Few-body resonances from finite-volume calculations

Sebastian König

FRIB TA Workshop
“Connecting bound state calculations with scattering and reactions”

NSCL, Michigan State University

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P. Klos, SK, J. Lynn, H.-W. Hammer, and A. Schwenk, arXiv:1805.02029 [nucl-th]

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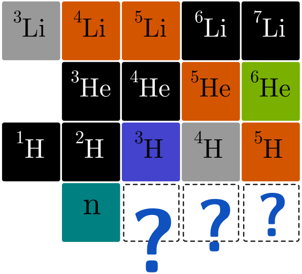
Motivation

terra incognita
at the doorstep. . .



- bound dineutron state not excluded by pionless EFT
  Hammer + SK, PLB **736** 208 (2014)
- recent indications for a three-neutron resonance state. . .
  Gandolfi *et al.*, PRL **118** 232501 (2017)
- . . . although excluded by previous theoretical work
  Offermann + Glöckle, NPA **318**, 138 (1979); Lazauskas + Carbonell, PRC **71** 044004 (2005)
- **possible evidence for tetraneutron resonance**
  Kisamori *et al.*, PRL **116** 052501 (2016)

Short (recent) history of tetraneutron states

1. **2002:** experimental claim of bound tetraneutron Marques *et al.*, PRC **65** 044006
2. **2003:** several studies indicate unbound four-neutron system
   Bertulani *et al.*. JPG **29** 2431; Timofeyuk, JPG **29** L9; Pieper, PRL **90** 252501
3. **2005:** observable tetraneutron resonance excluded Lazauskas PRC **72** 034003

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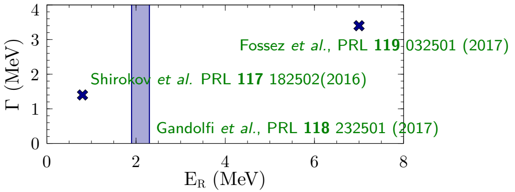
3. **2005:** observable tetraneutron resonance excluded — Lazauskas PRC **72** 034003
4. **2016: RIKEN experiment: possible tetraneutron resonance**
   $E_R = (0.83 \pm 0.65_{\text{stat.}} \pm 1.25_{\text{syst.}})$ MeV, $\Gamma \lesssim 2.6$ MeV — Kisamori *et al.*, PRL **116** 052501
5. **following this:** several new theoretical investigations
   - complex scaling → need unphys. $T = {}^3\!/_2$ 3N force or strong rescaling
     Hiyama *et al.*, PRC **93** 044004 (2016),; Deltuva, PLB **782** 238 (2018)
   - incompatible predictions:



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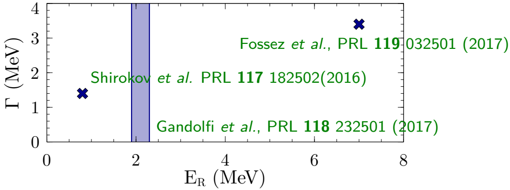
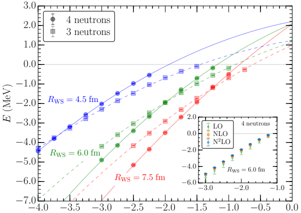




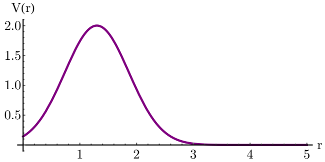
- **indications for three-neutron resonance. . .**
- **. . . lower in energy than tetraneutron state**

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

How to tackle resonances?

