Variation of multiple configurations for cluster structures in light nuclei

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TOAMD Collaboration

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科研費 KAKENHI

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Akinobu Doté	土手　昭伸	KEK、つくば

Motivation

- Configuration mixing (Configuration interaction) is a general concept in many-body quantum systems in atomic, molecular, and nuclear physics.
- Nuclear WF: $\Psi = \sum_n^N C_n \Phi_n$, $\Phi_n = \mathcal{A}\{\prod_{i=1}^A \phi_{n,i}(\boldsymbol{r}_i)\}$ Slater determinant
- Purpose: Determine the optimal single-particle WF $\{\phi_{n,i}\}$ for Ψ
- Usual energy-variation: Single configuration Φ_n + Constraints (β,γ,radius…)

Generator Coordinate

- Question from Lyu-san : How to determine many parameters in Ψ?
- IDEA: energy-variation of "Ψ" directly, $E = \langle \Psi | H | \Psi \rangle / \langle \Psi | \Psi \rangle$, $\delta E = 0$
- Nuclear model : Antisymmetrized Molecular Dynamics (AMD)
- In AMD, nucleon WF: $\phi(\boldsymbol{r}) \propto e^{-\nu(\boldsymbol{r}-\boldsymbol{Z})^2}$, $\boldsymbol{Z}$: variational parameter

History : Variation of multiple configurations

- Hartree-Fock approach
  - Atomic and Molecular physics, Chemistry (1960s -)
  - Faessler, Schmid, Plastino   Nucl. Phys. A174, 26 (1971)
  - Ogawa, Toki   Annals of Physics 326, 209 (2011)
    2p-2h mixing with high-momentum from tensor force (pion-exchange)
  - Pillet, Robin, Dupuis, Hupin, Berger   Eur. Phys. J. A53, 49 (2017)
    Many-particle many-hole in Gogny-HF with truncation
  - Matsumoto, Tanimura, Hagino   Phys. Rev. C108, L051302 (2023)
    Optimal Generator coordinate in Skyrme-HF
- Shell model : Monte-Carlo SM, Conjugate Gradient Method, Shimizu et al.
  Physics 2022, 1081 (2022)
- Cluster model : Generate multi-bases with Neural Network, Lyu et al.,

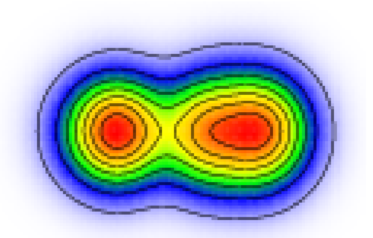
Motivation

- Purpose : Optimize multi AMD bases simultaneously in the superposition
- Future application to ab-initio type methods with realistic nuclear force
- TOAMD: Tensor-Optimized AMD

  Myo et al., Phys. Lett. B769 (2017) 213, Lyu et al., Phys. Lett. B805 (2020) 135421

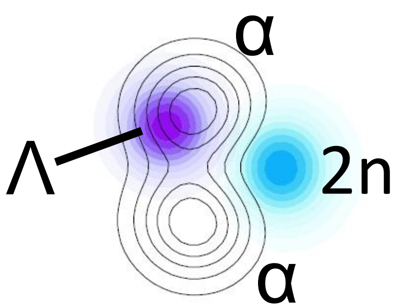
- Present results : p-shell nuclei with effective interaction
- ^{10}Be : various clustering such as linear chain shape

  Phys. Rev. C 108 (2023) 064314

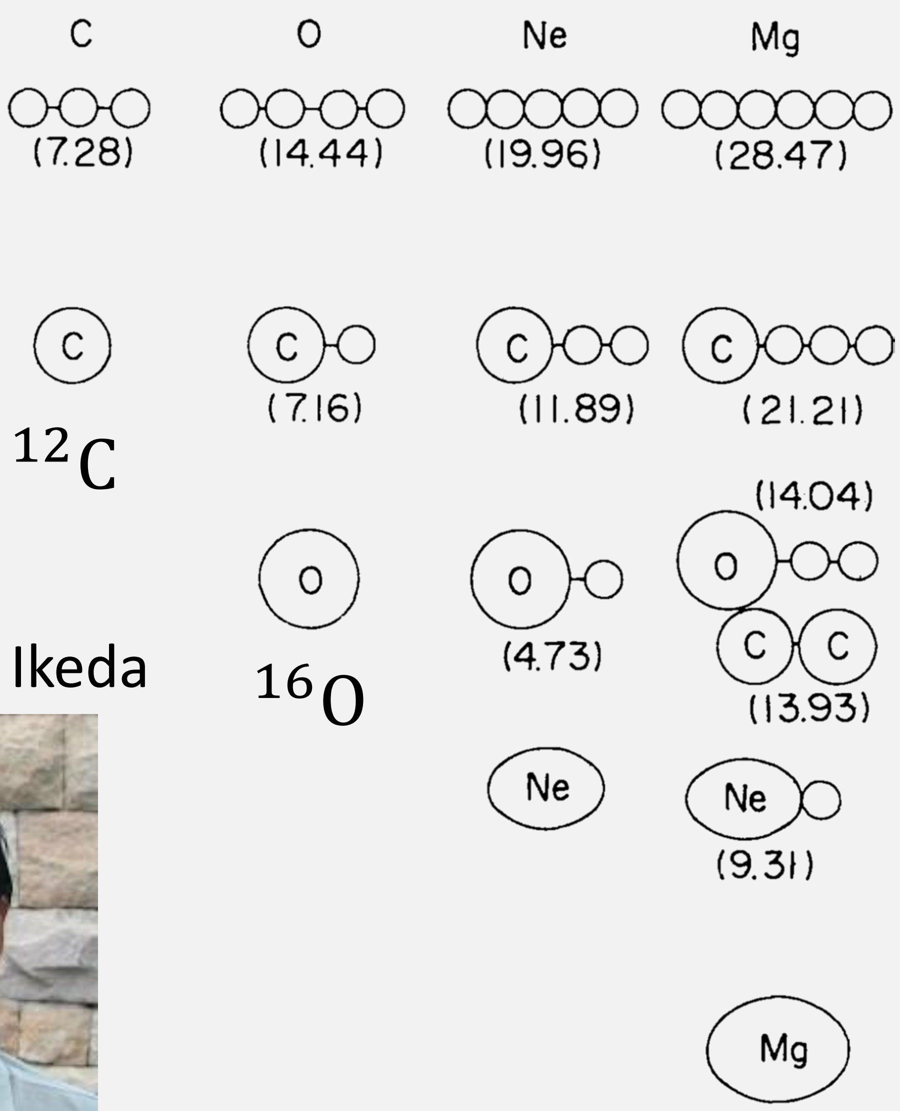


- Cluster configurations in Li isotopes PTEP 2025 (2025) 013D01
- Λ-hypernuclei in Be, B isotopes predicted via Neural Network

  by Lyu et al. Phys. Lett. B855 (2024) 138816, B862 (2025) 139338



Nuclear cluster states indicated by Ikeda diagram

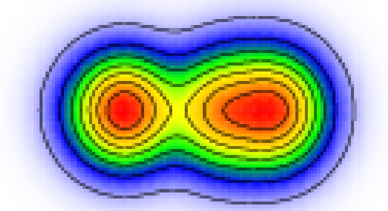


Prof. Kiyomi Ikeda

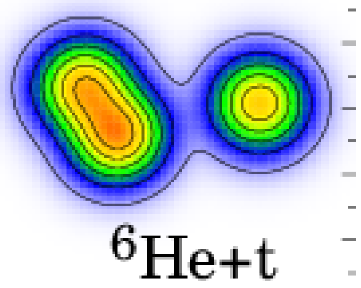
- Ikeda, Takigawa, Horiuchi, Prog. Theor. Phys. Suppl. E68, 464 (1968).
- Systematic Structure-Change into the **Molecule-like Structures** in the Self-Conjugate 4N Nuclei
- Numbers are threshold energies of cluster emissions
- **Threshold Rule :** It is suggested that cluster states can appear near the threshold energies due to weak binding in relative motions.

Motivation

- In Ikeda-diagram, Prof. Ikeda discussed **Threshold Rule** for α cluster states
- How about the unstable nuclei with excess protons/neutrons?
- Threshold energies of nucleon/cluster emissions.
- ^{10}Be : ^{9}Be+n (6.8 MeV), ^{6}He+α (7.4 MeV), 2α+2n (8.5 MeV)
- ^{9}Li : ^{8}Li+n (4.1 MeV), ^{7}Li+2n (6.1 MeV), ^{6}He+t (7.6 MeV), α+t+2n (8.6 MeV)
- The present work is worthy to examine the threshold rule for unstable nuclei.



α+6He



Single AMD Basis

Kanada-En’yo, Kimura, Horiuchi, Compt. Rendus Phys. **4**, 497 (2003)

Variation (Cooling) in AMD : Single basis

- $\Phi_{\rm AMD} = \det\{\prod_{i=1}^{A} \phi_{\tau_i}(\boldsymbol{r}_i, \boldsymbol{Z}_i, \alpha_i)\}$ i: particle index
- $\boldsymbol{Z}_i$: Centroid vector, α_i: spin (up/down) , τ_i: isospin
- $\phi_\tau(\boldsymbol{r}, \boldsymbol{Z}, \alpha) = \left(\frac{2\pi}{\nu}\right)^{3/4} e^{-\nu(\boldsymbol{r}-\boldsymbol{Z})^2} \chi_{\sigma\alpha}\chi_\tau$, $\chi_{\sigma\alpha} = \alpha_+|\uparrow\rangle + \alpha_-|\downarrow\rangle$, χ_τ : p, n
- $E = \frac{\langle\Phi|H|\Phi\rangle}{\langle\Phi|\Phi\rangle} = E[\boldsymbol{Z}, \alpha]$
- $\hbar \frac{d\boldsymbol{Z}_i}{d\tau} = -\frac{\partial E}{\partial \boldsymbol{Z}_i^*}$, $\hbar \frac{d\boldsymbol{Z}_i^*}{d\tau} = -\frac{\partial E}{\partial \boldsymbol{Z}_i}$, τ: imaginary time
- $\frac{dE}{d\tau} = \sum_{i=1}^{A}\left(\frac{\partial E}{\partial \boldsymbol{Z}_i}\frac{d\boldsymbol{Z}_i}{d\tau} + \frac{\partial E}{\partial \boldsymbol{Z}_i^*}\frac{d\boldsymbol{Z}_i^*}{d\tau}\right) = -2\hbar\sum_{i=1}^{A}\frac{d\boldsymbol{Z}_i}{d\tau}\frac{d\boldsymbol{Z}_i^*}{d\tau} < 0$: energy minimization

Similar to Gradient Descent Method

Cooling equation

Multiple AMD Bases

- T. Myo et al. , ^{10}Be Phys. Rev. C 108 (2023) 064314

  Li isotopes PTEP 2025 (2025) 013D01

- $^{9-11}_{\Lambda}$Be, $^{12}_{\Lambda}$B by M. Lyu et al.

  Phys. Lett. B855 (2024) 138816 , Phys. Lett. B862 (2025) 139338

Multi bases cooling : Multiple Cooling (Multicool)

- $\Phi = C_1\Phi_1 + C_2\Phi_2 + \cdots C_N\Phi_N,\quad N_{mn} := \langle\Phi_m|\Phi_n\rangle \neq 0$: non-orthogonal norm
- $E = \dfrac{\langle\Phi|H|\Phi\rangle}{\langle\Phi|\Phi\rangle} = \dfrac{\sum_{m,n} C_m^* C_n H_{mn}}{\sum_{m,n} C_m^* C_n N_{mn}} = E[\boldsymbol{X}_1, \boldsymbol{X}_2, \cdots, \boldsymbol{X}_N]$
- $X_{n,i} = \{C_n, \boldsymbol{Z}_{n,i}, \alpha_{n,i}\},\quad n$: basis index, i: particle index
- $\hbar \dfrac{dX_{n,i}}{d\tau} = -\dfrac{\partial E}{\partial X_{n,i}^*},\quad \hbar \dfrac{dX_{n,i}^*}{d\tau} = -\dfrac{\partial E}{\partial X_{n,i}},$ satisfying $\dfrac{dE}{d\tau} < 0$
- Same technique is used to determine the correlation function F in TOAMD
  - $F = \sum_{i<j}^{A} f(r_{ij})$: make 2p-2h excitations
  - $\{a_n\}$ in $f(r) = \sum_n C_n e^{-a_n r^2}$ with Gaussian expansion

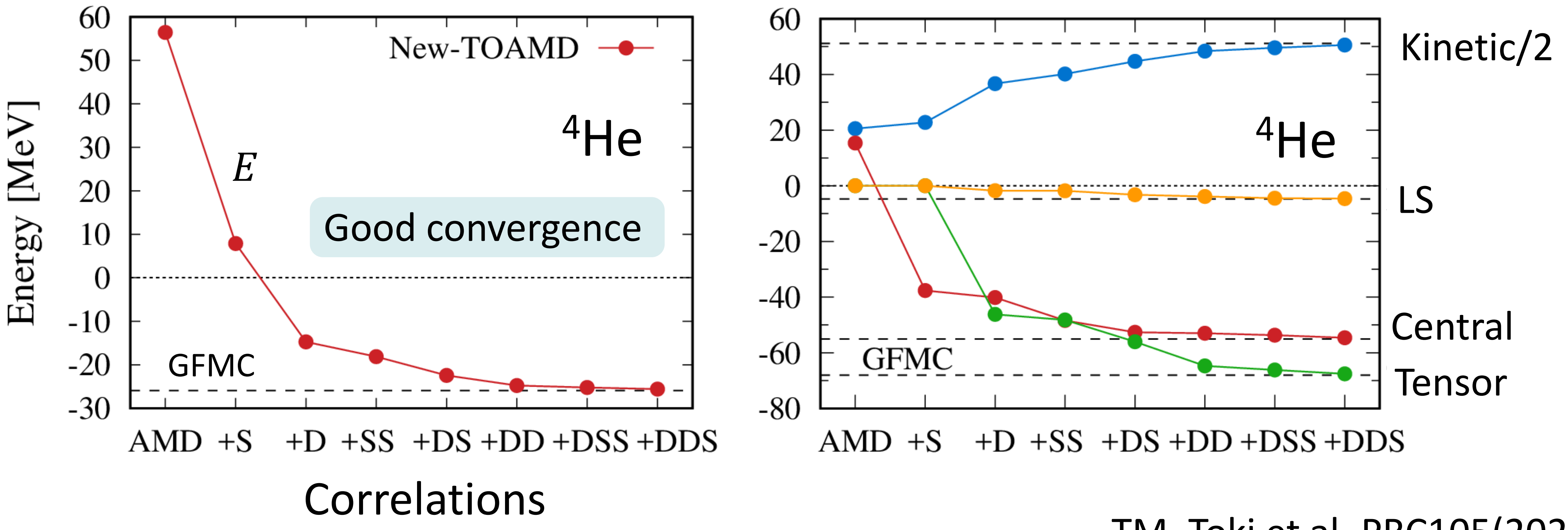
TM et al., PLB769 (2017)

