Volume dependence of quantum bound states and resonances

Sebastian König

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

Hirschegg, January 18, 2024

Thanks...

...to my students and collaborators...

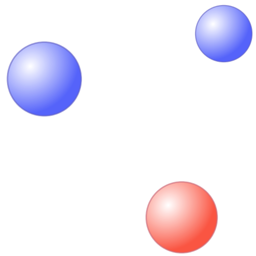
- **H. Yu, N. Yapa, A. Taurence, A. Andis (NCSU)**
- D. Lee (FRIB/MSU), K. Fossez (FSU)
- S. Dietz, H.-W. Hammer, A. Schwenk (TU Darmstadt)
- U.-G. Meißner (U Bonn)
- P. Klos, J. Lynn, S. Bour, ...

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

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

- Jülich Supercomputing Center
- NCSU High-Performance Computing Services

Quantum systems in a box



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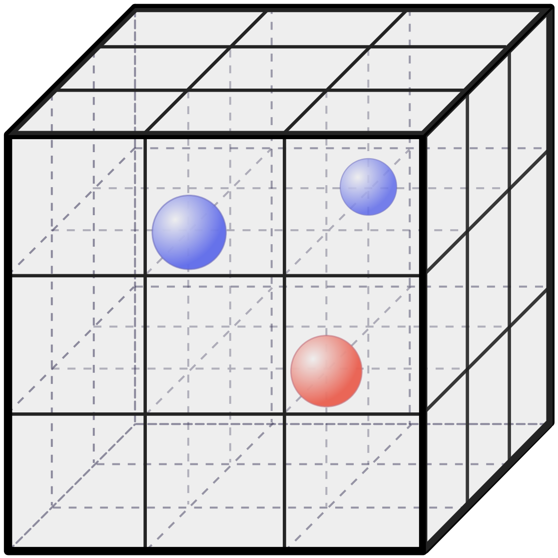

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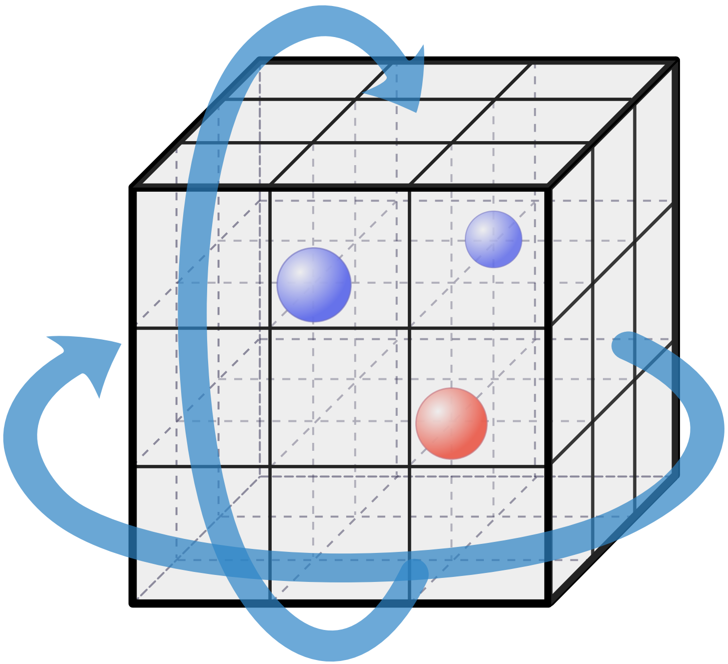

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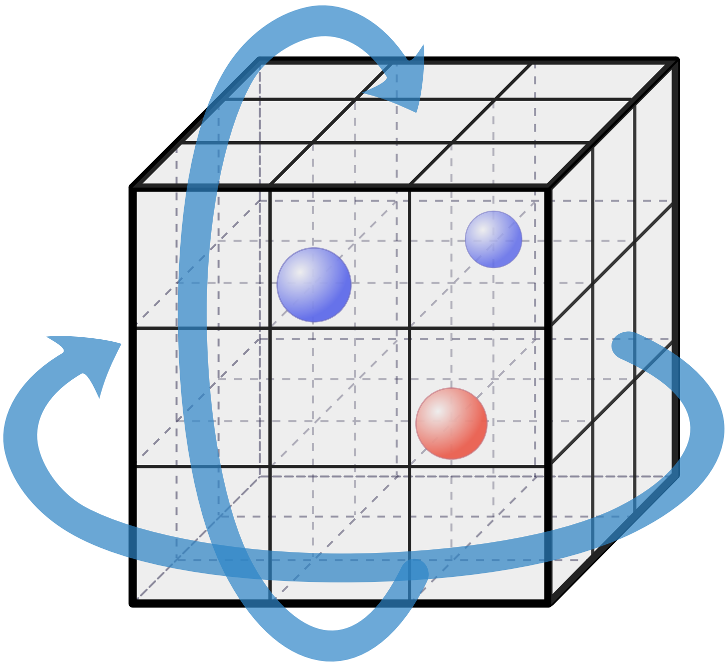

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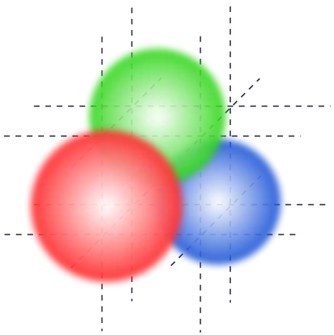
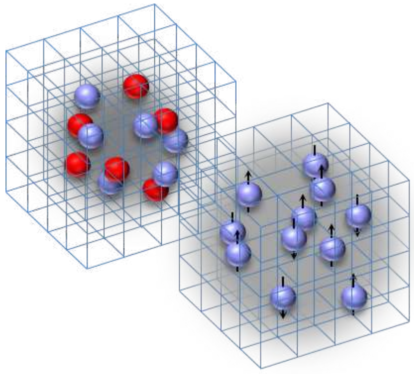
- place them in a finite cubic geometry...
- ...and impose periodic boundary conditions

- lattice spacing (if any): UV effects; **box size: IR effects $\rightsquigarrow$ physics**

Relevance of finite-volume relations

Lattice simulations





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- **lattice QCD:** few baryons, small volumes
- **lattice EFT:** larger volumes, many more particles

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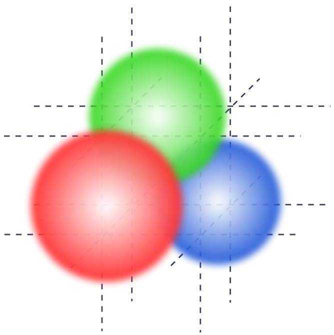

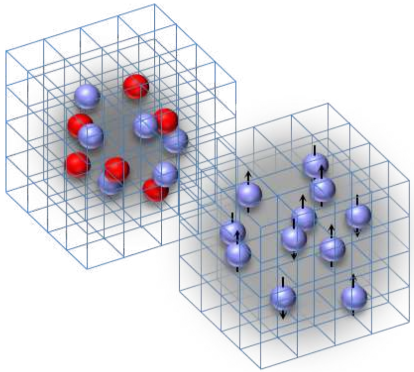

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Harmonic oscillator calculations

- infrared basis extrapolation

More et al, PRC **87** 044326 (2013); ...

- Busch formula: extraction of scattering phase shifts

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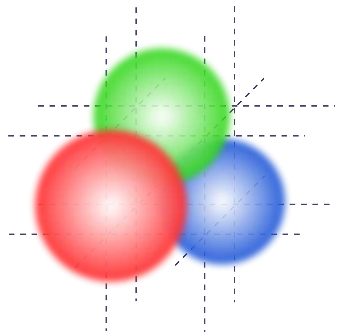

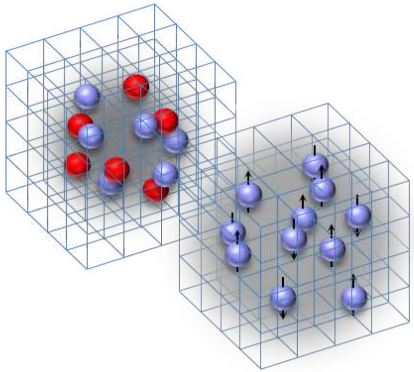

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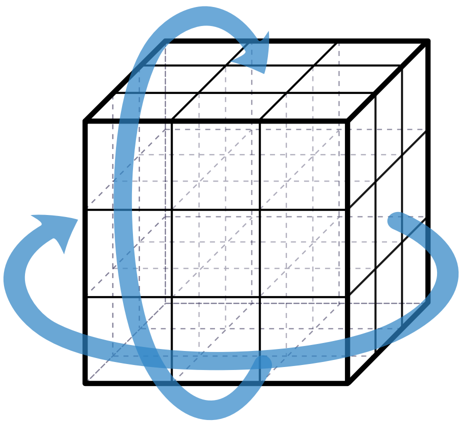
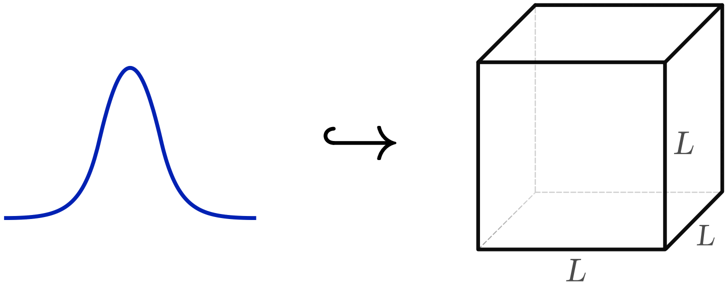
Dedicated finite-volume few-body simulations

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

Bound states

Resonances

Outlook

Bound states

SK et al., PRL **107** 112001 (2011); Annals Phys. **327**, 1450 (2012)

SK + Lee, PLB **779** 9 (2018)

H. Yu, SK, D. Lee, PRL **131** 212502 (2023)

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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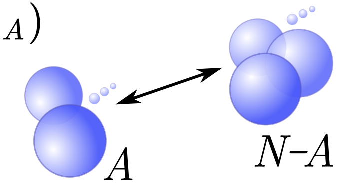

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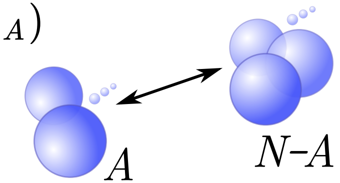

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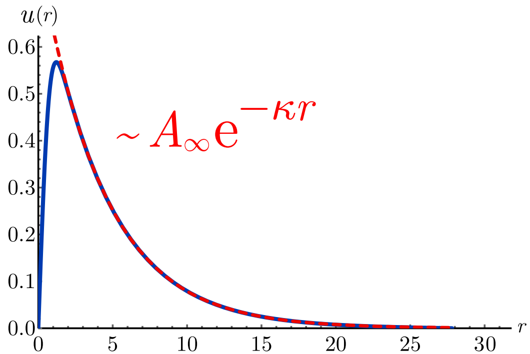
- **ANCs describe the bound-state wave function at large distances**
  - **important input quantities for reaction calculations**



Low-energy capture reactions

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

  Wulf et al., PRC **58** 517 (1998)
- $\alpha + {}^{12}\mathrm{C} \to {}^{16}\mathrm{O}^* + \gamma$

  deBoer et al., RMP **89** 035007 (2017), ...
- $\ldots$

  SK et al., JPG **40** 045106 (2013)

Higher partial waves

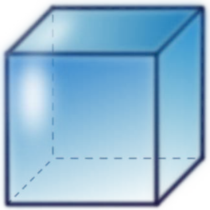
- **general result:** $\Delta E(L) = \alpha\left(\frac{1}{\kappa L}\right) \times |A_\infty|^2 \frac{\mathrm{e}^{-\kappa L}}{\mu L} + \mathcal{O}\left(\mathrm{e}^{-\sqrt{2}\kappa L}\right)$

ℓ	Γ	$\alpha(x)$
0	A_1^+	-3
1	T_1^-	$+3$
2	T_2^+	$30x + 135x^2 + 315x^3 + 315x^4$
2	E^+	$-1/2\,(15 + 90x + 405x^2 + 945x^3 + 945x^4)$

SK et al., PRL **107** 112001 (2011); Annals Phys. **327**, 1450 (2012)

