Universal Relations for Identical Bosons from Three-Body Physics

Eric Braaten,[1,*] Daekyoung Kang,[1,†] and Lucas Platter[2,3,‡]

[1]Department of Physics, The Ohio State University, Columbus, Ohio 43210, USA
[2]Institute for Nuclear Theory, University of Washington, Seattle Washington 98195 USA
[3]Fundamental Physics, Chalmers University of Technology, 41296 Göteborg, Sweden

(Received 14 January 2011; published 15 April 2011)

Systems consisting of identical bosons with a large scattering length satisfy universal relations determined by 2-body physics that are similar to those for fermions with two spin states. They require the momentum distribution to have a large-momentum $1/k^4$ tail and the radio-frequency transition rate to have a high-frequency $1/\omega^{3/2}$ tail, both of which are proportional to the 2-body contact. Identical bosons also satisfy additional universal relations that are determined by 3-body physics and involve the 3-body contact, which measures the probability of 3 particles being very close together. The coefficients of the 3-body contact in the $1/k^5$ tail of the momentum distribution and in the $1/\omega^2$ tail of the radio-frequency transition rate are log-periodic functions of k and ω that depend on the Efimov parameter.

DOI: 10.1103/PhysRevLett.106.153005 PACS numbers: 31.15.−p, 03.75.Nt, 34.50.−s, 67.85.Lm

Strongly interacting systems present a challenging problem in theoretical physics. Some of the simplest of such systems consist of particles with short-range interactions and large scattering lengths. They arise in almost all branches of physics, including atomic, condensed matter, high energy, and nuclear physics. Ultracold trapped atoms with large scattering lengths are particularly pristine examples of such systems. In addition to the exquisite probes that are available in atomic physics, the ability to control the scattering length by using Feshbach resonances makes this dimension of the system accessible experimentally.

The simplest many-body systems of particles that interact through a large scattering length consist of fermions with two spin states. In the past decade, such systems have been the subject of intensive investigations, both theoretical and experimental, using ultracold trapped atoms [1]. A powerful tool for studying these systems is universal relations that are determined by 2-body physics but hold for any state of the system [2]. These relations involve the *contact*, an extensive property of the system that measures the probability for a pair of particles in the two spin states to be very close together. The first such relations were derived by Shina Tan [3]. Universal relations were subsequently derived for radio-frequency spectroscopy [4–6], photoassociation [7], structure factors [8], and correlation functions related to the viscocity [9]. An exciting recent development is the experimental confirmation of some of the universal relations [10].

In this Letter, we present universal relations for identical bosons with large scattering length. Like those for fermions with two spin states, these new universal relations involve the *2-body contact*. They also involve the *3-body contact*, an extensive property of the system that measures the probability for triples of identical bosons to be very close together.

For identical bosons in the zero-range limit, there are two interaction parameters: the large scattering length a and an Efimov parameter κ_* that is defined below [11]. Observables can depend only log periodically on κ_* with discrete scaling factor $e^{\pi/s_0} \approx 22.7$, where $s_0 \approx 1.006\,24$ is the solution to a transcendental equation. In the unitary limit $a \to \pm\infty$, there are infinitely many Efimov trimers with an accumulation point at the 3-atom threshold. The parameter κ_* can be defined by the trimer spectrum near the threshold in the unitary limit: $-(e^{-2\pi/s_0})^n \hbar^2 \kappa_*^2/m$, where n is an integer.

The 2-body contact C_2 and the 3-body contact C_3 for a state with energy E can be defined operationally in terms of derivatives of the energy

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

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

For a many-body state at nonzero temperature, the derivatives should be evaluated at fixed entropy. The normalization of C_2 in Eq. (1a) has been chosen so that the tail of the momentum distribution at large wavenumber k (given below in Eq. (2)) is C_2/k^4. The coefficient on the right side of Eq. (1a) then differs by a factor of 1/2 from that for fermions with two spin states. The normalization of C_3 in Eq. (1b) has been chosen so that the 3-body contacts for the Efimov trimers in the unitary limit are $(e^{-2\pi/s_0})^n \kappa_*^2$. Werner and Castin have expressed the derivative of E in Eq. (1b) in terms of the 3-body Schrödinger wave function at small hyperradius [12].

