Few-Body Physics in Finite Volume

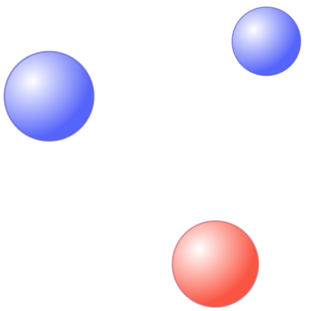
Sebastian König, NC State University

13th International Spring Seminar on Nuclear Physics

May 19, 2022

Yu, Lee, SK in preparation
Yapa, SK, arXiv:2201.08313 (2022)

Nuclear physics in a box



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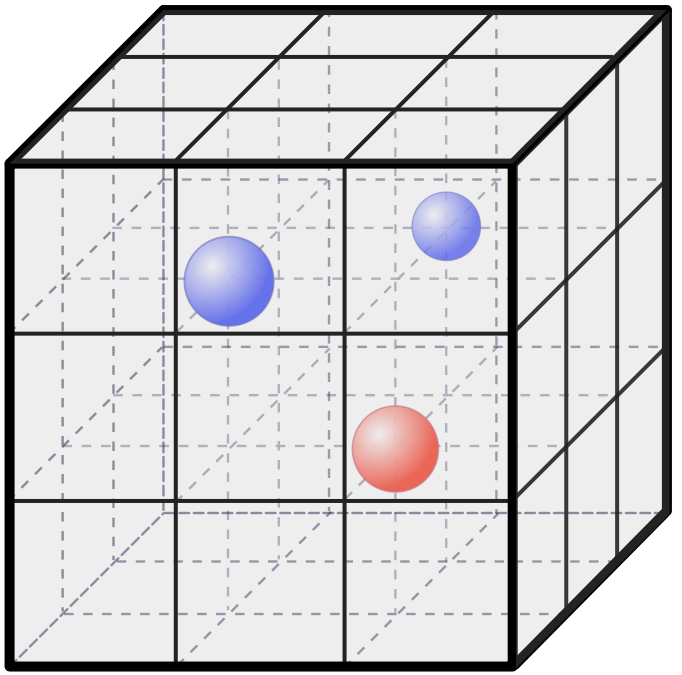

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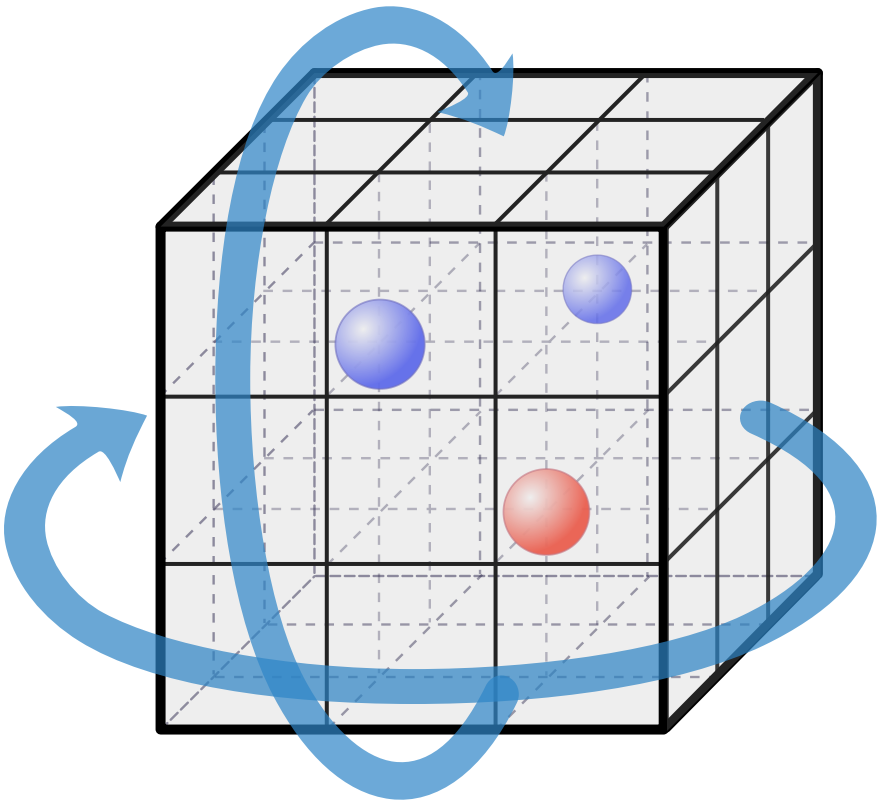
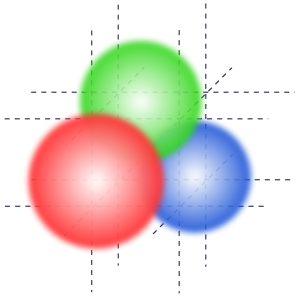
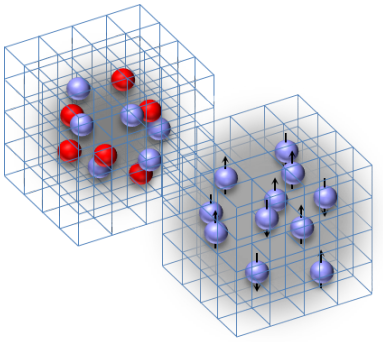


Relevance of finite-volume relations

Lattice simulations





D. Lee

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

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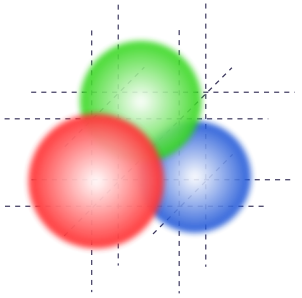

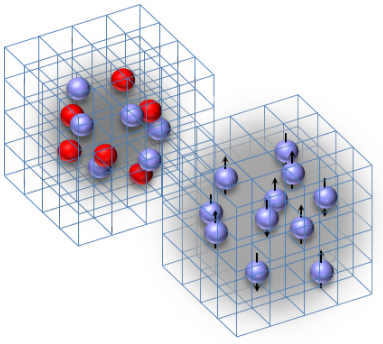

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Harmonic oscillator calculations

- infrared basis extrapolation — More et al, PRC **87** 044326 (2013); ...
- Busch formula: extraction of scattering phase shifts — Busch et al., Found. Phys. **28** 549 (1998); ...; Zhang et al., PRL **125** 112503 (2020);...

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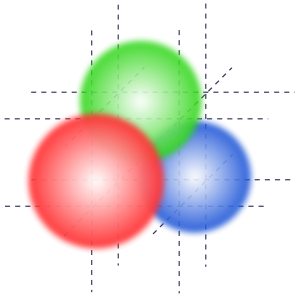

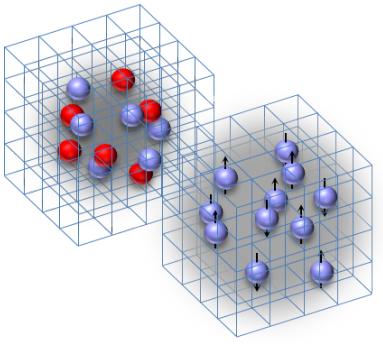

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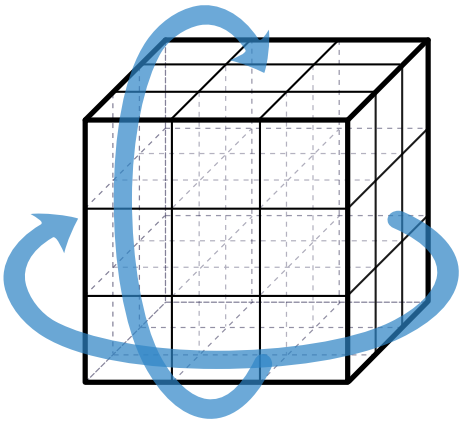
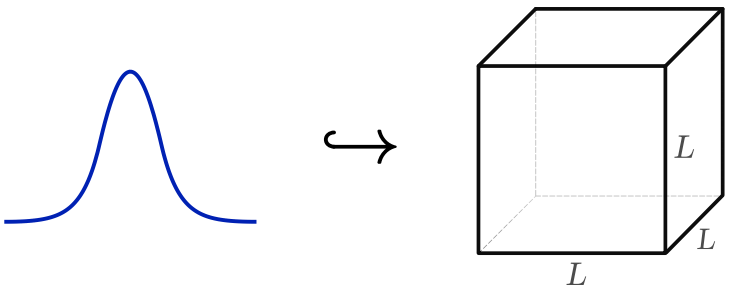
As direct tool to study nuclear states and reactions

