Universal molecules trapped with discrete scaling symmetries

Yusuke Nishida\textsuperscript{1} and Dean Lee\textsuperscript{2}

\textsuperscript{1}Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA
\textsuperscript{2}Department of Physics, North Carolina State University, Raleigh, North Carolina 27695, USA

(Dated: February 2012)

When the scattering length is proportional to distance from the center of the system, two particles are shown to be trapped about the center. Furthermore, their spectrum exhibits discrete scale invariance whose scale factor is controlled by the slope of the scattering length. We also elucidate how the emergent discrete scaling symmetry is violated for more than two bosons, which may shed new light on Efimov physics. Our system thus serves as a tunable model system to investigate universal physics involving scale invariance, quantum anomaly, and renormalization group limit cycle, which are important in a broad range of quantum physics.

PACS numbers: 03.65.Ge, 37.10.Pq

Introduction

When particles attract by a short-range interaction with large scattering length, their low-energy physics becomes universal \cite{1}. Ultracold atoms are ideal to study such universal physics because of the tunability of interatomic interactions and can provide insights applicable in a broad range of physics. One of the most striking phenomena in universal systems is the Efimov effect, i.e., formation of an infinite tower of three-body bound states characterized by discrete scale invariance \cite{2}. Although the Efimov effect was originally predicted in the context of nuclear physics, it is now subject to extensive research in ultracold atoms \cite{3}.

In this Letter, we propose novel systems in which two particles exhibit discrete scale invariance in their spectrum. In order for this to happen, their interaction needs to be scale invariant \cite{4}. It is usually considered that the short-range interaction can be scale invariant only when the scattering length $a$ is set to be zero or infinite. However, there is another possibility: The scattering length is made space-dependent and tuned to be proportional to distance from the center of the system; $a(x) = c|x|$. This interaction is scale invariant because there is no dimensionful parameter in it.

The emergence of the discrete scale invariance can be understood intuitively by using the Born-Oppenheimer approximation. Suppose one particle is much heavier than the other particle. With the heavy particle fixed at $x$, the light particle forms a bound state with binding energy $\hbar^2/2\mu a(x)^2$, which in turn acts as an effective potential for the heavy particle. Therefore, one can design any attractive potential by tuning the space-dependence of the scattering length. In particular, when $a(x) = c|x|$, the effective potential becomes a inverse square potential, for which it is well known that the spectrum exhibits discrete scale invariance. Since two particles are trapped about the center of the system with the discrete scaling symmetry, we shall call our system as a scaling trap.

This conclusion can be established for any mass ratio by solving the two-body problem exactly with the space-dependent scattering length. While our idea works in any spatial dimensions, we shall give extensive and detailed analyses in one dimension and then present key results in two and three dimensions.

Two particles in one dimension

Two interacting particles in one dimension are described by the Schrödinger equation (hereafter $\hbar = 1$):

$$\left[\frac{\nabla_X^2}{2M} - \frac{\nabla_x^2}{2\mu} + V(X,x)\right] \psi(X,x) = E \psi(X,x). \quad (1)$$

Here $M = m_1 + m_2$ and $\mu = m_1 m_2/(m_1 + m_2)$ are total and reduced masses and $X = (m_1 x_1 + m_2 x_2)/M$ and $x = x_1 - x_2$ are center-of-mass and relative coordinates. For a zero-range interaction whose strength depends on the position $X$, the interaction potential is written as $V(X,x) = -\frac{1}{\mu a(X)} \delta(x)$, where $a(X)$ is the space-dependent scattering length. For a bound state solution with $E \equiv -\kappa^2/(2M)$, the Schrödinger equation is formally solved by

$$\tilde{\psi}(P,p) = \frac{1}{\sqrt{p^2 + \kappa^2}} \frac{1}{\mu} \int \frac{dP'}{2\pi} \frac{1}{\tilde{a}(P-P')} \tilde{\chi}(P'), \quad (2)$$

where $\tilde{\psi}(P,p)$ is the wave function in momentum space and $\frac{1}{\tilde{a}(P)} \equiv \int dX e^{-iPx} \frac{1}{\mu a(X)}$ is the Fourier transform of the inverse scattering length. By integrating both sides of Eq. (2) over $p$, we obtain an integral equation solved by $\tilde{\chi}(P) \equiv \int \frac{dp}{2\pi} \tilde{\psi}(P,p)$:

$$\tilde{\chi}(P) = \frac{1}{\sqrt{P^2 + \kappa^2}} \mu \int \frac{dP'}{2\pi} \frac{1}{\tilde{a}(P-P')} \tilde{\chi}(P'). \quad (3)$$

We note that when $a(X) = a > 0$ is uniform, there is a single bound state with binding energy $|E| = 1/(2\mu a^2)$.

