Effective field theory for atomic ^{4}He clusters (and matter)

Lucas Madeira [1]
European Centre for Theoretical Studies in Nuclear Physics and Related Areas (ECT*)
Trento Institute for Fundamental Physics and Applications (TIFPA)

Pan-American Few-Body Physics Boot Camp: Fostering Collaboration

Projects: IsCc7_EFTANS and INF25_monstre

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1 lmadeira@ectstar.eu

Francesco Pederiva
University of Trento, TIFPA-INFN

Bira van Kolck
University of Arizona, Institut de Physique Nucléaire d'Orsay, ECT*

Objective

- To investigate the ground-state properties of ^{4}He clusters and matter using an Effective Field Theory (EFT) approach

- Work in progress!

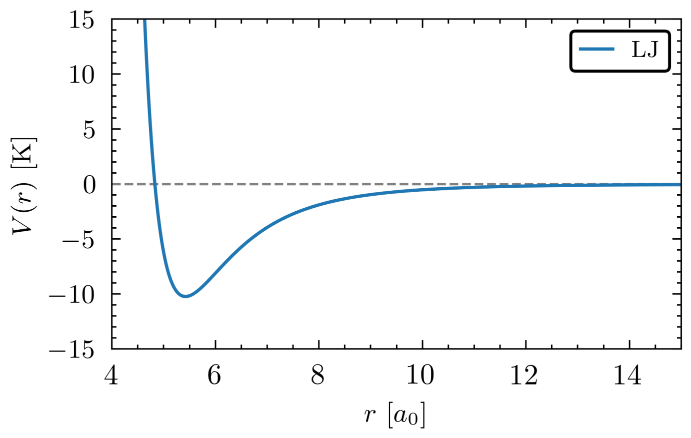
- ^{4}He –^{4}He interatomic potentials
- Two-body low-energy scattering
- ^{4}He beyond atomic physics
- ^{4}He: from $N = 3$ to $N \to \infty$
- This work

Lennard-Jones

- Lennard-Jones potential

$$\boxed{V(r) = 4\varepsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right]}$$

- Number of parameters: **2**
  - $\sigma = 2.556\,\text{Å}$
  - $\varepsilon / k_B = 10.22\,\text{K}$



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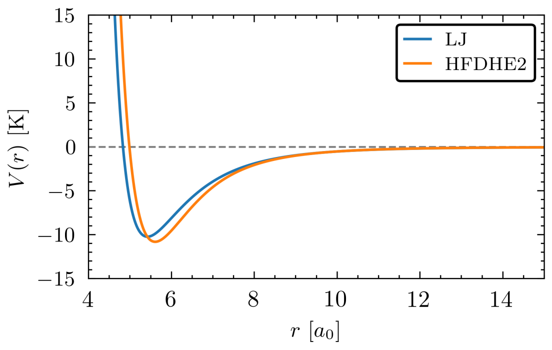
Aziz, Nain, Carley, Taylor, and McConville. An accurate intermolecular potential for helium. *J. Chem. Phys.*, 1979

HFDHE2

- Lennard-Jones potential
  - r^{-12}: represents poorly the Pauli repulsion
  - r^{-6}: misses higher-order multipolar contributions
- HFDHE2 (Hartree-Fock Dispersion, HElium, 2nd generation):

$$\boxed{V(r) = \varepsilon\left[Ae^{-\alpha x} - F(x)\sum_{n=3}^{5}\frac{C_{2n}}{x^{2n}}\right]}$$

- $x = r/r_m$
- $F(x)$ has one parameter
- “Simple” and “realistic” potential
- Number of parameters: **8**



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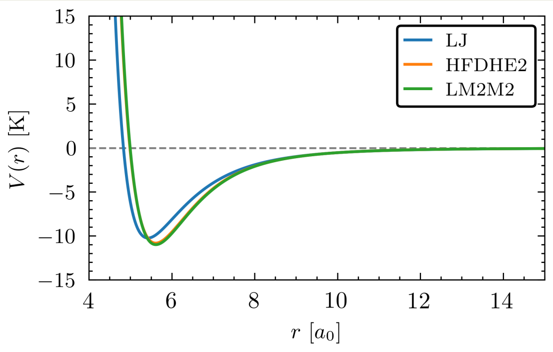
LM2M2

- LM2M2 (Liu and McLean 2, Mimic 2):

$$\boxed{V(r) = \varepsilon \left[A e^{-\alpha x + \beta x^2} - F(x) \sum_{n=3}^{5} \frac{C_{2n}}{x^{2n}} \right]}$$

- $x = r/r_m$
- $F(x)$ has one parameter
- Improvement on HFDHE2
- Number of parameters: **9**



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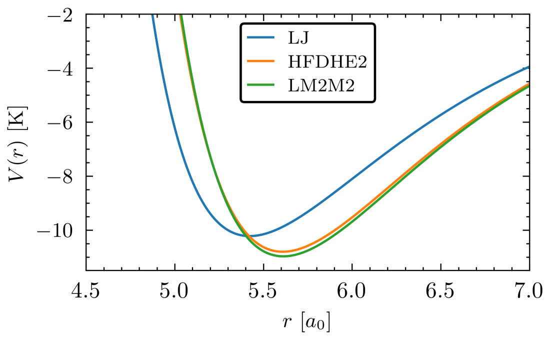

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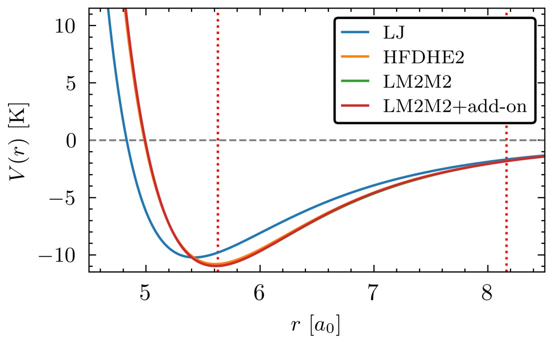
LM2M2 + add-on

- LM2M2 + add-on:

$$V(r) = V_{\mathrm{LM2M2}}(r) + \varepsilon V_a(r)$$

$$V_a(r) = \begin{cases} A_a \left\{ \sin\left[\frac{2\pi(x-x_1)}{x_2-x_1} - \frac{\pi}{2}\right] + 1 \right\}, & x_1 \leqslant x \leqslant x_2 \\ 0, & \text{otherwise} \end{cases}$$



- Improvement on LM2M2
- Number of parameters: **9+3=12**

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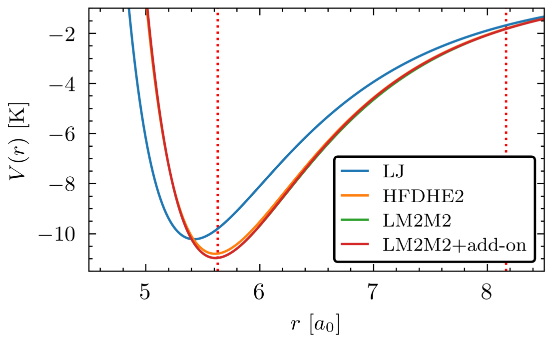