AMD with bare nuclear force using Triple F

$F = \sum_{i<j}^{A} f_{ij}$

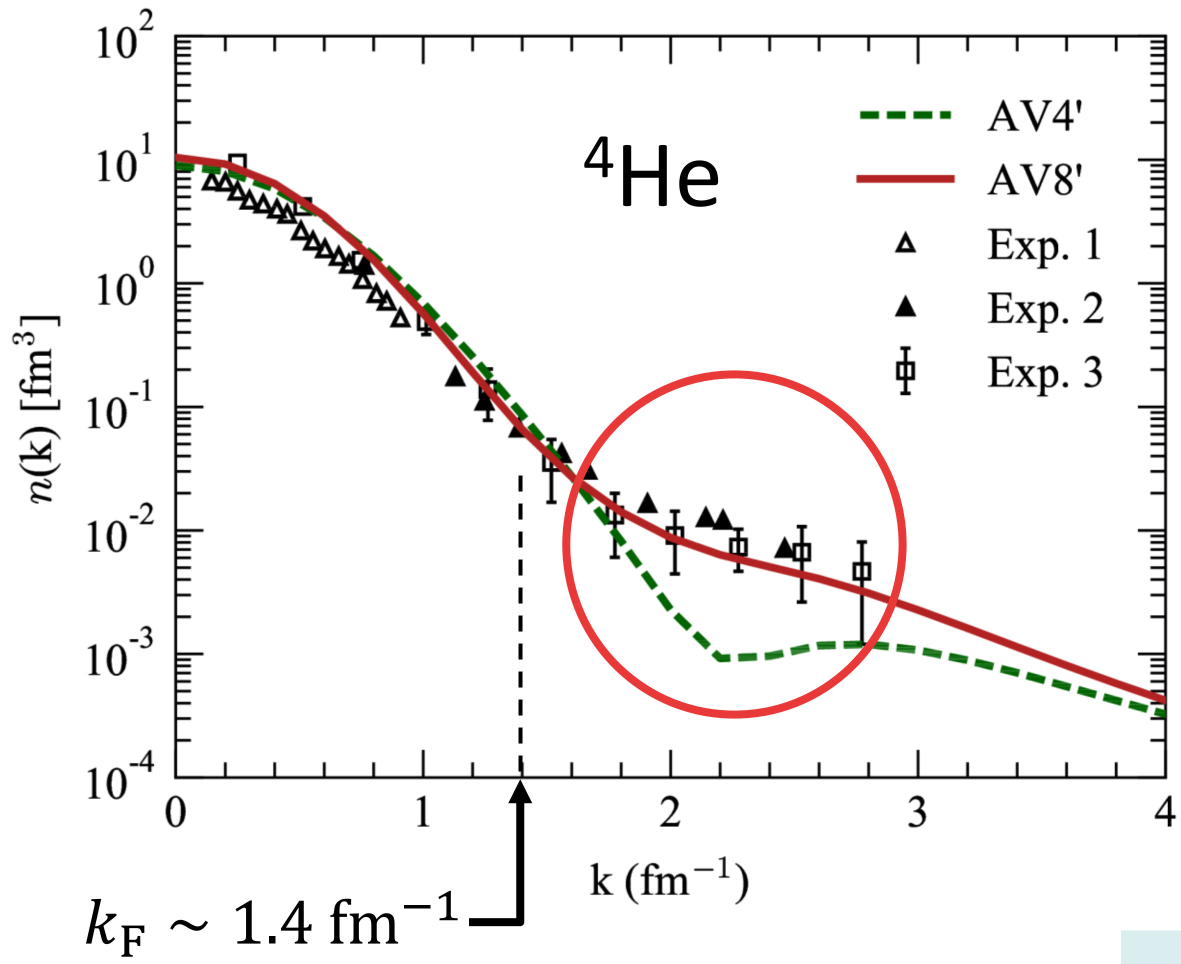
2p-2h

- $(1 + F_S + F_D + F_S F_S + F_D F_S + F_D F_D + F_D F_S F_S + F_D F_D F_S)|\Phi_{\mathrm{AMD}}\rangle$
- AV8' realistic potential, F_S: Short-range correlation, F_D: Tensor correlation with D-wave ($\Delta L=2$)



TM, Toki et al.,PRC105(2022)

Lyu's work : Nucleon Momentum Distribution



- ^{4}He in TOAMD
- **AV4'** Central V_{NN} with SR-repulsion (NO tensor)
- **AV8'** Realistic V_{NN}
- Manifestation of tensor correlation around k=2 fm^{-1}

Lyu, Myo, Toki et al. PLB 805 (2020) 135421

Calculation procedure

1. Set initial values: $X_n^{\mathrm{init}} = \{C_n^{\mathrm{init}}, \boldsymbol{Z}_{n,i}^{\mathrm{init}}, \alpha_{n,i}^{\mathrm{init}}\}$ and obtain E_{init}
2. Calculate energy-derivatives $\frac{\partial E}{\partial X_{n,i}^*} = \{\frac{\partial E}{\partial C_n^*}, \frac{\partial E}{\partial \boldsymbol{Z}_{n,i}^*}, \frac{\partial E}{\partial \alpha_{n,i}^*}\}$ to change $\{X_{n,i}\}$
3. Calculate Matrix elements H_{mn}, N_{mn} and obtain $E = \langle H \rangle$
4. Repeat 2.-3. until getting the converging results.
5. Projection to total spin J with parity for matrix elements $H_{mn}^{J\pi}$, $N_{mn}^{J\pi}$
6. $\delta E^{J\pi} = 0 \rightarrow$ Solve eigenvalue problem: $\sum_n^N (H_{mn}^{J\pi} - E^{J\pi} N_{mn}^{J\pi}) C_n^{J\pi} = 0$

For ground state

7. Extension : Impose orthogonal condition to generate the excited states

Generate the excited-state configurations

- Use projection operator method, often utilized in nuclear cluster model
- Ground state : Configurations $\{\Phi_n\}$ obtained in multiple cooling
- $\tilde{\Phi}_n \coloneqq \hat{O}\Phi_n, \quad \hat{O} \coloneqq \{1,\ R_{xyz\to zxy},\ R_{xyz\to yzx}\}$: add two rotations
- $H_\lambda = H + V_\lambda, \quad V_\lambda = \lambda \sum_n^{3N} |\tilde{\Phi}_n\rangle\langle\tilde{\Phi}_n|$, Strength λ [MeV] (Repulsive)
- Multicool calculation using H_λ from small to large values of λ
- For large λ, excited state $\Phi_{\rm ex} = \sum_n^N C_{{\rm ex},n}\Phi_{{\rm ex},n}$ with $\langle \Phi_{\rm ex} | \tilde{\Phi}_n \rangle = 0$
- Superpose Φ_n and $\Phi_{{\rm ex},n}$ with various λ (500-600 bases)

Results

- ^{10}Be Phys. Rev. C 108 (2023) 064314
- Li isotopes   PTEP 2025 (2025) 013D01

Inputs in the multicool calculation

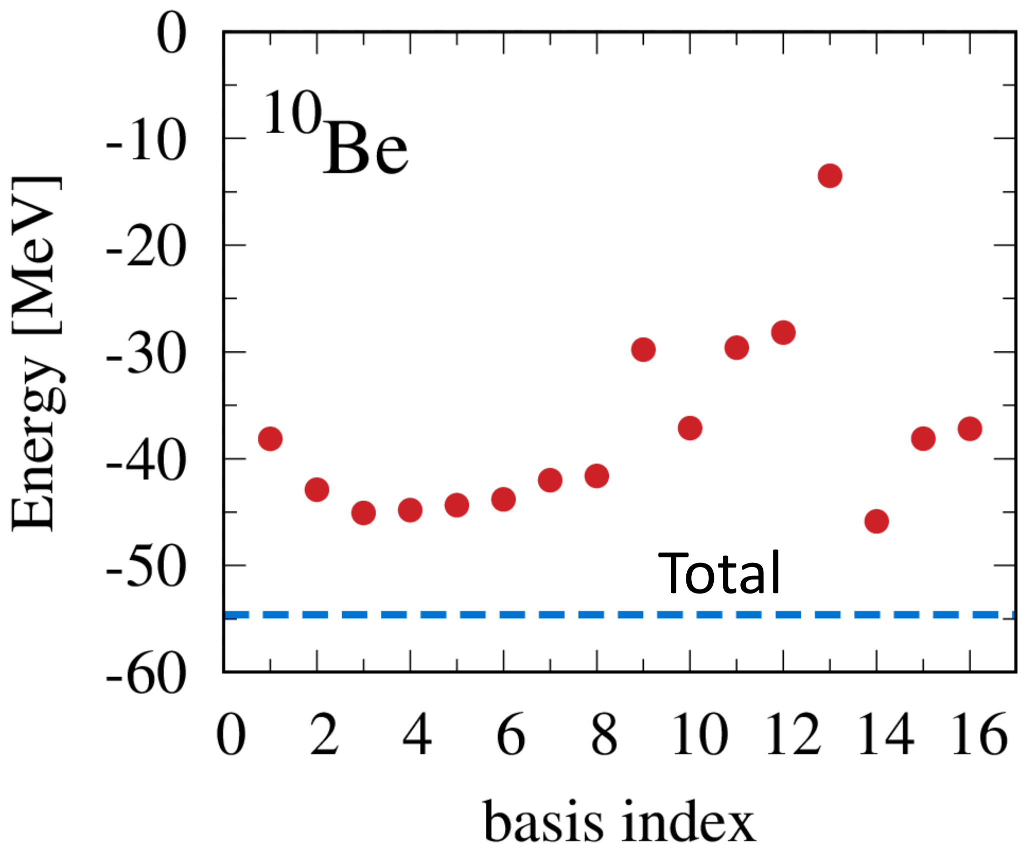
- In AMD, Gaussian $\nu = 0.235\ \mathrm{fm}^{-2}$
- Effective two-body force
  - Central : Volkov No.2 with (W,M,B,H)=(0,4, 0.6, 0.125, 0.125)
  - LS : G3RS with a strength of 1600 MeV (Reproduce LS splitting in ^{5}He)
- Reproduce the binding energy of deuteron (2.2 MeV)
- Variation of intrinsic WF after parity projection
- Basis number is typically 10-20 in multiple cooling

N. Itagaki and S. Okabe, Phys. Rev. C 61, 044306 (2000)
T. Suhara and Y. Kanada-En'yo, Prog. Theor. Phys. 123, 303 (2010)

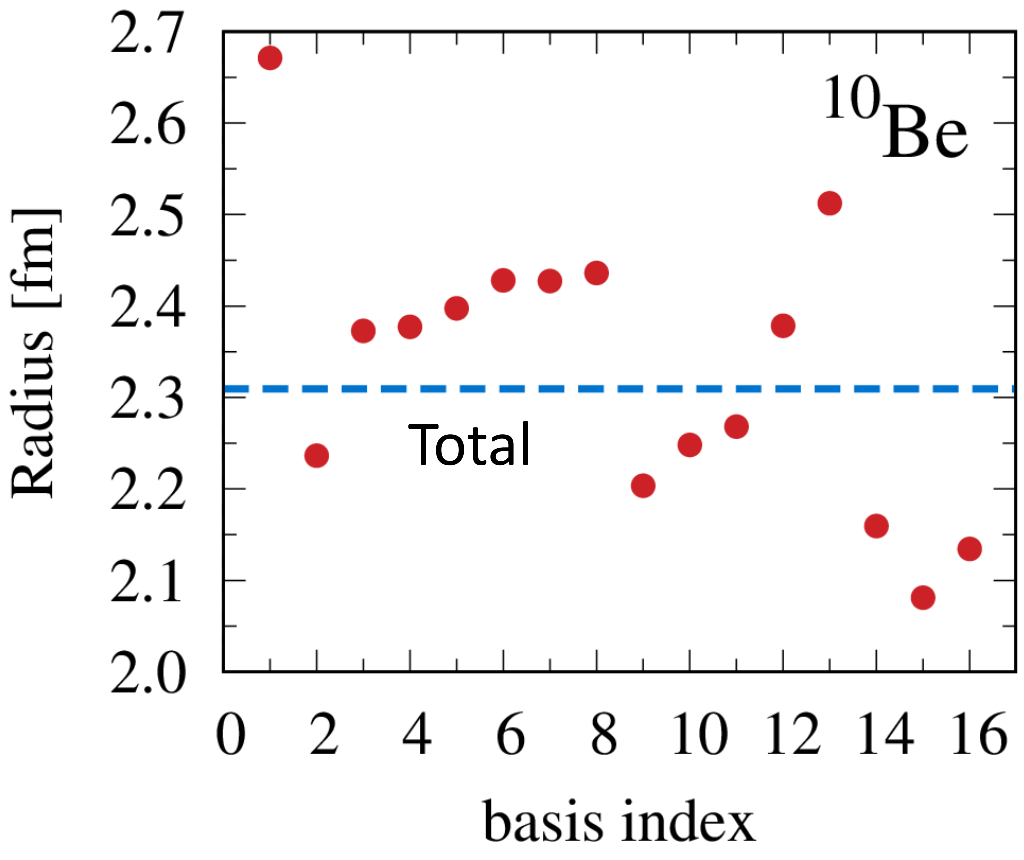
^{10}Be: Ground state with 16 bases

$\Phi_{\text{total}} = \sum_n^N C_n \Phi_n$

Intrinsic energies (MeV)

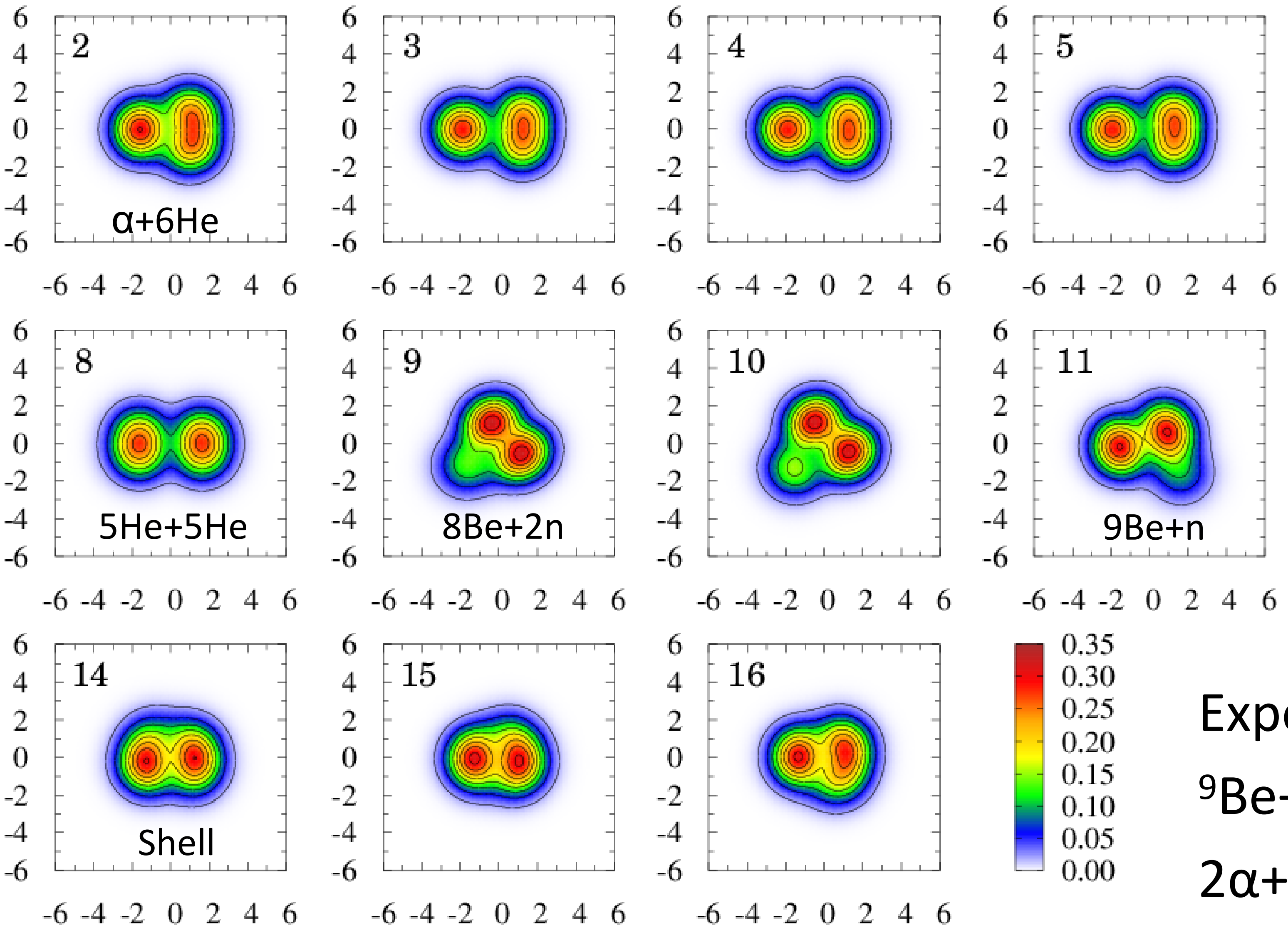


Radius (fm)