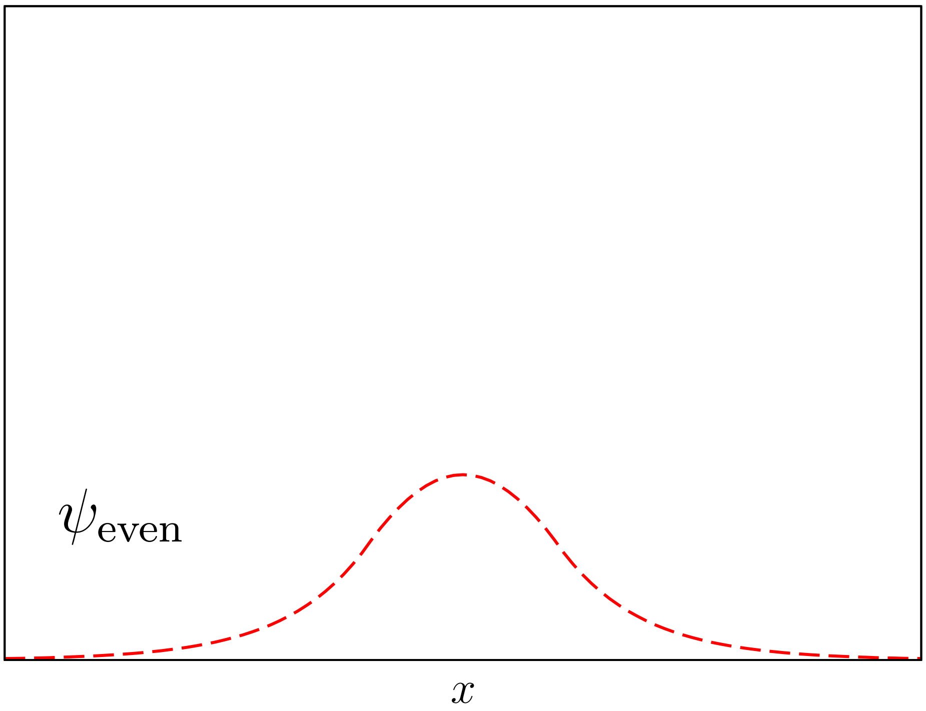
- prefactor for any bound state is polynomial in $1/(\kappa L)$
- depends in general on irreducible representation of the cubic group

rotation group $SO(3)$ $\longrightarrow$



cubic group O

Sign of the energy shift



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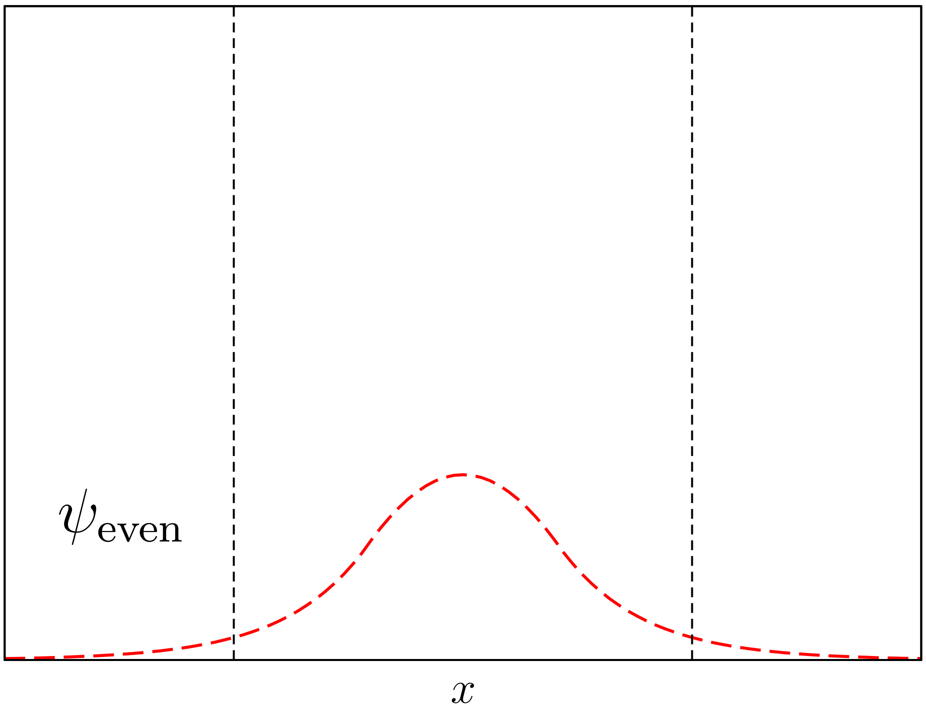

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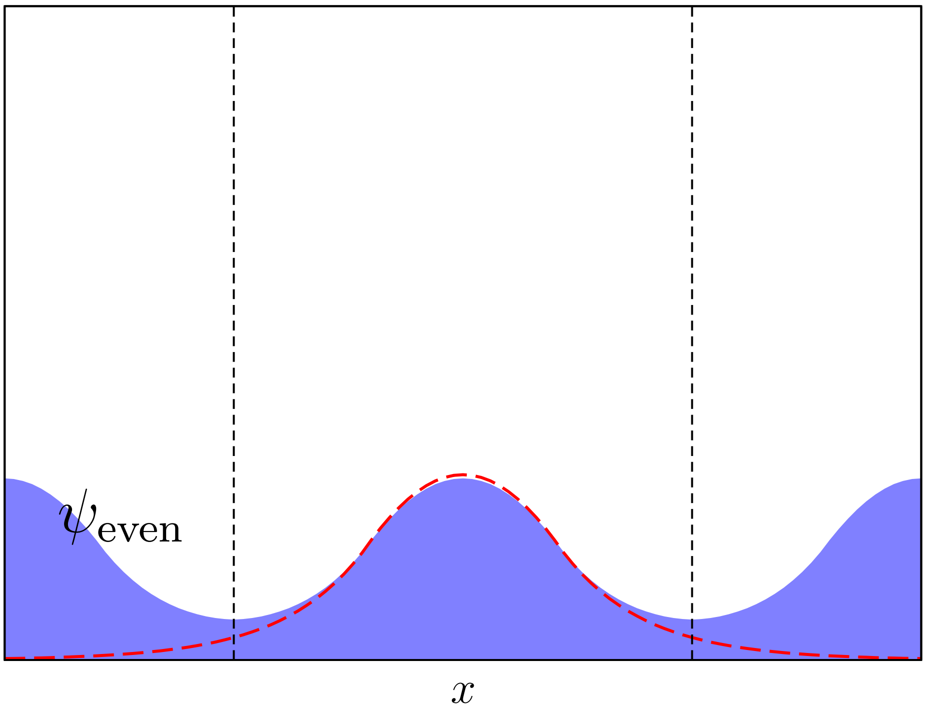

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even parity $\to$ WF profile relaxed $\to$ less curvarture $\rightsquigarrow$ **more deeply bound**

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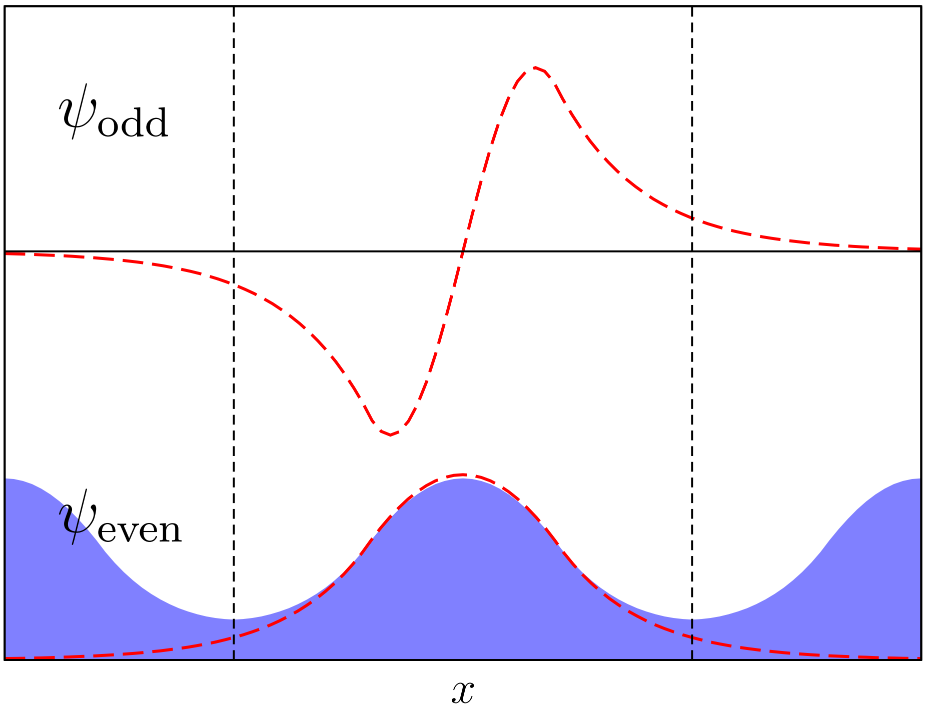

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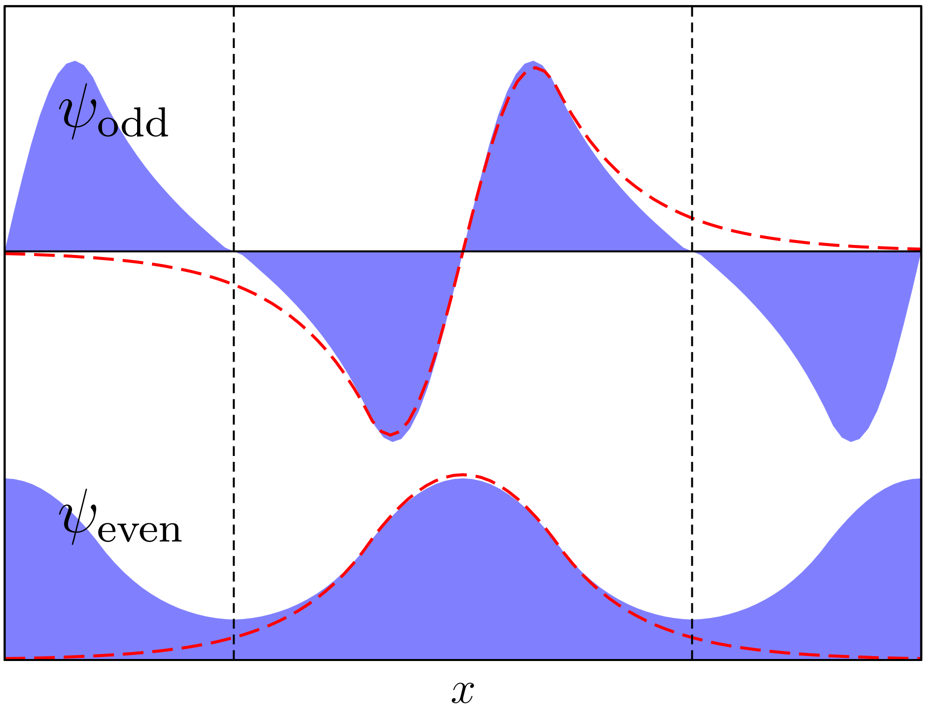
Sign of the energy shift

odd parity $\rightarrow$ WF profile compressed $\rightarrow$ more curvarture $\rightsquigarrow$ **less deeply bound**



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Charged-particle systems

Most nuclear systems involve multiple charged particles!

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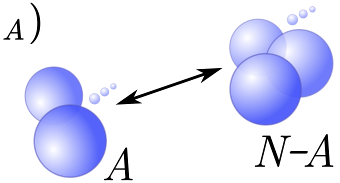

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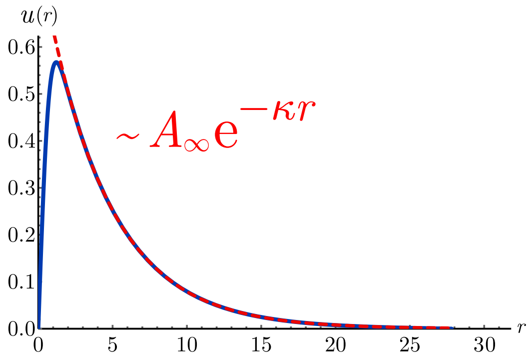

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- nonrelativistic description with short-range interaction + long-range Coulomb force

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

- 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, PRL **131** 212502 (2023)

Coulomb = exp $\longrightarrow$ Whittaker function?

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Yes, but not quite so simple...

