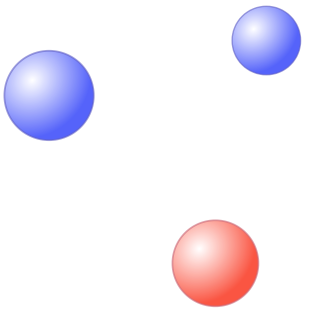
Few-Body Physics in Finite Volume

Sebastian König

25th European Few-Body Conference

Mainz, August 3, 2023

Few-body physics in finite volume



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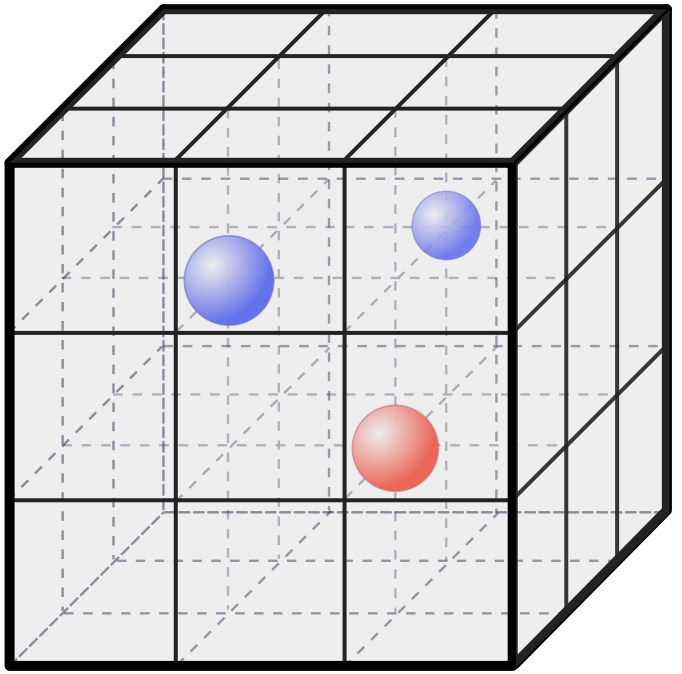

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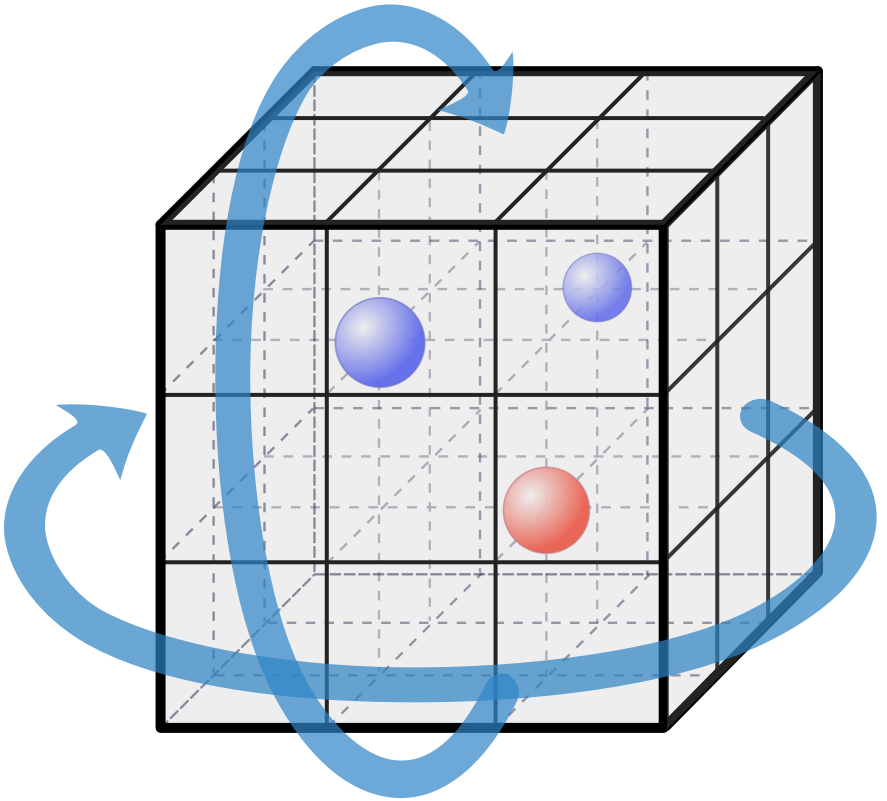
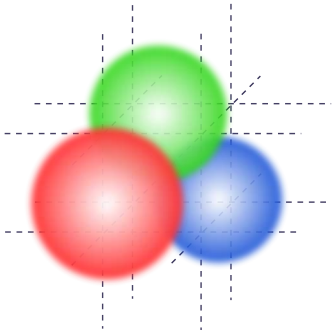
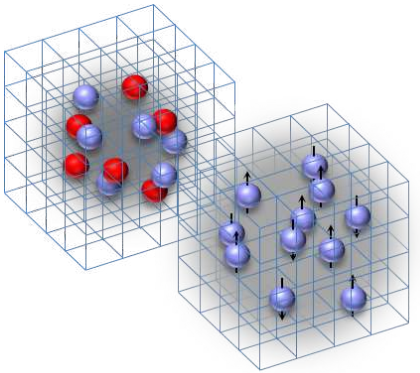


Relevance of finite-volume relations

Lattice simulations





D. Lee

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

talk by H. Wittig yesterday

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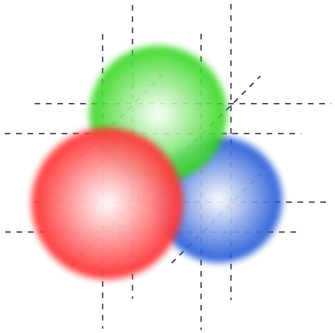

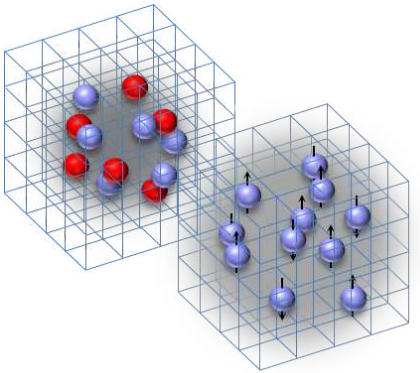

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Harmonic oscillator calculations

- infrared basis extrapolation
- Busch formula: extraction of scattering phase shifts

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

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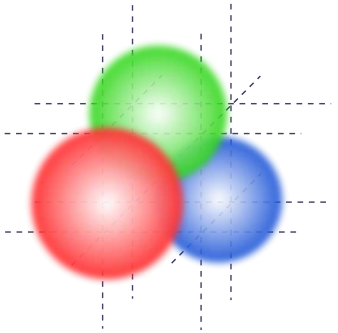

