

Resonances, currents, and medium mass nuclei

Sebastian König

SFB 1245 Workshop 2017

Mainz

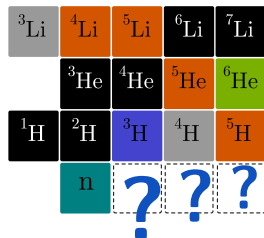
July 4, 2018



Signatures of few-body resonances in finite volume

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

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)
- **conflicting theoretical results!**
Hiyama *et al.*, PRC **93** 044004 (2016); Deltuva, PLB **782** 238 (2018)
Shirokov *et al.* PRL **117** 182502(2016); Gandolfi *et al.*, PRL **118** 232501 (2017); Fossez *et al.*, PRL **119** 032501 (2017)

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**

Wiese, Nucl. Phys. B (Proc. Suppl.) **9**, 609 (1989); ...

Finite-volume resonance signatures

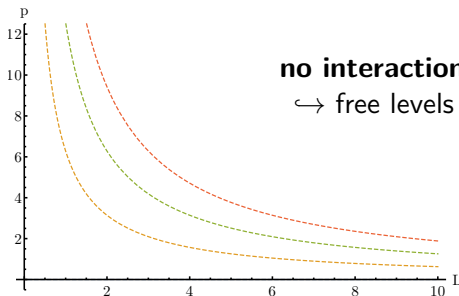
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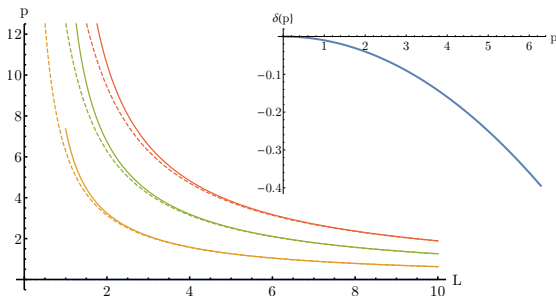
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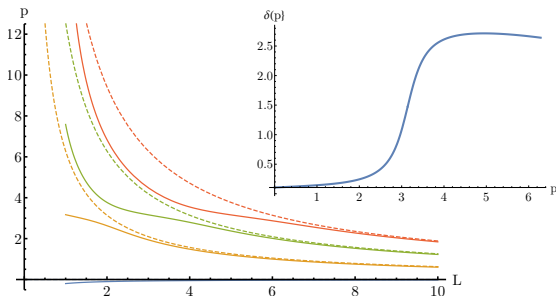
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Discrete variable representation

Needed: calculation of several few-body energy levels

- difficult to achieve with QMC methods
- direct discretization possible, but not very efficient

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

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

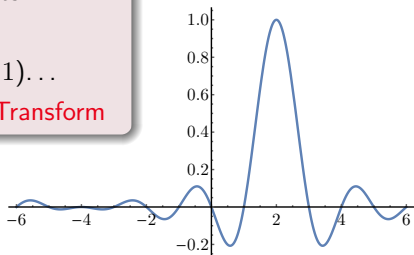
well established in quantum chemistry, suggested for nuclear physics by Bulgac+Forbes, PRC **87** 87, 051301 (2013)

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



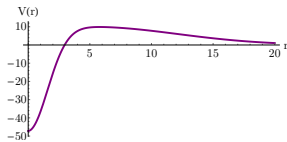
Three-body check

Take established three-body resonance from literature:

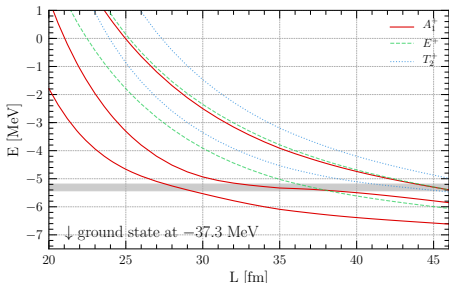
Fedorov *et al.*, *Few-Body Syst.* P 33 153 (2003); Blandon *et al.*, *PRA* 75 042508 (2007)

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

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



- three spinless bosons with mass $m = 939.0 \text{ MeV}$
- two- and three-body bound states at -6.76 MeV and -37.22 MeV
- three-body resonance at $-5.31 - i0.12 \text{ MeV}$ (Blandon *et al.*), $-5.96 - i0.40 \text{ MeV}$ (Fedorov *et al.*)

