Few-body resonances from finite-volume calculations

Sebastian König

in collaboration with P. Klos, J. Lynn, H.-W. Hammer, and A. Schwenk

Nuclear Theory Workshop

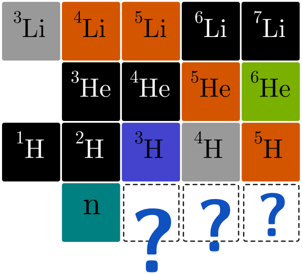
TRIUMF, Vancouver, BC

February 28, 2018

work in progress

Few-neutron systems

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)

Tetraneutron evidence

Physics ABOUT BROWSE PRESS COLLECTIONS

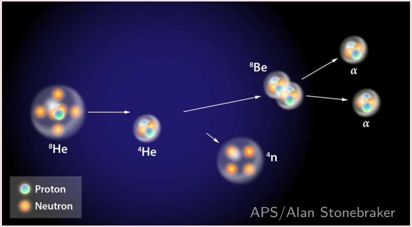
Viewpoint: Can Four Neutrons Tango?

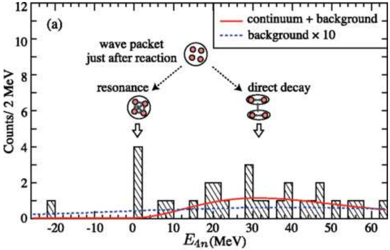
Nigel Orr, Laboratoire de Physique Corpusculaire de Caen, ENSICAEN, IN2P3/CNRS et Université de Caen Normandie, 14050 Caen cedex, France

February 3, 2016 • *Physics* 9, 14

Evidence that the four-neutron system known as the tetraneutron exists as a resonance has been uncovered in an experiment at the RIKEN Radioactive Ion Beam Factory.

Experimental setup





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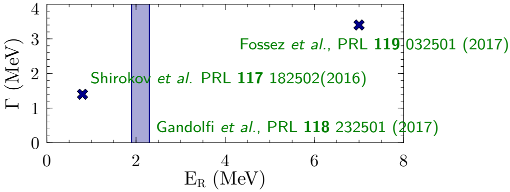
4. **2016: RIKEN experiment: possible tetraneutron resonance**
   $E_R = (0.83 \pm 0.65_{\text{stat.}} \pm 1.25_{\text{syst.}})$ MeV, $\Gamma \lesssim 2.6$ MeV — Kisamori *et al.*, PRL **116** 052501
5. **following this:** several new theoretical investigations
   - complex scaling → need unphys. $T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



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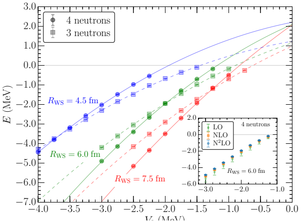
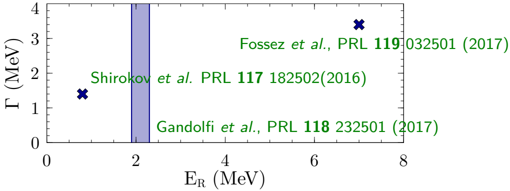




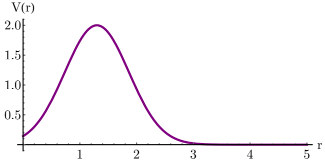
- **indications for three-neutron resonance. . .**
- **. . . lower in energy than tetraneutron state**

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

How to tackle resonances?

Resonances

- metastable states
- decay width $\leftrightarrow$ lifetime



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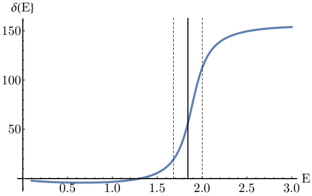
   ✓simple ✗ possibly ambiguous (background), need 2-cluster system



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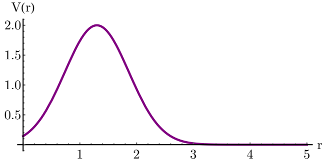