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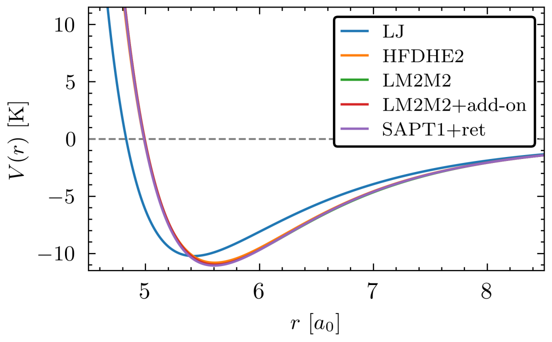
SAPT1

- Symmetry-Adapted Perturbation Theory (SAPT):

$$\boxed{V(r) = Ae^{-\alpha r+\beta r^2} + \sum_{n=3}^{8} f_{2n}(r,b)\frac{C_{2n}}{r^{2n}}}$$

$$f_{2n}(r,b) = 1 - \left(\sum_{k=0}^{2n} \frac{(br)^k}{k!}\right)\exp(-br)$$

- Number of parameters: **10**
- Retardation effects → introduce a function of r multiplying C_6/r^6 → **+30** parameters



Korona, Williams, Bukowski, Jeziorski, and Szalewicz. Helium dimer potential from symmetry-adapted perturbation theory calculations using large Gaussian geminal and orbital basis sets. *J. Chem. Phys.*, 1997.

Janzen and Aziz. An accurate potential energy curve for helium based on ab initio calculations. *J. Chem. Phys.*, 1997.

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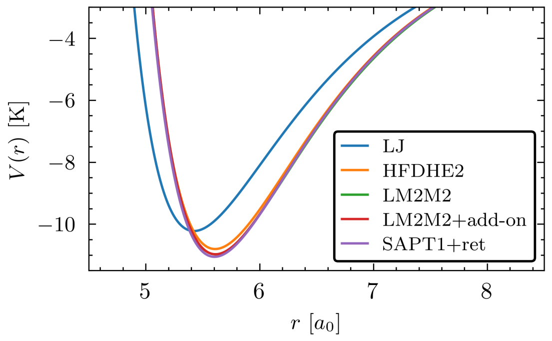

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What kind of ^{4}He am I having today?

- What makes helium ...well...helium?
- We want a simple model that can explain the key features of ^{4}He
- Goal: ground-state properties of ^{4}He clusters and bulk matter
- Let us start at the beginning: the helium dimer
    - Low-energy scattering theory works remarkably well!

- ^{4}He –^{4}He interatomic potentials
- Two-body low-energy scattering
- ^{4}He beyond atomic physics
- ^{4}He: from $N = 3$ to $N \to \infty$
- This work

Two-body scattering: the effective range expansion

- The s-wave scattering length and effective range are related to the low-energy phase shift $\delta_0(k)$ through:

$$\boxed{k \cot \delta_0(k) = -\frac{1}{a} + \frac{r_0 k^2}{2} + \mathcal{O}(k^4)}$$

- The two-body s-wave scattering amplitude is given by

$$f(k) = \frac{1}{k \cot \delta_0 - ik}$$

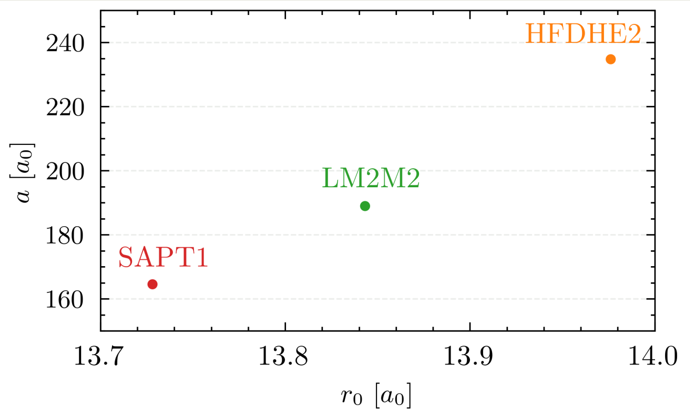
- From the pole of the s-wave scattering amplitude:

$$\boxed{E_2 = -\frac{\hbar^2}{2m_r a^2} \quad \text{(zero-range)}} \qquad \text{or} \qquad \boxed{E_2 = -\frac{\hbar^2}{2m_r r_0^2}\left(1 - \sqrt{1 - \frac{2r_0}{a}}\right)^2 \quad \text{(finite-range)}}$$

Bethe. Theory of the Effective Range in Nuclear Scattering. *Phys. Rev.*, 1949.
Macêdo-Lima and **Madeira**. Scattering length and effective range of microscopic two-body potentials. *RBEF*, 2023.

^{4}He dimer: scattering length and effective range

- LJ with the parameters presented before: not even bound! ($a \sim -300\, a_0$)
- Similar effective ranges
- Scattering lengths differ, but $\boxed{a \gg r_0}$



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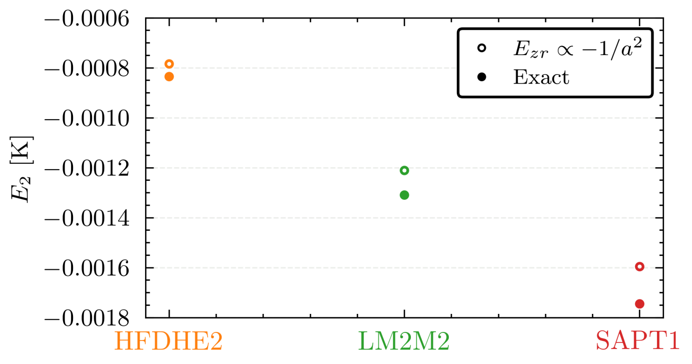
Janzen and Aziz. An accurate potential energy curve for helium based on ab initio calculations. *J. Chem. Phys.*, 1997.

Kievsky, Garrido, Romero-Redondo, and Barletta. The Helium Trimer with Soft-Core Potentials. *Few-Body Syst.*, 2011.

^{4}He dimer: binding energy (zero range)

- Zero-range approximation:

$$\boxed{E_{zr} = -\frac{\hbar^2}{2m_r a^2}}$$



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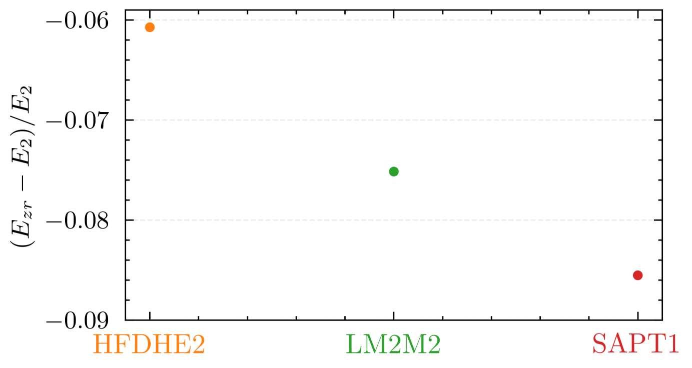
^{4}He dimer: binding energy (zero range)

- Zero-range approximation:

$$\boxed{E_{zr} = -\frac{\hbar^2}{2m_r a^2}}$$

- Less than 10% error!