The importance of the contacts C_2 and C_3 is that there are other properties of the system that depend linearly on these quantities with universal coefficients that are determined by few-body physics. One of these universal relations gives the *tail of the momentum distribution* at large wave vector $\boldsymbol{k}$. We normalize the distribution $n(k)$ so that $\int d^3kn(k)/(2\pi)^3$ is the total number of atoms. We will show below that the tail of $n(k)$ can be expressed as

$$n(k) \to \frac{1}{k^4}C_2 + \frac{F(k)}{k^5}C_3, \tag{2}$$

where $F(k)$ is a universal log-periodic function

$$F(k) = A\sin[2s_0\ln(k/\kappa_*) + 2\phi]. \tag{3}$$

The numerical constants are $A = 89.2626$ and $\phi = -0.669\,064$. The dependence on the state enters only through the contacts C_2 and C_3. Their coefficients can be determined by matching the tail of the momentum distribution for any convenient state. Werner and Castin have calculated C_2 and $F(k)C_3$ for an Efimov trimer in the unitary limit $a \to \pm\infty$ [12]. The 2-body contact for the trimer with binding momentum κ_* is $C_2 = 53.0972\kappa_*$. By our definition in Eq. (1b), the 3-body contact is $C_3 = \kappa_*^2$. We determined A and ϕ by matching the precise results of Ref. [12]. A connection between the $1/k^5$ tail in Eq. (2) and the derivative of the energy in Eq. (1b) was conjectured in Ref. [12].

Another universal relation for identical bosons is an *Energy Relation* that expresses the energy of a system in terms of $n(k)$, C_2, and C_3. The total energy E is the sum of the kinetic energy T, the interaction energy U, and the energy V associated with an external trapping potential. The kinetic energy can be expressed as an integral over $n(k)$. Because of the k^{-4} tail in Eq. (2), the integral is linearly ultraviolet divergent. If the k^{-4} tail were subtracted, the integral would be ultraviolet finite, but it would still depend log periodically on the ultraviolet momentum cutoff because of the k^{-5} tail. The linear and log-periodic dependence on the ultraviolet cutoff are both cancelled by U. The energy relation, which is derived below, expresses the sum $T + U$ in a form that is insensitive to the ultraviolet cutoff

$$T + U = \int \frac{d^3k}{(2\pi)^3}\frac{\hbar^2k^2}{2m}\left[n(k) - \frac{C_2}{k^4} - \theta(k-k_0)\frac{F(k)C_3}{k^5}\right] + \frac{\hbar^2}{8\pi ma}C_2 + \frac{[F(e^{\pi/4s_0}k_0) + f_0]\hbar^2}{8\pi^2 s_0 m}C_3, \tag{4}$$

where $f_0 = -8.424\,27$. The lower limit $k > k_0$ in the k^{-5} subtraction term avoids an ambiguity in the value of the integral over the infrared region. The dependence on the arbitrary wave number k_0 is cancelled by the remaining C_3 term, whose coefficient depends explicitly on k_0. The universal constant f_0 in Eq. (4) was determined by matching an expression for the energy of an Efimov trimer in the unitary limit derived by Werner and Castin [12].

Tan's Energy Relation for fermions with two spin states is similar to Eq. (4) except that there are no terms proportional to C_3 [3]. Combescot, Alzetto, and Leyronas proposed that such a relation should also apply to identical bosons [13]. Werner and Castin demonstrated that such a relation does not hold for an Efimov trimer in the unitary limit [12]. Our universal relation in Eq. (4) demonstrates that it fails for any state for which the 3-body contact C_3 is nonzero.

Another universal relation is the virial theorem for identical bosons trapped in the harmonic potential $V(r) = \frac{1}{2}m\omega^2r^2$, which was derived by Werner [14]:

$$T + U - V = -\frac{\hbar^2}{16\pi ma}C_2 - \frac{\hbar^2}{m}C_3. \tag{5}$$

This can be derived by using dimensional analysis, which implies that the differential operator $2\omega\partial/\partial\omega - a\partial/\partial a + \kappa_*\partial/\partial\kappa_*$ is equal to 2 when acting on the total energy $E = T + U + V$. The Feynman-Hellmann theorem and the definitions in Eqs. (1) imply that the three partial derivatives are proportional to V, C_2, and C_3, respectively.

