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# Breaking and restoration of rotational symmetry in the spectrum of $\alpha$ -conjugate nuclei on the lattice

**PRESENTATION SESSION** 

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#### Motivation

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

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

on a cubic lattice G.S. et al. EPJ A 54, 232 (2018). 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)

♣ exploring the dependence of physical observables on spacing and size  $\implies$  PRD 90, 034507 (2014), PRD 92, 014506 (2015)

developing memory-saving and fast algorithms for the diagonalization of the lattice Hamiltonian

testing techniques for the suppression of discretization artifacts

 $\implies$  Lect. Notes in Phys. 788 (2010)

#### Applications

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

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#### The Hamiltonian of the system

The macroscopic  $\alpha$ -cluster model<sup>1</sup> of B. Lu et al. PR D 90, 034507 (2014) is adopted  $\implies$  nuclei are decomposed into *M* structureless  $\alpha$ -particles

$$H = -\frac{\hbar^2}{2m_\alpha} \sum_{i=1}^M \nabla_i^2 + \sum_{i>j=1}^M V_C(\mathbf{r}_{ij}) + V_{AB}(\mathbf{r}_{ij}) + \sum_{i>j>k=1}^M V_T(\mathbf{r}_{ij}, \mathbf{r}_{ik}, \mathbf{r}_{jk})$$

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

#### Gaussian Ali-Bodmer<sup>2</sup> Coulomb<sup>2</sup> $V_0 e^{-\lambda (r_{ij}^2 + r_{ik}^2 + r_{jk}^2)}$ $V_a f e^{-\eta_a^2 r_{ij}^2} + V_r e^{-\eta_r^2 r_{ij}^2}$ $\frac{4e^2}{4\pi\epsilon_0}\frac{1}{r_{ii}}\operatorname{erf}\left(\frac{\sqrt{3}r_{ij}}{2R_{\alpha}}\right)$ with $\lambda = 0.00506 \text{ fm}^{-2}$ , with $\eta_r^{-1} = 1.89036$ fm, with $R_{\alpha} = 1.44$ fm $V_0 = -4.41$ MeV for ${}^{12}C^3$ $V_r = 353.508 \text{ MeV}$ and $\eta_a^{-1} = 2.29358 \text{ fm}$ , rms radius of the <sup>4</sup>He s.t. $E_{g.s.} = -\Delta E_{Hoyle}$ NB: Erf adsorbs the $V_a = -216.346 \,\mathrm{MeV}$ and $V_0 = -11.91$ MeV for ${}^{16}O^4$ singularity at r = 0auxiliary param. f = 1s.t. $E_{g,s_1} = -\Delta E_{4\alpha}$

<sup>1</sup>G.S. et al. JP G 43, 8 (2016), <sup>2</sup>NP 80, 99-112 (1966) , <sup>3</sup>Z. Physik A 290, 93-105 (1979) , <sup>4</sup>G.S. (2017)

Breaking and restoration of rotational symmetry on the lattice

#### The lattice environment

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

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

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

#### Consequences: discretization effects

- the action of differential operators is represented via finite differences: ⇒ Lect. Notes in Phys. 788 (2010)
- 2. breaking of Galiean invariance
- 3. breaking of continuous translational invariance (free-particle case)



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and **finite-volume effects** on physical observables

With periodic boundary conditions:

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



#### Symmetries

On the lattice SO(3) symmetry reduces to the invariance under the cubic group O.

#### 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 assignents and mass predictions it seems necessary to follow all the relevant irreps simultaneously to the continuum limit. »

R.C. Johnson, Phys. Lett. B 114, 147-151, (1982).

Integer spin irreps  $D^{\ell}$  of SO(3) decompose into irreps of  $\mathcal{O}$  as follows:

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

$$D^{1} = T_{1}$$

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

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

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

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

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

## Symmetries

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

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

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  $\Gamma$  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 bosonic states with reduced mass  $\mu$ , angular momentum  $\ell$  and belonging to the  $\Gamma$  irrep of O are given by PRL 107, 112011 (2011)

$$\Delta E_{B}^{(\ell,\Gamma)} \equiv E_{B}^{(\ell,\Gamma)}(\infty) - E_{B}^{(\ell,\Gamma)}(L) = \beta \left(\frac{1}{\kappa_{0}L}\right) |\gamma|^{2} \frac{e^{-\kappa_{0}L}}{\mu L} + \mathcal{O}\left(e^{-\sqrt{2}\kappa_{0}N}\right)$$

with

 $\gamma \Rightarrow$  asymptotic normalization constant

 $\kappa_0 \Rightarrow$  binding momentum and  $\beta(x) \Rightarrow$  a polynomial