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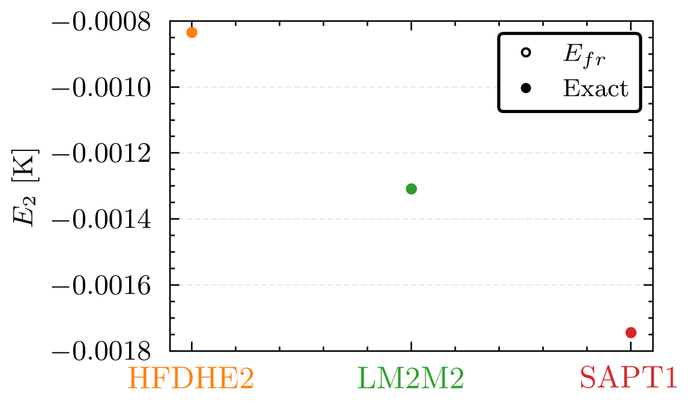
^{4}He dimer: binding energy (finite range)

- Finite-range approximation:

$$\boxed{E_{fr} = -\frac{\hbar^2}{2m_r r_0^2}\left(1 - \sqrt{1 - \frac{2r_0}{a}}\right)^2}$$

- Low-energy scattering theory
  - Less than 10% error if we use only the scattering length
  - Excellent results if we include range corrections
- **The agreement is independent of the potential we choose**



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- ^{4}He –^{4}He interatomic potentials
- Two-body low-energy scattering
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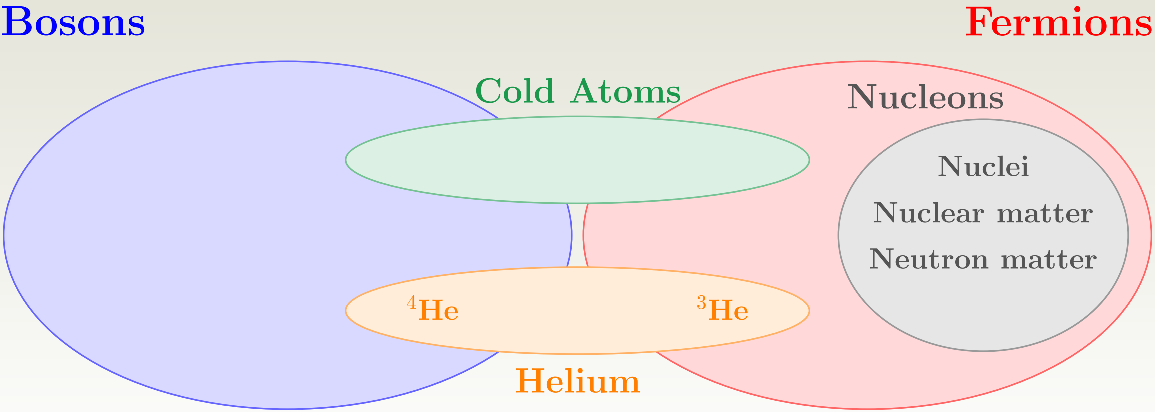
- ^{4}He: from $N = 3$ to $N \to \infty$
- This work

Themes of this workshop

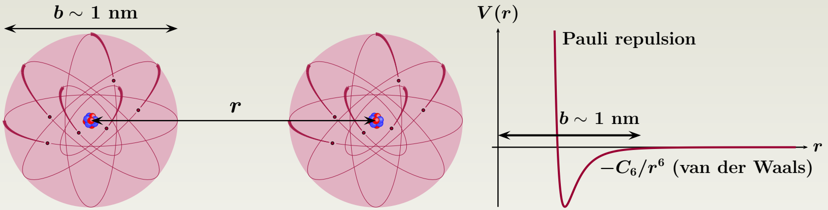
- How to connect this broad range of systems?



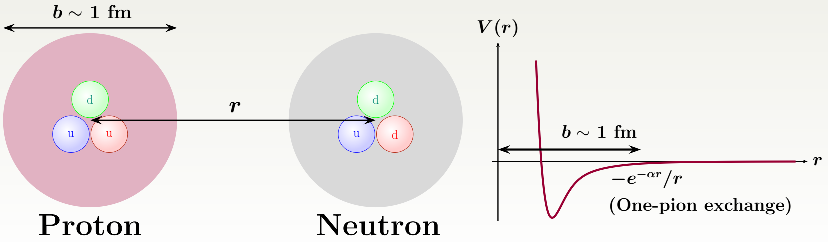
Physical systems

Universality is not apparent in these systems!

- Atomic physics
- Electromagnetic force



- Nuclear physics
- Residual strong force



Two-body scattering: zero-range *vs* physical systems

$$k \cot \delta_0(k) = -\frac{1}{a} + \mathcal{O}(k^2)$$

- From the pole of the *s*-wave scattering amplitude:

$$\boxed{E_{zr} = -\frac{\hbar^2}{2m_r a^2} \quad \text{(zero-range)}}$$

- This can be compared with physical systems:

$$\boxed{E_B = -\frac{\hbar^2}{2m_r a_B^2}}$$

Bethe. Theory of the Effective Range in Nuclear Scattering. *Phys. Rev.*, 1949.
Kievsky, Gattobigio, Girlanda, and Viviani. Efimov Physics and Connections to Nuclear Physics. *Annu. Rev. Nucl. Part. Sci.*, 2021.
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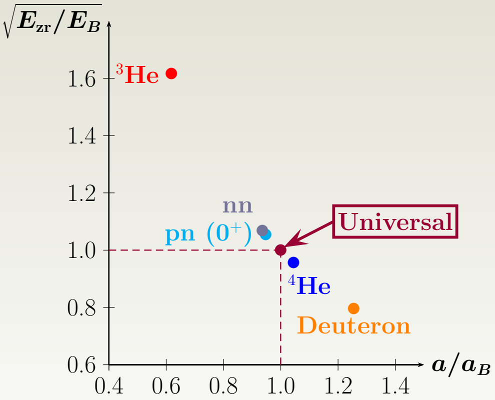
Zero-range universality

- He: HFDHE2
- Nucleon-nucleon: AV18

System	a	a_B
Atomic Physics (nm)		
^{4}He dimer	9.04	8.65
^{3}He dimer	−0.70	−1.13
Nuclear Physics (fm)		
deuteron [p-n (1^+)]	5.42	4.32
proton-neutron (0^+)	−23.74	−25.05
neutron-neutron (0^+)	−18.90	−20.19



Gutiérrez, de Llano, and Stwalley. Accurate direct determination of effective-range expansion parameters for several central potentials. *PRB*, 1984.

