EFT calculations and finite-volume techniques for nuclear few-body systems

Sebastian König

EMMI Workshop and International Workshop XLIX on Gross Properties of Nuclei and Nuclear Excitations

Hirschegg, January 18, 2023

S. Dietz, H.-W. Hammer, SK, A. Schwenk, PRC **105** 064002 (2022)
N. Yapa, SK, PRC **106** 014309 (2022)
H. Yu, SK, D. Lee, arXiv:2212.14379 [nucl-th]

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Thanks...

...to my students and collaborators...

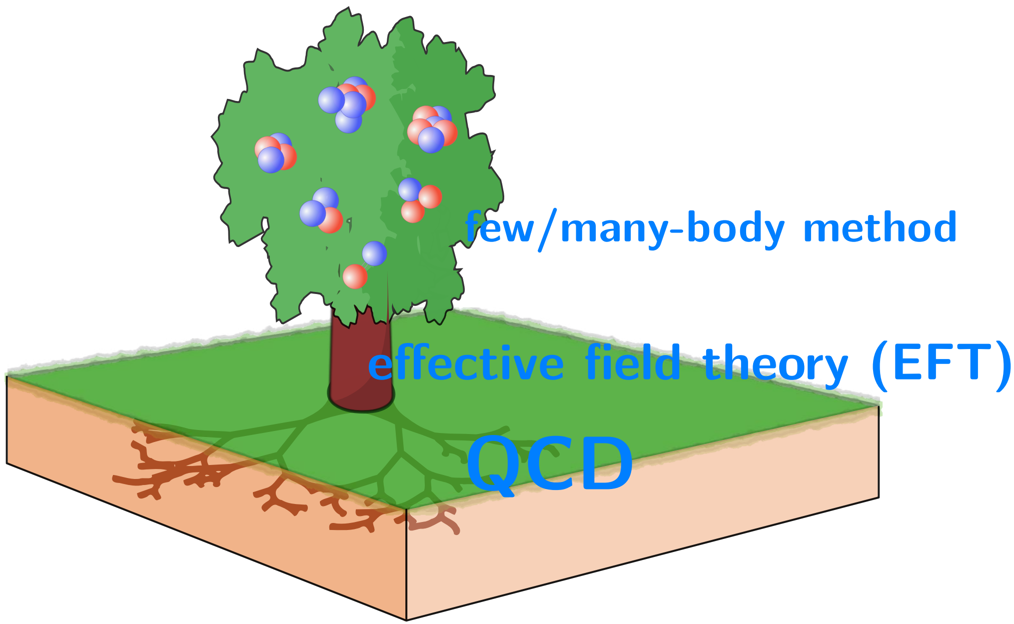
- S. Dietz, H.-W. Hammer, A. Schwenk (TU Darmstadt)
- H. Yu, N. Yapa (NCSU)
- D. Lee (FRIB/MSU)
- ...

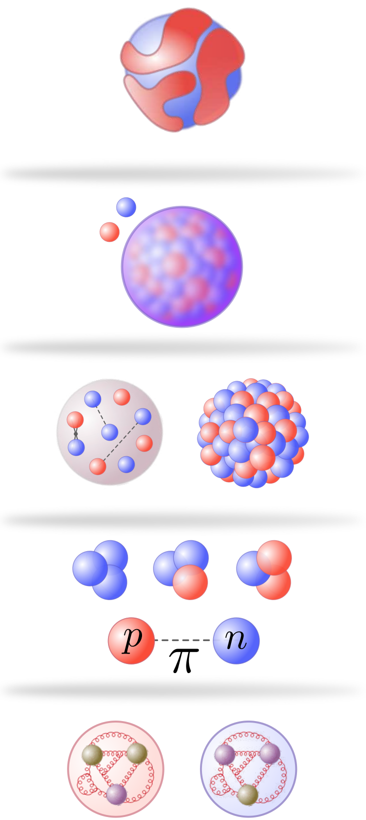
...for support, funding, and computing time...

FRIB Theory Alliance — U.S. DEPARTMENT OF ENERGY | Office of Science — NSF

- Jülich Supercomputing Center

Nuclear theory tower



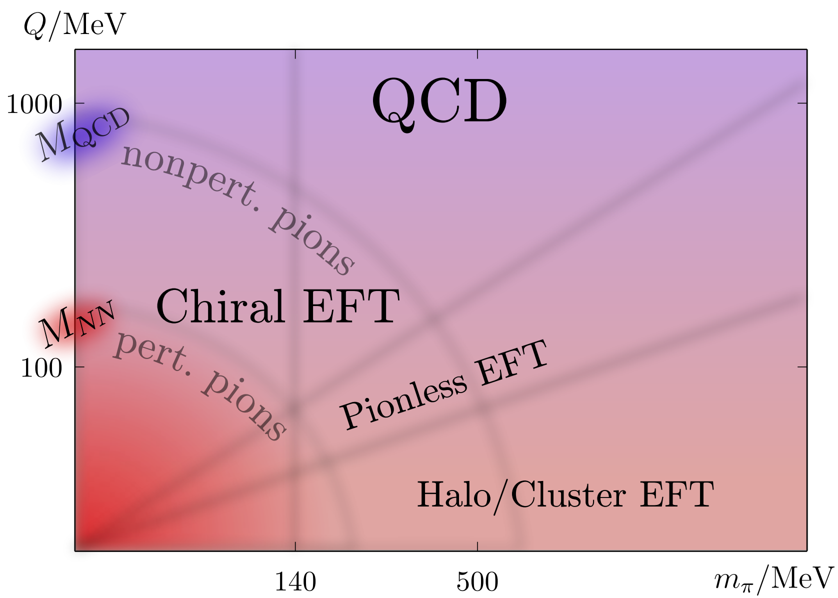


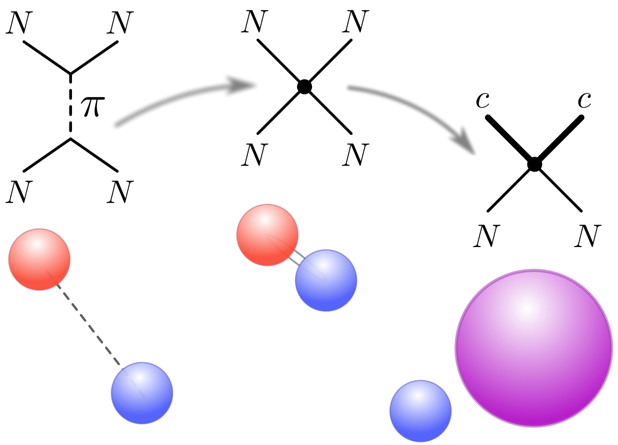
- **QCD** = underlying theory of strong interaction
- **EFT** = effective description in terms of hadrons
- **degrees of freedom depend on resolution scale**

Nuclear effective field theories

- choose **degrees of freedom** approriate to energy scale
- only restricted by **symmetry**, ordered by **power counting**

Hammer, SK, van Kolck, RMP **92** 025004 (2020)



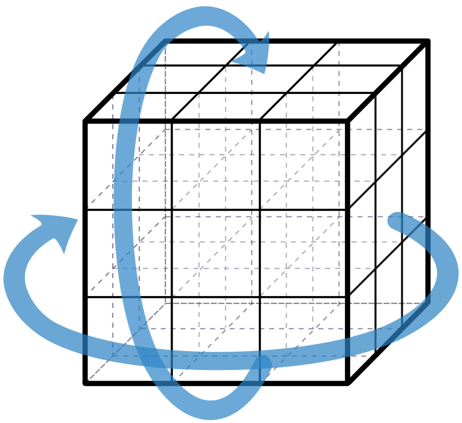


- degrees of freedom here: nucleons (and/or clusters thereof)
- even more effective d.o.f.: rotations, vibrations

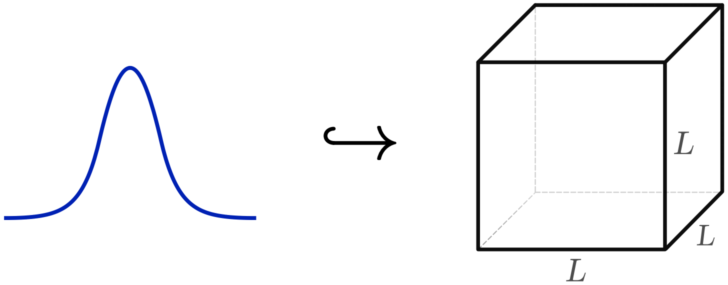
Papenbrock, NPA **852** 36 (2011); ...

- most effective theory depends on energy scale and nucleus of interest

Finite periodic boxes



- physical system enclosed in finite volume (box)
- typically used: periodic boundary conditions
- **leads to volume-dependent energies**



Lüscher formalism

- physical properties encoded in the volume-dependent energy levels
- infinite-volume S-matrix governs discrete finite-volume spectrum
- **finite volume used as theoretical tool**

Lüscher, Commun. Math. Phys. **104** 177 (1986); ...