Resonances

- metastable states
- decay width $\leftrightarrow$ lifetime



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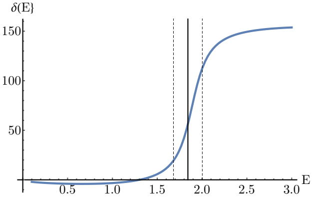
   ✓simple ✗ possibly ambiguous (background), need 2-cluster system



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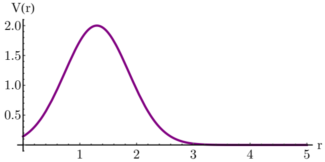

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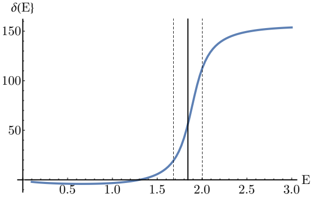

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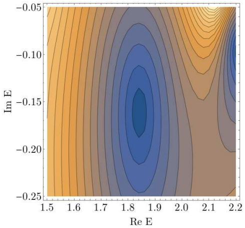

2. **Find complex poles in S-matrix:**

e.g., Glöckle, PRC **18** 564 (1978); Borasoy *et al.*, PRC **74** 055201 (2006); . . .

✓direct, clear signature ✗ technically challenging, needs analytic pot.

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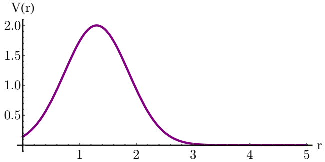

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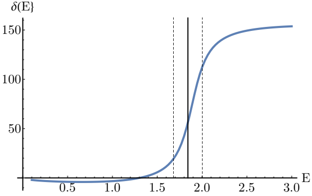

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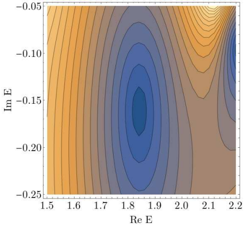

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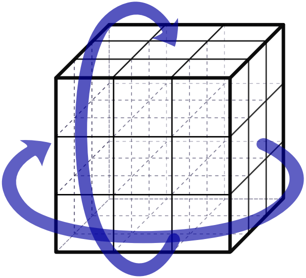
3. **Put system into periodic box!**

Finite periodic boxes



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

$\rightsquigarrow$ **volume-dependent energies**

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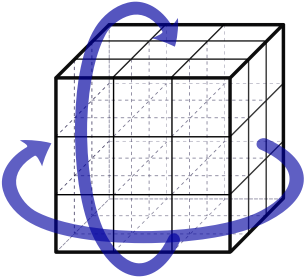

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⇝ **volume-dependent energies**

Lüscher formalism

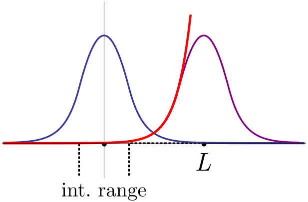
Physical properties encoded in the L-dependent energy levels!

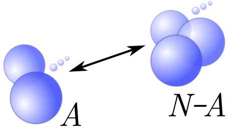
- infinite-volume S-matrix governs discrete finite-volume spectrum
- PBC natural for lattice calculations. . .
- . . . but can also be implemented with other methods

General bound-state volume dependence

volume dependence $\leftrightarrow$ overlap of asymptotic wave functions

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





$$\kappa_{A|N-A} = \sqrt{2\mu_{A|N-A}(B_N - B_A - B_{N-A})}$$

Volume dependence of N-body bound state

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

$$\sim \exp\left(-\kappa_{A|N-A} L\right) / L^{(d-1)/2} \quad \text{as} \quad L \to \infty$$

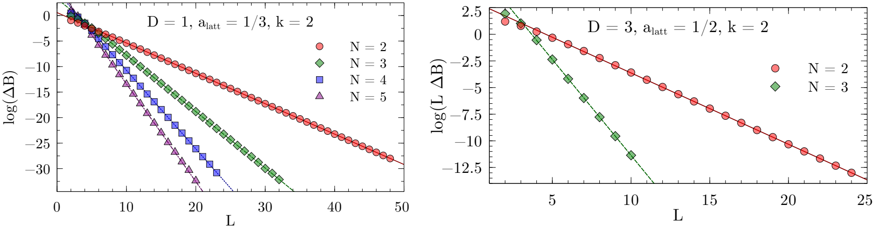
(L = box size, d no. of spatial dimensions, K_n = Bessel function)