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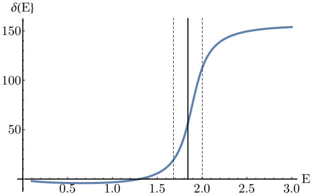
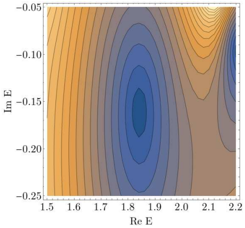


$\leftrightarrow$



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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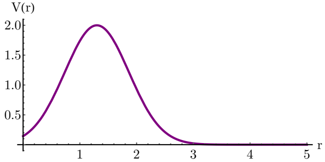

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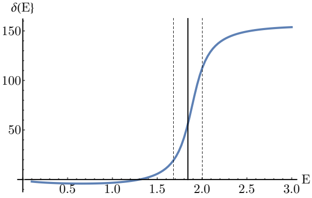

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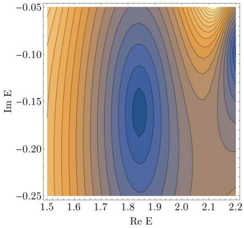

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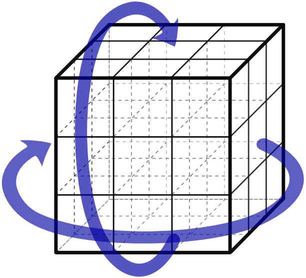
3. **Put system into periodic box!**

Finite periodic boxes



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

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

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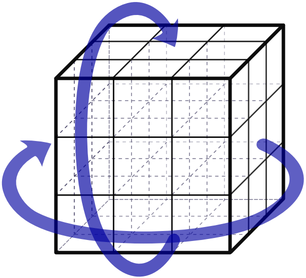

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$\rightsquigarrow$ **volume-dependent energies**

Lüscher formalism

Physical properties encoded in the L-dependent energy levels!

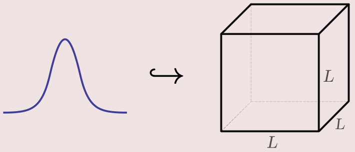
- infinite-volume S-matrix governs discrete finite-volume spectrum
- PBC natural for lattice calculations. . .
- . . . but can also be implemented with other methods

Bound states

$$\hat{H}\,|\psi_B\rangle = -\frac{\kappa^2}{2\mu}\,|\psi_B\rangle$$

binding momentum κ

$\leftrightarrow$ intrinsic length scale



Asymptotic wavefunction overlap

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

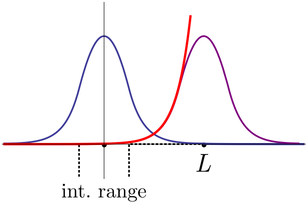
M. Lüscher, Commun. Math. Phys. **104** 177 (1986)

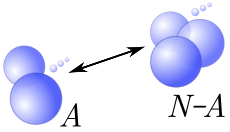
- for S-wave states, one finds $\Delta B(L) = -3\pi|\gamma|^2 \frac{\mathrm{e}^{-\kappa L}}{\mu L} + \mathcal{O}(\mathrm{e}^{-\sqrt{2}\kappa L})$
- in general, the prefactor is a polynomial in $1/\kappa L$

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

General bound-state volume dependence

volume dependence $\leftrightarrow$ overlap of asymptotic wave functions





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

Volume dependence of N-body bound state

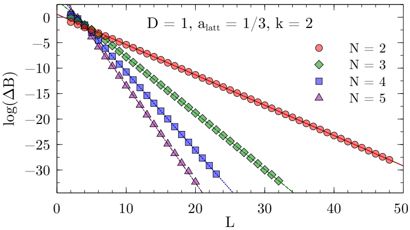
$$\Delta B_N(L) \propto (\kappa_{A|N-A} L)^{1-d/2} K_{d/2-1}(\kappa_{A|N-A} L)$$
$$\sim \exp\left(-\kappa_{A|N-A} L\right) / L^{(d-1)/2} \quad \text{as} \quad L \to \infty$$

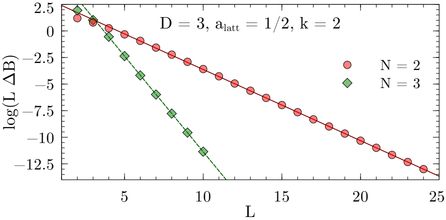
(L = box size, d no. of spatial dimensions, K_n = Bessel function)

