

# Few nucleons and other stories

**Sebastian König**

**24th European Few-Body Conference**

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TECHNISCHE  
UNIVERSITÄT  
DARMSTADT



# Thanks...

## ...to my mentors and collaborators

- P. Klos, J. Lynn, H.-W. Hammer, A. Schwenk, K. Hebeler (TU Darmstadt)
- H.W. Griebhammer (G. Washington U.), U. van Kolck (IPN Orsay, U. of Arizona)
- D. Lee, S. Bogner (FRIB, Michigan State U.)
- R.J. Furnstahl (Ohio State U), T. Papenrock (UTK)
- S. Wesolowski (Salsbury U.), D. Phillips (Ohio U.), A. Ekström (Chalmers U.)
- B. Bazak, N. Barnea (Hebrew U. Jerusalem), J. Kirscher (Manchester U.),  
M. Pavon Valderrama (Beihang U.), ...

## ...for funding and computing time:



- Jülich Supercomputing Centre

- Lichtenberg Cluster (Darmstadt)

# Outline

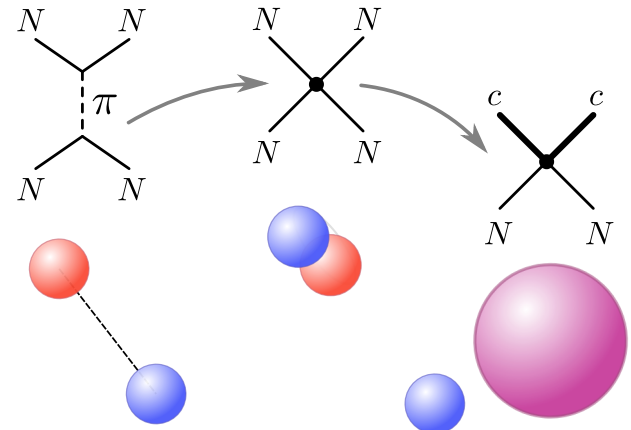
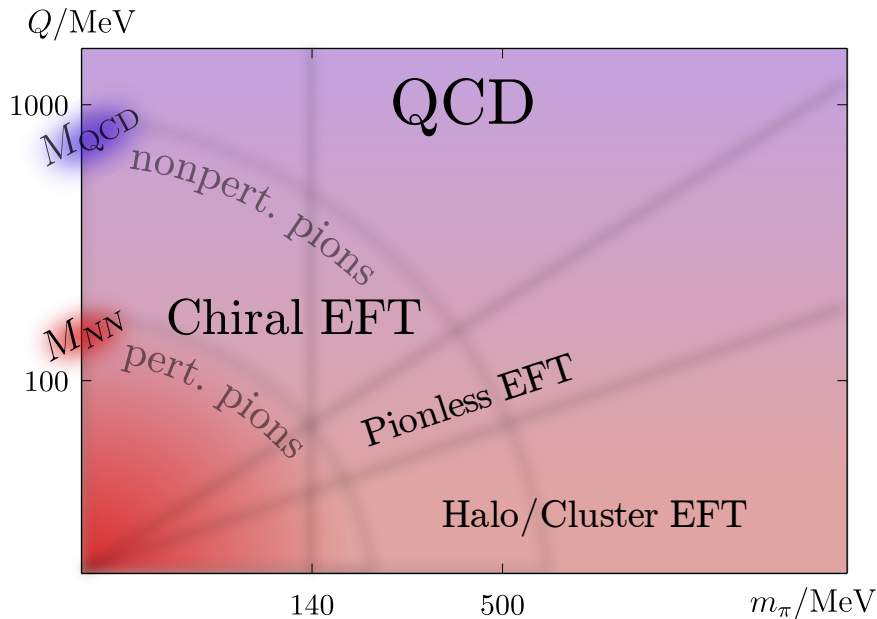
[...] the **Few-Body Systems Award for Young Researchers**  
has been assigned to you "For contributions to  
**effective field theories**  
and  
**finite-volume techniques**  
in the description of few-body systems."

# Part I

## The unitarity expansion

# Effective field theory

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



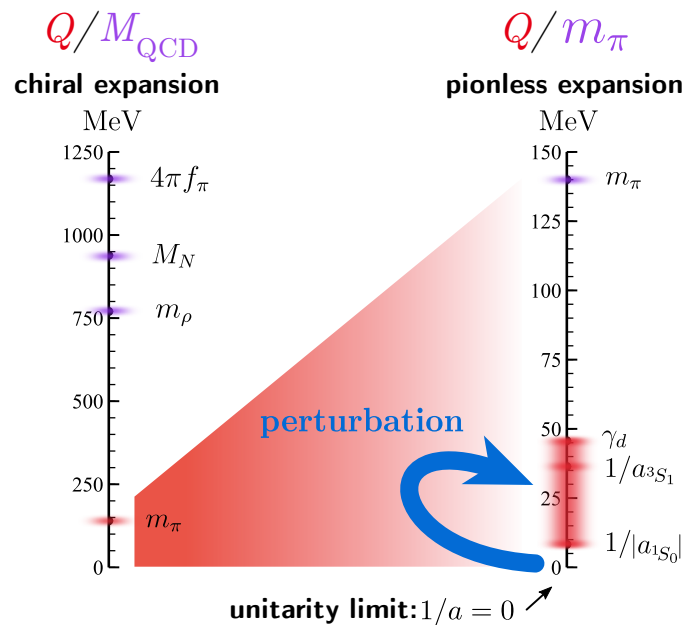
- unified discussion in recent review
- even more effective d.o.f.: rotations, vibrations

Hammer, SK, van Kolck, arXiv:1906:12122

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

# The unitarity expansion

Capture **gross features at leading order**, build up the rest as **perturbative “fine structure!”**



- take unitarity limit as leading order
  - infinite S-wave scattering lengths
  - deuteron at zero energy
- shift focus away from two-body details
- physics in universality regime

# The unitarity expansion

Capture **gross features at leading order**, build up the rest as **perturbative “fine structure!”**

## Nuclear sweet spot

- $1/a < Q_A < 1/R \sim m_\pi$
- $Q_A = \sqrt{2M_N B_A/A}$

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

A	2	3	4	...	56
$Q_A R$	0.3	0.5	0.8	...	0.9

↪ iron not much different from  ${}^4\text{He}$

van Kolck (2018)

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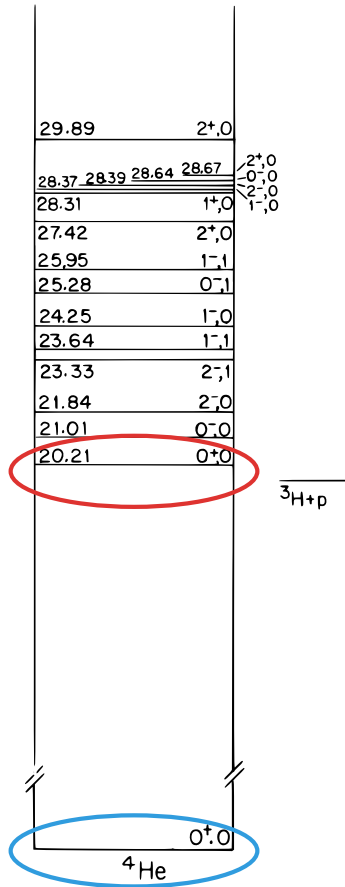
- **discrete scale invariance as guiding principle (Efimov effect!)**
  - ▶ near equivalence to bosonic clusters, exact  $SU(4)$  symmetry

Wigner, Phys. Rev. **51** 106 (1937); Mehen et al., PRL **83** 931 (1999); Bedaque et al., NPA **676** 357 (2000)  
Vanasse+Phillips, FB Syst. **58** 26 (2017)

cf. also Kievsky+Gattobigio, EPJ Web Conf. **113** 03001 (2016), ...  
A. Kievsky, talk on Monday; D. Lee, talk on Tuesday

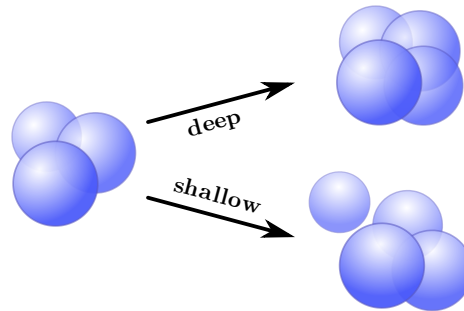


# Efimov trimers and tetramers



TUNL nuclear data

- $^3\text{H}$  as Efimov state Efimov, PLB **33** 563 (1970); Bedaque et al.(2000)
- **two associated tetramers for each Efimov state**  
Hammer+Platter, EPJA **32** 13 (2007); von Stecher, JPB **43** 101002 (2010); ...



- **at unitarity**
  - ▶  $B_4/B_3 \simeq 4.611$ ,  $B_{4^*}/B_3 \simeq 1.002$  Deltuva, PRA **82** 040701 (2010)
- **in  $^4\text{He}$** 
  - ▶ ground state at  $B_\alpha/B_H \simeq 3.66$
  - ▶ resonance at  $B_{\alpha^*}/B_H \simeq 1.05$  (where  $B_H = 7.72$ )

# Unitarity prescription

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

## (1) describe strong force with contact interaction

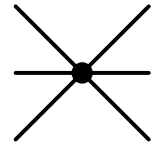
$$C_0 = \underbrace{C_0^{(0)}}_{\text{leading order (LO)}} + C_0^{(1)} + \dots$$

- momentum cutoff  $\Lambda$  gives "smearing"
- fit  $C_0^{(0)}$  to get  $a = \infty$  in both NN S-wave channels

## (2) fix Efimov spectrum to physical triton energy

- pionless LO three-body force
- triton as "anchor" at each order

Bedaque et al., NPA **676** 357 (2000)



## (3) include in perturbation theory

- finite  $a$ , Coulomb
- range corrections
- all further higher-order corrections

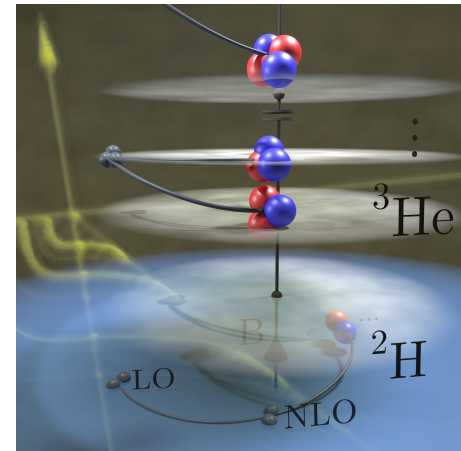
Leading order has a single parameter,  
all the rest is a perturbation!