$\Delta E_{\text{GCM}} = 10$ MeV (-45 → -55)

^{10}Be density



Main configurations for ground state

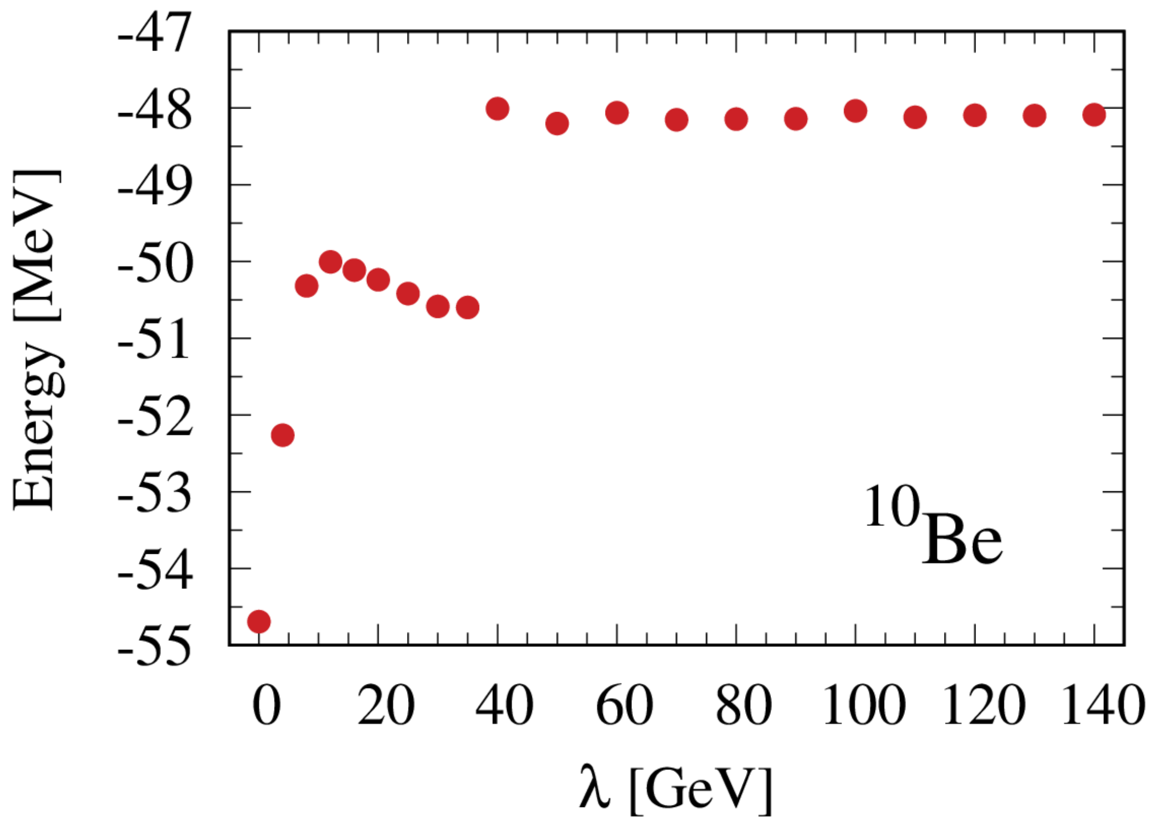
α+^{6}He, ^{5}He+^{5}He
^{8}Be+2n, ^{9}Be+n
Shell

Experimental threshold energies:
^{9}Be+n (6.8 MeV), ^{6}He+α (7.4 MeV)
2α+2n (8.5 MeV)

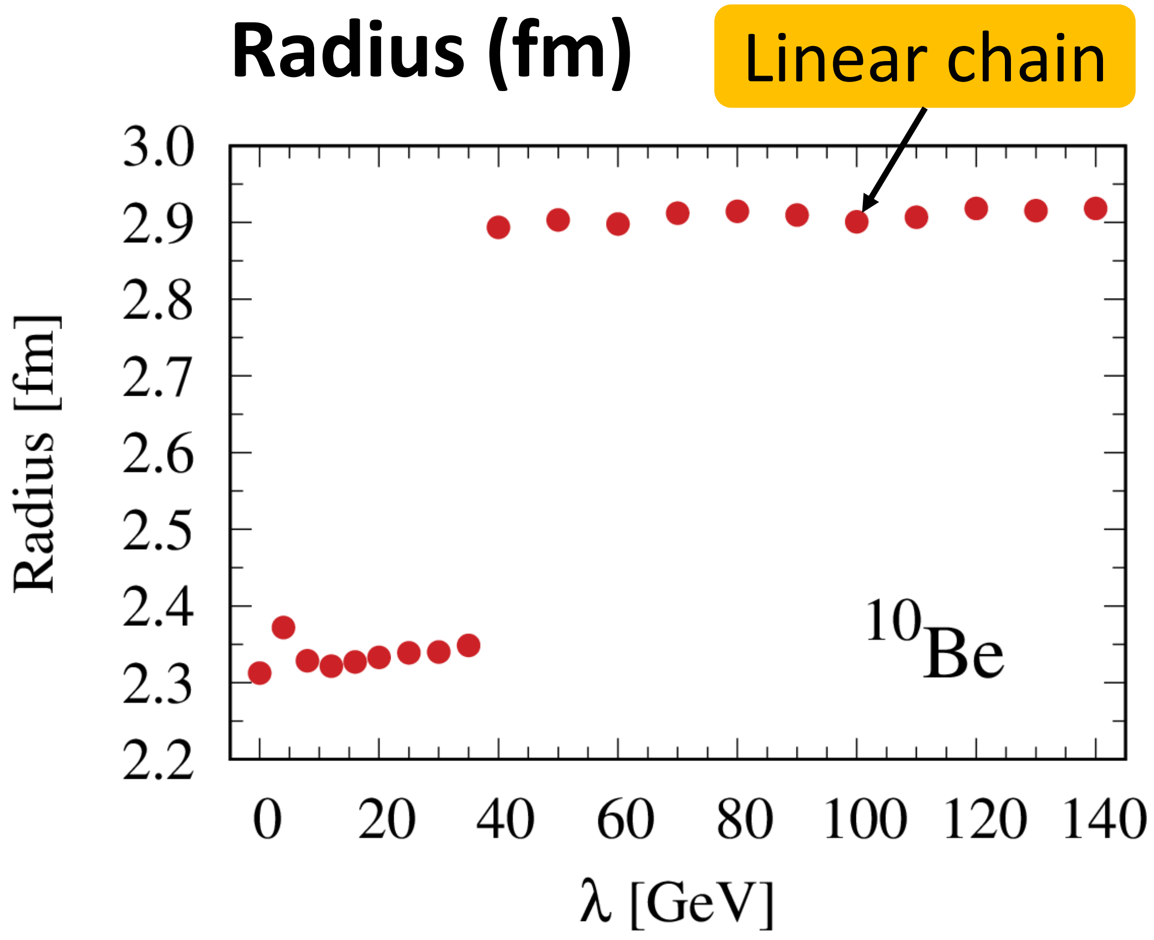
^{10}Be: excited state

$$\Phi_{\text{ex}} = \sum_n^N C_{\text{ex},n} \Phi_{\text{ex},n}$$

Intrinsic energy (MeV)

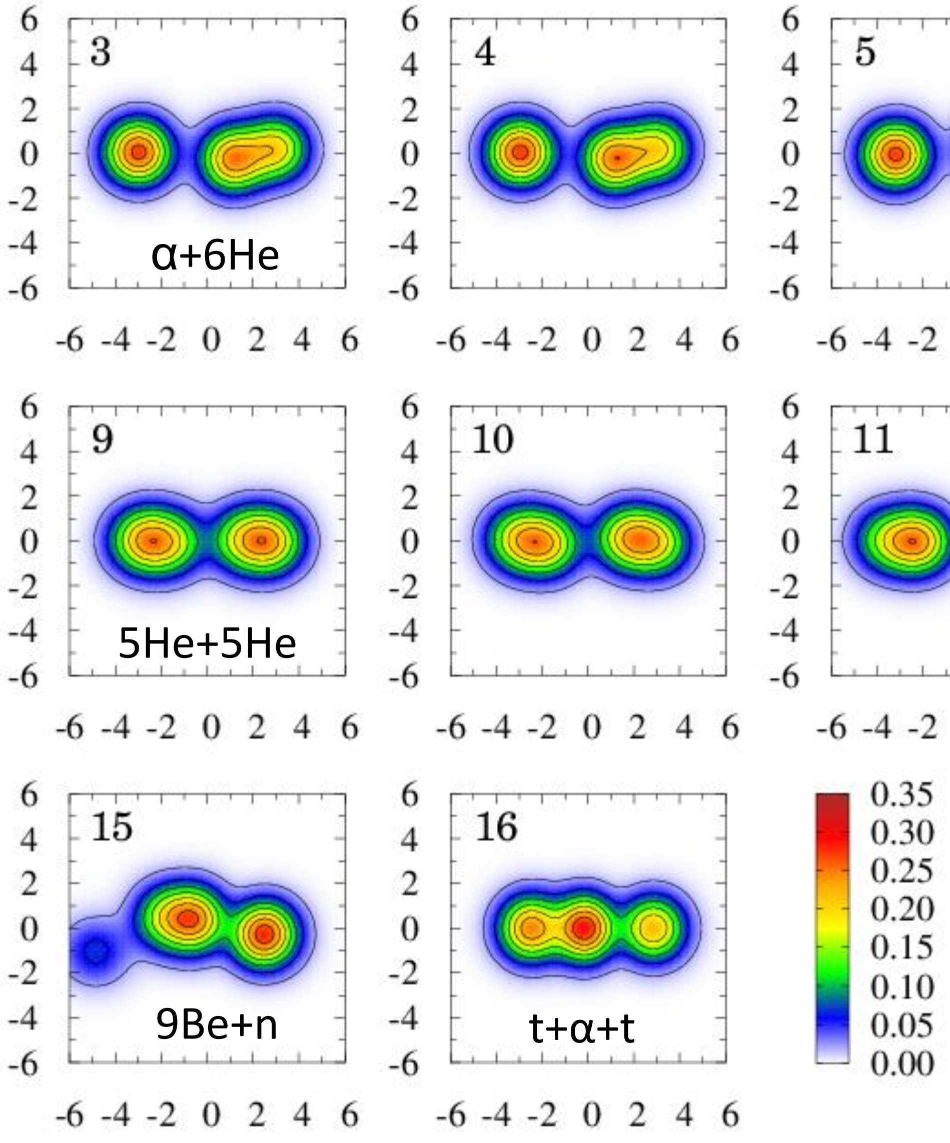


Radius (fm)



$$H_\lambda = H + V_\lambda, \quad V_\lambda = \lambda \sum_n^{3N} |\tilde{\Phi}_n\rangle\langle\tilde{\Phi}_n|$$

^{10}Be: excited state density with λ=100 GeV

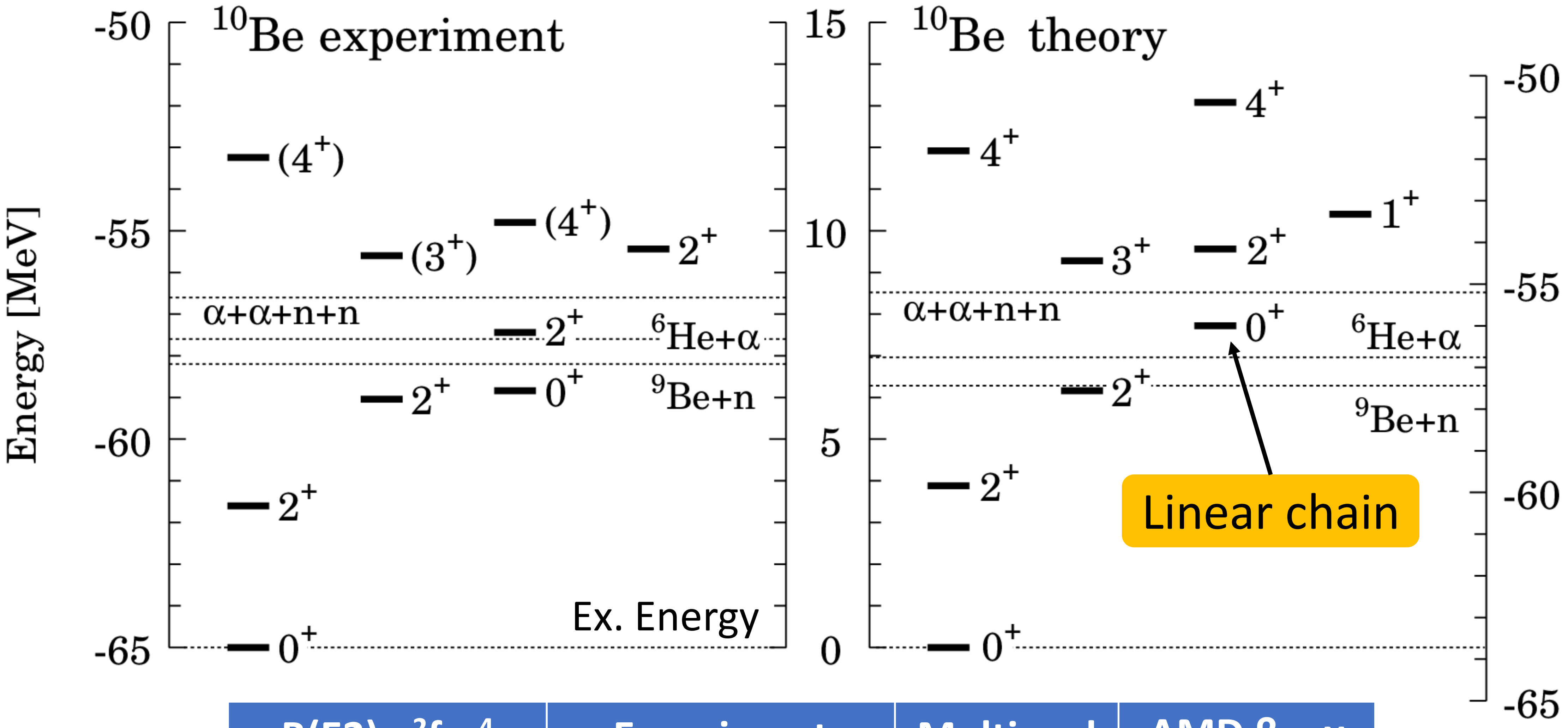


Linear chain

α+^{6}He, ^{5}He+^{5}He
^{8}Be+2n, ^{9}Be+n
t+α+t

^{10}Be : energy levels

Phys. Rev. C 108 (2023) 064314



B(E2) e^2fm^4	Experiment	Multicool	AMD $\beta-\gamma$
2^+ 1st → 0^+ 1st	10.5(1.0) / 9.2(3)	7.9	9.4

^{10}Be: Comparison with other cluster models

Excitation Energy in MeV (total energy)