One of the most important probes of ultracold atoms is radio-frequency (rf) spectroscopy, in which an rf signal is used to transfer atoms to a different spin state. In the case of fermions with two spin states, there are universal relations that provide sum rules for the rf transition rate [4] and control its high-frequency tail [5,6]. In the case of identical bosons, the universal relations for rf spectroscopy also involve the 3-body contact. The high-frequency tail of the rf transition rate is

$$\Gamma(\omega) \to \Omega^2\left[\frac{\hbar^{1/2}}{4\pi m^{1/2}\omega^{3/2}}C_2 + \frac{G_{\rm rf}(\omega)\hbar}{2m\omega^2}C_3\right], \tag{6}$$

where Ω is the Rabi frequency associated with the transition. The transition rate is normalized so that it satisfies the sum rule $\int d\omega\Gamma(\omega) = \pi\Omega^2 N$, where N is the number of identical bosons. The log-periodic function $G_{\rm rf}(\omega)$ is calculated below

$$G_{\rm rf}(\omega) = B_1 + B_2\sin[s_0\ln(m\omega/\hbar\kappa_*^2) + 2\phi_{\rm rf}], \tag{7}$$

where $B_1 = 9.23$, $B_2 = -13.6$, and $\phi_{\rm rf} = 1.33$.

Quantum field theory is a particularly powerful formalism for deriving universal relations [15]. The universal zero-range limit for identical bosons can be described by a quantum field theory with atom field ψ. The Hamiltonian density consists of the kinetic term for ψ and the interaction term

$$\mathcal{H}_{\rm int} = \frac{g_2}{4m}d^\dagger d + \frac{g_3}{36m}t^\dagger t, \tag{8}$$

where $d = \psi\psi$ and $t = \psi\psi\psi$ are local composite operators. We set $\hbar = 1$ for simplicity. To obtain scattering length a and Efimov parameter κ_*, the bare coupling constants g_2 and g_3 must be tuned as functions of the ultraviolet momentum cutoff Λ [16]. If we use a sharp cutoff on the momenta of virtual particles, the bare coupling constants must be chosen to be

$$g_2 = 8\pi/[1/a - 2\Lambda/\pi], \tag{9a}$$
$$g_3 = -9g_2^2(H + J/a\Lambda)/\Lambda^2, \tag{9b}$$
$$H = h_0(C - s_0 S)/(C + s_0 S), \tag{9c}$$
$$J = [j_0 + j_1(2SC) + j_2(C^2 - S^2)]/(C + s_0 S)^2, \tag{9d}$$

where $C = \cos[s_0 \ln(\Lambda/\Lambda_*)]$ and $S = \sin[s_0 \ln(\Lambda/\Lambda_*)]$. In the renormalization prescription for g_3 in Eq. (9b), H must be a log-periodic function of Λ. The analytic approximation for H derived in Ref. [16] is Eq. (9c) with $h_0 = 1$. We find that to within our numerical accuracy of about 10^{-3}, H is given by this analytic expression multiplied by the numerical constant $h_0 = 0.879$. The renormalization scale Λ_* introduced by this prescription differs from κ_* by a multiplicative factor that is only known numerically: $s_0 \ln(\Lambda_*/\kappa_*) = 0.971 \mod \pi$ [11]. The function J in Eq. (9b) is not essential for renormalization, but it is needed to derive the energy relation in Eq. (4).