# Unitarity expansion summary

- **novel approach to few-nucleon systems**
  - leading order at **unitarity limit** (infinite scattering length)
  - everything else as **perturbative fine structure**

SK et al., PRL **118** 202501 (2017); SK, JPG **44** 064007 (2017)

	LO	NLO*	N <sup>2</sup> LO	exp.
$^2\text{H}$	0	0	1.4(1.1)	2.22
$^3\text{H}$	8.48	8.48	8.48	8.48
$^3\text{He}$	8.48	7.6(2)	7.72	7.72
$^4\text{He}$	39(12)	30(9)		28.3



- **part of greater nuclear simplification trend**
- demonstrates feasibility of perturbative EFT calculations for  $A > 3$ 
  - unified Faddeev/Faddeev-Yakubowsky framework

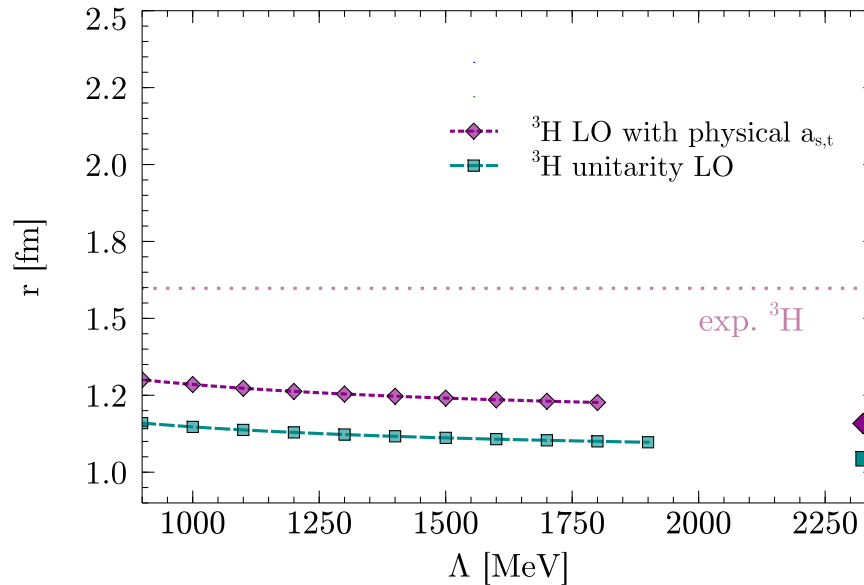
C. Elster, talk on Monday; D. Lee, talk on Tuesday

Kamada + Glöckle, NPA **548** 205 (1992); Platter (2005)

# Recent developments

# Charge radii

- calculate charge form factors  $F_C(q) = \langle \Psi | \rho(q) | \Psi \rangle \rightsquigarrow \langle r^2 \rangle = -\frac{1}{6} \frac{d^2}{dq^2} F_C, q \rightarrow 0$

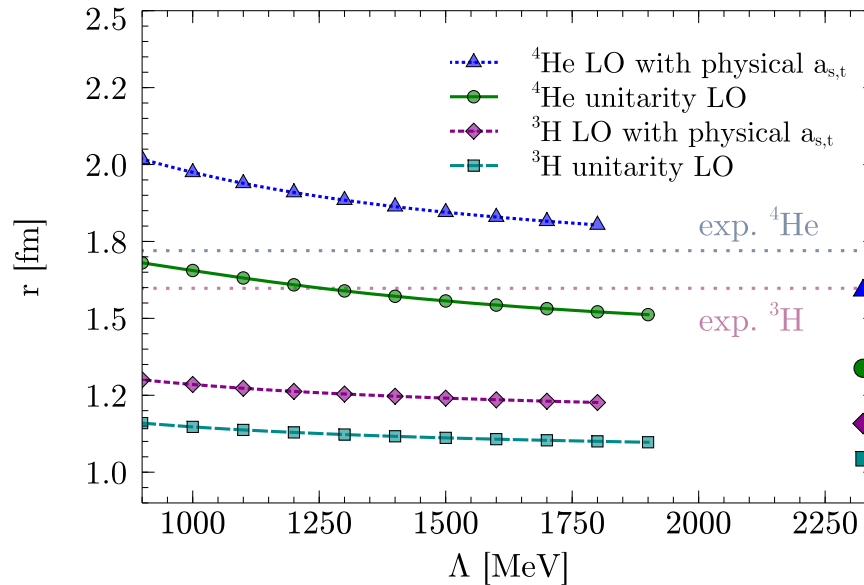


- point charge radii: subtract effects from  $r_p$  and  $r_n$
- **triton result in excellent agreement with pionless calculations**
  - range corrections known to be large

Vanasse, PRC **95** 024002 (2017); Vanasse+Phillips, FB Syst. **58** 26 (2017)

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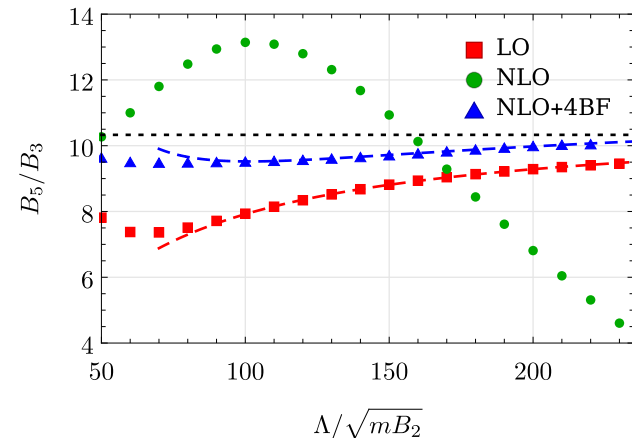
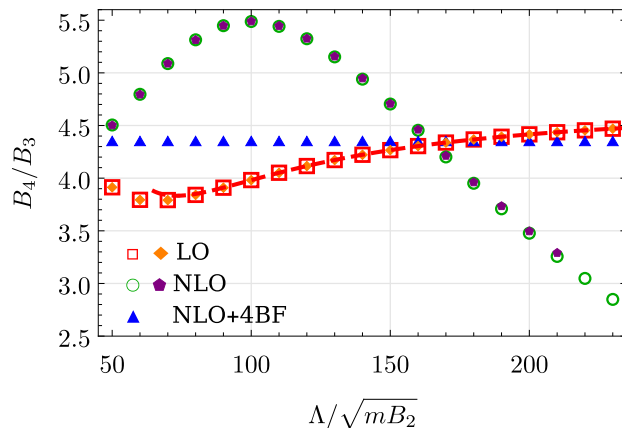
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# NLO four-body force

- full next-to-leading order includes range corrections  $\sim C_2 (k^2 + k'^2)$
- cancel in trinucleon energy splitting, but not in general
- four-boson energy does not converge with cutoff
- **promotion of four-body force to NLO**

Bazak, Kirscher, SK et al., PRL **122** 143001 (2019)



- **inclusion of four-body force stabilized five- and six-body system as well**
- general prediction for promotion of many-body forces (for bosons!)

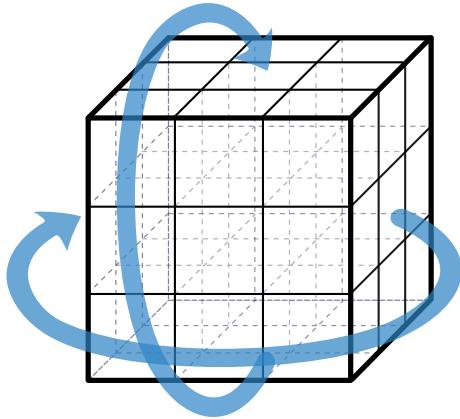
see talk by J. Kirscher tomorrow



# Part II

## Few-body states in finite volume

# 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 vol.-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); ...

# Few-body states in finite volume

## Bound states

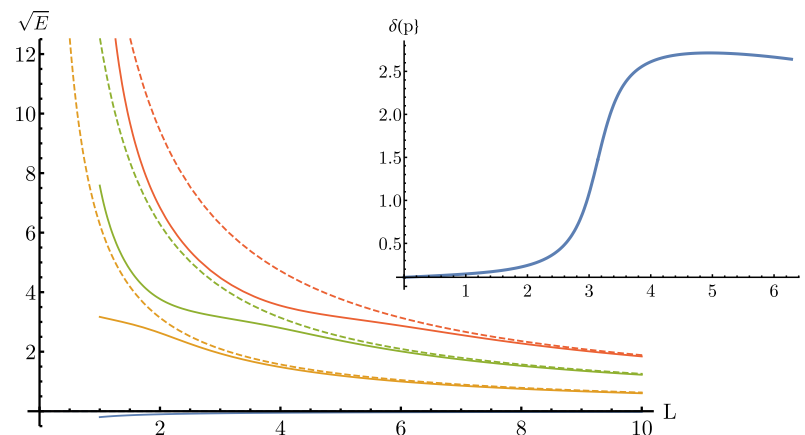
- exponential volume dependence
- physics encoded in prefactor and fall-off scale