Periodic Coulomb potential

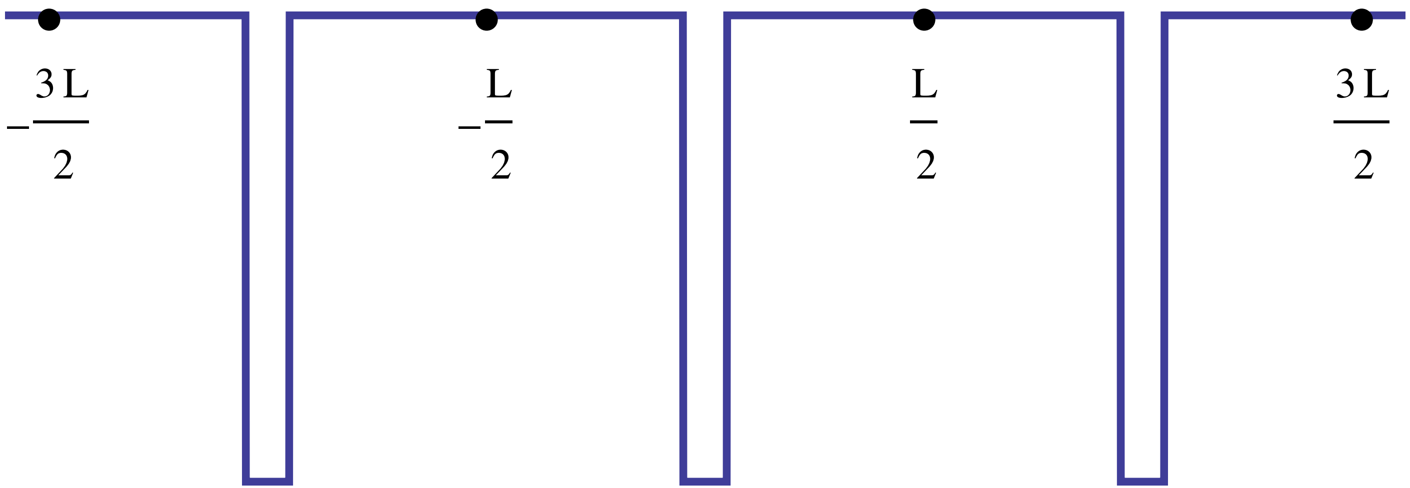
- **short-range interaction easy to extend periodically:** $V_L(\mathbf{r}) = \sum_{\mathbf{n}} V(\mathbf{r} + \mathbf{n}L)$
  - trivial for finite-range potental V
  - converging sum, negligible corrections for V falling faster than power law

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: $R = \text{range}(V) \ll L$



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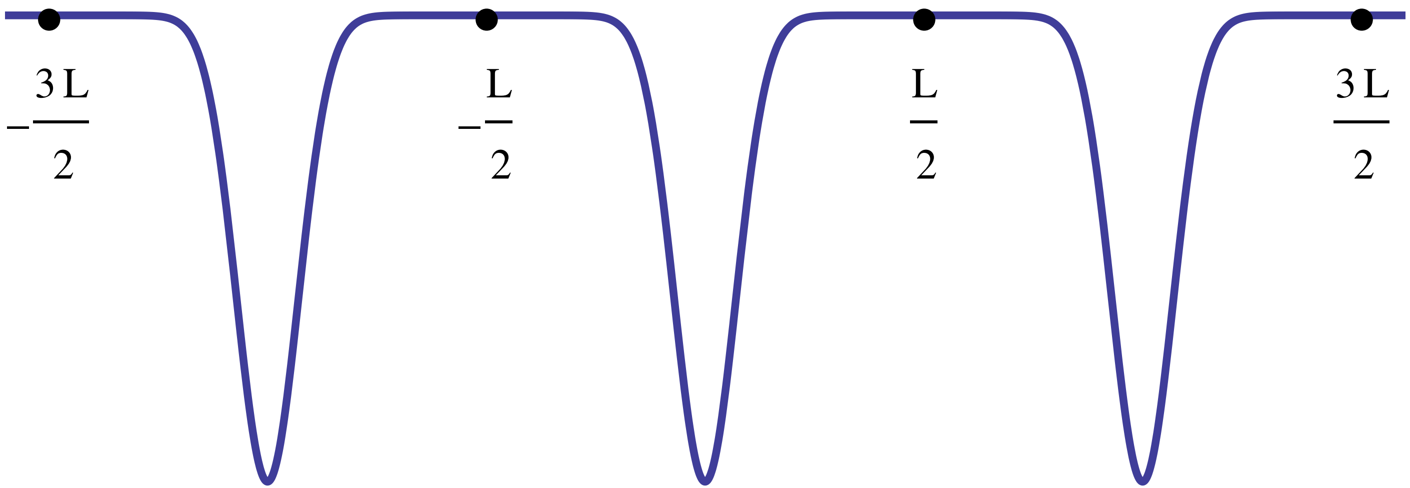

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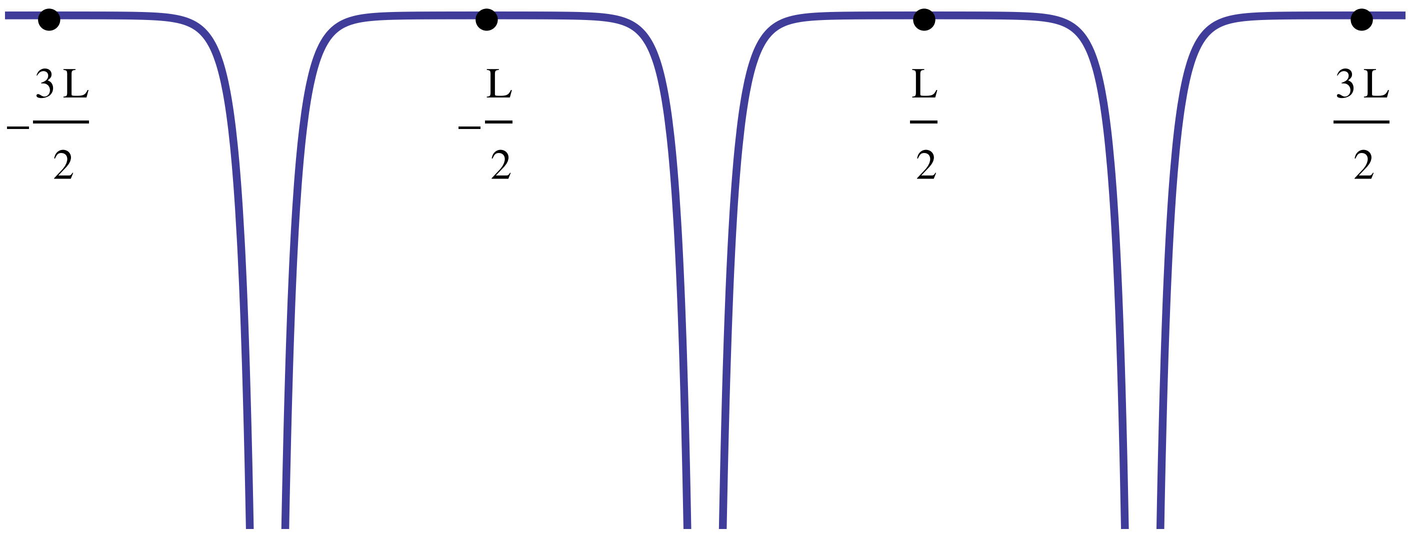

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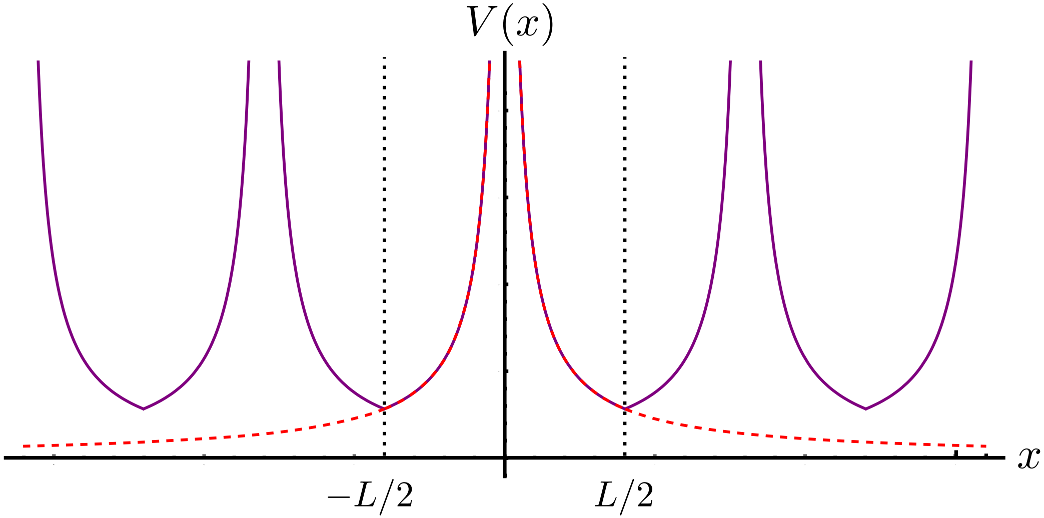
Solution

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



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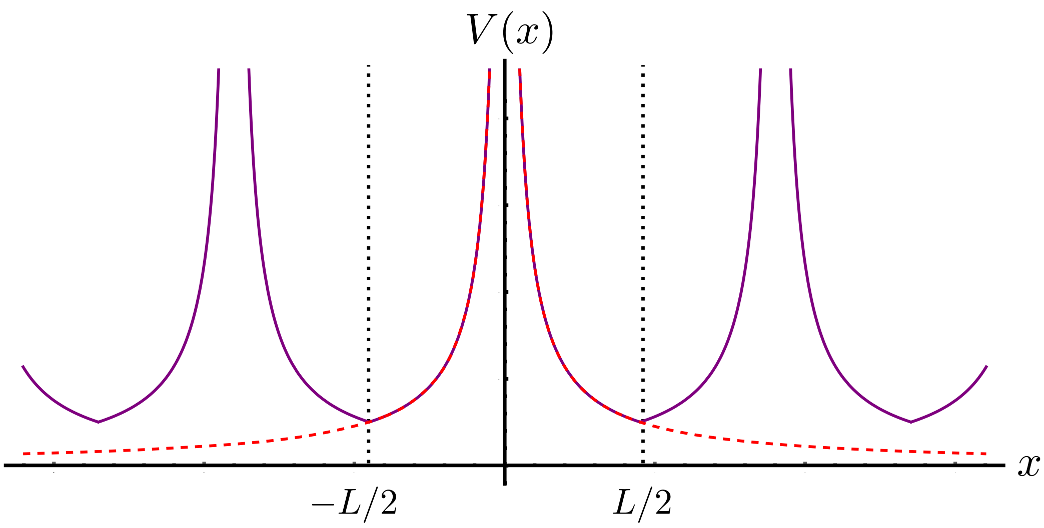

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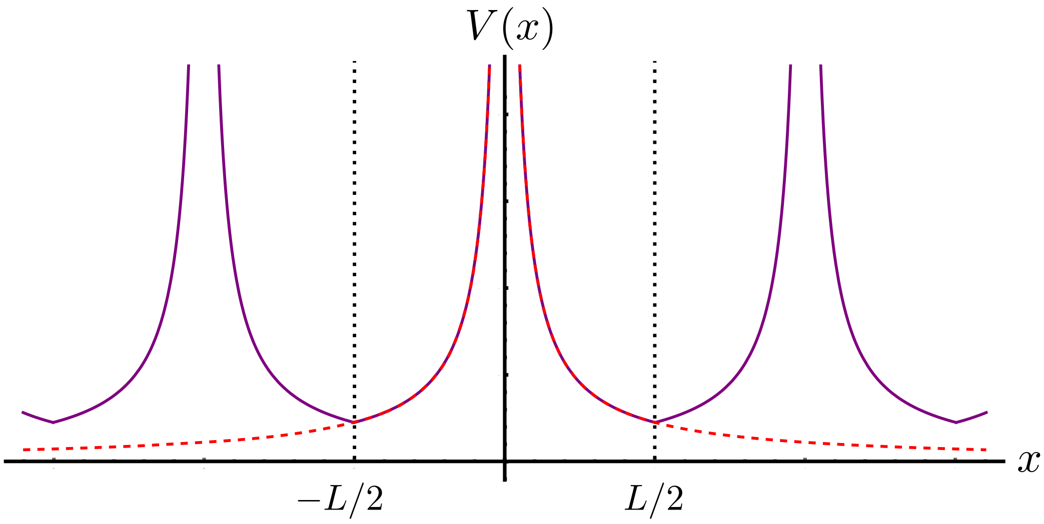