Now for the linearly space-dependent scattering length $1/a(X) = 1/(c|X|)$, $1/\tilde{a}(P)$ is ill defined because of the divergence at $X = 0$. This divergence needs to be regularized, for example, by a sharp cutoff $1/a(X) = \theta(|X| - \epsilon)/(c|X|)$ or by a smooth cutoff $1/a(X) = \kappa$,

$$\frac{1}{\mu} \int \frac{dP'}{2\pi} \frac{1}{\tilde{a}(P-P')} \tilde{\chi}(P'). \quad \text{We note that when a(X) = a > 0 is uniform, there is a single bound state with binding energy |E| = 1/(2\mu a^2).}$$

Now for the linearly space-dependent scattering length $1/a(X) = 1/(c|X|)$, $1/\tilde{a}(P)$ is ill defined because of the divergence at $X = 0$. This divergence needs to be regularized, for example, by a sharp cutoff $1/a(X) = \theta(|X| - \epsilon)/(c|X|)$ or by a smooth cutoff $1/a(X) = \kappa$.
The upper (lower) sign corresponds to the even (odd) infinite tower of two-body bound states characterized by Eqs. (2)–(4), the density distribution of a particle with equal masses \( m_1 = m_2 \).

\[
1/(c\sqrt{X^2 + \epsilon^2}).
\]

In either case, the limit of an infinitesimal cutoff \( \epsilon \to 0 \) leads to \( 1/\tilde{a}(P) \to -(2/c) \ln(\epsilon|P|) \), for which the analytic solution to Eq. (3) is obtained as

\[
\tilde{\chi}_\pm(P) = N_\pm \frac{\sin[s_\pm \arcsinh(P/\kappa) + \pi(1 \pm 1)/4]}{\sqrt{(P/\kappa)^2 + 1}}. \tag{4}
\]

The upper (lower) sign corresponds to the even (odd) parity channel and \( |N_\pm|^2 = \frac{2\pi}{1 - \tanh(s_\pm)} \) is the normalization constant and \( s_\pm \) solves

\[
1 = \frac{1}{c} \sqrt{\frac{M}{\mu}} \tanh \frac{\pi s_+}{2} \quad \text{or} \quad 1 = \frac{1}{c} \sqrt{\frac{M}{\mu}} \tanh \frac{\pi s_-}{2}. \tag{5}
\]

Note that \( s_+ \) has a solution for any \( c > 0 \), while \( s_- \) has a solution only for \( 0 < c < \frac{\pi}{2} \sqrt{\frac{2}{\mu}} \). The latter range of \( c \) is assumed below unless otherwise stated.

Then the inverse Fourier transform of \( \tilde{\chi}_\pm(P) \) leads to the wave function with two particles at the same point: \( \chi_\pm(X) = \psi_\pm(X,0) \propto K_{s_\pm}(\kappa|X|) \). An important observation is that this wave function toward the origin \( X \to 0 \) oscillates as \( \psi_\pm(X,0) \to \cos(s_\pm \ln(\kappa|X|/2) - \arg \Gamma(i{s_\pm})) \).

This oscillation is fixed by the precise behavior of \( a(X) \) near \( X = 0 \), which is not universal and depends on experimental setups. However, what is universal is that because of the logarithmic periodicity in \( \kappa \), if \( \kappa = \kappa_\pm \) is a solution, then \( \kappa = e^{-n\pi/2} \kappa_{\pm} \) are all solutions. Therefore, in each parity channel, there exists an infinite tower of two-body bound states characterized by discrete scale invariance: \( E_{\pm}^{(n)} = -e^{-2n\pi/2}|\kappa_\pm|^2/(2M) \).