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

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

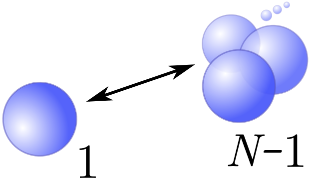
Numerical results





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

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



Bound-state summary

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

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2. reproduces known results, **checked numerically**
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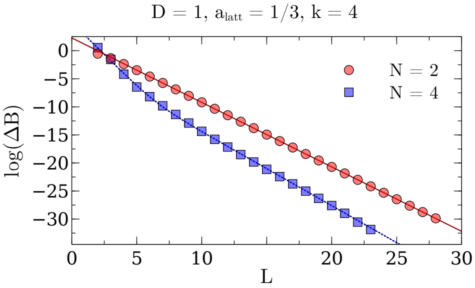
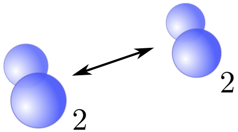
4. applications to lattice QCD, EFT, cold-atomic systems
5. **typically, one exponential dominates, but not necessarily:**





- **three-body system unbound**
- asymptotic slope from $2|2$ separation

Finite-volume resonance signatures

Lüscher formalism: phase shift $\leftrightarrow$ 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 $\rightsquigarrow$ **avoided level crossing**

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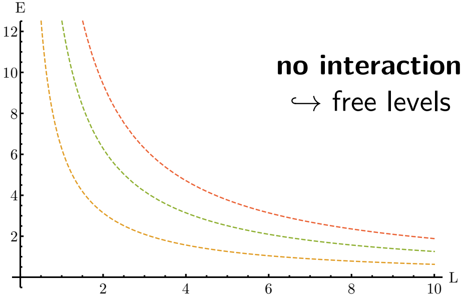

no interaction, $\delta(p) = 0$

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

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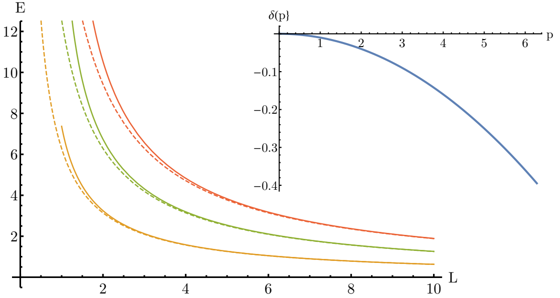

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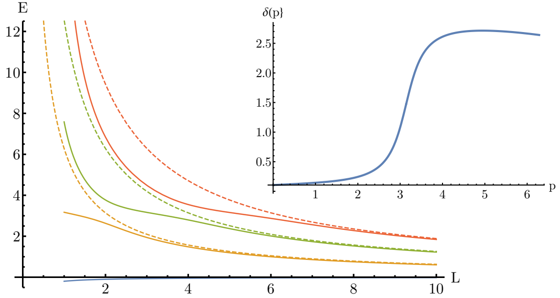

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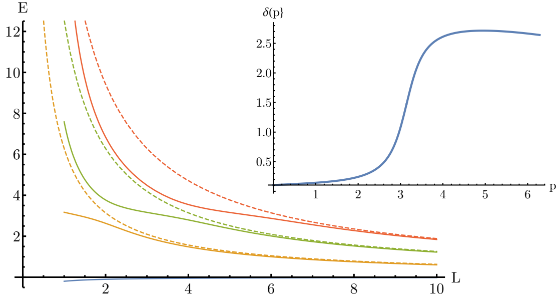


Effect can be very subtle in practice...