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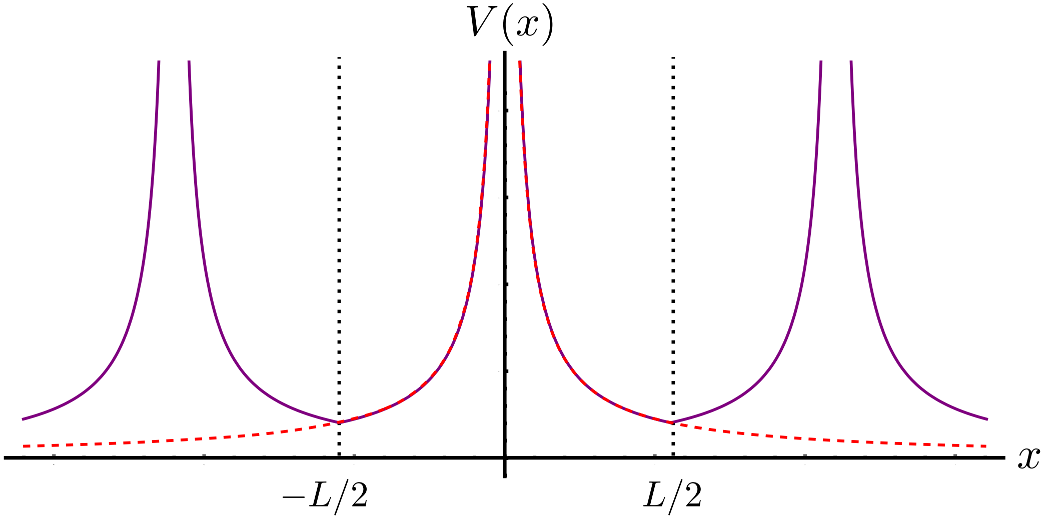

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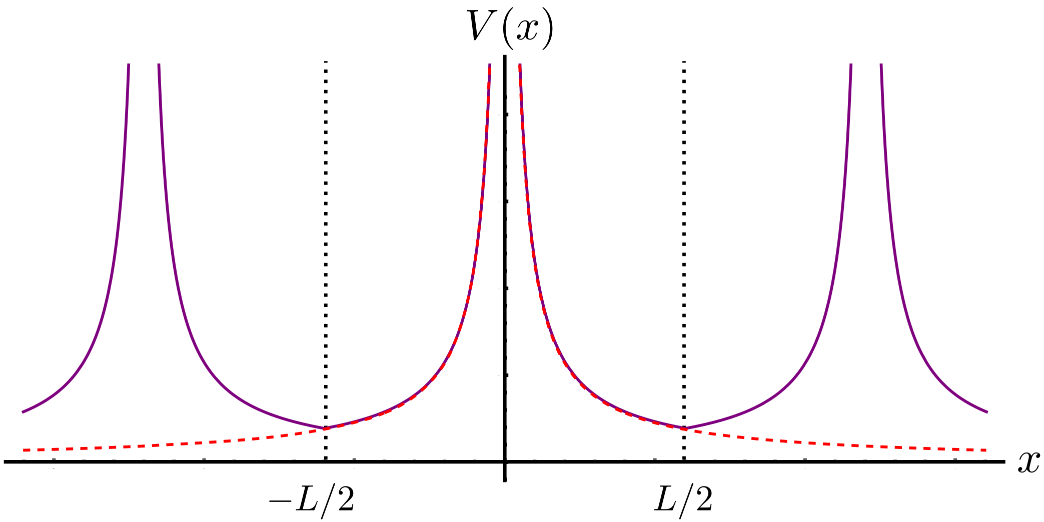
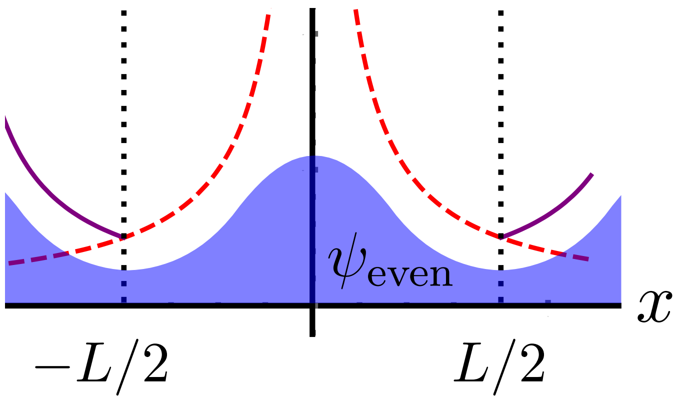


Exact result in one dimension

- **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)
  - $\Delta E(L) = 2\kappa\Delta\kappa(L)$



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

- 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 complicated due to **nontrival boundary condition**
  - can be done with two-step procedure based on formal perturbation theory
  - intricate details worked out by Hang Yu
  - $\rightsquigarrow$ leading result for S-wave states (cubic A_1^+ representation)

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

Correction terms

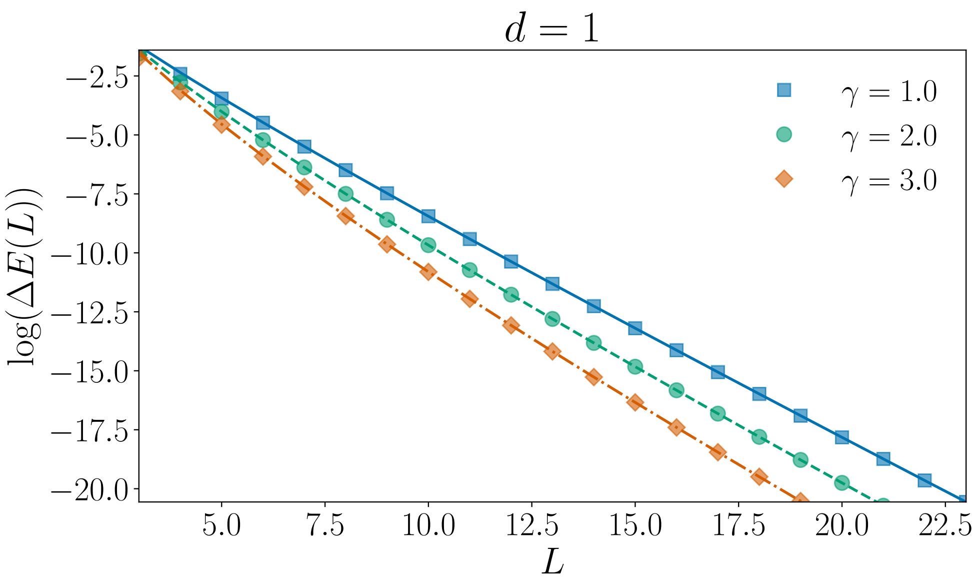
- in addition to exponentially suppressed corrections, there are two other terms
- these arise from the Coulomb potential and vanish for $\gamma \to 0$
- the perturbative approach makes it possible to derive their behavior

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

Yu, Lee, SK, PRL **131** 212502 (2023)

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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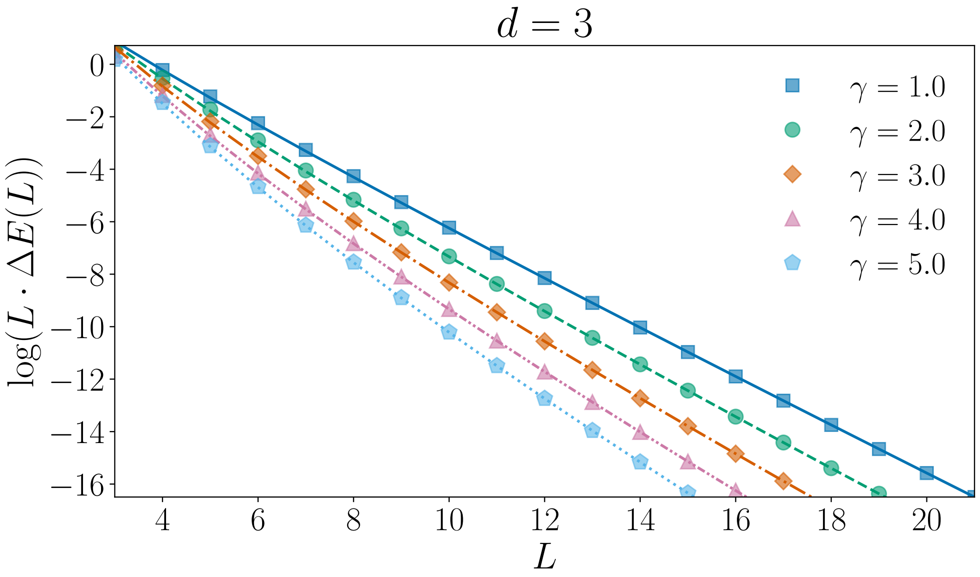

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	Finite-volume fit			Continuum result	
γ	κ_∞	A_∞	L range	κ_∞	A_∞
			$d = 1$		
1.0	0.861110(3)	2.1286(1)	$12 \sim 24$	0.860	2.1284
2.0	0.861125(9)	4.4740(9)	$12 \sim 23$	0.860	4.4782
3.0	0.86108(6)	10.386(2)	$12 \sim 20$	0.858	10.435
			$d = 3$		
1.0	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

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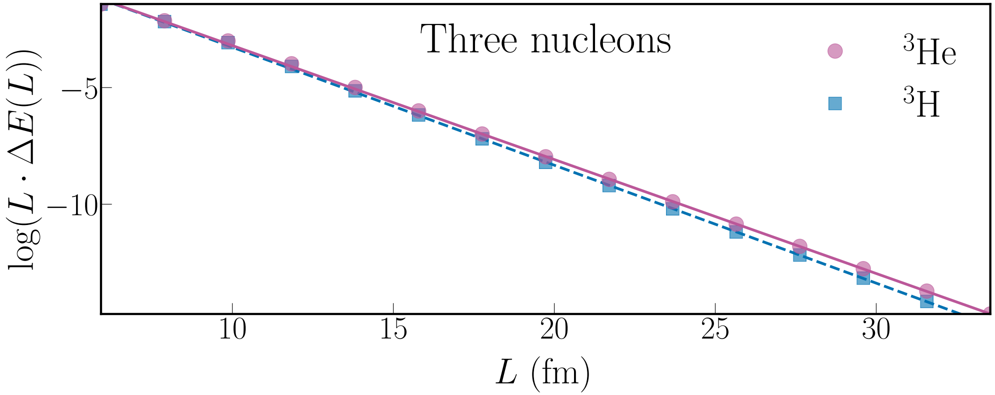
- **excellent agreement with direct continuum calculations**
  - obtained by solving the radial Schrödinger equation

Three-nucleon system: ^{3}He vs. ^{3}H

- **consider pionless EFT with SU(4) symmetric contact interaction**
- parameters tuned in infinite volume (very large box)
  - two-body interaction to produce 1 MeV deuteron
  - three-body interaction to produce physical triton
  - add Coulomb and short-range pp counterterm to also produce physical ^{3}He



- extract proton-deuteron ANC as $A_\infty = 1.44(1)\,\mathrm{fm}^{-1/2}$
- **would be off by 5% with pure short-range volume dependence fit**
  - significant effect given that Coulomb strengh $\gamma \sim 0.05\,\mathrm{fm}^{-1}$ is pretty small here!