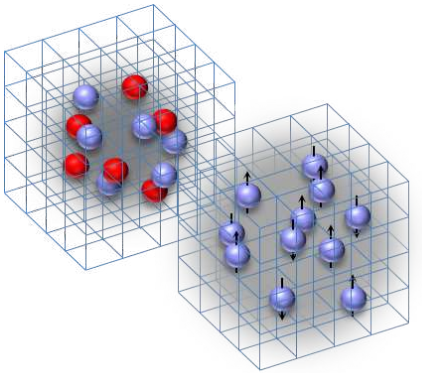

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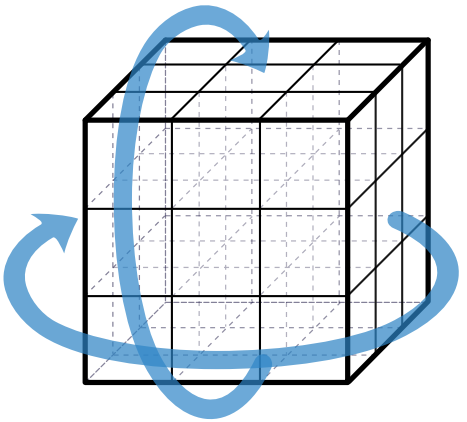
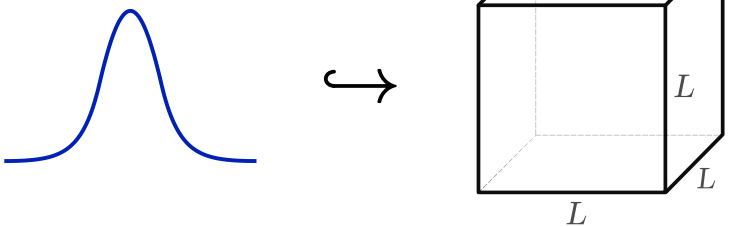
Dedicated finite-volume few-body simulations

Finite volume relations



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



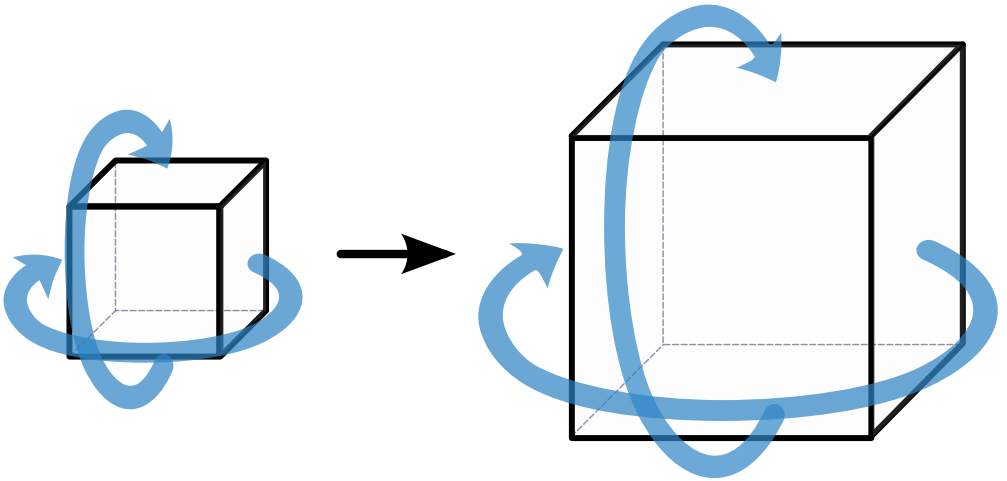
Lüscher formalism

- 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); ...

Leading-order outline

Two aspects of volume extrapolation...



$L_1 \qquad \rightarrow \qquad L_2 \gg L_1$

Part I: Analytical formula

Part II: Numerical technique

Outline @ NLO

(Introduction ✔)

Charged particles in a box

Finite-volume eigenvector continuation

(Summary and outlook)

Part I

Volume dependence of charged-particle bound states

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

Bound-state volume dependence

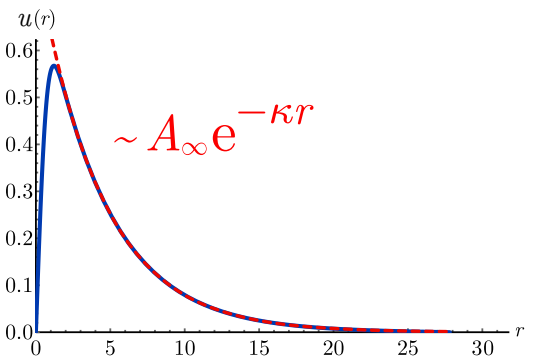
- **finite volume affects the binding energy of states:** $E_B \to E_B(L)$

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

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

- volume dependence determined by universal wavefunction tail — talk by D. Blume on Monday
  - binding momentum κ, **asymptotic normalization constant (ANC)** $\boldsymbol{A_\infty}$
- 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 quantity for reaction calculations ($\to$ S-factors)**

talks by Ch. Hebborn (yesterday), B. Acharya (Tuesday)



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 nuclear systems involve multiple charged particles!

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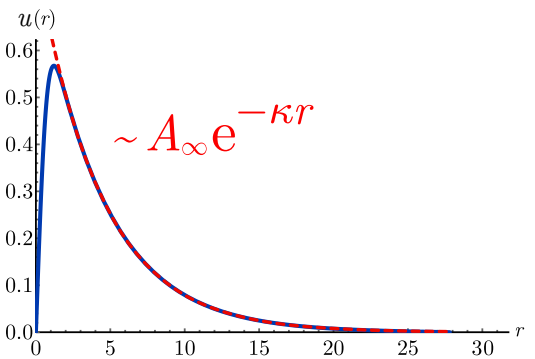

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- nonrelativistic description with short-range interaction + long-range Coulomb force

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

- 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, arXiv:2212.14379 [nucl-th]

Coulomb = exp $\longrightarrow$ Whittaker function?

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Yes, but not quite so simple...

Periodic Coulomb potential

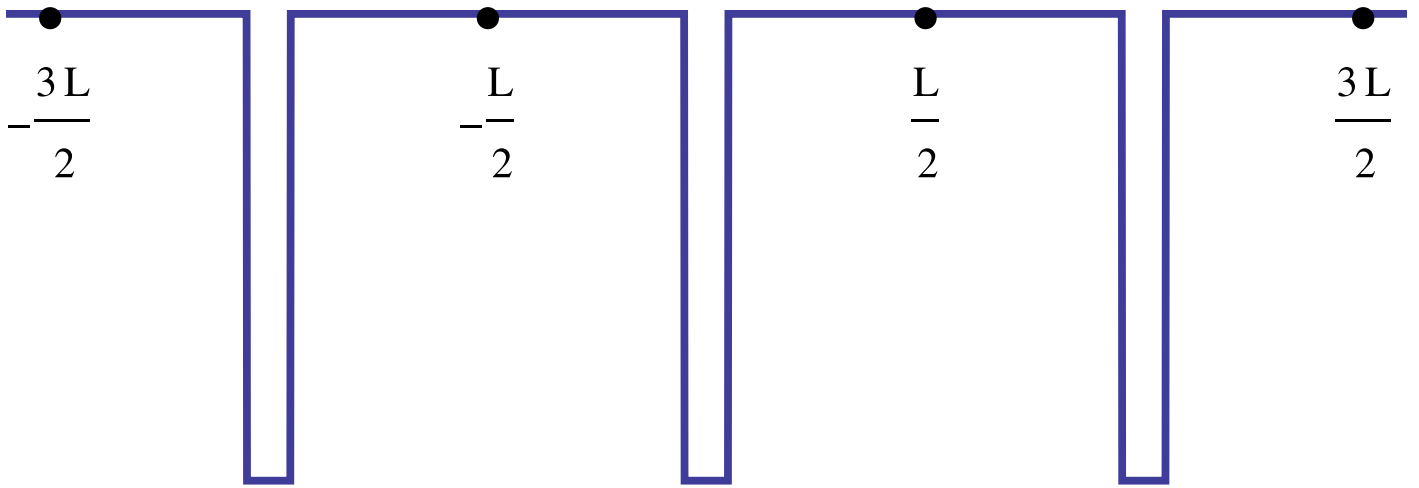
- **short-range interaction easy to extend periodically:** $V_L(\mathbf{r}) = \sum_{\mathbf{n}} V(\mathbf{r} + \mathbf{n}L)$
  - trivial for finite-range potental V
  - converging sum, negligible corrections for V falling faster than power law

