Revealing the origin of super-Efimov states in the hyperspherical formalism

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Recently a field-theoretic calculation predicted a new kind of universal three-body bound states for three identical fermions with p-wave resonant interactions in two dimensions [Phys. Rev. Lett. 110, 235301 (2013)]. These states were called “super-Efimov” states due to their binding energies $E_n = E_s e^{-2\pi n/s_0 + \theta}$ obeying a dramatic double exponential scaling. The scaling $s_0 = 4/3$ was found to be universal while $E_s$ and $\theta$ are the three-body parameters. Here we use the hyperspherical formalism and show that the super-Efimov states originate from an emergent effective potential $-1/4p^2 - (s_0^2 + 4)/\rho^2 \ln^2(\rho)$ at large hyperradius $\rho$. Moreover, for pairwise interparticle potentials with van der Waals tails, our numerical calculation indicates that the three-body parameters $E_s$ and $\theta$ are also universal and the ground super-Efimov state shall cross the threshold when the 2D p-wave scattering area is about $-42.0 l^2_{vdW}$ with $l_{vdW}$ the van der Waals length.

A landmark result of few-body physics is the Efimov bound states predicted theoretically in 1970 for three-body systems with s-wave resonant interactions in three dimensions [1]. The binding energy of the $n$th Efimov state scales as $E_n = E_s e^{-2\pi n/s_0}$ with $s_0$ a universal number and $E_s$ the three-body parameter [1][2]. This peculiar scaling is given rise to by an emergent effective potential of the form $-(s_0^2 + 4)/\rho^2$ in the hyperspherical formalism of the three-body problem at large hyperradius $\rho$. Only recently, extreme experimental controllability and versatility of ultra-cold atomic gases [3–6] provides a unique opportunity to detect evidences of the Efimov states for the very first time in atomic systems. Experimentalists succeeded in realizing s-wave resonant interactions in ultra-cold atomic gases by the technique of Feshbach resonance [7], and revealed the Efimov physics through measuring atom loss rate due to three-body recombinations [8–14], atom-dimer inelastic collisions [15–16] and radio-frequency spectroscopy [17–18]. Further studies showed that even the three-body parameter $E_s$, which determines the absolute energy levels of the Efimov states has a universal feature for different atomic species [10, 13, 25].

The quest for universal physics at resonances beyond the paradigm of the Efimov states brought about a recent quantum field theory calculation predicting that universal bound states exist for three identical fermions with p-wave resonant interactions in two dimensions [26]. These new states have angular momentum $\ell = \pm 1$ and are called “super-Efimov” due to the fascinating scaling of their binding energies $E_n = E_s e^{-2\pi n/s_0 + \theta}$ with $s_0 = 4/3$ a universal number, and $E_s$ and $\theta$ the three-body parameters. While the prediction of the super-Efimov states agrees with a recently proved theorem [27], understanding the origin of such universal states requests further investigation.

In this work, we use the hyperspherical formalism to study three identical fermions with p-wave resonant interactions in two dimensions. In the angular momentum $\ell = \pm 1$ channel, we show that the super-Efimov states are due to an emergent effective potential $U_{eff} \sim -1/4p^2 - (s_0^2 + 4)/\rho^2 \ln^2(\rho)$ in the large hyperradius $\rho$ limit. We extract $s_0$ from $U_{eff}$ calculated numerically at the first three p-wave resonances of three different kinds of model potentials; the extracted values of $s_0$ agree well with 4/3 as predicted by the field theory [26]. For pairwise interparticle potentials with a van der Waals tail, the numerically obtained binding energies of the lowest two super-Efimov states indicate that the three-body parameters $E_s$ and $\theta$ are also universal; the ground super-Efimov state is predicted to emerge at the threshold when the 2D scattering area is about $-42.0 l^2_{vdW}$ with $l_{vdW}$ the van de Waals length.