Using the operational definition of C_2 and C_3 in Eqs. (1) together with the Feynman-Hellman theorem, we can identify the 2-body and 3-body contact densities in the quantum field theory

$$\mathcal{C}_2 = \frac{g_2^2}{4}\langle d^\dagger d\rangle - \frac{g_2^3}{2\Lambda^2}\left(H + \frac{J}{\pi} + \frac{J}{2a\Lambda}\right)\langle t^\dagger t\rangle, \tag{10a}$$
$$\mathcal{C}_3 = -\frac{g_2^2}{8\Lambda^2}\left(H' + \frac{J'}{a\Lambda}\right)\langle t^\dagger t\rangle, \tag{10b}$$

where H' and J' are the derivatives of H and J with respect to $\ln(\Lambda/\Lambda_*)$. The contacts C_2 and C_3 are obtained by integrating these densities over all space. We have used the identity $(a\partial/\partial a)g_2 = g_2^2/8\pi a$ as well as the expression for g_3 in Eq. (9b). The condition that C_2 and C_3 have finite limits as $\Lambda \to \infty$ implies that the matrix elements $\langle d^\dagger d\rangle$ and $\langle t^\dagger t\rangle$ scale as Λ^2 and Λ^4, respectively. Thus the $\langle t^\dagger t\rangle$ term in Eq. (10a) and the J' term in Eq. (10b) can be omitted unless they are multiplied by a factor of Λ.

To derive the energy relation in Eq. (4), we express the interaction energy $U = \int d^3R\langle\mathcal{H}_{\rm int}\rangle$ in terms of the contacts defined by Eqs. (10):

$$U = \frac{1/a - 2\Lambda/\pi}{8\pi m}C_2 - \frac{2(H + 2J/\pi)}{mH'}C_3. \tag{11}$$

The coefficient of C_2 scales as Λ as $\Lambda \to \infty$, while the coefficient of C_3 is a log-period function of Λ. The subtraction terms proportional to C_2 and C_3 in the momentum integral on the right side of Eq. (4) can be evaluated explicitly in terms of the ultraviolet cutoff Λ. After subtracting these terms from U, we find that the dependence on the ultraviolet cutoff Λ cancels. The subtracted expression for U reduces to the last two terms proportional to C_2 and C_3 on the right side of Eq. (4). This proves the Energy Relation and determines the constants A, ϕ, and f_0 in terms of the coefficients h_0, j_0, j_1, and j_2.

The tail of the momentum distribution in Eq. (2) can also be derived by using the short-distance operator product expansion (OPE) [15]. The momentum distribution at wavevector $\boldsymbol{k}$ can be expressed in the quantum field theory as

$$n(\boldsymbol{k}) = \int d^3R\int d^3r e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}\left\langle\psi^\dagger\left(\boldsymbol{R} - \frac{1}{2}\boldsymbol{r}\right)\psi\left(\boldsymbol{R} + \frac{1}{2}\boldsymbol{r}\right)\right\rangle. \tag{12}$$

The coefficients in the OPE for $\psi^\dagger$ and ψ at equal times can be determined by matching matrix elements between asymptotic few-body states [15]. Alternatively, they can be determined by matching Green functions in the few-body sector. The simplest choice of Green functions for the matching are those that are one-particle-irreducible (1PI) with respect to the atom field ψ and the diatom field $d = \psi\psi$. The resulting OPE at large wavevector $\boldsymbol{k}$ can be expressed as

$$\int d^3r e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}\psi^\dagger\left(\boldsymbol{R} - \frac{1}{2}\boldsymbol{r}\right)\psi\left(\boldsymbol{R} + \frac{1}{2}\boldsymbol{r}\right) = \frac{1}{k^4}\frac{g_2^2}{4}d^\dagger d(\boldsymbol{R}) - \frac{F(k)}{k^5}\frac{g_2^2H'}{8\Lambda^2}t^\dagger t(\boldsymbol{R}) + \ldots, \tag{13}$$

where $F(k)$ is the log-periodic function in Eq. (3) and the additional terms are all suppressed by at least k^{-6}. The Wilson coefficient of $d^\dagger d$ was determined analytically by matching the diatom Green function. The Wilson coefficient of $t^\dagger t$ was subsequently detemined by matching the atom + diatom Green function. This Green function can be expressed as a sum of loop diagrams involving the connected atom + diatom Green function, which can be calculated by solving the Skorniakov–ter-Martyrosian integral equation numerically. Inserting the OPE in Eq. (13) into the expression for the momentum distribution $n(\boldsymbol{k})$ in Eq. (12), we obtain the result for the tail of the momentum distribution in Eq. (2). Our direct calculation gives constants A and ϕ that agree to within a few percent with the precise results given after Eq. (3).