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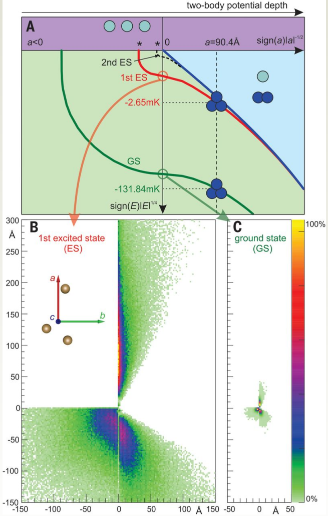
^{4}He trimer and Efimov physics

- **Efimov trimer**
  - Predicted by Efimov for three identical bosons with large two-body scattering lengths
  - Requires resonant (or near-resonant) s-wave interactions and short-range forces
  - Characterized by discrete scale invariance and a universal three-body parameter
  - Exhibits a geometric spectrum: $E^{(n)} \propto E^{(0)} e^{-2\pi n/|s_0|}$
- **Helium trimer**
  - First real-world realization of an Efimov state in a naturally occurring system



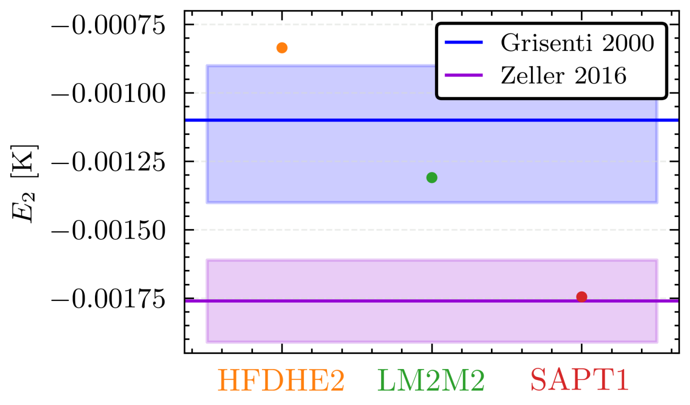
Efimov. Energy levels arising from resonant two-body forces in a three-body system. *Phys. Lett. B*, 1970

Efimov. Weakly-bound states of 3 resonantly-interacting particles. *Sov. J. Nucl. Phys.*, 1971

Kunitski, Zeller, Voigtsberger, Kalinin, Schmidt, Schoffler, Czasch, Schollkopf, Grisenti, Jahnke, Blume, and Dorner. Observation of the Efimov state of the helium trimer. *Science*, 2015

Experimental measurements

- Binding energy
  - Dimer
  - Trimer excited state: 2.6(2) mK
- Equation of state (of the bulk)
  - Energy per particle as a function of the density
- If we want to study ground-state properties of $N \geqslant 3$ clusters, we have to perform "*numerical experiments*"



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Grisenti, Schöllkopf, Toennies, Hegerfeldt, Köhler, and Stoll. Determination of the Bond Length and Binding Energy of the Helium Dimer by Diffraction from a Transmission Grating. *PRL*, 2000

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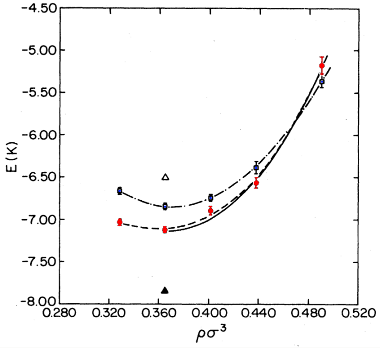
Zeller et al. Imaging the He 2 quantum halo state using a free electron laser. *PNAS*, 2016

Ground-state ^{4}He properties: Quantum Monte Carlo methods

- **Clusters**: HFDHE2

N	E/N (K) GFMC	E/N (K) VMC	r_0 (Å) GFMC	T (Å) GFMC
3	−0.0391(1)	⋯	5.35	5.0
4	−0.1333(5)	−0.128	4.20	4.5
8	−0.6165(6)	−0.597	3.19	4.4
20	−1.627(3)	−1.570	2.71	5.5
40	−2.487(3)	−2.396	2.57	5.6
70	−3.12(4)	−3.02	2.47	6.1
112	−3.60(1)	−3.52	2.44	7.3
240	⋯	−4.19	2.36[a]	6.8[a]
728	⋯	−4.95	2.32[a]	7.2[a]
∞	−7.11(2)	−6.88	2.22	⋯

- **Matter**: Lennard-Jones, HFDHE2, Expt. (solid line)



Kalos, Lee, Whitlock, and Chester. Modern potentials and the properties of condensed He 4. *PRB*, 1981.
Pandharipande, Zabolitzky, Pieper, Wiringa, and Helmbrecht. Calculations of Ground-State Properties of Liquid 4He Droplets. *PRL*, 1983.

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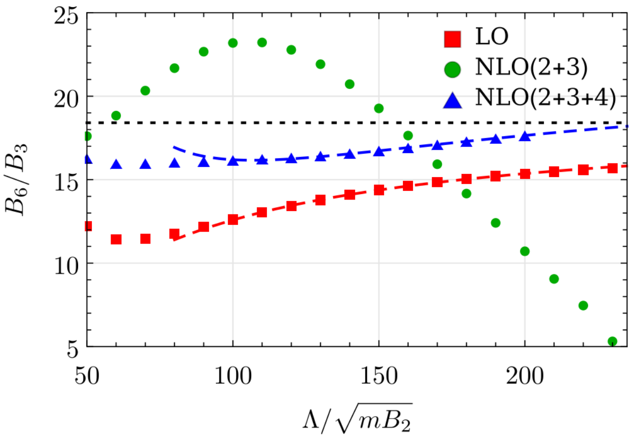
Motivation

- Success of EFT describing properties of ^{4}He clusters with $N \leqslant 6$
- Universal properties of unitary bosons
  - Clusters (up to $N = 60$)
  - Matter
- Objective: apply EFT to ^{4}He **clusters** (the largest N within our computational capabilities) and **matter**



Bazak, Eliyahu, and van Kolck. Effective field theory for few-boson systems. *PRA*, 2016.
Bazak, Kirscher, König, Valderrama, Barnea, and van Kolck. Four-Body Scale in Universal Few-Boson Systems. *PRL*, 2019.

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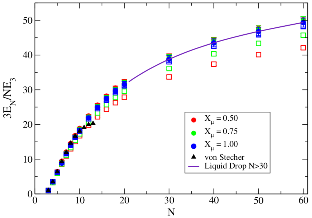
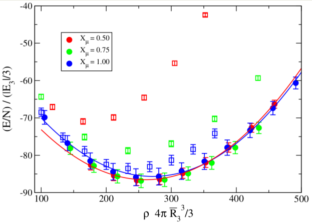


Clusters



Matter

Carlson, Gandolfi, van Kolck, and Vitiello. Ground-State Properties of Unitary Bosons: From Clusters to Matter. *PRL*, 2017.

