Universal and non-universal effective N-body interactions for ultracold harmonically-trapped few-atom systems

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We derive the ground-state energy for a small number of ultracold atoms in an isotropic harmonic trap using effective quantum field theory (EFT). Atoms are assumed to interact through pairwise energy-independent and energy-dependent delta-function potentials with strengths proportional to the scattering length a and effective range volume V, respectively. The calculations are performed systematically up to order l^{-4}, where l denotes the harmonic oscillator length. The effective three-body interaction contains a logarithmic divergence in the cutoff energy, giving rise to a non-universal three-body interaction in the EFT. Our EFT results are confirmed by nonperturbative numerical calculations for a Hamiltonian with finite-range two-body Gaussian interactions. For this model Hamiltonian, we explicitly calculate the non-universal effective three-body contribution to the energy.

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I. INTRODUCTION

The properties of dilute Bose gases are to leading order determined by the two-body free-space s-wave scattering length a [1]. Two-body contact interactions between each pair of bosons are typically assumed, and used to derive expansions around the non-interacting [2–17] or strongly-interacting unitary limit [14, 15, 18–21]. Both few- and many-body systems have been considered and, in some cases, the two limits have been connected using the local density approximation [1, 19, 22, 23]. If the expansion is carried out to sufficiently high order in a or $1/a$, respectively, corrections due to the two-body effective range volume V have to be accounted for if a consistent description that allows one to connect to atomic systems with realistic interaction potentials is desired [2, 4, 10–14, 17, 24].

A question that has intrigued researchers for decades is how three-body interactions come into play [7, 10–13, 20, 25–28]. In the strongly-interacting regime, three-body physics manifests itself in the Efimov effect. Signatures of the Efimov effect are seen by detecting atom losses governed by the three-body recombination rate [20, 29]. In contrast, we investigate in this work elastic three-body scattering processes. We consider N identical bosons with mass M in a spherically symmetric harmonic trap with angular frequency ω and harmonic oscillator length $l=\sqrt{\hbar/(M\omega)}$ in the regime where the two-body s-wave scattering length a and two-body effective range volume V are small compared to the harmonic oscillator length l and volume l^3, respectively. The effective range volume V is related to the effective range $r_{\rm eff}$ by

$$V=\frac{1}{2}r_{\rm eff}a^2. \tag{1}$$

Earlier work developed a perturbative effective field theory (EFT) and derived a low-energy Hamiltonian that accounts for terms up to order $(a/l)^3$ and V/l^3 [17]. The resulting ground-state energy was interpreted in terms of universal effective two-, three-, and four-body interactions. The present paper extends this earlier work and determines universal and non-universal contributions of the terms proportional to $(a/l)^4$, aV/l^4, and $g_3^{(0)}/l^4$ to the ground-state energy; here, $g_3^{(0)}$ denotes a three-body coupling constant. Throughout this paper, the term universal is used to indicate that the quantity under consideration is fully determined by the low-energy two-body scattering observables. The term non-universal, in contrast, is used to indicate that the quantity under consideration cannot, in general, be determined from the low-energy two-body scattering observables.

Our key findings are the following. (*i*) The $(a/l)^4$ term contains effective five-, four-, three- and two-body interactions. The aV/l^4 term contains effective three- and two-body interactions. (*ii*) The effective three-body interaction at order l^{-4} contains a logarithmic divergence in a cutoff energy Λ, introduced to regularize the EFT, which signals a fundamental difference in character between the two- and three-body interactions. Specifically, our results imply that the effective three-body interaction contains a non-universal contribution that cannot be predicted from the low-energy two-body scattering observables. Similar physics has previously been seen for the homogeneous system [8, 9, 30] and for few-body systems confined to a periodic box [10–13]. (*iii*) We extract the non-universal three-body contribution from numerical ground state energies for $N=3-5$ bosons interacting via a short-range two-body Gaussian model potential.

Section II introduces the system Hamiltonian and summarizes our final expression for the ground-state energy of the trapped N-boson system. Sections III and IV dis-

cuss the structure of the terms at order l^{-4}. In addition, Sec. IV elucidates that the field theoretical treatment indicates the presence of a non-universal three-body interaction. Lastly, Section V summarizes our results and discusses implications.

II. SYSTEM HAMILTONIAN AND GROUND-STATE ENERGY

We consider N identical bosons with mass M in a three-dimensional isotropic harmonic trap with angular trapping frequency ω. Our aim is to derive an expression for the ground-state energy of the N-boson system, applicable in the low energy regime, using quantum field theory [31]. Our Hamiltonian is

$$H = H_1 + \sum_{p=2}^{N} \sum_{m=0,2,\ldots} H_{p,\text{bare}}^{(m)}, \tag{2}$$

where H_1 denotes the single-particle Hamiltonian

$$H_1 = \int \hat{\psi}^\dagger(\vec{r}_1) \left(-\frac{\hbar^2}{2M} \overrightarrow{\nabla}_1^2 + \frac{1}{2} M\omega^2 \vec{r}_1^{\,2} \right) \hat{\psi}(\vec{r}_1)\, d\vec{r}_1 \tag{3}$$