In a quantum field theory, rf transitions of an atom to a different spin state can be represented by an operator $\psi_2^\dagger\psi$, where $\psi_2^\dagger$ creates an atom in the second spin state. The rf transition rate can be expressed as

$$\Gamma(\omega) = \Omega^2 {\rm Im}\, i\int dt e^{i(\omega+i\epsilon)t}\int d^3R\int d^3r \times\left\langle T\psi^\dagger\psi_2\left(\boldsymbol{R} + \frac{1}{2}\boldsymbol{r}, t\right)\psi_2^\dagger\psi\left(\boldsymbol{R} - \frac{1}{2}\boldsymbol{r}, 0\right)\right\rangle. \tag{14}$$

We assume for simplicity that the scattering length for the second spin state and the pair scattering length for the first and second spin states are negligible compared to a. We can therefore take ψ_2 to be a noninteracting field. The rf transition rate at large ω can be determined by using the short-time operator product expansion for $\psi^\dagger\psi_2$ and $\psi_2^\dagger\psi$ [6]. The leading terms in the OPE at large ω can be expressed as

$$\int dt e^{i\omega t} \int d^3r \psi^\dagger \psi_2\left(\boldsymbol{R} + \frac{1}{2}\boldsymbol{r}, t\right)\psi_2^\dagger \psi\left(\boldsymbol{R} - \frac{1}{2}\boldsymbol{r}, 0\right) = \frac{i}{\omega}\psi^\dagger \psi(\boldsymbol{R}) + \frac{i[(-m\omega)^{1/2} - a^{-1}]}{4\pi m\omega^2}\frac{g_2^2}{4}d^\dagger d(\boldsymbol{R}) + \frac{iF_{\rm rf}(\omega)}{m\omega^2}\frac{g_2^2 H'}{8\Lambda^2}t^\dagger t(\boldsymbol{R}) + \ldots, \quad (15)$$

where $F_{\rm rf}(\omega)$ is a dimensionless function and the additional terms are all suppressed by at least $\omega^{-5/2}$. The Wilson coefficients for $\psi^\dagger \psi$ and $d^\dagger d$ were determined analytically by matching the atom and diatom Green functions, respectively. The Wilson coefficient of $t^\dagger t$ was subsequently determined by matching the atom + diatom Green function. The function $F_{\rm rf}(\omega)$ in Eq. (15) has the form

$$F_{\rm rf}(\omega) = D_0 + D_1 \ln((-m\omega)^{1/2}/\Lambda) + D_2 \sin^2[s_0 \ln((-m\omega)^{1/2}/\kappa_*) + \phi_{\rm rf}], \quad (16)$$

where Λ is the ultraviolet momentum cutoff. Note that $F_{\rm rf}(\omega)$ is logarithmically ultraviolet divergent. The numerical constants in Eq. (16) are $D_0 = 0.670$, $D_1 = -2.94$, $D_2 = 1.16$, and $\phi_{\rm rf} = 1.33$. To obtain the high-frequency tail in the rf transition rate, we insert the OPE in Eq. (15) into the expression for $\Gamma(\omega)$ in Eq. (14) and take the imaginary part. Terms that are analytic functions of ω, such as $1/\omega$ and $1/\omega^2$, do not contribute to the imaginary part. The leading terms at large ω are given by Eq. (6), where $G_{\rm rf}(\omega) = 2\,{\rm Im} F_{\rm rf}(\omega + i\epsilon)$. Using our result for $F_{\rm rf}(\omega)$ in Eq. (16), we obtain the result for $G_{\rm rf}(\omega)$ in Eq. (7).