Finite periodic boxes



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

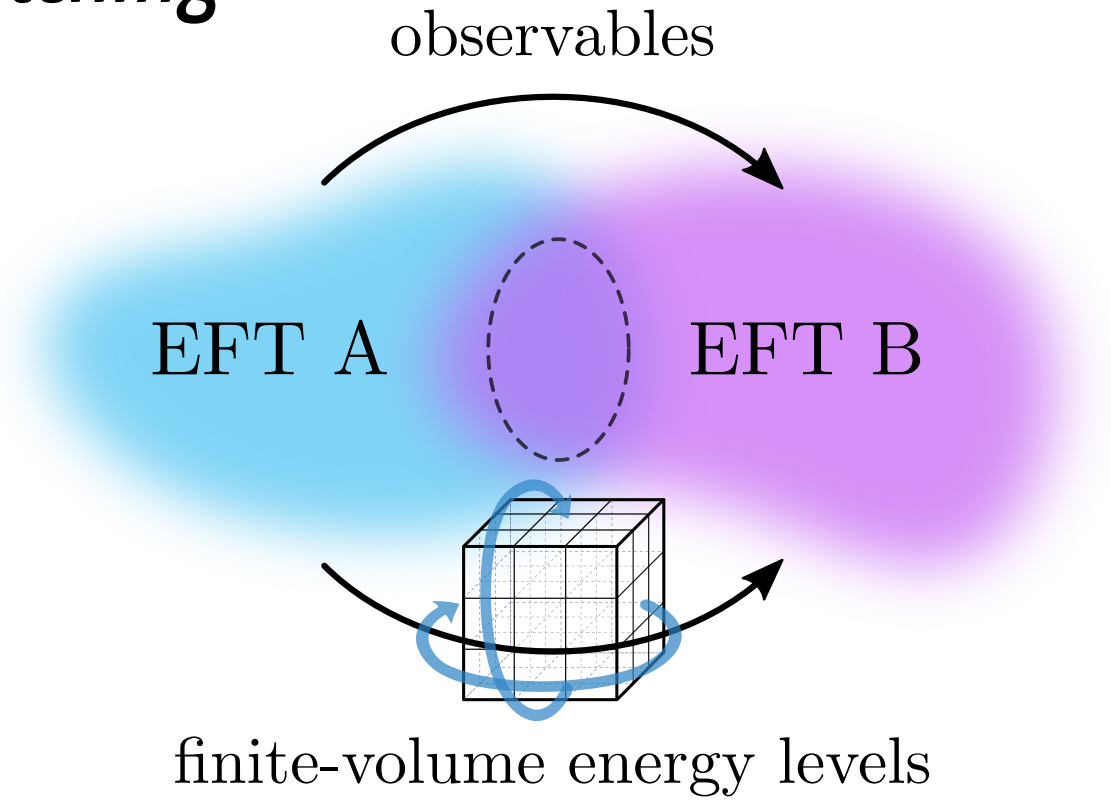


Lüscher formalism

- 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); ...

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)

Outline

Introduction ✔

Charged particles

Volume extrapolation

Part I

Volume dependence of charged-particle bound states

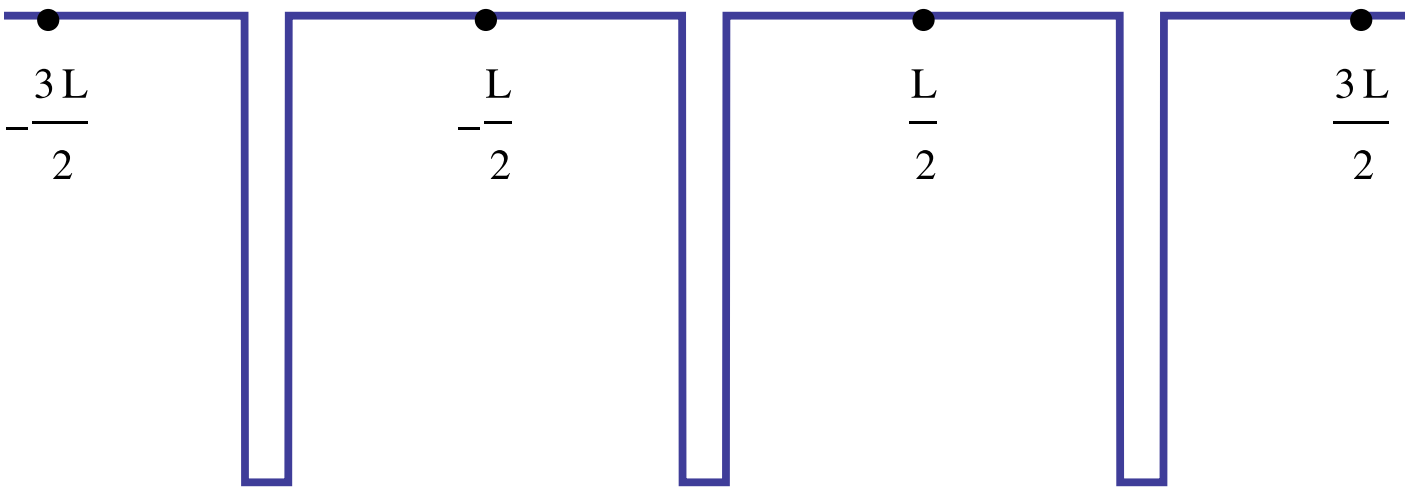
H. Yu, D. Lee, SK, in preparation

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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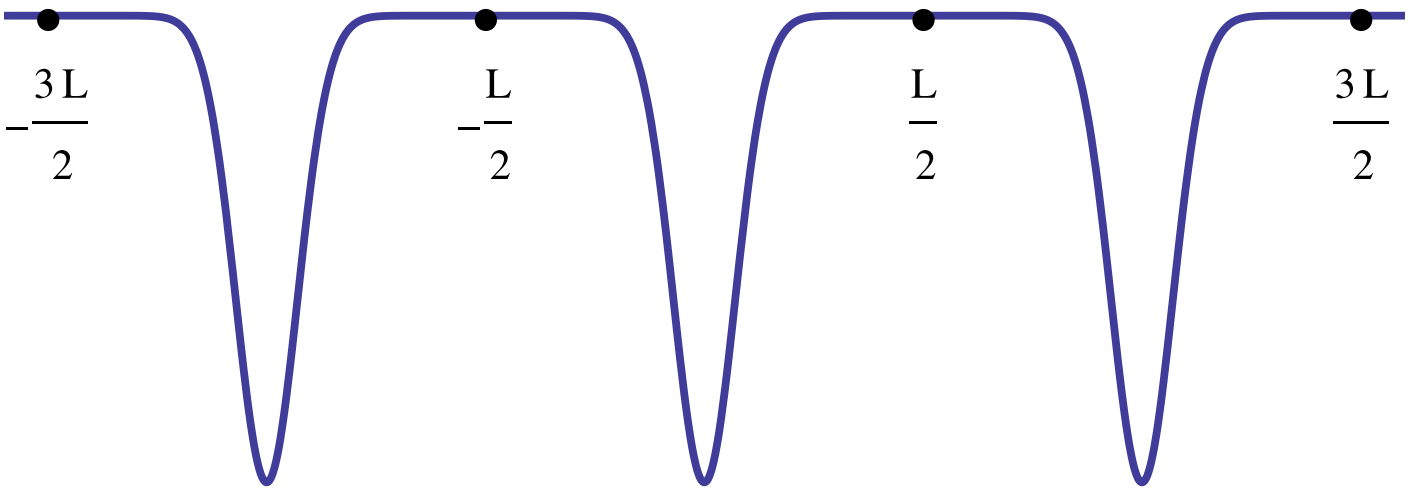

