

Introduction





9th Quantum Phase Transitions in Nuclei and Many-Body Systems

Breaking and restoration of rotational symmetry in the spectrum of α —conjugate nuclei on the lattice

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24th May 2018



Motivation

We investigate rotational symmetry breaking in the low-energy spectra of

light
$$\alpha$$
-conjugate nuclei: 8 Be, 12 C, 16 O, ...

on a cubic lattice. In particular, we aim at

- ♣ identifying lattice eigenstates in terms of SO(3) irreps
 - ⇒ Phys. Lett. B 114, 147-151 (1982), PRL 103, 261001 (2009)
- \clubsuit exploring the dependence of physical observables on spacing and size
 - ⇒ PR D 90, 034507 (2014), PR D 92, 014506 (2015)
- testing techniques for the suppression of discretization artifacts
 - ⇒ Symanzik improvement scheme Lect. Notes in Phys. 788 (2010)

Applications

Nuclear Lattice EFT: ab initio nuclear structure PRL 104, 142501 (2010), PRL 106, 192501 (2011), PRL 112, 102501 (2014), PRL 117, 132501 (2016) and scattering Nature 528, 111-114 (2015)



The Hamiltonian of the system

The macroscopic α -cluster model¹ of B. Lu et al. PR D 90, 034507 (2014) is adopted \implies nuclei are decomposed into M structureless α -particles

$$H = -rac{\hbar^2}{2m_lpha}\sum_{i=1}^{M}
abla_i^2 + \sum_{i>j=1}^{M} V_{\mathsf{C}}(\mathbf{r}_{ij}) + V_{AB}(\mathbf{r}_{ij}) + \sum_{i>j>k=1}^{M} V_{T}(\mathbf{r}_{ij},\mathbf{r}_{ik},\mathbf{r}_{jk})$$

with $r_{ii} = |\mathbf{r}_i - \mathbf{r}_i|$. The potentials are of the type

Erf-Coulomb²

$$\frac{4e^2}{4\pi\epsilon_0}\frac{1}{r_{ij}}\mathrm{erf}\left(\frac{\sqrt{3}r_{ij}}{2R_{\alpha}}\right)$$

with $R_{\alpha} = 1.44$ fm rms radius of the 4He NB: Erf adsorbs the singularity at r = 0

Ali-Bodmer²

$$V_a f e^{-\eta_a^2 r_{ij}^2} + V_r e^{-\eta_r^2 r_{ij}^2}$$

with $\eta_r^{-1} = 1.89036$ fm, $V_r = 353.508 \text{ MeV}$ and $\eta_a^{-1} = 2.29358$ fm, $V_a = -216.346 \text{MeV},$ auxiliary param. f = 1

Gaussian

$$V_0e^{-\lambda(r_{ij}^2+r_{ik}^2+r_{jk}^2)}$$

with $\lambda = 0.00506 \text{ fm}^{-2}$ $V_0 = -4.41 \text{ MeV for}^{12}\text{C}^3$ s.t. $E_{g.s.} = -\Delta E_{Houle}$ and $V_0 = -11.91$ MeV for $^{16}O^4$ s.t. $E_{\sigma.s.} = -\Delta E_{4\alpha}$



Introduction

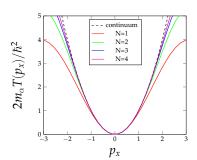
The configuration space in relative d.o.f. of an M - body physical system into a cubic lattice reduces to

 $\mathbb{R}^{3M-3} \longrightarrow L^{3M-3}$

 $L \Longrightarrow$ number of points per dimension (\equiv lattice size) where: $a \Longrightarrow$ lattice spacing

Consequences: discretization effects

- the action of differential operators is represented via finite differences: ⇒ Symanzik improvement scheme
- breaking of Galiean invariance
- breaking of continuous translational invariance (free-particle case)



The lattice environment

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The lattice environment

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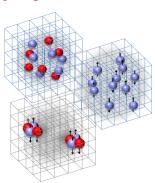
$$\mathbb{R}^{3M-3} \longrightarrow L^{3M-3}$$

where: $L \Longrightarrow$ number of points per dimension (\equiv lattice size) $a \Longrightarrow$ lattice spacing

and finite-volume effects on physical observables

With periodic boundary conditions:

- configuration space becomes isomorphic to a torus in 3M - 3-dimensions
- 2 lattice momenta become $\mathbf{p} = \hbar \frac{2\pi \mathbf{n}}{La}$ where \mathbf{n} is a vector of integers