De-Leon and Pederiva. Equation of State of a Strongly Interacting many-Boson System from an Effective Interaction. arXiv:2211.00165. 2022.

EFT approach

- The LO EFT Hamiltonian for non-relativistic bosons with large scattering lengths is:

$$\boxed{H = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\nabla_i^2 + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk}}$$

- The contact interactions are regularized:

$$V_{ij} = V_2(\Lambda) e^{-r_{ij}^2\Lambda^2/4} \qquad \text{and} \qquad V_{ijk} = V_3(\Lambda) e^{-(r_{ij}^2 + r_{ik}^2 + r_{jk}^2)\Lambda^2/6}$$

- where we introduced the low-energy constants (LECs)
- Typical momentum scale of the N particle system:

$$Q_N = \frac{1}{\hbar}\sqrt{\frac{-2mE_N}{N}}$$

- Extrapolating quantities to infinite cutoff:

$$\boxed{O_N(\Lambda) = O_N(\Lambda \to \infty)\left[1 + \alpha_N\left(\frac{Q_N}{\Lambda}\right) + \beta_N\left(\frac{Q_N}{\Lambda}\right)^2 + \ldots\right]}$$

- α_N and β_N should be of order 1

Quantum Monte Carlo

- QMC: *ab-initio* many-body methods used to compute ground-state properties of strongly-interacting systems
- Trial wave function:

$$\Psi_T = \prod_i f^{(1)}(r_i) \prod_{i<j} f^{(2)}(r_{ij}) \prod_{i<j<k} f^{(3)}(R_{ijk})$$

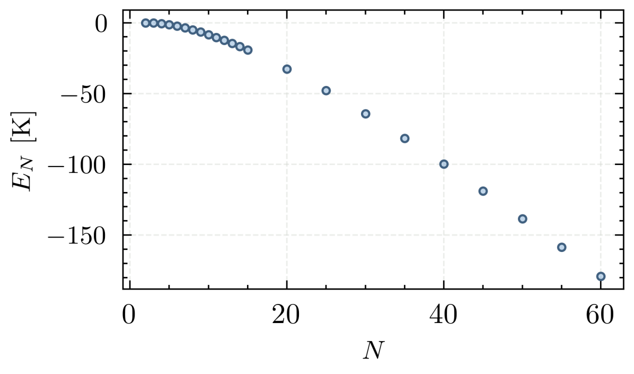
- Variational Monte Carlo (VMC) is used to optimize the parameters
- Diffusion Monte Carlo (DMC): Ground-state energy
  - Method for solving the imaginary-time many-body Schrödinger equation
  - Projects out the lowest energy eigenstate that has non-zero overlap with the initial state

$$\boxed{|\Phi_0\rangle \propto \lim_{\tau\to\infty} \exp\left[-(H - E_T)\tau\right] |\Psi_T\rangle}$$

- Exact for bosons, but with controllable statistical uncertainties

Numerical experiments

- HFDHE2 potential
- Data is used to:
  - determine the LECs ($N = 2$ and $N = 3$)
  - compare with EFT predictions for $N \geqslant 4$
- $V_2(\Lambda)$ reproduces $E_2 = -0.8348$ mK
- $V_3(\Lambda)$ reproduces $E_3 = -117.2$ mK

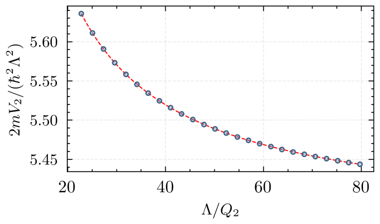


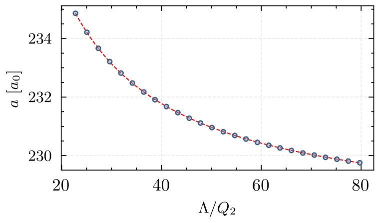
Madeira, Pederiva, and van Kolck. In preparation.

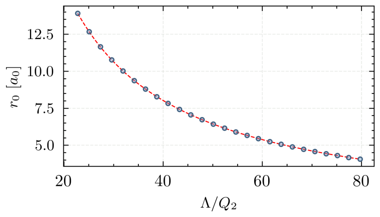
EFT and the two-body sector

$$O(\Lambda) = O(\Lambda \to \infty)\left[1 + \alpha\left(\frac{Q_2}{\Lambda}\right) + \beta\left(\frac{Q_2}{\Lambda}\right)^2\right]$$

$$r_0(\Lambda) = r_{0,\infty} + \alpha\left(\frac{Q_2}{\Lambda}\right) + \beta\left(\frac{Q_2}{\Lambda}\right)^2$$







- $2mV_2/(\hbar^2\Lambda^2) \xrightarrow{\Lambda\to\infty} 5.368011(1)$
- $\alpha = 1.12031(2)$
- $\beta = 0.3642(3)$

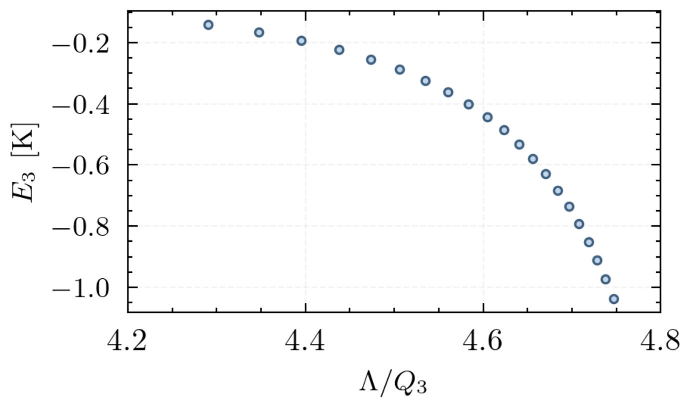
- $a_\infty = 227.723(2)\ a_0$ $(-\hbar^2/ma_\infty^2 = E_2)$
- $\alpha = 0.710(1)$
- $\beta = 0.09(1)$

- $r_{0,\infty} = 0.0028(3)\ a_0$
- $\alpha = 326.44(2)\ a_0$
- $\beta = -222.2(5)\ a_0$

Madeira, Pederiva, and van Kolck. In preparation.

The Thomas collapse

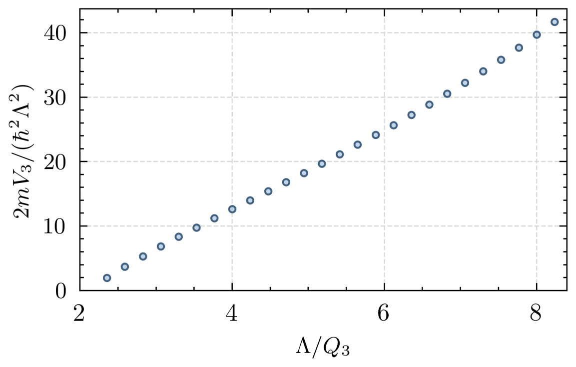
- What happens if we do not include a three-body force?