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

## Resonances

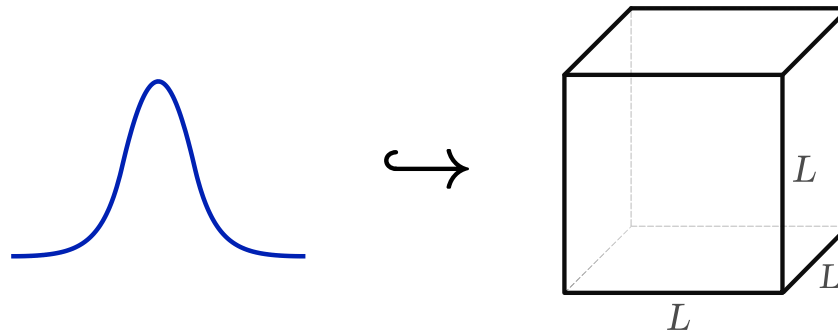
- continuum discretized into states with power-law volume dependence
- resonances show up as **avoided crossings**

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



# Two-body bound states

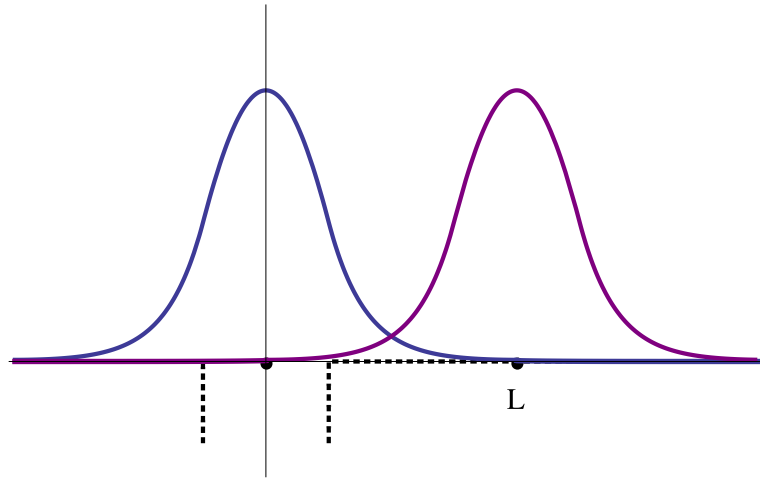
- consider bound state with energy  $E_B = -\kappa^2/(2\mu)$
- binding momentum  $\kappa$  corresponds to intrinsic length scale
- **finite volume affects the binding energy:  $E_B(L)$**



- for S-wave states, one finds  $\Delta B(L) \sim -|\gamma|^2 \exp(-\kappa L)/L + \dots$ ,  $\gamma = \mathbf{ANC}$   
Lüscher, Commun. Math. Phys. **104** 177 (1986); ...
- in general, the prefactor is a polynomial in  $1/\kappa L$   
SK et al., PRL **107** 112001 (2011); Annals Phys. 327, 1450 (2012)
- **asymptotic wavefunction determines volume dependence**

# Two-body bound states

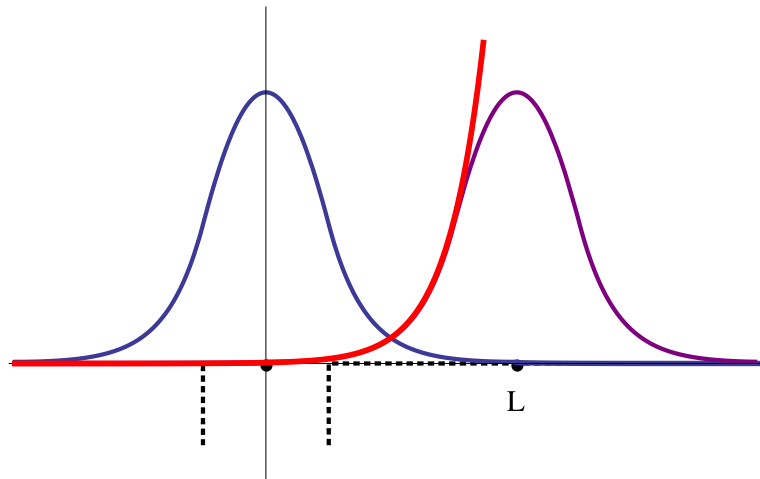
$$\Delta B(L) = \sum_{|\mathbf{n}|=1} \int d^3r \psi_B^*(\mathbf{r}) V(\mathbf{r}) \psi_B(\mathbf{r} + \mathbf{n}L) + \mathcal{O}(e^{-\sqrt{2}\kappa L})$$



- periodic boundary: sum over nearest neighbour overlapping wavefunctions
- contribution to integral only inside potential range
- use Schrödinger equation to eliminate potential:  $\psi(\mathbf{r})V(\mathbf{r}) = [\Delta_r - \kappa^2]\psi(\mathbf{r})$

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- only asymptotic tail matters:  $\psi(\mathbf{r}) \sim \gamma \times \exp(-\kappa r)/r$

Now consider the general case

$N$  particles

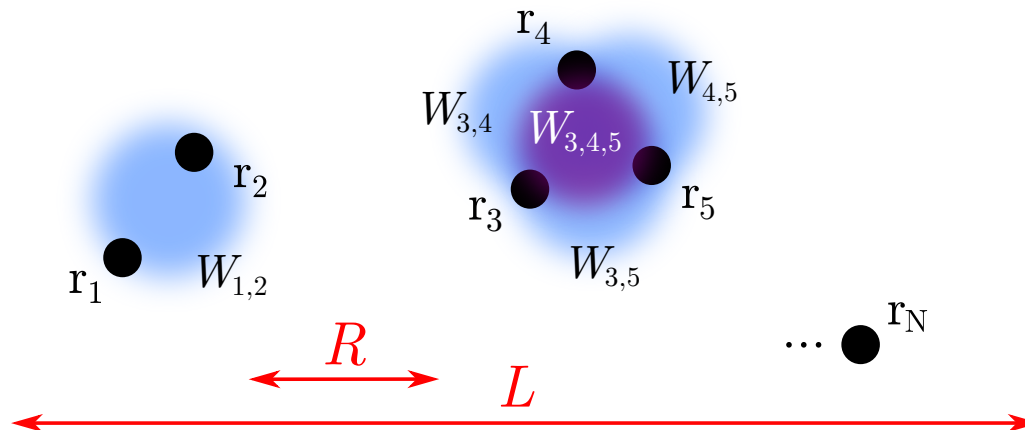
$d$  spatial dimensions

# N-body setup

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

$$V_{1\dots N}(\mathbf{r}_1, \dots, \mathbf{r}_N; \mathbf{r}'_1, \dots, \mathbf{r}'_N) = \sum_{i < j} W_{i,j}(\mathbf{r}_i, \mathbf{r}_j; \mathbf{r}'_i, \mathbf{r}'_j) 1_{R_{i,j}} + \dots$$

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

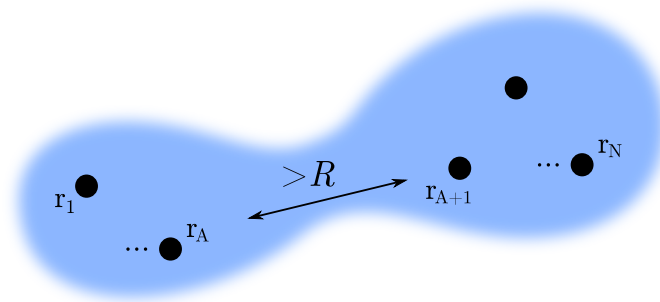




# General result

Separate  $A$  particles and **factorize wavefunction**

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



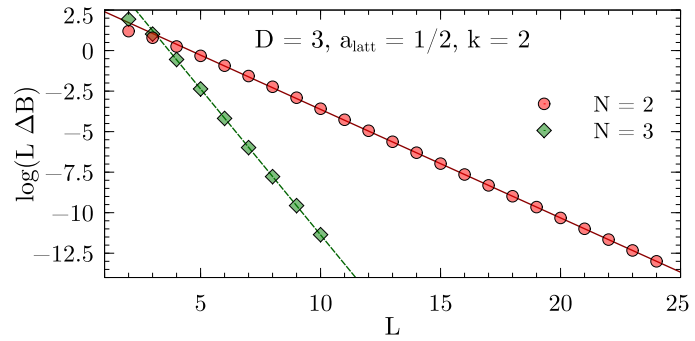
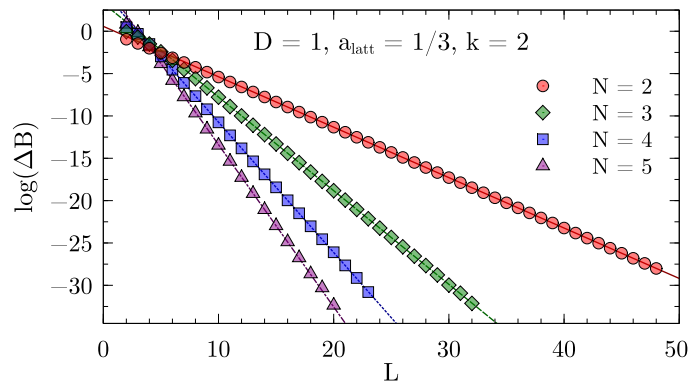
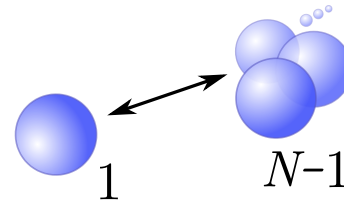
$$\psi_N^B(\mathbf{r}_1, \dots, \mathbf{r}_N) \sim \psi_A^B(\mathbf{r}_1, \dots, \mathbf{r}_A) \psi_{N-A}^B(\mathbf{r}_{A+1}, \dots, \mathbf{r}_N) \\ \times (\kappa_{A|N-A} r_{A|N-A})^{1-d/2} K_{d/2-1}(\kappa_{A|N-A} r_{A|N-A})$$

