

Few-body resonances from finite-volume calculations

Sebastian König

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

**International Workshop XLVI on Gross Properties of Nuclei and Nuclear Excitations:
Multiparticle resonances in hadrons, nuclei, and ultracold gases**

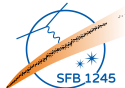
Hirschegg, Austria

January 18, 2018

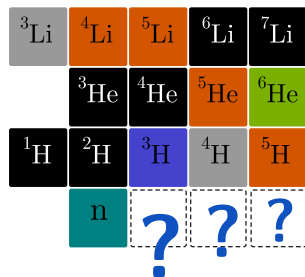
work in progress



TECHNISCHE
UNIVERSITÄT
DARMSTADT



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)

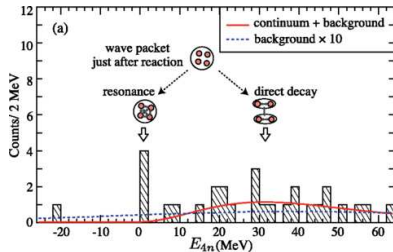
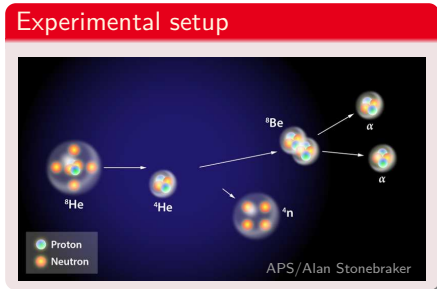
Tetraneutron evidence

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.



Kisamori *et al.*, PRL 116 052501 (2016)

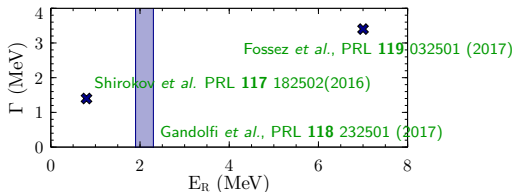
Short (recent) history of tetra-neutron states

- ① **2002:** experimental claim of **bound tetra-neutron** 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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 $E_R = (0.83 \pm 0.65_{\text{stat.}} \pm 1.25_{\text{syst.}}) \text{ MeV}$, $\Gamma \lesssim 2.6 \text{ MeV}$ Kisamori *et al.*, PRL **116** 052501
- 5 **following this:** several new theoretical investigations
 - complex scaling \rightarrow **need unphys. $T = 3/2$ 3N force** Hiyama *et al.*, PRC **93** 044004 (2016)

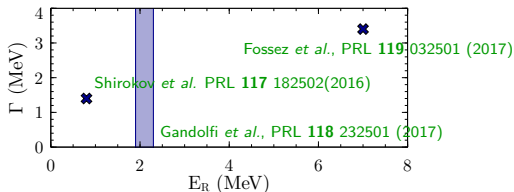
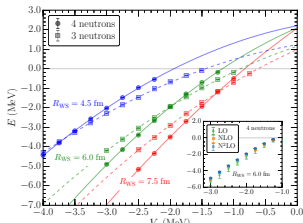
- incompatible predictions:



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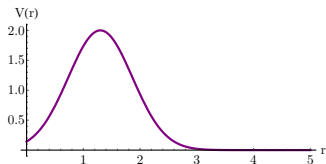
- **indications for three-neutron resonance...**
- **...lower in energy than tetra-neutron state**

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

How to tackle resonances?

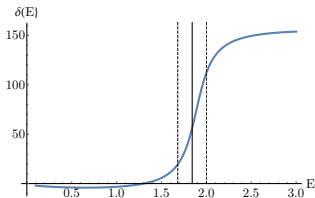
Resonances

- metastable states
- decay width \leftrightarrow lifetime



- 1 Look for jump by π in scattering phase shift:

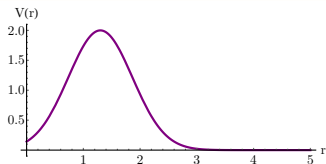
simple possibly ambiguous (background), need 2-cluster system



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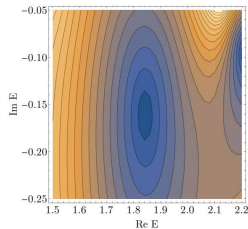
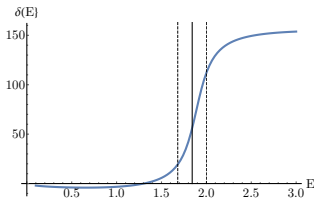
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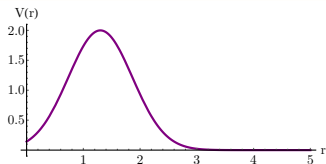
e.g., Glöckle, PRC **18** 564 (1978); Borasoy *et al.*, PRC **74** 055201 (2006); ...

direct, clear signature technically challenging, needs analytic pot.