Resonances

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

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

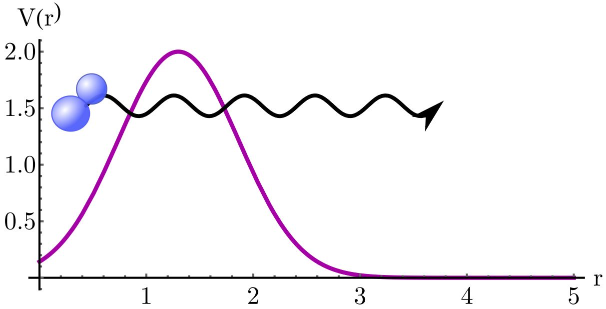
Yapa, SK, PRC **106** 014309 (2022)

Yu, Yapa, SK, PRC **109** 014316 (2024)

Resonances

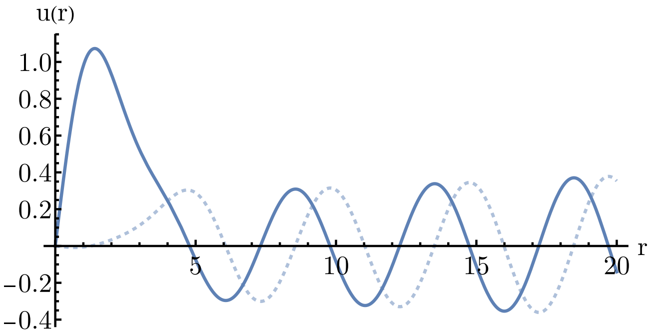
Intuitive

- **metastable state (finite lifetime)**
- tunneling through potential barrier



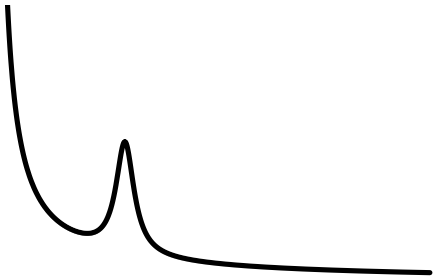
Formally

- **S-matrix pole at complex energy**
- wavefunction similar to bound state...
- ...but not quite normalizable



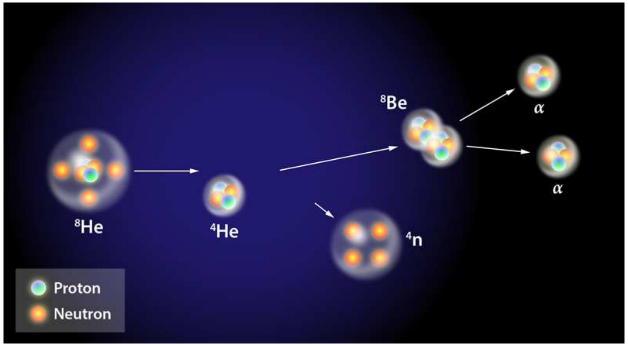
Experimentally

- **enhancement in cross section**
- related to sharp jump in scattering phase shift
- $\sigma \sim \dfrac{\Gamma^2}{(E - E_R)^2 + \Gamma^2/4}$

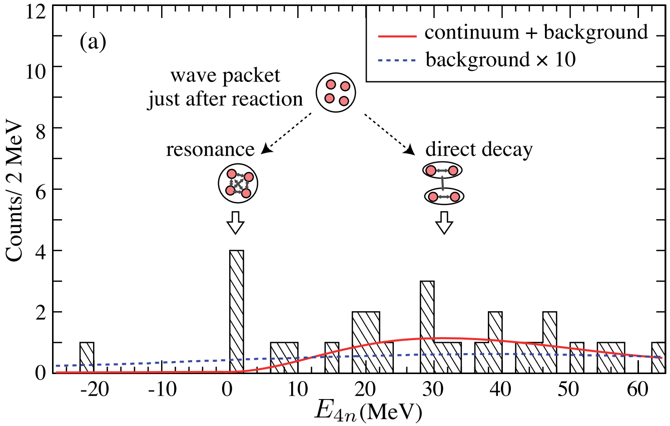


Tetraneutron situation (I)

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 (II)

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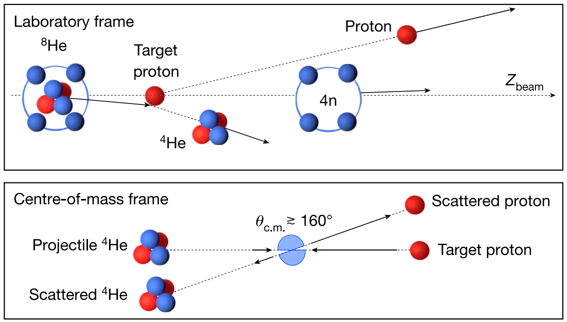
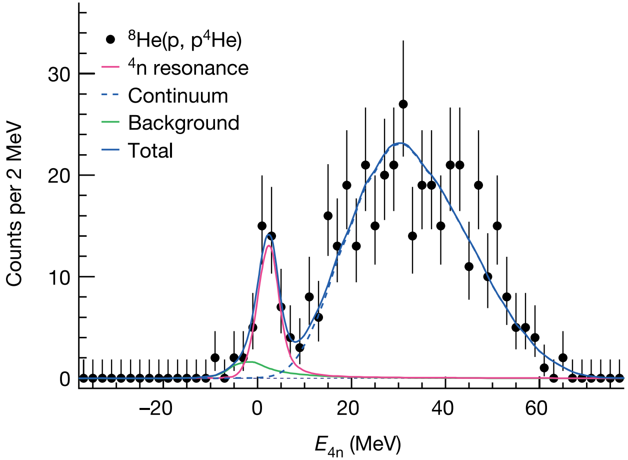


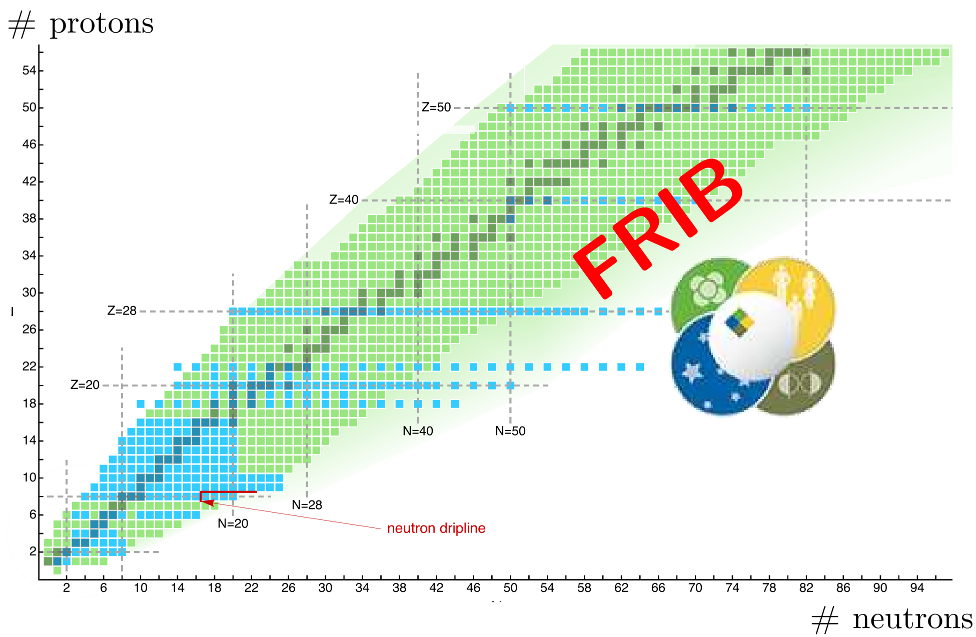
Duer et al., Nature **606** 678 (2022)



- 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., PRL **130** 102501 (2023)

More exotic nuclei



original chart: Hergert et al., Phys. Rep. **621** 165 (2016)

- **FRIB will discover a host of unknown nuclei near the edge of stability**
  - among those there are likely exotic states
  - halos, clusters ⇝ few-body resonances

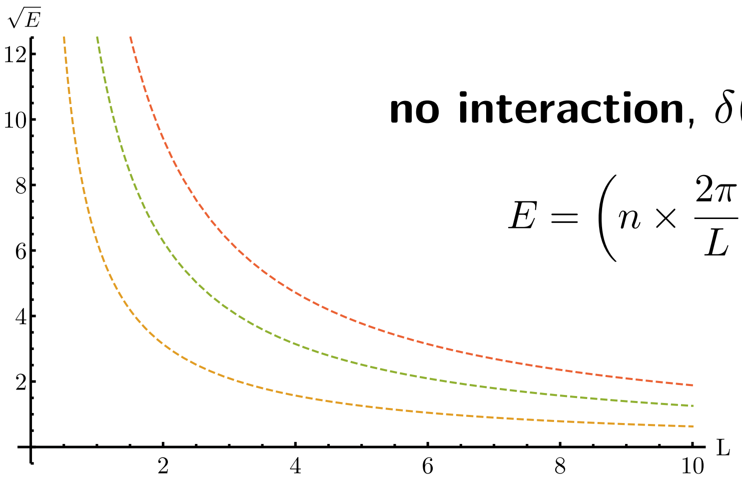
Finite-volume resonance signatures

Lüscher formalism

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

Lüscher, NPB **354** 531 (1991); ...

Wiese, NPB (Proc. Suppl.) **9** 609 (1989); ...



no interaction, $\delta(p) = 0$

$$E = \left(n \times \frac{2\pi}{L}\right)^2$$

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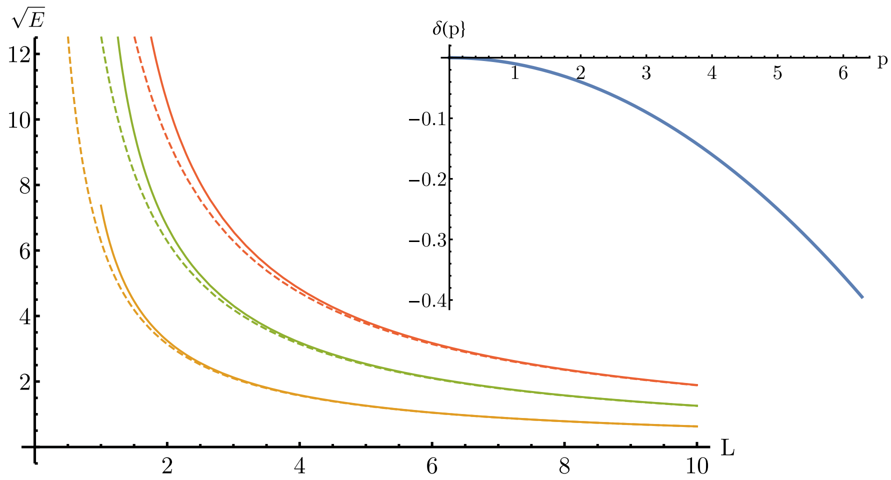

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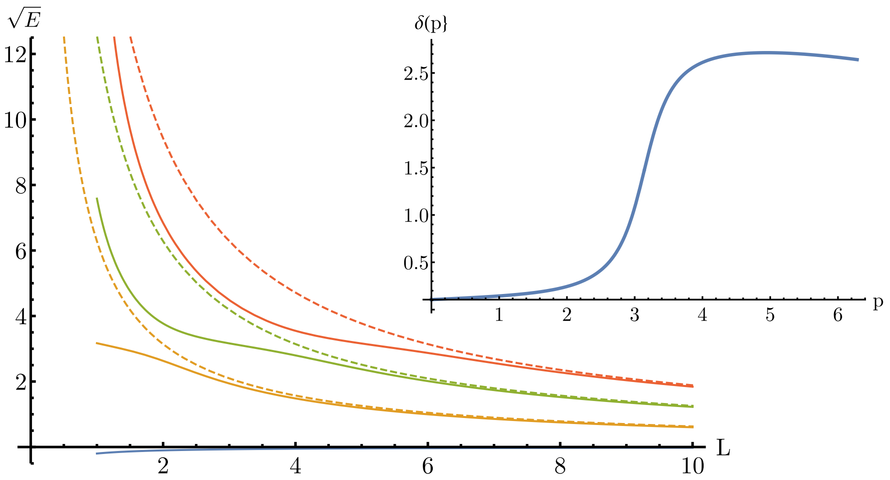

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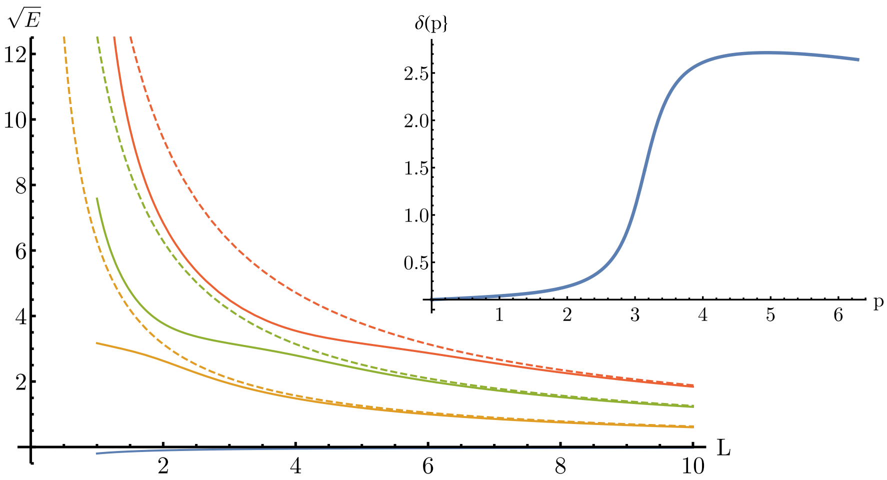