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

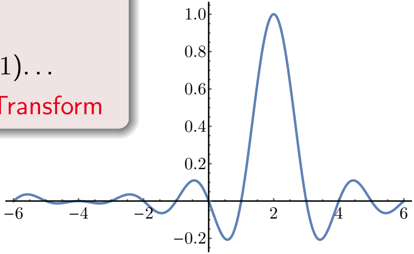
$\hookrightarrow$ **use a Discrete Variable Representation (DVR)**

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 states and features

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

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1. **potential energy is diagonal!**

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

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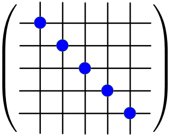

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- number N of DVR states controls quadrature approximation

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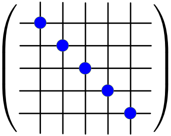

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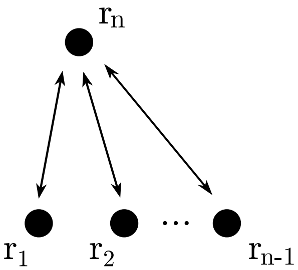
2. **kinetic energy is simple (via FFT) or sparse (in $d > 1$)!**

- 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

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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Distributed implementation

- written from scratch in C++ (and Haskell), together with P. Klos
- can handle arbitrary n_{dim}, n_{body}, and spin
- hybrid parallelism: TBB + MPI, threaded libraries (`FFTW`, `librsb`; MKL)

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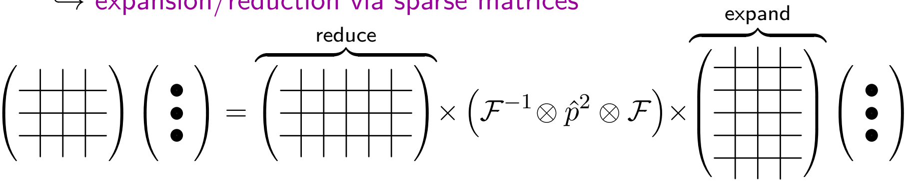
- diagonalization via distributed Lanczos algorithm (`PARPACK`)

  $\rightsquigarrow$ 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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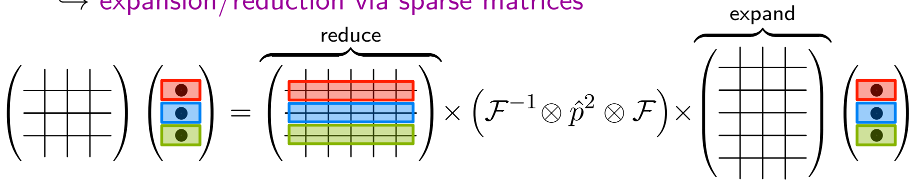

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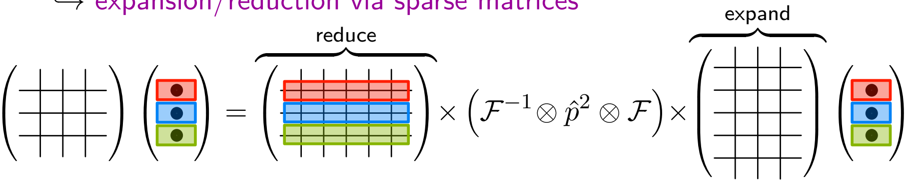


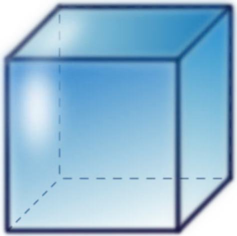
(note: kinetic matrix diagonal in spin-configurations space)

- potential part still diagonal in symmetry-reduced basis

Broken symmetry

The finite volume breaks the symmetry of the system:

$\longrightarrow$



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

Cubic projection

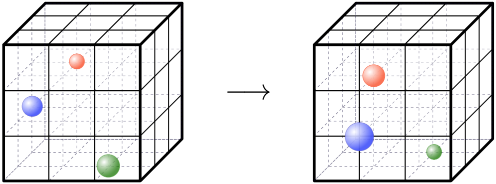
Cubic projector

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

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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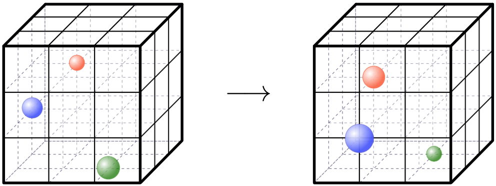
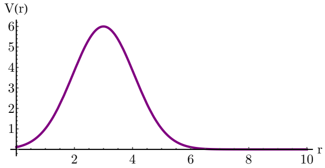
e.g. 