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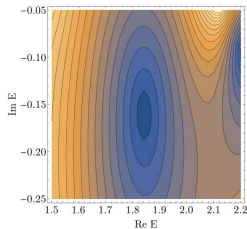
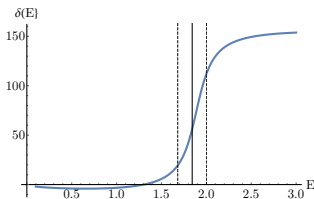
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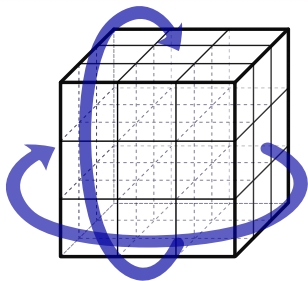
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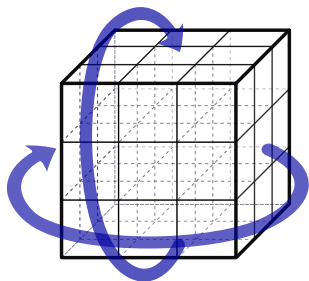
3 Put system into periodic box!

Finite periodic boxes



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

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Lüscher formalism

Physical properties encoded in the L -dependent energy levels!

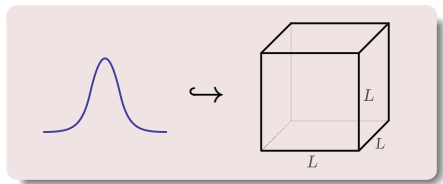
- infinite-volume S-matrix governs **discrete** finite-volume spectrum
- PBC natural for lattice calculations. . .
- . . . but can also be implemented with other methods

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

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

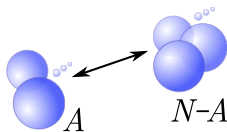
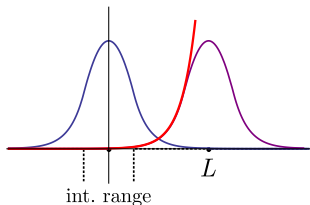
M. Lüscher, *Commun. Math. Phys.* **104** 177 (1986)

- for S-wave states, one finds $\Delta B(L) = -3\pi|\gamma|^2 \frac{e^{-\kappa L}}{\mu L} + \mathcal{O}(e^{-\sqrt{2}\kappa L})$
- 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

$$\begin{aligned}\Delta B_N(L) &\propto (\kappa_{A|N-A} L)^{1-d/2} K_{d/2-1}(\kappa_{A|N-A} L) \\ &\sim \exp(-\kappa_{A|N-A} L) / L^{(d-1)/2} \quad \text{as } L \rightarrow \infty\end{aligned}$$

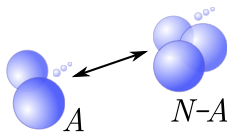
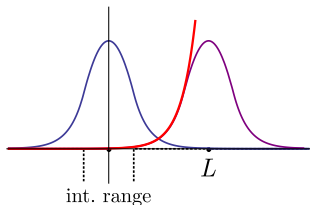
(L = box size, d no. of spatial dimensions, K_n = Bessel function)

SK and D. Lee, arXiv:1701.00279 [hep-lat]

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

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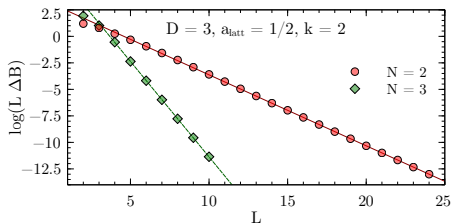
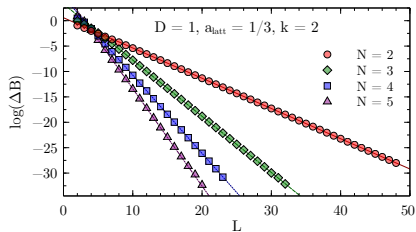
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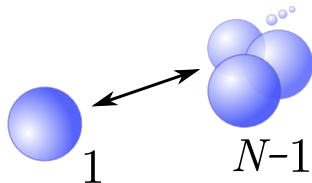
- channel with **smallest** $\kappa_{A|N-A}$ determines asymptotic behavior
- $\Delta B_N(L)$ prop. to ANC of $A|N-A$ system \rightsquigarrow **extract from L -dep.!**

