Approaching universality in weakly-bound three-body systems

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Atom-dimer scattering below the three-body break-up threshold is studied for a system of three identical bosons. The atom-dimer scattering length and the energy of the most weakly-bound three-body state are shown to be strongly correlated. An appropriate rescaling of the observables reveals the subtlety of the correlation, and serves to identify universal trends in the unitary limit of divergent two-body scattering length. The correlation provides a new quantitative measure of the degree of universality in three-body systems with short-ranged interactions, as well as a consistency check of effective field theories and other theoretical models.

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Among the most striking results of recent experimentation with supercooled atomic gases is the demonstration that trap loss rates are extraordinarily sensitive to few-body interactions within a trapped many-body system. The experiments of many groups [1] show signatures of few-body correlations within a trapped ensemble of Bose alkali vapors at nano-Kelvin temperatures. This discovery has stimulated a large number of theoretical and experimental investigations, particularly in the unitarity limit of a divergent two-body scattering length, where the system has no natural length scale beyond that of the trapping potential.

It is widely anticipated that in the vicinity of unitarity, supercooled Bose gases display universal collective properties. However, criteria for the onset of universality and measures of the degree of universality have not yet emerged. The primary purpose of this Letter is to provide such a measure through a thorough investigation of atom-dimer scattering for a wide variety of two-body short-ranged potentials and the zero-range interaction model.

Weakly-bound few-body systems with relatively large two-body scattering lengths have long been studied in nuclear physics. A salient example is a result published by Phillips in 1968 [2] which puzzled nuclear theorists for more than a decade. Phillips compared results of calculations of the neutron-deuteron scattering length and the energy of the triton bound state made with different two-body potentials. He found that, unlike two-body scattering in which the energy of the last bound state scales as the inverse squared scattering length \( E \sim -1/a^2 \), the bound state energy of the triton \( n-n-p \) appears approximately proportional to the scattering length of the neutron-deuteron collision. The data illustrating this correlation is shown in Figure 1.

Many subsequent works [3] confirmed that a strong linear correlation between these two observables exists. Two decades later a simple and elegant explanation of the Phillips line was given by Efimov and Tkachenko [4], who simply noted that the apparent linearity derives from the fact that the two-body potentials used sample only a small portion of the space of scattering parameters; that is, they yield similar values for the neutron-deuteron scattering lengths.

While the origin of Phillips’ observation is now well understood, modern experiments with ultracold gases are able to sample a much wider range of scattering parameters by magnetic field tuning through a Fano-Feshbach resonance. This suggests that the correlation between two- and three-body parameters can be investigated in far greater detail than in earlier nuclear physics studies. Theoretical and experimental works related to universality in ultracold Bose gases have been concentrated on three-body recombination in the close vicinity of the three-body threshold. In this work we discuss the properties of the three-body system at the two-body threshold and below.

In this work we introduce a new parametrization of the relationship between the three-body (atom-dimer) scattering length and the energy of the last three-body bound state for the specific case of three identical Bosons. This relationship is referred to below as the modified Phillips line. In contrast to the original Phillips line, this relationship is found to be linear over a large range of interaction parameters and more directly reflects the well known threshold law for single-channel scattering, namely \( E \approx \frac{1}{a_{\text{min}}} \). It also provides a simple test for universality of three-body systems.

\begin{figure}
\centering
\includegraphics[width=0.5\textwidth]{Phillips_line}
\caption{The Phillips line, showing the unexpected linear correlation between the triton bound state energy and the neutron-deuteron scattering length (data from ref. [4]).}
\end{figure}
As pointed out by Efimov and Tkachenko [4], for a weakly-bound three-body state the following approximate correlation should hold

\[ E_2 - E_3 \approx \frac{1}{2m_{12}a_3^2} \]  

(1)

where \( E_2 \) is the dimer binding energy and \( m_{12} \) is the reduced mass of the particle-dimer system. A more transparent representation of the strength of the correlation is obtained by rewriting Eq. 1 in terms of the scaled dimensionless variables

\[ \alpha \equiv \frac{a_3\sqrt{-2m_{12}E_2}}{\omega} \]

\[ \omega \equiv 1/\sqrt{E_3/E_2 - 1} \]  

(2)

The variable \( \alpha \) can be thought of as a dimensionless scattering length, and \( \omega \) characterizes the three-body binding energy. If the three-body state nearest to the threshold is deeply bound, \( \omega \) is small; large values of \( \omega \) indicate the existence of a weakly-bound three-body state.