There are universal relations involving the 3-body contact for any system in which the Efimov effect arises in the 3-body problem. Another such system consists of fermions with three spin states, which we label 1, 2, and 3. In the zero-range limit, the interactions are described by three large pair scattering lengths a_{12}, a_{13}, and a_{23} and an Efimov parameter κ_*. The discrete scaling factor has the same value $e^{\pi/s_0} \approx 22.7$ as for identical bosons. There are 2-body contacts C_{12}, C_{13}, and C_{23} associated with each pair of spin states and a 3-body contact C_{123}. The tail of the number distribution $n_1(k)$ for spin state 1 is given by Eq. (2) with C_2 and C_3 replaced by $C_{12} + C_{13}$ and C_{123}. An operational definition of C_{12} is given by Eq. (1a) with a and C_2 replaced by a_{12} and $2C_{12}$. An operational definition of C_{123} is given by Eq. (1b) with C_3 replaced by C_{123}. It is straightforward to derive the analogs of the Energy Relation in Eq. (4) and the universal relation for the rf transition rate in Eq. (6).

Many-body systems consisting of identical bosonic atoms or of fermonic atoms with three or more spin states are unstable due to recombination into deeply-bound dimers. The rates for these loss processes scale as a^4 for large a, which makes it difficult to test universal relations for global equilibrium properties of the system, such as the virial theorem in Eq. (5). However, universal relations that govern the short-time behavior of the system, such as the tails of the momentum distribution in Eq. (2) and the tail of the rf transition rate in Eq. (6), can be tested experimentally by using short-time probes of ultracold atoms, such as those that have already been applied to fermions with two spin states [10]. These universal relations involve log-periodic functions, so they provide a new probe of Efimov physics in ultracold atoms.

This research was supported in part by a joint grant from the Army Research Office and the Air Force Office of Scientific Research and by a grant from the Department of Energy.

*braaten@mps.ohio-state.edu
†kang@mps.ohio-state.edu
‡platter@chalmers.se

[1] S. Giorgini, L. Pitaevskii, and S. Stringari, Rev. Mod. Phys. **80**, 1215 (2008); W. Ketterle and M. W. Zwierlein, in *Ultracold Fermi Gases*, edited by M. Inguscio, W. Ketterle, and C. Salomon (IOS Press, 2008).
[2] E. Braaten, arXiv:1008.2922.
[3] S. Tan, Ann. Phys. (N.Y.) **323**, 2952 (2008); **323**, 2971 (2008); **323**, 2987 (2008).
[4] M. Punk and W. Zwerger, Phys. Rev. Lett. **99**, 170404 (2007); G. Baym, C. J. Pethick, Z. Yu, and M. W. Zwierlein, Phys. Rev. Lett. **99**, 190407 (2007).
[5] W. Schneider and M. Randeria, Phys. Rev. A **81**, 021601 (R) (2010).
[6] E. Braaten, D. Kang, and L. Platter, Phys. Rev. Lett. **104**, 223004 (2010).
[7] F. Werner, L. Tarruell, and Y. Castin, Eur. Phys. J. B **68**, 401 (2009); S. Zhang and A. J. Leggett, Phys. Rev. A **79**, 023601 (2009).
[8] D. T. Son and E. G. Thompson, Phys. Rev. A **81**, 063634 (2010); H. Hu, X.-J. Liu, and P. D. Drummond, Europhys. Lett. **91**, 20005 (2010); W. D. Goldberger and I. Z. Rothstein, arXiv:1012.5975.
[9] E. Taylor and M. Randeria, Phys. Rev. A **81**, 053610 (2010); T. Enss, R. Haussmann, and W. Zwerger, Ann. Phys. (N.Y.) **326**, 770 (2011).
[10] E. D. Kuhnle *et al.*, Phys. Rev. Lett. **105**, 070402 (2010); J. T. Stewart *et al.*, Phys. Rev. Lett. **104**, 235301 (2010).
[11] E. Braaten and H. W. Hammer, Phys. Rep. **428**, 259 (2006).
[12] F. Werner and Y. Castin, arXiv:1001.0774.
[13] R. Combescot, F. Alzetto, and X. Leyronas, Phys. Rev. A **79**, 053640 (2009).
[14] F. Werner, Phys. Rev. A **78**, 025601 (2008).
[15] E. Braaten and L. Platter, Phys. Rev. Lett. **100**, 205301 (2008).
[16] P. F. Bedaque, H. W. Hammer and U. van Kolck, Phys. Rev. Lett. **82**, 463 (1999).