$\ell$	Г	$\beta(x)$
0	$A_1^+$	-3
1	$T_{1}^{-}$	+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	$T_2^{-}$	$-\frac{1}{2}(105x + 945x^2 + 5355x^3 + 19530x^4 + 42525x^5 + 42525x^6)$
	$T_{1}^{2}$	$-\frac{1}{2}(14 + 105x + 735x^2 + 3465x^3 + 11340x^4 + 23625x^5 + 23625x^6)$

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

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with  $\gamma \Rightarrow$  asymptotic normalization constant  $\kappa_0 \Rightarrow$  binding momentum and  $\beta(x) \Rightarrow$  a polynomial **Multiplet averaging** of the energies.  $\Rightarrow$  the finite volume energy corrections assume an universal form, independent in magnitude on the SO(3) irreps

$$\begin{split} E_{\infty}(\ell_A^p) - E_L(\ell_A^p) \Big|_{L^0}^{L^0} &= (-1)^{\ell+1} 3 |\gamma|^2 \frac{e^{-\kappa_0 L}}{\mu L} \quad \text{with} \quad E(\ell_A^p) \equiv \sum_{\Gamma \in \mathcal{O}} \frac{\chi^{\Gamma}(1)}{2\ell+1} E_B^{(\ell^p, \Gamma)}(L) \\ \text{at LO, i.e. order } \exp(-\kappa_0 L). \end{split}$$

where:  $\Gamma \Rightarrow$  irrep of the cubic group  $\chi^{\Gamma}(\mathbb{1}) \Rightarrow$  character of  $\Gamma$  w.r.t. the identity conjugacy class ( $\equiv \dim \Gamma$ )  $P \Rightarrow$  eigenvalue of the inversion operator  $\mathscr{P}$ 

Finite volume energy corrections including Coulomb interaction Leading Coulomb corrections for the energies of states with  $\ell = 0$  ( $A_1$ ) describing two spinless singly-charged particles in a finite volume are given by  $\Delta E_{B,QED}^{(0,A_1)} \equiv E_{B,QED}^{(0,A_1)}(\infty) - E_{B,QED}^{(0,A_1)}(L) = \frac{\alpha}{\pi L} \mathcal{I} + \mathcal{O}(\alpha^2) \qquad \Longrightarrow \text{PRD 90, 074511 (2014)} \\ \mathcal{I} = \sum_{n\neq 0}^{\Lambda_n} \frac{1}{|\mathbf{n}|^2} - 4\pi \Lambda_n = -8.9136$ where:  $\alpha = e^2/4\pi \Rightarrow \text{fine structure constant} \\ \Lambda_n = N\Lambda/2\pi \text{ with } \Lambda \Rightarrow \text{UV lattice momentum cutoff}$  $\mathbf{n} \Rightarrow \text{three-vector of integers}$ 

As in the case without QED, FV corrections for the  $\ell = 0$  state are negative

In presence of Coulomb interaction, the infinite-volume bound state energy  $E \equiv -E_B^{(0,A_1)}(\infty) = -\kappa_0^2/2\mu$  and binding momentum  $\kappa_0$  is modified into

$$E_{B,\text{QED}}^{(0,A_1)}(\infty) = \frac{\kappa_0^2}{2\mu} - \frac{2\alpha\kappa_0}{1-\kappa_0r_0} \left[\gamma_E + \log\left(\frac{\alpha\mu}{2\kappa_0}\right)\right]$$

where:  $r_0 \Rightarrow$  effective range of strong interactions  $\gamma_E \approx 0.57721 \Rightarrow$  Euler-Mascheroni constant

Remark: in absence of further forces there's no QED contribution at  $O(\alpha)$ Outlook: extension of the Coulomb FVEC formula to states with  $\ell \ge 1$ 

