -\frac{\hbar}{2\pi m}\text{Im}(1/a)(C_2+\cdots). \tag{3}$$

The coefficient of C_2 is the same as for fermions with two spin states in Ref. [17]. The additional terms in Eq. (3) come from the integral of the normal-ordered correlator, which is zero in a system consisting of fewer than three atoms. If these terms are suppressed, the C_2 term in Eq. (3) alone provides a good estimate for the loss rate.

If the effects of 2-atom inelastic scattering are negligible, the dominant mechanism for atom loss should be 3-atom inelastic scattering. The effects of three-particle inelastic scattering with large energy release on a system of low-energy particles can be taken into account through an anti-Hermitian term in the Hamiltonian that allows three particles to disappear if they are all sufficiently close together. In a quantum field theory framework, the anti-Hermitian term in the Hamiltonian density can be chosen to be the local operator $\psi^\dagger\psi^\dagger\psi^\dagger\psi\psi\psi$ multiplied by an imaginary coefficient. This same operator multiplied by an appropriate ultraviolet-sensitive coefficient is the three-body contact density operator [15]. Using the methods of Ref. [17], dN/dt can be expressed as the double integral over space of a correlator of $\psi^\dagger\psi$ and the three-body contact density. Using the commutation relations for ψ, the loss rate can be expressed in the form

$$\frac{dN}{dt} = -\frac{12\eta_*\hbar}{s_0 m}(C_3 + \cdots). \tag{4}$$

The leading term in the expansion was first given by Werner and Castin [18]. The additional terms come from the integral of the normal-ordered correlator, which is zero in a system consisting of fewer than four atoms. If these terms are suppressed, the C_3 term in Eq. (4) alone provides a good estimate for the loss rate.

Contact densities.—The contacts C_2 and C_3 for a system of trapped atoms can be determined using the local density approximation if the contact densities $\mathcal{C}_2$ and $\mathcal{C}_3$ are known for the corresponding homogeneous system. The contact densities for a homogeneous dilute BEC at zero temperature can be obtained analytically. The two-body contact density can be determined from the operational definition in Eq. (1a). The three-body contact density is most easily determined by matching Eq. (4) for the atom loss rate with the universal result for the loss rate from three-body recombination into deep dimers [4] in the limit $\eta_* \to 0$. The additional terms in Eq. (4) are suppressed by powers of na^3. The contact densities for the dilute BEC are

$$\mathcal{C}_2 = 16\pi^2 a^2 n^2, \tag{5a}$$

$$\mathcal{C}_3 \approx \frac{16\pi^2(4\pi - 3\sqrt{3})s_0 \cosh(\pi s_0)}{3\sinh^3(\pi s_0)} a^4 n^3. \tag{5b}$$

In Eq. (5b), we have neglected log-periodic effects that are numerically suppressed by powers of $e^{-2\pi s_0} \approx 1/557$. In Ref. [13], Wild *et al.* put an upper bound on C_3 for a dilute BEC of ^{85}Rb atoms. The three-body contact obtained using $\mathcal{C}_3$ in Eq. (5b) is a factor of 30 below that upper bound.

The contact densities for a homogeneous dilute thermal Bose gas at unitarity can also be obtained analytically. The two-body contact density in this limit can be obtained by adapting the analogous calculation for fermions in Ref. [17]. The three-body contact density is most easily determined by matching Eq. (4) for the atom loss rate with the exact universal result for the loss rate from three-body recombination into deep dimers [5] in the limit $\eta_* \to 0$. The additional terms in Eq. (4) are suppressed by powers of $n\lambda_T^3$, where $\lambda_T = (2\pi\hbar^2/mk_BT)^{1/2}$. The contact densities for the dilute thermal gas at unitarity are

$$\mathcal{C}_2 = 32\pi\lambda_T^2 n^2, \tag{6a}$$

$$\mathcal{C}_3 \approx 3\sqrt{3}s_0\lambda_T^4 n^3. \tag{6b}$$

In Eq. (6b), we have neglected log-periodic effects that are numerically suppressed by powers of $e^{-\pi s_0} \approx 1/24$.