- direct correspondence between phase-shift jump and avoided crossing only for two-body systems, but the **spectrum signature carries over to few-body systems**

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

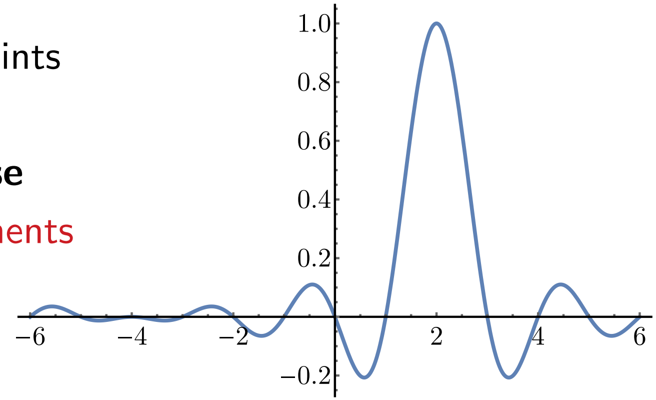
Discrete variable representation

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

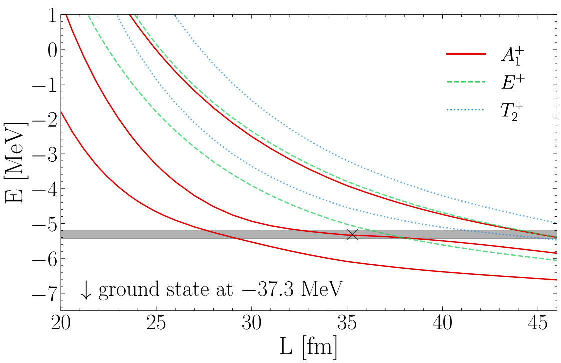
Dietz, SK et al., PRC **105** 064002 (2022); SK, arXiv:2211.00395 [nucl-th]

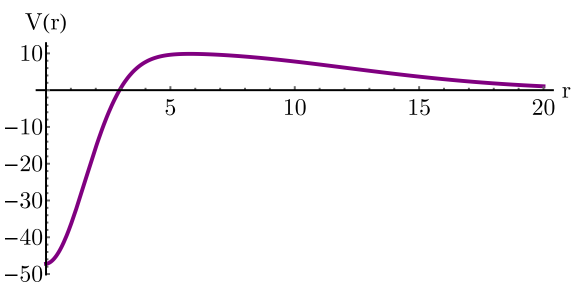
Three-body calculations

1. established three-body resonance from literature

Fedorov et al., Few-Body Syst. **33** 153 (2003); Blandon et al., PRA **75** 042508 (2007)

- three bosons with mass $m = 939.0$ MeV, potential = sum of two Gaussians
- three-body resonance at $-5.31 - i0.12$ MeV (Blandon et al.)





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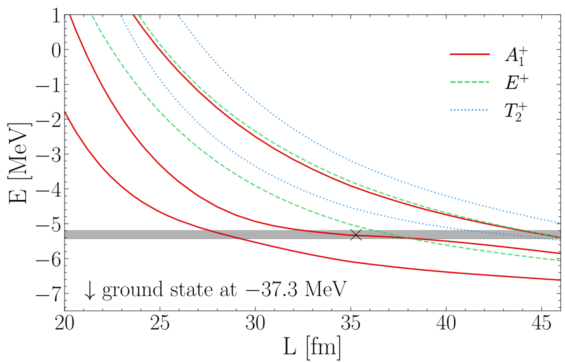

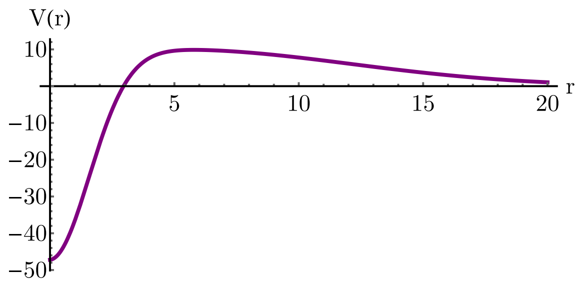

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Klos, SK et al., PRC **98** 034004 (2018)

2. three-neutron system studied in pionless EFT

- apply the same method to a simple neutron-neutron contact interaction
- no sign of a resonance in this system

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

Four-neutron calculations not yet fully conclusive...

- requires calculations in very large boxes $\rightsquigarrow$ numerically expensive!
- enabled by finite-volume eigenvector continuation... N. Yapa, SK, PRC **106** 014309 (2022)
- ...but still not quite sufficiently converged

More formal look at resonances

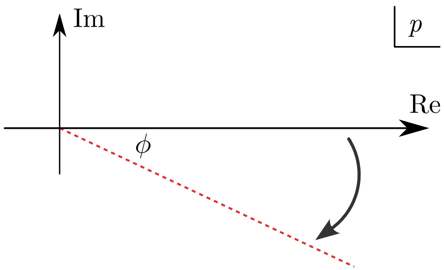
- in stationary scattering theory, resonances are described as generalized eigenstates
  - S-matrix poles at comples energies $E = E_R - \mathrm{i}\Gamma/2$ (lifetime $\sim 1/\Gamma$)
  - wave functions are not normalizable (exponentially growing in r-space)

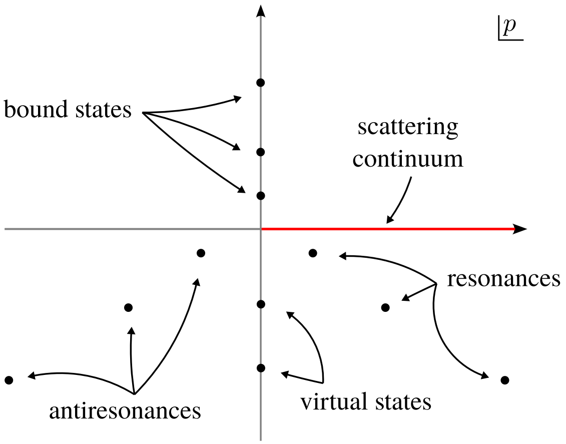
Complex scaling method

- one way to circumvent this problem is the complex scaling method:

$$r \to \mathrm{e}^{\mathrm{i}\phi} r \quad , \quad p \to \mathrm{e}^{-\mathrm{i}\phi} p$$

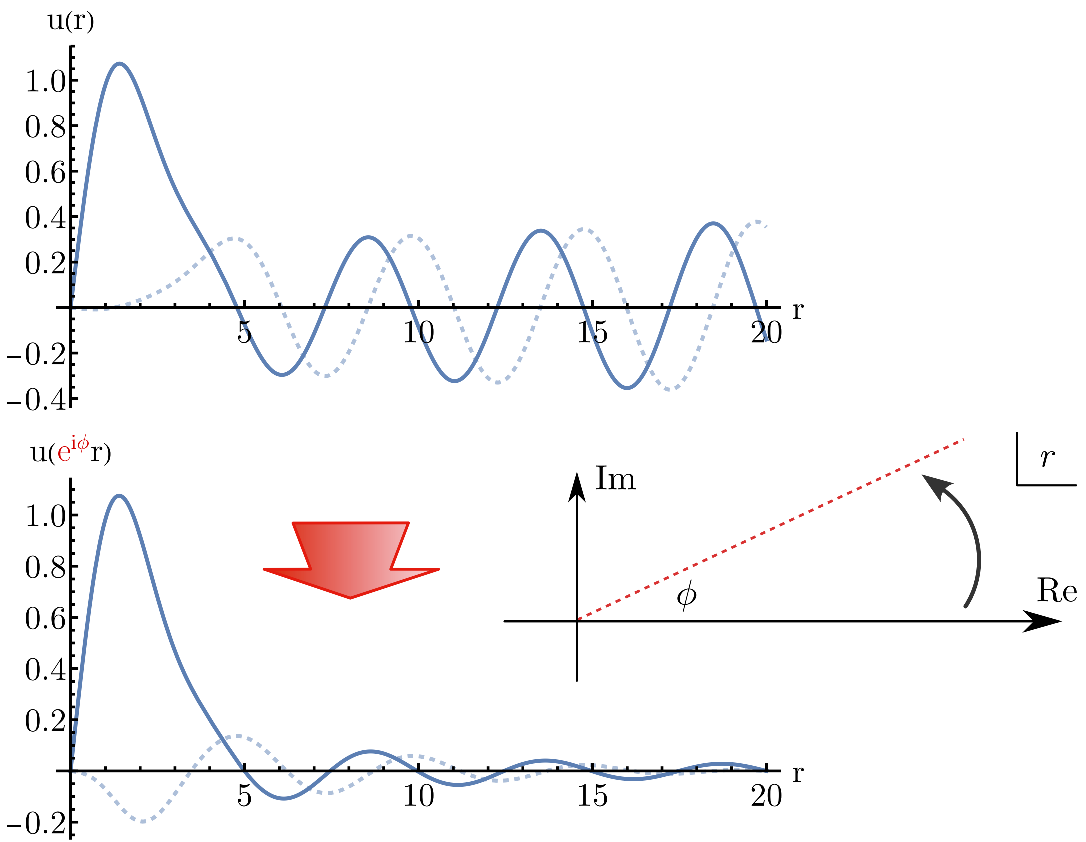
$\rightsquigarrow$ **"reveals" the resonance regime**





Complex-scaled resonance wave functions

- complex scaling suppresses the exponentially growing tail of the wave function



calculations by Nuwan Yapa

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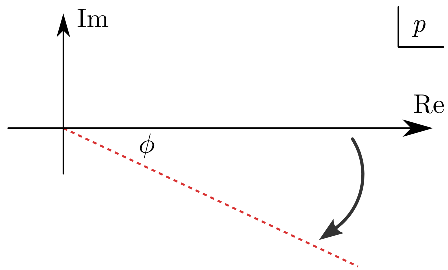

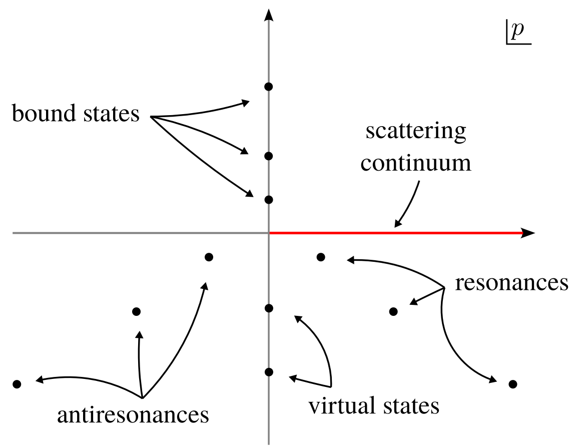

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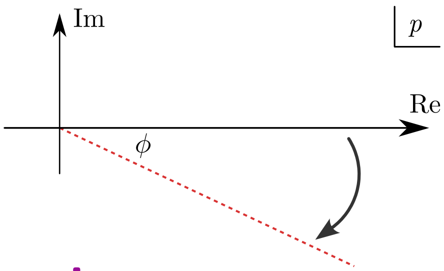
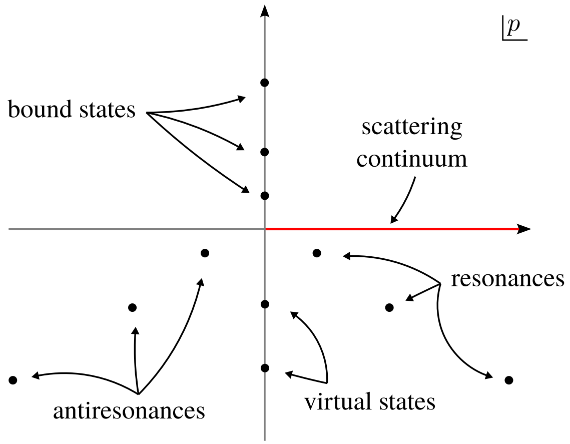




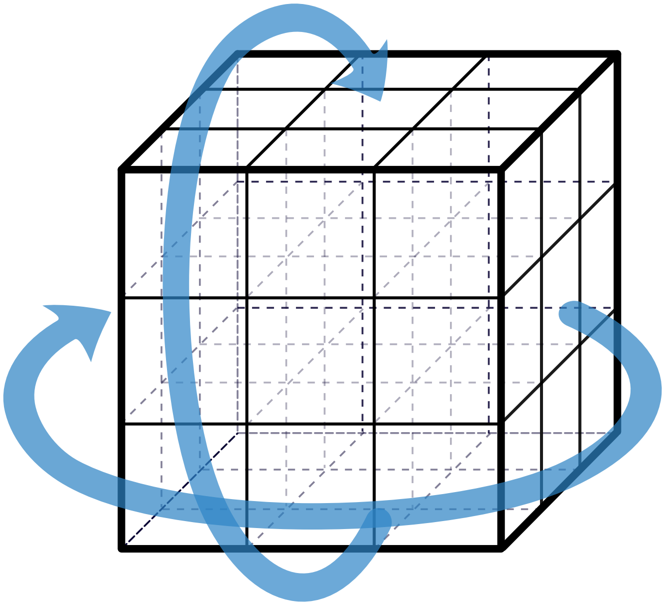
Advertisement

- as the interaction changes, bound states can evolve into resonances
- resonance eigenvector continuation enables extrapolations along such trajectories

Yapa, SK, Fossez, PRC **107** 064316 (2023)

Back to the box

Consider again the peridioc boundary condition...