and the bosonic field operators $\hat{\psi}(\vec{r})$ and $\hat{\psi}^\dagger(\vec{r})$ destroy and create particles at position $\vec{r}$, respectively. The term $H_{p,\text{bare}}^{(m)}$ denotes p-body contact interactions

$$H_{p,\text{bare}}^{(m)} = \frac{1}{p!} \int \hat{\psi}^\dagger(\vec{r}_1) \cdots \hat{\psi}^\dagger(\vec{r}_p) W_p^{(m)}(\vec{r}_1, \vec{r}_2, \cdots, \vec{r}_p) \times \hat{\psi}(\vec{r}_1) \cdots \hat{\psi}(\vec{r}_p)\, d\vec{r}_1 d\vec{r}_2 \cdots d\vec{r}_p. \tag{4}$$

The superscript "(m)" indicates the order of the derivative operator in the p-body potentials $W_p^{(m)}$. In our calculations, we expand the field operators in terms of the eigenstates of the single-particle harmonic oscillator Hamiltonian [16, 17].

Through order l^{-4}, we find that only three potentials are needed: $W_2^{(0)}(\vec{r}_1, \vec{r}_2)$, $W_2^{(2)}(\vec{r}_1, \vec{r}_2)$, and $W_3^{(0)}(\vec{r}_1, \vec{r}_2, \vec{r}_3)$; no local four- or higher-body potentials are necessary. The two-body potential $W_2^{(0)}(\vec{r}_1, \vec{r}_2)$ corresponds to the "usual" δ-function pseudopotential [32]

$$W_2^{(0)}(\vec{r}_1, \vec{r}_2) = g_{2,\text{bare}}^{(0)} \delta(\vec{r}_1 - \vec{r}_2), \tag{5}$$

where $g_{2,\text{bare}}^{(0)}$ is the two-body bare coupling constant. The $m = 2$ two-body potential $W_2^{(2)}(\vec{r}_1, \vec{r}_2)$ depends on the energy through the second-derivative operators [11, 17]

$$W_2^{(2)}(\vec{r}_1, \vec{r}_2) = \frac{1}{2} g_{2,\text{bare}}^{(2)} \times \left[\overleftarrow{\nabla}_{12}^2 \delta(\vec{r}_1 - \vec{r}_2) + \delta(\vec{r}_1 - \vec{r}_2) \overrightarrow{\nabla}_{12}^2 \right], \tag{6}$$

where $g_{2,\text{bare}}^{(2)}$ is another two-body bare coupling constant. The operators $\overleftarrow{\nabla}_{12}$ and $\overrightarrow{\nabla}_{12}$ are gradients with respect to the relative distance vector $\vec{r}_1 - \vec{r}_2$ that act to the left and right, respectively. Note that the two-body interaction with $m = 1$ is absent due to symmetry constraints. The lowest order three-body potential is modeled by the product of two δ-functions,

$$W_3^{(0)}(\vec{r}_1, \vec{r}_2, \vec{r}_3) = g_{3,\text{bare}}^{(0)} \delta(\vec{r}_1 - \vec{r}_2) \delta(\vec{r}_2 - \vec{r}_3), \tag{7}$$

where $g_{3,\text{bare}}^{(0)}$ is the three-body bare coupling constant. The three-body potential acts only when three particles are at the same position.

We calculate the N-boson ground-state energy using renormalized Rayleigh-Schrödinger perturbation theory. Divergences arise at second- and higher-order in perturbation theory [31]. To obtain physical results we include counterterm interactions for each p and m combination. Specifically, we write the bare coupling constant as [16, 17]

$$g_{p,\text{bare}}^{(m)} = g_p^{(m)} + g_{p,\text{ct}}^{(m)}, \tag{8}$$

where $g_p^{(m)}$ is the *physical* coupling constant and $g_{p,\text{ct}}^{(m)}$ the counterterm coupling constant. The counterterms $g_{2,\text{ct}}^{(0)}$ and $g_{2,\text{ct}}^{(2)}$ are determined self-consistently such that the EFT energy shifts reproduce the ground-state energy for two harmonically-trapped bosons interacting through a short-range potential with free-space s-wave scattering length a and free-space effective range volume V up to order l^{-4} (see, e.g., Ref. [17]). In this renormalization scheme, the physical coupling constants are

$$g_2^{(0)} = \frac{4\pi\hbar^2}{M} a \quad \text{and} \quad g_2^{(2)} = -\frac{4\pi\hbar^2}{M} V. \tag{9}$$