Outline

Introduction ✔

Few-neutron systems

Charged particles

Summary and outlook

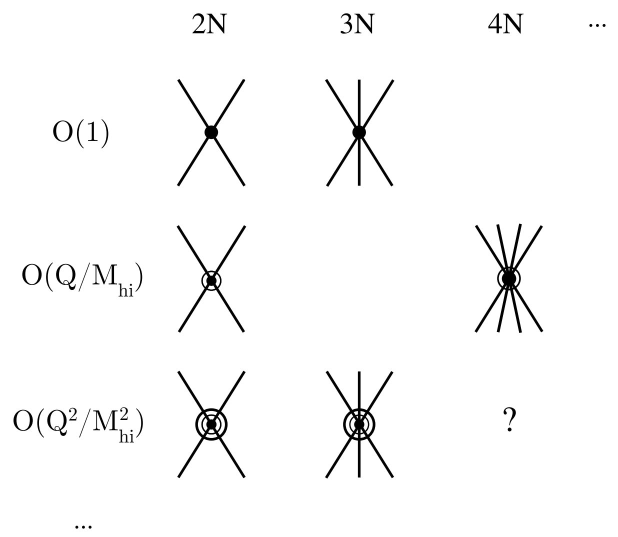
Part I

Pionless EFT calculations for few-neutron systems

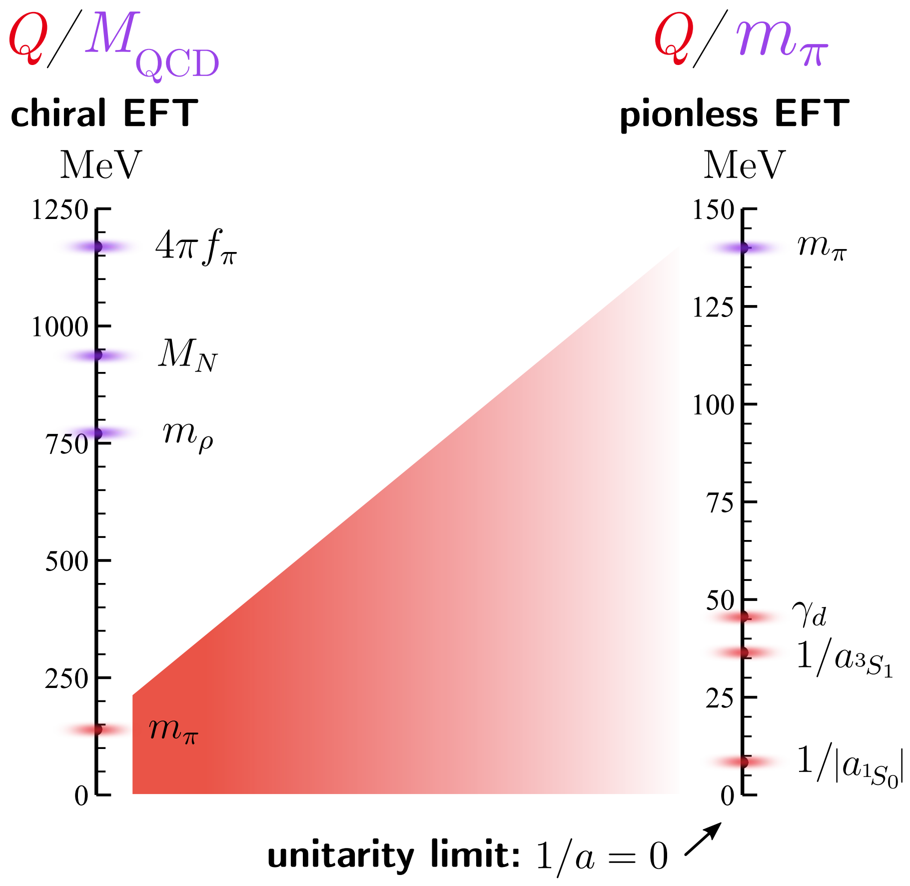
S. Dietz, H.-W. Hammer, SK, A. Schwenk, PRC **105** 064002 (2022)
N. Yapa, SK, PRC **106** 014309 (2022)
and work in progress

Pionless EFT

- only contact (zero-range) forces (plus electromagnetism)
- closely linked to universality for large scattering lengths
- excels at low energies, exact range of validity still an open question



Nuclear scales



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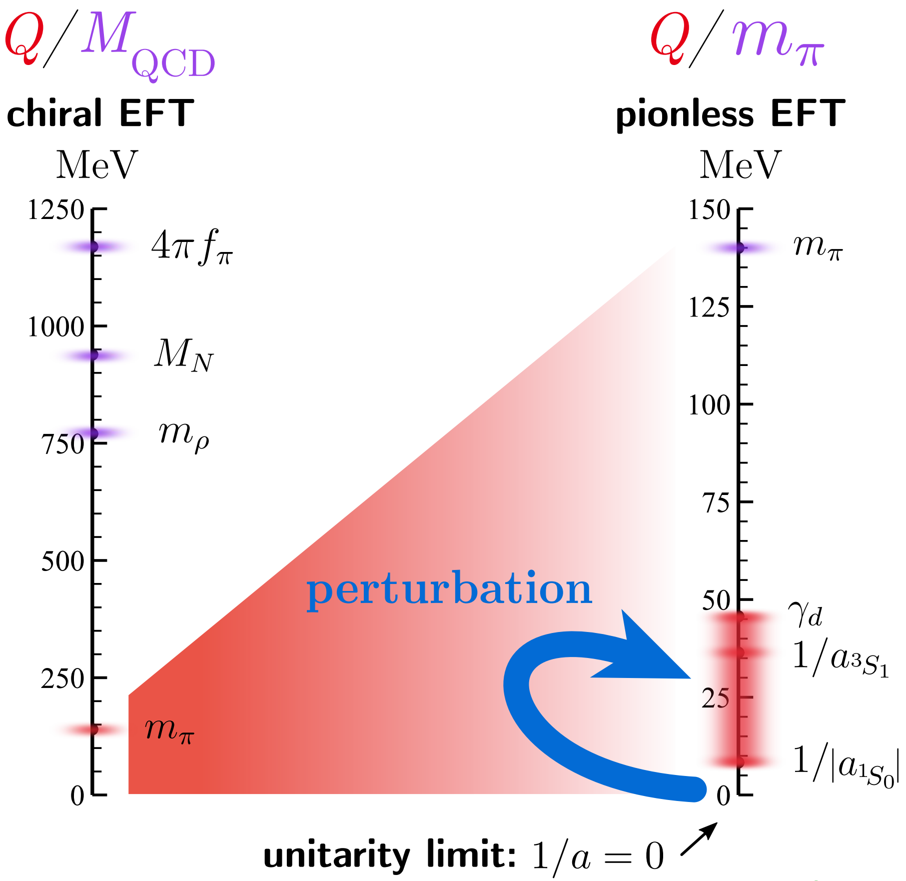

SK et al. PRL **118** 202501 (2017)

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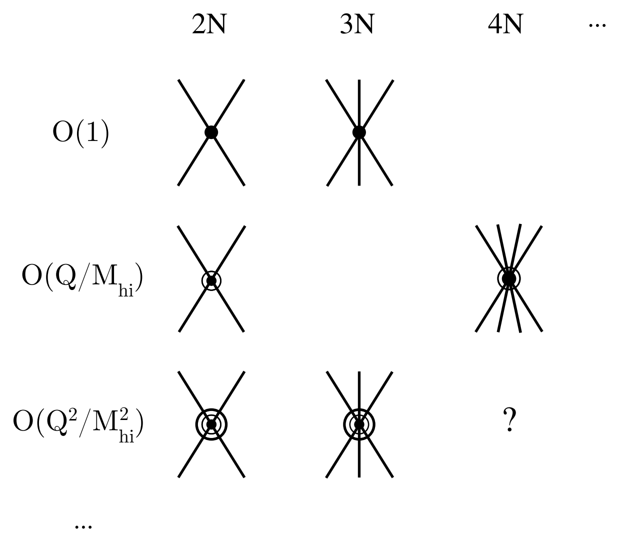
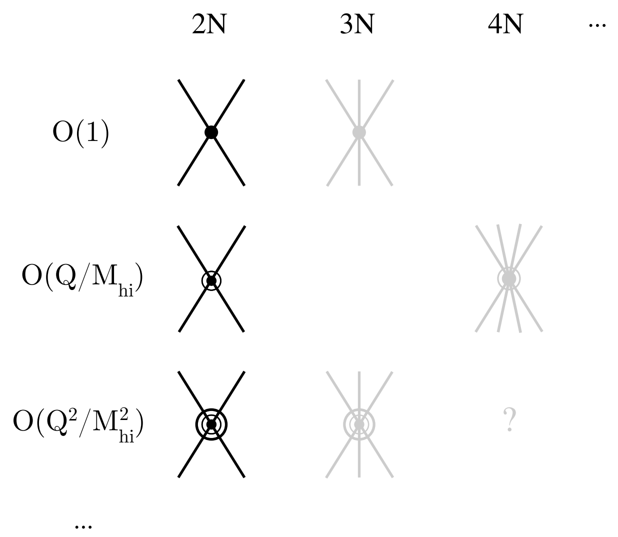


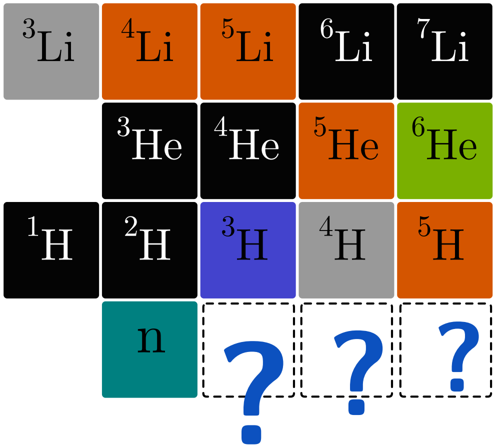
Pionless EFT

- only contact (zero-range) forces (plus electromagnetism)
- closely linked to universality for large scattering lengths
- excels at low energies, exact range of validity still an open question
- no leading-order 3n force for pure neutron systems



Few-neutron systems

Ongoing searches and speculations



- bound dineutron not excluded by pionless EFT

Kirscher + Phillips, PRC **84** 054004 (2011); SK et al., PLB **736** 208 (2014)

- new speculations about a three-neutron resonance...