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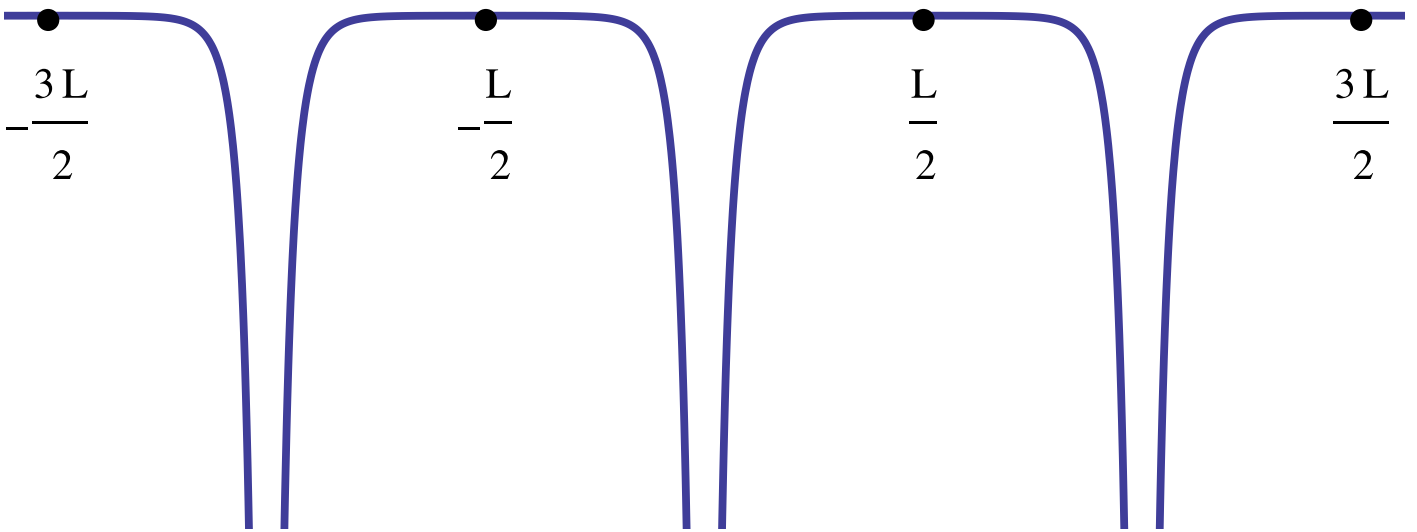


Bound-state volume dependence

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

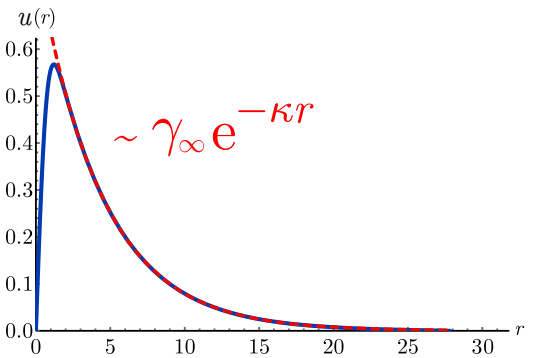
$$\Delta E_B(L) \sim -|\gamma_\infty|^2 \exp\big(-\kappa L\big)/L + \cdots, \; \gamma_\infty \text{ = ANC}$$

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

- infinite-volume properties determine volume dependence
  - binding momentum κ, asymptotic normalization constant (ANC) γ_∞
- in general, the prefactor is a polynomial in $1/\kappa L$

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

- 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**

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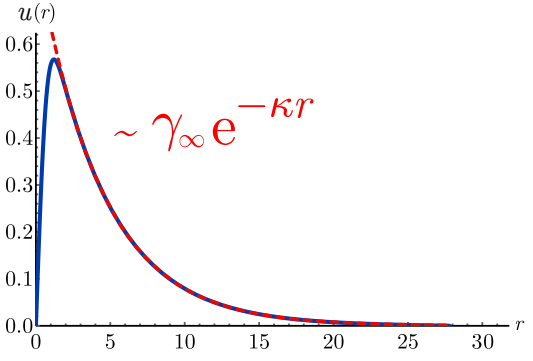

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- nonrelativistic description with short-range interaction + long-range Coulomb force

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

- 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

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
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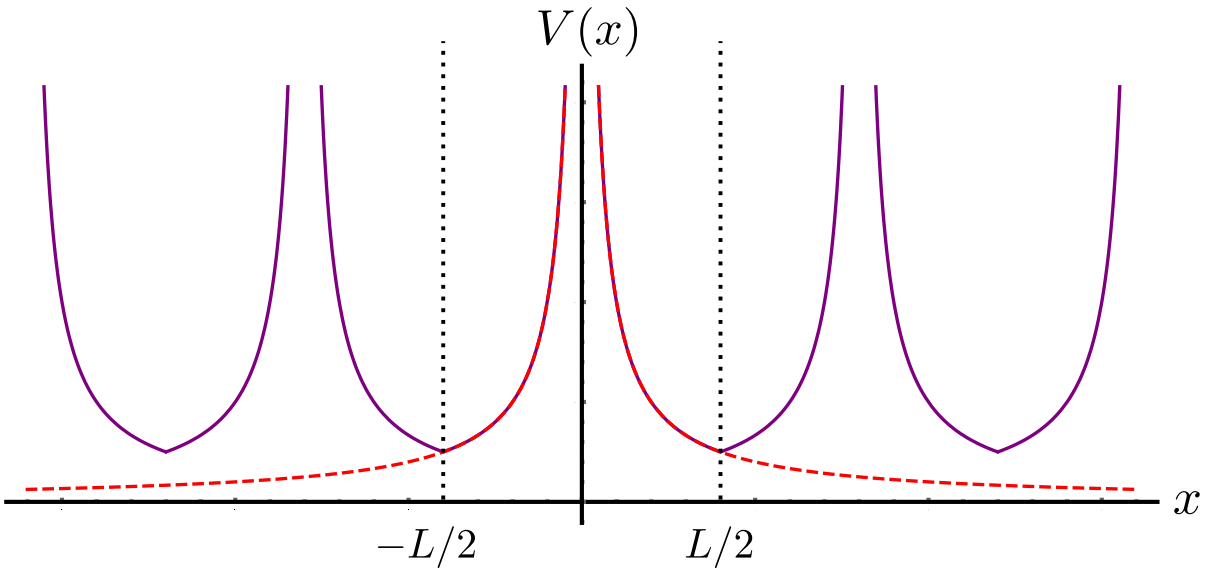
↪ **cut off at box boundary, grow Coulomb tail with L**



Charged-particle volume dependence

- **exact form in one spatial dimension can be found from boundary condition**
- **3D derivation is more involved due to nontrival geometry**

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

- this result is for S-wave (A_1^+ cubic rep.) states
- based on two-step procedure: first account for Coulomb potential in PT
- surface integrals lead to additional **power-law correction terms**
  - first term can be explicitly evaluated numerically
  - second term is more tricky, depends on short-range potential

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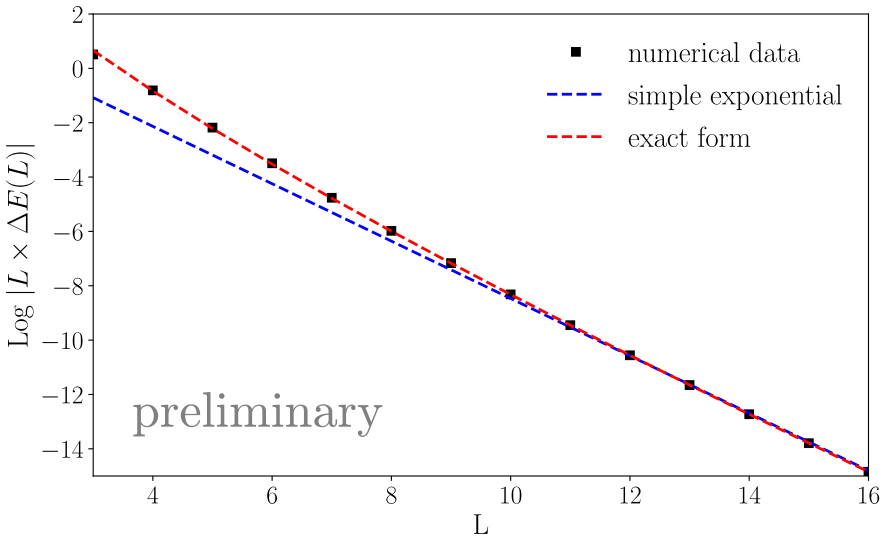
Asymptotic bounds