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



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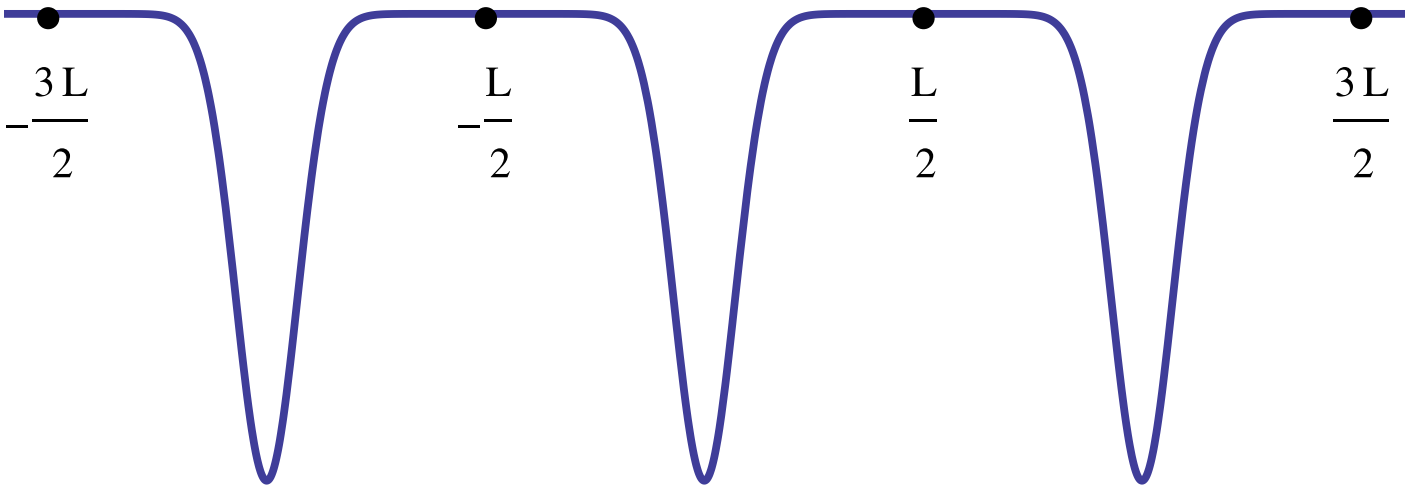

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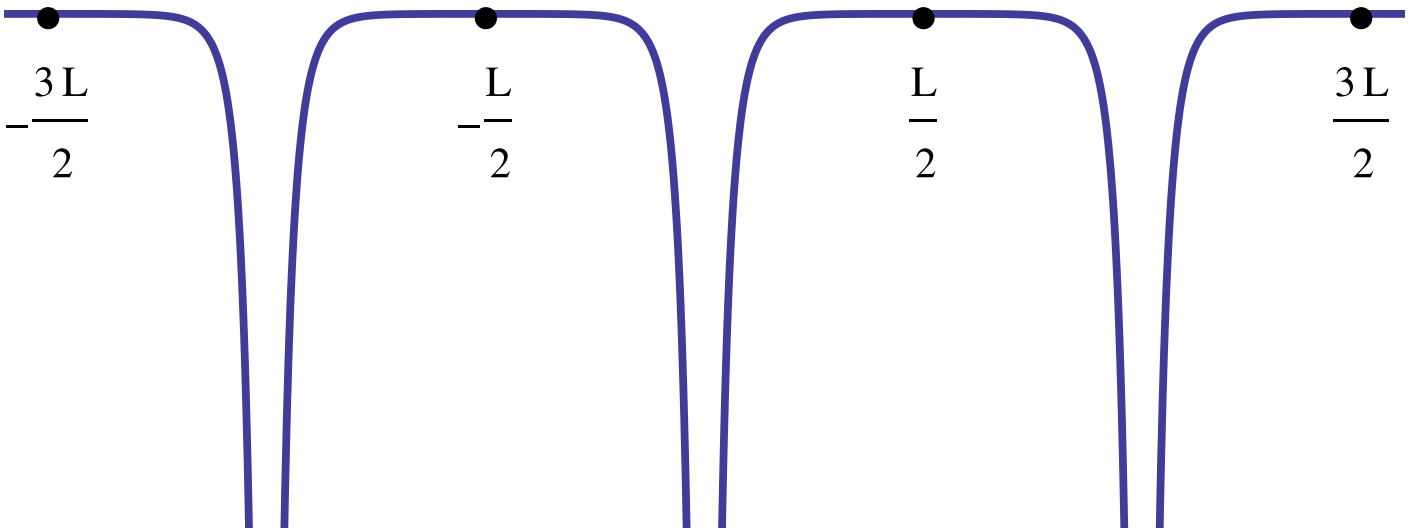

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Solution

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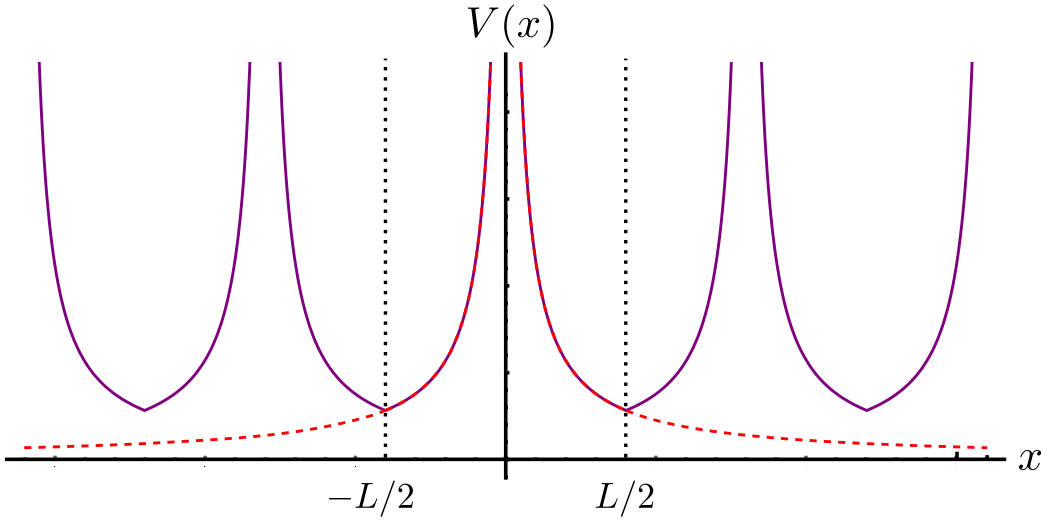
- nicely matches practical implementation (e.g. in Lattice EFT)