Gandolfi et al., PRL **118** 232501 (2017)

- ...although excluded by previous work

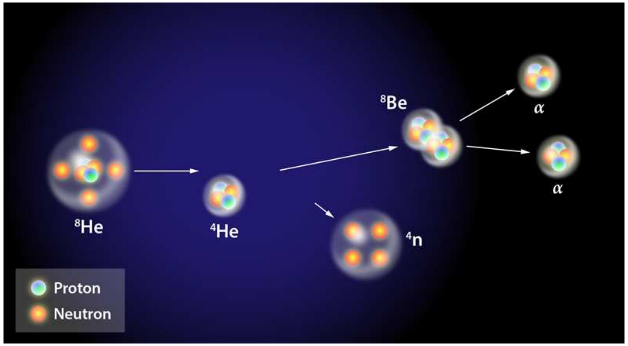
Lazauskas + Carbonell, PRC **71** 044004 (2005); Offermann + Glöckle, NPA **318** 138 (1979)

- **experimental evidence for tetraneutron resonance (or even bound state?)**

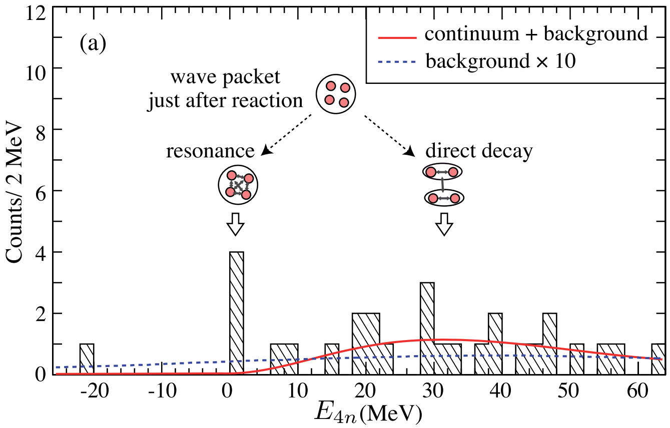
Kisamori et al., PRL **116** 052501 (2016), Duer et al., Nature **606** 678 (2022), Faestermann et al., PLB **824** 136799 (2022)

Tetraneutron situation

Observation at RIKEN (2016)



APS/Alan Stonebraker

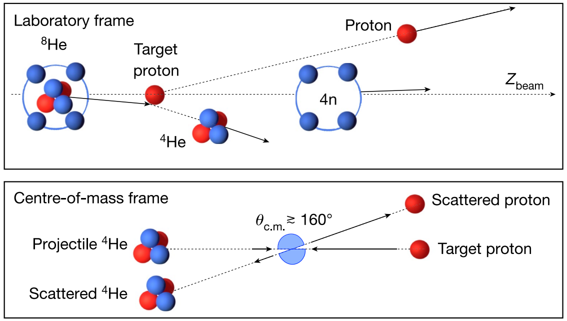


Kisamori et al., PRL **116** 052501 (2016)

- double-charge exchange reaction
- **excess of near threshold events hints at possible resonance**
- **motivated follow-up experiment**

Tetraneutron situation

Observation at RIKEN (2022)



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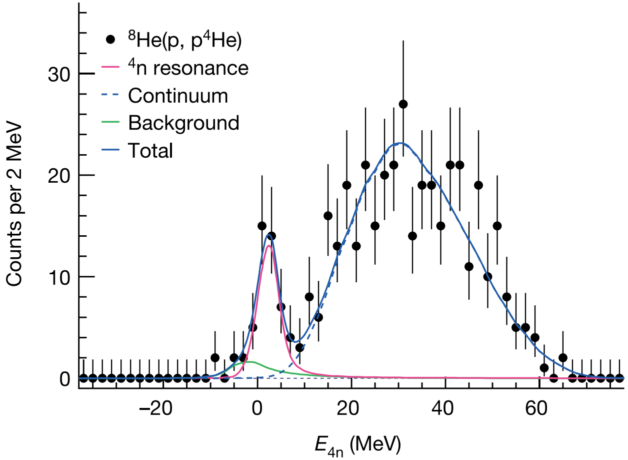


- knockout reaction: scattering ^{8}He beam off proton target
- **clear peak with resonance shape around 2 MeV**
- **theory suggests alternative explanations (time delay, phase space + FSI)**

Higgins et al., PRC **103** 024004 (2021), Lazauskas et al., arXiv:2207.07575 [nucl-th]

Overview

Search for resonance states with two different methods

Dietz, SK et al., PRC **105** 064002 (2022)

- **analytically continued Faddeev equations**

  following Glöckle, PRC **18** 564 (1978); Afnan, Aust. J. Phys. **44** 201 (1991)

  - calculation of S-matrix pole trajectories
  - application to three-boson and three-neutron system
  - three-neutron scaling exponents

  Dietz, Hammer, SK, work in progress

- **finite-volume energy levels in large periodic boxes**

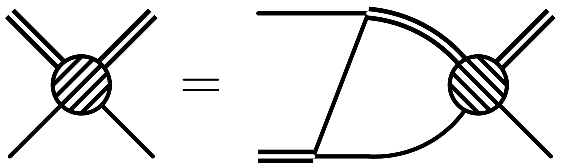
  following Klos, SK et al., PRC **98** 034004 (2018)

  - exact few-body calculation with discrete variable representation
  - application to three and four neutrons
  - efficient calculation enabled by finite-volume eigenvector continuation

  Yapa+König, PRC **106** 014309 (2022)

Three-body equation

- **consider the Faddeev equation with separable interaction**



$$F(q) = -\frac{1}{2}\int \mathrm{d}q' q'^2 \int_{-1}^{1} \mathrm{d}x\, g(\pi_1) G_0(E;\pi_2,q') \times g(\pi_2) P_1(x) \tau\left(E - \frac{3}{4}q'^2\right) F(q')$$

- effective two-body equation structure
- written here for three neutrons with $J^\pi = \frac{1}{2}^-$ or $\frac{3}{2}^-$ (degenerate)
  - very similar form (plus three-body force) for three bosons
- energies for which a solution exists correspond to S-matrix poles

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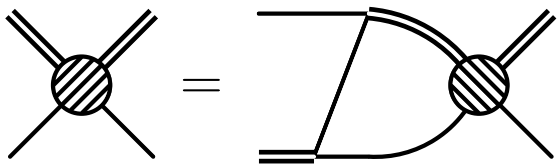

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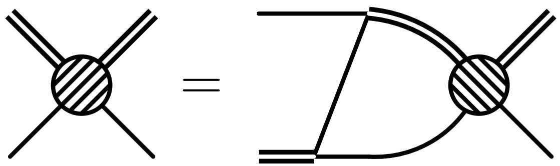

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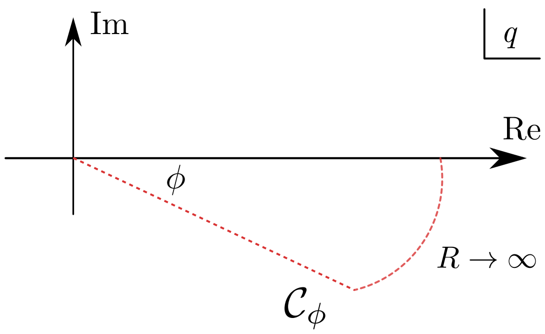
Analytic continuation

- rotate the integration contour: $q \to q\mathrm{e}^{-\mathrm{i}\phi}$
  - this exposes lower right quadrant

Afnan, Aust. J. Phys. **44** 201 (1991)

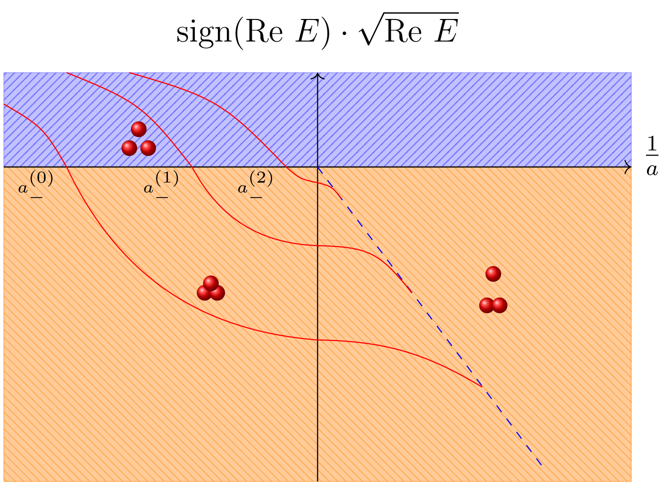
- possible to rotate back and pick up a residue
  - leads to modified effective interaction

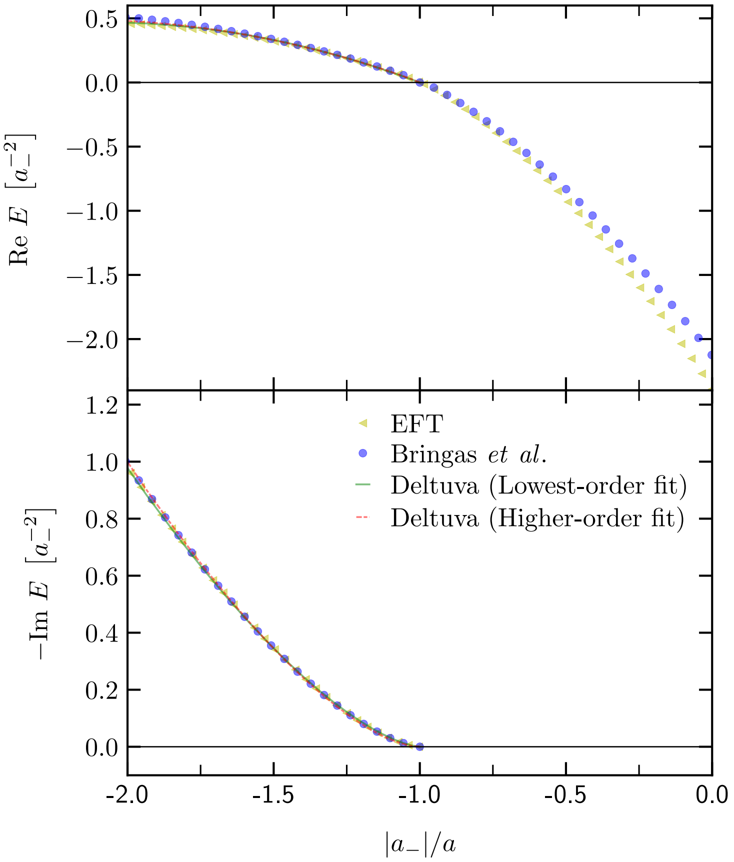
Glöckle, PRC **18** 564 (1978)