We find it convenient to organize the contributions to the ground-state energies E_N in terms of powers of $1/l$ [16, 17]. To understand this structure, it is instructive to perform a dimensional analysis. The coupling constants $g_{p,\text{bare}}^{(m)}$, and correspondingly $g_p^{(m)}$, have units of $energy \times (length)^{3p-3+m}$. For the scaled ground-state energy $E_N/(\hbar\omega)$ this implies that the first-order correction due to the Hamiltonian term proportional to $g_2^{(0)}$ corresponds to an energy shift of order $1/l$. Similarly, the term proportional to $(g_2^{(0)})^2$ corresponds to a shift of order $1/l^2$, and the terms proportional to $(g_2^{(0)})^3$ and $g_2^{(2)}$ correspond to shifts of order $1/l^3$. Finally, the contributions $(g_2^{(0)})^4$, $g_2^{(0)} g_2^{(2)}$, and $g_3^{(0)}$ lead to terms of order $1/l^4$. Thus, we can write the scaled energy as

$$\frac{E_N}{\hbar\omega} = \frac{3}{2} N + \sum_{p=2}^{N} \binom{N}{p} U_p\,, \tag{10}$$

where the dimensionless effective p-body interaction en-

ergies U_p are power series in $1/l$:

$$U_p = \sum_{K=1}^{\infty} \underbrace{\left[\sum_{\substack{k_{2,0},k_{2,2},k_{3,0} \\ k_{2,0}+3k_{2,2}+4k_{3,0}=K}} U_p^{(k_{2,0},k_{2,2},k_{3,0})} \right]}_{\mathcal{O}(l^{-K})} . \quad (11)$$

The notation $\mathcal{O}(l^{-K})$ indicates that the term is proportional to l^{-K}. The dimensionless partial energies

$$U_p^{(k_{2,0},k_{2,2},k_{3,0})} = c_p^{(k_{2,0},k_{2,2},k_{3,0})} \quad (12)$$
$$\times \left(\frac{g_2^{(0)}}{4\pi\hbar^2/M}\frac{1}{l} \right)^{k_{2,0}} \left(-\frac{g_2^{(2)}}{4\pi\hbar^2/M}\frac{1}{l^3} \right)^{k_{2,2}} \left(\frac{g_3^{(0)}}{\hbar^2/M}\frac{1}{l^4} \right)^{k_{3,0}}$$

are proportional to $(g_2^{(0)})^{k_{2,0}}(g_2^{(2)})^{k_{2,2}}(g_3^{(0)})^{k_{3,0}}$. The three superscripts $k_{p,m}$ take the values $0, 1, 2, \ldots$ subject to the constraint $k_{2,0} + 3k_{2,2} + 4k_{3,0} = K$; here, the prefactors of the $k_{p,m}$ are given by $3p + m - 5$. The factors of $\pm 4\pi$ in the first two terms in the second line of Eq. (12) are included for later convenience.

Equation (10) is valid when a/l, V/l^3, and $g_3^{(0)}/[(\hbar^2/M)l^4]$ are much smaller than one. The expansion coefficients $c_p^{(k_{2,0},k_{2,2},k_{3,0})}$ are summarized in Table I. After renormalization of the two-body interactions all coefficients are finite except $c_3^{(4,0,0)}$, which diverges logarithmically with the cutoff. The origin and implications of this logarithmic divergence are discussed in Sec. IV. The $p = 2$ coefficients agree with what one obtains by expanding the exact zero-range solution for two s-wave interacting particles in a harmonic trap [14, 33].

III. THE UNIVERSAL EFFECTIVE FOUR- AND FIVE-BODY INTERACTIONS

References [16, 17] showed that the renormalized perturbation theory treatment at orders $K = 2$ and 3 requires a counterterm coupling constant $g_{2,\mathrm{ct}}^{(0)}$, which cancels all divergences at these orders. As we discuss now, new physics emerges at order $K = 4$.

We start our discussion of the $K = 4$ terms by considering the effective four- and five-body interaction energies $U_4^{(4,0,0)}$ and $U_5^{(4,0,0)}$. The five-body term, which first arises at this order, is finite. The four-body term is finite after renormalization of the two-body interaction, with $g_{2,\mathrm{ct}}^{(0)}$ removing power-law divergences. Since $U_4^{(4,0,0)}$ and $U_5^{(4,0,0)}$ are fully determined by a/l, we refer to these effective interactions as universal. We were unable to evaluate the sums that give the coefficients $c_4^{(4,0,0)}$ and $c_5^{(4,0,0)}$ analytically. Numerical estimates and uncertainties are reported in Table I.

To validate our EFT results for the effective four- and five-body interactions, we compare to numerical simulations of $N = 2, 3, 4$, and 5 bosons interacting via a finite-range, non-singular potential. We consider a Hamiltonian with pairwise additive Gaussian model interaction