Hyperspherical formalism. — We consider three identical fermions with coordinates $r_1$, $r_2$ and $r_3$ interacting pairwisely through a central potential $V(r)$ of finite range $r_0$ in two dimensions. The potential is fine tuned such that it is at a p-wave resonance. We introduce the Jacobi coordinates $x_i = r_j - r_k$ and $y_i = 2(r_i - (r_j + r_k)/2)/\sqrt{3}$, where $\{i, j, k\}$ takes the values of $\{1, 2, 3\}$ cyclically. The hyperspherical radius is given by $\rho = \sqrt{x_1^2 + x_2^2}$, and the corresponding hyperspherical angles $\Omega_i = \{\alpha_i, \theta_{x_i}, \theta_{y_i}\}$ with $\alpha_i = \tan^{-1}(x_i/y_i)$. After separating out the center of mass part, we expand the wave-function of the system in terms of any set of hyperangles $\Omega_i$ as

$$\Psi = \sum_{\mu} \rho^{-3/2} f_{\mu}(\rho) \Phi_{\mu}(\rho, \Omega_i).$$

(1)
The angular part $\Phi_\mu(\rho, \Omega_i)$ is required to satisfy the eigenequation
\[
\hat{\Lambda}^2 + m^2 \rho^2 \sum_{j=1}^{3} V(\rho \sin \alpha_j) \Phi_\mu(\rho, \Omega_i) = \lambda_\mu(\rho) \Phi_\mu(\rho, \Omega_i),
\]
with $m$ the mass of each fermion. Here, the total angular momentum operator is given by
\[
\hat{\Lambda} = -\frac{\partial^2}{\partial \alpha_i^2} - 2 \cot(2\alpha_i) \frac{\partial}{\partial \alpha_i} + \frac{L_\alpha^2}{\sin^2 \alpha_i} + \frac{L_\beta^2}{\cos^2 \alpha_i}.
\]

Hereafter, we use units such that $\hbar = 1$ and $m = 1$ unless stated otherwise. Consequently, the hyperradial part satisfies the coupled equations of eigen-energy $E$ as
\[
\left[-\frac{d^2}{d\rho^2} - \frac{1}{4\rho^2} + U_\mu(\rho) - Q_{\mu\mu} - mE\right] f_\mu(\rho) = \sum_{\nu(\neq \mu)} \left[2P_{\mu\nu} \frac{d}{d\rho} + Q_{\mu\nu}\right] f_\nu(\rho),
\]
with $U_\mu(\rho) = [\lambda_\mu(\rho) + 1]/\rho^2$. The couplings $P_{\mu\nu} = \langle \Phi_\mu | \partial_{\rho} | \Phi_\nu \rangle$ and $Q_{\mu\nu} = \langle \Phi_\mu | \partial^2_{\rho} | \Phi_\nu \rangle$, with $\langle \ldots \rangle$ standing for the integration over the hyperangles, are expected to be negligible for $\mu \neq \nu$ in the large $\rho$ limit [28] as Eq. (2) becomes decoupled, the three-body problem is reduced to a one dimensional equation, and the eigenstates with $E \rightarrow 0^+$ shall be governed by the effective potential $U_{\text{eff}} = -1/4\rho^2 + U_0 - Q_{00}$ of the shallowest attractive channel $\mu = 0$ at large hyperradius [28].

We focus on the states with total angular momentum $|\ell| = |\ell_x, \ell_y| = 1$ for which the super-Efimov states were predicted [26]. We solve the Faddeev equations derived from Eq. (2) in the regime $r_0/\rho < 1$ [28], and find for the shallowest attractive channel
\[
\lambda_0(\rho) + 1 = -\frac{Y}{\ln(\rho/r_0)} + O\left(\frac{1}{\ln^2(\rho/r_0)}\right),
\]
where the dimensionless parameter $Y$ is given by
\[
Y = -1 - m \int_0^\infty dr \left[\frac{V(r) u_0^2(r)}{\lim_{r \to \infty} |r u_0(r)|^2}\right] dr
\]
with $u_0$ the zero energy $p$-wave two-body wave-function satisfying $[-\partial^2/(1/r) \partial_r + 1/r^2 + mV(r)] u_0(r) = 0$. An alternative expression is
\[
Y = \int_0^\infty \frac{dr \left[|\partial_r u_0(r)|^2 \right]}{\lim_{r \to \infty} |r u_0(r)|^2},
\]
which shows $Y$ positive definite. Note that a similar logarithmic structure also appears in the scattering $T$-matrix in two dimensions [32].