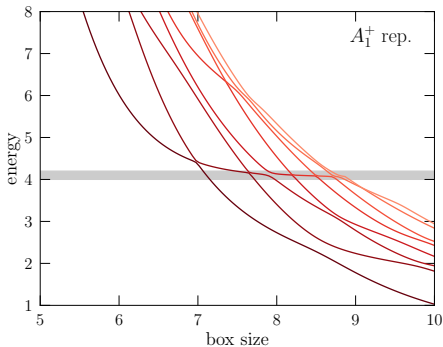
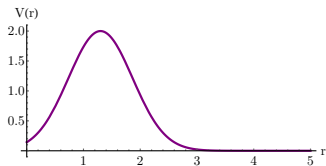


- fit inflection point(s) to extract resonance energy $\rightsquigarrow E_R = -5.32(1) \text{ MeV}$

Three bosons with shifted Gaussian interaction

three-boson system

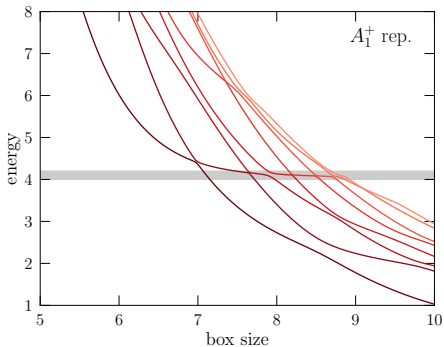
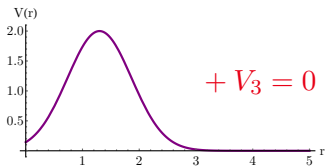
- shifted Gaussian 2-body potential
- **note:** no 2-body bound state!



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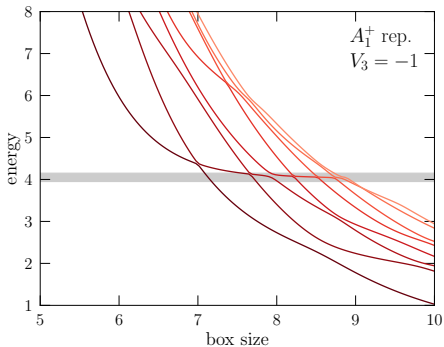
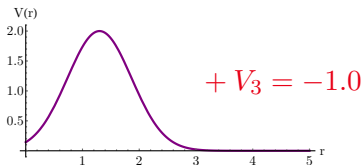
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- add short-range 3-body force



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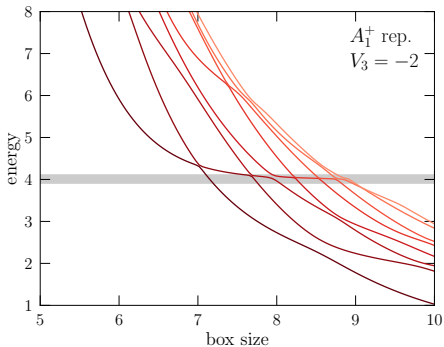
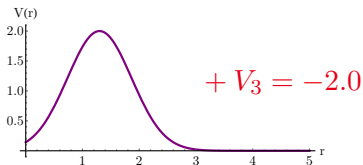
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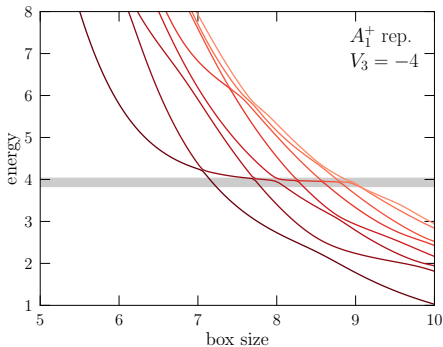
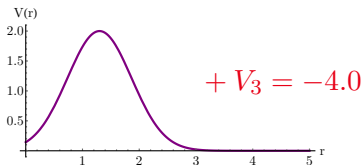
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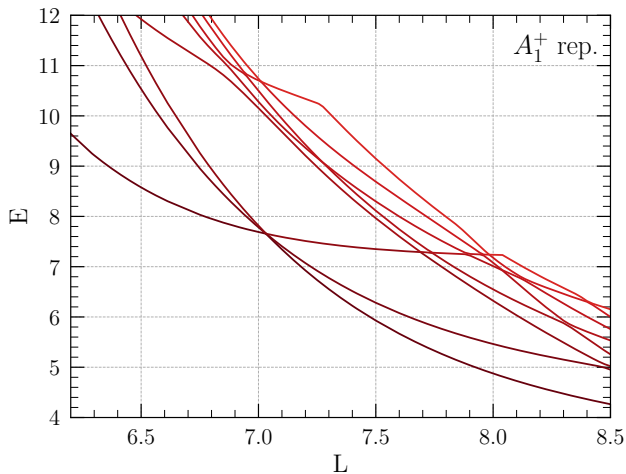
- shifted Gaussian 2-body potential
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↪ possible to move three-body state ↔ spatially localized wf.