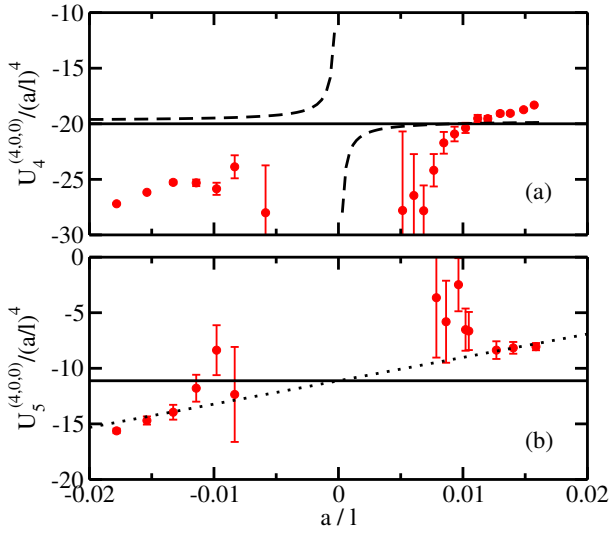

FIG. 1. (Color online) (a) and (b) show the effective four- and five-body contributions $U_4^{(4,0,0)}$ and $U_5^{(4,0,0)}$, respectively, as a function of a/l. The interaction energies are scaled by $(a/l)^{-4}$, such that the EFT predictions at order $K = 4$ are given by the solid horizontal lines. Circles show numerical values for a model Hamiltonian with a pairwise Gaussian interaction with $r_0 = 0.01l$. The numerical data is unreliable in the regime $|a/l| \lesssim 0.007$ and $|a/l| \lesssim 0.11$ for (a) and (b), respectively, as the numerical uncertainty becomes comparable to or larger than 0.3 times the quantity of interest. The dashed line in panel (a) includes the scaled $K = 5$ effective range volume dependent contribution, which is proportional to $c_4^{(2,1,0)}V/a^2$. We use the numerically obtained effective range volume, as a function of a, for the Gaussian potential with $r_0 = 0.01l$, and $c_4^{(2,1,0)} = 25.422472$ as determined within the EFT. The dotted line in panel (b) shows a linear fit of the form $c_5^{(4,0,0)} + c_5^{(5,0,0)}a/l$ to the numerically determined energies in the regime $|a/l| > 0.11$, with $c_5^{(4,0,0)}$ fixed at our EFT value of -11.12. We find $c_4^{(5,0,0)} \approx 210$. The error bars, which are one standard deviation, are estimated from the basis set extrapolation errors of the numerically determined $N = 3, 4$, and 5 energies E_N.

$V_{\mathrm{g}}(r) = V_0 \exp[-(r/r_0)^2/2]$, with depth V_0 and width r_0, and determine the energies E_N, $N > 2$, numerically using an explicitly correlated Gaussian basis set [17, 34, 35]. For $N = 2$, we use a grid-based B-spline approach. For a given width r_0, we adjust the depth V_0 ($V_0 < 0$ and $V_0 > 0$) such that $V_{\mathrm{g}}(r)$ reproduces the desired physical free-space s-wave scattering length a at zero collision energy. The parameters are chosen such that $V_{\mathrm{g}}(r)$ supports at most one bound state.

The effective range volume for the Gaussian potential as a function of V_0 and thus scattering length a was previously numerically calculated by us. The result is shown in Fig. 3 of Ref. [17]. Crucial here is that in the limit of zero scattering length the effective range volume approaches zero. In fact, we have $V = -ar_0^2 + \mathcal{O}(a^2)$ from a perturbative Born calculation of the two-body free-space scattering amplitude.

TABLE I. Expansion coefficients $c_p^{(k_{2,0},k_{2,2},k_{3,0})}$, defined in Eq. (12), of the effective p-body interactions for N bosons in an isotropic harmonic trap, up to order l^{-4}. Columns 4 and 5 give analytic expressions and numerical values, respectively, obtained using renormalized perturbation theory. The numbers in round brackets in column 5 denote the numerical uncertainty; those without error bars have been rounded. After renormalization of the two-body interactions, all coefficients are finite except for the logarithmically diverging $c_3^{(4,0,0)}$. The terms $D_\mathrm{a}, D_\mathrm{b}, D_\mathrm{c}$, and D_d are defined in the text. To interpret Fig. 1(a), we calculate the $K = 5$ effective four-body contribution proportional to Va^2. This gives $c_4^{(2,1,0)} = 25.42247$. No other $K = 5$ contributions are calculated in the present paper. The function $\zeta(z)$ is the Riemann Zeta function.

p	$(k_{2,0}, k_{2,2}, k_{3,0})$	K	compact expression / comment	numerical value
2	$(1,0,0)$	1	$(2/\pi)^{1/2}$	0.797884561
	$(2,0,0)$	2	$(2/\pi)(1-\log 2)$	0.195348572
	$(3,0,0)$	3	$(2/\pi)^{3/2}(1-\frac{\pi^2}{24}-3\log 2+\frac{3}{2}\log^2 2)$	−0.391118531
	$(0,1,0)$	3	$(3/2)(2/\pi)^{1/2}$	1.196826841
	$(4,0,0)$	4	$\frac{1}{3\pi^2}[12+\pi^2(-2+\log 4)-4(-3+\log 4)^2\log 4-3\zeta(3)]$	−0.408766776
	$(1,1,0)$	4	$(1/\pi)(8-6\log 2)$	1.222665489
3	$(2,0,0)$	2	$(2/\pi)[-4\sqrt{3}+6-12\log 2-6\log(2-\sqrt{3})]$	−0.855758313
	$(3,0,0)$	3	see Ref. [17] (sum evaluated numerically)	2.7921(1)
	$(4,0,0)$	4	$10.8629(1)-12(2D_\mathrm{a}+D_\mathrm{b}+2D_\mathrm{c}-3D_\mathrm{d})$	log-divergent
	$(1,1,0)$	4	$-(4/3\pi)[-36+26\sqrt{3}+9\log 64-27\log(2+\sqrt{3})]$	−4.628397857
	$(0,0,1)$	4	$16/(3\sqrt{3}\pi)$	0.980140259
4	$(3,0,0)$	3	see Ref. [17] (sum evaluated numerically)	2.433174845
	$(4,0,0)$	4	sum evaluated numerically	−20.0(2)
5	$(4,0,0)$	4	sum evaluated numerically	−11.12(2)