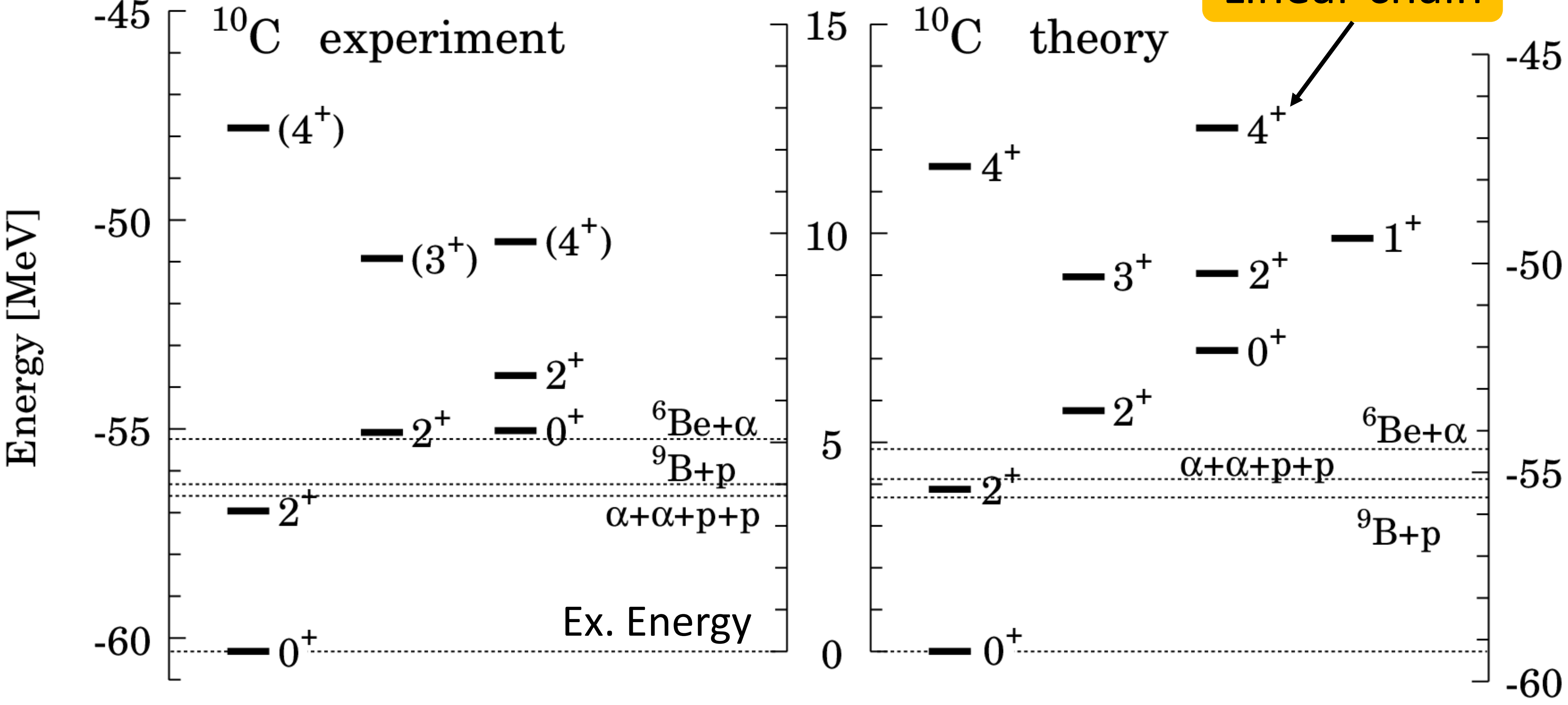
	Multicool	MO[23]	β-γ[24]	DC[25]	β-γK[26]
0_1^+	0 (−63.7)	0 (−61.4)	0 (−59.2)	0 (−60.4)	0 (−63)
0_2^+	7.7 (−56.0)	8.1 (−53.3)	8.0 (−51.2)	9.5 (−50.9)	12 (−51)
1^+	10.4	10.1	–	–	–
2_1^+	3.9	3.3	3.3	–	–
2_2^+	6.2	5.7	5.8	–	–
2_3^+	9.6	9.5	9.9	–	–

Radius in fm (matter, p, n, charge)

		Expt.	Multicool
0_1^+	r_m	2.30(2)	2.33
	r_p	–	2.21
	r_n	–	2.40
	r_ch	2.357(18)	2.36
0_2^+	r_m	–	2.88
	r_p	–	2.70
	r_n	–	2.99
	r_ch	–	2.82

Multicool gives the lowest energies among the calculations

^{10}C



Linear chain

Mirror of ^{10}Be

B(E2) e^2fm^4	Experiment	Multicool	Shell model
2+ 1st → 0+ 1st	8.8(3)	8.82	9.30

Li isotopes

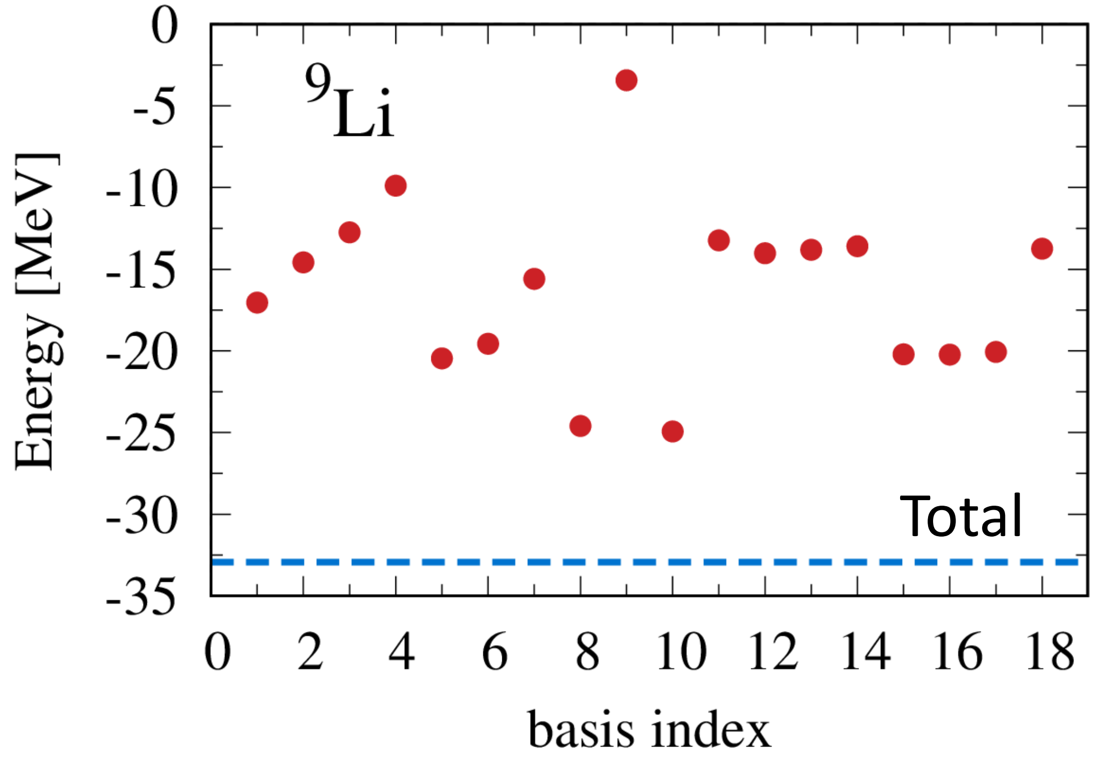
^{4}He, ^{5}Li-^{9}Li PTEP 2025 (2025) 013D01

^{9}Li : Ground state (isotone of ^{10}Be)

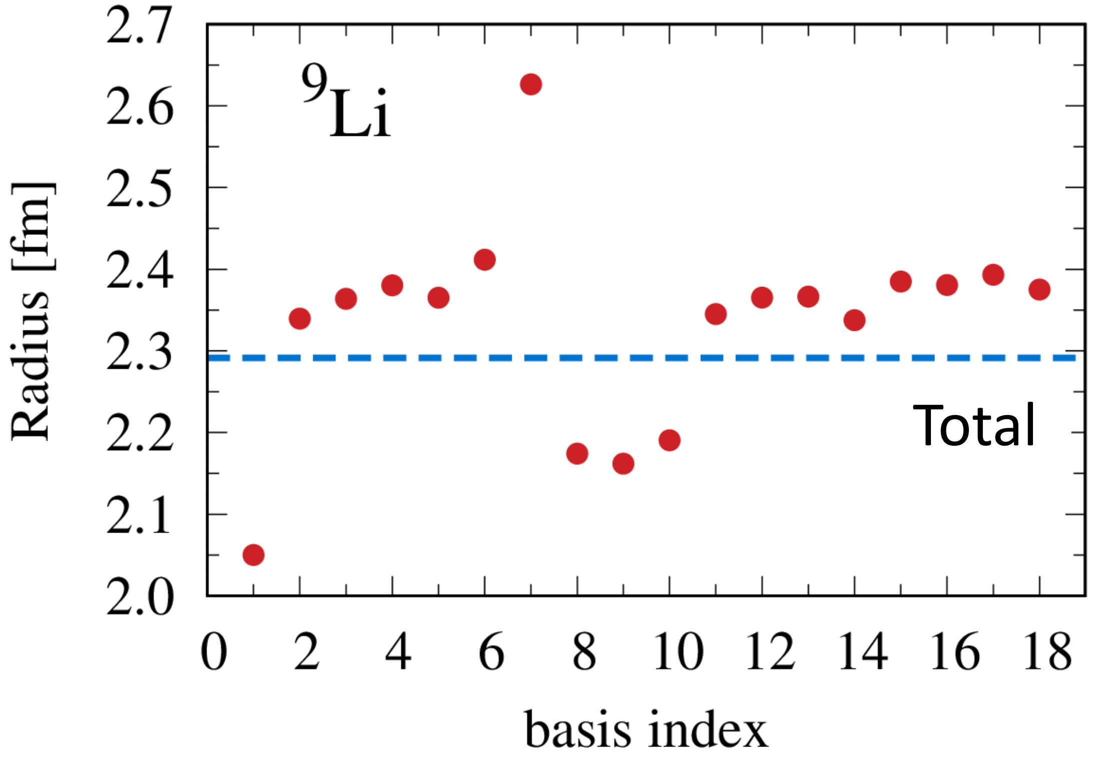
$$\Phi_{\text{total}} = \sum_n^N C_n \Phi_n$$

18 bases

Intrinsic energies (MeV)



Radius (fm)

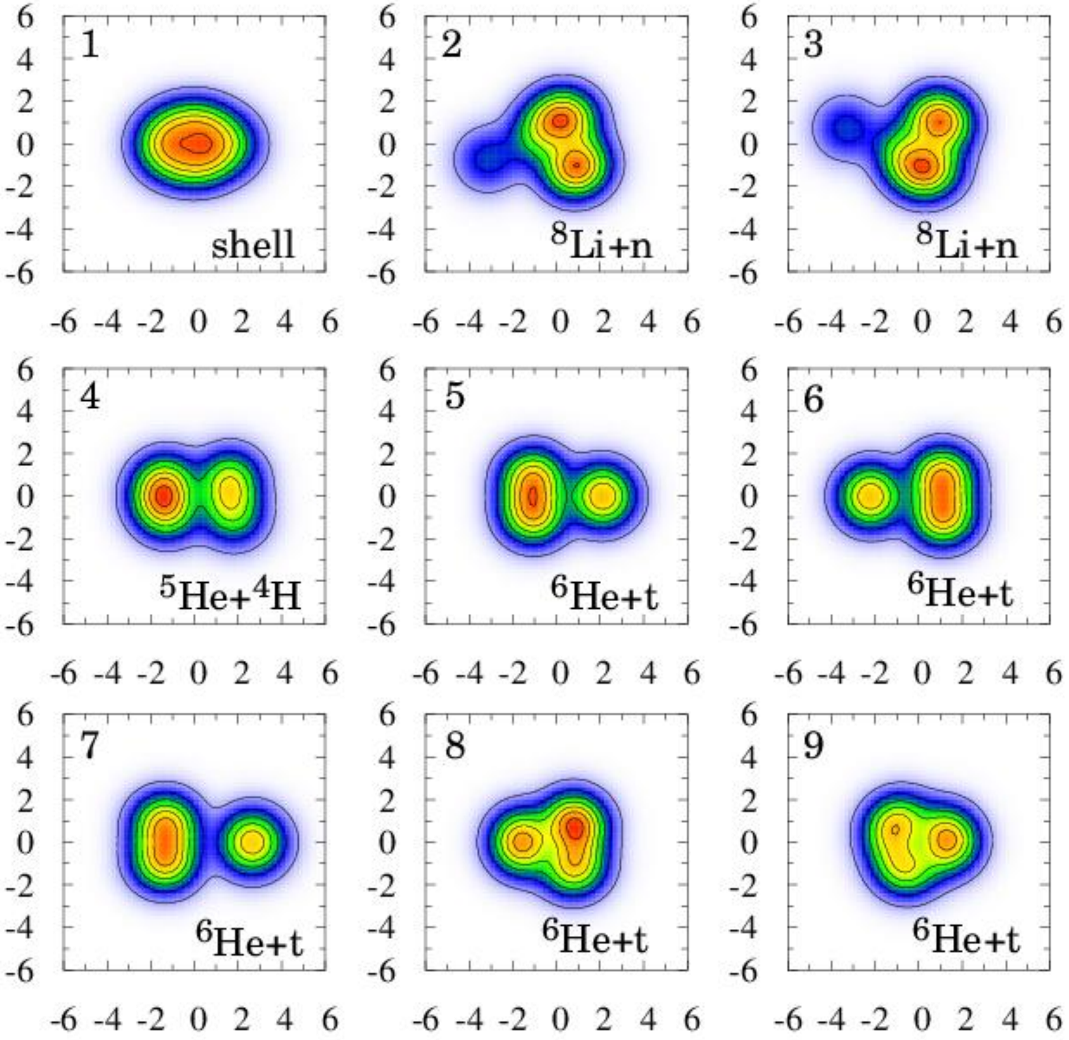


$\Delta E_{\text{GCM}} = 8$ MeV (-25 to -33)