SK and D. Lee, PLB **779**, 9 (2018)

channel with smallest $\kappa_{A|N-A}$ determines asymptotic behavior

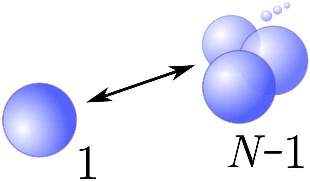
Numerical results

SK and D. Lee, PLB **779**, 9 (2018)



$\hookrightarrow$ **straight lines** $\leftrightarrow$ **excellent agreement with prediction**

N	B_N	$L_{\mathsf{min}} \ldots L_{\mathsf{max}}$	κ_{fit}	$\kappa_{1\|N-1}$
$d = 1,\ V_0 = -1.0,\ R = 1.0$				
2	0.356	$20 \ldots 48$	0.59536(3)	0.59625
3	1.275	$15 \ldots 32$	1.1062(14)	1.1070
4	2.859	$12 \ldots 24$	1.539(3)	1.541
5	5.163	$12 \ldots 20$	1.916(21)	1.920
$d = 3,\ V_0 = -5.0,\ R = 1.0$				
2	0.449	$15 \ldots 24$	0.6694(2)	0.6700
3	2.916	$4 \ldots 14$	1.798(3)	1.814



Finite-volume resonance signatures

Lüscher formalism: phase shift ↔ box energy levels

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

Lüscher, Nucl. Phys. B **354** 531 (1991); ...

resonance contribution ⇝ **avoided level crossing**

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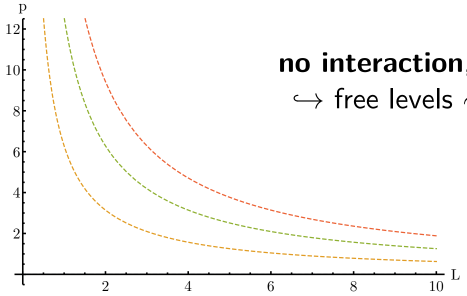

no interaction, $\delta(p) = 0$

$\hookrightarrow$ free levels $\sim 1/L$

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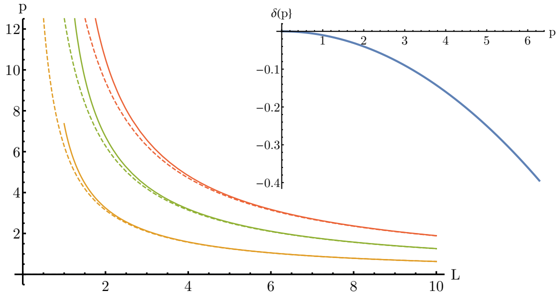

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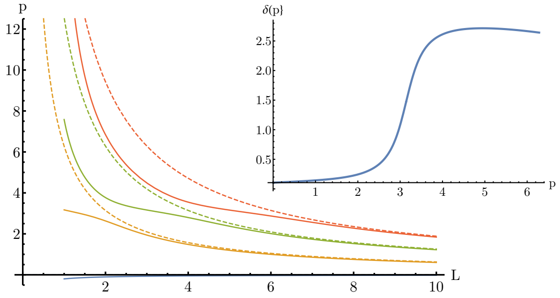

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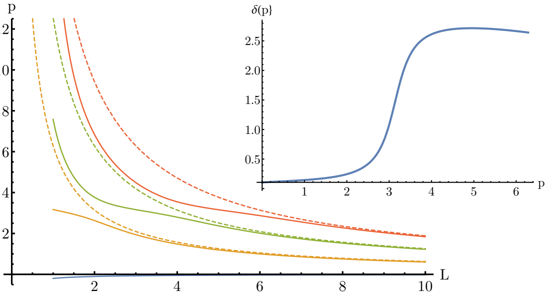


Effect can be very subtle in practice...

Bernard *et al.*, JHEP **0808** 024 (2008); Döring *et al.*, EPJA **47** 139 (2011); ...