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

- **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)
- **prefactor determined by asymptotic normalization constant (ANC)**

# Numerical results

- consider one particle separated from the rest



- diagonalization of discretized Hamiltonian
- interaction = short-range Gaussian two-body potentials
  - $L \gg R$  well satisfied for  $L \gtrsim 5$
- all quantities in natural units with mass = 1
- **straight lines indicate excellent agreement with analytical result**

# Finally: Few-body resonances

# Finite-volume resonance signatures

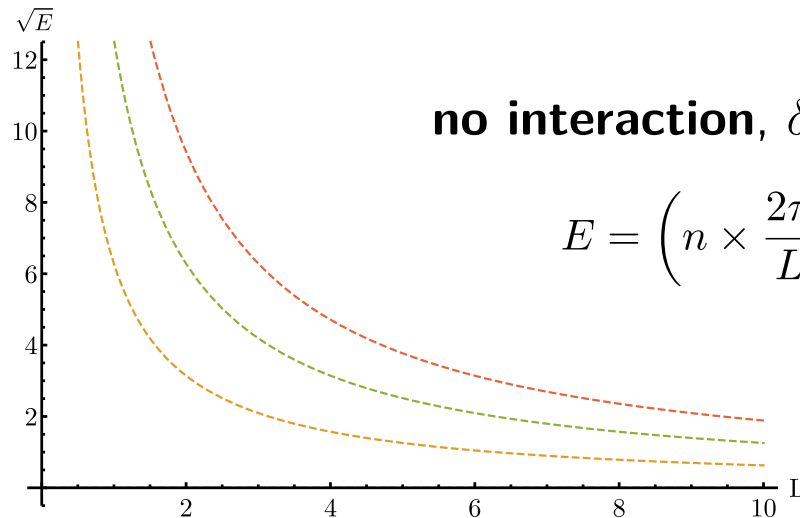
## Lüscher formalism

$$p \cot \delta_0(p) = \frac{1}{\pi L} S(\eta) \quad , \quad \eta = \left( \frac{Lp}{2\pi} \right)^2 \quad , \quad p = p(E(L))$$

Lüscher, NPB **354** 531 (1991); ...

- finite volume  $\rightarrow$  momentum quantization  $\rightarrow$  discrete energy levels
- **resonance contribution**  $\rightsquigarrow$  **avoided level crossing**

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



# Finite-volume resonance signatures

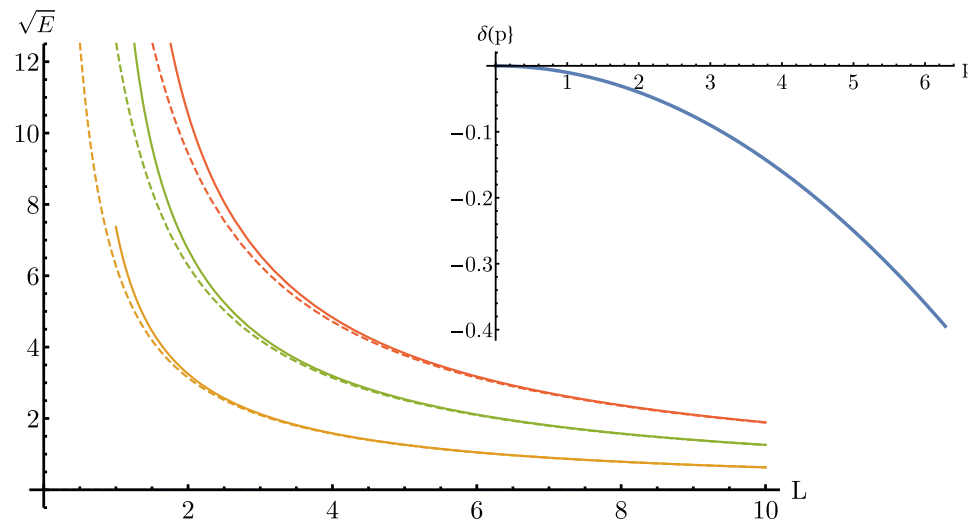
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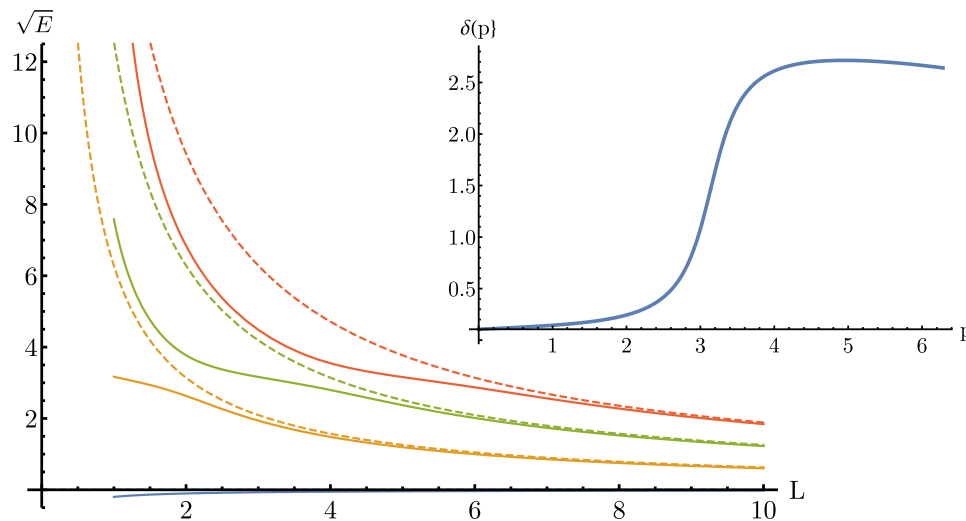
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# Discrete variable representation

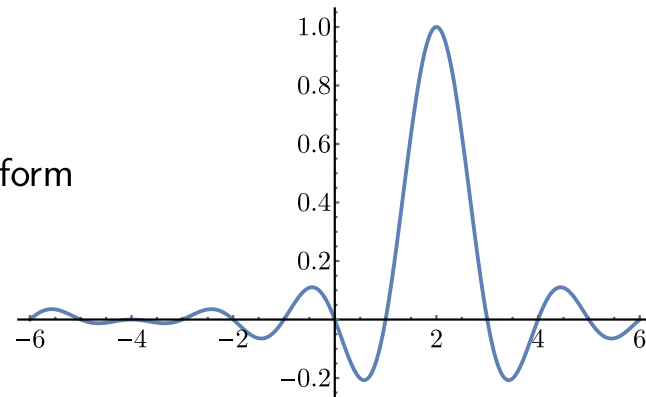
## Need calculation of **several** few-body energy levels

- difficult to achieve with QMC methods
- use a **Discrete Variable Representation (DVR)**

Klos et al., PRC **94** 054005 (2016)

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 sparse...
- ...or implemented via Fast Fourier Transform



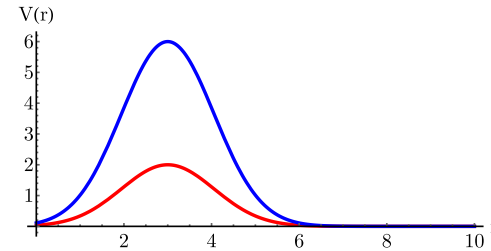
- periodic boundary conditions  $\leftrightarrow$  plane waves as starting point
- **implementation for large-scale calculations**
  - ▶ numerical framework scales from laptop to HPC clusters

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

# Two-body check

## Use model potential to produce S-wave resonance

- shifted gaussian barrier
  - $V(r) = V_0 \exp\left(-\left(\frac{r-a}{R_0}\right)^2\right)$
- tune parameters to generate resonances

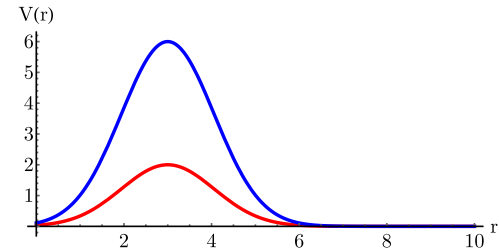




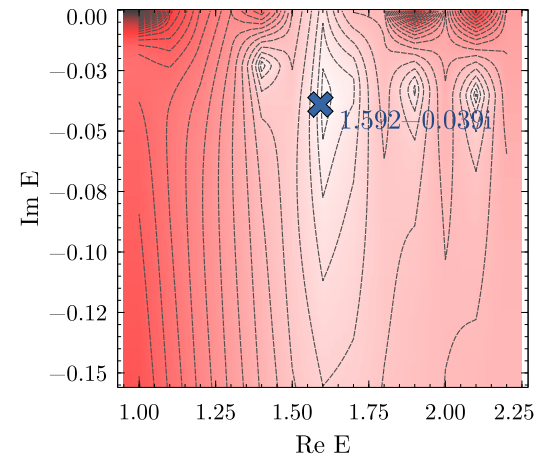
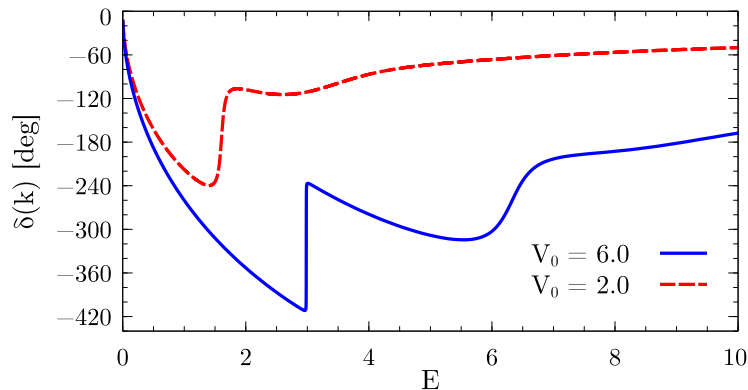
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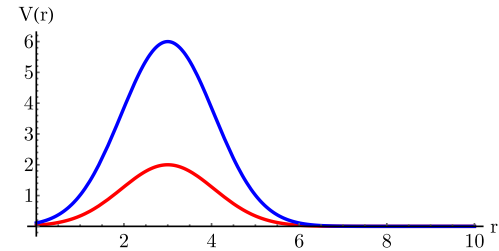
## Phase shifts and S-matrix pole