This is exactly the same physics as the Efimov effect, while the difference should be emphasized that our bound state consisting of two particles is trapped about the center of the system (see Fig. 1 below) and the scale factor \( \lambda_\pm \equiv e^{\pi/2} \) is tunable by the slope of the scattering length as seen in Eq. (4). We also note that the full scale invariance demonstrated by the classical Hamiltonian \( H \) with \( a(X) = c|X| \) is broken down to the discrete subset by the scale \( \kappa_\pm \) generated in quantum mechanics. This is known as a quantum anomaly.

With the use of the wave function obtained from Eqs. (2)–(4), the density distribution of a particle with mass \( m_1 \) and its momentum distribution \( \rho_{\pm}(p_1) \) are plotted in Figs. 1 and 2, respectively, for \( c = 0.5, 1, 1.5 \) with equal masses \( m_1 = m_2 \). In particular, the momentum distribution has an oscillatory large momentum tail \( \rho_{\pm}(p_1) \to \kappa^2 t_{\pm}(p_1) \) at \( |p_1|/\kappa \to \infty \) given by

\[
t_{\pm}(p_1) = \frac{|N_\pm|^2}{|p_1|^3} \left[ \frac{1}{2} \pm \frac{\Re \left\{ \frac{2\sqrt{2}}{|p_1|} \right\}}{2} \right] \times \frac{(1 - is_\pm) \cosh \frac{\pi s_\pm}{2} + s_\pm \sinh \frac{\pi s_\pm}{2}}{2 \cosh \frac{\pi s_\pm}{2}}. \tag{6}
\]

This logarithmic oscillation signals the discrete scale invariance and exactly the same tail emerges in any few-body and many-body states as we will show later. In contrast to the Efimov effect in which the oscillatory tail appears at the subleading order [3, 6], it appears at the leading order in our scaling trap. This will make its observation easier by a time-of-flight measurement in ultracold atom experiments.

**More than two particles**

A longstanding problem in Efimov physics is whether the discrete scale invariance demonstrated for three particles persists for larger numbers of particles [1, 3]. The scaling trap realizes a novel pattern of discrete scaling symmetry violation for bosons: Different particle sectors obey different scaling laws and incommensurable scalings among them result in the breakdown of discrete scale invariance.

This pattern can be explained easily in the limit \( c \ll 1 \) where the Born-Oppenheimer approximation is applicable. Recall that one-dimensional bosons form an \( N \)-body bound state with binding energy \(-N(N^2-1)/(6ma^2)\) [7]. For \( a = c|X| \), this binding energy acts as an effective potential for the center-of-mass motion of the \( N \)-body cluster. Accordingly, \( N \) bosons form an infinite tower of trapped states characterized by a discrete scaling symmetry set by a scale factor \( \lambda_N = e^{\pi s_N} \) with \( s_N = \sqrt{N^2(N^2-1)/(3c^2)} + \mathcal{O}(d^2) \). However, these \( N \)-body trapped states for \( N \geq 3 \) are actually unstable resonances coupled with a continuous spectrum. For example, when \( N = 3 \), there are continuum states composed of a free particle and two-body trapped state obeying a discrete scaling symmetry set by \( \lambda_2 \). Because dilatations with respect to \( \lambda_2 \approx e^{\pi c/2} \) and \( \lambda_3 \approx e^{\pi c/(2\sqrt{6})} \) are incom-
mensurate, the discrete scaling symmetry breaks down for three bosons and hence more.

Further insights into the nature of \( N \)-boson resonances can be obtained in the same limit \( c \ll 1 \). Because the local binding energy scales as \(-1/(c|\lambda X|)^2\), their relative wave function is localized within a separation \( \sim c|X|\). On the other hand, their center-of-mass wave function is \( \sim K_{inN}(\kappa_N|X|)\), which oscillates rapidly at \( \kappa_N|X| \ll 1 \) and decays exponentially at \( \kappa_N|X| \gg 1 \). This \( N \)-body cluster can decay into a deeper \( N' \)-body cluster with \( 2 \leq N' < N \) whose wave function also oscillates rapidly but with a different logarithmic period \( \pi/s_{N'} > \pi/s_N \). Because of the resulting small overlap between their wave functions, \( N \)-boson resonances are expected to have small decay widths and thus obey an approximate discrete scaling law set by \( \lambda_N \).