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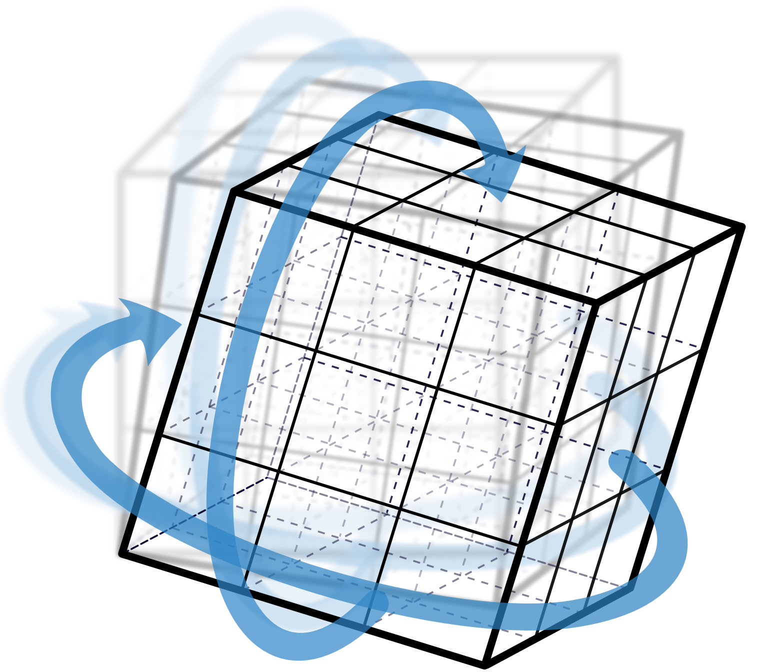

...but now in terms of complex-scaled coordinates!

Complex scaling in finite volume

Key idea

Yu, Yapa, SK, PRC **109** 014316 (2024)

- **put system into a box, apply peridioc boundary condition along rotated axes**

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Volume dependence

- resonances, like bound states, correspond to isolated S-matrix poles
- complex scaling renders their wave functions normalizable
- we can adapt bound-state techniques to derive their volume dependence

$$\Delta E(L) = \frac{3A_\infty^2}{\mu\zeta L}\left[\exp(\mathrm{i}\zeta p_\infty L) + \sqrt{2}\exp(\mathrm{i}\sqrt{2}\zeta p_\infty L) + \frac{4\exp(\mathrm{i}\zeta\sqrt{3}p_\infty L)}{3\sqrt{3}L}\right] + \mathcal{O}\left(\mathrm{e}^{\mathrm{i}2\zeta p_\infty L}\right)$$

- in this equation $\zeta = \mathrm{e}^{\mathrm{i}\phi}$, $p_\infty = \sqrt{2\mu E(\infty)}$
- explicit form for leading term (LO) and subleading corrections (NLO)
- **note:** dependence on volume L and complex-scaling angle ϕ

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Numerical implementation

- DVR method can be adapted to this scenario (scaling of $x, y, z \rightsquigarrow$ scaling of r)

Derivation

Leading-order expression

- possible to work with wave functions after complex scaling
  - derivation proceeds analogous to bound-state case
- based on ansatz for periodic finite-volume resonance wave function

$$\psi_{\zeta L,0}(x) = \sum_{n=-\infty}^{\infty} \psi_\infty(\zeta x + \zeta n L) \qquad \text{(1D)}$$

- energy shift $\sim \langle \psi_{\zeta L,0} | \eta \rangle$ with $|\eta\rangle = \sum_n \sum_{n' \neq n} V(\zeta x + \zeta n L) \psi_\infty(\zeta x + z n L)$
  - **note:** no complex conjugation for bra states (c-product)

Subleading corrections

- easiest to derive directly from quantization condition: $K_0(p) = \frac{\sqrt{4\pi}}{\pi L} \mathcal{Z}_{00}(1; q^2)$
- analytic continuation based on complex-scaled finite-volume Green's function

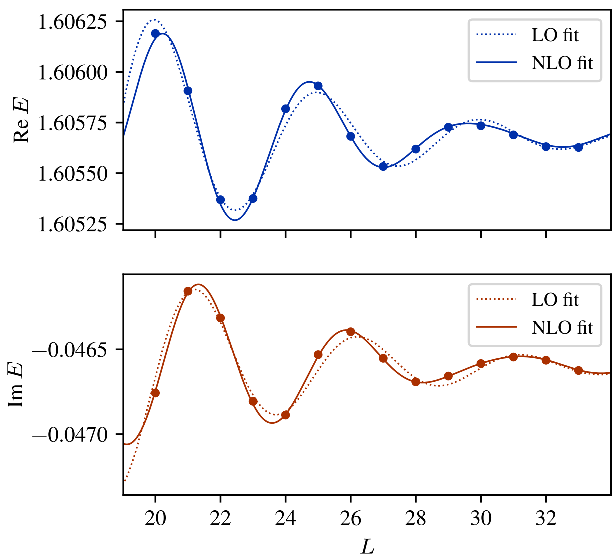
$$G_{\zeta L}(\zeta \mathbf{r}, E) = \zeta G_L(\mathbf{r}, \zeta^2 E)$$

  - see paper for details Yu, Yapa, SK, PRC **109** 014316 (2024)

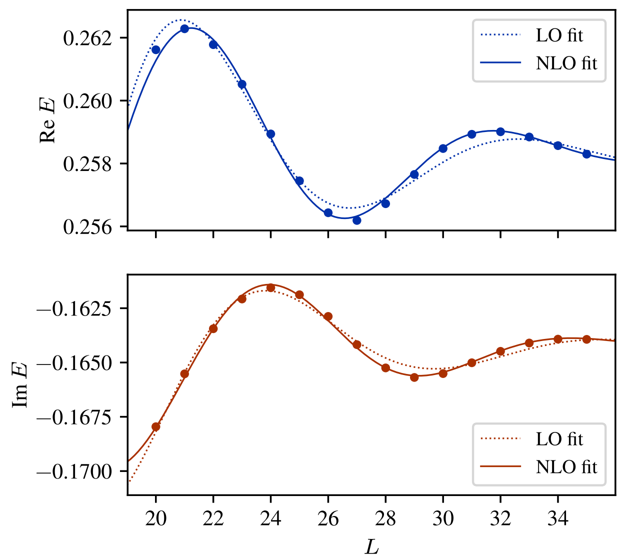
Resonance examples

- two-body calculations are in excellent agreement with derived volume dependence
  - S-wave resonance generated via explicit barrier
  - P-wave resonance from purely attractive potential

S-wave state



P-wave state

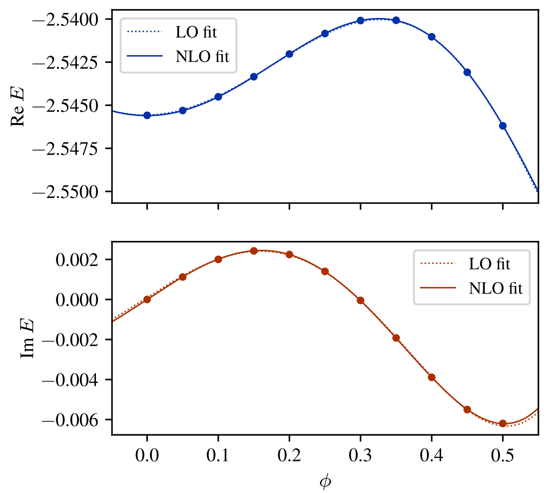


- **fitting the L dependence yields physical resonance position and lifetime!**

More applications

Single-volume bound-state fitting

- bound-state energies normally remain real under complex scaling (strictly true in infinite volume)
- the finite-volume, however, induces a non-zero imaginary part
- $\mathrm{Re}\,E$ and $\mathrm{Im}\,E$ oscillate as a function of L
  - **and also as a function of ϕ**
- possible to fit ϕ dependence at fixed volume!



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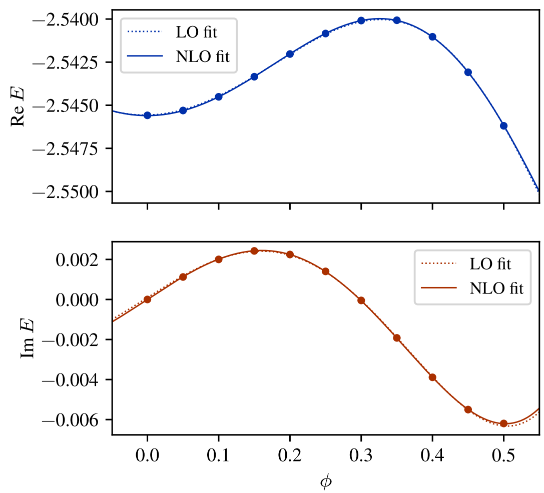
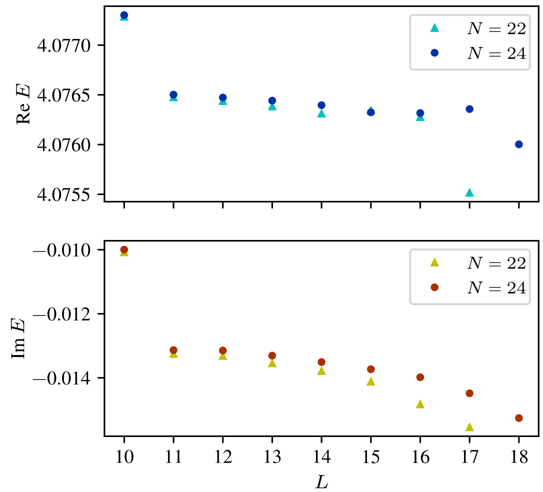


Three-body resonance

- the exact volume dependence is only known for two-body system
- the complex scaled FV-DVR can however be used to study more particles
- three-boson example in decent agreement with previous avoided-crossings analysis



Summary

Bound states

- wave function at large distances determines finite-volume energy shift
  - possible to extract asymptotic normalization coefficients
- volume dependence is known for arbitrary angular momentum and cluster states
- infinite-range Coulomb force complicates derivation
  - leading volume dependence derived for S-wave states