Four-boson resonance

Still same potential, look at four bosons...



↪ (supposedly) narrow resonance at $E_R = 7.31(8)$

Summary and outlook

- ✓ **method established** for up to four particles
- ✓ handle **large N_{DVR} for three-body systems** (current record: 32)
- ✓ efficient **symmetrization and antisymmetrization**
- ✓ projection onto **cubic irreps.** ($H \rightarrow H + \lambda(1 - P_{\Gamma})$, λ large)

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Work in progress

- ✓ **chiral interactions** (non-diagonal due to spin dependence!)
 - application to **few-neutron systems**
 - **further optimization** (especially for spin-dep. potentials)
 - ↪ 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)

Electroweak currents from chiral EFT in few-nucleon systems

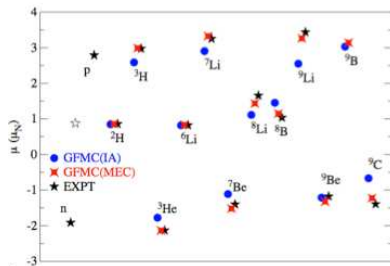
R. Seutin, SK, K. Hebeler, A. Schwenk *et al.*, work in progress

Chiral EFT currents

Chiral EFT predicts consistent electroweak 1+2-body currents

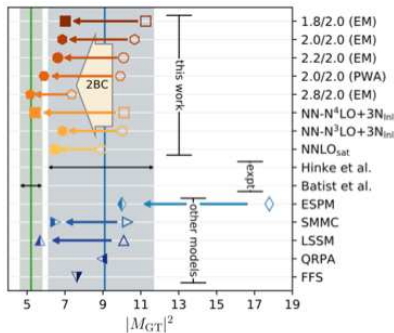
magnetic moments in light nuclei

Pastore et al. (2012-)



Gamow-Teller beta decay of ^{100}Sn

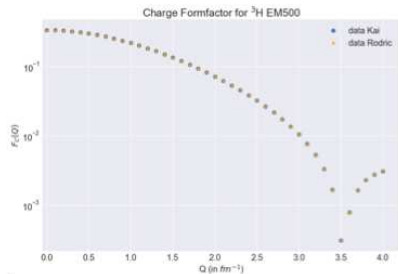
Gysbers, Hagen et al.



contributions from 2-body currents are key!

Chiral EFT currents

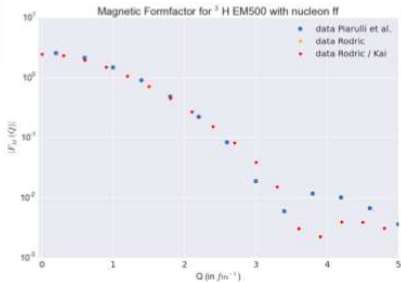
developing framework to include 1+2-body currents at finite q
in partial-wave basis, momentum basis, HO matrix elements



charge form factor for $A=3$
pw basis vs. mom basis check

magnetic form factor benchmarks
with literature not perfect

2-body current tests ongoing,
especially for cm-dependent part



Probing next-generation nuclear forces in medium-mass nuclei

J. Hoppe, J. Simonis, K. Hebeler, A. Schwenk *et al.*, work in progress

Shell-model interactions from chiral EFT: L. Huth, V. Durant, J. Simonis, A. Schwenk, arXiv:1804.04990

Nuclear forces and nuclear matter

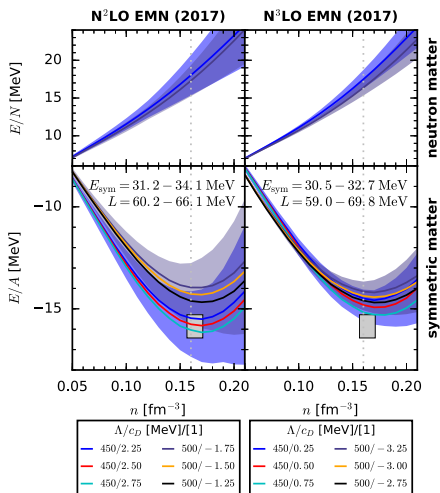
Monte-Carlo calculation of all energy diagrams
up to 4th order in MBPT