Efimov state trajectories

- Efimov bound states become resonances at certain negative scattering length
- possible to follow the trajectory
- **EFT reproduces potential models**

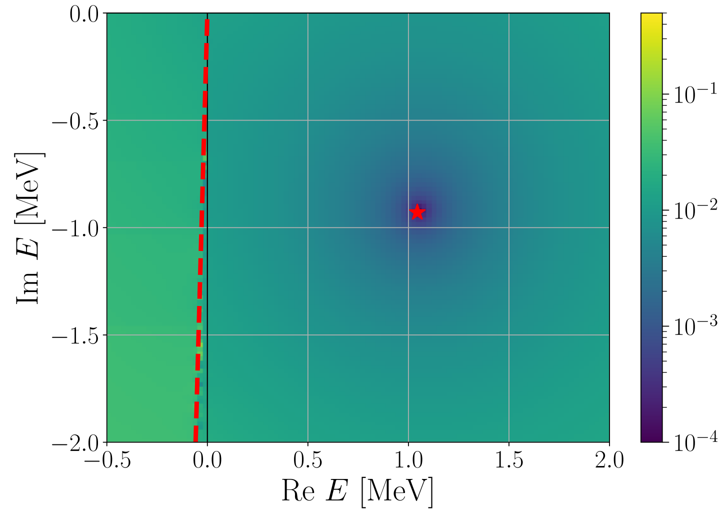


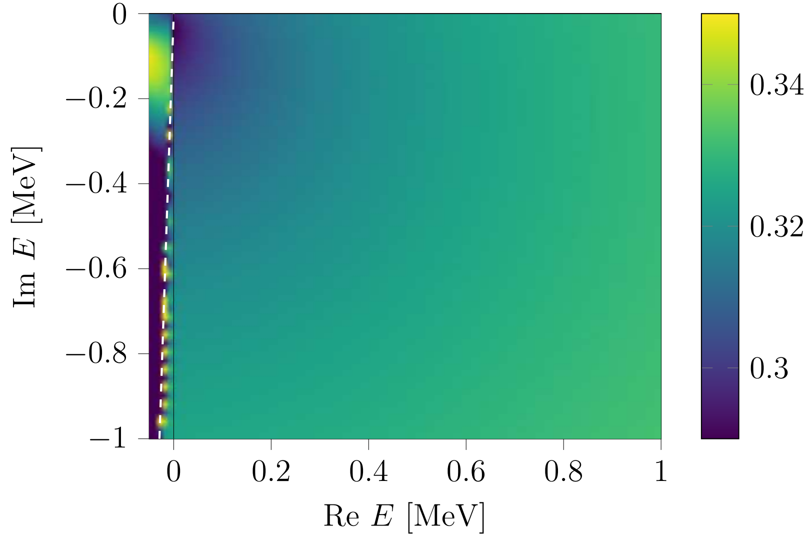


Dietz, SK et al., PRC **105** 064002 (2022)

Neutrons vs. bosons

- for three bosons we can follow the resonance trajectory of an Efimov state
  - consistent with previous work Bringas et al., PRA **69** 040702 (2004); Deltuva, PRC **102** 034003 (2020)
- for three neutrons, we can reproduce Glöckle's Yamaguchi model Glöckle, PRC **18** 564 (1978)
  - generates a $3n$ resonance with deep $2n$ bound state
- **no sign of a three-neutron resonance for physical nn scattering length**
  - consistent with related work
    Lazauskas + Carbonell, PRC **71** 044004 (2005); Deltuva + Lazauskas, PRL **123** 069201 (2019)





Dietz, SK et al., PRC **105** 064002 (2022)

Three-neutron point production

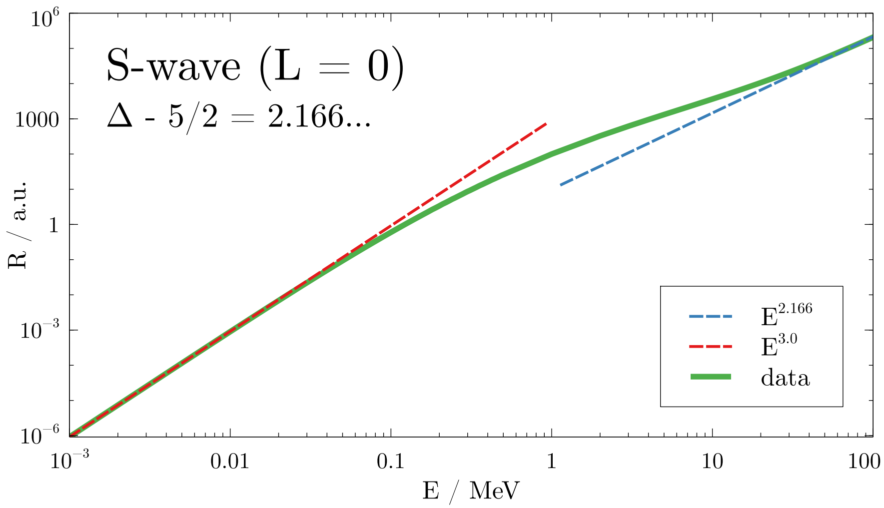
- assume that final-state neutrons in experiments are created effectively in a point
- possible to solve Faddeev equation for production amplitude
  - same interaction kernel as shown previously in this talk

Dietz, Hammer, SK, in preparation

- spectrum governed by conformal symmetry in universal regime: $\frac{1}{ma^2} \ll E \ll \frac{1}{mr^2}$
- cross section $\frac{d\sigma}{dE} \sim R(E) \sim E^{\Delta - 5/2}$

Hammer+Son, Proc. Natl. Acad. Sci. 118, e2108716118 (2021)

  - scaling dimension Δ depends on partial wave: 4.666 ($L = 0$), 4.273 ($L = 1$), ...



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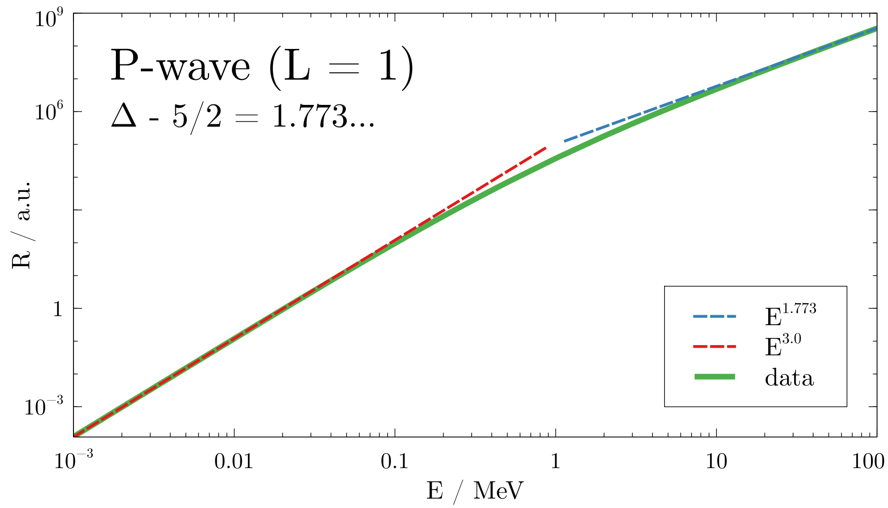
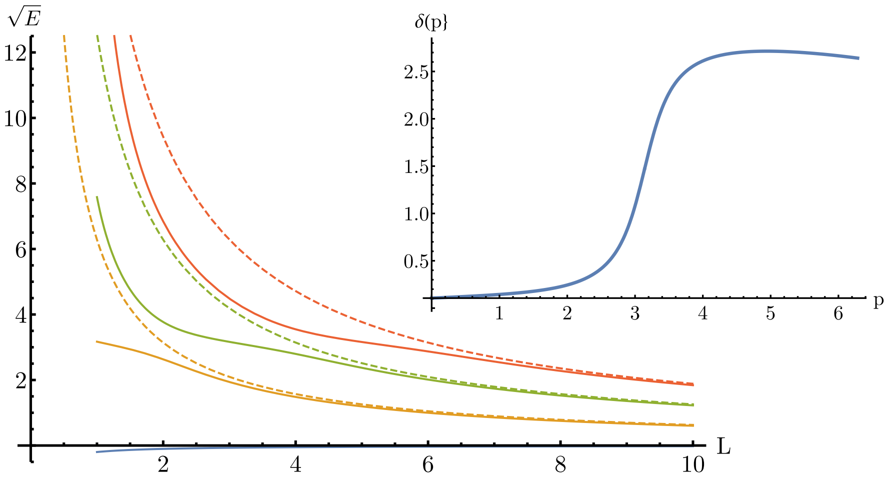


Finite-volume resonance signatures

Lüscher formalism

- finite volume $\rightarrow$ discrete energy levels $\rightarrow p\cot\delta_0(p) = \frac{1}{\pi L} S(E(L))$ $\rightarrow$ phase shift
- **resonance contribution $\leftrightarrow$ avoided level crossing**

Lüscher, NPB **354** 531 (1991); ...
Wiese, NPB (Proc. Suppl.) **9** 609 (1989); ...