Accordingly

«Only eight [five: A_1 , A_2 , E, T_1 , T_2] different possibilities exist for rotational classification of states on a cubic lattice. So, the question arises: how do these correspond to the angular momentum states in the continuum? [...] To be sure of higher spin assigments and mass predictions it seems necessary to follow all the relevant irreps simultaneously to the continuum limit. »

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SO(3) to \mathcal{O} irreps decomposition

$$D^{0} = A_{1}, D^{1} = T_{1}$$

$$D^{2} = E \oplus T_{2}$$

$$D^{3} = A_{2} \oplus T_{1} \oplus T_{2}$$

$$D^{4} = A_{1} \oplus E \oplus T_{1} \oplus T_{2}$$

$$D^{5} = E \oplus T_{1} \oplus T_{1} \oplus T_{2}$$

$$D^{6} = A_{1} \oplus A_{2} \oplus E \oplus T_{1} \oplus T_{2} \oplus T_{2}$$

Symmetries

Degenerate states belonging to the same \mathscr{O} irrep can be labeled with the irreps I_z of the cyclic group \mathscr{C}_4 , generated by an order-three element of \mathscr{O} (e.g. $\mathcal{R}_z^{\pi/2}$):

$$\begin{array}{ccc} \mathrm{SO}(3) &\supset & \mathrm{SO}(2) \\ \downarrow & & \downarrow \\ l & & m, \end{array} \implies \begin{array}{cccc} \mathcal{O} &\supset & \mathcal{C}_4 \\ \downarrow & & \downarrow \\ \Gamma & & I_z, \end{array}$$

Conversely, the discrete symmetries of the Hamiltonian are preserved:

time reversal, parity, exchange symmetry

Applications

Within an iterative approach for the diagonalization of \mathcal{H} , the states belonging to an irrep Γ of a point group \mathcal{G} can be extracted applying the projector

$$P_{\Gamma} = \sum_{g \in \mathcal{G}} \chi_{\Gamma}(g) D(g)$$

where D(g) is a representation of dimension 3M - 3 for the operation $g \in \mathcal{G}$



Finite-volume energy corrections

LO finite-volume energy corrections for relative two-body states with angular momentum ℓ and belonging to the Γ irrep of $\mathcal O$ PRL 107, 112011 (2011)

$$\Delta E_{B}^{(\ell,\Gamma)} = \alpha \left(\frac{1}{\kappa L}\right) \left|\gamma\right|^{2} \frac{e^{-\kappa L}}{\mu L} + \mathcal{O}\left(e^{-\sqrt{2}\kappa L}\right)$$

with γ the asymptotic normalization, κ the binding momentum and $\alpha(x)$ a polynomial:

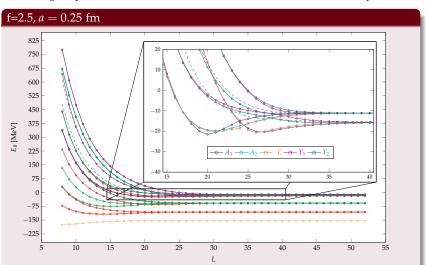
ℓ	Γ	$\alpha(x)$
0	A_1^+	-3
	T_1^-	+3
	T_2^+	$30x + 135x^2 + 315x^3 + 315x^4$
2	E^{-}	$-\frac{1}{2}(15+90x+405x^2+945x^3+945x^4)$
	A_2^-	$315x^2 + 2835x^3 + 122285x^4 + 28350x^5 + 28350x^6$
3	T_2^-	$-\frac{1}{2}(105x + 945x^2 + 5355x^3 + 19530x^4 + 42525x^5 + 42525x^6)$
	T_1^-	

Although no analythic LO FVEC formula for the three-body case exists, results for zero-range potentials PRL 114, 091602 (2015) and the asymptotic (\equiv large L) behaviour are available Phys. Lett. B 779, 9-15 (2018).

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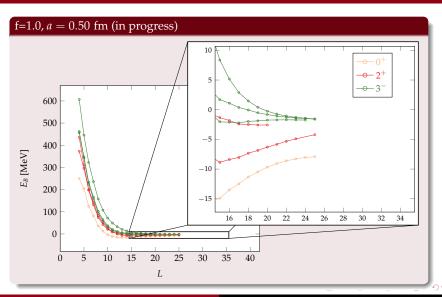
The low-energy ⁸Be spectrum

Increasing the parameter V_a of V_{AB} , a set of bosonic bound states can be analyzed.