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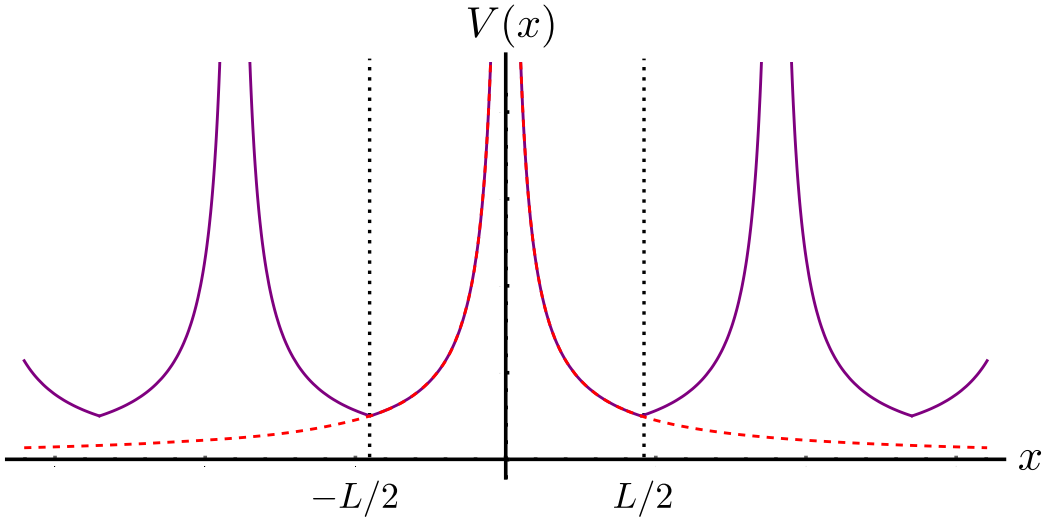

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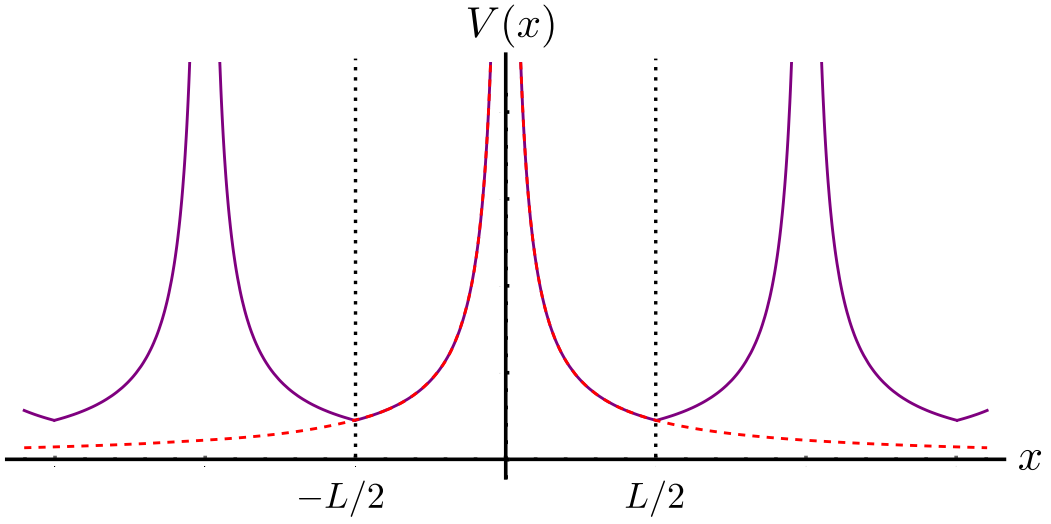

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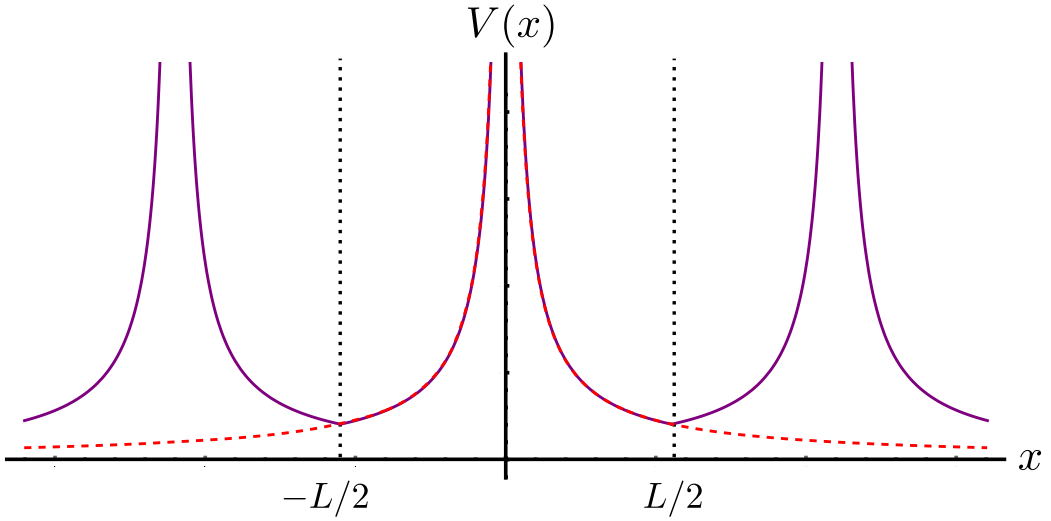

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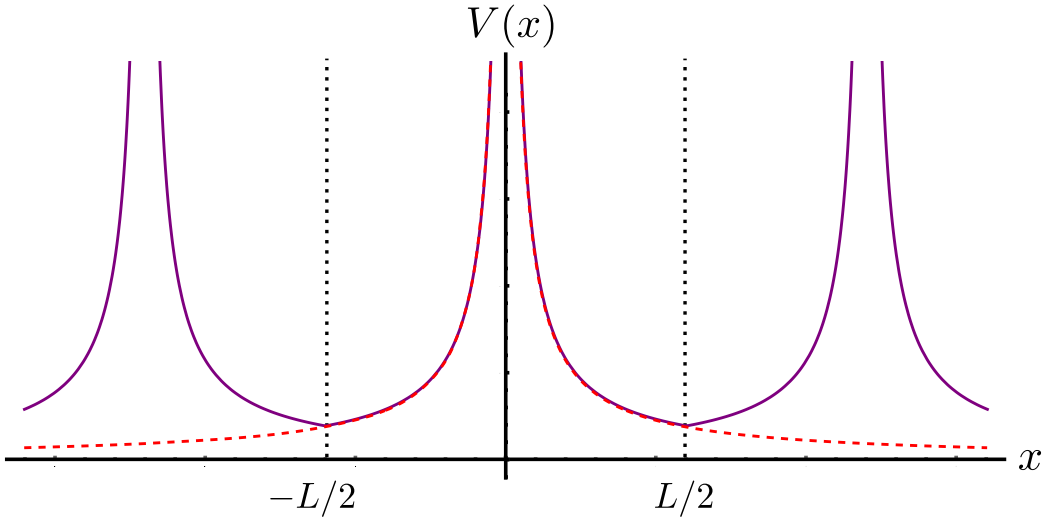
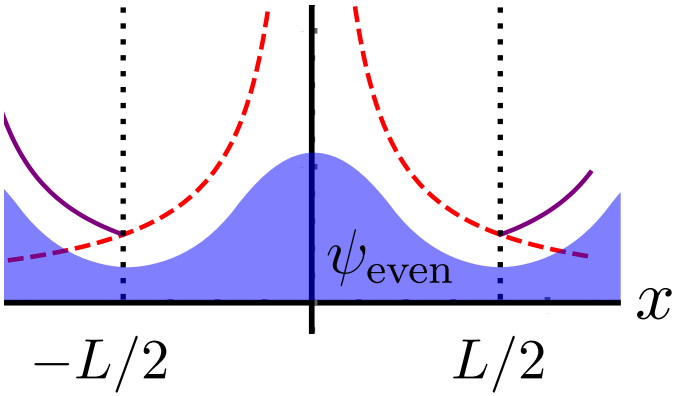