Numerical results



↪ **straight lines** ↔ **excellent agreement with prediction**

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

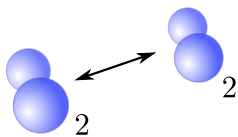
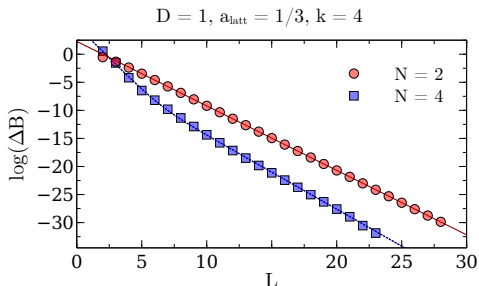


Bound-state summary

- 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**
- 3 calculate ANCs, **single-volume extrapolations possible!**
- 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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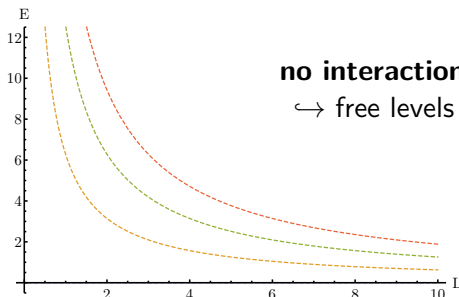
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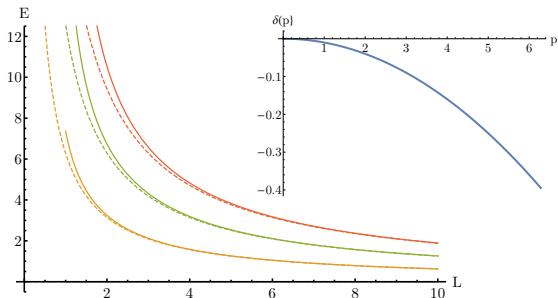
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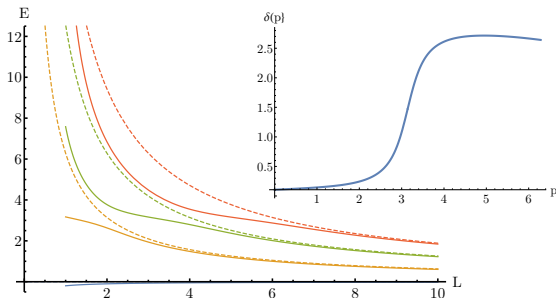
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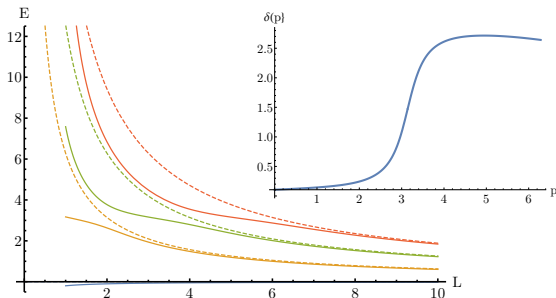
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Effect can be very subtle in practice...

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

Discrete variable representation

Needed: calculation of several few-body energy levels

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

↪ **use a Discrete Variable Representation (DVR)**

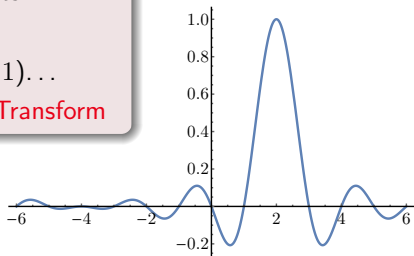
well established in quantum chemistry, suggested for nuclear physics by Bulgac+Forbes, PRC **87** 87, 051301 (2013)

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

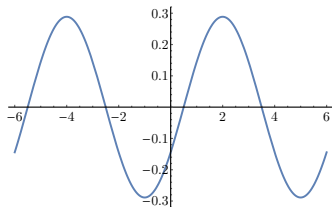
periodic boundary conditions

↔ **plane waves as starting point**



DVR construction

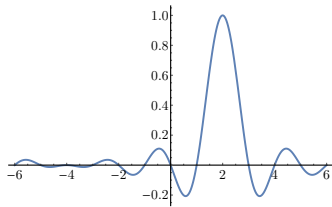
- start with some initial basis; here: $\phi_i(x) = \frac{1}{\sqrt{L}} \exp\left(i\frac{2\pi i}{L}x\right)$
- consider (x_k, w_k) such that
$$\sum_{k=-N/2}^{N/2-1} w_k \phi_i^*(x_k) \phi_j(x_k) = \delta_{ij}$$



unitary trans.