- dominant correction $= \mathcal{O}\left(\frac{\bar{\eta}}{(\kappa L)^2}\right) \times$ leading volume dependence
- second term has the same asymptotic dependence
  - but numerically observed to be smaller, practially not relevant

Example

- consider two particles (in three dimensions) with Coulomb strength $\gamma = 3.0$
  - bound state generated by short-range Gaussian potential
- determine **binding momentum** κ and **ANC** γ_∞ from volume dependence



- numerical values: $\kappa = 0.8611$, $\gamma_\infty = 8.78$
- from finite-volume fit: $\kappa = 0.8609$, $\gamma_\infty = 8.72$
- simple exponential fit would give $\kappa = 1.014$ instead

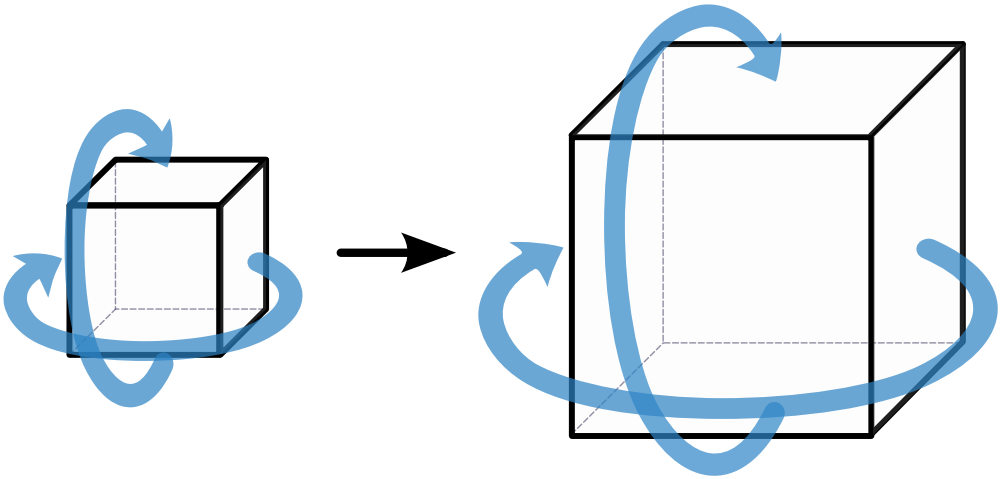
Hang Yu, Dean Lee, SK, in preparation (2021)

Part II

Volume extrapolation via eigenvector continuation

N. Yapa, SK, arXiv:2201.08313 (2022)

Volume extrapolation



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

Why?

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); ...
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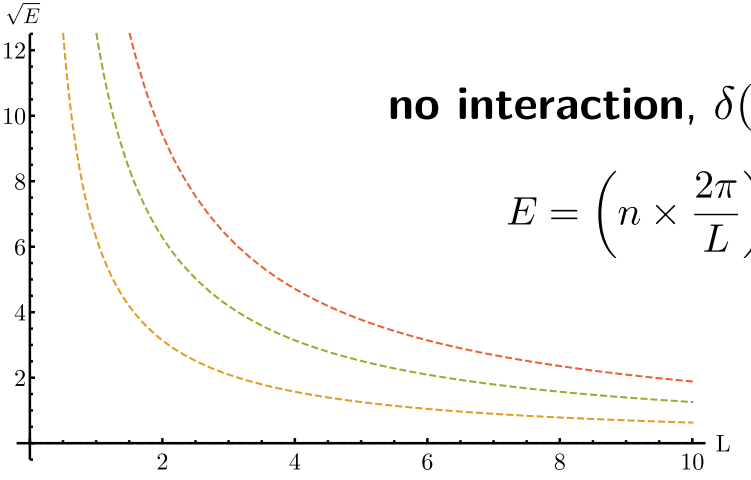

no interaction, $\delta(p) = 0$

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

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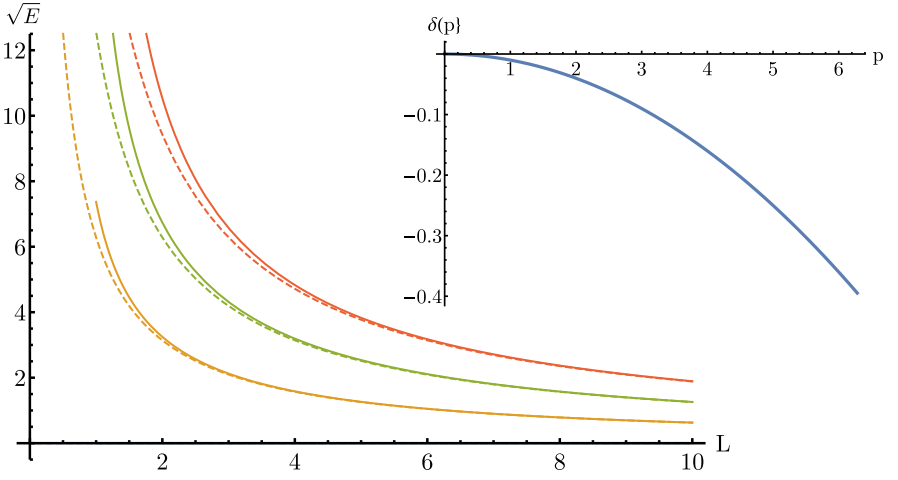

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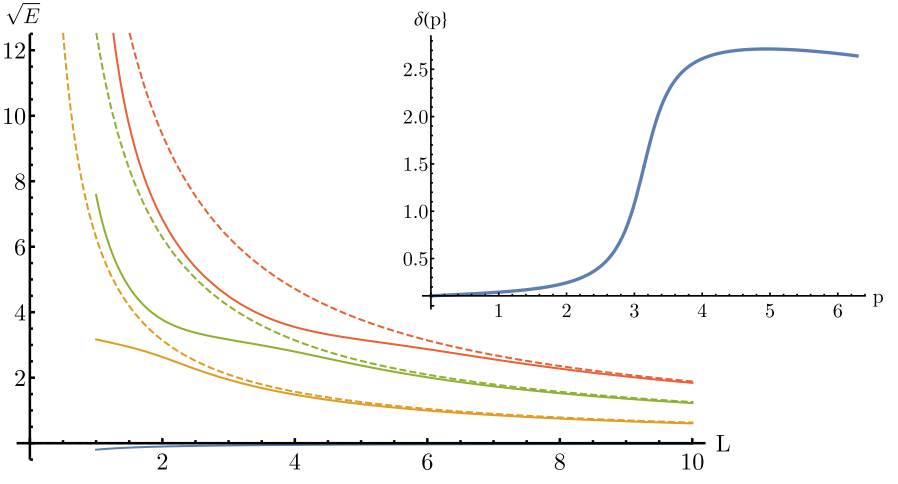

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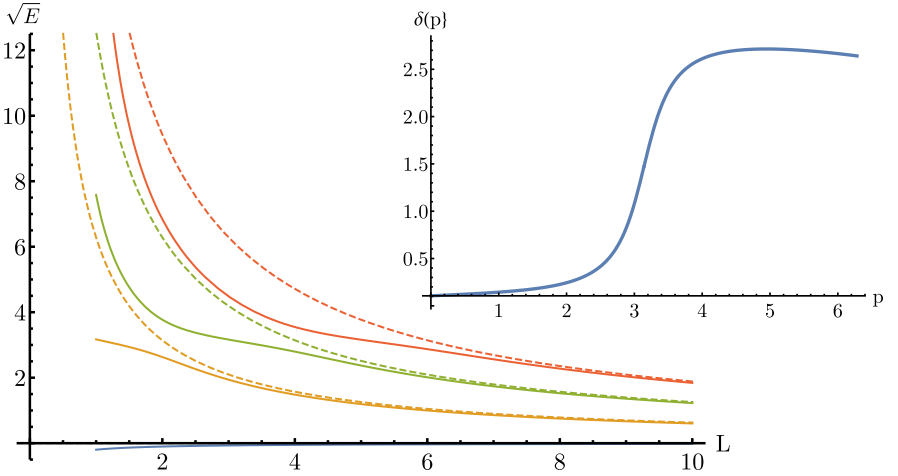

- direct correspondence between phase-shift jump and avoided crossing only for two-body systems, but the **spectrum signature carries over to few-body systems**

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, ...