Interestingly, following Refs. [11, 12], we can extract $U_4^{(4,0,0)}$ and $U_5^{(4,0,0)}$ from the numerically determined E_N using

$$U_4^{(4,0,0)} = -U_4^{(3,0,0)} - 6 + (E_4 - 4E_3 + 6E_2)/(\hbar\omega) + \mathcal{O}(l^{-5}) \tag{13}$$

and

$$U_5^{(4,0,0)} = 15/2 + (E_5 - 5E_4 + 10E_3 - 10E_2)/(\hbar\omega) + \mathcal{O}(l^{-5}), \tag{14}$$

where the dimensionless partial energy $U_4^{(3,0,0)}$ has been obtained and validated in Ref. [17].

Figure 1(a) compares the numerically extracted scaled $U_4^{(4,0,0)}/(a/l)^4$, for $r_0 = 0.01l$, to the EFT prediction $c_4^{(4,0,0)} = -20.0$ given in Table I, as a function of a/l. Similarly, Fig. 1(b) compares $U_5^{(4,0,0)}/(a/l)^4$ to the EFT prediction $c_5^{(4,0,0)} = -11.12$. In both cases, the EFT at order $K = 4$ predicts horizontal lines. Comparison to the numerics shows reasonable agreement, including the correct sign.

We can attempt to understand the deviations in Figs. 1(a) and 1(b) by looking at the $K = 5$ contributions. The effective four-body interaction contains terms proportional to a^5, a^2V, and $ag_3^{(0)}$. We have calculated the a^2V coefficient from the EFT. The dashed line in Fig. 1(a) shows the contribution proportional to $c_4^{(2,1,0)}a^2V$, using the effective range volume V for the Gaussian potential with $r_0 = 0.01l$. It can be seen that this effective range volume correction to the solid line is negligible in the regime for which our numerical data is reliable. Note that as $V \propto -a$ for very small $|a|$, the correction diverges as $|a| \to 0$. We conjecture that the deviation between the EFT predictions for the effective four-body interaction and the numerical data for $|a/l| \gtrsim 0.01$ is due to both the $(a/l)^5$ and $ag_3^{(0)}$ contributions. Moreover we expect that $g_3^{(0)}$ depends nontrivially on a/l (see also Sec. IV).

The effective five-body interaction at order $K = 5$ has only an $(a/l)^5$ contribution. As we have not calculated this contribution using EFT, the numerical data in Fig. 1(b) is fit to a line [see dotted line in Fig. 1(b)] with coefficients given in the caption of Fig. 1. From the slope we extract an estimate for $c_4^{(5,0,0)}$.

IV. THE NON-UNIVERSAL THREE-BODY INTERACTION

This section considers the effective three-body interaction. Unlike the four- and five-body terms, $U_3^{(4,0,0)}$ contains a logarithmic divergence that is not renormalized by $g_{2,\mathrm{ct}}^{(0)}$. To shed light on this behavior, Figs. 2(a)-2(d) diagrammatically represent the diverging sums D_a, D_b, D_c, and D_d that enter into $U_3^{(4,0,0)}$. Note that these are modified Rayleigh-Schrödinger perturbation theory diagrams, using the formalism described in Refs. [16, 17], and not Feynman diagrams. For brevity, we do not show the diagrams corresponding to convergent sums. Solid lines represent particles in the single-particle ground state. Dotted lines represent particles in single-particle excited states. Vertices represent interactions. The dot represents the two-body interaction with coupling constant $g_2^{(0)}$, while the circled dot represents the two-body counterterm with coupling constant $g_{2,\mathrm{ct}}^{(0)}$. We evaluate these

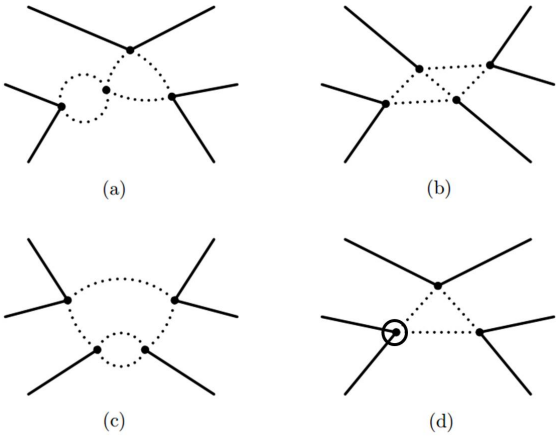

FIG. 2. Diagrammatic representation of the divergent sums that contribute to the effective three-body interaction $U_3^{(4,0,0)}$. Diagrams (a)-(d) represent the quantities $D_{\rm a}$, $D_{\rm b}$, $D_{\rm c}$, and $D_{\rm d}$, (see Table I and text). The dot represents the two-body interaction with coupling constant $g_2^{(0)}$. The circled dot represents the two-body counterterm with coupling constant $g_{2,{\rm ct}}^{(0)}$.