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



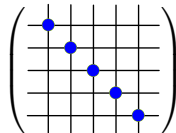
DVR states

- $\psi_k(x)$ 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!

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

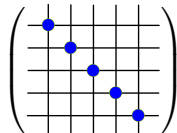


- no need to evaluate integrals
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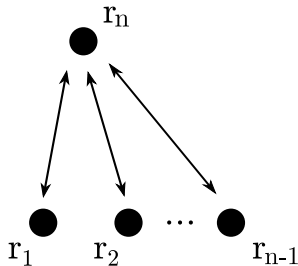
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2 kinetic energy is simple (via FFT) or sparse (in $d > 1$)!

- 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**



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

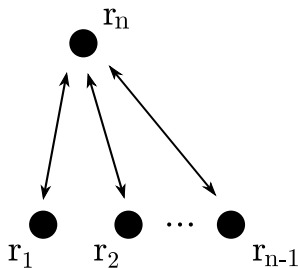
$$U_{ij} = \begin{cases} \delta_{ij} & \text{for } i, j < n \\ -1 & \text{for } i < n, j = n \\ 1/n & \text{for } i = n \end{cases}$$

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

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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 $|s\rangle_{\mathcal{A}} = \mathcal{N} \sum_{p \in S_n} \text{sgn}(p) D_n(p) |s\rangle$
- 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 PBC

(Anti-)symmetrization and parity

Permutation symmetry

- for each $|s\rangle \in B$, construct $|s\rangle_{\mathcal{A}} = \mathcal{N} \sum_{p \in S_n} \text{sgn}(p) D_n(p) |s\rangle$
- 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 PBC

This operation partitions the original 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!
- $B \rightarrow B_{\text{reduced}}$, significantly smaller: $N \rightarrow N_{\text{reduced}} \approx N/n!$

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

DVR computational aspects

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

- $N_{\text{spin}} = (2S + 1)^{n_{\text{body}}}$, $N_{\text{isospin}} = 1$ 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, multithreaded libraries (FFTW, librsb)

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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

$$\left(\begin{array}{|c|c|c|c|} \hline & & & \\ \hline & & & \\ \hline & & & \\ \hline & & & \\ \hline \end{array} \right) \begin{pmatrix} \bullet \\ \bullet \\ \bullet \end{pmatrix} = \overbrace{\left(\begin{array}{|c|c|c|c|} \hline & & & \\ \hline & & & \\ \hline & & & \\ \hline & & & \\ \hline \end{array} \right)}^{\text{reduce}} \times \left(\mathcal{F}^{-1} \otimes \hat{p}^2 \otimes \mathcal{F} \right) \times \overbrace{\left(\begin{array}{|c|c|c|c|} \hline & & & \\ \hline & & & \\ \hline & & & \\ \hline & & & \\ \hline \end{array} \right)}^{\text{expand}} \begin{pmatrix} \bullet \\ \bullet \\ \bullet \end{pmatrix}$$

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

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$$\left(\begin{array}{|c|} \hline \text{grid} \\ \hline \end{array} \right) \left(\begin{array}{|c|} \hline \text{red} \\ \hline \text{blue} \\ \hline \text{green} \\ \hline \end{array} \right) = \overbrace{\left(\begin{array}{|c|} \hline \text{red} \\ \hline \text{blue} \\ \hline \text{green} \\ \hline \end{array} \right)}^{\text{reduce}} \times \left(\mathcal{F}^{-1} \otimes \hat{p}^2 \otimes \mathcal{F} \right) \times \overbrace{\left(\begin{array}{|c|} \hline \text{grid} \\ \hline \end{array} \right)}^{\text{expand}} \left(\begin{array}{|c|} \hline \text{red} \\ \hline \text{blue} \\ \hline \text{green} \\ \hline \end{array} \right)$$

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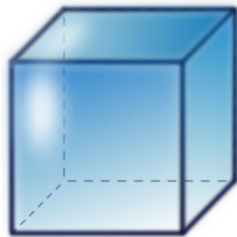
- potential part still diagonal in symmetry-reduced basis