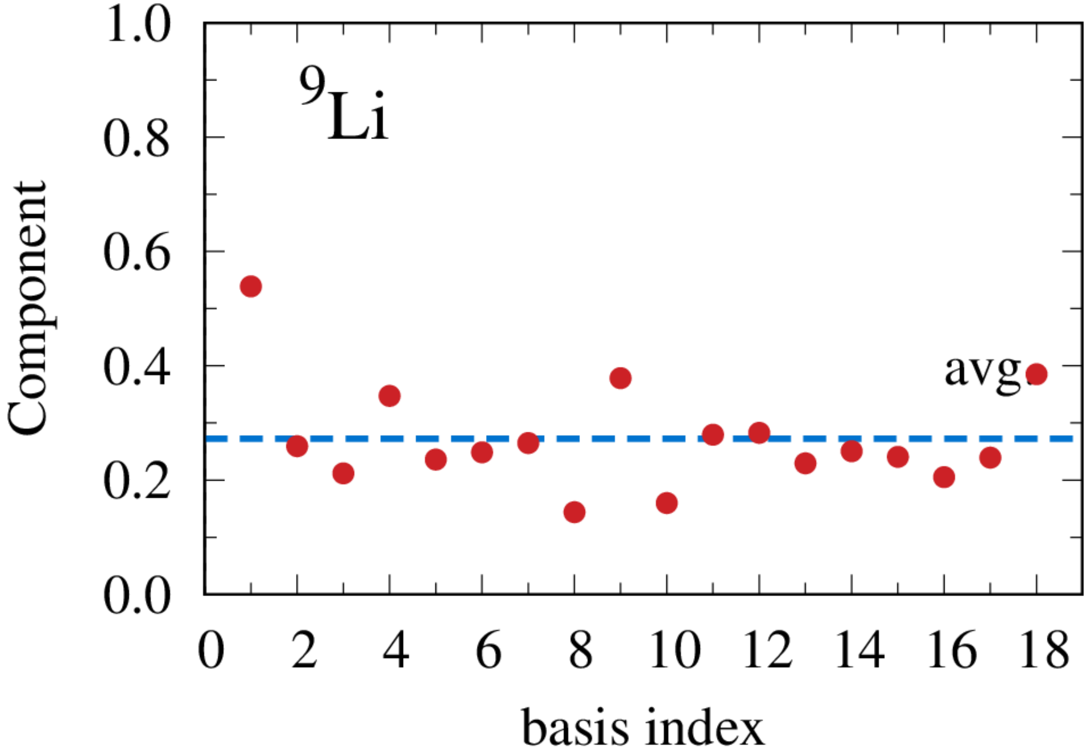
^{9}Li : Ground state

$$\Phi_{\mathrm{total}} = \sum_n^N C_n \Phi_n$$

Density distributions



Components: $\langle \Phi_n | \Phi \rangle^2$



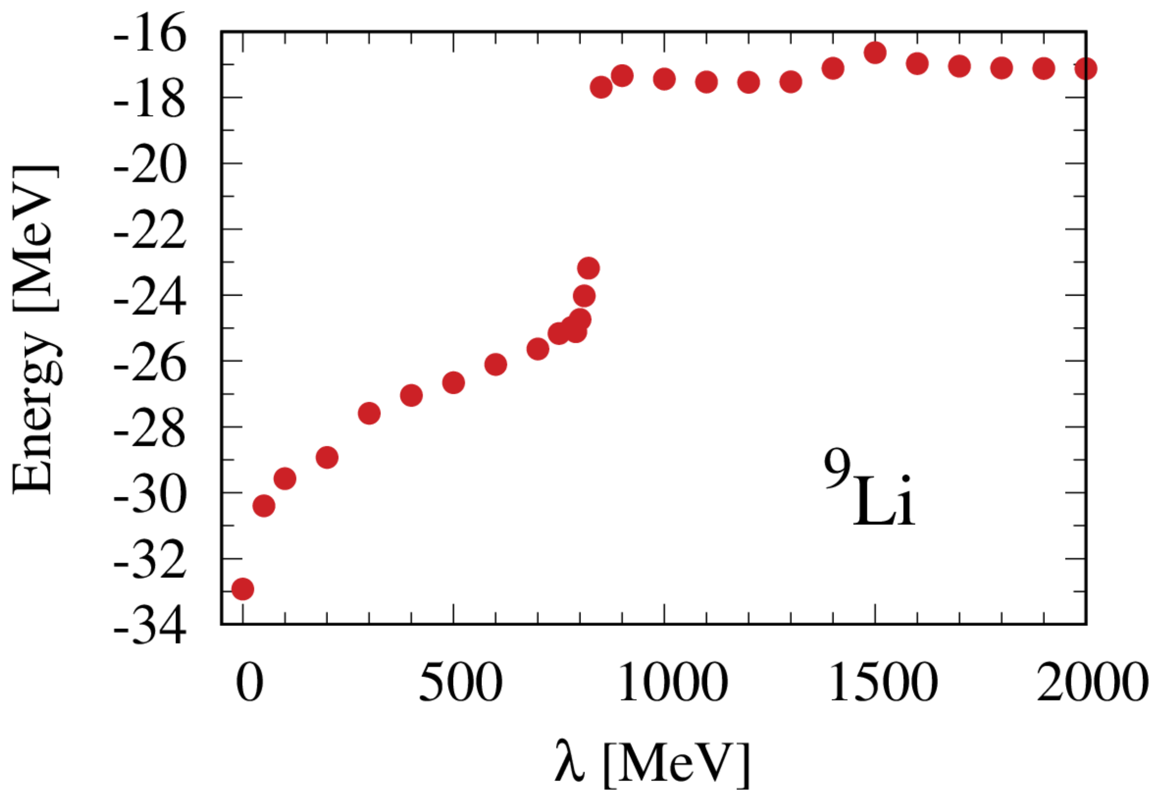
Experimental threshold energies:

^{8}Li+n (4.1 MeV), ^{6}He+t (7.6 MeV)

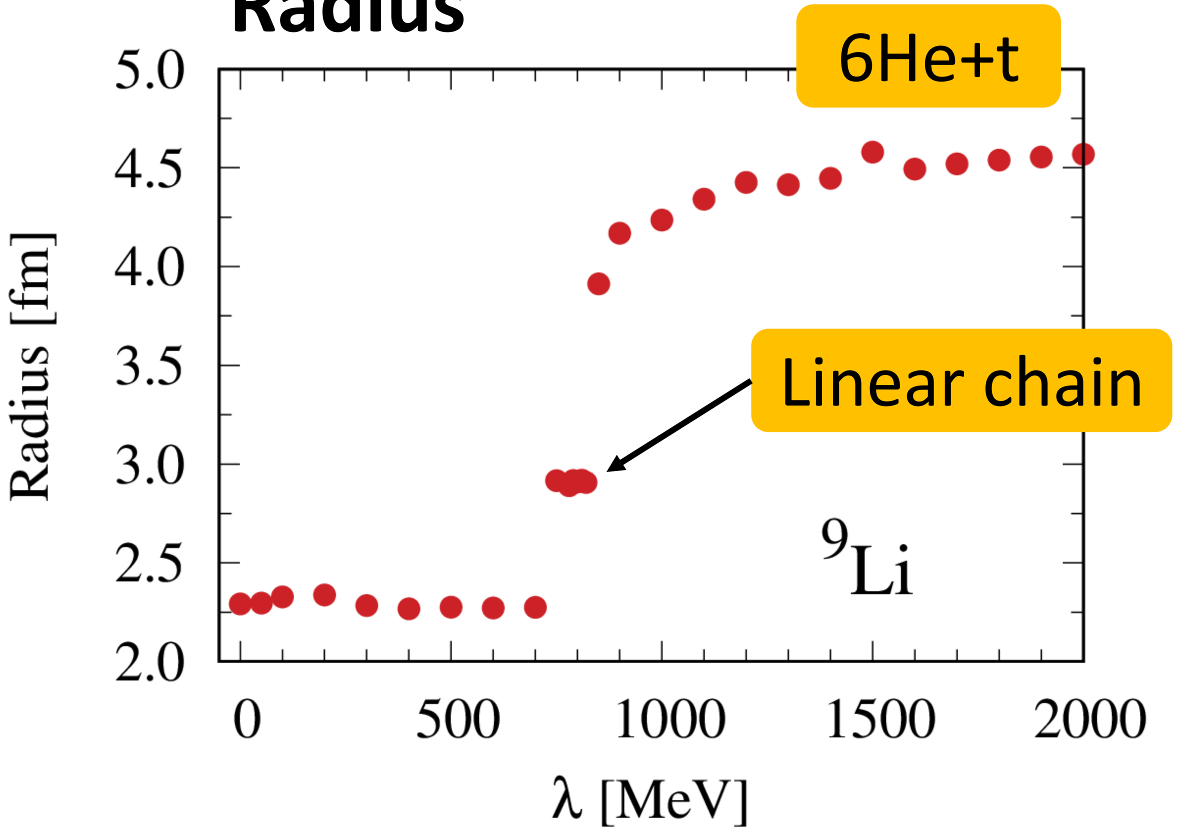
^{9}Li : excited states

$$\Phi_{\mathrm{ex}} = \sum_n^N C_{\mathrm{ex},n} \Phi_{\mathrm{ex},n}$$

Intrinsic energy



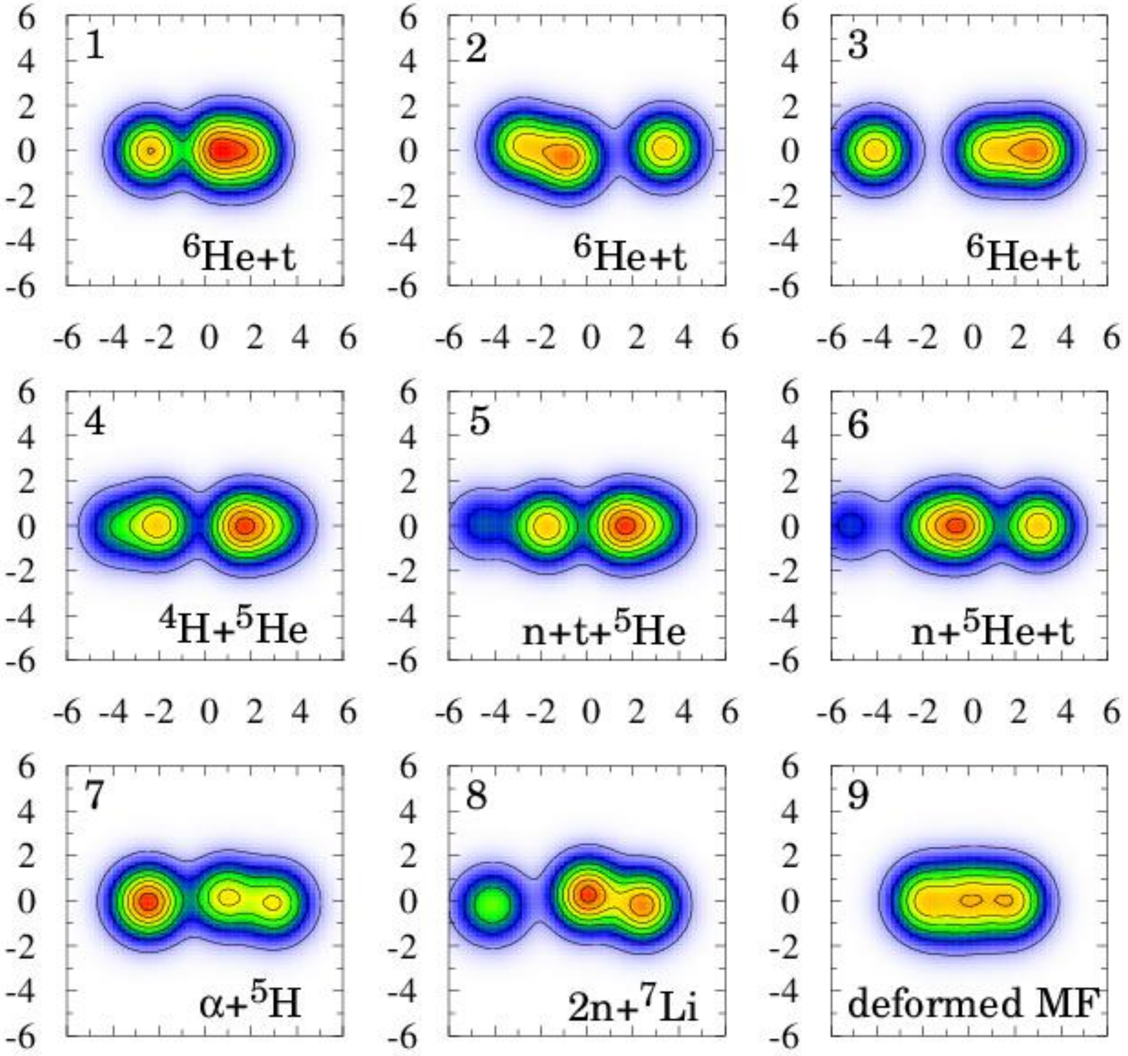
Radius



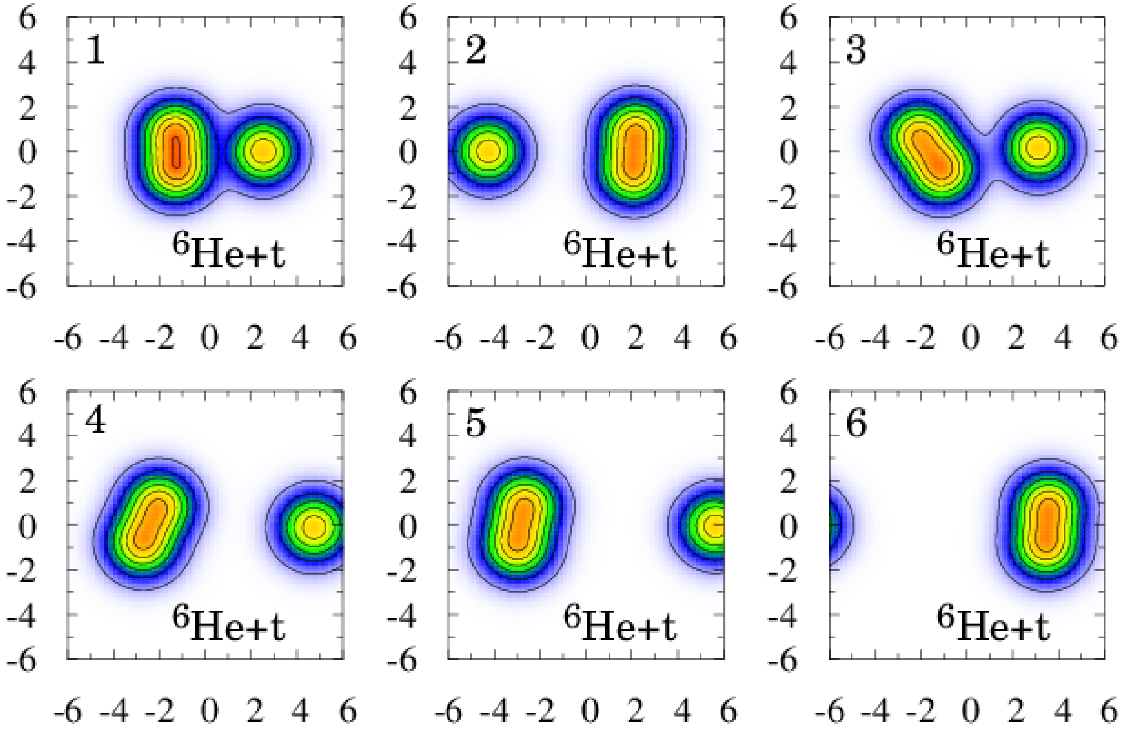
$$H_\lambda = H + V_\lambda, \quad V_\lambda = \lambda \sum_n^{3N} |\tilde{\Phi}_n\rangle\langle\tilde{\Phi}_n|$$