Madeira, Pederiva, and van Kolck. In preparation.

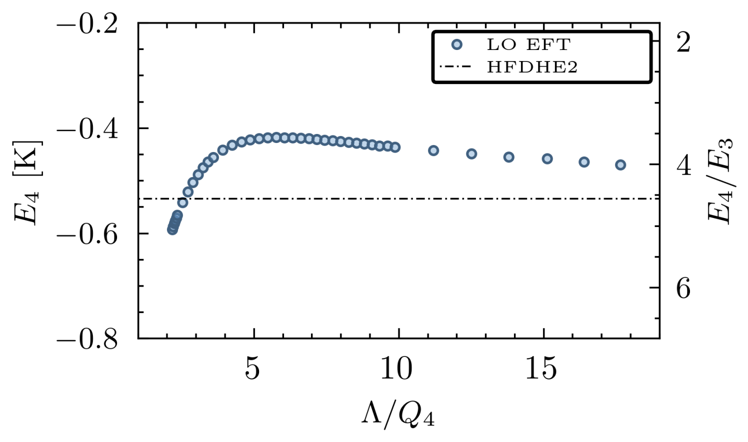
The ^{4}He trimer

- $V_3(\Lambda)$ reproduces $E_3 = -117.2$ mK
- At this point, the LO Hamiltonian is fully determined for N particles



Madeira, Pederiva, and van Kolck. In preparation.

Clusters - $N = 4$



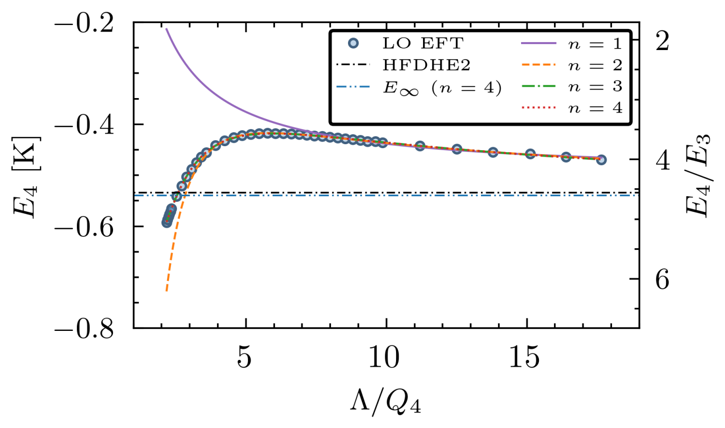
Madeira, Pederiva, and van Kolck. In preparation.

Clusters - $N = 4$

- Extrapolation:

$$E_4(\Lambda) = E_{4,\infty}\left[1 + \sum_{i=1}^{n} c_i \left(\frac{Q_4}{\Lambda}\right)^i\right]$$

- 1% relative difference!

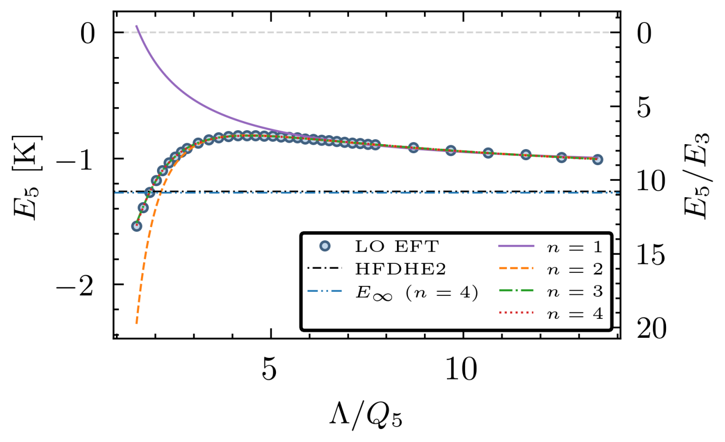


Madeira, Pederiva, and van Kolck. In preparation.

Clusters - $N = 5$

- Extrapolation:

$$E_N(\Lambda) = E_{N,\infty}\left[1 + \sum_{i=1}^{n} c_i \left(\frac{Q_N}{\Lambda}\right)^i\right]$$

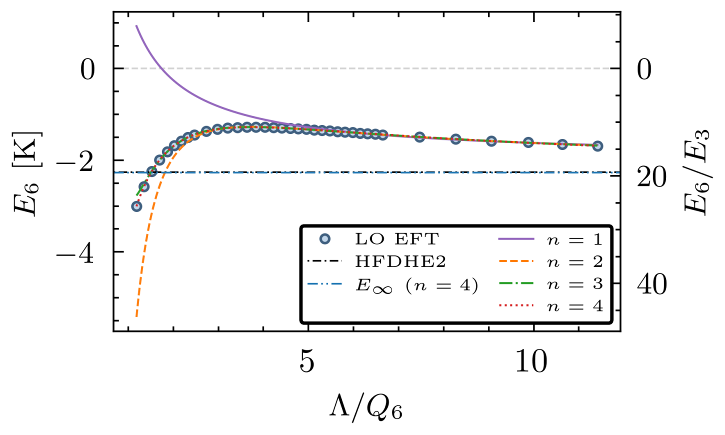


Madeira, Pederiva, and van Kolck. In preparation.

Clusters - $N = 6$

- Extrapolation:

$$E_N(\Lambda) = E_{N,\infty}\left[1 + \sum_{i=1}^{n} c_i \left(\frac{Q_N}{\Lambda}\right)^i\right]$$

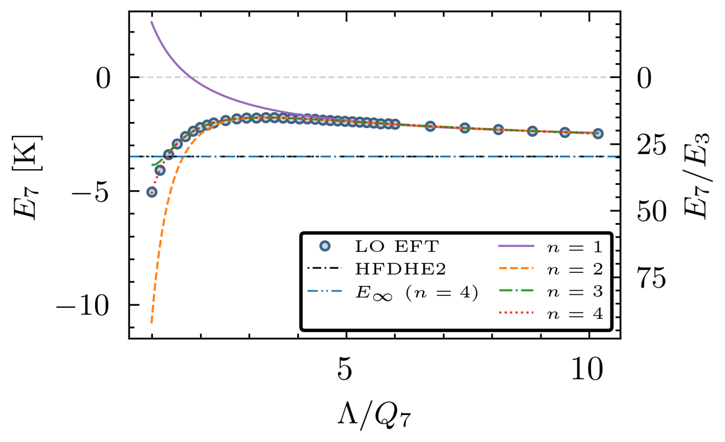


Madeira, Pederiva, and van Kolck. In preparation.