Broken symmetry

The finite volume breaks the 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

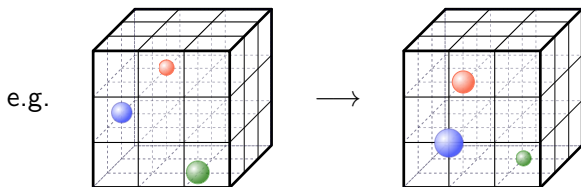
Cubic projection

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 wrapped back into range $-N/2, \dots, N/2 - 1$



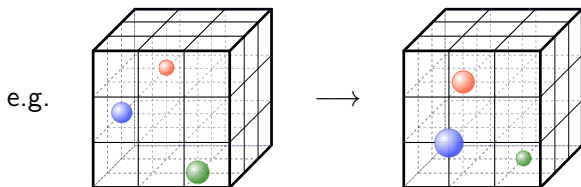
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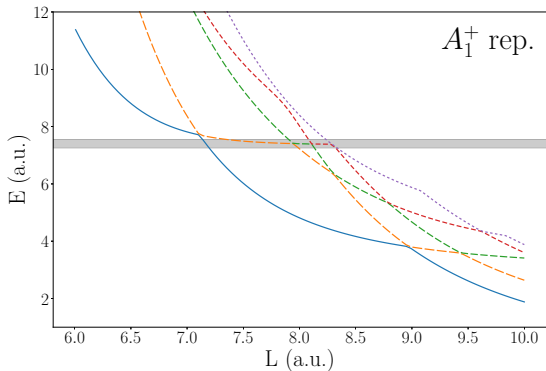
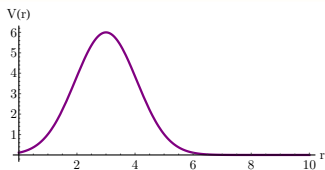


numerical implementation: $\hat{H} \rightarrow \hat{H} + \lambda(1 - \mathcal{P}_\Gamma)$, $\lambda \gg E$

Three-body resonance example

three-boson system

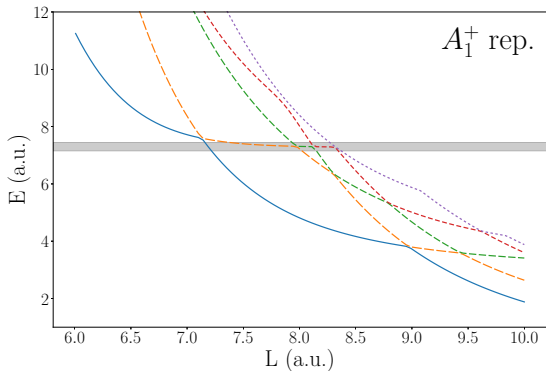
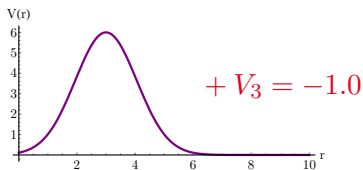
- shifted Gaussian 2-body potential