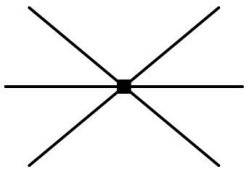

FIG. 3. Diagrammatic representation of the non-universal three-body interaction. The square represents the three-body interaction with coupling constant $g_3^{(0)}$.

diagrams numerically as a function of the cutoff energy Λ, where terms corresponding to intermediate states with total energy greater than Λ are not included in the sums. We find that the diagrams shown in Figs. 2(a), 2(b), and 2(d) diverge as $(\Lambda/\hbar\omega)^{1/2}$, $\log(\Lambda/\hbar\omega)$, and $(\Lambda/\hbar\omega)^{1/2}$, respectively. The diagram shown in Fig. 2(c) contains terms that diverge as $(\Lambda/\hbar\omega)^{1/2}$ and $\log(\Lambda/\hbar\omega)$.

The power-law divergences contained in the diagrams $D_{\rm a}$ and $D_{\rm c}$ [see Figs. 2(a) and 2(c)] are renormalized by the two-body counterterm diagram $D_{\rm d}$ [see Fig. 2(d)]. The $\log(\Lambda/\hbar\omega)$ divergences contained in the diagrams $D_{\rm b}$ and $D_{\rm c}$ remain, however, and the properly weighted diagrams $D_{\rm a}$-$D_{\rm d}$ evaluate to a term of the form $q_0 + q_1 \log(\Lambda/\hbar\omega)$, where q_0 and q_1 are constants. This signals that a non-universal, local three-body interaction with cutoff dependent coupling constant $g_3^{(0)}$, represented diagrammatically in Fig. 3, is needed [8, 10, 12]. Specifically, renormalization requires a three-body interaction energy $U_3^{(0,0,1)}$, generated by $g_3^{(0)}$, which cancels the logarithmic divergence in $U_3^{(4,0,0)}$. The corresponding $c_3^{(0,0,1)}$ value can be found in Table I.

The above discussion motivates us to define a renormalization-scheme-independent three-body contribution (see also Refs. [11, 12])

$$\bar{U}_3^{K=4} = U_3^{(4,0,0)} + U_3^{(0,0,1)}. \tag{15}$$

As $g_3^{(0)}$ is a new, undetermined parameter in the Hamiltonian, the EFT does not make a unique prediction for $\bar{U}_3^{K=4}$ based on the values of $g_2^{(0)}$ and $g_2^{(2)}$. Instead, $\bar{U}_3^{K=4}$ depends on the short-range features of the true, "intrinsic" underlying interaction potentials. The interaction energy $\bar{U}_3^{K=4}$ must therefore either be obtained by measurement or by accurate numerical simulation of an N-body system ($N > 2$). We can extract the value of $\bar{U}_3^{K=4}$, to order l^{-4}, using the numerically determined N-body ground state energies E_N,

$$\begin{aligned}\binom{N}{3}\bar{U}_3^{K=4} = \frac{E_N}{\hbar\omega} - \frac{3}{2}N \\ -\binom{N}{2}\left[\sum_{k=1}^{4} U_2^{(k,0,0)} + U_2^{(0,1,0)} + U_2^{(1,1,0)}\right] \\ -\binom{N}{3}\left[\sum_{k=2}^{3} U_3^{(k,0,0)} + U_3^{(1,1,0)}\right] \\ -\binom{N}{4}\left[\sum_{k=3}^{4} U_4^{(k,0,0)}\right] - \binom{N}{5} U_5^{(4,0,0)} + \mathcal{O}\big(l^{-5}\big).\end{aligned} \tag{16}$$

The key point is that the $U_p^{(k_{2,0},k_{2,2},k_{3,0})}$ quantities on the right hand side of Eq. (16) are known from the EFT (see Table I). This implies that we can calculate $\bar{U}_3^{K=4}$ for $N = 3, 4, 5\cdots$, provided the E_N are known.