Discrete variable representation

Needed: calculation of <u>several</u> few-body energy levels

- difficult to achieve with QMC methods — Klos *et al.*, PRC **94** 054005 (2016)
- direct discretization possible, but not very efficient

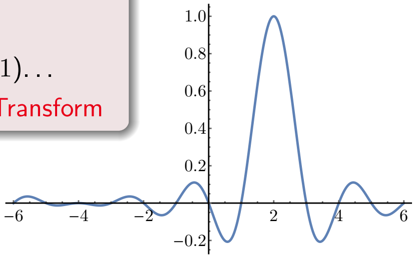
$\hookrightarrow$ **use a Discrete Variable Representation (DVR)**

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

Main features

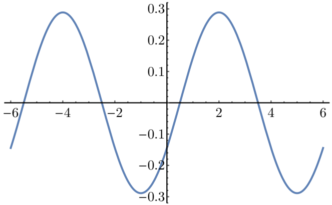
- basis functions localized at grid points
- potential energy matrix diagonal
- kinetic energy matrix sparse (in $d > 1$)...
- ...or implemented via Fast Fourier Transform

periodic boundary condistions
$\leftrightarrow$ **plane waves as starting point**



DVR construction

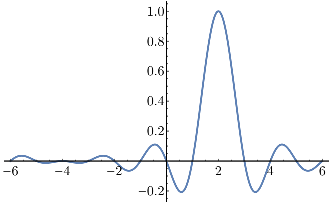
- start with some initial basis; here: $\phi_i(x) = \frac{1}{\sqrt{L}} \exp\left(\mathrm{i}\frac{2\pi i}{L}x\right)$
- consider (x_k, w_k) such that $\sum_{k=-N/2}^{N/2-1} w_k\, \phi_i^*(x_k)\phi_j(x_k) = \delta_{ij}$



unitary trans.

$\longrightarrow$

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



DVR states

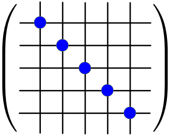
- $\psi_k(x)$ localized at x_k, $\psi_k(x_j) = \delta_{kj}/\sqrt{w_k}$
- **note:** momentum mode $\phi_i \leftrightarrow$ spatial mode ψ_k

DVR features

1. **potential energy is diagonal!**

$$\langle\psi_k|V|\psi_l\rangle = \int \mathrm{d}x\,\psi_k(x)\,V(x)\,\psi_l(x)$$

$$\approx \sum_{n=-N/2}^{N/2-1} w_n\,\psi_k(x_n)\,V(x_n)\,\psi_l(x_n) = V(x_k)\delta_{kl}$$



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- number N of DVR states controls quadrature approximation

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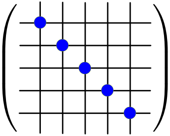

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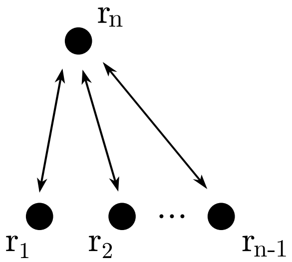
2. **kinetic energy is simple (via FFT) or sparse (in $d > 1$)!**

- plane waves ϕ_i are momentum eigenstates $\rightsquigarrow \hat{T}\,|\psi_k\rangle \sim \mathcal{F}^{-1} \otimes \hat{p}^2 \otimes \mathcal{F}\,|\psi_k\rangle$
- $\langle\psi_k|\hat{T}|\psi_l\rangle =$ known in closed form

  $\hookrightarrow$ replicated for each coordinate, with Kronecker deltas for the rest

General 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



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

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

General DVR state

$$|s\rangle = |(k_{1,1}, \cdots, k_{1,d}), \cdots, (k_{n-1,1}, \cdots); \text{spins}\rangle \in B$$

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 PBC

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This operation partitions the orginal basis, *i.e.*, each state appears in at most one (anti-)symmetric combination.