Exact result in one dimension

- **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) ✓

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

Charged-particle volume dependence in 3D

- three-dimensional derivation is more involved due to **nontrival boundary condition**
- **can be done with two-step procedure based on formal perturbation theory**
  - consider periodicity first only for Coulomb potential
  - formally define eigenstates for this scenario
  - then construct ansatz based on these states to derive volume dependence

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

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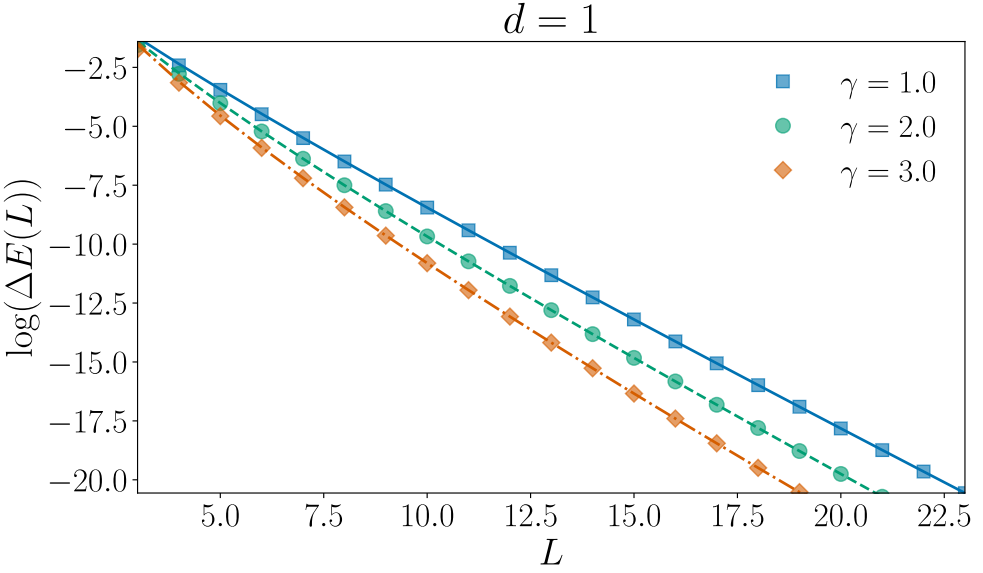
Correction terms

- 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 bound their behavior**

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

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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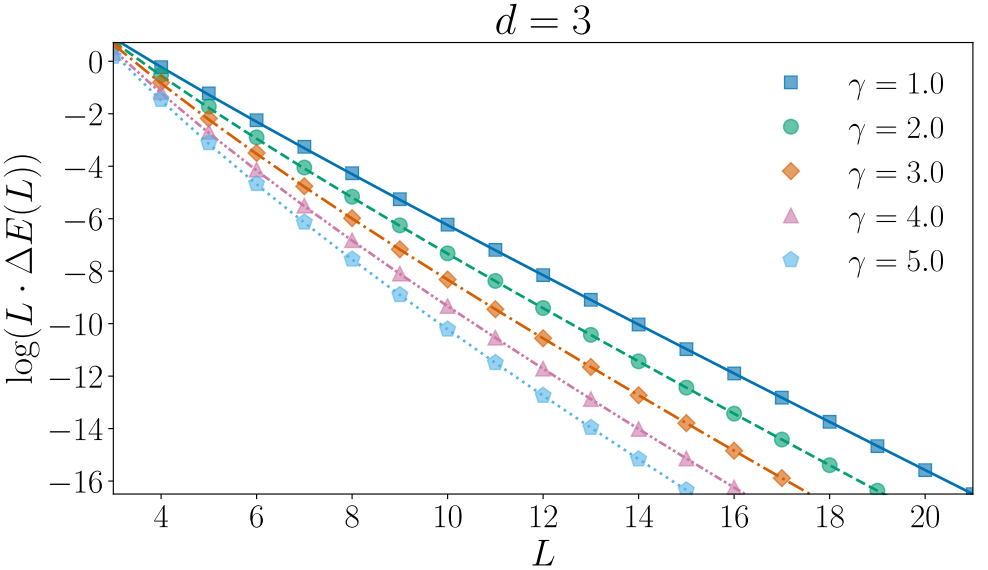

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	Finite-volume fit			Continuum result	
γ	κ_∞	A_∞	L range	κ_∞	A_∞
			$d=1$		
1.0	0.861110(3)	2.1286(1)	$12 \sim 24$	0.860	2.1284
2.0	0.861125(9)	4.4740(9)	$12 \sim 23$	0.860	4.4782
3.0	0.86108(6)	10.386(2)	$12 \sim 20$	0.858	10.435
			$d=3$		
1.0	0.8610(3)	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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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]

Part II

Volume extrapolation via eigenvector continuation

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

Motivation

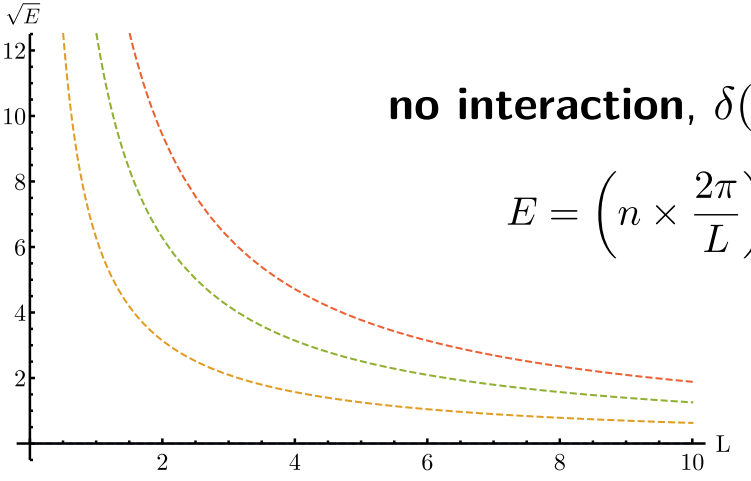
Lüscher formalism and resonances

- 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); ...

talk by A. Saentz on Monday



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

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

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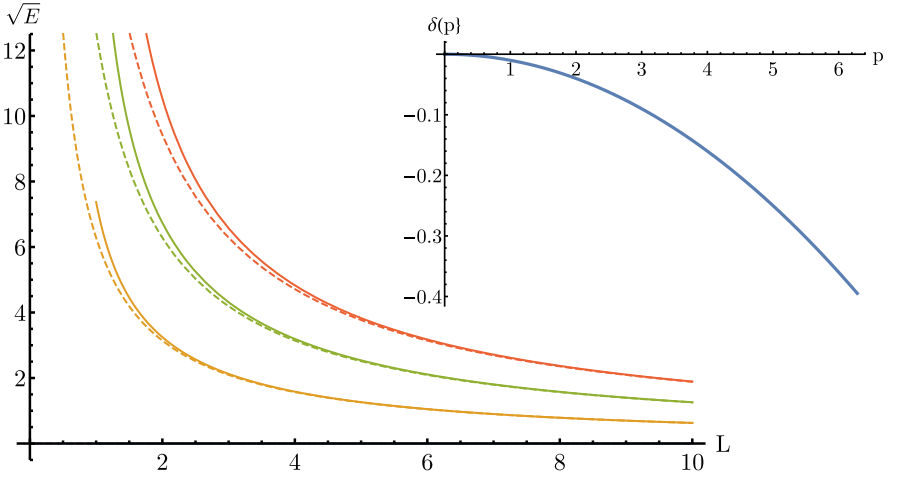