Figure 4 shows $\bar{U}_3^{K=4}/(a/l)^4$ as a function of a/l determined from Eq. (16) for $N = 3$, 4, and 5 using the numerically determined ground-state energies for the Hamiltonian with pairwise Gaussian interactions with width $r_0 = 0.01l$. We make two observations. First, for a fixed potential width r_0, the $\bar{U}_3^{K=4}$ calculated for $N = 3$, 4, and 5 collapse, to a good approximation, to a single curve. This confirms that the extracted value of $\bar{U}_3^{K=4}$ scales with the number of trimers in the system, i.e., that the physics seen is indeed a three-body effect. Second, the fact that $\bar{U}_3^{K=4}/(a/l)^4$ is not independent of a shows that $\bar{U}_3^{K=4}$ is not simply proportional to a^4. This, combined with other analysis, indicates that the three-body physics at order $K = 4$ is not fully described by the two-body s-wave scattering length and two-body effective range volume.

To investigate the dependence of the non-universal three-body interaction on the short-range interaction scale of the Gaussian model interaction, we additionally calculated $\bar{U}_3^{K=4}/(a/l)^4$ for $r_0 = 0.005l$, $0.0075l$, and $0.0125l$. We find that the $\bar{U}_3^{K=4}$ for fixed a but different r_0 differ on the negative scattering length side where one expects the formation of three-body bound states to be sensitive to the details of the underlying two-body interaction model. On the positive scattering length side, the $\bar{U}_3^{K=4}$ shows a comparatively weak dependence on r_0. We believe that this can be attributed to the fact that

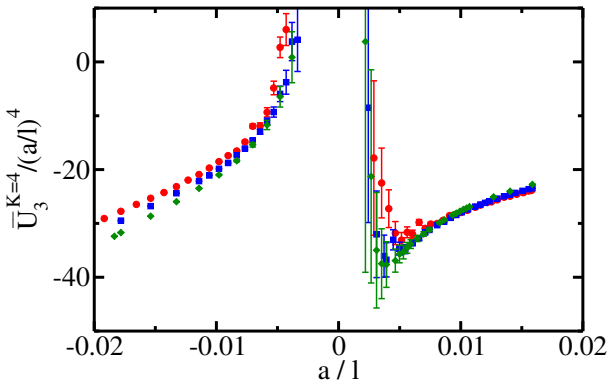

FIG. 4. (Color online) Scaled three-body interaction $\bar{U}_3^{K=4}/(a/l)^4$ as a function of a/l, extracted from numerical N-body ground-state energies for the Gaussian two-body potential with width $r_0 = 0.01l$ and using Eq. (16). Circles, squares and diamonds are determined from Eq. (16) for $N = 3, 4$, and 5, respectively. The numerical data is unreliable for $|a/l| \lesssim 0.005$, as the numerical uncertainty becomes comparable to or larger than 0.3 times the quantity of interest. The error bars, which are one standard deviation, are estimated from the basis set extrapolation errors of the numerically determined $N = 3, 4$, and 5 energies E_N.

the purely repulsive Gaussian interaction model behaves similar to a hard core potential, especially for relatively "large" a/l. For the hardcore potential, $\bar{U}_3^{K=4}$ has been shown to scale as a^4 [10].

If non-perturbative numerical N-body energies are not available, we can still make rough, order-of-magnitude, estimates of $\bar{U}_3^{K=4}$ by evaluating the logarithmically diverging sums in the EFT up to the characteristic energy scale of the two-body system, i.e., up to $\Lambda = \hbar^2/(mr_0^2)$. In practice, one might want to use the scale corresponding to the van der Waals length as suggested in Ref. [8]. In the present work, however, it seems more appropriate to use the energy scale corresponding to the Gaussian potential. For $r_0 = 0.01l$, this corresponds to $\Lambda = 10,000\hbar\omega$. Because we are unable to numerically evaluate the necessary sums in diagrams $D_{\rm a}, D_{\rm b}, D_{\rm c}$ and $D_{\rm d}$ of the EFT to a value of Λ this large, we instead extrapolate to $\Lambda = 10,000\hbar\omega$ using numerically determined estimates with smaller Λ and the expected power-law and logarithmic divergences. This approach yields $\bar{U}_3^{K=4}/(a/l)^4 \approx -8.6$. Comparison with Fig. 4 shows that this estimate gives the correct sign and order of magnitude of the true $\bar{U}_3^{K=4}$ for the Gaussian model potential with $r_0 = 0.01l$.

Finally, we note that at order $K = 4$, the effective three- and two-body interactions $U_3^{(1,1,0)}$ and $U_2^{(1,1,0)}$ also depend on the effective range volume. These universal contributions have been determined analytically and are given in Table I. Following the convention introduced in Sec. I, we refer to $U_3^{(1,1,0)}$ and $U_2^{(1,1,0)}$ as universal as they are fully determined by the low-energy two-body scattering properties, expressed in harmonic oscillator units.

V. CONCLUSION

In this paper, we utilized a quantum field theory approach to derive the ground-state energy for a small number of bosons in a spherically-symmetric harmonic trap up to order l^{-4}, where l is the harmonic oscillator length. We showed that the ground-state energy at this order depends on two two-body parameters (the scattering length a and effective range volume V) and one emergent non-universal three-body interaction strength ($g_3^{(0)}$). In the spirit of effective field theory, these parameters can be determined by performing measurements at two trap frequencies of the ground-state energy of the two-body system and one measurement on the three-body system. Using these three data points as input, the ground-state energy up to order l^{-4} is then known for any trapping frequency and any number of particles.