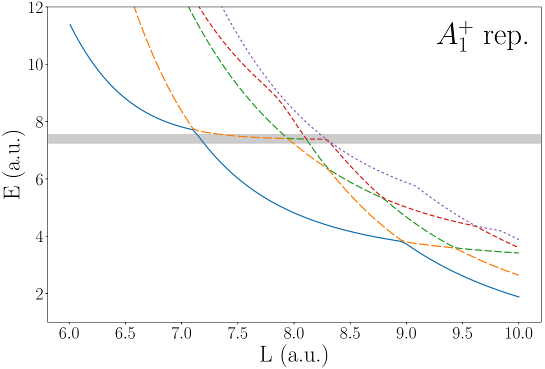
numerical implementation: $\hat{H} \to \hat{H} + \lambda(\mathbf{1} - \mathcal{P}_\Gamma) \quad , \quad \lambda \gg E$

Three-body resonance example

three-boson system

- shifted Gaussian 2-body potential





Three-body resonance example

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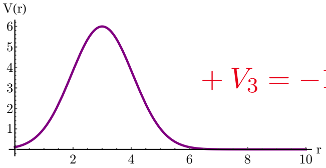
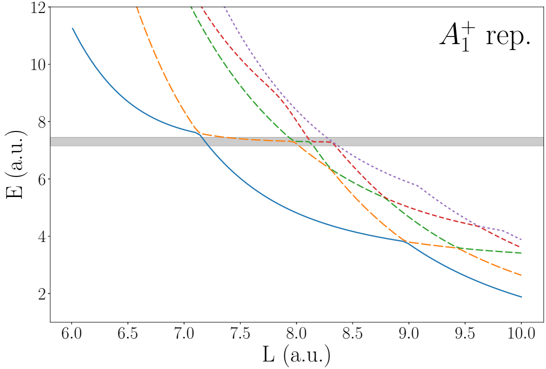
- shifted Gaussian 2-body potential
- plus short-range 3-body force



$+ V_3 = -1.0$



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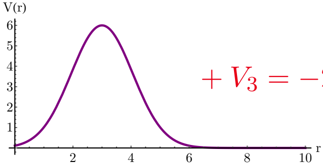
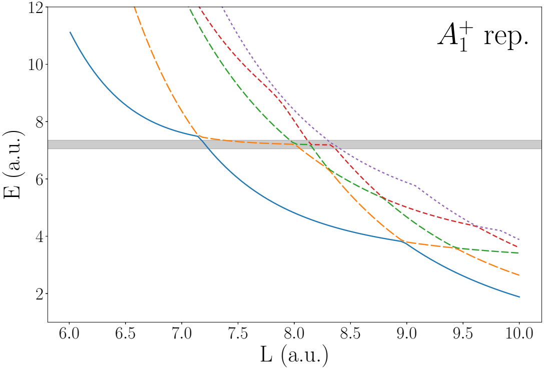


$+ V_3 = -2.0$



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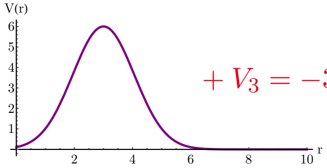
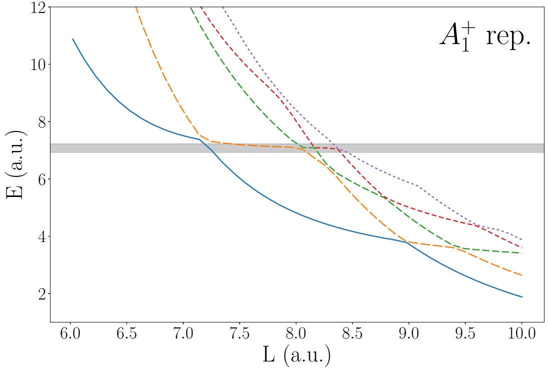


$+V_3 = -3.0$



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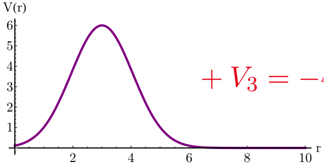
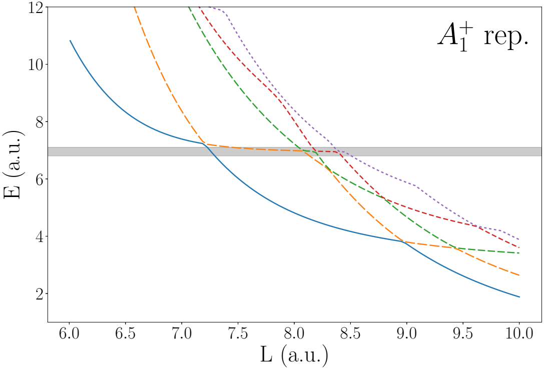