Breaking and restoration of rotational symmetry on the lattice

## The low-energy <sup>8</sup>Be spectrum

Increasing the parameter  $V_a$  of  $V_{AB}$  up to 130% of its eigenvalue (f = 1.3), the finite volume behaviour of the energies of the  $0_1^+$  and  $2_1^+$  bound states can be inspected:



♣ Remark: for  $N \gtrsim 27$  the sign of the FVECs agrees with the  $\Delta E_B^{(\ell,\Gamma)}$  formulas for  $\ell = 0$ and 2, even if Coulomb corrections dominate outside the strong interaction region

Introduction

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## The low-energy <sup>8</sup>Be spectrum

The further increase of the parameter  $V_a$  of  $V_{AB}$  up to 250% (f = 2.5) permits to extend the FV analysis to the  $\ell = 4$  and 6 states  $\implies$  the  $4^+_2$  and  $6^+_1$  multiplets (cf. magnification)



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## The low-energy <sup>12</sup>C spectrum

Since the nucleus is naturally bound, no artificial increase of the strength parameter  $V_0$  of  $V_{AB}$  is necessary for the study of the lowest  $0^+_1$ ,  $2^+_1$  and  $3^-_1$  states.



♣ Remark: the spacing is larger (a = 0.5 fm)  $\implies$  discretization effects:  $10^{-2}$ - $10^{-3}$  MeV.

Breaking and restoration of rotational symmetry on the lattice

## The low-energy <sup>8</sup>Be spectrum: the $0_1^+$ and $2_1^+$ multiplets Now we consider the average values of the squared total angular momentum operator $\mathcal{L}^2$ , in relative coordinates. Fixing a = 0.5 fm, for the $0_1^+$ and $2_1^+$ states (f = 1.3) we find:



**A** Remark: The average values of  $\mathcal{L}^2$  for the  $0^+_{A_1}$ ,  $2^+_E$  and  $2^+_{T_2}$  states smoothly converge to the eigenvalues equal to 0 and  $6\hbar^2$ , modulo residual discretization errors:  $\langle \Xi \rangle = \Xi$ 

### The low-energy <sup>8</sup>Be spectrum: the $4^+_2$ multiplet

In the f = 2.5 case, by fixing a = 0.25 fm discretization effects for the  $4_2^+$  multiplets reduce to  $\approx 10^{-4} \hbar^2$ . Multiplet-averaging enhances convergence.



## The low-energy <sup>8</sup>Be spectrum: the $6_1^+$ multiplet

In the f = 2.5 case, fixing a = 0.25 fm residual discretization effects for the  $6_1^+$  multiplets amount to  $\approx 10^{-4}\hbar^2$ . Multiplet-averaging enhances convergence.



Remark: for  $L \gtrsim 25$   $|\Delta \mathcal{L}^2| \propto \exp(m_{\kappa}L)$  with  $m_{\kappa} < 0$ 

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## The low-energy <sup>12</sup>C spectrum

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

Restoring the  $V_a$  parameter of the Ali-Bodmer potential to its default value (f = 1.0) and fixing the spacing to a = 0.50 fm, we compute the average values of  $\mathcal{L}^2$  on the  $0^+_1$ ,  $2^+_1$  and  $3^-_1$  multiplets of states.



Remark: residual discretization errors are sensibly larger ( $\approx 10^{-1} - 10^{-2}\hbar^2$ ).

#### Discretization effects: a cover story...



#### 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  $d^*$ 

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#### 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  $|\Psi_B^{\text{Max}}|^2 \gg |\Psi_B(\mathbf{r})|^2$  where  $|\mathbf{r}| = nd^*$  and  $n \ge 2 \Longrightarrow \langle \mathcal{R} \rangle \approx d^*$  and  $\langle V \rangle$  is approximately minimized



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 $2^+_1 \to (I_z = 0)$ 

Appendix

## Discretization on <sup>8</sup>Be: the $2^+_1 E$ states

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

$$\implies E_B(a)$$
 minima are, then, predicted to lie at

$$a = \frac{d^*}{n}$$
 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



Breaking and restoration of rotational symmetry on the lattice

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### Discretization on <sup>8</sup>Be: the $2^+_1$ *E* states

 $I_z = 2 \text{ Pdf}$ : 4 principal maxima on the x and y axes, 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







Still:

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

## Discretization on <sup>8</sup>Be: the $2^+_1$ *E* states

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## Discretization on <sup>8</sup>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.