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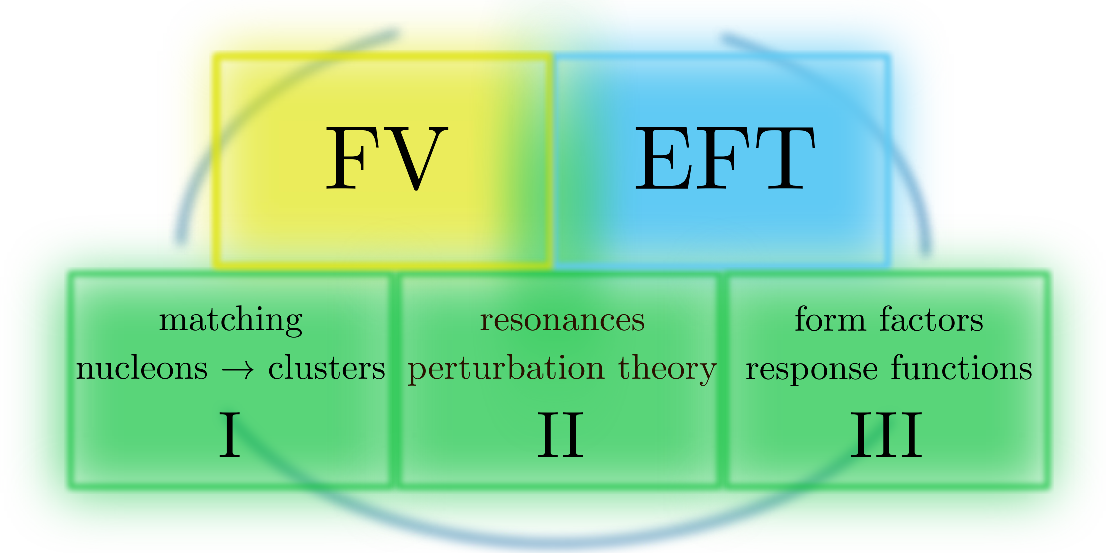
Resonances

- DVR method can handle few-nucleon EFT calculations in large boxes
- pionless EFT excludes a low-energy three-neutron resonance
- four-neutron calculations possible with more recent developments
  - but still too difficult to converge to be fully conclusive
- complex scaling method can be implemented in finite volume
  - gives direct access to resonance positions and lifetimes
  - leading volume dependence derived for two-cluster resonances

Outlook

Finite-volume research program

- simulations of quantum systems in **Finite Volume (FV)** can be used to elegantly extract physical properties
- **Effective Field Theory (EFT)** provides a model-independent descriptions of nuclear interactions
- the combination of these two concepts can be used to study a number of questions



Radius volume dependence

- binding energy volume dependence is governed by asymptotic tails
- other observables can be more sensitive to details of the wave function
- simplest example: **mean squared radius**

$$\langle r^2\rangle(L) = \frac{1}{2}\frac{\langle\psi_L|\mathbf{r}^2\chi_C(\mathbf{r})|\psi_L\rangle}{\langle\psi_L|\chi_C(\mathbf{r})|\psi_L\rangle} = \langle r^2_\infty\rangle + \Delta\langle r^2\rangle(L)$$

  - $|\psi_L\rangle$ is the periodic state at volume L
  - χ_C projects onto the central box

- $\Delta\langle r^2\rangle(L)$ has been worked out by undergraduate student Anderson Taurence
  - explicit expressions for S- and P-wave states, e.g.:

Taurence + SK, arXiv:2401.00107 [nucl-th]

$$\Delta\langle r^2\rangle_0^{A_1^+}(L) = |A_\infty|^2 \mathrm{e}^{-\kappa L}\left(\frac{L^2}{2\kappa} + \frac{3\left(1-4\kappa^2\langle r^2_\infty\rangle\right)}{4\kappa^3} + \frac{a}{\kappa^4 L}\right) + \frac{3}{8}|\gamma|^2 L^3\,\mathrm{Ei}(-\kappa L) + \mathcal{O}(\mathrm{e}^{-\sqrt{2}\kappa L}) \quad (1)$$

Radius volume dependence

Naive expectation

- typically, more tightly bound states tend to be smaller spatially
- recall, FV energy shift positive for S-wave states, negative for P-wave states
  - in general, "leading parity" determines the sign of the energy shift
- based on this, one would expect a negative FV radius shift for S-wave states

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- the explicit calculation however yields a positive shift for S-waves...
- ...and the opposite sign for P-wave states

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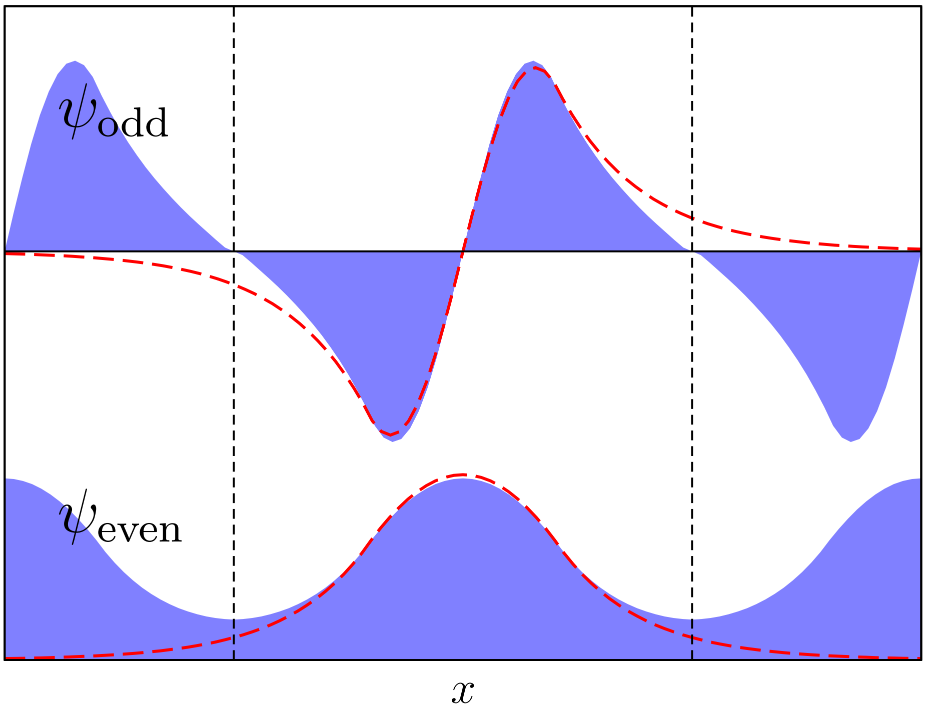
Explanation

- the operator $\sim r^2$ emphasizes the large-distance behavior of the wave function
- **the relaxed profile for even parity then yields a larger radius in FV**

Sign of the energy shift

odd parity → WF profile compressed → more curvarture ⇝ **less deeply bound**



$\Delta E_B(L) < 0$

$\Delta E_B(L) > 0$

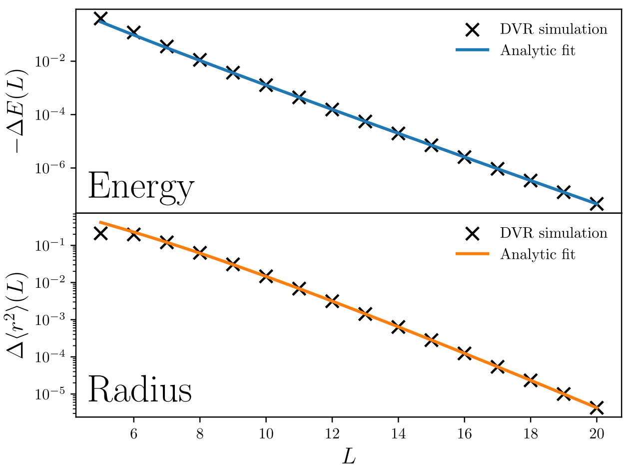
even parity → WF profile relaxed → less curvarture ⇝ **more deeply bound**

Radius volume dependence

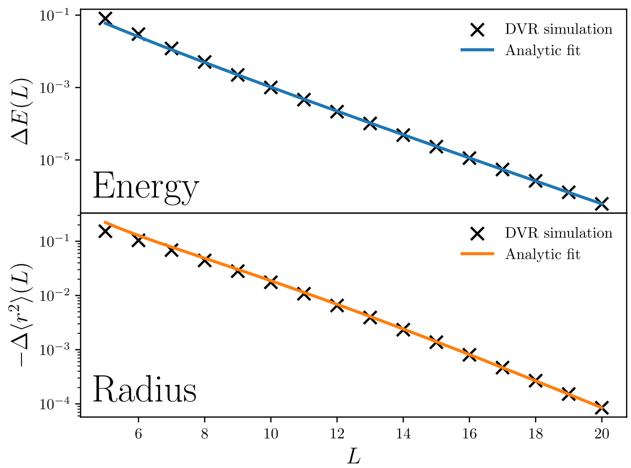
Numerical checks

- consider again bound states generated by attractive Gaussian potentials
- calculate radius in finite volume, fit known functional form
  - **one-parameter radius fit** when ANC and κ are extracted from energy fit

S-wave state

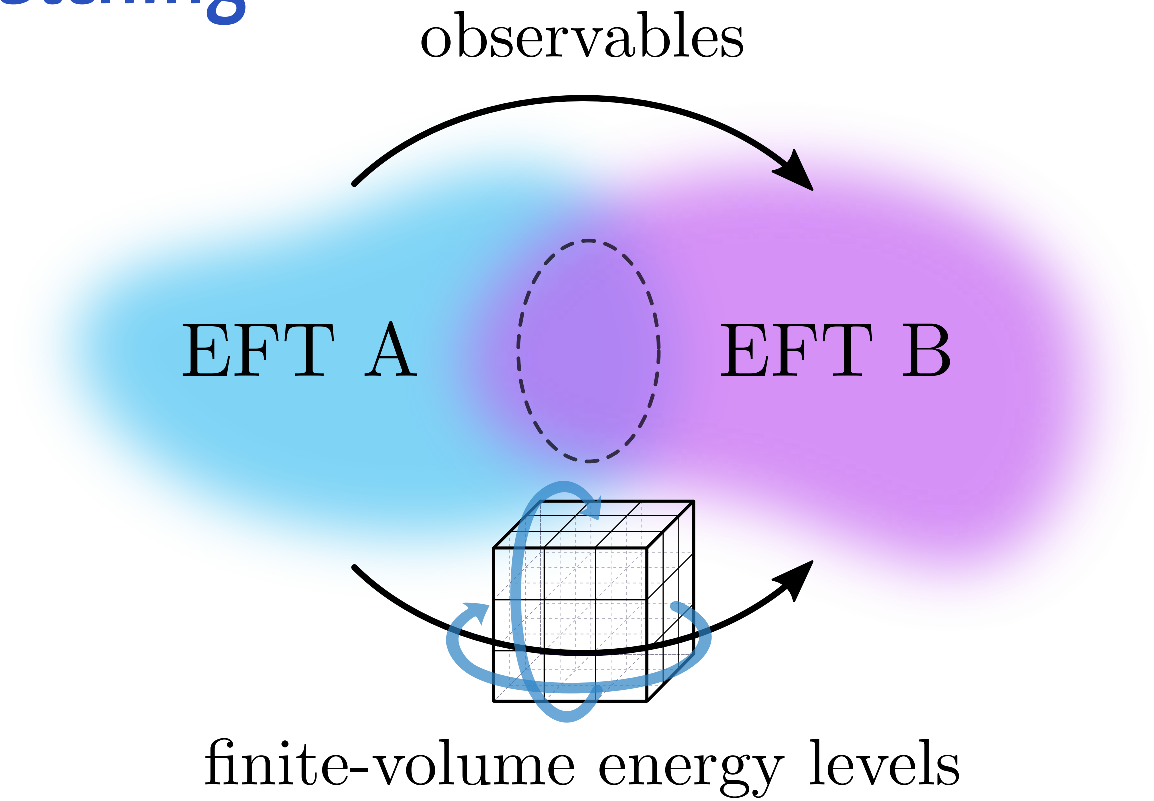


P-wave state



- radius fits work as well as energy fits
- extracted infinite-volume radii agree well with direct benchmark calculations

EFT matching



- (E)FTs can be **matched** in their **overlapping regime of applicability**
  - "analytic continuation" of theories

recent application: Detmold+Shanahan, PRD **103** 074503 (2021)

- specifically, the Chiral EFT (Lattice) input can inform Halo/Cluster EFT (FV DVR)

Thanks...

...to my students and collaborators...

- **H. Yu, N. Yapa, A. Taurence, A. Andis (NCSU)**
- D. Lee (FRIB/MSU), K. Fossez (FSU)
- S. Dietz, H.-W. Hammer, A. Schwenk (TU Darmstadt)
- U.-G. Meißner (U Bonn)
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...and to you, for your attention!