Exact results for the contact densities at unitarity for a homogeneous quantum-degenerate Bose gas at zero temperature are not known. If we assume that log-periodic effects are numerically suppressed, as they are in Eqs. (5b) and (6b), the only important length scale for the homogeneous system is provided by the number density. If we assume that the contact densities depend weakly on κ_*, they must, by dimensional analysis, have the form

$$\mathcal{C}_2 \approx \alpha n^{4/3}, \tag{7a}$$

$$\mathcal{C}_3 \approx \beta n^{5/3}, \tag{7b}$$

where α and β are numerical constants. Some values of α obtained in previous attempts to calculate $\mathcal{C}_2$ for the unitary Bose gas are 10.3 [19], 32 [20], 160 [21], and 12 [22]. The values in Refs. [19,20] were calculated for an equilibrium system, while those in Refs. [21,22] were calculated for a system quenched to unitarity. All of these calculations used uncontrolled approximations. The local density approximations for the contacts of trapped atoms are $C_2 = \alpha N\langle n^{1/3}\rangle$ and $C_3 = \beta N\langle n^{2/3}\rangle$.

Momentum distributions.—In the experiment of Ref. [7], a BEC of ^{85}Rb atoms was quickly ramped to unitarity. The resulting clouds had approximately Thomas-Fermi distributions with about 60 000 atoms and an average number density $\langle n\rangle$ of either $5.5\times10^{12}/\mathrm{cm}^3$ or $1.6\times10^{12}/\mathrm{cm}^3$. The JILA group measured the momentum distribution $n(k)$ after a variable holding time at unitarity. They observed that $n(k)$ saturates in approximately 0.1 ms at the higher density and 0.2 ms at the lower density, both of which are significantly shorter than the atom-loss time scale, 0.6 ms. The distributions $k^4 n(k)$ are plotted in Fig. 1 using dimensionless variables obtained by scaling by $k_F = (6\pi^2\langle n\rangle)^{1/3}$. The scaled distributions for the two densities agree well for $k < 1.1k_F$, but they differ dramatically for $k > 1.1k_F$, indicating large scaling violations in the tails of the momentum distributions. According to Eq. (2), $k^4 n(k)$ should asymptotically approach the constant C_2 at large k, but the distributions in Fig. 1 do not appear to be approaching a constant for either density.

We assume that the data for $k > 1.5k_F$ in Fig. 1 are part of the tail of the momentum distribution that is determined

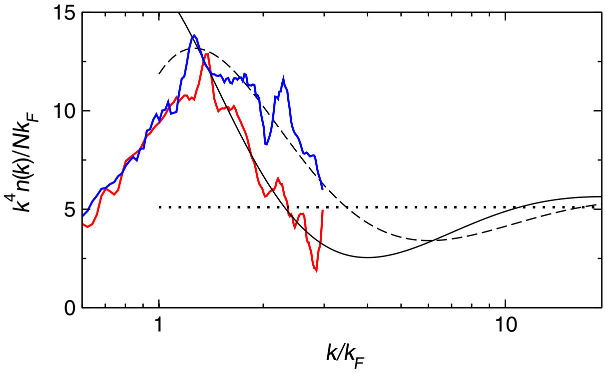

FIG. 1 (color online). Momentum distributions for the unitary Bose gas. The dimensionless quantity $k^4 n(k)/N k_F$, where $k_F = (6\pi^2 \langle n \rangle)^{1/3}$, is plotted as a function of k/k_F. The data from the JILA group in Ref. [7] are for two average densities: $\langle n \rangle = 5.5 \times 10^{12}/\mathrm{cm}^3$ (red line with lower tail) and $1.6 \times 10^{12}/\mathrm{cm}^3$ (blue line with higher tail) [7]. The solid curve through the higher-$\langle n \rangle$ data is a two-parameter fit obtained by adjusting C_2 and C_3. The dashed curve through the lower-$\langle n \rangle$ data is a parameter-free prediction obtained by scaling C_2 and C_3 from the higher-$\langle n \rangle$ fit. The horizontal dotted line is the contribution to both distributions from C_2.