Effective potential.— In the regime $r_0/\rho \ll 1$, if $Q_{00}$ can be neglected, $U_{\text{eff}} + 1/4\rho^2 \sim -Y/\rho^2 \ln(\rho/r_0)$ would give rise to shallow bound states whose energies $E_n$, scale as $\ln |E_n| \sim -(n\pi)^2/2Y$. Surprisingly Ref. [30] argued that $Q_{00} \sim -Y/\rho^2 \ln(\rho/r_0)$; the leading orders of $U_0$ and $Q_{00}$ shall cancel. This cancellation would result in $U_{\text{eff}} + 1/4\rho^2 = U_0 - Q_{00} \sim 1/\rho^2 \ln^2(\rho/r_0)$ in which case super-Efimov states become possible.

The involved hyperangle integral of $Q_{00}$ seems to preclude evaluating it analytically to order $1/\rho^2 \ln^2(\rho/r_0)$. Hence we obtain $U_{\text{eff}}$ by calculating $U_0$ and $Q_{00}$ numerically with three kinds of model potentials: the Leonard-Jones (LJ), Gaussian (GS), Pöschl-Teller (PT).

The red solid lines are for the first $p$-wave resonances of the three potentials, and the blue ones for the second, and the green ones for the third. The dashed line is $\rho^2 U_{\text{eff}} + 1/4 = -[(4/3)^2 + 1/4]/\ln^2(\rho/r_0)$. The model potentials are all tuned at a shallow resonance. We solve Eq. (2) by using the modified Smith-Whitten coordinates, which have been successfully applied to three-body systems in both three dimensions [33–37] and two dimensions [38, 39]. The details of constructing the Smith-Whitten coordinates and the corresponding hyperspherical representation can be found in Refs. [38] and [40].

Figure (1) shows the resultant numerical results of $U_{\text{eff}}$ at the first three $p$-wave resonances of the three model potentials, which all converge to a universal form $-1/4\rho^2 - [(4/3)^2 + 1/4]/\rho^2 \ln^2(\rho/r_0)$ when $\rho/r_0$ is large. We fit the data of $\rho^2 U_{\text{eff}} + 1/4$ by the series $-\sum_{n=2}^4 c_n \ln^{-n}(\rho/r_0)$ in the range $\rho/r_0 \in [30, 500]$. We define $s_0^2 \equiv c_2 - 1/4$. Likewise Tab. (1) shows that all fitted values of $s_0$ agree with $4/3$ within $\sim 4\%$. Similarly we fit the data for
\(\rho^2 U_0\) and \(\rho^2 Q_{00}\) separately by \(-\sum_{n=1}^{3} c_n \ln^{-n}(\rho/r_0)\) in the same range. As shown in Tab. 1, fitted \(c_1\) of both \(U_0\) and \(Q_{00}\) and \(Y\) calculated by the analytic result Eq. (6) show good agreement within \(\sim 6\%\), the difference between which nevertheless quantifies the overall error of our numerical data and the fitting scheme.

Our calculation indicates that when \(\rho/r_0\) is large, the three-body system is subject to an emergent effective potential

\[
U_{\text{eff}}(\rho) = -\frac{1}{4\rho^2} - \frac{s_0^2 + 1/4}{\rho^2 \ln^{-2}(\rho/r_0)}.
\]

Given such a potential, one can use the WKB approximation (or other methods) to show that the binding energies of shallow bound states have the super-Efimov form \(E_n = E_\ast \exp(-2\rho/n_s + \theta)\). Our numerical results of \(s_0\) agrees well with the universal scaling factor 4/3 predicted by Ref. [20]. Thus we show that the universal super-Efimov states originate from the universal effective potential Eq. (3).