$+V_3 = -4.0$



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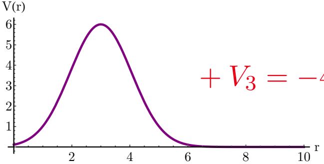

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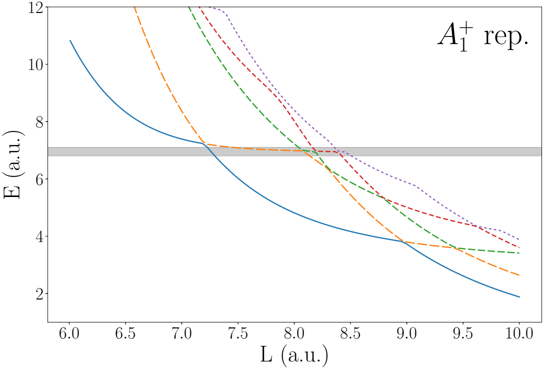
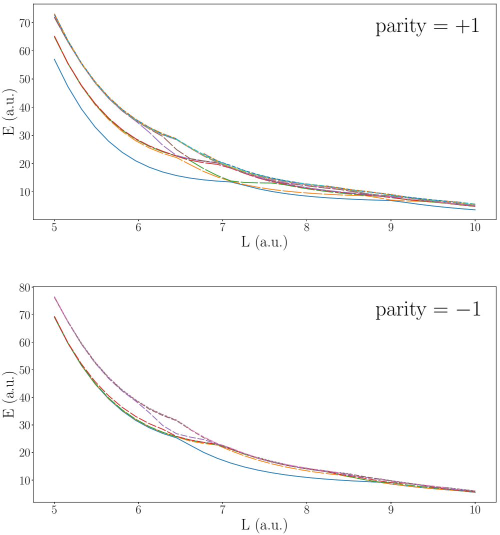
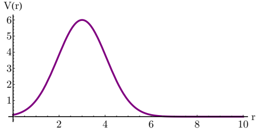


$\hookrightarrow$ **possible to move three-body resonance**

Four-body spectra (very preliminary)



four bosons



crossings need not be avoided!

Current status

- ✓ handle **large N_{DVR} for three-body systems** (current record: 28)
- ✓ **chiral interactions** (non-diagonal due to spin dependence!)
- ✓ projection onto **cubic irreps.** ($H \to H + \lambda(1 - P_\Gamma)$, λ large)

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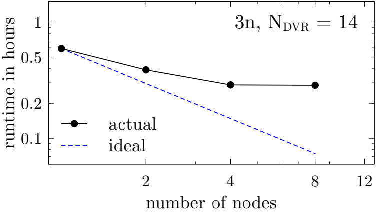

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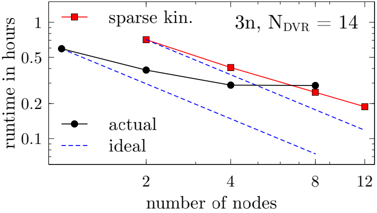

Work in progress

- **further optimization** (sparse-matrix kin. energy instead of FFT)
  $\hookrightarrow$ need to reach decent N_{DVR} for four-neutron calculation!
- isospin degrees of freedom $\rightsquigarrow$ **treat general nuclear systems**
- **different boundary conditions** (e.g., antiperiodic)

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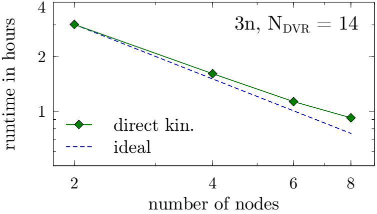

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Thank you!

. . . and thanks to my collaborators:

- Philipp Klos, Joel Lynn
- Hans-Werner Hammer, Achim Schwenk
- Dean Lee

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