The emergence of the non-universal three-body interaction derived here for harmonically-trapped atoms has been discussed for other systems. For few-boson systems confined to a periodic box [10–13], the ground-state energy can be organized, similar to the harmonically-trapped system, in terms of powers of $1/L$ and p-body interactions, where L is the length of the cubic box. Interestingly, the leading order three-, four-, and five-body energy contributions for N bosons in the periodic box are proportional to a^3, a^4, and a^5, respectively [10–13], rather than the leading order contributions a^2, a^3, and a^4 for bosons in a harmonic trap. Just as for the harmonically trapped system, the non-universal three-body interaction is renormalization scheme dependent. Similar physics has also been observed in the homogeneous system [8]. Our analysis extends the EFT approach to non-universal few-body interactions of harmonically trapped bosons.

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[1] F. Dalfovo, S. Giorgini, L. P. Pitaevskii, and S. Stringari, Rev. Mod. Phys. **71**, 463 (1999).

[2] K. Huang and C. N. Yang, Phys. Rev. **105**, 767 (1957).

[3] T. D. Lee, K. Huang, and C. N. Yang, Phys. Rev. **106**, 1135 (1957).
[4] K. Huang, Phys. Rev. **115**, 765 (1959).
[5] M. Lüscher, Commun. Math. Phys. **105**, 153 (1986).
[6] M. Lüscher, Nucl. Phys. B **354**, 531 (1991).
[7] T. T. Wu, Phys. Rev. **115**, 1390 (1959).
[8] E. Braaten and A. Nieto, EPJ B **11**, 143 (1999).
[9] E. Braaten, H.-W. Hammer, and S. Hermans, Phys. Rev. A **63**, 063609 (2001).
[10] S. Tan, Phys. Rev. A **78**, 013636 (2008).
[11] S. R. Beane, W. Detmold, and M. J. Savage, Phys. Rev. D **76**, 074507 (2007).
[12] S. R. Beane, W. Detmold, T. C. Luu, K. Orginos, M. J. Savage, and A. Torok, Phys. Rev. Lett. **100**, 082004 (2008).
[13] W. Detmold and M. J. Savage, Phys. Rev. D **77**, 057502 (2008).
[14] K. M. Daily, X. Y. Yin, and D. Blume, Phys. Rev. A **85**, 053614 (2012).
[15] F. Werner and Y. Castin, Phys. Rev. A **86**, 053633 (2012).
[16] P. R. Johnson, E. Tiesinga, J. V. Porto, and C. J. Williams, New J. Phys. **11**, 093022 (2009).
[17] P. R. Johnson, D. Blume, X. Y. Yin, W. F. Flynn, and E. Tiesinga, New J. Phys. **14**, 053037 (2012).
[18] D. B. Kaplan, M. J. Savage, and M. B. Wise, Phys. Lett. B **424**, 390 (1998).
[19] S. Jonsell, H. Heiselberg, and C. J. Pethick, Phys. Rev. Lett. **89**, 250401 (2002).
[20] E. Braaten and H.-W. Hammer, Phys. Rep. **428**, 259 (2006).
[21] C. Ji, D. R. Phillips, and L. Platter, Annals Phys. **327**, 1803 (2012).
[22] A. Fabrocini and A. Polls, Phys. Rev. A **60**, 2319 (1999).
[23] H. Fu, Y. Wang, and B. Gao, Phys. Rev. A **67**, 053612 (2003).
[24] F. Werner and Y. Castin, Phys. Rev. A **86**, 013626 (2012).
[25] V. Efimov, Phys. Lett. B **33**, 563 (1970).
[26] E. Braaten and A. Nieto, Phys. Rev. B **55**, 8090 (1997).
[27] E. Epelbaum, A. Nogga, W. Glöckle, H. Kamada, U.-G. Meißner, and H. Witała, Phys. Rev. C **66**, 064001 (2002).
[28] D. S. Petrov, Phys. Rev. Lett. **112**, 103201 (2014).
[29] B. D. Esry, C. H. Greene, and J. P. Burke, Phys. Rev. Lett. **83**, 1751 (1999).
[30] E. Braaten, H.-W. Hammer, and T. Mehen, Phys. Rev. Lett. **88**, 040401 (2002).
[31] M. Srednicki, *Quantum Field Theory* (Cambridge University Press, 2007).
[32] E. Fermi, Nuovo Cimento **11**, 157 (1934).
[33] T. Busch, B.-G. Englert, K. Rzaewski, and M. Wilkens, Found. of Phys. **28**, 549 (1998).
[34] J. Mitroy, S. Bubin, W. Horiuchi, Y. Suzuki, L. Adamowicz, W. Cencek, K. Szalewicz, J. Komasa, D. Blume, and K. Varga, Rev. Mod. Phys. **85**, 693 (2013).
[35] Y. Suzuki and K. Varga, *Stochastic Variational Approach to Quantum-Mechanical Few-Body Problems* (Springer, 1998).