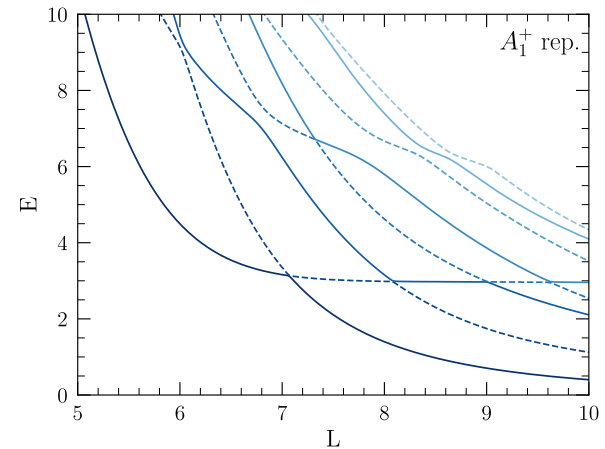
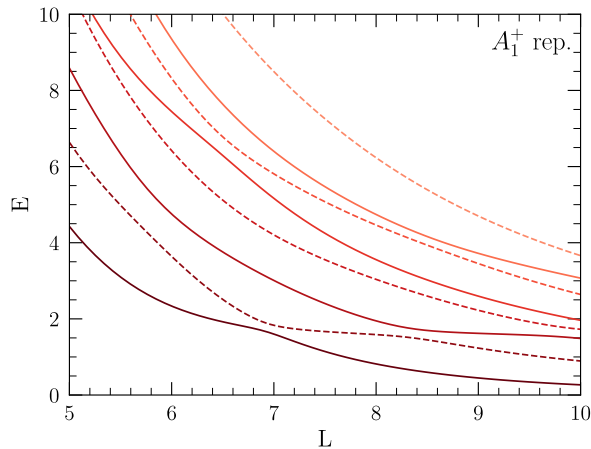
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## Finite-volume spectra

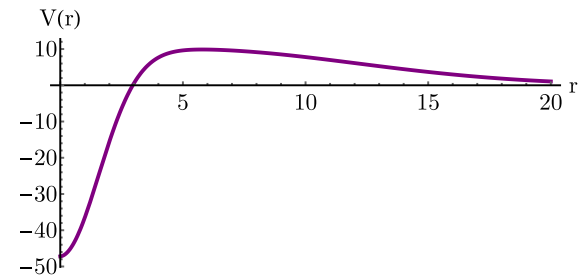
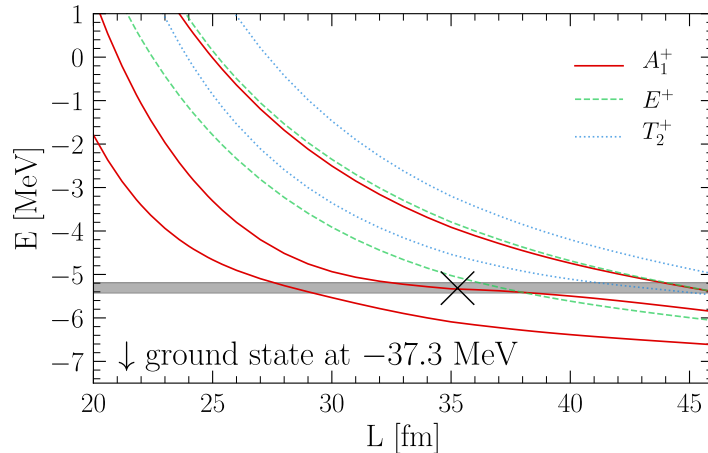


# Three-body check

## Study 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.)
  - ▶  $-5.96 - i0.40$  MeV (Fedorov et al.)



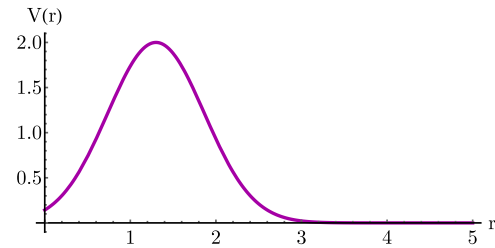
- **fit inflection point(s) to extract resonance energy:  $E_R = -5.32(1)$  MeV**

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

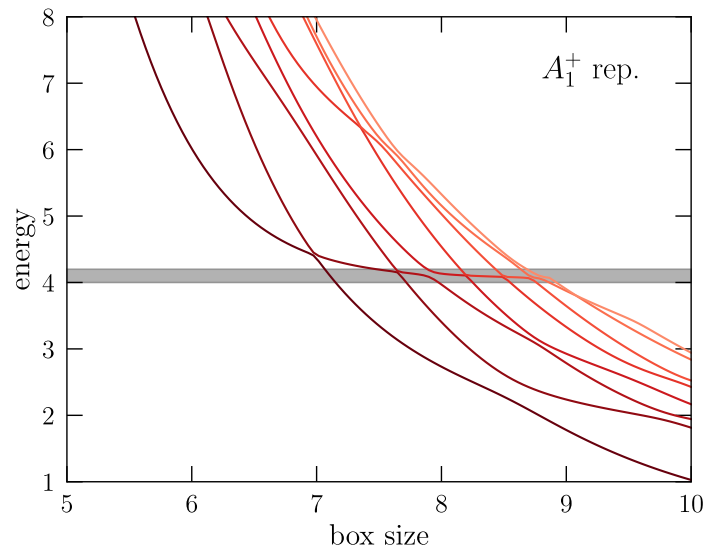
# Genuine three-body resonance

## Three-boson system

- shifted Gaussian two-body potential
- **no two-body bound state!**
- **add short-range three-body force**



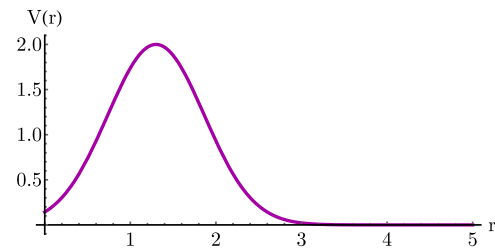
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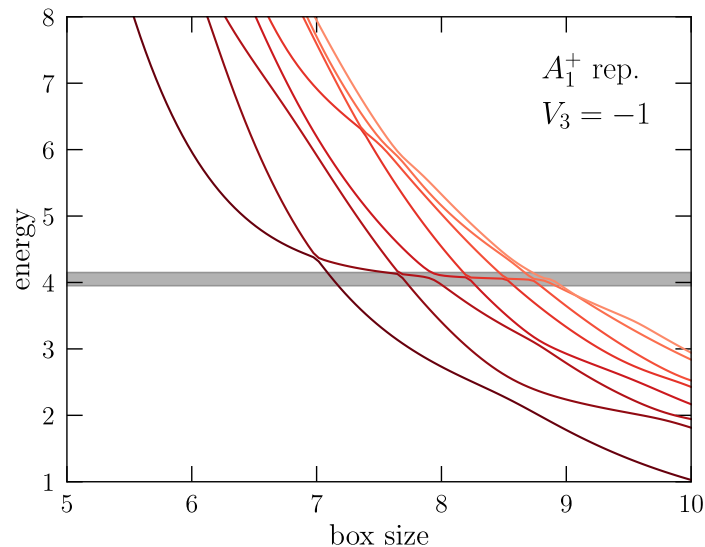
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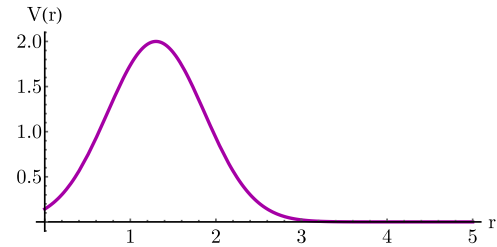
SK et al., PRC **98** 034004 (2018)



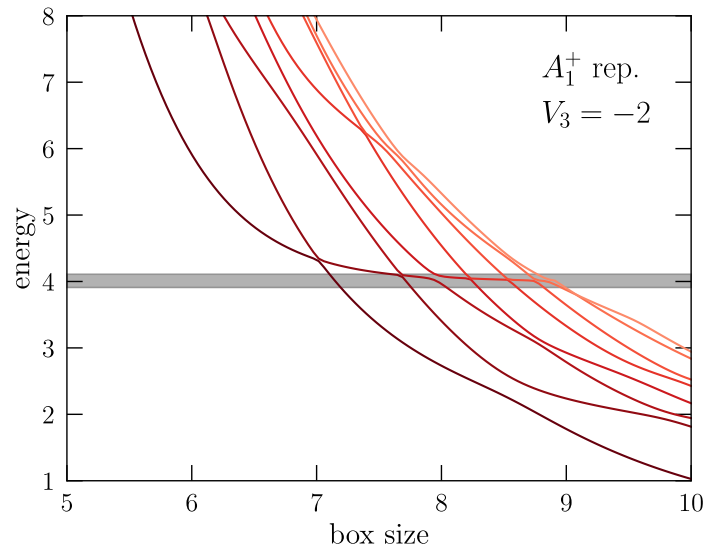
# Genuine three-body resonance

## Three-boson system

- shifted Gaussian two-body potential
- **no two-body bound state!**
- **add short-range three-body force**