- efficient reduction to (anti-)symmetrized orthonormal basis
  $\hookrightarrow$ no need for numerically expensive diagonalization!
- $B \to B_{\text{reduced}}$, significantly smaller: $N \to N_{\text{reduced}} \approx N/n!$

Note: parity (with projector $\mathcal{P}_{\pm} = 1 \pm \mathcal{P}$) can be handled analogously.

DVR computational aspects

DVR basis size $N = N_{\text{spin}} \, (\times N_{\text{isospin}}) \times N_{\text{DVR}}^{n_{\text{dim}} \times (n_{\text{body}}-1)}$

- $N_{\text{spin}} = (2S+1)^{n_{\text{body}}}$, $N_{\text{isospin}} = 1$ for neutrons only
- $3n$: $8 \times N_{\text{DVR}}^6$, $4n$: $16 \times N_{\text{DVR}}^9$ $\rightsquigarrow$ **large-scale calculation**

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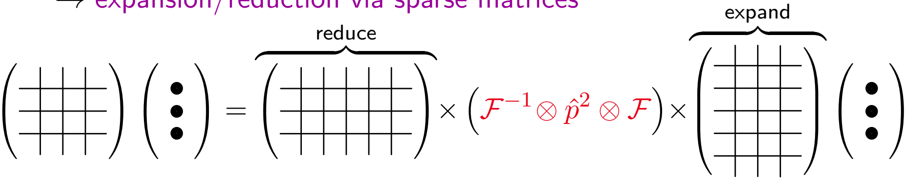
- diagonalization via distributed Lanczos algorithm (`PARPACK`)
  $\rightsquigarrow$ large matrix-vector products
- kinetic part (via FFT) in original basis (before reduction)
  $\hookrightarrow$ expansion/reduction via sparse matrices



(note: kinetic matrix diagonal in spin-configurations space)

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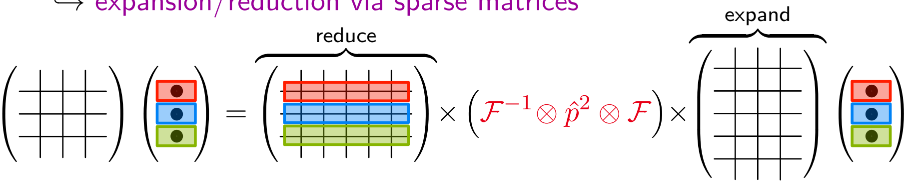

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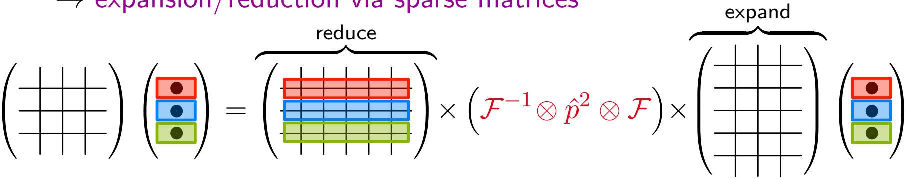
DVR computational aspects

DVR basis size $N = N_{\text{spin}} \; (\times N_{\text{isospin}}) \times N_{\text{DVR}}^{n_{\text{dim}} \times (n_{\text{body}} - 1)}$

- $N_{\text{spin}} = (2S+1)^{n_{\text{body}}}$, $N_{\text{isospin}} = 1$ for neutrons only
- $3n$: $8 \times N_{\text{DVR}}^6$, $4n$: $16 \times N_{\text{DVR}}^9$ $\rightsquigarrow$ **large-scale calculation**
- diagonalization via distributed Lanczos algorithm (`PARPACK`)

  $\rightsquigarrow$ large matrix-vector products
- kinetic part (via FFT) in original basis (before reduction)

  $\hookrightarrow$ expansion/reduction via sparse matrices



(note: kinetic matrix diagonal in spin-configurations space)

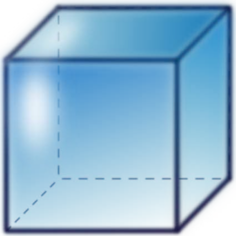
- potential part still diagonal in symmetry-reduced basis