Drischler, Hebeler, AS, arXiv:1710.08220

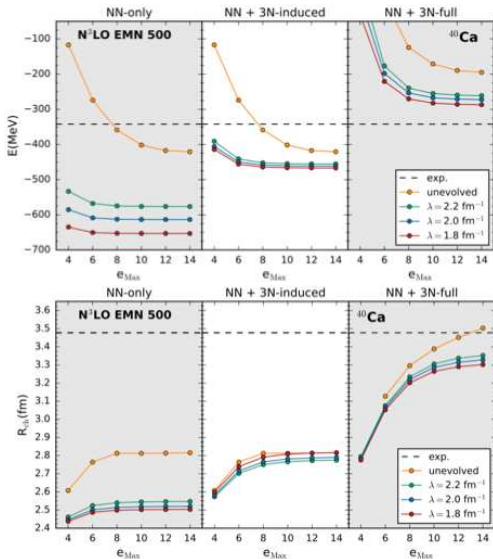
including NN, 3N, 4N
3N fit to saturation region

systematic improvement
from N²LO to N³LO

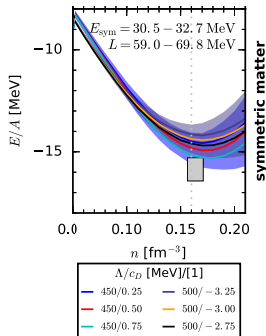
first full N³LO Hamiltonians
for use in nuclear structure!



First (preliminary) N³LO results for nuclei



energy and radius trends as expected from nuclear matter saturation, but more studies needed!



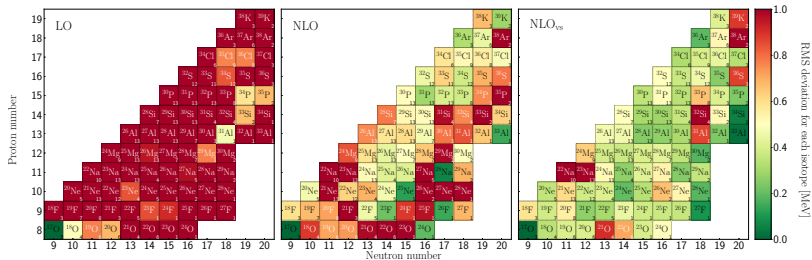
Chiral shell model interactions

use chiral EFT interactions as basis and fit in sd shell directly

Huth, Durant et al., arXiv:1804.04990

includes new valence-space (vs) operators

all LECs turn out natural



The end

Thank you!

Backup slides

Chiral shell model interactions

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Huth, Durant et al., arXiv:1804.04990

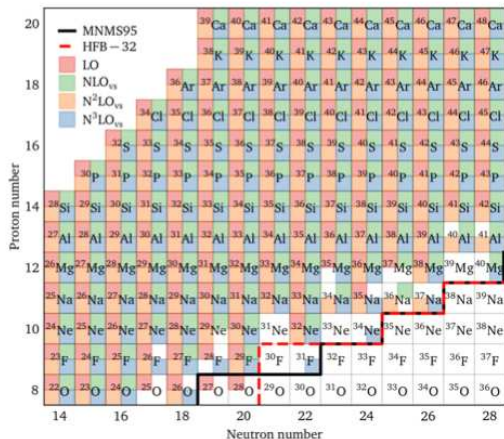
includes new valence-space (vs) operators

all LECs turn out natural

explore dripline

in $sdf_{7/2}$ space

Huth et al., in prep.



Tetraneutron evidence

Physics

ABOUT BROWSE PRESS COLLECTIONS

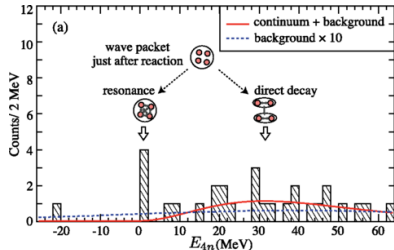
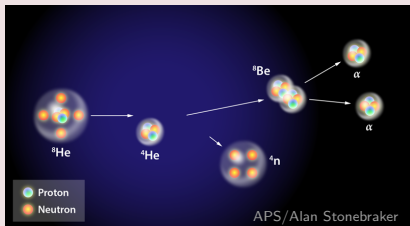
Viewpoint: Can Four Neutrons Tango?