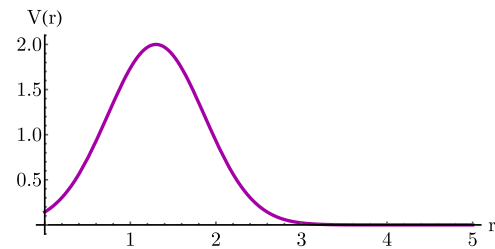
SK et al., PRC **98** 034004 (2018)



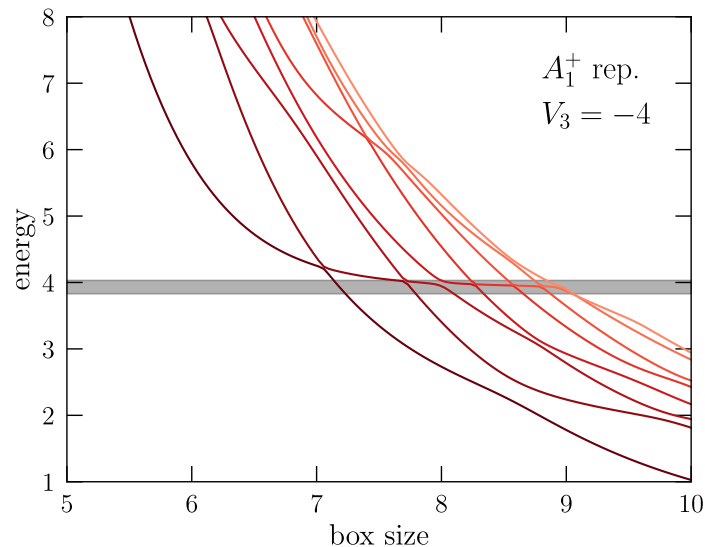
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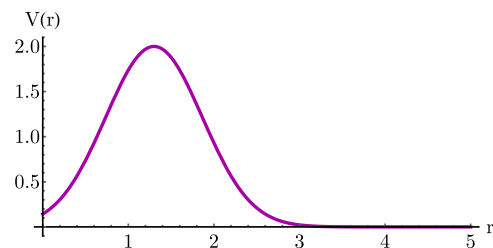
SK et al., PRC **98** 034004 (2018)



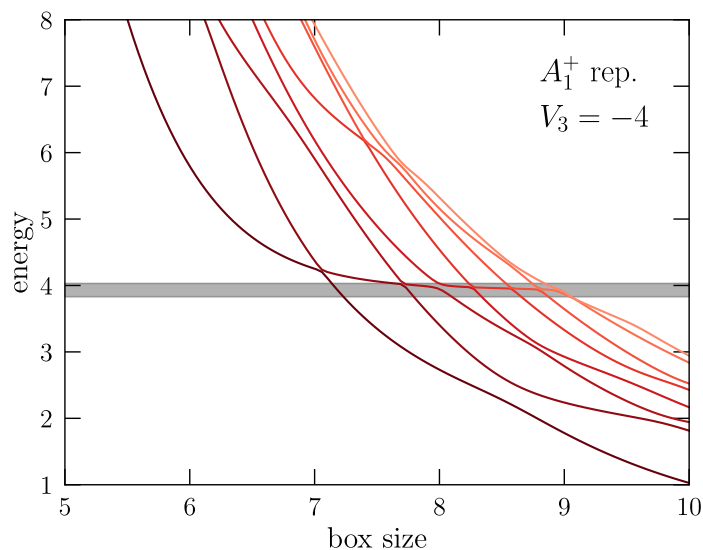
# Genuine three-body resonance

## Three-boson system

- shifted Gaussian two-body potential
- **no two-body bound state!**
- **add short-range three-body force**



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



- **possible to move three-body state  $\leftrightarrow$  spatially localized wavefunction**

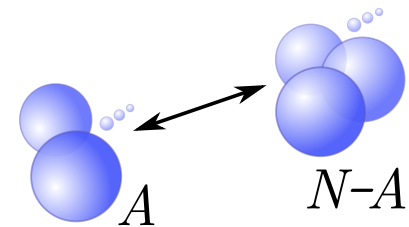


# Finite-volume summary

## Bound states

- leading volume dependence known for **arbitrary bound states**
- reproduces known results, **checked numerically**
- calculate ANCs, **single-volume extrapolations possible!**
- applications to lattice QCD, EFT, cold-atomic systems

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



## Resonances

- explicit proof of concept for **up to four particles**
- efficient **large-scale numerical implementation (DVR)**
- different concrete **physics applications**
  - ▶ **few-neutron systems**, alpha clusters, atomic resonances, ...

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

Thank you

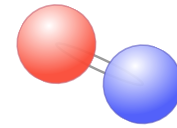
# Backup slides

# Implementation

## Unified (2-, 3-, 4-body) numerical framework

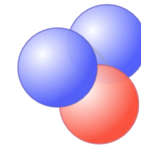
### Two-nucleon system

- separable regulator for contact interactions:  $V = C_0|g\rangle\langle g|$
- can be **solved analytically** to get scattering amplitudes



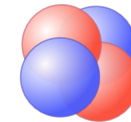
### Three-nucleon system

- **Faddeev equations**:  $|\psi\rangle = G_0 t_2 P |\psi\rangle + G_0 t_2 |\psi_3\rangle$
- used to fit three-body force



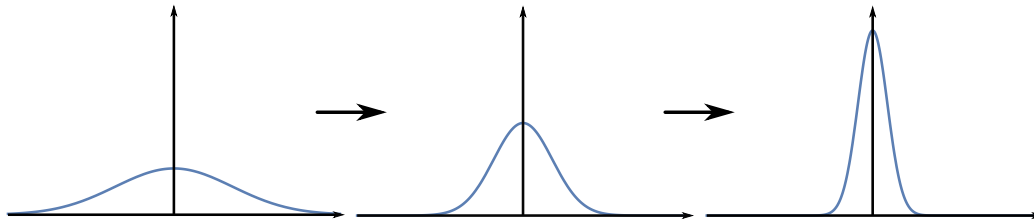
### Four-nucleon system

- **Faddeev-Yakubowsky equations**: two components  $|\psi_{A,B}\rangle$
- need full wavefunction for perturbation theory:
  - $|\Psi\rangle = (1 - P_{34} - P P_{34})(1 + P)|\psi_A\rangle + (1 + P)(1 + \tilde{P})|\psi_B\rangle$



# The cutoff

- increasing the **momentum cutoff  $\Lambda$**  decreases interaction range
- **RG invariance:** fix  $C = C(\Lambda)$  to keep input observables invariant

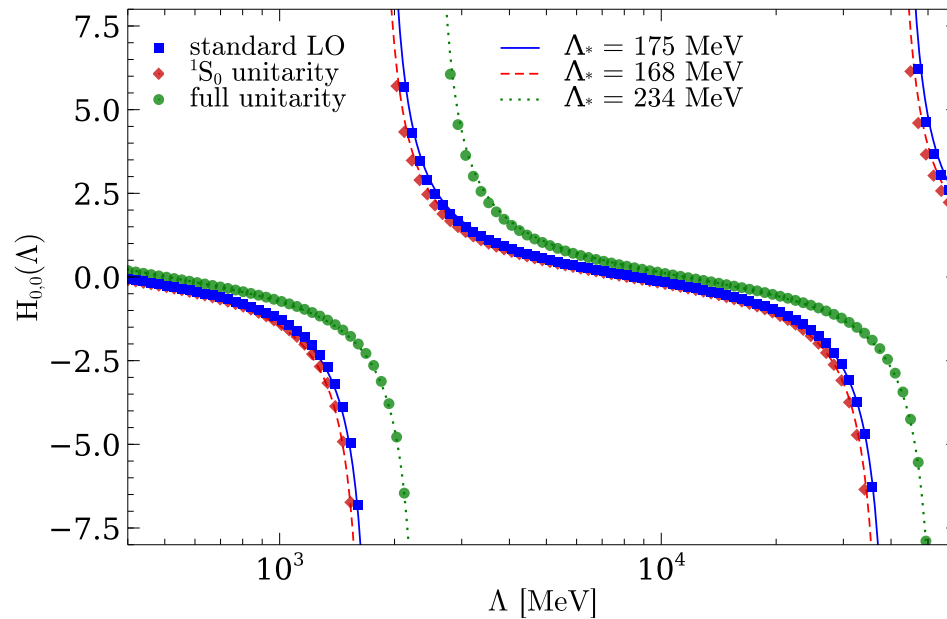


- predicted observables should converge as  $\Lambda$  increases...
- **...but individual contributions generally do not, e.g.:**

$\Lambda / \text{MeV}$	800	1000	1200	1400
$E_{\text{kin}} / \text{MeV}$	+113.67	+140.58	+168.44	+197.09
$E_{\text{pot}} / \text{MeV}$	-139.77	-167.47	-195.76	-224.62

# Three-body force running

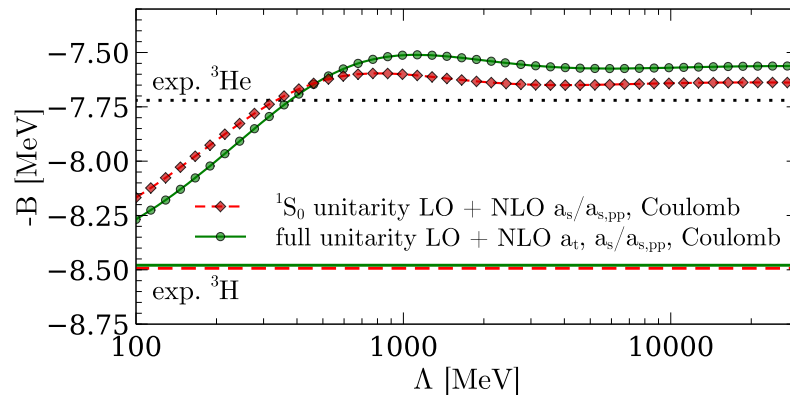
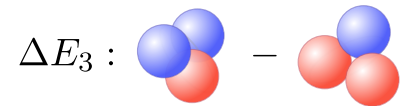
- three-body force  $D_0^{(0)}(\Lambda)$  depends on a single parameter  $\Lambda_*$
- fit to triton binding energy (in this case)