### Three-body parameters

In the case of Efimov states, the three-body parameter \(\tilde{E}_\ast\) is originally believed to be not universal and to be determined by short-range interaction details [2]. Surprisingly recent experiments of ultracold atomic gases found \(\tilde{E}_\ast\) rather universal (in van der Waals units) [21]. Subsequent theoretical calculations [21, 24-25] inspired by this new discovery soon confirmed that when the long range tail of the two-body interaction is dominated by the van der Waals form \(V(\rho) \rightarrow -C_6/\rho^6\), \(\tilde{E}_\ast\) is universally determined by the van der Waals length \(\ell_{vdW} \equiv (m C_6)^{1/4}/2\) or equivalently the van der Waals energy \(E_{vdW} \equiv -1/m\ell_{vdW}^2\). It is natural to ask the question: whether the three-body parameters for super-Efimov states \(E_\ast\) and \(\theta\) are also universal, if the two-body interaction has the long-range tail \(-C_6/\rho^6\)?

We use two-body model potentials \(V_k^\ast(r) = -C_6/r^6 [1 - (\beta_n/r)^k]\) to study the three-body parameters numerically. The short-range parameter \(\beta_n\) is tuned such that there are \(n\) \(p\)-wave two-body bound states including the shallowest one at threshold. These two-body model potentials have the same long-range van der Waals tail, but very different short-range interactions determined by \(\beta_n\) and \(k\). The first evidence of universality is the effective potential \(U_{\text{eff}}\) at short range as shown in Fig. 2, where a universal repulsive core rises up at about \(\rho \approx 2.2\ell_{vdW}\); it seems that the short range details of these different two-body model potentials have little effect on those of the three-body effective potential \(U_{\text{eff}}\).

Applying the numerical treatment similar to Ref. [37], we obtain the three-body super-Efimov ground state energies \(E_g\) for different \(V_k^\ast(r)\) which are shown to be quite universal in Fig. 3. Interestingly, the values of \(E_g \approx -0.05 E_{vdW}\) is close to the universal Efimov ground state energies [21]. In addition, we extrapolate \(U_{\text{eff}}\) to very large distances and calculate the energies \(E_{g,1}^{\text{ad}}\) and \(E_{g,1}^{\text{vd}}\) of both the ground and the first excited super-Efimov states for \(V_k^\ast(r)\) within the adiabatic hyperspherical approximation (neglecting \(P_0\) and \(Q_{00}\) for \(\nu \neq 0\)). Table [IV] shows that while the ground state energies \(E_{g,1}^{\text{ad}}\) have good agreement with the full calculations \(E_g\), the first excited state energies \(E_{g,1}^{\text{vd}}\) have extremely small values (of order \(10^{-14} E_{vdW}\)), implying that a full calculation will be extremely challenging. Nevertheless, from \(E_{g,1}^{\text{ad}}\) and \(E_{g,1}^{\text{vd}}\), the three-body parameters \(\theta\) and \(\xi [\equiv \ln(\tilde{E}_\ast/E_{vdW})]\) are shown in the inset of Fig. 3 to be very universal, if we express the super-Efimov energies as \(E/E_{vdW} = \exp[-2\exp(4\pi r/3 + \theta) + \xi]\). We attribute the universality of \(\theta\) and \(\xi\) to the same mechanism as in Efimov states that the three-body wave functions of super-Efimov states have so small amplitude at small \(\rho(\lesssim \ell_{vdW})\) that other than the van de Waals tail of \(V(r)\), short distance details of interactions have negligible effect [21].
-4.651 \times 10^{-2}  -4.254 \times 10^{-2}  -0.969 \times 10^{-14}  -1.496  -2.709
-4.415 \times 10^{-2}  -4.429 \times 10^{-2}  -1.232 \times 10^{-14}  -1.502  -2.672
-3.941 \times 10^{-2}  -4.785 \times 10^{-2}  -1.995 \times 10^{-14}  -1.517  -2.601

old, we find that the crossing point $A$ three-body continuum. Extrapolating $p$ to approximately $-5.0$, the error bars of $E_g$ for $n = 2, 3$ quantify the finite lifetime of the state due to its decaying into atom-dimer states.