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



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

Short (recent) history of tetra-neutron states

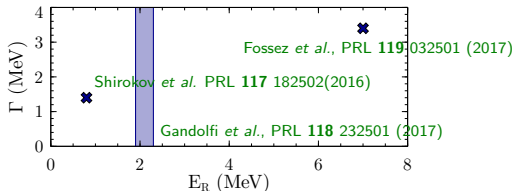
- 1 **2002:** experimental claim of **bound tetra-neutron** Marques *et al.*, PRC **65** 044006
- 2 **2003:** several studies indicate unbound four-neutron system
Bertulani *et al.*, JPG **29** 2431; Timofeyuk, JPG **29** L9; Pieper, PRL **90** 252501
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- 4 **2016: RIKEN experiment: possible tetra-neutron resonance**
 $E_R = (0.83 \pm 0.65_{\text{stat.}} \pm 1.25_{\text{sys.}}) \text{ MeV}$, $\Gamma \lesssim 2.6 \text{ MeV}$ Kisamori *et al.*, PRL **116** 052501
- 5 **following this:** several new theoretical investigations
 - complex scaling \rightarrow **need unphys. $T = 3/2$ 3N force or strong rescaling**

Hiyama *et al.*, PRC **93** 044004 (2016); Deltuva, PLB **782** 238 (2018)

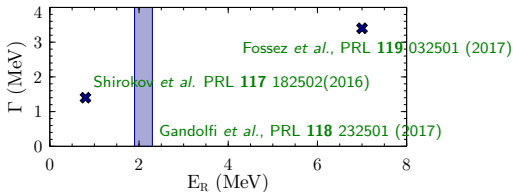
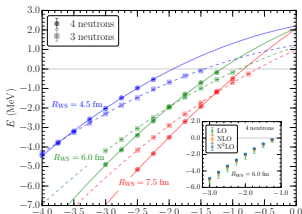
- incompatible predictions:



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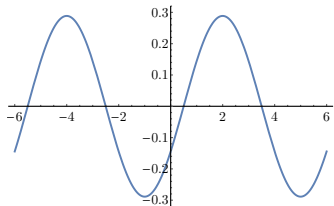


- **indications for three-neutron resonance...**
- **... lower in energy than tetra-neutron state**

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

DVR construction

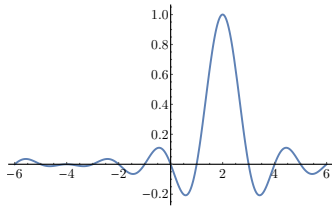
- start with some initial basis; here: $\phi_i(x) = \frac{1}{\sqrt{L}} \exp\left(i \frac{2\pi i}{L} x\right)$
- consider (x_k, w_k) such that $\sum_{k=-N/2}^{N/2-1} w_k \phi_i^*(x_k) \phi_j(x_k) = \delta_{ij}$



unitary trans.



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



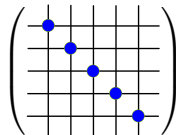
DVR states

- $\psi_k(x)$ 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!

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

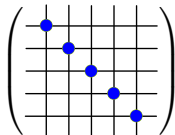


- no need to evaluate integrals
- number N of DVR states controls quadrature approximation

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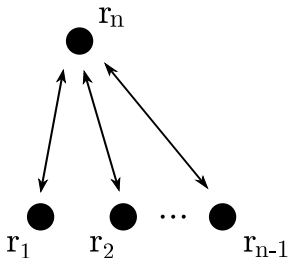
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2 kinetic energy is **simple** (via FFT) or **sparse** (in $d > 1$)!