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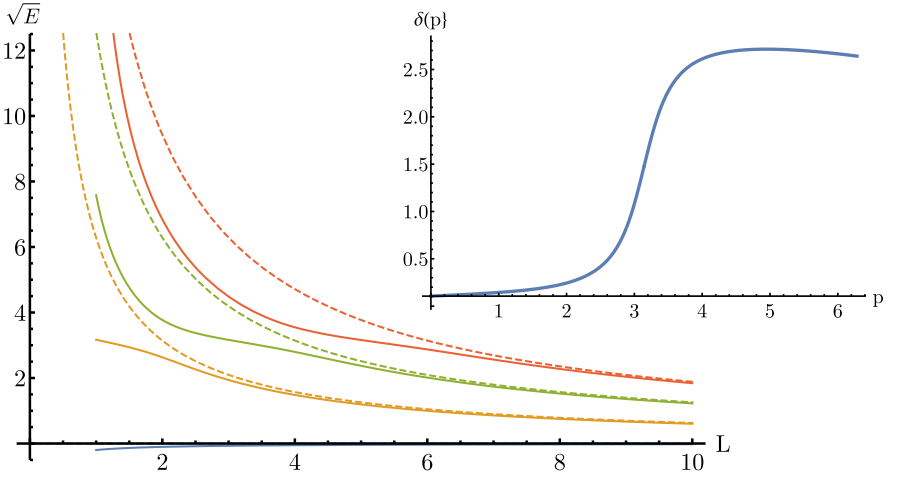

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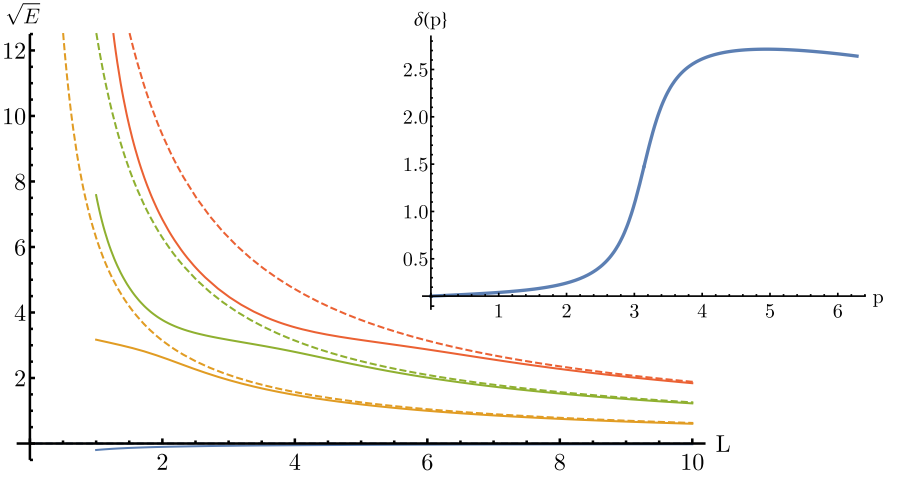


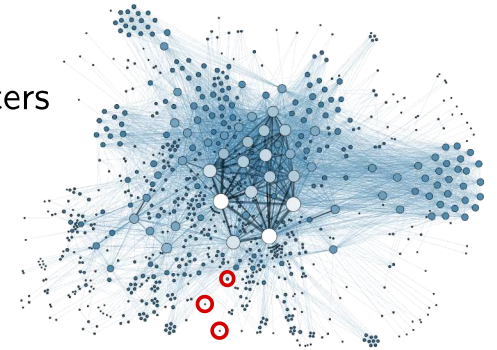
- direct correspondence between phase-shift jump and avoided crossing only for two-body systems, but the **spectrum signature carries over to few-body systems**

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

Eigenvector continuation

Many physics problems are tremendously difficult...

- huge matrices, possibly too large to store
  - ever more so given the evolution of typical HPC clusters
- most exact methods suffer from exponential scaling
- **interest only in a few (lowest) eigenvalues**



Martin Grandjean, via Wikimedia Commons (CC-AS 3.0)

Introducing eigenvector continuation

D. Lee, TRIUMF Ab Initio Workshop 2018; Frame et al., PRL **121** 032501 (2018)

KDE Oxygen Theme

- **novel numerical technique, broadly applicable**
  - emulators, perturbation theory, ...

  Duguet, Ekström, Furnstahl, SK, Lee, review in preparation
- **amazingly simple in practice**
- special case of "reduced basis method" (RBM)

  Bonila et al., arXiv:2203.05282; Melendez et al., arXiv:2203.05528

General idea

Scenario

Frame et al., PRL **121** 032501 (2018)

- consider physical state (eigenvector) in a large space
- **parametric dependence of Hamiltonian $H(c)$ traces only small subspace**

Procedure

- calculate $|\psi(c_i)\rangle$, $i = 1, \ldots N_{\mathrm{EC}}$ in "training" regime
- solve generalized eigenvalue problem $H|\psi\rangle = \lambda N|\psi\rangle$ with
  - $H_{ij} = \langle\psi_i|H(c_{\mathrm{target}})|\psi_j\rangle$
  - $N_{ij} = \langle\psi_i|\psi_j\rangle$

Prerequisite

- smooth dependence of $H(c)$ on c

Result

- construction of highly efficient, tailored variational basis
- enables analytic continuation of $|\psi(c)\rangle$ from $\{c_i\}$ to c_{target}

Finite-volume eigenvector continuation

Naive setup

- consider states $|\psi_{L_i}\rangle$ at volume L_i
- want to use these to extrapolate via EC to target volume L_*
- to that end, we'd consider Hamiltonian and norm matrices like this:

$$H_{ij} = \langle \psi_{L_i} | H_{L_*} | \psi_{L_j} \rangle$$
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However...

All the $|\psi_{L_i}\rangle$ are defined in different Hilbert spaces!

- parametric dependence now not only in the Hamiltonian...
- ...but inherent in the basis
- **need to generalize EC to deal with this scenario**
- work together with graduate student Nuwan Yapa

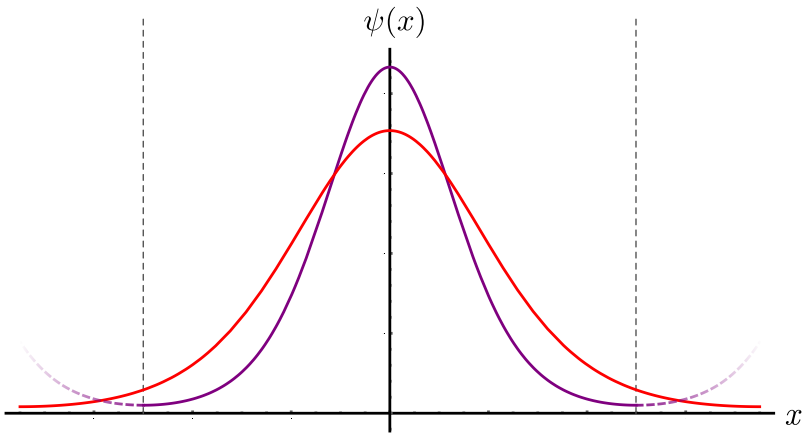
Dilatations

- consider a function f with period L, $f \in \mathcal{H}_L$
- this can be mapped onto a function with period L' by means of a dilatation:

$$(D_{L,L'} f)(x) = \sqrt{\frac{L}{L'}}\, f\left(\frac{L}{L'} x\right)$$

- this provides a bijection between the Hilbert spaces $\mathcal{H}_L$ and $\mathcal{H}'_L$