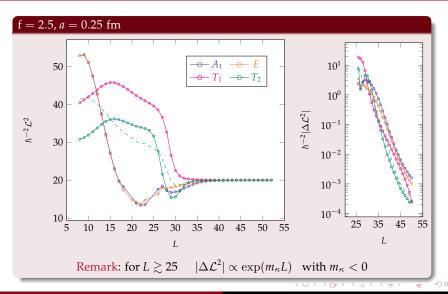


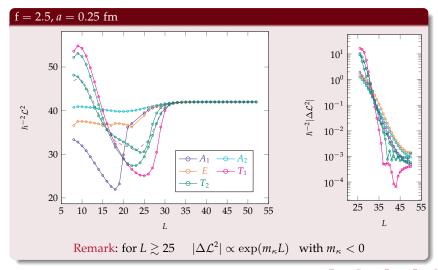
Energy

The low-energy ¹²C spectrum



The low-energy 8 Be spectrum: the ${}^{4}_{2}$ multiplet

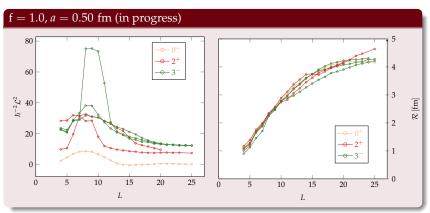






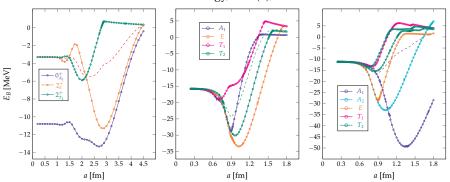
The low-energy ¹²C spectrum

As a consequence of the isotropy of the potentials, the nucleus has an equilateral triangular equilibrium configuration, i.e. $\langle r_{12} \rangle = \langle r_{23} \rangle = \langle r_{13} \rangle \equiv \mathcal{R}$.



Discretization effects on energy

Unlike finite-volume effects, the dominant behaviour of dicretization corrections on energy, $\Delta E_B(a)$, is unknown.



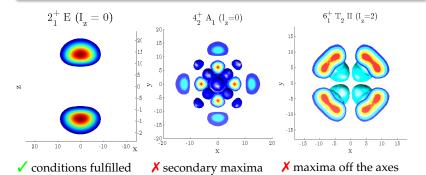
Nevertheless: some extrema of $E_B(a)$ can be associated to the maxima of the probability density function corresponding to the given energy eigenstate.

NB: If the primary maxima of the pdf lie at distance d^* w.r.t. the origin, the most probable $\alpha - \alpha$ separation \mathcal{R}^* is given by d^*

Discretization effects on energy

If the all pdf maxima are absolute and lie along the coordinate axes, \exists a value of a s.t. all the maxima of the pdf are included in the cubic lattice.

In particular: for
$$a=d^*\Longrightarrow E_B(a)$$
 is minimized and if $|\Psi_B^{\mathrm{Max}}|^2\gg |\Psi_B(\mathbf{r})|^2$ where $|\mathbf{r}|=nd^*$ and $n\geq 2\Longrightarrow \langle\mathcal{R}\rangle\approx d^*$ and $\langle V\rangle$ is approximately minimized

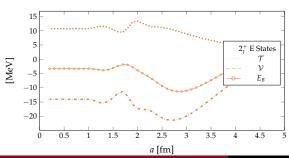


 $I_z = 0 \text{ Pdf}$: two principal maxima along the z axis, located at a distance $d^* = 2.83$ fm from the origin.

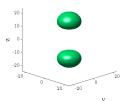
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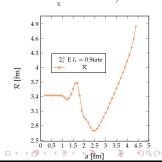
$$a = \frac{d^*}{n}$$
 with $n \ge 1$, i.e. $a \approx 2.83, 1.42, 0.94, ...$

In practice: two E_B minima at $a \approx 1.36$ and 2.85 fm are observed







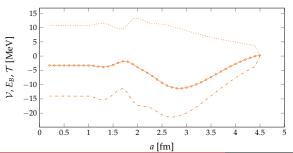


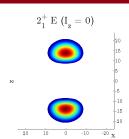
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In addition:

$$\mathcal{V} \approx -21.21 \text{ MeV } @ a = d^*$$

 $e^{min} \approx -21.40 \text{ MeV } @ a \approx 2.70 \text{ fm}$
and
 $\mathcal{R} \approx 2.88 \text{ fm } @ a = d^*$