To confirm this consideration, we numerically computed \( N \)-boson resonance energies for \( N = 2, 3, 4 \). Here a Hamiltonian lattice formalism and iterative eigenvector methods were used in a semi-infinite system with a hard wall boundary at the origin. At \( c = 0.25 \), decay widths of resonances are indeed found to be negligible and associated behaviors of resonance energies are clearly seen in Fig. 3 Their scale factors are extracted as \( \lambda_2 \approx 1.482(2), \lambda_3 \approx 1.172(2), \) and \( \lambda_4 \approx 1.102(2)\), which are in good agreement with the Born-Oppenheimer approximation; 
\[
\lambda_N \approx e^{\pi c/\sqrt{2N(N^2-1)}}/N.
\]

In contrast to bosons, we did not observe any resonances in the spectrum of three fermions (two of one component and one of the other) with equal masses. This is indeed expected because two-component fermions with equal masses do not form any bound states with more than two fermions. Therefore, their discrete scaling symmetry cannot be violated by the pattern elucidated above.

On the other hand, there exists another pattern of discrete scaling symmetry violation which is common to bosons and fermions. For more than two particles, both of even and odd parity two-particle states contribute in general. Because they obey incommensurate scalings set by \( \lambda_+ \) and \( \lambda_- \), the discrete scaling symmetry breaks down. However, this pattern does not take place in the range \( c > \pi \) where only the even parity channel exhibits the discrete scale invariance [see Eq. (4)]. Here it is possible that an arbitrary number of fermions maintains the discrete scaling symmetry set by \( \lambda_+ \). Accordingly, we expect two-component fermions with equal masses to exhibit three phases with distinct symmetries as a function of the inverse slope; phases with full scale invariance at \( c^{-1} < 0 \), discrete scale invariance at \( 0 < c^{-1} < 1/\pi \), and no scale invariance at \( 1/\pi < c^{-1} \). Their many-body physics and phase transitions in between will be extremely interesting and to be explored in the future.

**Effective field theory**

The scaling trap can be formulated in the language of effective field theories. A local field theory to be considered is
\[
H = \int dx \left[ -\psi_1^\dagger \frac{\nabla^2}{2m} \psi_1(x) - \frac{1}{\mu c |x|} \psi_1^\dagger \psi_2^\dagger \psi_2 \right] + \frac{g}{\mu} \psi_1^\dagger \psi_2^\dagger \psi_2 \psi_1(0) + \frac{g}{\mu} \nabla [\psi_1^\dagger \psi_2^\dagger] \nabla [\psi_2 \psi_1](0),
\]
where \( i = 1, 2 \) is summed and the space argument \( x \) acts on all operators on its left. The first part describes particles interacting by the zero-range interaction with the linearly space-dependent scattering length. As we discussed above, such an interaction is singular at the origin and needs to be regularized by introducing a cutoff. The independence of physical quantities from the cutoff is ensured by counter-terms. According to the above argument of discrete scaling symmetry violation, \( N \)-body counter-terms, \( \psi_1^N \psi_2^N (0) \) and \( \nabla [\psi_1^N] \nabla [\psi_2^N](0) \), are needed for bosons with each \( N \geq 2 \). On the other hand, two counter-terms \( g_2^\Lambda \) are expected to be sufficient for an arbitrary number of two-component fermions with equal masses.