Example: periodic bound-state wavefunction



Periodic matching

- consider the union of all periodic Hilbert spaces: $\mathcal{H} = \bigcup_{L>0} \mathcal{H}_L$
  - not a Hilbert space with normal pointwise addition
- define a new operation for $f \in \mathcal{H}_L$, $g \in \mathcal{H}_{L'}$, $L' > L$:

$$(f \overset{\max}{+} g)(x) = (D_{L,L'} f)(x) + g(x)$$

- similarly, define inner products between different periodicities:

$$\langle f, g \rangle_{\max} = \langle D_{L,L'} f, g \rangle_{\mathcal{H}_{L'}} = \int_{-L'/2}^{L'/2} (D_{L,L'} f)(x)^* g(x) \, \mathrm{d}x$$

- **together, these make $\mathcal{H}$ a vector space with inner product**

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Truncated periodic bases

- let $S_{L,N}$ be a truncated basis of plane-wave states
- then for $\psi \in S_{L,N}$ and $\psi' \in S_{L',N}$, **the $\mathbb{R}^N$ inner product of coefficient vectors is the same as $\langle \cdot, \cdot \rangle_{\max}$**

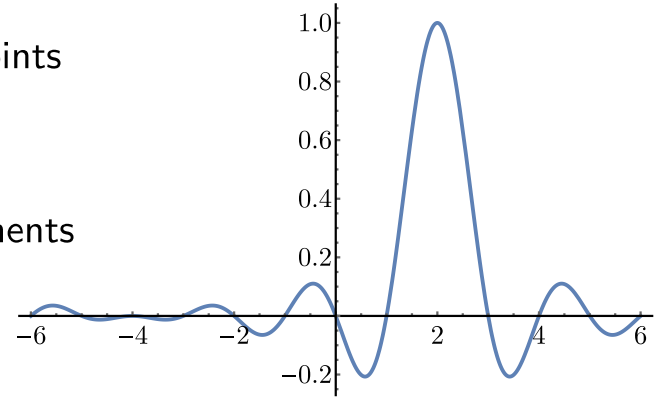
Discrete variable representation

Efficient 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



- **related via unitary transformation to truncated plane-wave basis!**

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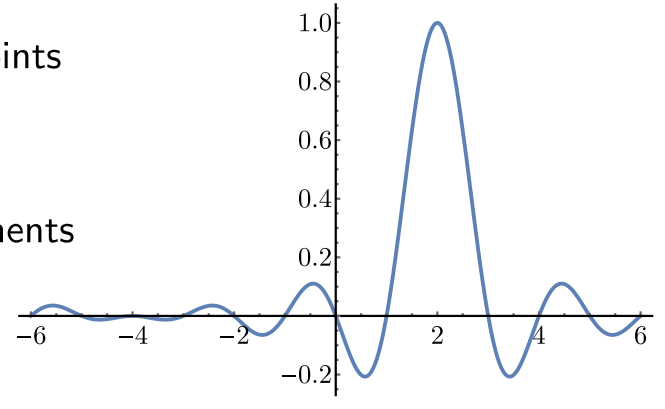


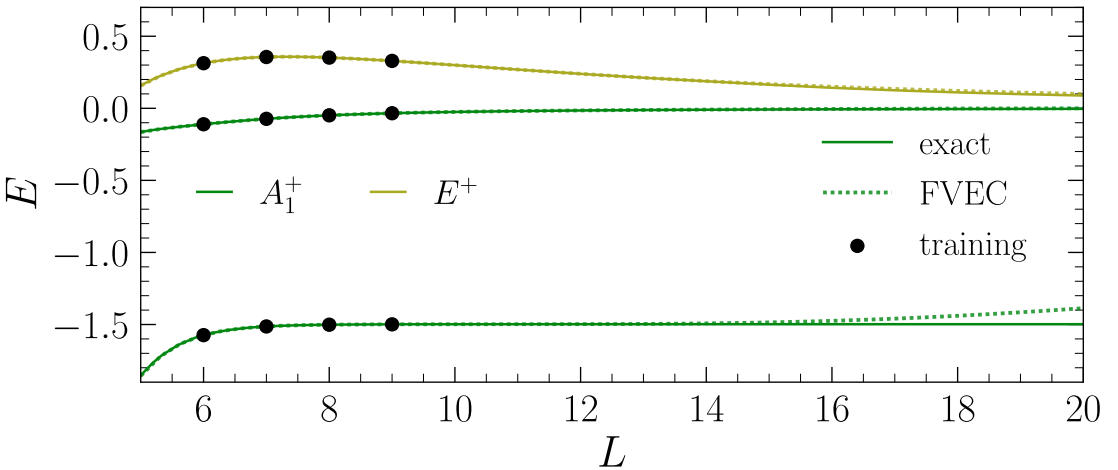
- **related via unitary transformation to truncated plane-wave basis!**
- **efficient implementation for large-scale calculations**
  - handle arbitrary number of particles (and spatial dimensions)
  - numerical framework scales from laptop to HPC clusters

    SK et al., PRC **98** 034004 (2018)
  - recent extensions: GPU acceleration, separable interactions

    Dietz, SK et al., PRC **105** 064002 (2022); SK, J. Phys. Conf. Ser. **2453** 012025 (2023)

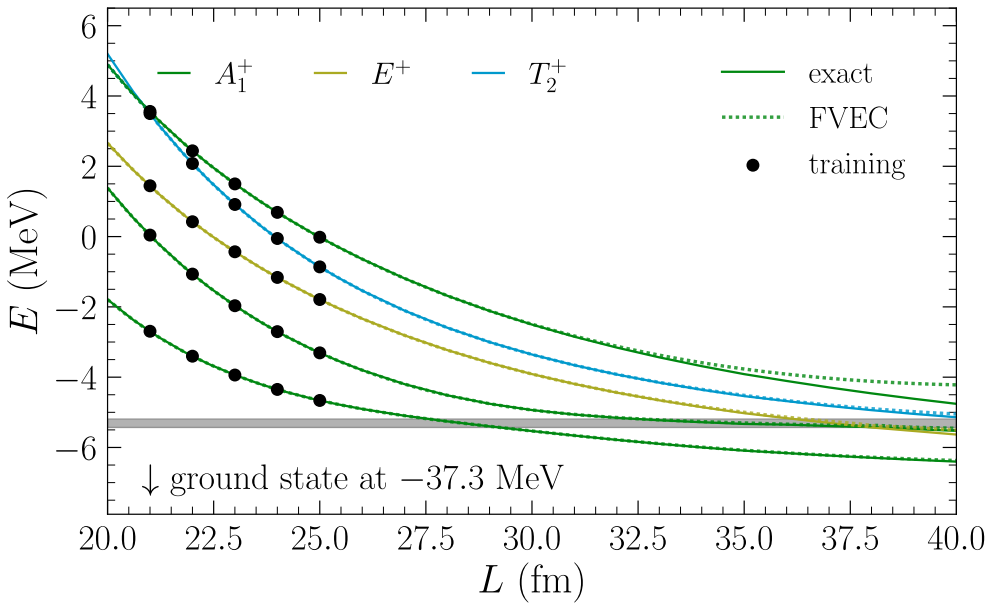
Two-body proof of concept

- consider a simple two-body system as first example
  - attractive Gaussian interaction: $V(r) = V_0 \exp\left(-\left(\frac{r}{R}\right)^2\right)$, $R = 2$, $V_0 = -4$
- **note: cubic finite volume breaks spherical symmetry**
  - angular momentum no longer good quantum number
  - instead: cubic irreducible representations $\Gamma \in A_1, A_2, E, T_1, T_2$
  - to good approximation, S-wave states $\sim A_1^+$ irrep. (positive parity)



Three-boson resonance

- 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., PRA **75** 042508 (2007))
  - $-5.96 - i0.40$ MeV (Fedorov et al., FB Syst. **33** 153 (2003)) (potential S-wave projected!)