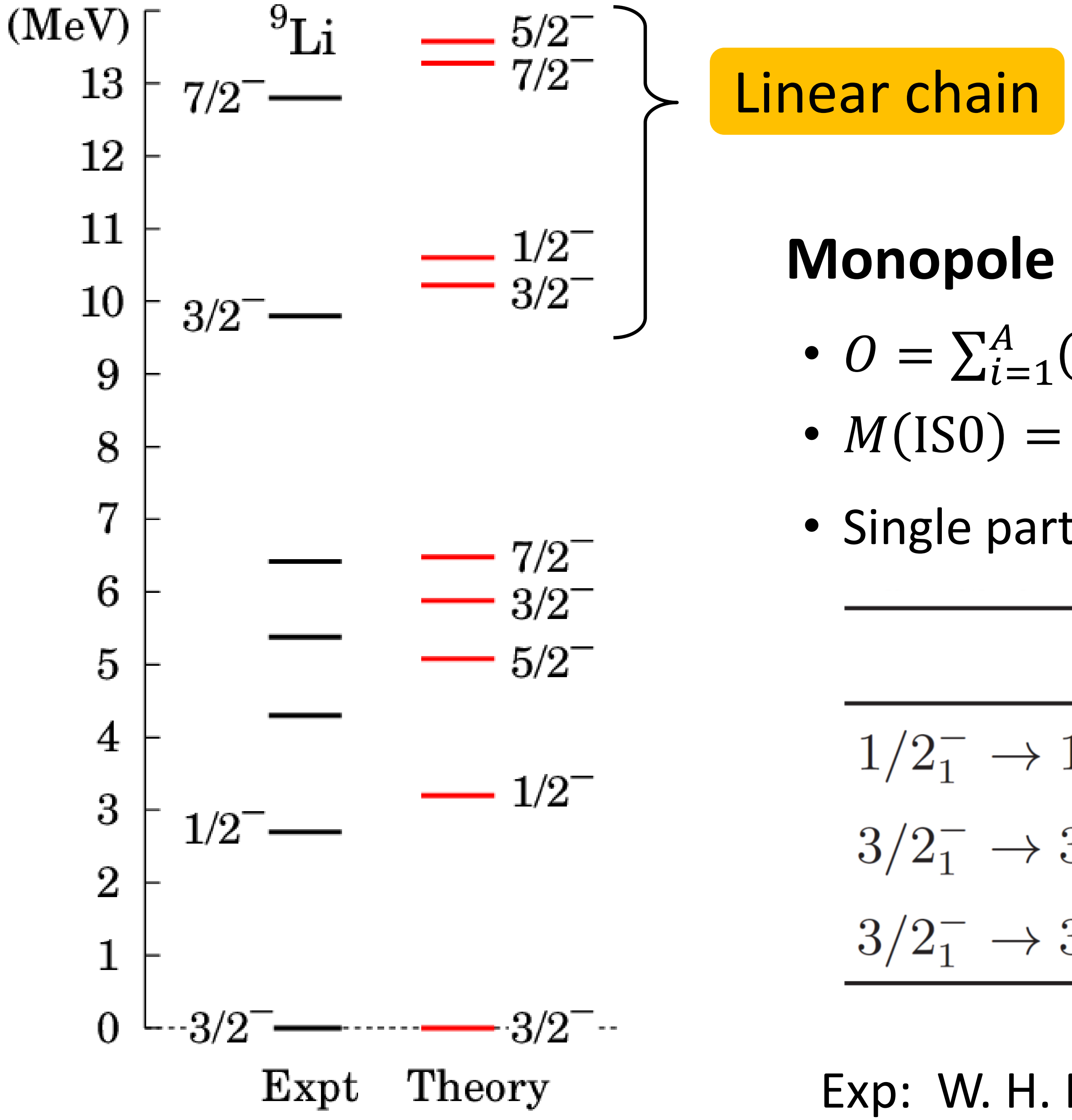
^{9}Li excited state density

λ=800 MeV, Linear-chain



λ=1600 MeV, ^{6}He+t





^{9}Li : Energy levels

Monopole strength (fm^2)

- $O = \sum_{i=1}^{A} (\boldsymbol{r}_i - \boldsymbol{r}_G)^2$: isoscalar (IS0)
- $M(\mathrm{IS0}) = \langle \Phi_F | O | \Phi_I \rangle = M(E0) + M(\mathrm{neutron})$
- Single particle $\langle 1p | r^2 | 0p \rangle = \sqrt{5/(8\nu^2)} = 3.4\ \mathrm{fm}^2$

	IS0	$E0$	Neutron
$1/2_1^- \to 1/2_2^-$	4.27	1.11	3.17
$3/2_1^- \to 3/2_2^-$	0.42	0.07	0.35
$3/2_1^- \to 3/2_3^-$	3.57 [8.1(8)]	0.98	2.58

Exp: W. H. Ma *et al.*, Phys. Rev. C **103**, L061302 (2021)

Energy & Radius of GS

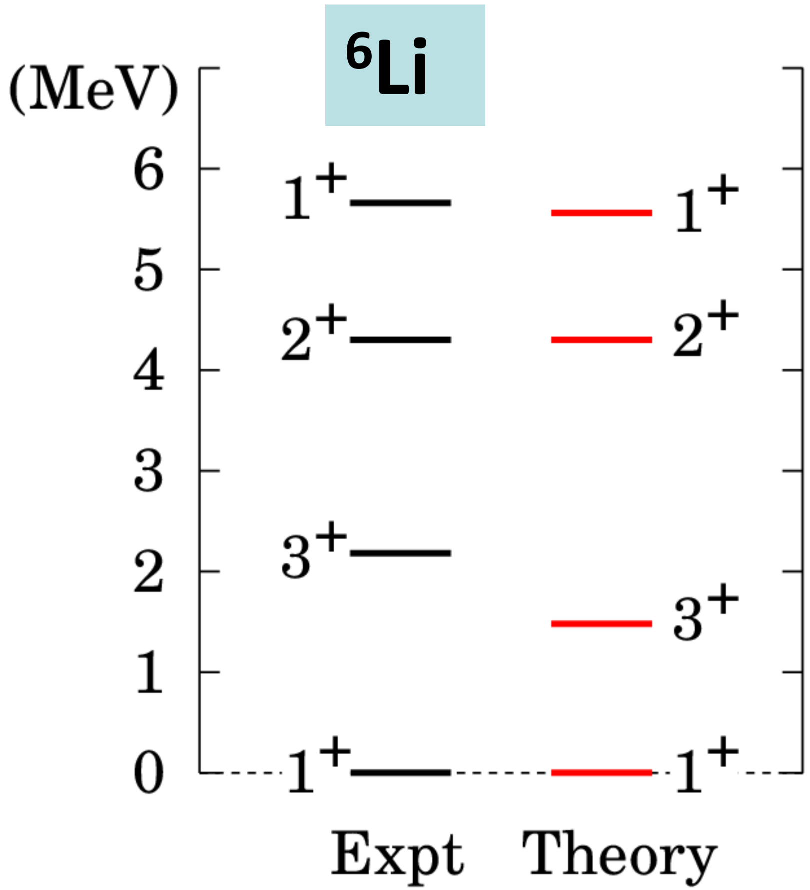
	Energy	r_m	r_p	r_n	r_{ch}
$^6He(0^+)$	−29.2 [−29.3]	2.38	1.88	2.59	2.04 [2.068(11)]
$^9Be(3/2^-)$	−57.5 [−58.2]	2.44	2.37	2.50	2.51 [2.519(12)]

Li isotopes

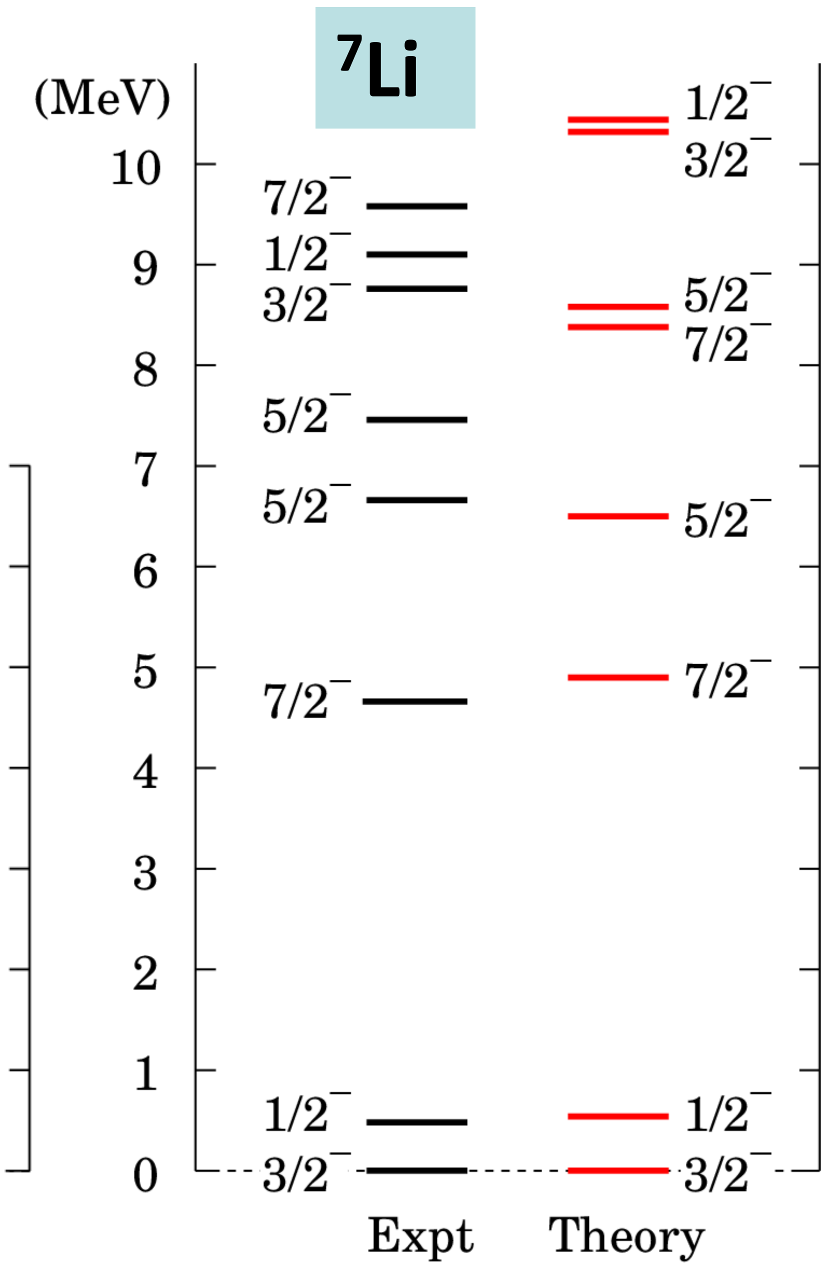
	Energy	r_m	r_p	r_n	r_{ch}
$^5Li\ (3/2^-)$	−26.87 [−26.61]	–	–	–	–
$^5Li\ (1/2^-)$	−25.34 [−25.12]	–	–	–	–
$^6Li\ (1^+)$	−31.41 [−32.00]	2.31	2.31	2.30	2.46 [2.59(4)]
$^7Li\ (3/2^-)$	−38.99 [−39.25]	2.39	2.30	2.46	2.44 [2.44(4)]
$^8Li\ (2^+)$	−38.07 [−41.28]	2.33	2.16	2.42	2.30 [2.34(5)]
$^9Li\ (3/2^-)$	−41.55 [−45.34]	2.29	2.06	2.40	2.20 [2.25(5)]

experiment experiment

Li isotopes



6Li
(MeV)
6
5
4
3
2
1
0
1+
2+
3+
1+
1+
2+
3+
1+
Expt
Theory



7Li
(MeV)
10
9
8
7
6
5
4
3
2
1
0
7/2−
1/2−
3/2−
5/2−
5/2−
7/2−
1/2−
3/2−
1/2−
3/2−
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7/2−
5/2−
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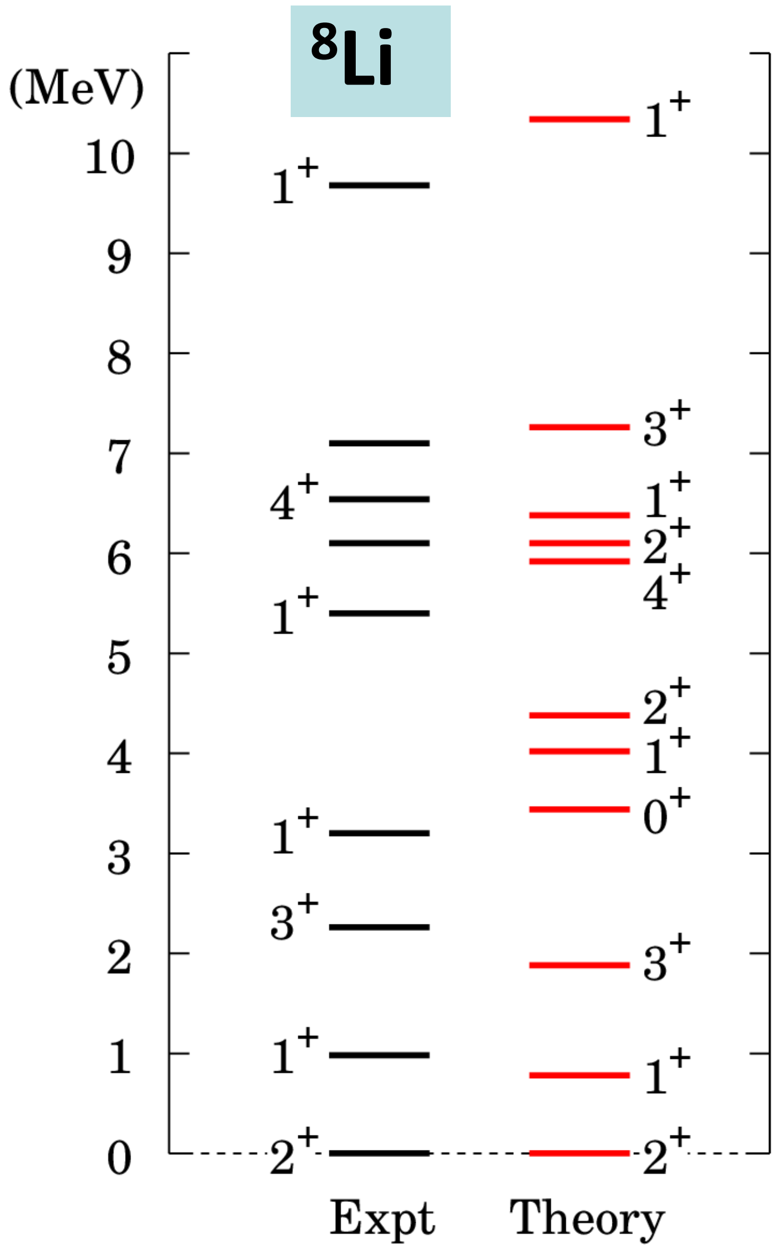
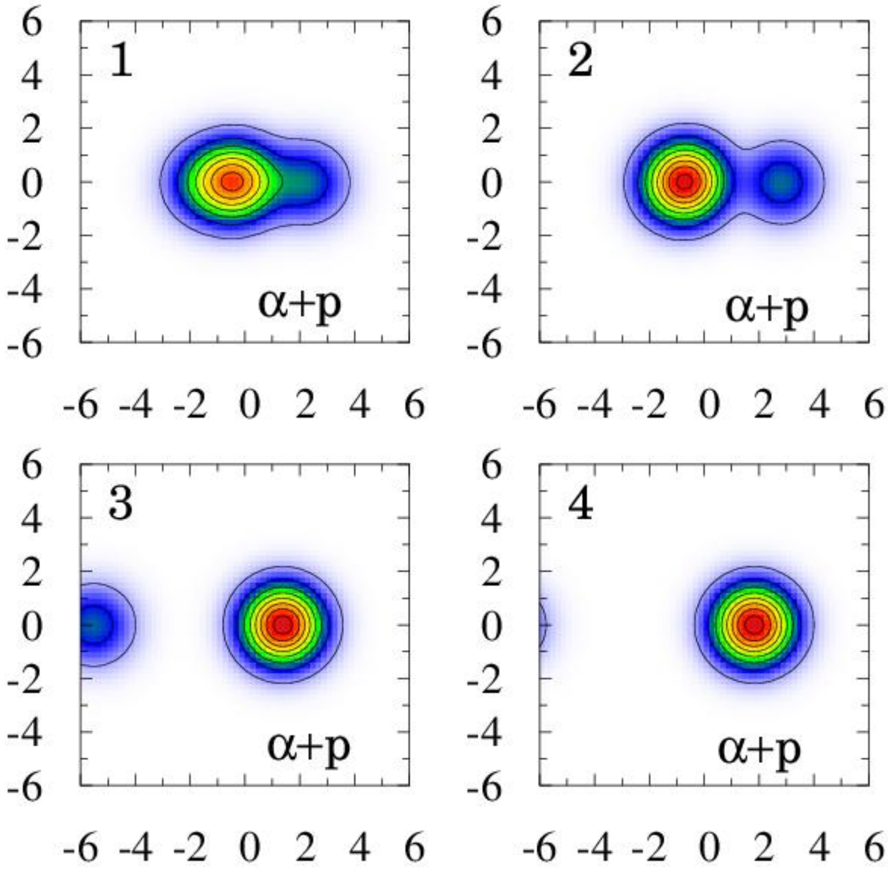
1/2−
3/2−
Expt
Theory