- spectrum signature **carries over to few-body systems**
  - need considerable range of volumes for such studies!

Klos, SK et al., PRC **98** 034004 (2018)

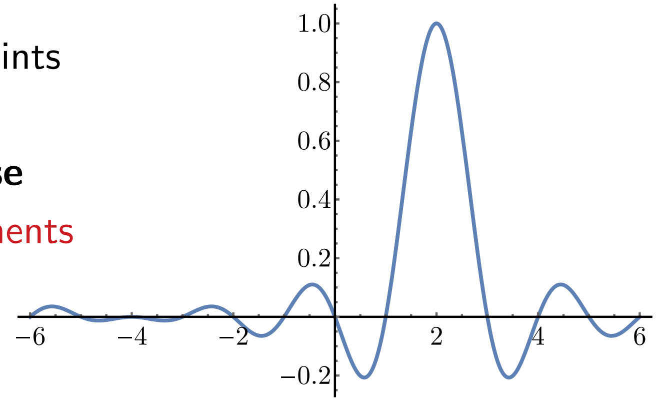
Discrete variable representation

Need calculation of several few-body energy levels

- **use a Discrete Variable Representation (DVR)**

well established in quantum chemistry, suggested for nuclear physics by Bulgac+Forbes, PRC **87** 051301 (2013)

- basis functions localized at grid points
- potential energy matrix diagonal
- **kinetic energy matrix very sparse**
  - precalculate only 1D matrix elements



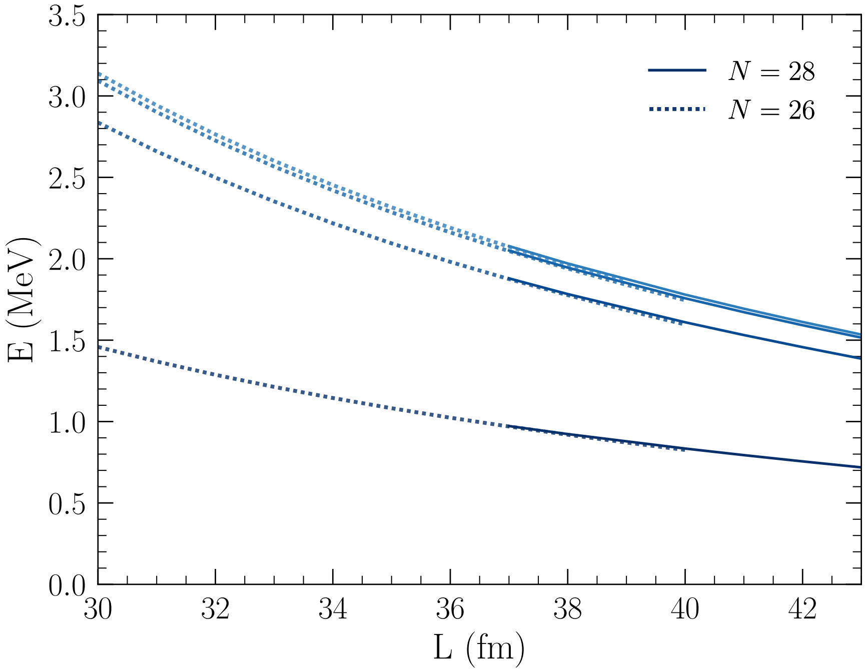
- periodic boundary condistions ↔ plane waves as starting point
- **efficient implementation for large-scale calculations**
  - handle arbitrary number of particles (and spatial dimensions)
  - numerical framework scales from laptop to HPC clusters Klos, SK et al., PRC **98** 034004 (2018)
  - recent extensions: GPU acceleration, separable interactions

Dietz, SK et al., PRC **105** 064002 (2022); SK, arXiv:2211.00395 [nucl-th]

Three-neutron energy levels

Physical n-n scattering length $a_{nn} = -18.9\ \text{fm}$

- interacting levels with positive parity, $S_z = 1/2$



- good convergence up to very large boxes ✓
- **no sign of a three-neutron resonance**

Dietz, SK et al., PRC **105** 064002 (2022)

Three-neutron energy levels

Positive n-n scattering length $a_{nn} = +18.9 \text{ fm}$

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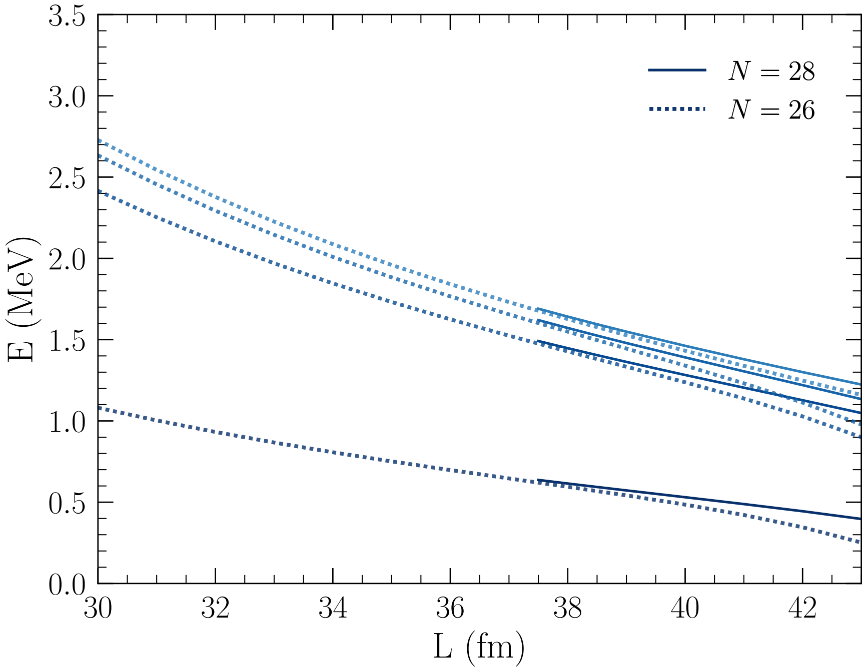

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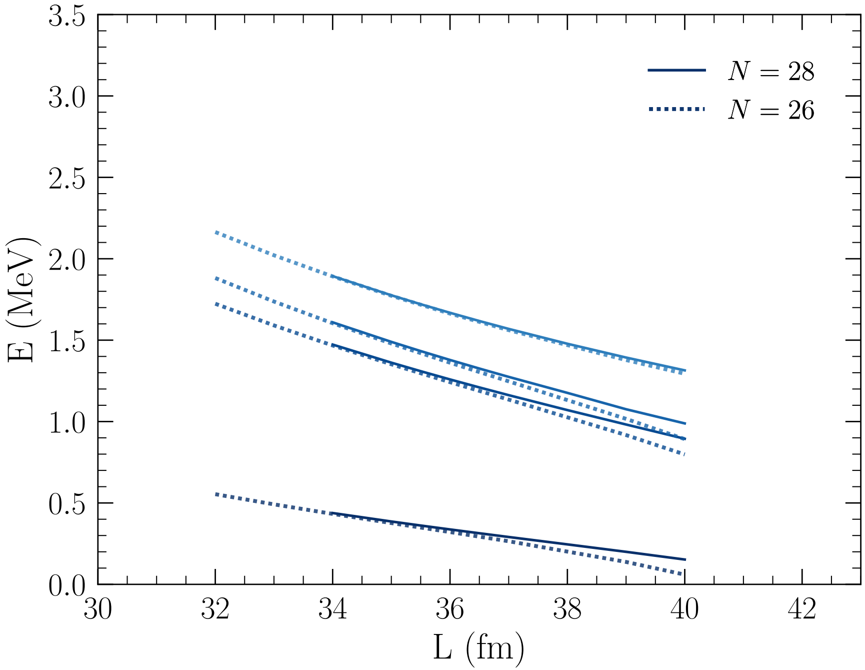
Dietz, SK et al., PRC **105** 064002 (2022)

Three-neutron energy levels

Positive n-n scattering length $a_{nn} = +10.0\text{ fm}$

- interacting levels with positive parity, $S_z = 1/2$



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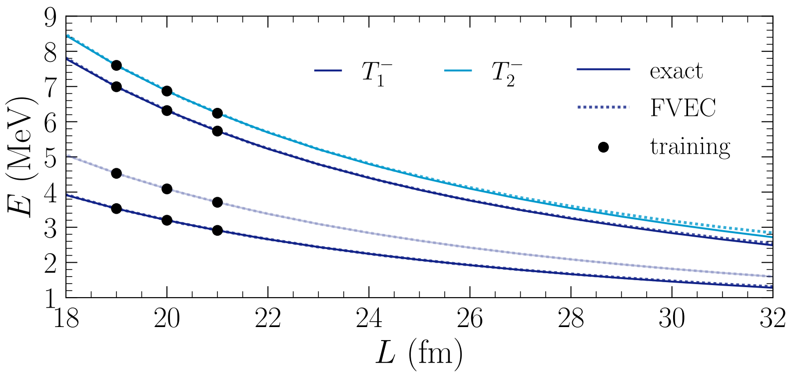
Dietz, SK et al., PRC **105** 064002 (2022)