by C_2 and C_3 according to Eq. (2). The positions of the local maxima and minima in the tail are predicted in terms of κ_*, which is determined by the Efimov loss resonance observed in Ref. [13]. In particular, there should be a minimum at $0.71\kappa_*$, which is $3.9k_F$ for the higher $\langle n \rangle$ and $5.8k_F$ for the lower $\langle n \rangle$. Fitting Eq. (2) to the momentum distribution for $\langle n \rangle = 5.5 \times 10^{12}/\mathrm{cm}^3$ from $k = 1.5k_F$ to $k = 3.0k_F$, we obtain $\alpha = 22(1)$ and $\beta = 2.1(1)$. The errors are lower bounds on the uncertainties, because there are systematic errors in the JILA experiment that were not quantified. The value of α agrees to within a factor of 2 with the previous estimates of Refs. [19,20,22]. The fitted curve in Fig. 1 predicts that, beyond the range of the measured data, $k^4 n(k)$ should increase and asymptotically approach C_2. Having fit α and β to the higher-$\langle n \rangle$ data, the tail of the momentum distribution for other values of $\langle n \rangle$ can be predicted without any adjustable parameters. The prediction for $\langle n \rangle = 1.6 \times 10^{12}/\mathrm{cm}^3$ is shown in Fig. 1 and is in good agreement with the data. Thus, the observed scaling violations in the tails of the momentum distributions are explained by the log-periodic dependence of the coefficient of the C_3/k^5 term in Eq. (2) on k/κ_*.

Atom loss rate.—The loss of ^{85}Rb atoms from a trapping potential comes from inelastic 2-atom collisions, which gives the C_2 term in Eq. (3), and from inelastic 3-atom collisions, which gives the C_3 term in Eq. (4). The initial loss rate for trapped atoms determines a time constant τ defined by $dN/dt = -(1/\tau)N$. In the JILA experiment in Ref. [7], τ was determined to be 0.63 ± 0.03 ms for $\langle n \rangle = 5.5 \times 10^{12}/\mathrm{cm}^3$. If we assume the dominant loss mechanism is 2-atom inelastic collisions as in Eq. (3) and use τ to estimate C_2, we obtain $\alpha \sim 6000$. This is more than 30 times larger than any of the estimates in Refs. [19–22], which suggests that 2-atom inelastic collisions are unlikely to give a significant contribution to the observed atom losses. If we assume the dominant loss mechanism is 3-atom inelastic collisions as in Eq. (4) and use τ to estimate C_3, we obtain $\beta \sim 1$. This is within a factor of 2 of the value we obtained by fitting the momentum distributions. This makes it plausible that 3-atom inelastic collisions are the dominant mechanism for the observed atom losses. The time constant τ is increased by the suppression factor of $\eta_* = 0.06$ in the expression for the loss rate in Eq. (4).

Other probes of the contacts.—The virial theorem for identical bosons trapped in a harmonic potential was first derived by Werner [23]:

$$(T + U) - V = -\frac{\hbar^2}{16\pi m a} C_2 - \frac{\hbar^2}{m} C_3, \tag{8}$$

where T, U, and V are the kinetic, interaction, and potential energies, respectively. This implies that C_3 at unitarity can be determined from the difference between $T + U$ and V and that C_2 can be determined from the slope of that difference as a function of $1/a$. The virial theorem for fermions with two spin states is Eq. (8) with $C_3 = 0$. This universal relation has been tested by a group at JILA by measuring $T + U$, V, and C_2 separately as functions of a for ultracold trapped ^{40}K atoms [24]. Similar measurements of $T + U$ and V for identical bosons near unitarity could be used to determine C_2 and C_3.

Another way to determine C_2 and C_3 is using rf spectroscopy, in which a radio-frequency signal transfers atoms to a different hyperfine state. Universal relations for the rf spectroscopy of identical bosons were derived in Ref. [15]. They predict scaling violations in the high-frequency tail. The observation of such scaling violations would add to the theoretical evidence presented in this letter that the experiment in Ref. [7] was studying a locally equilibrated metastable state of the unitary Bose gas.

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