**Threshold crossing.**— In ultra-cold atomic gases, the three-body recombination resonances observed experimentally in the vicinity of Feshbach resonances occur where Efimov state energies cross the three-body continuum threshold, and serve as first evidences of Efimov physics [8–14, 19]. Here we tune the depth of the Lenard-Jones two-body model potential around the $n$th $p$-wave resonance, and calculate the ground super-Efimov state energy $E_g$ as a function of 2D $p$-wave scattering area $A$. For small scattering wave vector $q$, the 2D $p$-wave scattering phase shift $\delta(q)$ is given by $\cot \delta(q) = -1/Aq^2$. Figure 4 shows that when $A$ is tuned to large and negative values, $E_g$ becomes shallower and eventually hit the three-body continuum. Extrapolating $E_g$ to the threshold, we find that the crossing point $A_g^{(-)}$ is at $-45.9_{\text{vdW}}^2$, $-42.1_{\text{vdW}}^2$, and $-42.0_{\text{vdW}}^2$ near the 1st, 2nd, and 3rd $p$-wave resonance respectively. The magnitude of $A_g^{(-)}$ complies with the linear dimension of the ground super-Efimov state at resonance. The convergence of $A_g^{(-)}$ to approximately $-42.0_{\text{vdW}}^2$ is reminiscent of the Efimov physics in which the three-body parameters becomes more universal for two-body potentials that can support more bound states [21]. Recent successful realization of “quasi” 2D Fermi gases [42, 44] opens up the prospect of experimental study of the super-Efimov physics in atomic gases. It will be worth examining how the super-Efimov physics would be affected by the strong confinement applied to produce the “quasi” 2D gases in future investigations.