Finite-volume eigenvector continuation

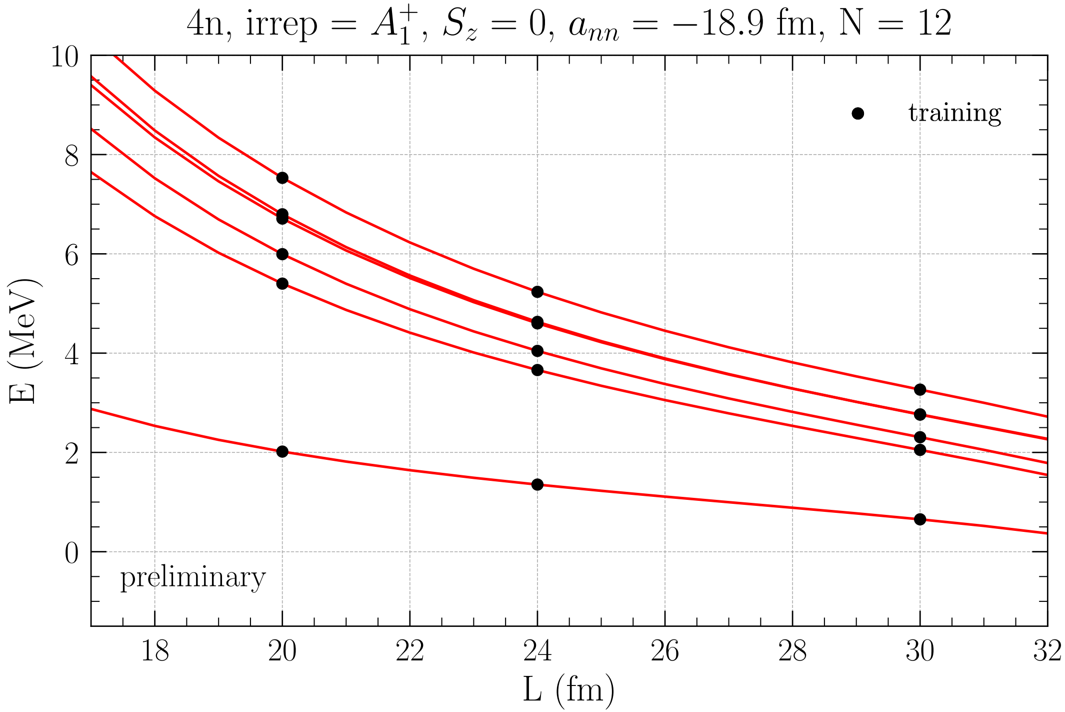
- parametric dependence of Hamiltonian $H(c)$ traces only small subspace
- this can be exploited to construct a powerful extrapolation method called eigenvector continuation Frame et al., PRL **121** 032501 (2018)
- special case of "reduced basis method" (RBM) Bonila et al., arXiv:2203.05282; Melendez et al., arXiv:2203.05528
- method extended to handle parametric dependence in model space directly
  - **enables highly efficient volume extrapolation** Yapa+König, PRC **106** 014309 (2022)



- total number of training data: $3 \times 8 = 24$ (partly covering cubic group multiplets)
- **four-neutron finite-volume resonance search finally feasible with FVEC!**

Four-neutron energy levels

- **preliminary results for four-neutron energy levels**
- calculated with separable Gaussian interaction, cutoff = 150 MeV



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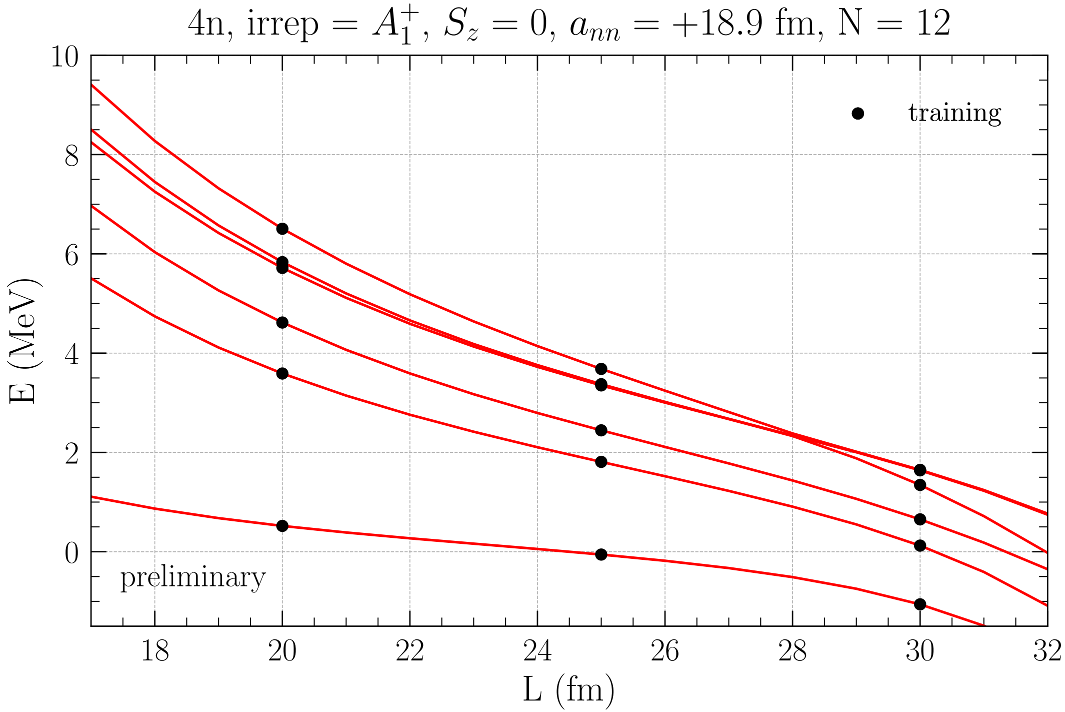


Part II

Volume dependence of charged-particle bound states

N. Yapa, D. Lee, SK, arXiv:2212.14379 [nucl-th]

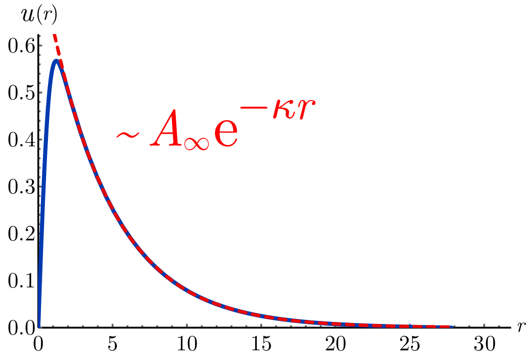
Bound-state volume dependence

- **finite volume affects the binding energy of states:** $E_B \to E_B(L)$

$$\Delta E_B(L) \sim -|A_\infty|^2 \exp\big(-\kappa L\big)/L + \cdots,\quad \boldsymbol{A_\infty} = \textbf{ANC}$$

Lüscher, Commun. Math. Phys. **104** 177 (1986); ...

- infinite-volume properties determine volume dependence
  - binding momentum κ, asymptotic normalization constant (ANC) A_∞
- general prefactor is a polynomial in $1/\kappa L$ SK et al., PRL **107** 112001 (2011); A. Phys. **327**, 1450 (2012)
- relation has been extented to arbitrary two-cluster states SK + Lee, PLB **779** 9 (2018)
- ANCs describe the bound-state wavefunction at large distances
  - **important input quantities for reaction calculations**



Low-energy capture reactions

- $p + {}^9\mathrm{Be} \to {}^{10}\mathrm{B} + \gamma$

Wulf et al., PRC **58** 517 (1998)

- $\alpha + {}^{12}\mathrm{C} \to {}^{16}\mathrm{O}^* + \gamma$
- $\cdots$

deBoer et al., RMP **89** 035007 (2017), ...
SK et al., JPG **40** 045106 (2013)

Charged-particle systems

- **most systems of interest in nuclear physics involve charged particles**

Bound-state volume dependence

- **finite volume affects the binding energy of states:** $E_B \to E_B(L)$

$$\Delta E_B(L) \sim -|A_\infty|^2 \exp\big(-\kappa L\big)/L + \cdots,\ \boldsymbol{A_\infty = \text{ANC}}$$

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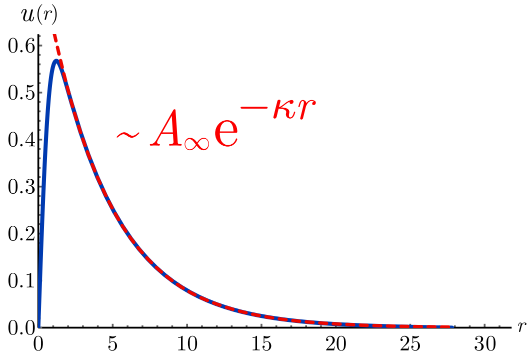

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- $p + {}^9\mathrm{Be} \to {}^{10}\mathrm{B} + \gamma$

Wulf et al., PRC **58** 517 (1998)

- $\alpha + {}^{12}\mathrm{C} \to {}^{16}\mathrm{O}^* + \gamma$
- $\cdots$

deBoer et al., RMP **89** 035007 (2017), ...
SK et al., JPG **40** 045106 (2013)

Charged-particle systems

- **most systems of interest in nuclear physics involve charged particles**

Charged-particle systems

- **most systems of interest in nuclear physics involve charged particles**
- nonrelativistic description with short-range interaction + long-range Coulomb force

$$H + H_0 + V + V_C \ , \ V_C(r) = \frac{\gamma}{r} = \frac{2\mu\alpha Z_1 Z_2}{r}$$

- charged bound-state wavefunctions have **Whittaker tails**:

$$\psi_\infty(r) \sim W_{-\bar{\eta},\frac{1}{2}}(2\kappa r)/r \sim \frac{\mathrm{e}^{-\kappa r}}{(\kappa r)^{\bar{\eta}}}$$

  - these govern the asymptotic volume dependence
  - additional suppression at large distances
  - depends on Coulomb strength: $\bar{\eta} = \gamma/(2\kappa)$
  - for $\alpha - \alpha$ system: $\gamma \approx 0.55 \ \mathrm{fm}^{-1}$

- details worked out by graduate student Hang Yu

Yu, Lee, SK, arXiv:2212.14379 [nucl-th]

Coulomb = exp $\rightarrow$ Whittaker function?