- **not much shift in  $\Lambda_*$  due to unitarity limit**

# Trinucleon energy difference

- at LO  ${}^3\text{H}$  and  ${}^3\text{He}$  are degenerate (exact isospin symmetry)
- Coulomb correction enters together with  $1/a_{s,pp}$  at NLO
- predict binding energy **difference**



	LO	NLO	exp.
${}^3\text{H}$	8.48	8.48	8.48
${}^3\text{He}$	8.48	7.6(2)	7.72

(red = input)

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

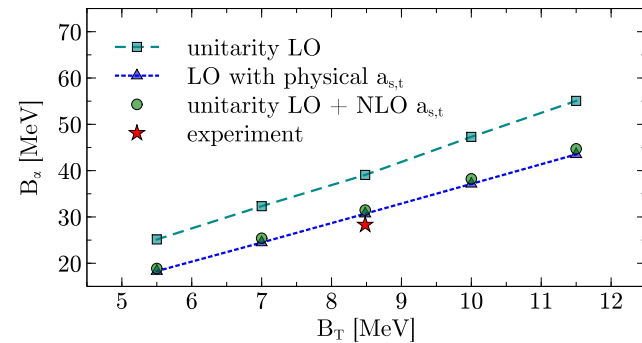
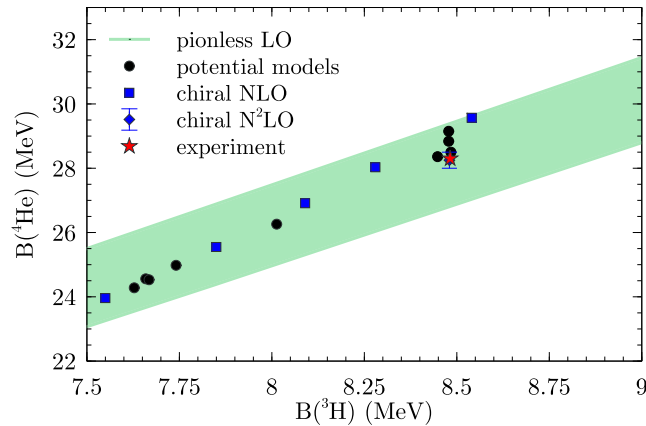
- **range corrections cancel at NLO**

- ▶ leading order is isospin symmetric
- ▶ small isospin breaking  $r_{pp} \neq r_{np}$  (5%) relegated to next higher order

SK et al. JPG **43** 055106 (2016)

# Tjon line

## Correlation between ${}^3\text{H}$ and ${}^4\text{He}$ binding energies



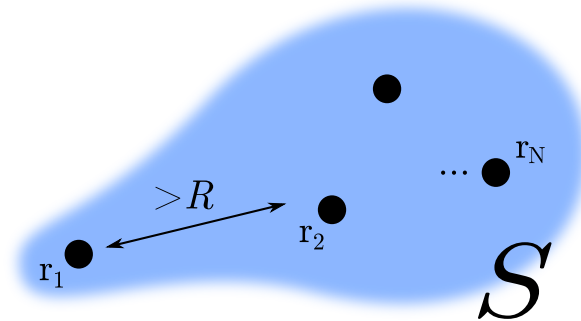
- originally observed comparing different potential models
- well reproduced by unitarity expansion
- perturbativeness of  $1/a$  persists off the physical point

Tjon, PLB 56 217 (1975)



# Cluster separation

- consider one particle separated from all others



$$S = \{(\mathbf{r}_1, \dots, \mathbf{r}_N) : |\mathbf{r}_1 - \mathbf{r}_i| > R \quad \forall i = 2, \dots, N\}$$

- look at Hamiltonian restricted to  $S$

$$\hat{H}|_S = \sum_{i=2}^N \left[ \hat{K}_i - \hat{K}_{2\dots N}^{\text{CM}} + \hat{V}_{2\dots N} \right] + \hat{K}_{1|N-1}^{\text{rel}} \quad \text{no interaction } \hat{V}_{1\dots!}$$

- separation ansatz:  $\Psi(\mathbf{r}_1, \dots, \mathbf{r}_N) = \sum_{\alpha} f_{\alpha}(\mathbf{r}_2, \dots, \mathbf{r}_N) g_{\alpha}(\mathbf{r}_{1|N-1})$ 
  - lowest  $f_0$  is eigenstate of sub-Hamiltonian with energy  $-B_{N-1}$
  - $g_0$  is Bessel function with scale set by  $B_N - B_{N-1}$

# Analytical examples

## Three bosons at unitarity

- two-body interaction with zero range and infinite scattering length

$$\begin{aligned}\Delta B_3(L) &\propto (\kappa_{1|2}L)^{-1/2} K_{1/2}(\kappa_{1|2}L) P(\kappa_{1|2}L) \\ &\sim \exp\left(-\sqrt{\frac{4mB_3}{3}}L\right) \left(\sqrt{\frac{4mB_3}{3}}L\right)^{-1} P(\kappa_{1|2}L)\end{aligned}$$

- same exp. dependence as exact result ✓
- by comparison, power-law factor  $P(x) = x^{-1/2}$

Meißner et al., PRL **114** 091602 (2015)

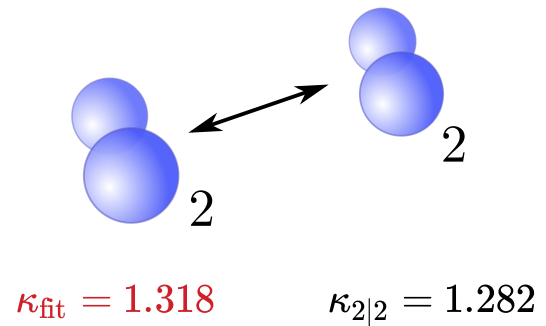
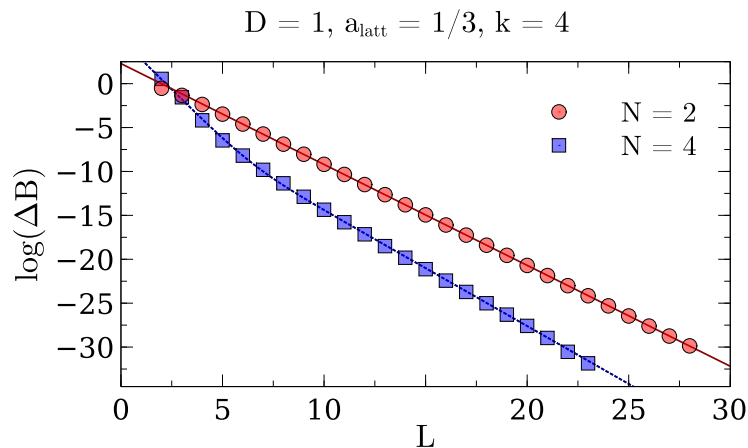
## $N$ particles with $N$ -body interaction only

- spinless  $N$ -particle bound state with only an  $N$ -particle interaction
- $\psi(\mathbf{r}_1, \dots) \propto (\kappa_{1|N-1} r_{1|N-1})^{1-d(N-1)/2} K_{d(N-1)/2-1}(\kappa_{1|N-1} r_{1|N-1})$
- again leads exactly to expected exp. dependence ✓
- read off power-law factor  $P(x) = x^{-d(N-2)/2}$

# More complicated example

Typically one channel dominates, but not necessarily...

- take an attractive two-body force  $\rightsquigarrow B_2 < 0$
- add a repulsive three-body force  $\rightsquigarrow$  no three-body bound state
- add attractive four-body force  $\rightsquigarrow B_4 < 0$



- contributions from two channels clearly visible
- asymptotic slope in good agreement with  $2|2$  separation

# Further possibilities

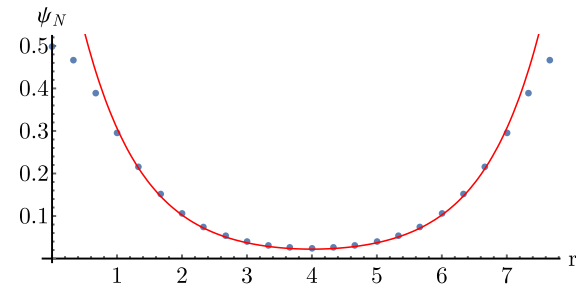
## (a) Extract ANC from volume dependence

$$\Delta B_N(L) = \frac{(-1)^{\ell+1} \sqrt{\frac{2}{\pi}} f(d) |\gamma|^2}{\mu_{A|N-A}} \kappa_{A|N-A}^{2-d/2} L^{1-d/2} K_{d/2-1}(\kappa_{A|N-A} L)$$

- ANC  $\gamma$  relevant for low-energy capture reactions
- notoriously difficult to measure experimentally (especially for charged systems)
- possible to extract ANC for arbitrary cluster systems

## (b) Extrapolate from single-volume calculations

- get  $N$ -body and  $(N-A)$ -body wavefunctions
  - look along fixed direction
  - mind periodic boundary condition
- $\kappa_{A|N-A}$  obtained from same fit
- $\hookrightarrow$  directly calculate  $\Delta B_N(L)$