Broken symmetry

The finite volume breaks the symmetry of the system:

rotation group $SO(3)$

$\rightarrow$



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

Cubic projection

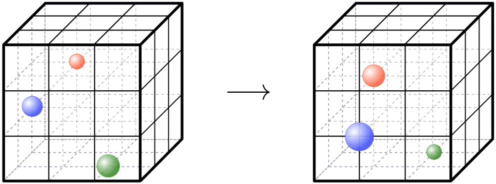
Cubic projector

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

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 wrappen back into range $-N/2,\ldots,N/2-1$

e.g.



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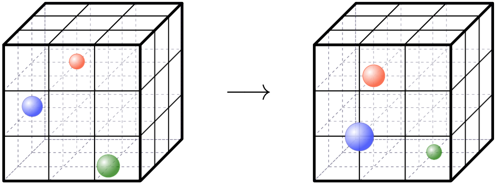
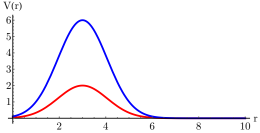


numerical implementation: $\hat{H} \to \hat{H} + \lambda(\mathbf{1} - \mathcal{P}_\Gamma) \quad , \quad \lambda \gg E$

Two-body check: anything goes

$$V(r) = V_0 \exp\left(-\left(\frac{r-a}{R_0}\right)^2\right)$$

$\hookrightarrow$ use barrier to produce S-wave resonance



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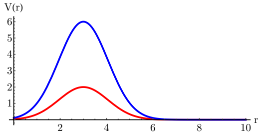

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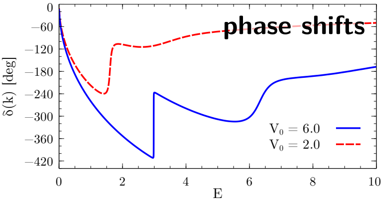

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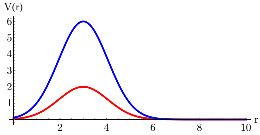

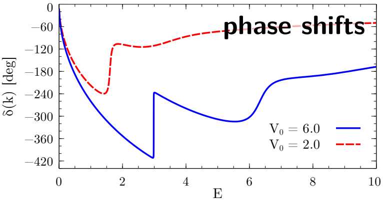

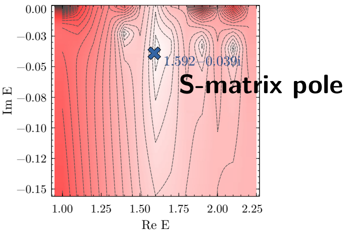

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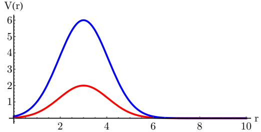

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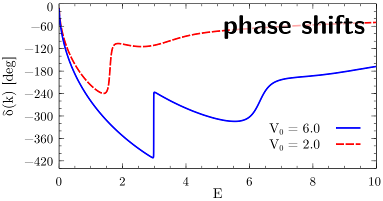
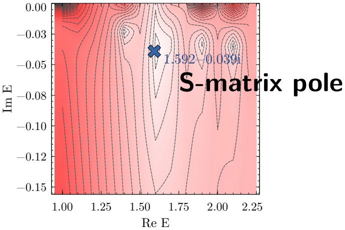
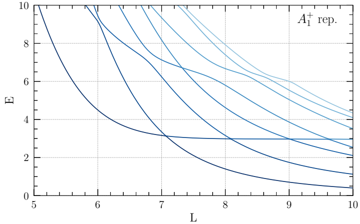
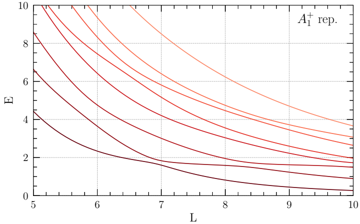




finite-volume spectra





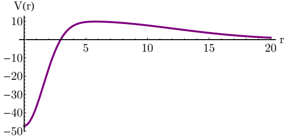
Three-body check

Take established three-body resonance from literature:

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

$$V(r) = V_0 \exp\left(-\left(\frac{r}{R_0}\right)^2\right) + V_1 \exp\left(-\left(\frac{r-a}{R_1}\right)^2\right)$$

$V_0 = -55$ MeV, $V_1 = 1.5$ MeV, $R_0 = \sqrt{5}$ fm, $R_1 = 10$ fm, $a = 5$ fm



- three spinless bosons with mass $m = 939.0$ MeV
- two- and three-body bound states at -6.76 MeV and -37.22 MeV
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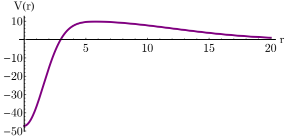

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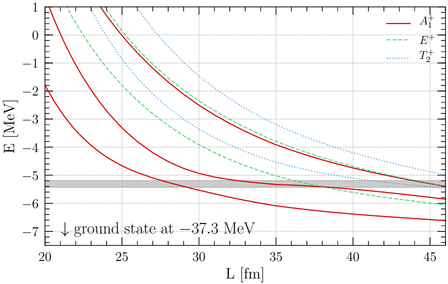
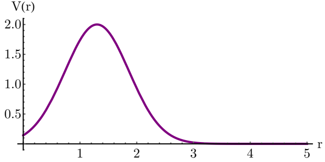


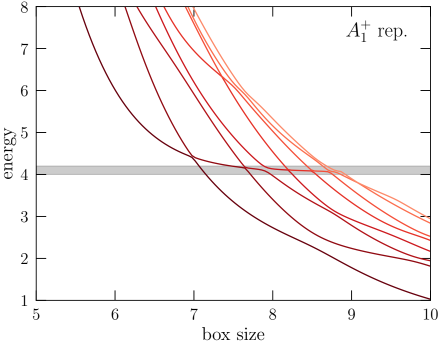
- **fit inflection point(s)** to extract resonance energy ⇝ $E_R = -5.32(1)$ MeV

Three bosons with shifted Gaussian interaction

three-boson system

- shifted Gaussian 2-body potential
- **note:** no 2-body bound state!





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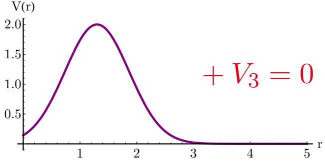
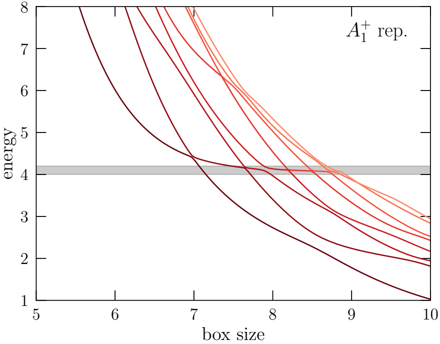


$+ V_3 = 0$



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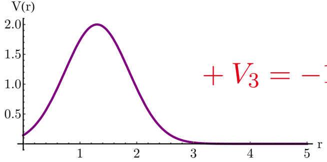
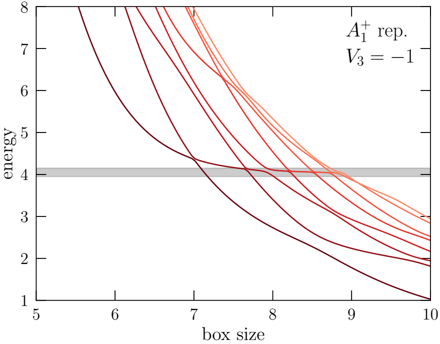