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Yes, but not quite so simple...

Periodic Coulomb potential

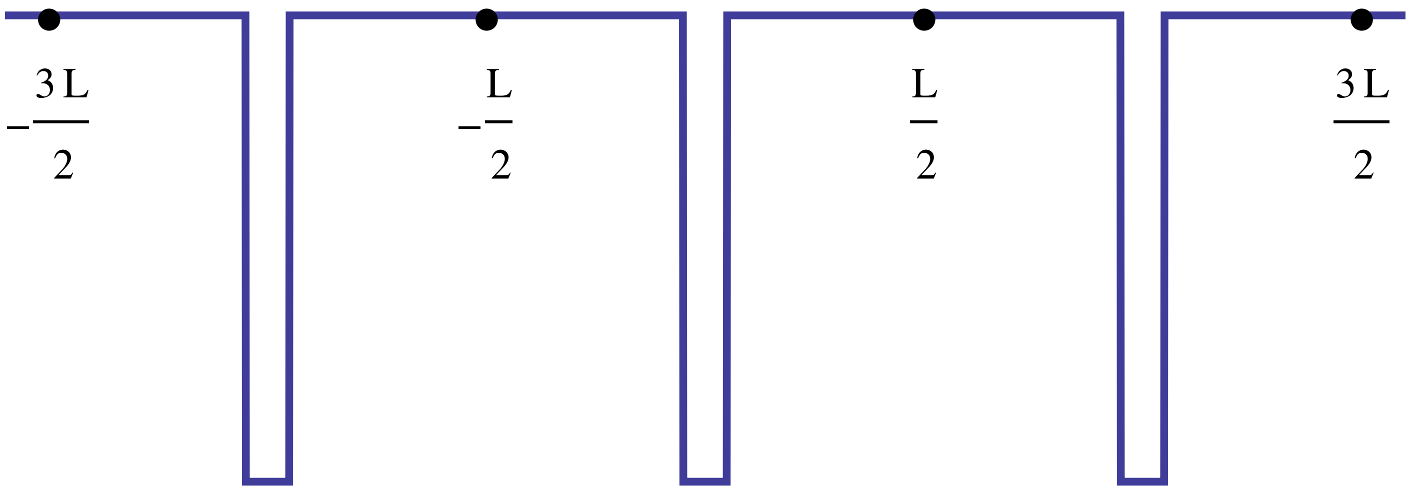
- short-range interaction easy to extend periodically: $V_L(\mathbf{r}) = \sum_{\mathbf{n}} V(\mathbf{r} + \mathbf{n}L)$
  - trivial for finite-range potental V
  - converging sum, negligible corrections for V falling faster than power law

Periodic short-range potentials

- implement periodic boundary condition via shifted potentials copies:

$$V_L(\mathbf{r}) = \sum_{\mathbf{n}\in\mathbb{Z}^3} V(\mathbf{r} + \mathbf{n}L)$$

- necessary condition for this: $R = \mathrm{range}(V) \ll L$



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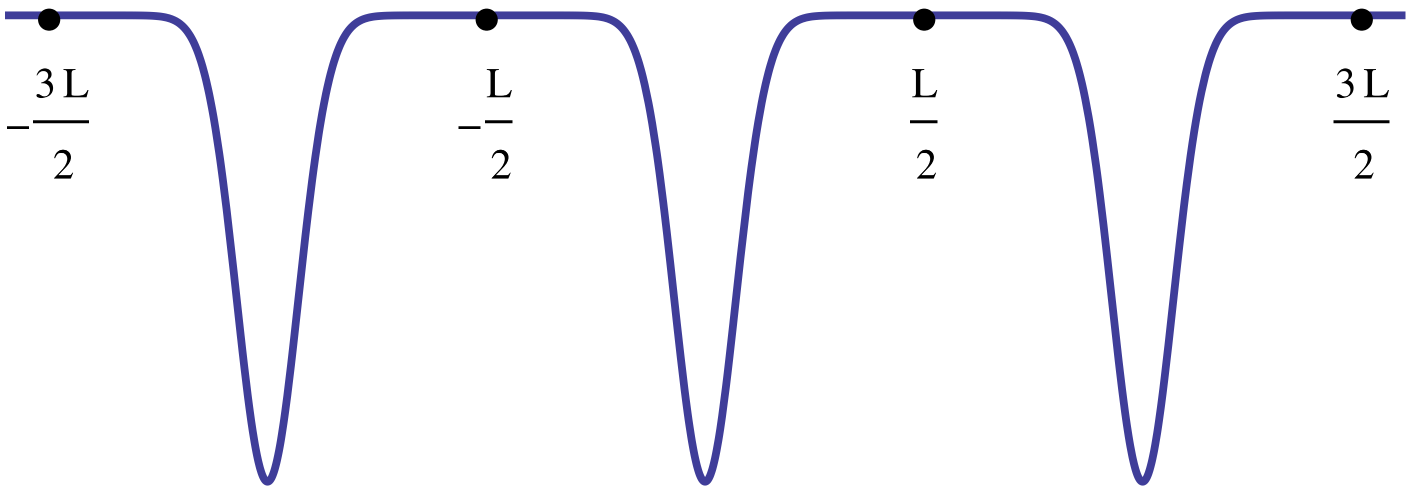

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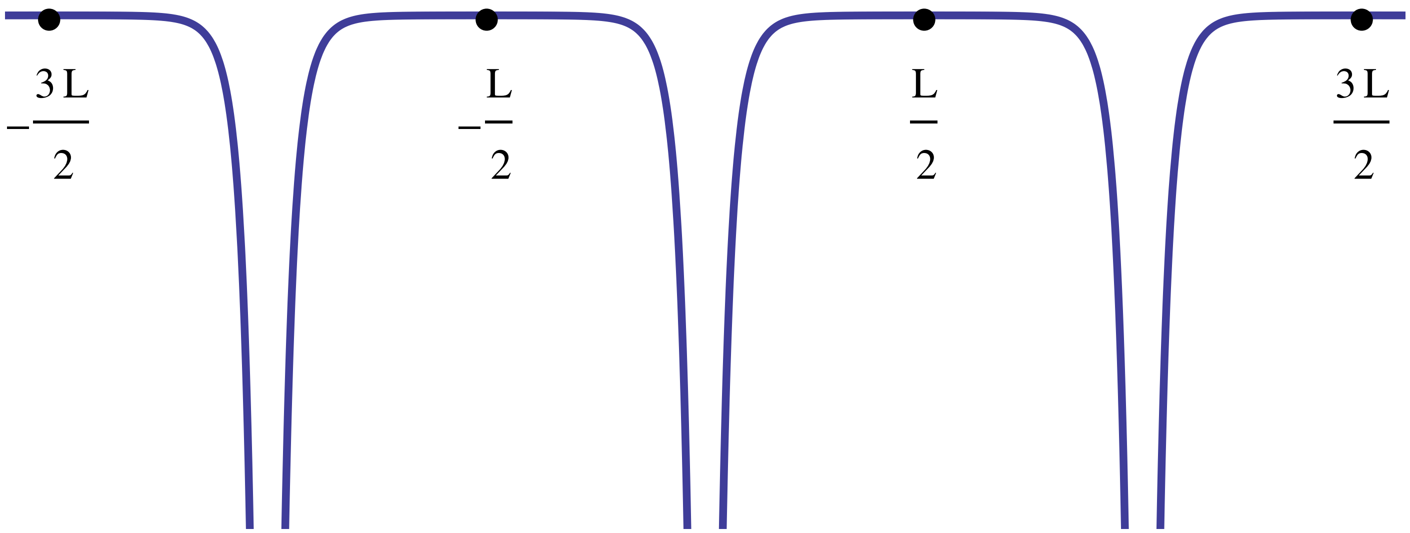

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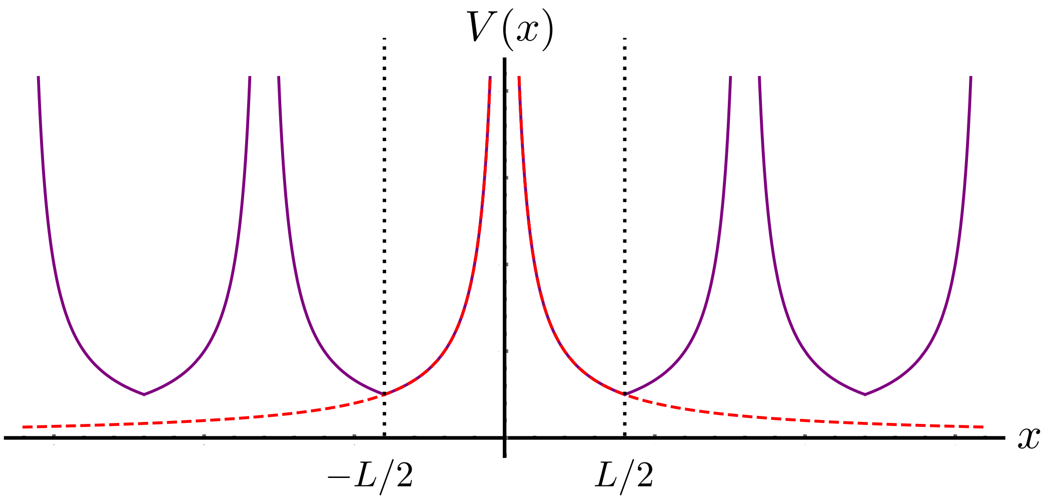
Solution