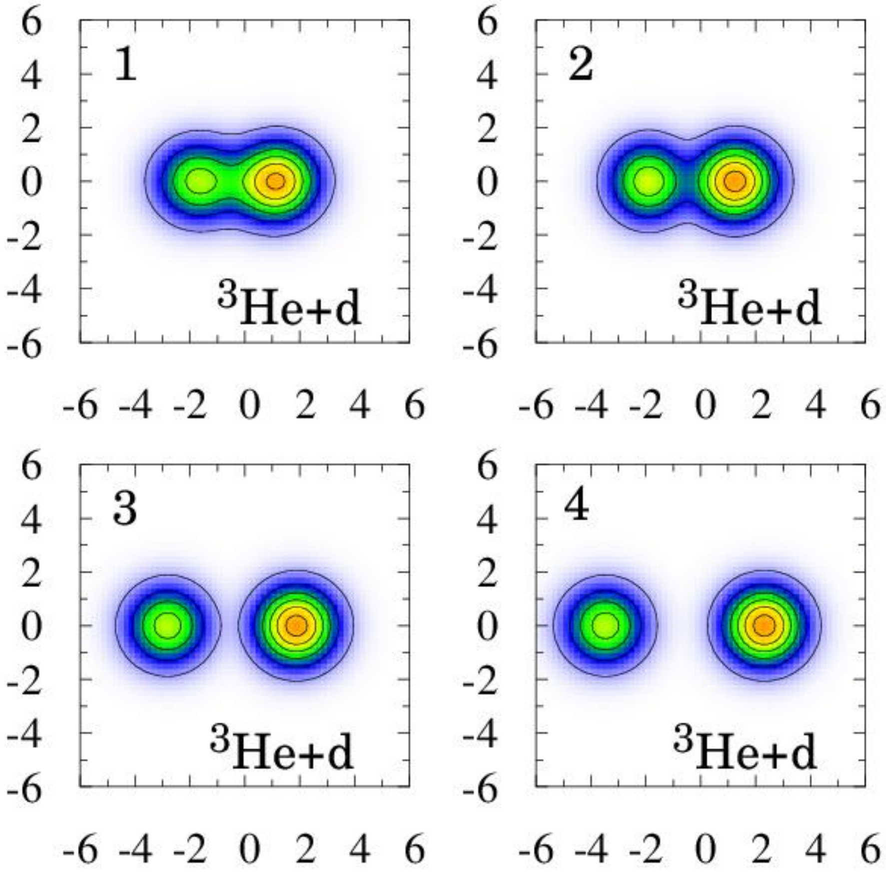
8Li
(MeV)
10
9
8
7
6
5
4
3
2
1
0
1+
4+
1+
1+
3+
1+
2+
1+
3+
1+
2+
4+
2+
1+
0+
3+
1+
2+
Expt
Theory

^5Li

Ground State (α+p resonance)

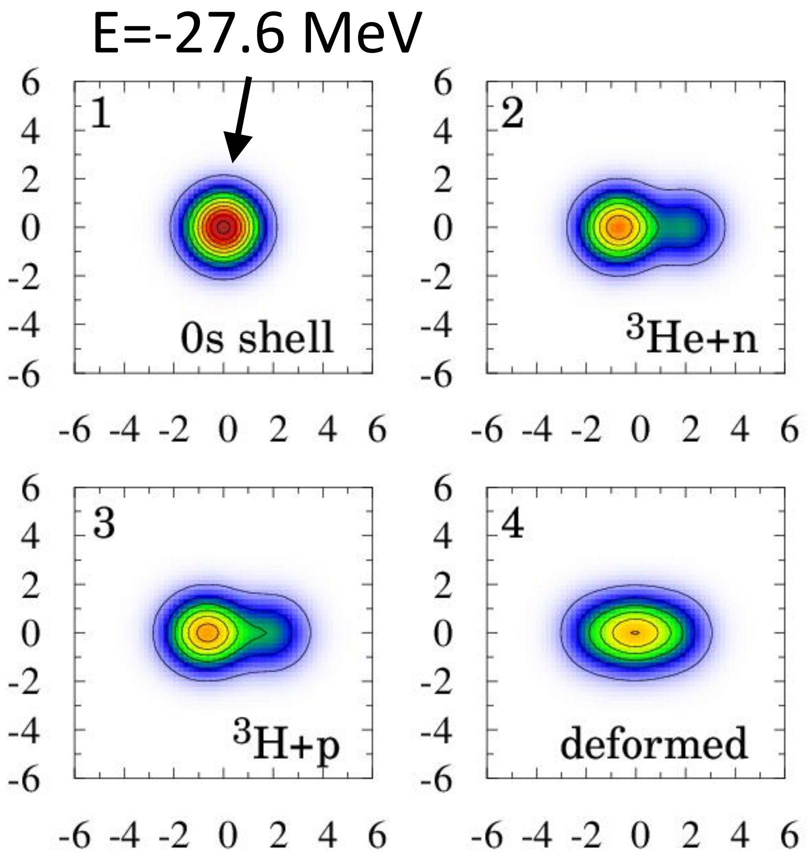


Excited States (3/2+ resonance)

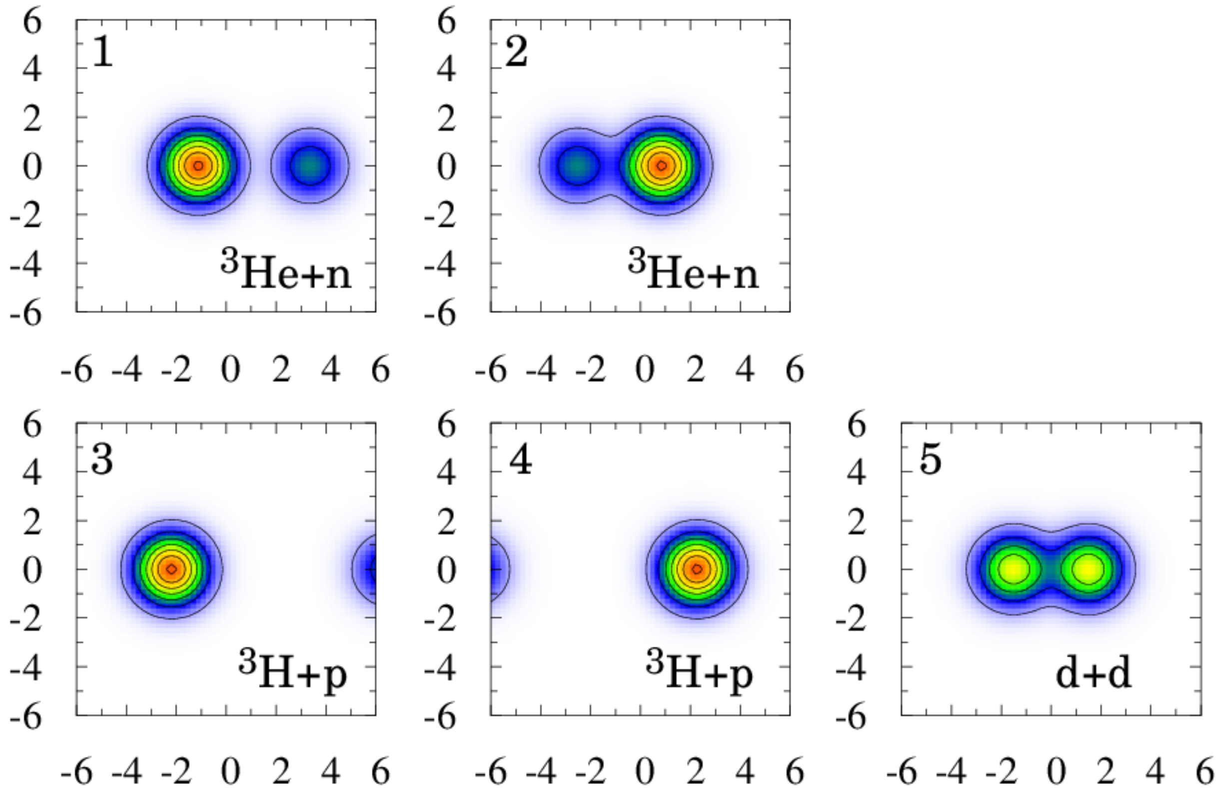


^{4}He

Ground 0^+ State E=-28.9 MeV

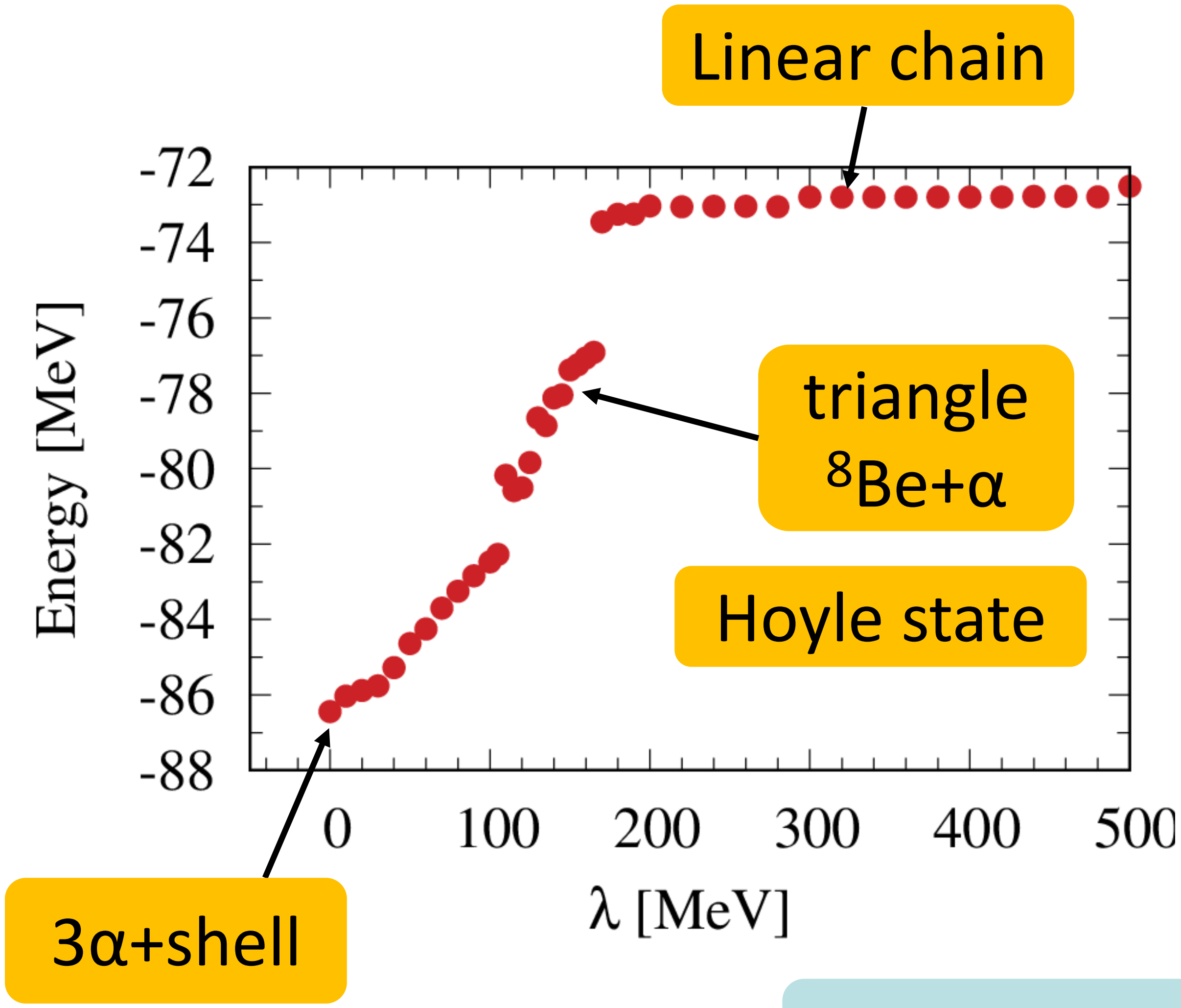


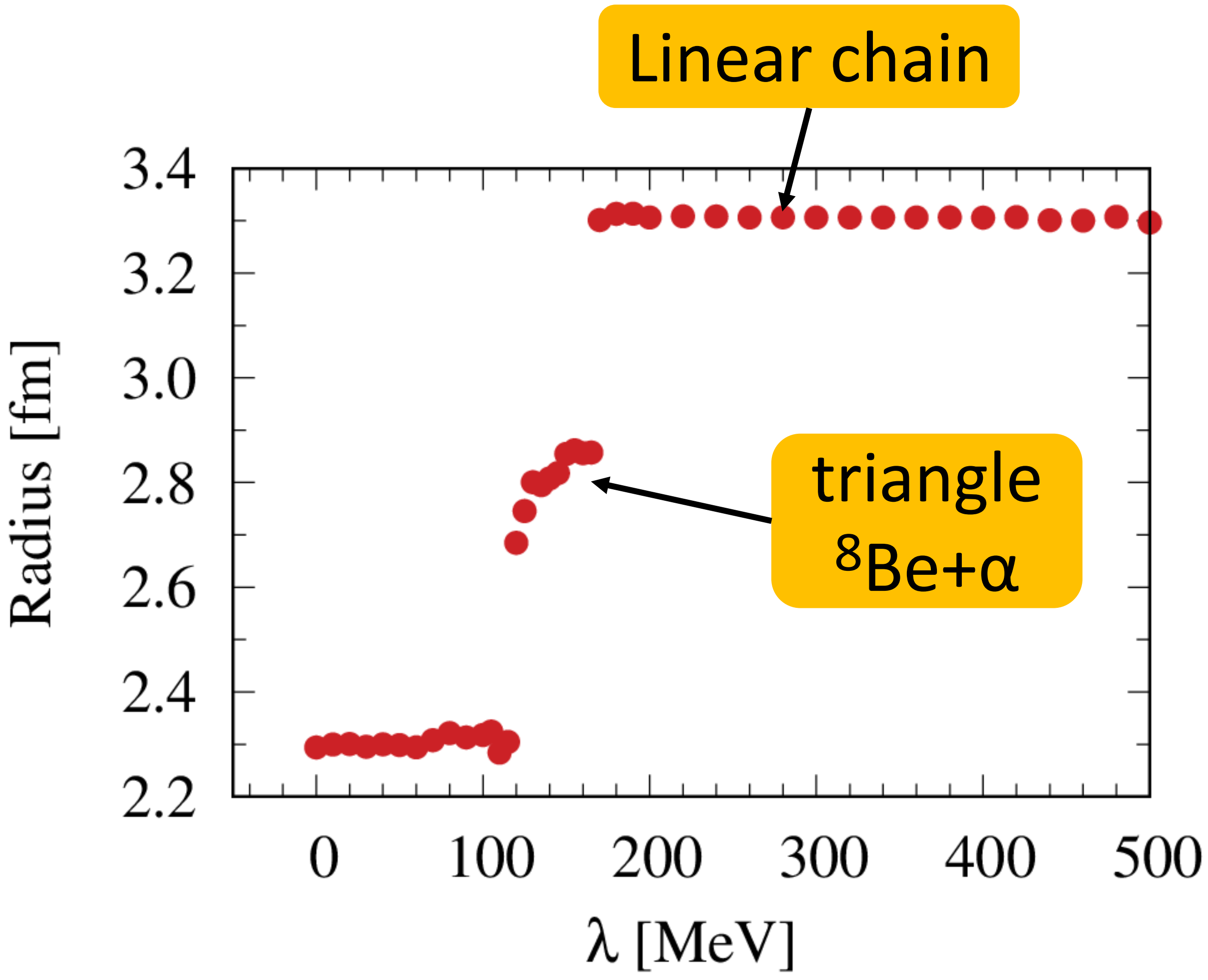
Excited 0^+ State E=-7.0 MeV



^{12}C (preliminary)