Three-body resonance example

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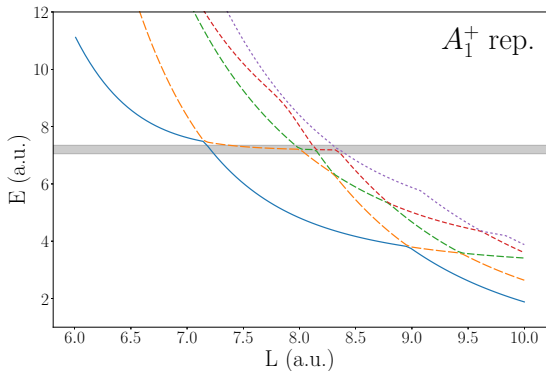
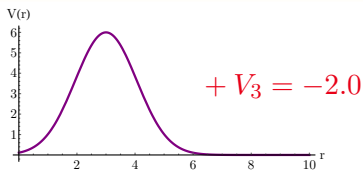
- shifted Gaussian 2-body potential
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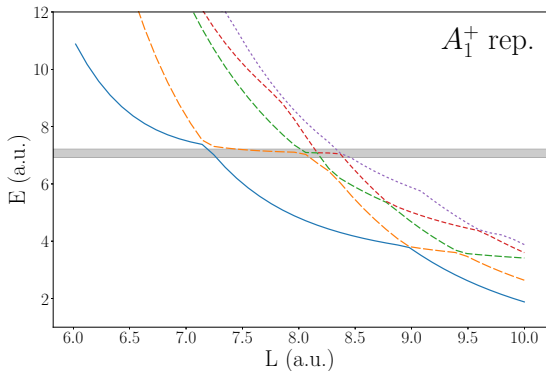
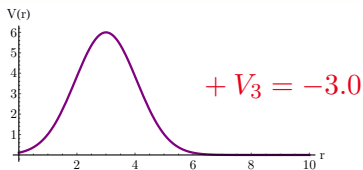
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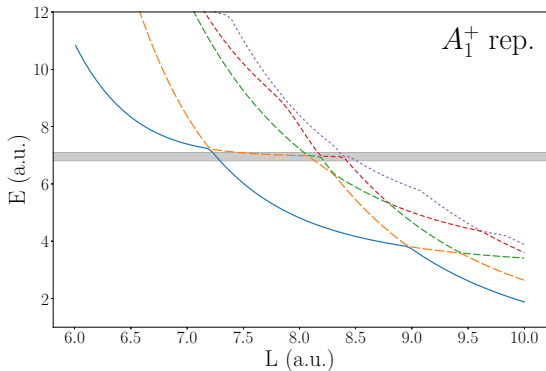
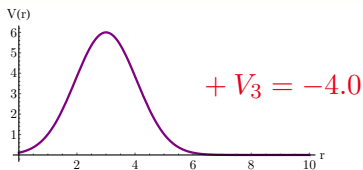
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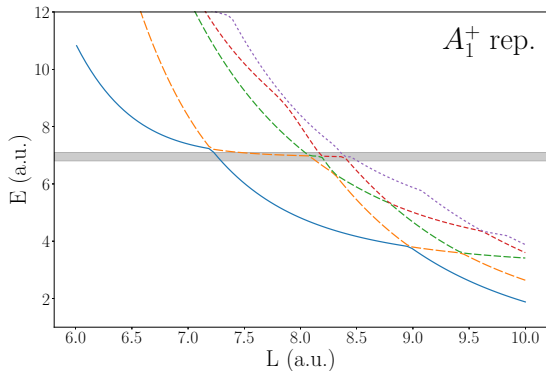
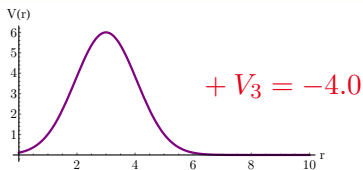
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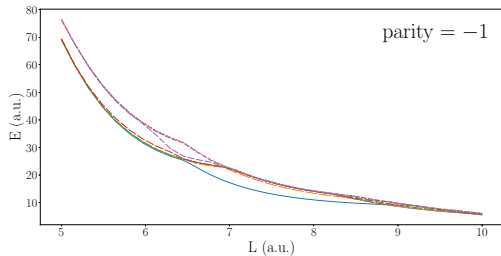
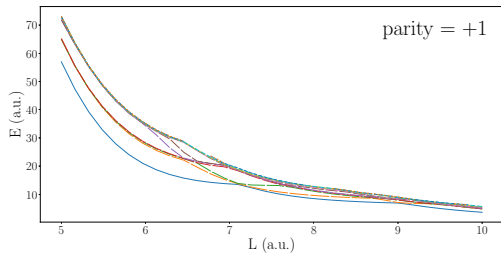
three-boson system

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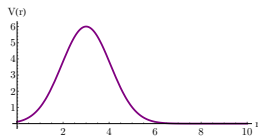


↪ possible to move three-body resonance

Four-body spectra (very preliminary)



four bosons



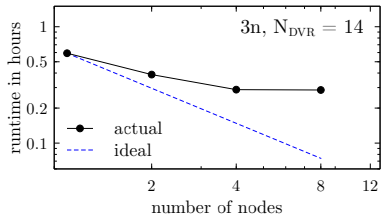
**crossings need not
be avoided!**

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**. ($H \rightarrow H + \lambda(1 - P_{\Gamma})$, λ large)



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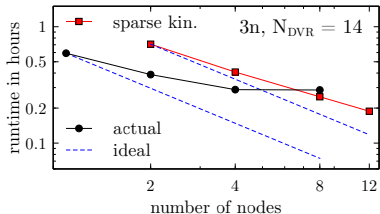


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Work in progress

- **further optimization** (sparse-matrix kin. energy instead of FFT)
↪ 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)

Thank you!

... and thanks to my collaborators:

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



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