Clusters - $N = 7$

- Extrapolation:

$$E_N(\Lambda) = E_{N,\infty}\left[1 + \sum_{i=1}^{n} c_i \left(\frac{Q_N}{\Lambda}\right)^i\right]$$

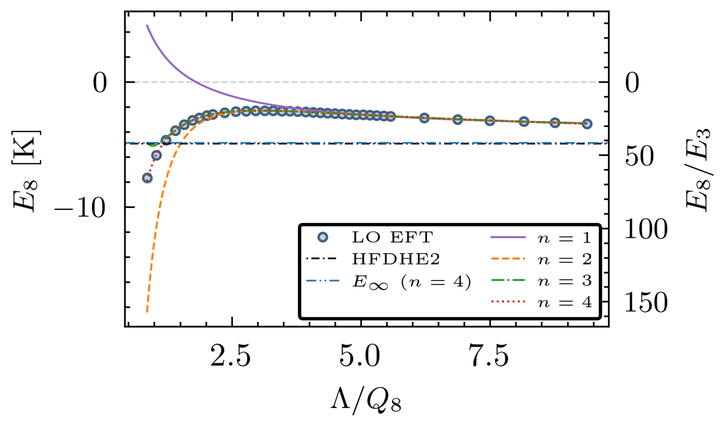


Madeira, Pederiva, and van Kolck. In preparation.

Clusters - $N = 8$

- Extrapolation:

$$E_N(\Lambda) = E_{N,\infty}\left[1 + \sum_{i=1}^{n} c_i \left(\frac{Q_N}{\Lambda}\right)^i\right]$$

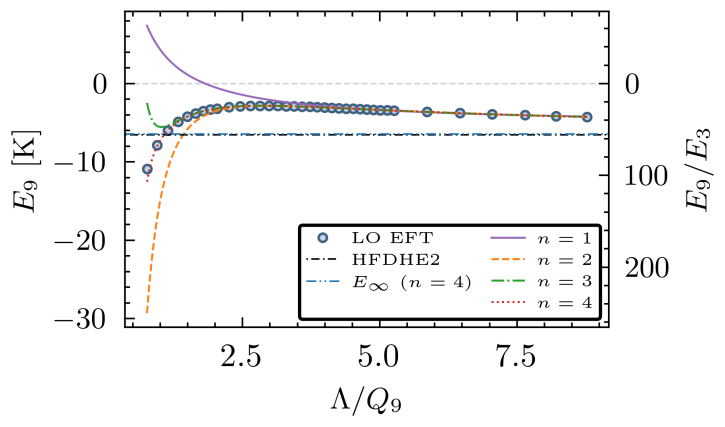


Madeira, Pederiva, and van Kolck. In preparation.

Clusters - $N = 9$

- Extrapolation:

$$E_N(\Lambda) = E_{N,\infty}\left[1 + \sum_{i=1}^{n} c_i \left(\frac{Q_N}{\Lambda}\right)^i\right]$$

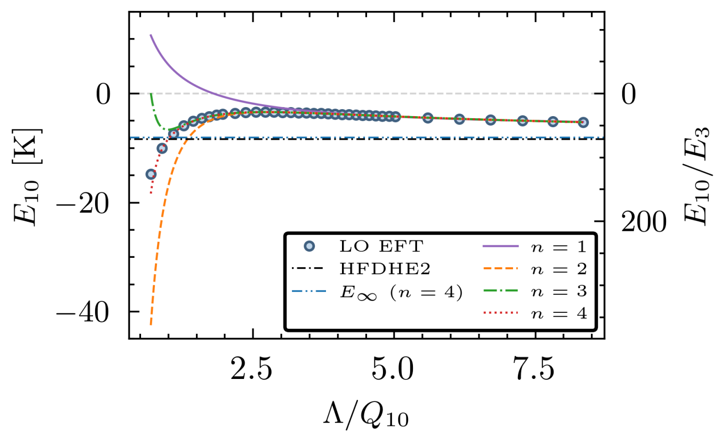


Madeira, Pederiva, and van Kolck. In preparation.

Clusters - $N = 10$

- Extrapolation:

$$E_N(\Lambda) = E_{N,\infty}\left[1 + \sum_{i=1}^{n} c_i \left(\frac{Q_N}{\Lambda}\right)^i\right]$$

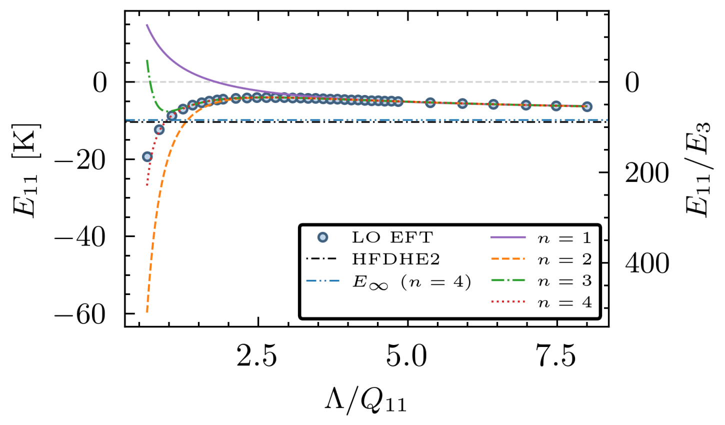


Madeira, Pederiva, and van Kolck. In preparation.

Clusters - $N = 11$

- Extrapolation:

$$E_N(\Lambda) = E_{N,\infty}\left[1 + \sum_{i=1}^{n} c_i \left(\frac{Q_N}{\Lambda}\right)^i\right]$$

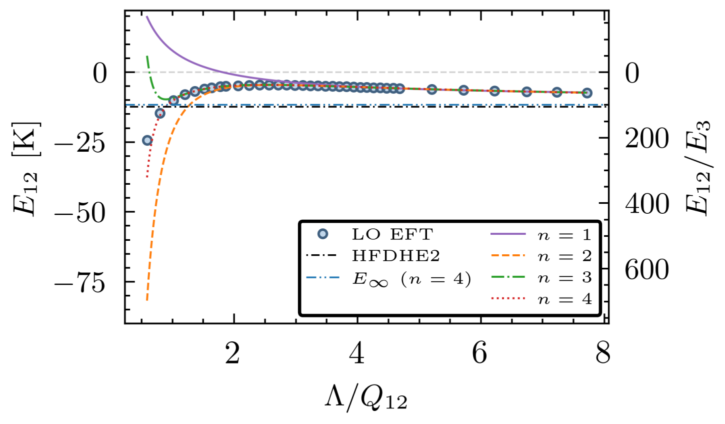


Madeira, Pederiva, and van Kolck. In preparation.