- **avoided crossing well reproduced by FVEC calculation**

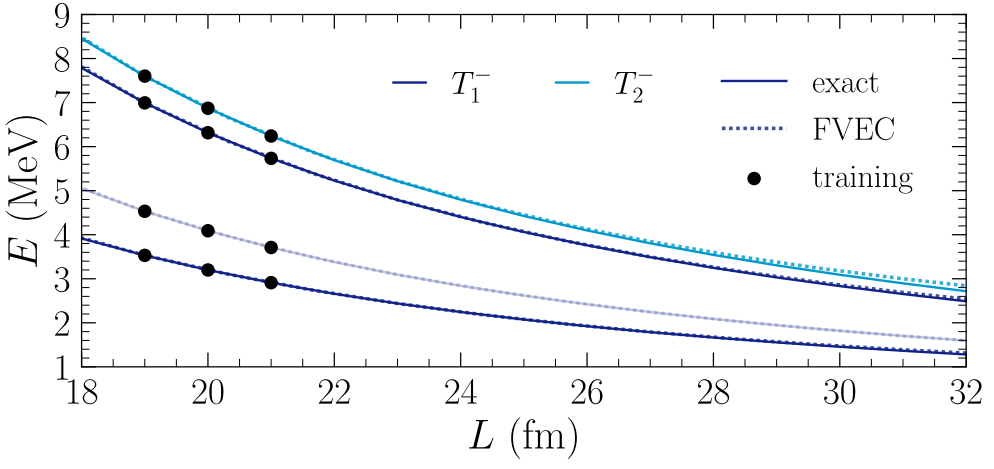
Three neutrons

- now consider three neutrons with Pionless EFT leading-order interaction

$$V(q,q') = C\, g(q) g(q') \quad , \quad g(q) = \exp(-q^{2n}/\Lambda^{2n})$$

- separable super-Gaussian form with $n = 2$ and $\Lambda = 250$ MeV
- efficiently implemented within DVR framework

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

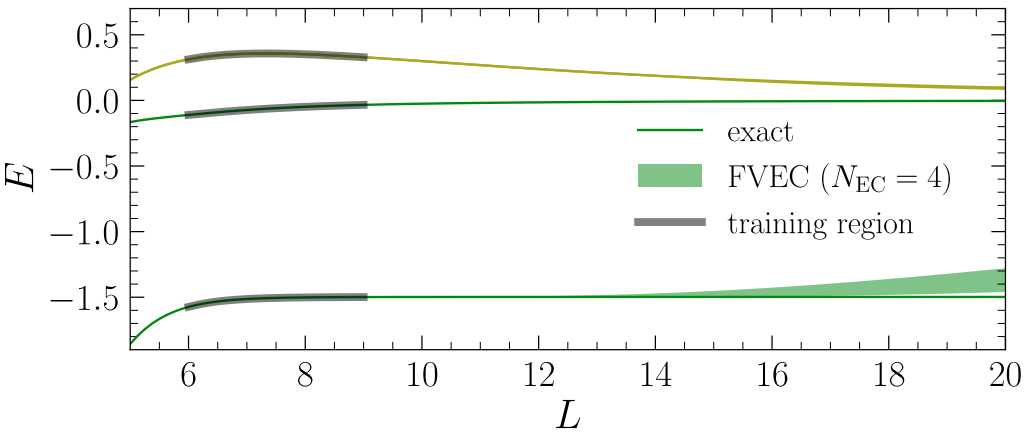


- total number of training data: $3 \times 8 = 24$ (partly covering cubic group multiplets)

Uncertainty quantification

- **FVEC uncertainty depends on choice of training data**
  - domain to choose from (note also: extrapolation vs. interpolation)
  - number N_{EC} of training space (controls dimension of FVEC subspace)
- use this dependence to estimate uncertainty
  - calculate initial pool of training data
  - from that pool, consider combinations with fixed N_{EC}

Application to two-body system



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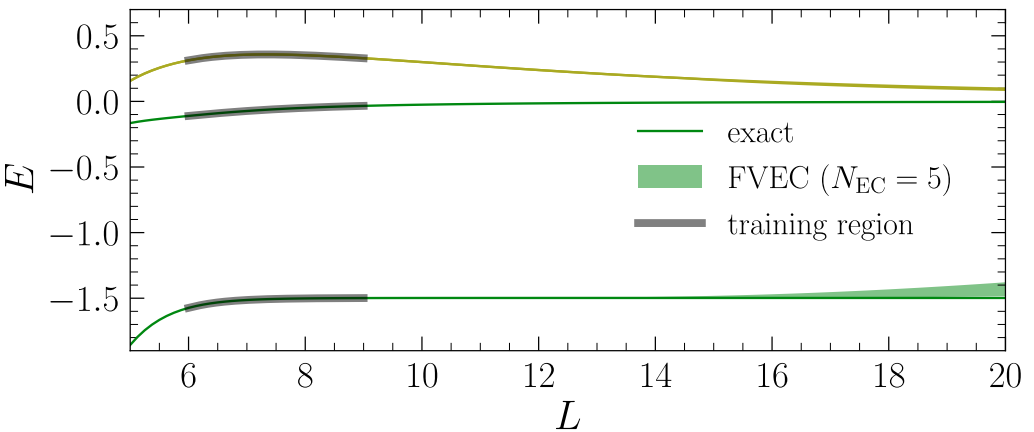

Summary and outlook

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
- planned work: ANC calculations based on lattice EFT

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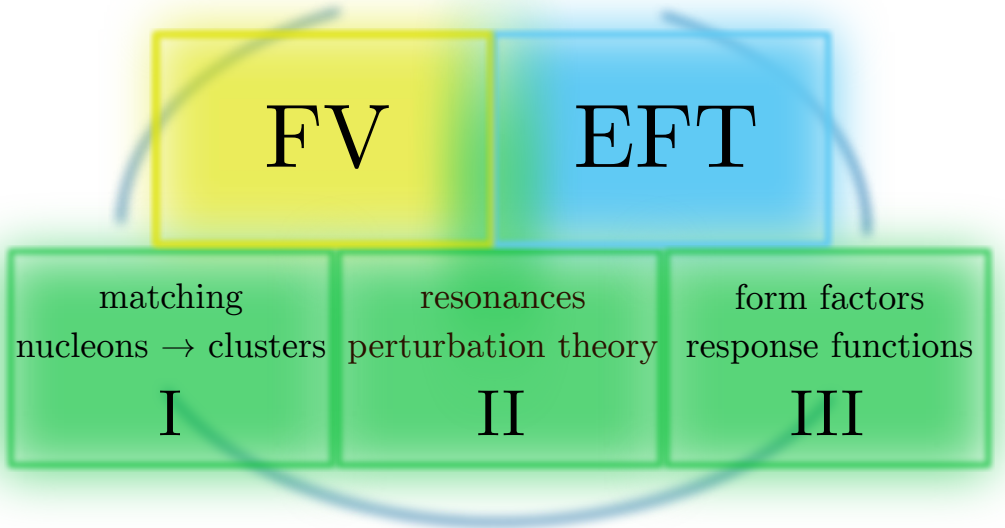
Volume extrapolation via eigenvector continuation

- extension of EC to handle parametric dependence direcly in basis
- justified by periodic matching construction
- makes it possible to extrapolate reliably over large volume ranges
- DVR method can handle few-nucleon EFT calculations in large boxes
- in progress: application to four-neutron system

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



Thanks...

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