- 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**



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

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

General DVR state

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

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

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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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- $3n$: $8 \times N_{\text{DVR}}^6$, $4n$: $16 \times N_{\text{DVR}}^9 \rightsquigarrow$ **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

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

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

DVR computational aspects

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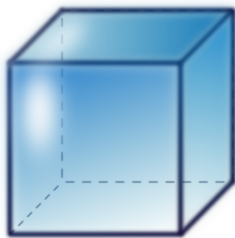
- potential part still diagonal in symmetry-reduced basis

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

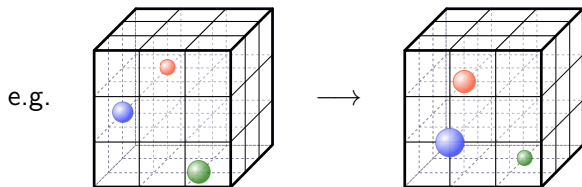
Cubic projection

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 $-N/2, \dots, N/2 - 1$



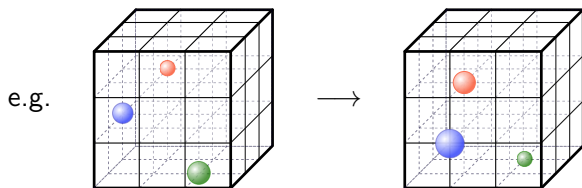
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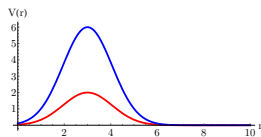


numerical implementation: $\hat{H} \rightarrow \hat{H} + \lambda(\mathbf{1} - \mathcal{P}_\Gamma)$, $\lambda \gg E$

Two-body check: anything goes

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

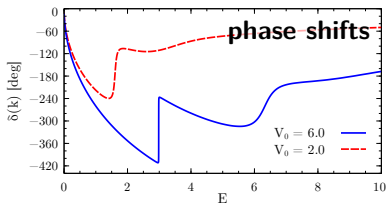
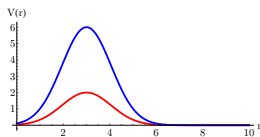
↪ use barrier to produce S-wave resonance



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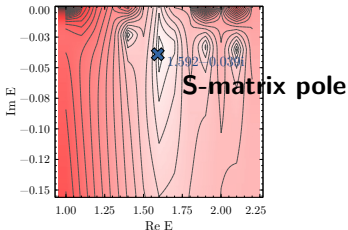
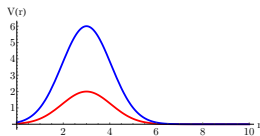
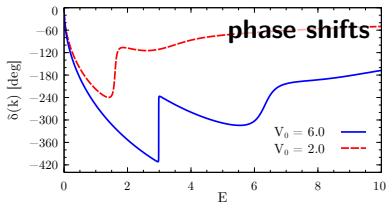
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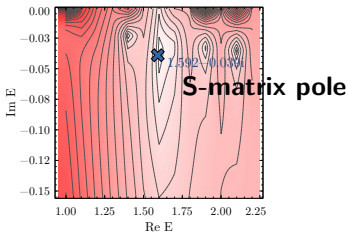
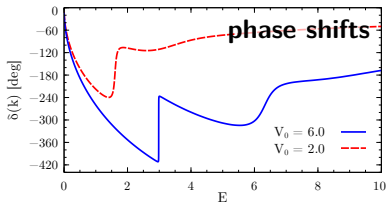
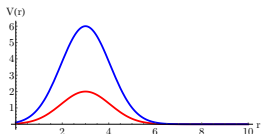
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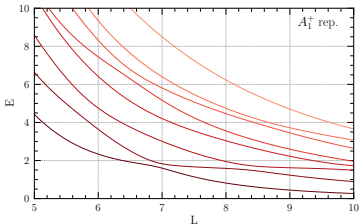
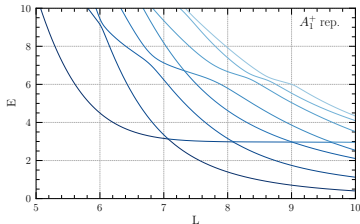
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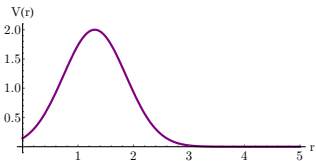
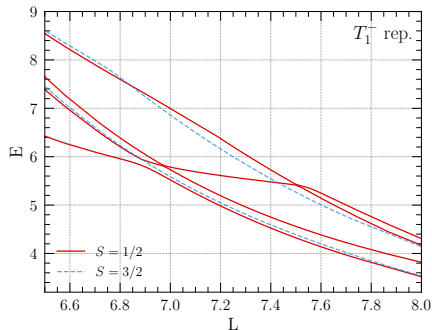
finite-volume spectra



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: $E_R = 5.7(2)$