    SK et al., PLB **810** 135814 (2020); Demol, ..., SK et al., PRC **101** 041302 (2020); ...
- **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 $|\psi(c_i)\rangle$, $i = 1, \dots N_{\mathrm{EC}}$ 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

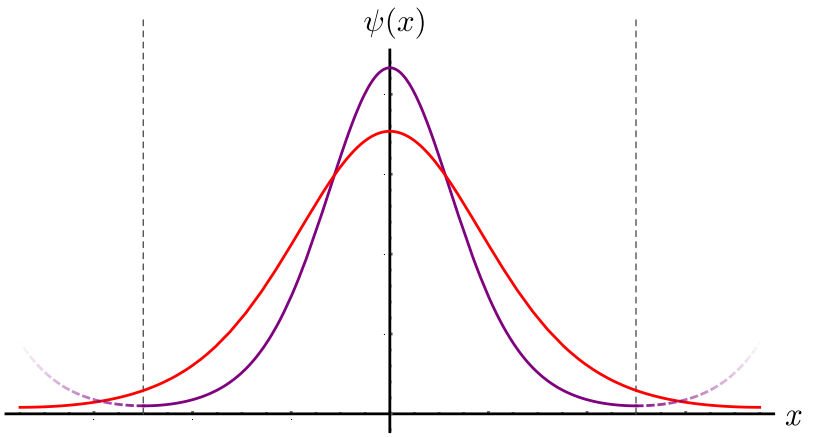
Dilatations

- 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 $\langle \cdot, \cdot \rangle_{\max}$**

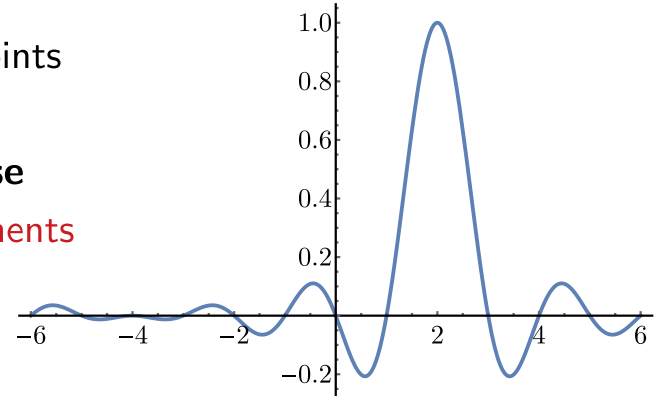
Discrete variable representation

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

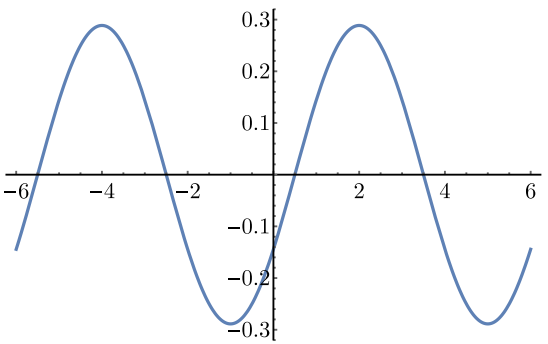


- periodic boundary condistions $\leftrightarrow$ plane waves as starting point
- **efficient implementation for large-scale calculations**
  - handle arbitrary number of particles (and spatial dimensions)
  - numerical framework scales from laptop to HPC clusters — SK et al., PRC **98** 034004 (2018)
  - recent extensions: GPU acceleration, separable interactions — Dietz, SK et al. arXiv:2109.11356

DVR construction

Basic idea

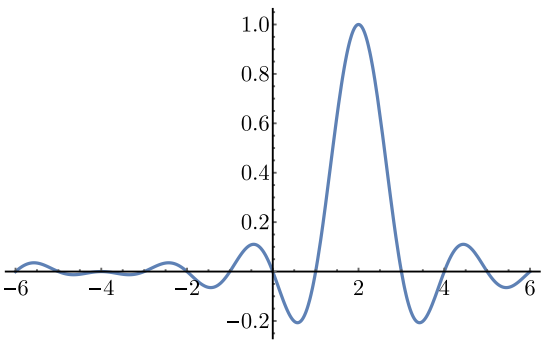
- start with some initial basis; here: plane waves $\phi_i(x) = \dfrac{1}{\sqrt{L}} \exp\left(\mathrm{i}\dfrac{2\pi i}{L} x\right)$
- consider (x_k, w_k) such that $\sum_{k=-N/2}^{N/2-1} w_k\, \phi_i^*(x_k)\phi_j(x_k) = \delta_{ij}$



unitary trans.

$\longrightarrow$

$\mathcal{U}_{ki} = \sqrt{w_k}\phi_i(x_k)$

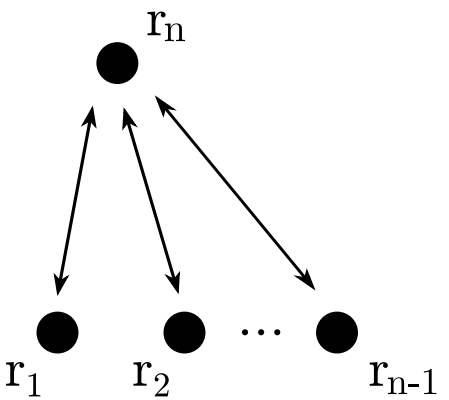


DVR states

- $\psi_k(x)$ localized at x_k, $\psi_k(x_j) = \delta_{kj}/\sqrt{w_k}$
- **note duality:** momentum mode ϕ_i $\leftrightarrow$ spatial mode ψ_k

DVR basis states

- construct DVR basis in simple relative coordinates
  - because Jacobi coordinates would complicate the boundary conditions
- separate center-of-mass energy (choose $\mathbf{P} = \mathbf{0}$)
- mixed derivatives in kinetic energy operator



$$\mathbf{x}_i = \sum_{i=1}^{n} U_{ij} \mathbf{r}_i$$

$$U_{ij} = \begin{cases} \delta_{ij} & \text{for} \quad i,j < n \\ -1 & \text{for} \quad i < n,\ j = n \\ 1/n & \text{for} \quad i = n \end{cases}$$

- **general DVR state for n particles in d dimensions**
  - $|s\rangle = |(k_{1,1}, \cdots, k_{1,d}), \cdots, (k_{n-1,1}, \cdots); \text{spins}\rangle \in B$
- basis size: $\dim B = (2S+1)^n \times N^{d \times (n-1)}$

(Anti-)symmetrization and parity

Permutation symmetry

- for each $|s\rangle \in B$, construct $|s\rangle_{\mathcal{A}} = \mathcal{N} \sum_{p \in S_n} \operatorname{sgn}(p)\, D_n(p)|s\rangle$
  - then $|s\rangle_{\mathcal{A}}$ is antisymmetric: $\mathcal{A}|s\rangle_{\mathcal{A}} = |s\rangle_{\mathcal{A}}$
  - for bosons, leave out $\operatorname{sgn}(p)$ $\rightsquigarrow$ symmetric state
  - $D_n(p)|s\rangle =$ some other $|s'\rangle \in B$, modulo periodic boundary

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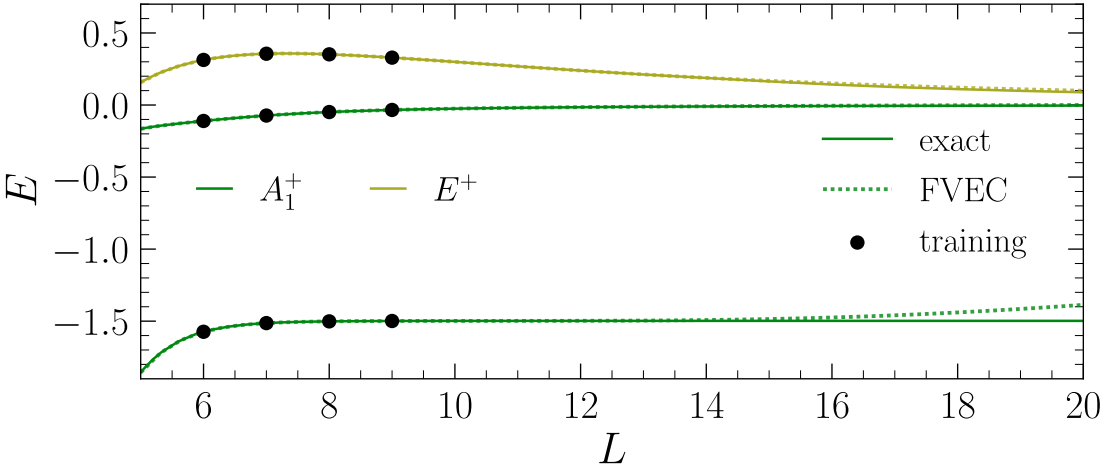
This operation partitions the orginal basis!