Using a recently developed three-body code, we have strenuously tested the well studied case of three bosonic \(^4\)He atoms [6], and so we will use the helium trimer as a first illustration of our improved parameterization. The traditional Phillips line for helium trimer states calculated with four commonly used two-body potentials is plotted in Figure 2a, where \( E_3 \) is the energy of the \( He_3 \) threshold bound state (relative to the three-body breakup threshold), and \( a_3 \) is the scattering length for a helium atom and a bound helium dimer. Figure 2a shows the modified Phillips line obtained using the suggested scaling with the dimer binding energy. Note that the scaling results in an improved fit.

Equation 1 derives from the fact that atom-dimer scattering is dominated by the pole of the \( t \)-matrix corresponding to the near-threshold state of the trimer. Generally speaking, we should expect the linear relation of

\[ E_2 - E_3 \approx \frac{1}{2m_{12}a_3^2} \]

(1)

The near-linearity over a wide range of \( \omega \) is apparent in the figure, though deviations can be seen, especially for small values of the 3-body scattering length, magnified in the inset of Figure 3, where the complexity of the correlation is revealed. An interesting aspect of the plot, which we had not anticipated, is the emergence of a universal behavior as the 3-body scattering length approaches zero.

To better understand the complex correlation revealed in Figure 3, we show in Figure 4 the same correlation plot using a single two-body potential (the Bargmann potential with the effective range \( r_0 = 1 \) a.u.), but with large variations of the two-body scattering length. We have also shown the three-body data generated by solving the regularized Skornyakov/Ter-Martirosyan equations (STM) [7, 8] corresponding to a zero-range interaction model.

We can identify two distinctive regimes: a universal regime and a strong coupling regime. In the strong coupling regime (characterized by relatively small two-body scattering length) the shape of the modified Phillips line depends on the potential (inset Fig. 5) and, typically,
forms an elongated half-loop above the universal curve. First, as the two-body scattering length increases, the points on the Phillips line move right along the correlation plot reaching a local maximum, and then turn left as they approach the universal regime.

In the universal regime, as the two-body scattering length increases, the points along the Phillips line move left along the universal curve. The shape of the universal correlation plot stems from the interplay of poles of the three-body \( t \)-matrix corresponding to the formation of near-threshold bound and virtual states.

We can distinguish three characteristic parts of the universal curve. The linear part at the right end corresponds to large positive particle-dimer scattering length and a very shallow three-body bound state. The diverging part at the left end of the correlation plot corresponds to large negative particle-dimer scattering length and indicates the formation of a near-threshold virtual state. With increasing two-body scattering length this virtual state turns into a bound state, and the corresponding point on the modified Phillips line jumps to the far end of the positive linear part of the universal curve. There is also a transitional nonlinear regime, when the scaled particle-dimer scattering length \( \alpha \) is small, and both poles contribute to the shape of the universal curve.

The most transparent interpretation for the shape of the universal part of the correlation plot can be obtained from a simple analysis of the spectrum of the Faddeev operator

\[
\hat{K}(E) = \hat{G}_2(E)V(\hat{P}^+ + \hat{P}^-),
\]

where \( \hat{G}_2(E) = (\hat{H}_0 + V - E)^{-1} \) is the Green’s function for the three-body cluster Hamiltonian, \( \hat{H}_0 \) is the Hamiltonian for three free particles, \( V \) is the two-body pairwise potential and \( \hat{P}^\pm \) are Jacobi coordinate transformation operators. The equation for the component of the scattering wave function then reads

\[
[1 + \hat{K}(E)] \Phi = -V(\hat{P}^+ + \hat{P}^-)\chi_0,
\]

where \( \chi_0 \) stands for the atom-dimer plane wave. The component of the bound state wave function satisfies the homogeneous equation

\[
[1 + \hat{K}(E)] \Phi = 0.
\]

The Faddeev operator \( \hat{K}(E) \) for short-range potentials has a discrete spectrum with eigenvalues \( \lambda_n(E) \). For \( E \leq E_2 \) the eigenvalues \( \lambda_n(E) \) are real.