An expression for the cutoff-dependent coupling \( g_{\pm}^\Lambda \) is obtained in the same spirit of Ref. [8]: We employ a sharp momentum cutoff \( |P| < \Lambda \) and require that two-body physics becomes independent from the choice of \( \Lambda \). The two-body sector of our field theory is equivalent to the Schrödinger equation in Eq. (1) but with the interaction potential; \( V(X, x) = [-1/(|cX|)] + g_4 \delta(X) + g_5 \nabla X \delta(X)^2 \delta(x)/\mu. \) Accordingly, the integral equation in Eq. (3) is modified into that in which \( 1/\delta(P - P') \) is replaced by \( -(2/c) \ln(|P - P'|/\Lambda) - g_5 g_4 P P' \). Then we require that its solution \( \chi_{\pm}^\Lambda \) for \( |P| < \Lambda \) in Eq. (1) does not change when the cutoff is changed from \( \Lambda \) to \( \Lambda' \). This requirement is satisfied by choosing
\[
g_{+}^\Lambda(\Lambda) = \alpha_+ - \frac{2}{c} \cot[\phi_+^\Lambda(\Lambda)]/s_+,
\]
\[
\Lambda^2 g_{-}^\Lambda(\Lambda) = \alpha_- \frac{\sin[\phi_-^\Lambda(\Lambda)] + s_- \cos[\phi_-^\Lambda(\Lambda)]}{\sin[\phi_-^\Lambda(\Lambda)] - s_- \cos[\phi_-^\Lambda(\Lambda)]},
\]
where \( \phi_{\pm}^\Lambda(\Lambda) = s_\pm \ln(2\Lambda/|\kappa_\pm|) + \beta_\pm \). With numerical constants \( \alpha_{\pm} \) and \( \beta_{\pm} \), the analytic expression fits to a numerical solution accurately. An important observation is
that these couplings run in logarithmically periodic ways as functions of the cutoff. This is known as a renormalization group limit cycle and the Efimov effect is its rare manifestation in physics. Our scaling trap is newly added to a short list of systems demonstrating the limit cycle.

The field-theoretical formulation is useful to derive universal relationships valid in an arbitrary few-body and many-body state. An operator product expansion of \( \langle dx_1 e^{-ip_1 x_1^2} | \psi_1(X_1 - \frac{\kappa}{p} x_1) \psi_1(X_1 + \frac{\kappa}{p} x_1) \rangle \) at \( |p_1| \to \infty \) is dominated by two lowest local operators: \( \mathcal{O}_+(X_1) \equiv \psi_1^\dagger \psi_2^\dagger \psi_1 \) and \( \mathcal{O}_-(X_1) \equiv \nabla \psi_1^\dagger \nabla \psi_2 \psi_1(X_1) \). By matching their matrix elements with respect to two-particle trapped states with even and odd parities, a Wilson coefficient of the state under consideration changes with respect to \( \kappa \) defined so that when \( a|X| \to \pm \pi \delta(p_1) (p_1) \delta(X_1) \). Accordingly, the momentum distribution of a particle with mass \( m_1 \) exhibits the oscillatory large momentum tail: \( \rho(p_1) \to t_+(p_1) \mathcal{C}_+ + t_-(p_1) \mathcal{C}_- \) in any state of the scaling trap. The form of each term is fixed by \( \mathcal{C}_\pm \) obtained in Eq. (6) for equal masses, while its magnitude is set by a local contact density: \( \mathcal{C}_\pm \equiv -\frac{M}{2} \left( \partial_{\ln \kappa} \mathcal{O}_\pm (0) \right) \). By applying the Hellmann-Feynman theorem to the Hamiltonian, we find that \( \mathcal{C}_\pm \) measures how an energy of the state under consideration changes with respect to \( \kappa \): \( \kappa \partial E/\partial \kappa = -\mathcal{C}_\pm /M \).

**Scaling traps in two and three dimensions**

So far we have focused on physics in one dimension but our idea works equally in two and three dimensions. A two-body bound state problem in an arbitrary spatial dimension \( d \) reduces to solving an integral equation which is an analog of Eq. (3) in real space:

\[
\chi_d(X) = \int \frac{dX' dP}{(2\pi)^d} \frac{e^{iP(X-X')}}{\sqrt{2\pi} |P|^2 + \kappa^2} a(X')^{2-d}. \tag{9}
\]