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[1] V. Efimov, Phys. Lett. B 33 563 (1970); Yad. Fiz. 12, 1080 (1970) [Sov. J. Nucl. Phys. 12, 589 (1971)]; Nucl. Phys. A 210, 157 (1973).
[2] E. Braaten, and H.-W. Hammer, Phys. Rep. 428, 259 (2006).
[3] D. S. Petrov, arXiv:1206.5752
[4] I. Bloch, J. Dalibard, and W. Zwerger, Rev. Mod. Phys. 80, 885 (2008).
[5] M. Saffman, T. G. Walker and K. Mølmer, Rev. Mod. Phys. 82, 2313 (2010).
[6] J. Dalibard, F. Gerbier, and G. Juzeliunas, and P. Öhberg, Rev. Mod. Phys. 83, 1523 (2011).
[7] C. Chin, R. Grimm, P. Julienne, and E. Tiesinga, Rev. Mod. Phys. 82, 1225 (2010).
[8] T. Kraemer, M. Mark, P. Waldburger, J.G. Danzl, C. Chin, B. Engeser, A.D. Lange, K. Pilch, A. Jaakkola,
H.-C. Nägerl and R. Grimm, Nature **440**, 315 (2006).
[9] T. B. Ottenstein, T. Lompe, M. Kohnen, A.N. Wenz, and S. Jochim, Phys. Rev. Lett. **101**, 203202 (2008).
[10] S. E. Pollack, D. Dries, and R.G. Hulet, Science **326**, 1683 (2009).
[11] N. Gross, Z. Shotan, S. Kokkelmans, and L. Khaykovich, Phys. Rev. Lett. **103**, 163202 (2009).
[12] J. H. Huckans, J. R. Williams, E. L. Hazlett, R. W. Stites, and K. M. O’Hara, Phys. Rev. Lett. **102**, 165302 (2009).
[13] J. R. Williams, E. L. Hazlett, J. H. Huckans, R. W. Stites, Y. Zhang, and K. M. O’Hara, Phys. Rev. Lett. **103**, 130404 (2009).
[14] R. J. Wild, P. Makotyn, J. M. Pino, E. A. Cornell, and D. S. Jin, Phys. Rev. Lett. **108**, 145305 (2012).
[15] S. Knoop, F. Ferlaino, M. Mark, M. Berninger, H. Schöbel, H.-C. Nägerl, R. Grimm, Nature Phys. **5**, 227 (2009).
[16] T. Lompe, T. B. Ottenstein, F. Serwane, K. Viering, A. N. Wenz, G. Zürn, S. Jochim, Phys. Rev. Lett. **105**, 103201 (2010).
[17] T. Lompe, T. B. Ottenstein, F. Serwane, A. N. Wenz, G. Zürn, S. Jochim, Science **330**, 940 (2010).
[18] S. Nakajima, M. Horikoshi, T. Mukaiyama, P. Naidon, and M. Ueda, Phys. Rev. Lett. **106**, 143201 (2011).
[19] N. Gross, Z. Shotan, S. Kokkelmans, and L. Khaykovich, Phys. Rev. Lett. **105**, 103203 (2010).
[20] M Berninger, A Zenesini, B. Huang, W. Harm, H.-C. Nägerl, F. Ferlaino, R. Grimm, Phys. Rev. Lett. **107**, 120401 (2011).
[21] J. Wang, J. P. D’Incao, B.D. Esry, and C. H. Greene, Phys. Rev. Lett. **108**, 263001 (2012).
[22] Y. Wang, J. Wang, J. P. D’Incao, and C.H. Greene, Phys. Rev. Lett. **109**, 243201 (2012).
[23] C. Chin, arXiv:1111.1484
[24] R. Schmidt, S. P. Rath, and W. Zwerger, Eur. Phys. J. B **85**, 886 (2012).
[25] P. Naidon, S. Endo, and M. Ueda, Phys. Rev. Lett. **112**, 105301 (2014).
[26] Y. Nishida, S. Moroz, and D. T. Son, Phys. Rev. Lett. **110**, 235301 (2013).
[27] D. K. Gridnev, J. Phys. A **47**, 505204 (2014).
[28] E. Nielsen, D. V. Fedorov, A. S. Jensen, and E. Garrido, Phys. Rep. **347**, 373 (2001).
[29] For the Leonard-Jones, Gaussian, and Pöschl-Teller two-body model potentials, we find numerically $P_\nu \sim 1/\rho \ln^2(\rho)$ and $Q_\nu \sim 1/\rho^2 \ln^2(\rho)$ for $\nu \neq 0$ when $\rho$ is large; the effect of these channel couplings shall be equivalent to introduce corrections $\sim 1/\rho^2 \ln^2(\rho)$ to $U_{\text{eff}}$, which thus is negligible.
[30] A.G. Volosniev, D. V. Fedorov, A. S. Jensen and N. T. Zinner, J. Phys. B **47**, 185302 (2014).
[31] Y. Castin, private communication.
[32] J. Levinsen, N. R. Cooper, and V. Gurarie, Phys. Rev. A **78**, 063616 (2008).
[33] B. R. Johnson, J. Chem. Phys. **73**, 5051 (1980).
[34] B. Lepetit, Z. Peng, A. Kuppermann, Chem. Phys. Lett. **166**, 572 (1990).
[35] C. D. Lin, Phys. Rep. **257**, 1 (1995).
[36] H. Suno and B. D. Esry, Phys. Rev. A **78**, 062701 (2008).
[37] J. Wang, J. P. D’Incao and C. H. Greene Phys. Rev. A **84**, 052721 (2011).
[38] J. P. D’Incao and B. D. Esry, Phys. Rev. A **90**, 042707 (2014).
[39] J. P. D’Incao, F. Anis, and B. D. Esry, arXiv: 1411.2321.
[40] J. Wang, J. P. D’Incao, Y. Wang and C. H. Greene, Phys. Rev. A **86**, 062511 (2012).
[41] C. M. Bender and S. A Orszag, *Advanced Mathematical Methods for Scientists and Engineers*, (McGraw-Hill Book Company, 1978).
[42] K. Martyianov, V. Makhalov, and A. Turlapov, Phys. Rev. Lett. **105**, 030404 (2010).
[43] P. Dyke, E. D. Kuhnle, S. Whitlock, H. Hu, M. Mark, S. Hoinka, M. Lingham, P. Hannaford, C.J. Vale, Phys. Rev. Lett. **106**, 105304 (2011).
[44] B. Fröhlich, M. Feld, E. Vogt, M. Koschorreck, W. Zwerger, and M. Köhl, Phys. Rev. Lett. **106**, 105301 (2011).