Clusters - $N = 12$

- Extrapolation:

$$E_N(\Lambda) = E_{N,\infty}\left[1 + \sum_{i=1}^{n} c_i \left(\frac{Q_N}{\Lambda}\right)^i\right]$$

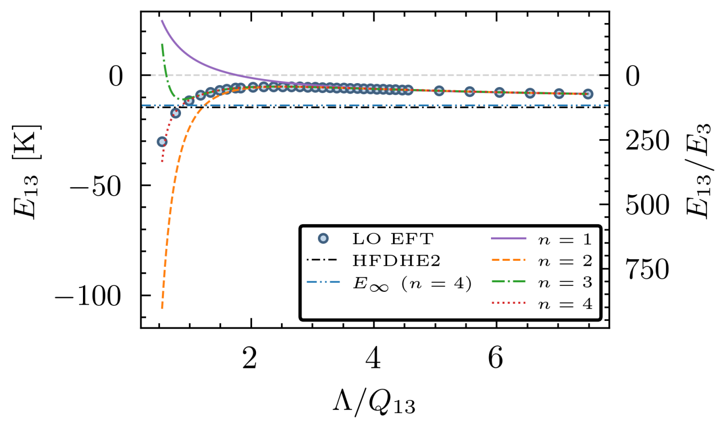


Madeira, Pederiva, and van Kolck. In preparation.

Clusters - $N = 13$

- Extrapolation:

$$E_N(\Lambda) = E_{N,\infty}\left[1 + \sum_{i=1}^{n} c_i \left(\frac{Q_N}{\Lambda}\right)^i\right]$$

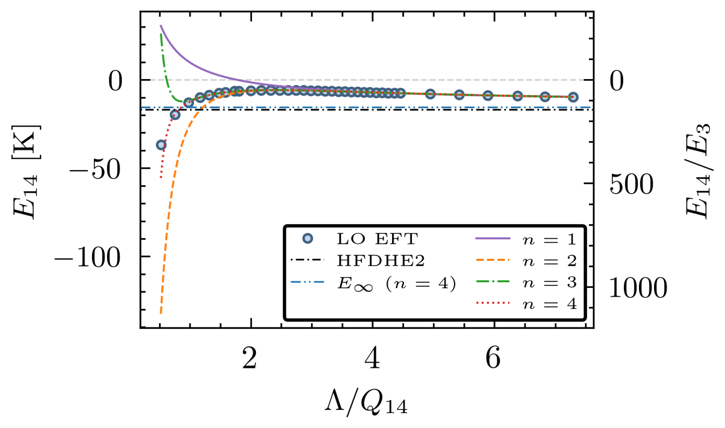


Madeira, Pederiva, and van Kolck. In preparation.

Clusters - $N = 14$

- Extrapolation:

$$E_N(\Lambda) = E_{N,\infty}\left[1 + \sum_{i=1}^{n} c_i \left(\frac{Q_N}{\Lambda}\right)^i\right]$$

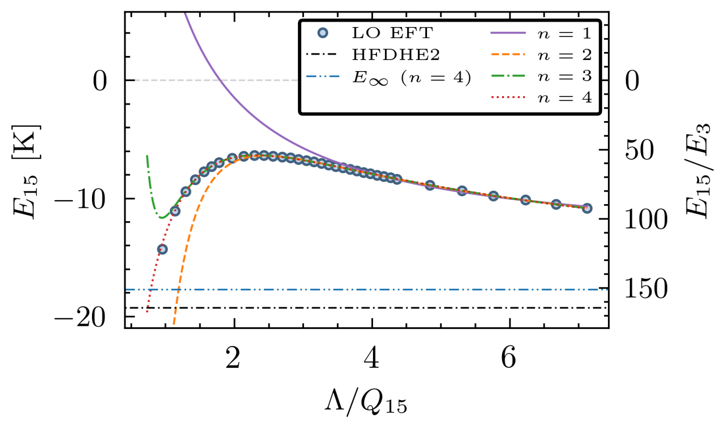


Madeira, Pederiva, and van Kolck. In preparation.

Clusters - $N = 15$

- Extrapolation:

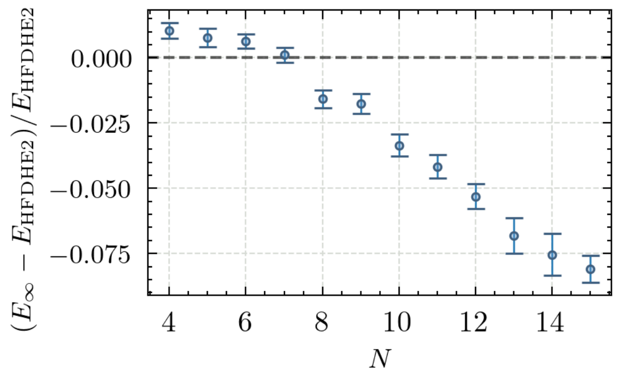
$$E_N(\Lambda) = E_{N,\infty}\left[1 + \sum_{i=1}^{n} c_i \left(\frac{Q_N}{\Lambda}\right)^i\right]$$



Madeira, Pederiva, and van Kolck. In preparation.

Clusters - comparison with the HFDHE2 potential

- Compare $E_N(\Lambda \to \infty)$ with $E_{N,\mathrm{HFDHE2}}$
- Relative difference
  - 1% ($N = 4$)
  - 8% ($N = 15$)



Madeira, Pederiva, and van Kolck. In preparation.

Conclusions

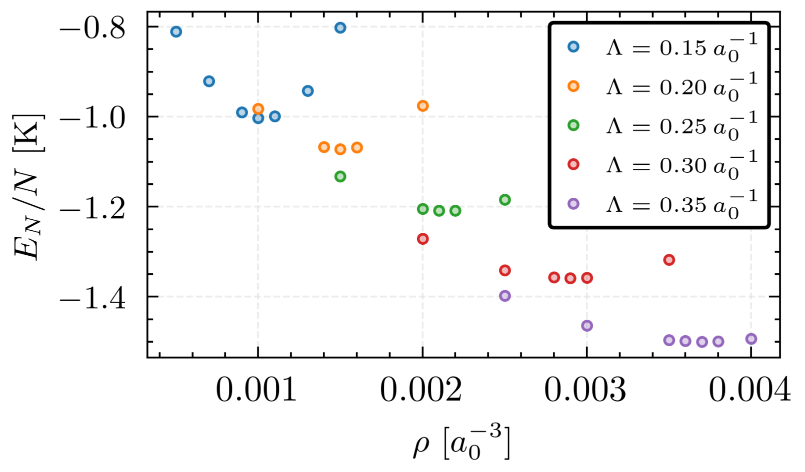
- Motivation and advantages of using an EFT description of ^{4}He
- Leading Order: only two inputs
  - E_2
  - E_3
- Clusters: relative differences to the "numerical experiment"
  - 1% ($N = 4$)
  - 8% ($N = 15$)

Outlook

- Next-to-Leading-Order (NLO)
  - Four-body scale
- Uncertainty quantification
- Matter

Bazak, Kirscher, König, Valderrama, Barnea, and van Kolck. Four-Body Scale in Universal Few-Boson Systems. *PRL*, 2019.

Matter



Madeira, Pederiva, and van Kolck. In preparation.