 $6^+ A_2 (I_2 = 2)$ 



 $6^+ A_2 (I_z=2)$ 

Appendix

## Discretization on <sup>8</sup>Be: the $6_1^+ A_2$ state

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

$$a_x = \frac{d^*}{n} \cos\left(\frac{\pi}{4} - \frac{\gamma}{2}\right),$$
 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 !





a [fm]

1.2 1.4 1.6 1.8 2



0 0.2 0.4 0.6 0.8

2.5

2.25

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## Other low-energy <sup>8</sup>Be wavefunctions





#### Conclusions & Outlook

The macroscopic  $\alpha$ -cluster model in PRD 90, 034507 (2014) has been applied to the <sup>8</sup>Be and <sup>12</sup>C on the lattice. A fully-parallel method based on the Lanczos iteration has been adopted for the diagonalization of the Hamiltonian, allowing for

1. the exploration of SO(3) breaking effects on a sample of bound eigenstates:  $0^+$ ,  $2^+$ ,  $4^+$  and  $6^+$  for the <sup>8</sup>Be and  $0^+$ ,  $2^+$  and  $3^-$  for the <sup>12</sup>C;



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- 2. a test for the capability of the squared total angular momentum operator of identifying the lattice eigenstates in terms of the label of SO(3) irreps;

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#### Perspectives and hints

- ♠ Extension of the analysis to the <sup>16</sup>O ⇒ usage of the existing *exact* GPU codes for small volumes (memory issues!) and benchmarks as well as Metropolis Monte Carlo wordline or auxiliary field algorithms for large volumes (under development);
- ♦ Derivation of an analytical formula for the leading order FV energy corrections for bound states with  $\ell \ge 1$  in presence of a Coulomb-type potential.

Conclusion



#### **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 :  $SO(3) \Longrightarrow [H, L^2] = 0, [H, L_{\alpha}] = 0$ 

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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 assignents and mass predictions it seems necessary to follow all the relevant irreps simultaneously to the continuum limit. »

R.C. Johnson, Phys. Lett. B 114, 147-151, (1982).

## Discretization on <sup>8</sup>Be: the $2^+_1 T_2$ states

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

 $\Rightarrow$   $E_B(a)$  minima are, then, predicted to lie at

$$a = \frac{\sqrt{2}}{2} \frac{d^*}{n}$$
 with  $n \ge 1$ , i.e.  $a \approx 2.02, 1.01, 0.67, ...$ 

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









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 $2^+_1 T_2 (I_z=2)$ 





 $2_{1}^{+} T_{2} (I_{a}=2)$ 

Appendix

## Discretization on <sup>8</sup>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.  $d^* = 2.83$  fm.

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Breaking and restoration of rotational symmetry on the lattice

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## Discretization on <sup>8</sup>Be: the $2^+_1 T_2$ states

 $I_z = 1,3$  Pdf: 2 circles of principal maxima about the z axis,

located at a distance  $d^* = 2.83$  fm from the origin.

 $\implies$   $E_B(a)$  minima are, then, predicted to lie at

$$a = \frac{\sqrt{2}}{2} \frac{d^*}{n}$$
 with  $n \ge 1$ , i.e.  $a \approx 2.02, 1.01, 0.67, ...$ 

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









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Breaking and restoration of rotational symmetry on the lattice

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## The low-energy <sup>8</sup>Be spectrum: the $4_2^+$ multiplet

In the f = 2.5 case, fixing  $Na \ge 12$  fm residual finite volume effects for the  $4_2^+$  multiplets amount to  $\approx 10^{-3}\hbar^2$ . Multiplet-averaging evens the spikes.



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## The low-energy <sup>8</sup>Be spectrum: the $6_1^+$ multiplet

In the f = 2.5 case, fixing  $Na \ge 12$  fm residual finite volume effects for the  $6_1^+$  multiplets amount to  $\approx 10^{-4} \hbar^2$ . Multiplet-averaging evens the spikes.



**Remark:** for  $a \leq 0.80$  fm  $|\Delta \mathcal{L}^2| \propto \exp(c_{\kappa} a)$  with  $c_{\kappa} > 0$ 

Breaking and restoration of rotational symmetry on the lattice