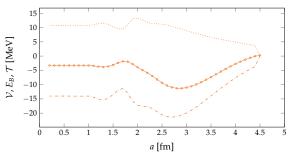
 $\mathcal{R}^{min} \approx 2.70 \text{ fm } @ a \approx 2.50 \text{ fm}$

 $I_z = 2 \text{ Pdf}$: 4 principal maxima on the x and y axes, $\overline{\text{located at a distance }}d^* = 2.83 \text{ fm from the origin.}$

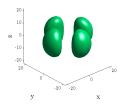
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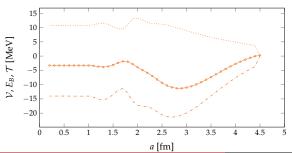
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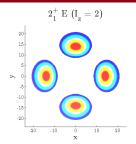
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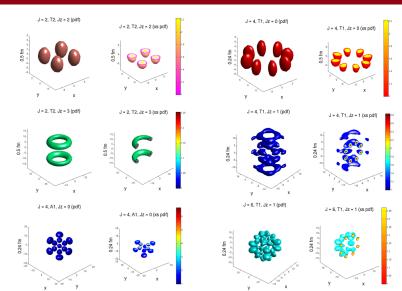


Still:

 $V \approx -21.21 \text{ MeV } @ a = d^*$ ≈ -21.40 MeV @ $a \approx 2.70$ fm

Energy

Other low-energy ⁸Be wavefunctions





Conclusions & Outlook

The macroscopic α -cluster model in PR D 90, 034507 (2014) has been applied to the 8 Be and 12 C on the lattice. A fully-parallel method based on the power iteration has been adopted for the diagonalization of the Hamiltonian, allowing for

 the reconstruction of a larger part of the low-energy spectrum of the two nuclei, made possible by the application of projectors;



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Perspectives and hints

- ♠ Extension of the analysis to the ¹⁶O ⇒ adaption of the present MPI diagonalization code to GPU calculations;
- ♠ Derivation of an analytical formula for the leading order FV energy corrections for bound states in presence of a Coulomb-type potential.



Rotational Symmetry

On the lattice 3-dim rotational symmetry reduces to a subgroup of SO(3), the cubic group \mathcal{O} . A process of descent in symmetry takes place: $\alpha = x$; y; z

continuum,
$$\infty$$
 – volume : $SO(3) \Longrightarrow [H, L^2] = 0, [H, L_{\alpha}] = 0$

continuum, finite volume :
$$\mathscr{O} \subset SO(3) \Longrightarrow [H, L^2] = 0, [H, L_{\alpha}] \neq 0$$

discrete, finite volume :
$$\mathscr{O} \subset SO(3) \Longrightarrow [\mathcal{H}, \mathcal{L}^2] \neq 0, [\mathcal{H}, \mathcal{L}_{\alpha}] \neq 0$$

Accordingly

«Only eight [five: A_1 , A_2 , E, T_1 , T_2] different possibilities exist for rotational classification of states on a cubic lattice. So, the question arises: how do these correspond to the angular momentum states in the continuum? [...] To be sure of higher spin assigments and mass predictions it seems necessary to follow all the relevant irreps simultaneously to the continuum limit. »

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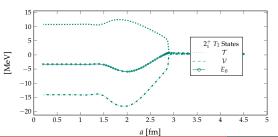
Discretization on ${}^{8}\text{Be}$: the 2_{1}^{+} T_{2} states

 $I_z = 2 \text{ Pdf}$: four principal maxima in the intersection betw. the z = 0 plane and the $x = \pm y$ planes, s.t. $d^* = 0$ 2.83 fm.

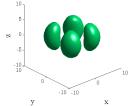
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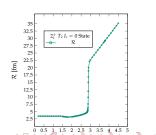
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In practice: two E_B minima at $a \approx 1.05$ and 2.02 fm are observed









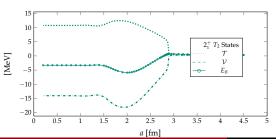
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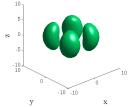
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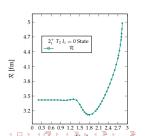
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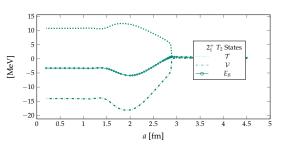
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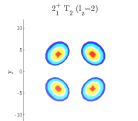
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$$\mathcal{V} \approx -5.43 \text{ MeV } @ a = d^*$$
 $\mathcal{V}^{min} \approx -18.05 \text{ MeV } @ a \approx 1.15 \text{ fm}$
and

$${\cal R} \approx 4.86 \,\, {\rm fm} \,\, @ \,\, a = d^* \ {\cal R}^{min} \approx 3.11 \,\, {\rm fm} \,\, @ \,\, a \approx 1.78 \,\, {\rm fm}$$