Here \( \chi_d(X) \equiv \psi(X,0)/\ln|\Delta a(X)| \) and \( \chi_d(X) \equiv \lim_{|x| \to 0} \frac{\partial}{\partial |x|} |x| \psi(x,x) \). The scattering length \( a(X) \) is defined so that when \( a(X) = a > 0 \) is uniform, there is a single bound state with binding energy \( |E| = 1/(2ma^2) \). The emergence of a scaling trap for \( a(X) = c|X| \) is deduced by whether there exist solutions that oscillate as \( \chi_d(X) \to |X|^{1-d+is} \) toward the origin \( \kappa |X| \to 0 \). By substituting an ansatz \( \chi_d(X) \sim |X|^{1+is} e^{iQX} \) or \( \chi_3(X) \sim |X|^{-2+is} P(\cos \theta X) \) into Eq. (9) with \( \kappa \to 0 \), we find that \( s_\ell \) solves \( \frac{1}{2\pi} \sqrt{\frac{M}{p}} = \text{Re} \left[ \Gamma \left( \frac{s_\ell + is_\ell}{2} \right) / \Gamma \left( \frac{s_\ell + is_\ell}{2} \right) \right] \) in \( d = 2 \) or \( \frac{1}{2\pi} \sqrt{\frac{M}{p}} = \left| \Gamma \left( \frac{s_\ell + is_\ell}{2} \right) / \Gamma \left( \frac{s_\ell + is_\ell}{2} \right) \right| \) in \( d = 3 \). For each angular momentum \( \ell \) where \( s_\ell \) has a solution, there exists an infinite tower of two-body states characterized by discrete scale invariance: \( E_{\ell N}^{(n)} = -e^{-2\pi n \pi/4} \kappa^2 / (2M) \). We expect similar patterns of discrete scaling symmetry violation for more than two particles as elucidated in one dimension.

**Remarks on experimental realization**

In this Letter, we proposed scaling traps in which two particles form an infinite tower of trapped states characterized by discrete scale invariance. The key idea is to make the scattering length proportional to distance from the center of the system. Such space-dependent interactions can be realized in ultracold atom experiments by spatially varying a magnetic- or optical-field intensity or by varying transverse confinement lengths along a longitudinal direction.

If two particles correspond to different spin states of an fermionic atom, our two-body bound states with Efimov character are long-lived because three-body recombinations are strongly suppressed by the Pauli exclusion principle. Furthermore, a scale factor can be easily controlled by the slope of the scattering length. This will greatly facilitate an observation of the discrete scale invariance, for example, by a radio-frequency spectroscopy or a time-of-flight measurement. Therefore, the scaling trap overcomes common difficulties in ultracold atom experiments of Efimov physics arising from an instability of three-body bound states and their sizable scale factor \( \approx 22.7 \).

We also elucidated that the discrete scaling symmetry emergent for two particles is inevitably violated for three or more bosons by the appearance of resonance states while not for fermions. It is possible that insights developed here shed new light on Efimov physics. Our scaling trap thus serves as a tunable model system to investigate universal physics involving scale invariance, quantum anomaly, and renormalization group limit cycle, which are important in a broad range of quantum physics.

This work was supported by a LANL Oppenheimer Fellowship and the U.S. Department of Energy under contract No. DE-FG02-03ER41260.

[1] E. Braaten and H.-W. Hammer, Phys. Rept. 428, 259 (2006).
[2] V. Efimov, Phys. Lett. B 33, 563 (1970).
[3] R. Grimm, Phys. 3, 9 (2010).
[4] Y. Nishida and S. Tan, Few-Body Syst. 51, 191 (2011).
[5] Y. Castin and F. Werner, Phys. Rev. A 83, 063614 (2011).
[6] E. Braaten, D. Kang, and L. Platter, Phys. Rev. Lett. 106, 153005 (2011).
[7] M. Takahashi, Thermodynamics of One-Dimensional Solvable Models (Cambridge University Press, 1999).
[8] P. Bedaque, H.-W. Hammer, and U. van Kolck, Phys. Rev. Lett. 82, 463 (1999); Nucl. Phys. A 646, 444 (1999).
[9] Another universal relationship involving \( \mathcal{C}_\pm \) is \( \mathcal{O}_\pm (X) \to \sum_{p \in \mathbb{Z}} \frac{\sqrt{2}}{2\pi} f_{\pm}(\pi s_\ell p) \Gamma(is_\ell) \cos[s_\ell \ln(is_\ell X)/2] \), where \( f_{\pm}(\pi s_\ell p) \) is defined as \( f_{\pm} \left( \frac{\pi s_\ell p}{2} \right) \).
[10] D. S. Petrov, C. Salomon, and G. V. Shlyapnikov, Phys. Rev. Lett. 93, 090404 (2004); Phys. Rev. A 71, 012708 (2005).