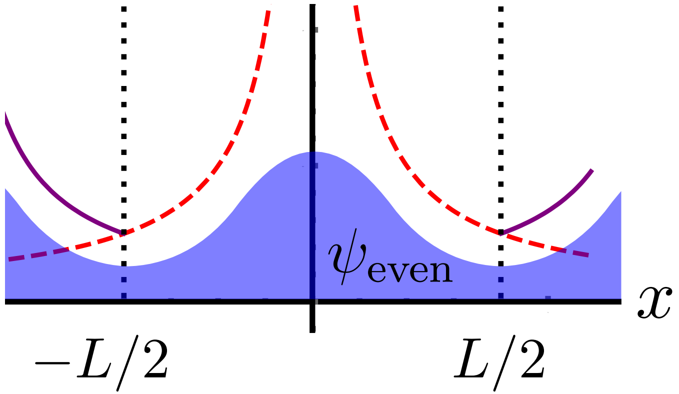
- **cut off at box boundary, grow Coulomb tail with L**
- nicely matches practical implementation (e.g. in Lattice EFT)



Exact result in one dimension

- **exact form in one spatial dimension can be found from boundary condition**
- derivative of wavefunction needs to vanish at boundary: $\psi'_\kappa(L/2) = 0$
- for fixed L this determines the binding momentum $\kappa = \kappa(L)$
  - linear combination of Jost functions
  - ANC from S-matrix residue

    Fäldt+Wilkin, Phys. Scr. **56** 566 (1997)
  - $\Delta E(L) = 2\kappa\Delta\kappa(L)$



$$\Delta E(L) = -\frac{\kappa}{\mu} A_\infty^2 e^{i\pi\bar{\eta}} \frac{W'_{-\bar{\eta},\frac{1}{2}}(\kappa L)}{W'_{\bar{\eta},\frac{1}{2}}(-\kappa L)} + \mathcal{O}\left[e^{-2\kappa L}\right] \qquad \text{(1D, even parity)}$$

- seemingly complex phase cancels against Whittaker functions ✓
- reduces to simple exponential for $\gamma \to 0$ (no Coulomb) ✓

Charged-particle volume dependence

- three-dimensional derivation is more involved due to **nontrival boundary condition**
  - can be done with two-step procedure, formal perturbation theory
  - introduce $\tilde{H}_L = H_0 + V_{C,\{L\}} + V = H + \Delta V_C \rightsquigarrow$ eigenstate $\tilde{\psi}_L$
  - for the exact solution, both potentials are periodic: $H_L = H_0 + V_{C,\{L\}} + V_{\{L\}}$
  - volume dependence follows from ansatz $\tilde{\psi}_{L,0}(\mathbf{x}) = \sum_{\mathbf{n}\in\mathbb{Z}^3} \tilde{\psi}_L(\mathbf{x} - \mathbf{n}L)$

$$\Delta E(L) = \underbrace{-\frac{3A_\infty^2}{\mu L}\left[W'_{-\bar{\eta},\frac{1}{2}}(\kappa L)\right]^2}_{\equiv \Delta E_0(L)} + \Delta\tilde{E}(L) + \Delta\tilde{E}'(L) + \mathcal{O}\left[e^{-\sqrt{2}\kappa L}\right] \qquad (3\mathrm{D},\ A_1^+)$$

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Correction terms

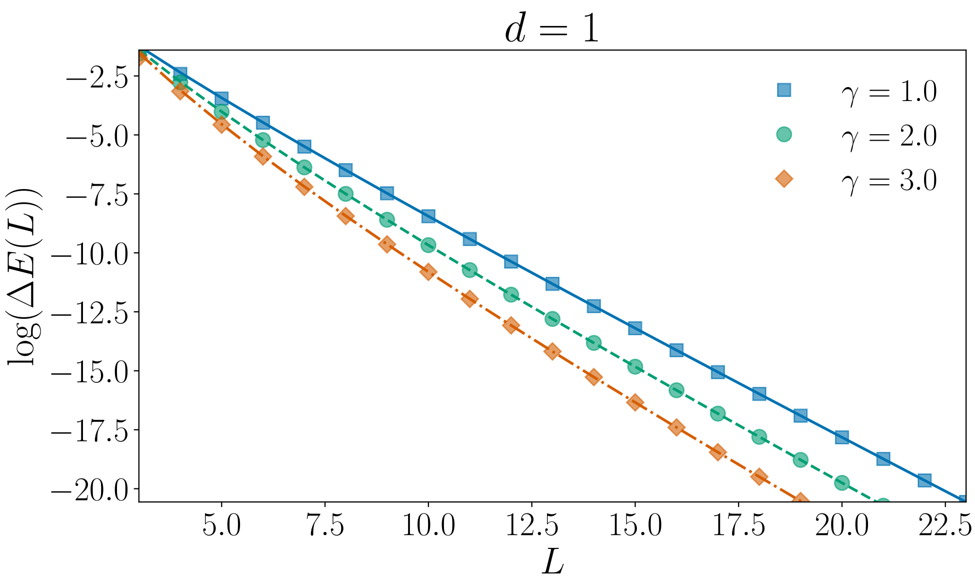
- in addition to exponentially suppressed corrections, there are two other terms
- these arise from the Coulomb potential and vanish for $\gamma \to 0$
- the perturbative approach makes it possible to deriver their behavior

Yu, Lee, SK, arXiv:2212.14379 [nucl-th]

$$\Delta\tilde{E}(L), \Delta\tilde{E}'(L) = \mathcal{O}\left(\frac{\bar{\eta}}{(\kappa L)^2}\right) \times \Delta E_0(L)$$

Numerical checks

- **the relations can be checked with explicit numerical calculations**
- simple lattice discretization with attrative Gaussian potentials
- the Coulomb singularity at the origin is also regularized: $V_{C,\mathrm{Gauss}}(r) \sim \dfrac{1 - \mathrm{e}^{-r^2/R_C^2}}{r}$
  - this is equivalent to a redefinition of the short-range potential



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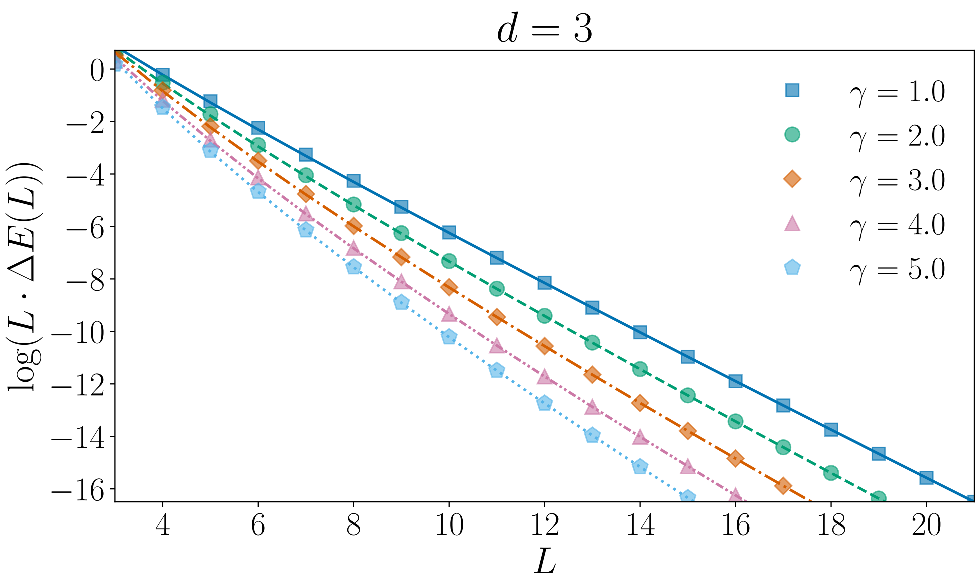

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	Finite-volume fit			Continuum result	
γ	κ_∞	A_∞	L range	κ_∞	A_∞
			$d = 1$		
1.0	0.861110(3)	2.1286(1)	$12 \sim 24$	0.860	2.1284
2.0	0.861125(9)	4.4740(9)	$12 \sim 23$	0.860	4.4782
3.0	0.86108(6)	10.386(2)	$12 \sim 20$	0.858	10.435
			$d = 3$		
1.0	0.8610(3)	5.039(2)	$17 \sim 28$	0.861	5.049
2.0	0.8607(3)	11.71(4)	$15 \sim 26$	0.860	11.79
3.0	0.8605(7)	29.95(20)	$14 \sim 24$	0.859	30.31
4.0	0.8604(1)	83.14(10)	$14 \sim 22$	0.858	84.76
5.0	0.8604(2)	247.9(5)	$14 \sim 18$	0.857	255.4

- **excellent agreement with direct continuum calculations**
  - obtained by solving the radial Schrödinger equation

Yu, Lee, SK, arXiv:2212.14379 [nucl-th]

Summary and outlook

Few-neutron systems in pionless EFT

- studied three- and four neutrons with separable contact interaction
- finite-volume simulations complement Faddeev equations for three neutrons
- no indication for three-neutron resonance with large nn scattering length
  - consistent with previous work
- finite-volume eigenvector continuation enables studies of larger system
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Volume dependence of charged-particle bound states

- wave function at large distances determines finite-volume energy shift
- possible to extract asymptotic normalization coefficients
- long-range Coulomb force complicates derivation
- leading volume dependence derived for 1D and 3D S-wave systems
- asymptotic bounds for additional correction terms
- **will be applied for ANC calculations based on lattice EFT**

Thanks...

...to my students and collaborators...

- S. Dietz, H.-W. Hammer, A. Schwenk (TU Darmstadt)
- H. Yu, N. Yapa (NCSU)
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...and to you, for your attention!