Discretization on ${}^{8}\text{Be}$: the 2_{1}^{+} T_{2} states

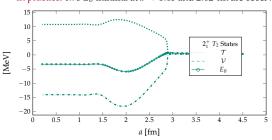
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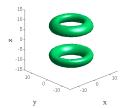
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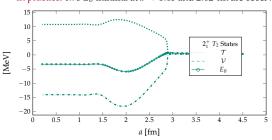
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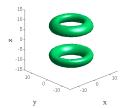
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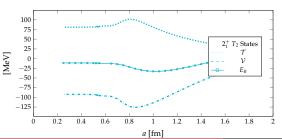


Discretization on ${}^{8}\text{Be}$: the 6_{1}^{+} A_{2} state

 $[I_z = 2 \text{ Pdf}]$: four equidistant couples of principal maxima separated by an angle $\gamma \approx 34.2^{\circ}$ and located at a distance $d^* \approx 2.31$ fm from the origin in the x, y and z = 0 planes.

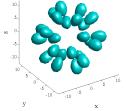


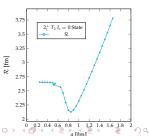
The 24 maxima cannot be included on the lattice





 6^{+} A_{2} $(I_{2}=2)$





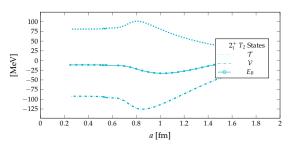
Discretization on ${}^{8}\text{Be}$: the 6_{1}^{+} A_{2} state

Considering the inclusion conditions of a couple of maxima in the 1st quadrant of the xy plane (n > 1):

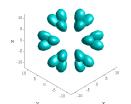
$$a_x = \frac{d^*}{n} \cos\left(\frac{\pi}{4} - \frac{\gamma}{2}\right)$$
, i.e $a_y \approx 2.04, 1.02, 0.68...$

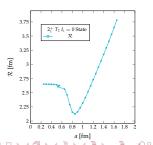
$$a_y = \frac{d^*}{n} \sin\left(\frac{\pi}{4} - \frac{\gamma}{2}\right), \text{ i.e. } a_y \approx 1.08, 0.54, 0.36...$$

In practice: an E_B minimum at $a \approx 1.03$ fm is observed!









Introduction

Discretization on 8Be

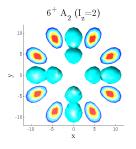
Discretization on ${}^{8}\text{Be}$: the 6_{1}^{+} A_{2} state

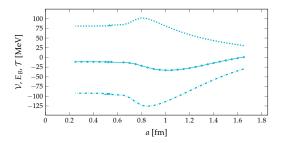
Considering the inclusion conditions of a couple of maxima in the 1st quadrant of the *xy* plane ($n \ge 1$):

$$a_x = \frac{d^*}{n} \cos\left(\frac{\pi}{4} - \frac{\gamma}{2}\right), \text{ i.e. } a_y \approx 2.04, 1.02, 0.68...$$

$$a_y = \frac{d^*}{n} \sin\left(\frac{\pi}{4} - \frac{\gamma}{2}\right), \text{ i.e. } a_y \approx 1.08, 0.54, 0.36...$$

In practice: an E_B minimum at $a \approx 1.03$ fm is observed!



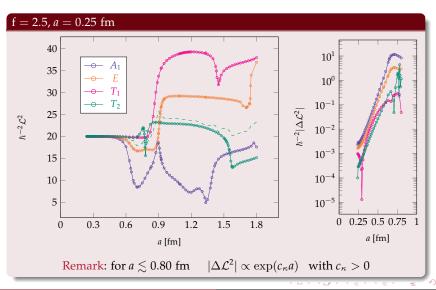


In addition:

 $V \approx 0.0 \text{ MeV } @ a = d^* \text{ (unbound)}$ $V^{min} \approx -125.85 \text{ MeV } @ a \approx 0.85 \text{ fm}$

$$\mathcal{R}\gg\mathcal{R}^{min}$$
 @ $a=d^*$ $\mathcal{R}^{min}\approx 2.13$ fm @ $a\approx 0.85$ fm

The low-energy 8 Be spectrum: the ${}^{4}_{2}$ multiplet



The low-energy ⁸Be spectrum: the 6⁺ multiplet