$+ V_3 = -1.0$



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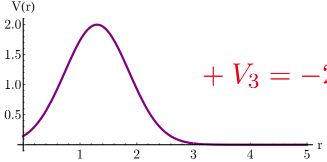
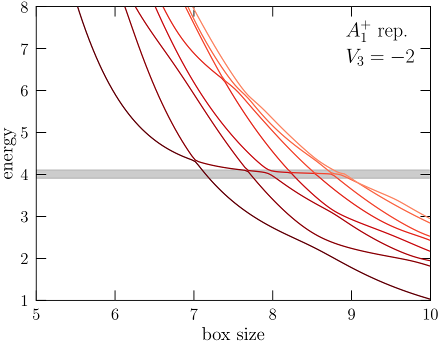


$+ V_3 = -2.0$



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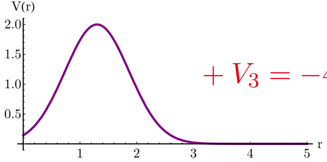
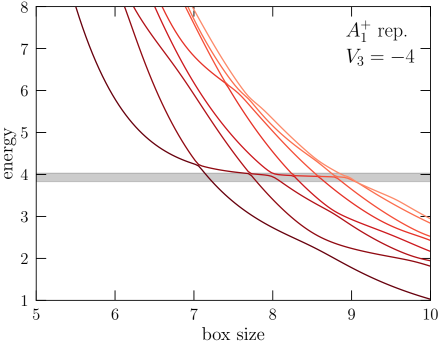


$+V_3 = -4.0$

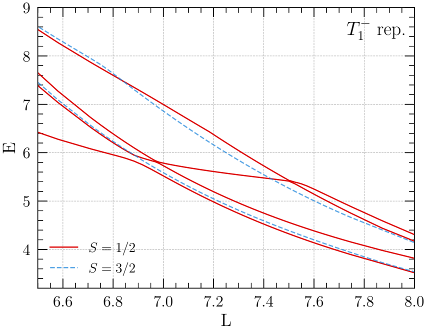


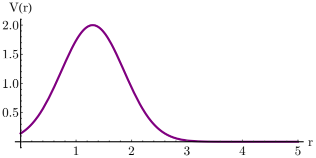
↪ **possible to move three-body state** ↔ **spatially localized wf.**

Three fermions

Consider same shifted Gaussian potential for three fermions. . .

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



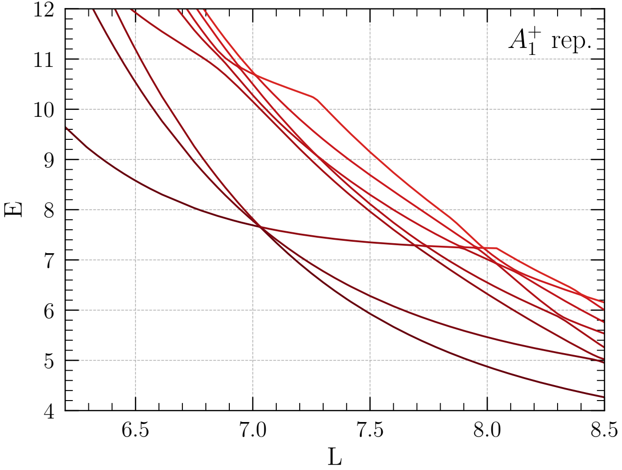


$V_0 = 2.0,\ a = 3.0,\ R = 1.5$

- all lowest states found to be in T_1^- irrep. ($\sim$ P-wave state)
- some remaining volume dependence (box not very large)
- extracted $S = 1/2$ resonance energy: $E_R = 5.7(2)$

Four-boson resonance

Still same potential, look at four bosons...



$\hookrightarrow$ (supposedly) narrow resonance at $E_R = 7.31(8)$

Summary and outlook

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- ✓ handle **large N_{DVR} for three-body systems** (current record: 32)
- ✓ efficient **symmetrization and antisymmetrization**
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- application to **few-neutron systems**
- **further optimization** (especially for spin-dep. potentials)
  $\hookrightarrow$ need to reach decent N_{DVR} for four-neutron calculation!
- isospin degrees of freedom $\rightsquigarrow$ **treat general nuclear systems**
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***** Thank you! *****