Reduced basis

- **each state appears in at most one (anti-)symmetric combination**
  - no need for expensive symmetry eigenspace determination
- significant reduction of basis size: $N \to N_{\mathrm{reduced}} \approx N/n!$
- parity (with projector $\mathcal{P}_{\pm} = 1 \pm \mathcal{P}$) can be handled analogously

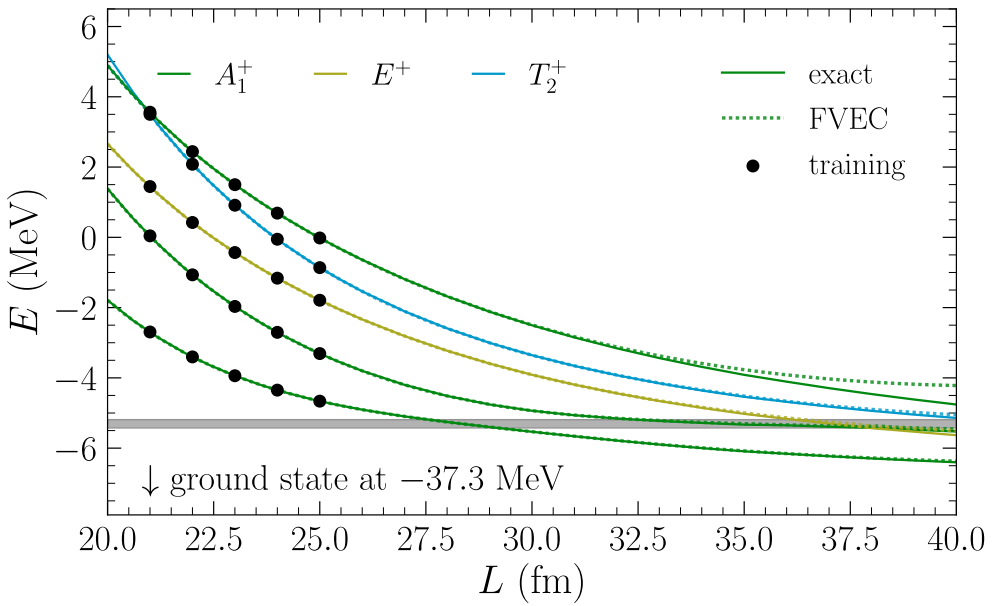
Two-body proof of concept

- 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**

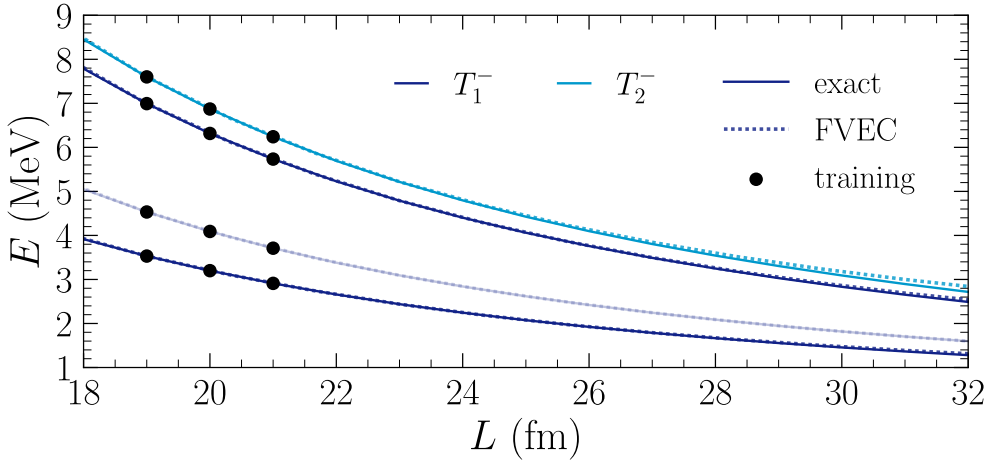
Three neutrons

- 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. arXiv:2109.11356

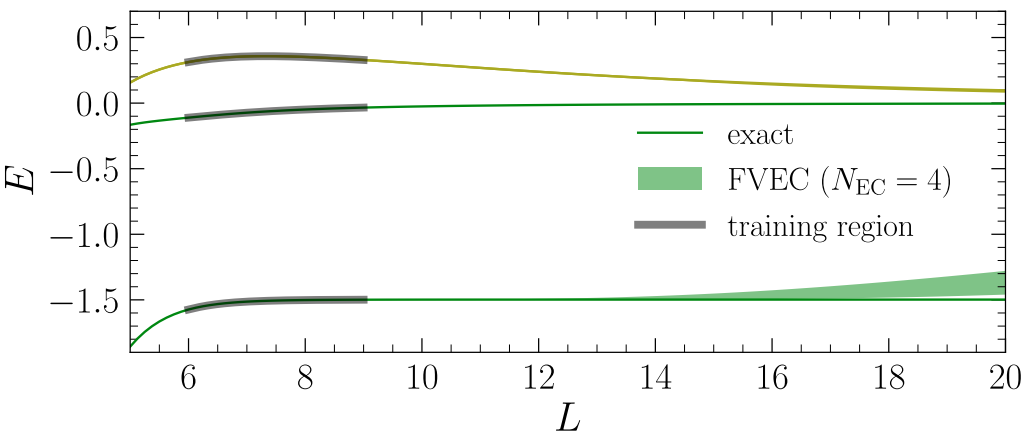


- total number of training data: $3 \times 8 = 24$ (partly covering cubic group multiplets)

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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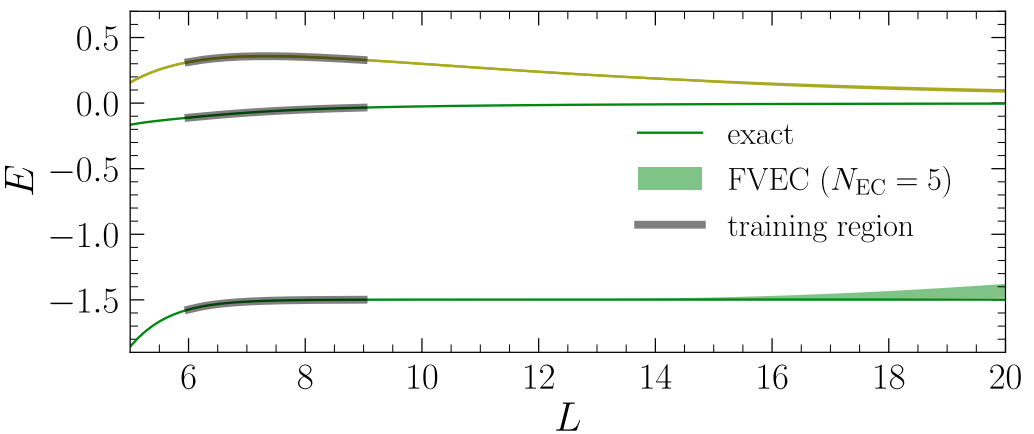

Summary and outlook

Volume dependence of charged-particle bound states

- wave function at large distances determines finite-volume energy shift
  - possible to extract asymptotic normalization coefficients
- 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
  - numerical calculation and/or bounds for additional correction terms

Volume extrapolation via eigenvector continuation

- DVR method can handle few-nucleon EFT calculations in large boxes
- 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
- in progress: application to four-neutron system

Thanks...

...to my students and collaborators...

- **H. Yu, N. Yapa, A. Andis (NCSU)**
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- A. Ekström (Chalmers U.)
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...and to you, for your attention!