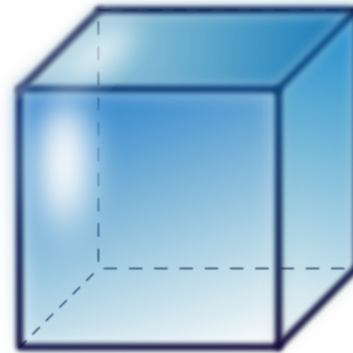


# Broken symmetry

- 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

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

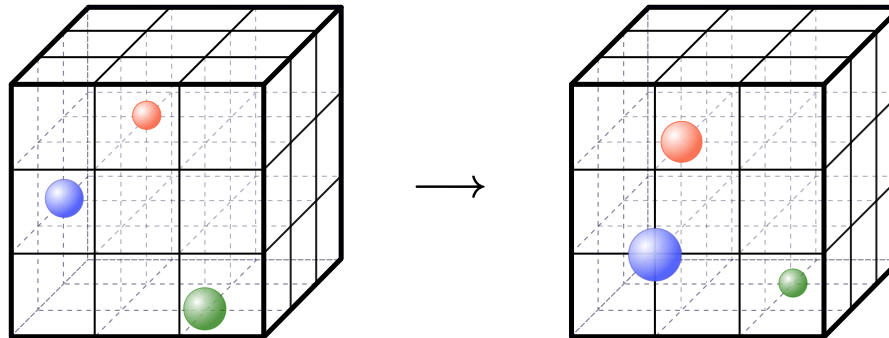
# Cubic projection

## Cubic projector

$$\mathcal{P}_\Gamma = \frac{\dim\Gamma}{24} \sum_{R \in \mathcal{O}\mathcal{O}} \chi_\Gamma(R) D_n(R), \quad \chi_\Gamma(R) = \text{character}$$

Johnson, PLB **114** 147 (1982)

- $D_n(R)$  realizes a cubic rotation  $R$  on the  $n$ -body DVR basis
- $\rightsquigarrow$  permutation/inversion of relative coordinate components
- indices are wrapped back into range  $-N/2, \dots, N/2 - 1$

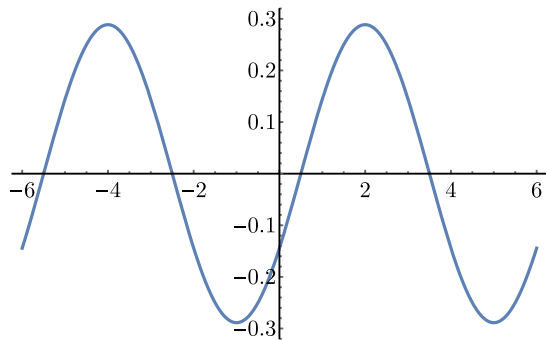


- numerical implementation:  $\hat{H} \rightarrow \hat{H} + \lambda(1 - \mathcal{P}_\Gamma)$ ,  $\lambda \gg E$

# DVR construction

## Basic idea

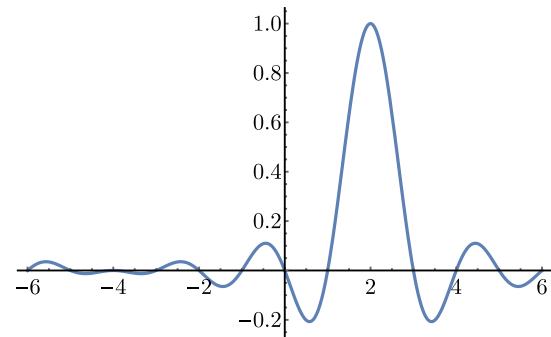
- start with some initial basis; here: plane waves  $\phi_i(x) = \frac{1}{\sqrt{L}} \exp\left(i \frac{2\pi i}{L} x\right)$
- consider  $(x_k, w_k)$  such that 
$$\sum_{k=-N/2}^{N/2-1} w_k \phi_i^*(x_k) \phi_j(x_k) = \delta_{ij}$$



unitary trans.



$$U_{ki} = \sqrt{w_k} \phi_i(x_k)$$



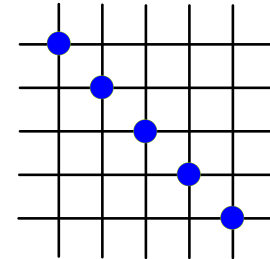
## DVR states

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

# DVR features

## Potential energy is diagonal

$$\begin{aligned}\langle \psi_k | V | \psi_l \rangle &= \int dx \psi_k(x) V(x) \psi_l(x) \\ &\approx \sum_{n=-N/2}^{N/2-1} w_n \psi_k(x_n) V(x_n) \psi_l(x_n) = V(x_k) \delta_{kl}\end{aligned}$$



- no need to evaluate integrals
- number  $N$  of DVR states controls quadrature approximation

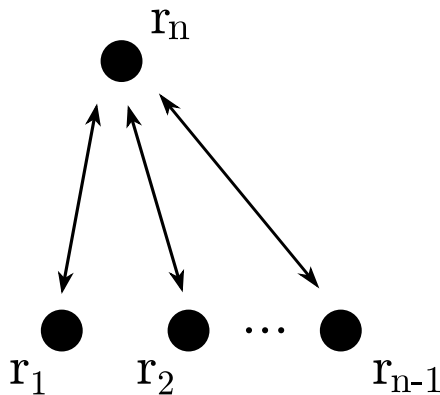
## Kinetic energy is **simple** (via FFT) or **sparse** (in $d > 1$ )

- plane waves are momentum eigenstates
  - evaluate kinetic energy in momentum space:  $\hat{T}|\psi_k\rangle \sim \mathcal{F}^{-1} \otimes \hat{p}^2 \otimes \mathcal{F}|\psi_k\rangle$
- $\langle \psi_k | T | \psi_l \rangle =$  known in closed form
  - replicated for each coordinate, with Kronecker deltas for the rest



# DVR basis states

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



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

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

- **general DVR state for  $n$  particles in  $d$  dimensions**
  - $|s\rangle = |(k_{1,1}, \dots, k_{1,d}), \dots, (k_{n-1,1}, \dots); \text{spins}\rangle \in B$
- **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  $|s\rangle_{\mathcal{A}} = \mathcal{N} \sum_{p \in \mathcal{S}_n} \text{sgn}(p) D_n(p) |s\rangle$ 
  - then  $|s\rangle_{\mathcal{A}}$  is antisymmetric:  $\mathcal{A}|s\rangle_{\mathcal{A}} = |s\rangle_{\mathcal{A}}$
  - for bosons, leave out  $\text{sgn}(p) \rightsquigarrow$  symmetric state
  - $D_n(p)|s\rangle =$  some other  $|s'\rangle \in B$ , **modulo periodic boundary**

**This operation partitions the original basis!**

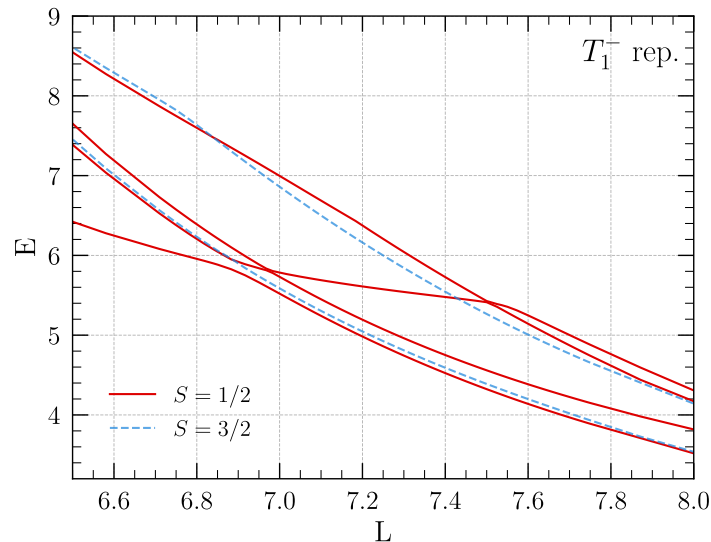
## Reduced basis

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

# Three fermions

## Consider shifted Gaussian potential now for three fermions

- add spin d.o.f., but no spin dependence in potential
  - total spin  $S$  good quantum number (fix  $S_z$  to filter states)
  - can also still consider simple cubic irreps.

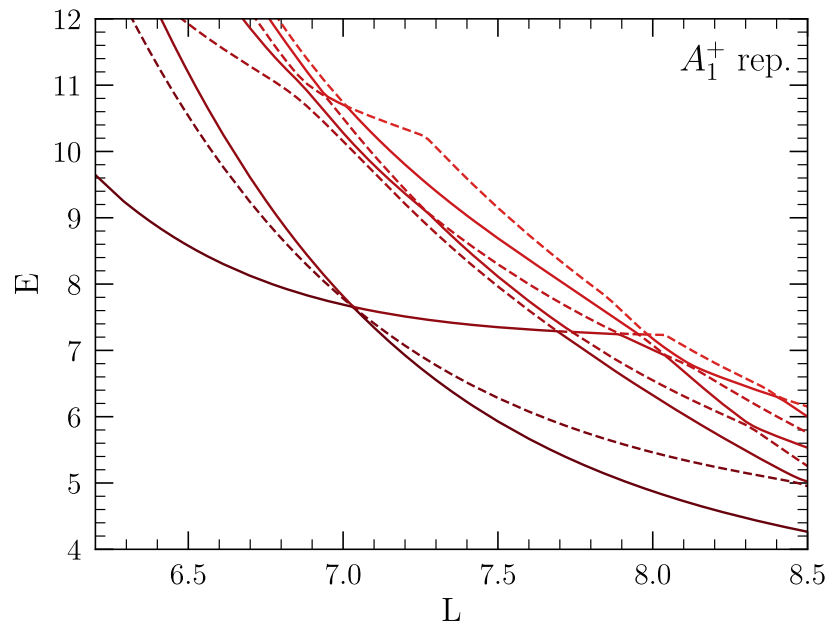


- all lowest states found to be in  $T_1^-$  irrep. ( $\sim$  P-wave state)
- **extract  $S = 1/2$  resonance at  $E_R = 5.7(2)$**

# Four-boson resonance

## Now look at four bosons...

- still the same shifted Gaussian potential ( $V_0 = 2.0$ )



- **clear horizontal sequence of avoided level crossings**
  - (supposedly narrow) resonance at  $E_R = 7.31(8)$