At the two-body threshold \( E = E_2 \) the Faddeev operator can be approximated by a sum of projectors on the states corresponding to eigenvalues \( \lambda^+ \) and \( \lambda^- \) closest to \(-1\), and the particle-dimer scattering length can be expressed as

\[
a_3 = \frac{a^+}{1 + \lambda^+(E_2)} + \frac{a^-}{1 + \lambda^-(E_2)}.
\]

There are two possible situations: 1) one of the eigenvalues – \( \lambda^+(E_2) \) or \( \lambda^-(E_2) \) – is very close to the critical value \( \lambda = -1 \) and the corresponding term gives the major contribution to the particle-dimer scattering length; 2) both of the terms contribute substantially. The first case is responsible for the “linear” and “singular” parts of the \( \alpha(\omega) \) universal correlation plot. The second case corresponds to the intermediate regime of small scaled particle-dimer scattering length \( \alpha \).

This interpretation is illustrated in Fig. 5 where we show the particle-dimer scattering length (top) and the three-body operator spectrum (bottom) as a function of the two-body scattering length. The poles in the three-body scattering length correspond to the eigenvalue of the three-body operator crossing the critical value \( \lambda(E_2) = -1 \), where a new three-body bound state is formed.

The universal part of the modified Phillips line is reproduced by the simple formula

\[
\alpha = \frac{\alpha_1}{\omega - \omega_0} + \omega + \alpha_0
\]

with \( \alpha_1 = 5.5 \), \( \omega_0 = 0.419 \) and \( \alpha_0 = 4 \). The first term here is responsible for the description of the large negative scattering length regime, the other two terms fit the large positive scattering length regime. Equation 4 can be used in practical calculations to estimate the trimer binding energy from the scattering length. A simpler empirical fit \( \alpha = \omega + \omega^2 (1 - 1/\omega^2) \) is suitable for positive three-body scattering length.

Careful analysis of the modified Phillips line reveals that in the universal, potential-independent regime the

\[ FIG. 4. \text{The modified Phillips line for the Bargmann potential and the zero-range model. For the Bargmann potential the effective range is held fixed at 1 a.u., while the scattering length varies from 2 to 460 a.u. . The values of the two-body scattering length \( a_2 \) are shown along the curve.} \]
scattering length for the atom-dimer collision approaches zero when $E_3/E_2 \approx 2.54$. The other special point on the plot corresponds to divergent negative scattering length, which corresponds to the universal ratio $E_3/E_2 \approx 6.7$.

The result demonstrates a novel form of universality in weakly bound systems. Simple in physical nature, the modified Phillips line provides an important test for numerical and theoretical analysis of 3-body systems. It affords the opportunity to check bound-state and scattering results for consistency and classifies 3-body systems according to distinct dynamical regimes. It also provides an opportunity to check estimates of 3-body bound states and atom-dimer scattering lengths for internal consistency; such as those obtained with regularized zero-range potential models. Correlation plots similar to the modified Phillips line for bosons can be constructed for three-body systems with nontrivial spin-isospin structure and nonidentical particles. Here we shall only mention that the data shown in Figure 1 is consistent with the universal part of the modified Phillips line constructed on the base of the zero-range interaction model.

All the calculations presented here have been performed using an original code for solving Faddeev equations. The code is currently capable of three-body bound state and scattering calculations below the first excitation threshold. It provides users a simple interface for preparing configuration files and for constructing optimized grids automatically. The computational kernel solves the system of Faddeev equations for bound or scattering states. It uses a numerically effective computational scheme which – in combination with an option of using multiple CPUs – makes it possible to calculate scattering amplitudes quickly (from a few seconds to a few minutes, depending on the desired numerical accuracy and physical parameters of the system).

The code is available from the authors by request and will be available online in the near future.

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FIG. 5. Atom-dimer scattering length and the spectrum of the kernel of the Faddeev (a) or STM (b) equation at the two-body threshold as a function of the two-body scattering length. a) Bargmann potential with $r_0 = 1$ a.u., b) zero-range interaction model.