Backup slides

Higher partial waves

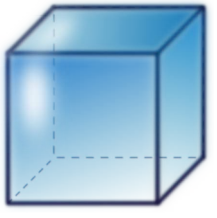
- **general result:** $\Delta E(L) = \alpha\left(\frac{1}{\kappa L}\right) \times |\gamma_\infty|^2 \frac{\mathrm{e}^{-\kappa L}}{\mu L} + \mathcal{O}\left(\mathrm{e}^{-\sqrt{2}\kappa L}\right)$

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 $SO(3)$

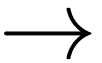


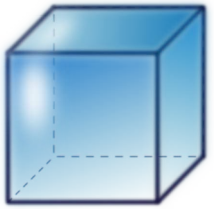
cubic group O

Broken symmetry

- **the finite volume breaks the spherical symmetry of the system**

rotation group $SO(3)$





cubic group O

- **irreducible representations of $SO(3)$ are reducible with respect to O**

  - finite subgroup of $SO(3)$
  - number of elements $= 24$
  - five irreducible representations

Γ	A_1	A_2	E	T_1	T_2
$\dim \Gamma$	1	1	2	3	3

- S waves contribute only to A_1, P waves only to T_1
- splitting first starts at D waves: $D^2 = T_2^+ \oplus E^+$

Higher partial waves

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

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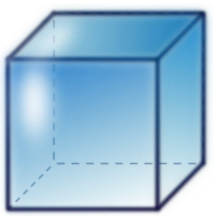
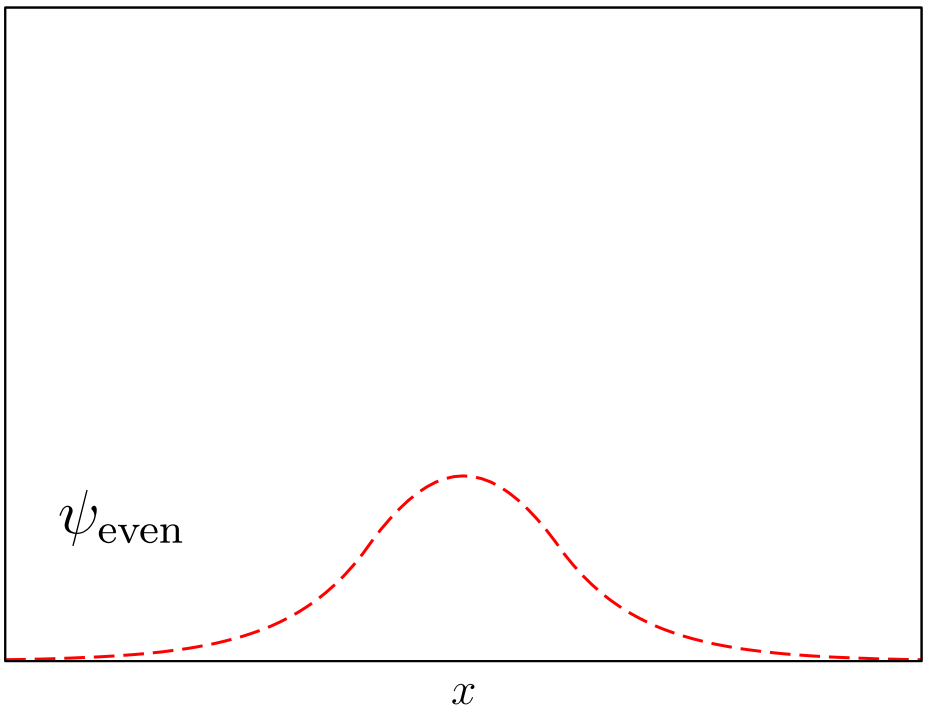


cubic group O

Sign of the energy shift



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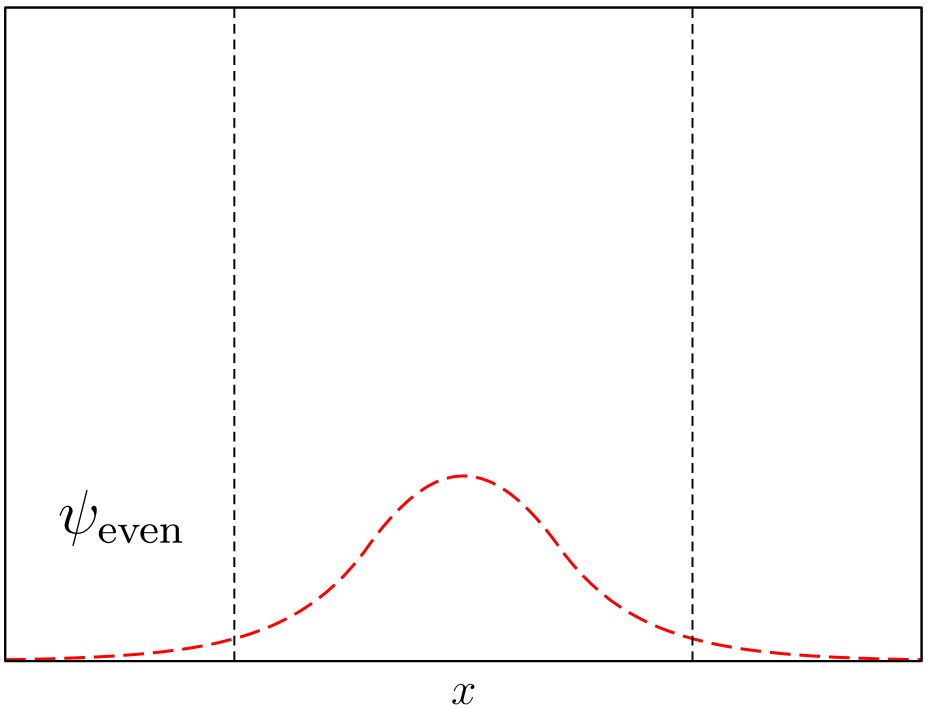

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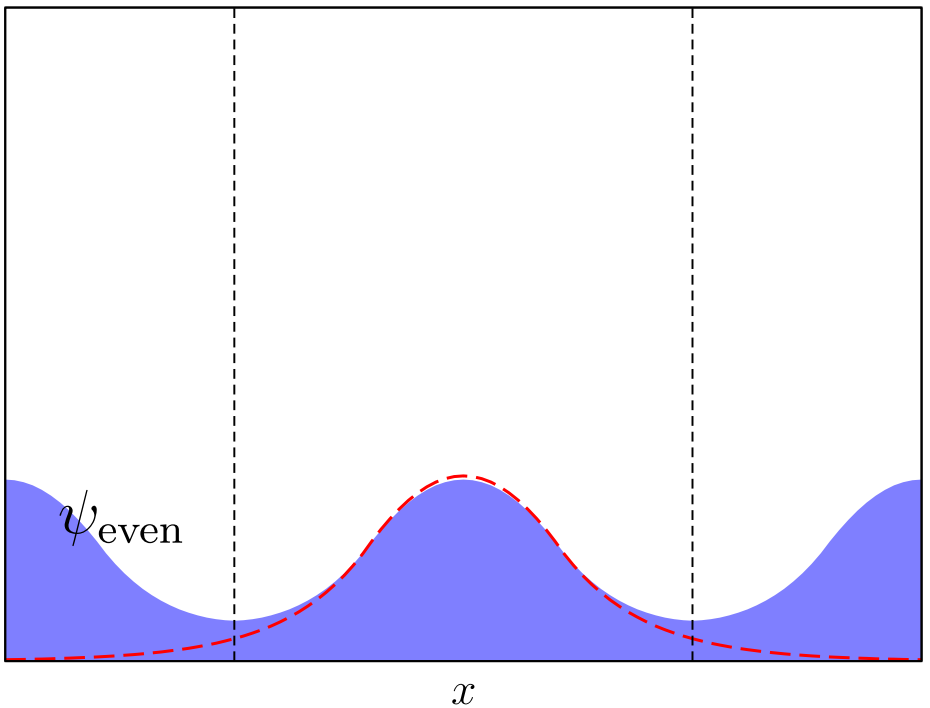
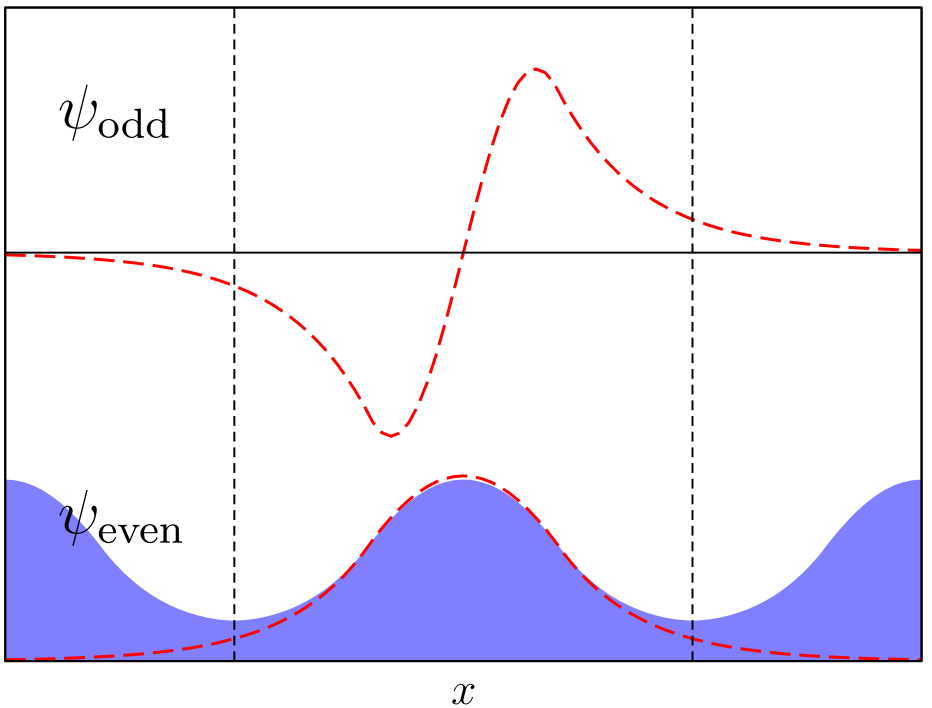


$$\Delta E_B(L) > 0$$

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

Sign of the energy shift

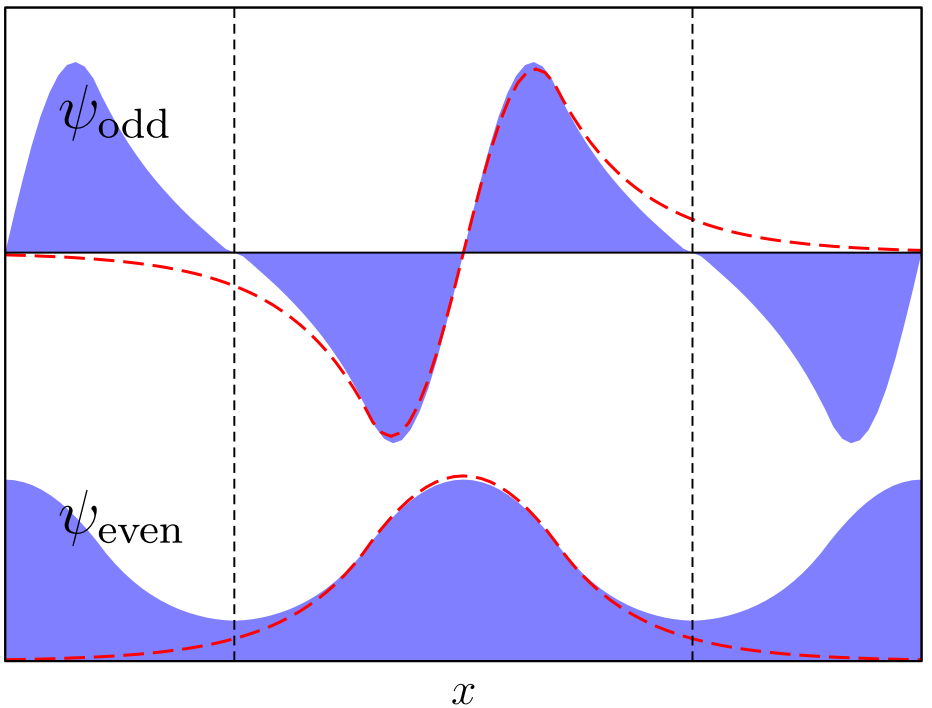


$$\Delta E_B(L) > 0$$

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

Sign of the energy shift

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



$\Delta E_B(L) < 0$

$\Delta E_B(L) > 0$

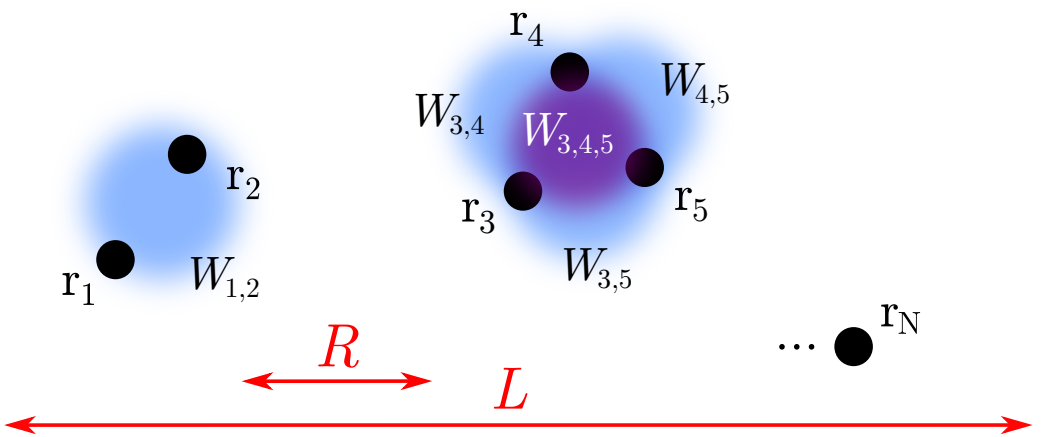
even parity $\rightarrow$ WF profile relaxed $\rightarrow$ less curvarture $\rightsquigarrow$ **more deeply bound**

N-body setup

- 2- up to N-body interactions, can be local or non-local

$$V_{1\cdots N}(\mathbf{r}_1,\cdots\mathbf{r}_N;\mathbf{r}'_1,\cdots\mathbf{r}'_N)=\sum_{i<j}W_{i,j}(\mathbf{r}_i,\mathbf{r}_j;\mathbf{r}'_i,\mathbf{r}'_j)1_{\not i,\not j}+\cdots$$

- all with finite range, set $R=\max\{R_{i,j},\cdots\}$
- assume asymptotically large volume: $L\gg R$

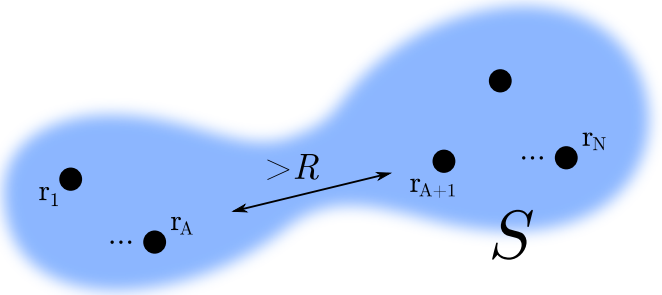


General result

- consider N particles (in d spatial dimensions), all interaction ranges $\leq R$
- separated into clusters $\rightsquigarrow$ set S in configuration space
- **restricted Hamiltonian determines asymptotic wavefunction**
- simplest example: $A = 1$

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

$$\hat{H}\big|_S = \sum_{i=2}^{N} \left[\hat{K}_i - \hat{K}^{\rm CM}_{2\cdots N} + \hat{V}_{2\cdots N}\right] + \hat{K}^{\rm rel}_{1|N-1}$$



$$\psi^B_N(\mathbf{r}_1, \cdots \mathbf{r}_N) \propto \psi^B_A(\mathbf{r}_1, \cdots \mathbf{r}_A)\psi^B_{N-A}(\mathbf{r}_{A+1}, \cdots \mathbf{r}_N) \times \left(\kappa_{A|N-A} r_{A|N-A}\right)^{1-d/2} K_{d/2-1}\left(\kappa_{A|N-A} r_{A|N-A}\right) \qquad (1)$$

$$\Delta E_N(L) \propto \left(\kappa_{A|N-A} L\right)^{1-d/2} K_{d/2-1}\left(\kappa_{A|N-A} L\right) \sim \exp\left(-\kappa_{A|N-A} L\right)/L^{(d-1)/2}$$

- **smallest** $\kappa_{A|N-A} = \sqrt{2\mu_{A|N-A}(B_N - B_A - B_{N-A})}$ **governs volume dependence**
- this assumes both clusters to be bound (otherwise: power-law correction factors)