^{12}C with projection operator

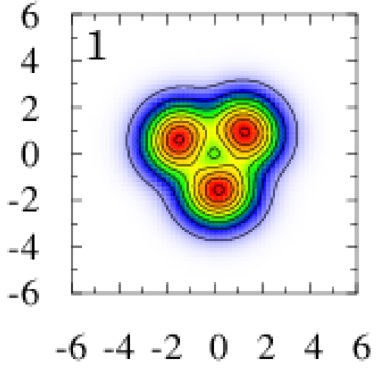




$$H_\lambda = H + V_\lambda,\quad V_\lambda = \lambda \sum_n^{3N} |\widetilde{\Phi}_n\rangle\langle\widetilde{\Phi}_n|$$

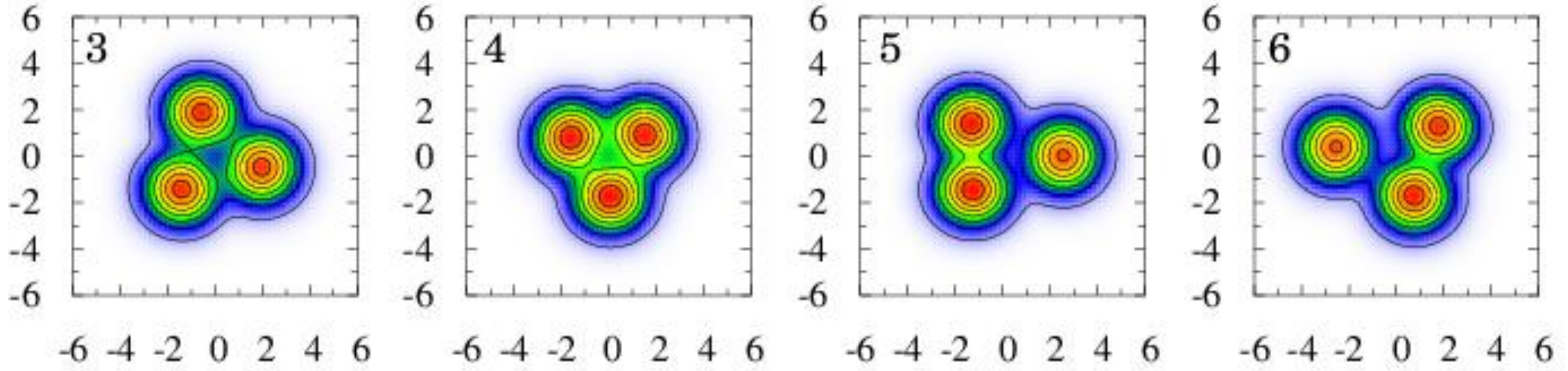
^{12}C Configurations

$1^{st}\ 0^+$



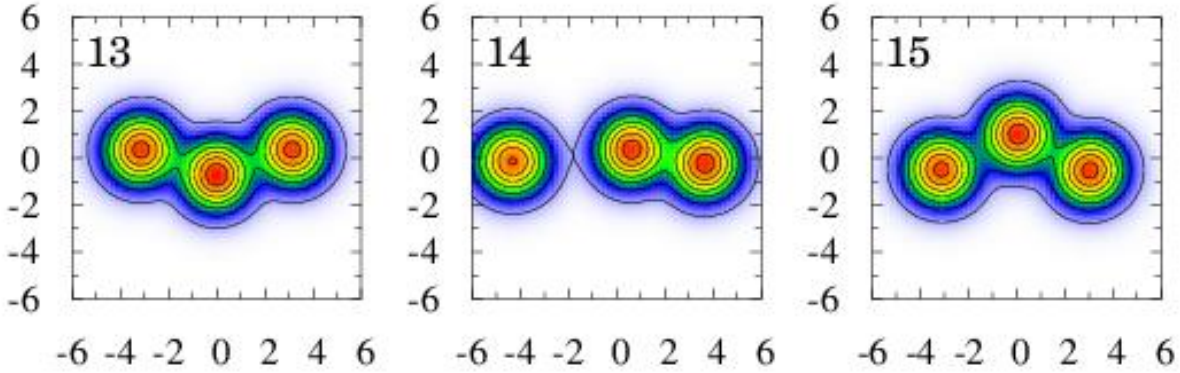
3α+shell

$2^{nd}\ 0^+$



triangle
$^8Be+\alpha$

$3^{rd}\ 0^+$



Linear chain

^{12}C Results (preliminary)

V_{LS}=1000 MeV

- E(1st 0$^+$) = -92.21 MeV (exp. -92.16 MeV)
- E(2nd 0$^+$)= -81.09 MeV : 3α Hoyle state, Ex=11.12 MeV (exp: 7 MeV)
- E(3rd 0$^+$) = -77.81 MeV : Linear-chain, Ex=14.4 MeV (exp: ~10 MeV)
- NO 4th 0$^+$ at present (breathing mode of Hoyle state)

- Radius (1st , 2nd , 3rd 0$^+$) = 2.35 / 3.05 / 3.34 fm , smaller than THSR

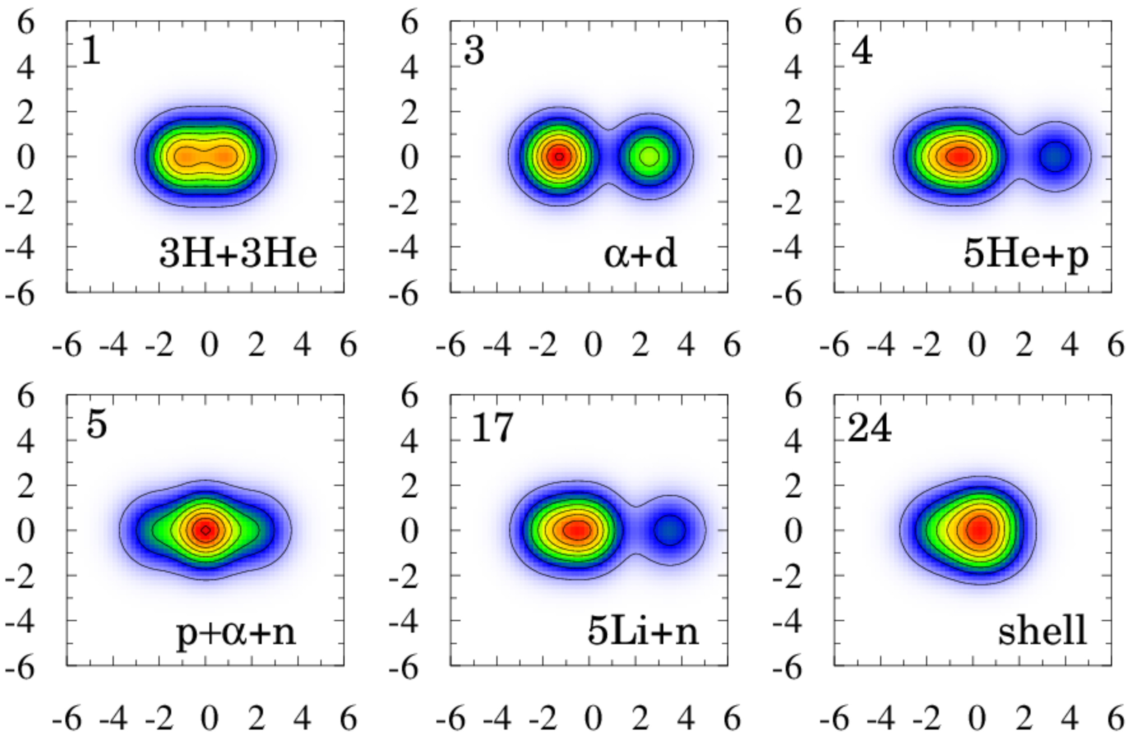
- 2$^+$: E_x=3.1 MeV (exp 4.4 MeV)
- 4$^+$: E_x =10.1 MeV (exp 14.1 MeV)
- B(E2, 1st 2$^+$ → 1st 0$^+$) = 8.17 e^2fm^4 (exp: 7.59)
- Monopole M(E0, 1st 0$^+$ → 2nd 0$^+$) = 6.90 e fm^2 (exp:5.4(2))

Summary

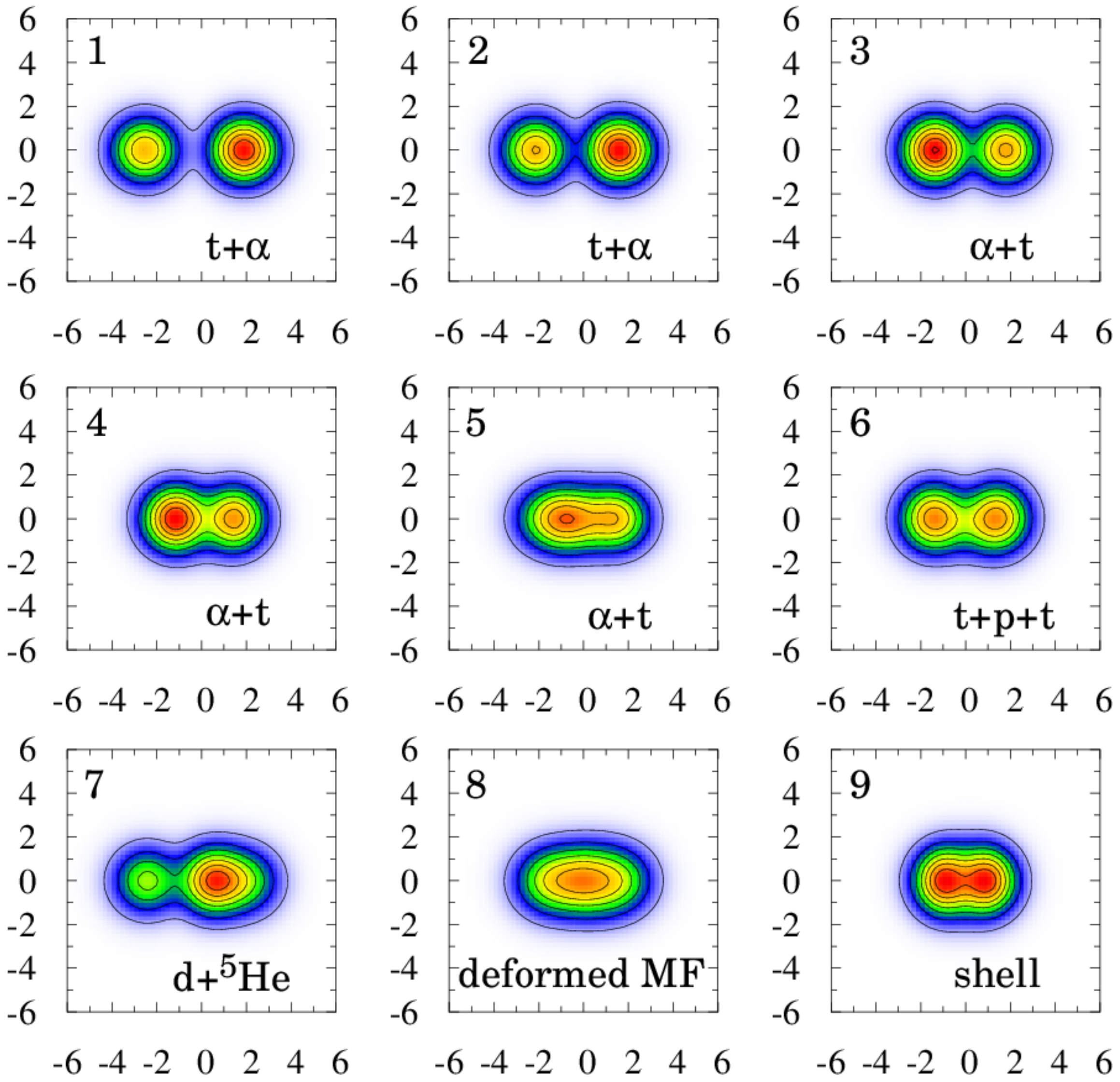
- Variation of multiple configurations with AMD
- Simultaneous optimization of multi-basis states : multiple cooling
- Shell structure, various combinations of sub-clusters (α,t,d)
- Future works
  - Spectroscopic factors of cluster configurations.
  - Heavier mass nuclei from p-shell (C, O) to sd-shell region (Ne, Mg)
  - Ab initio calculation with realistic nuclear force
  - Combine the framework with neural network (M. Lyu)

Backup

^{6}Li Ground State



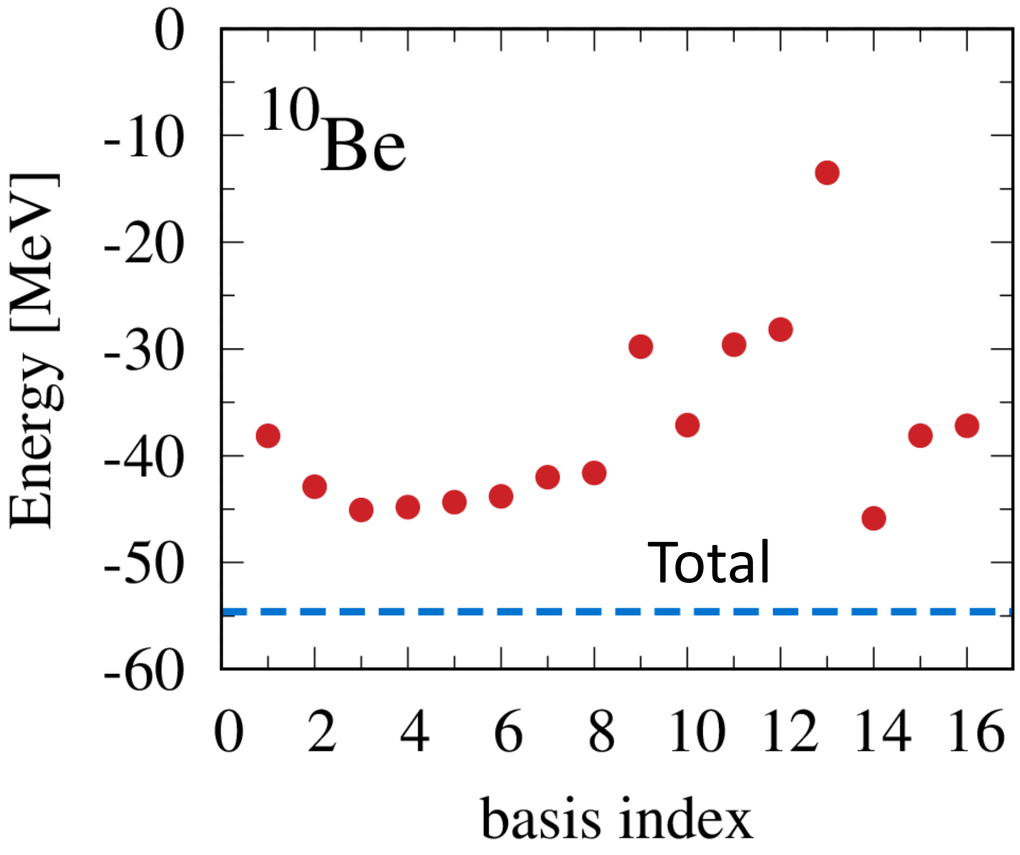
^{7}Li Ground State



^{10}Be Ground state with 16 bases

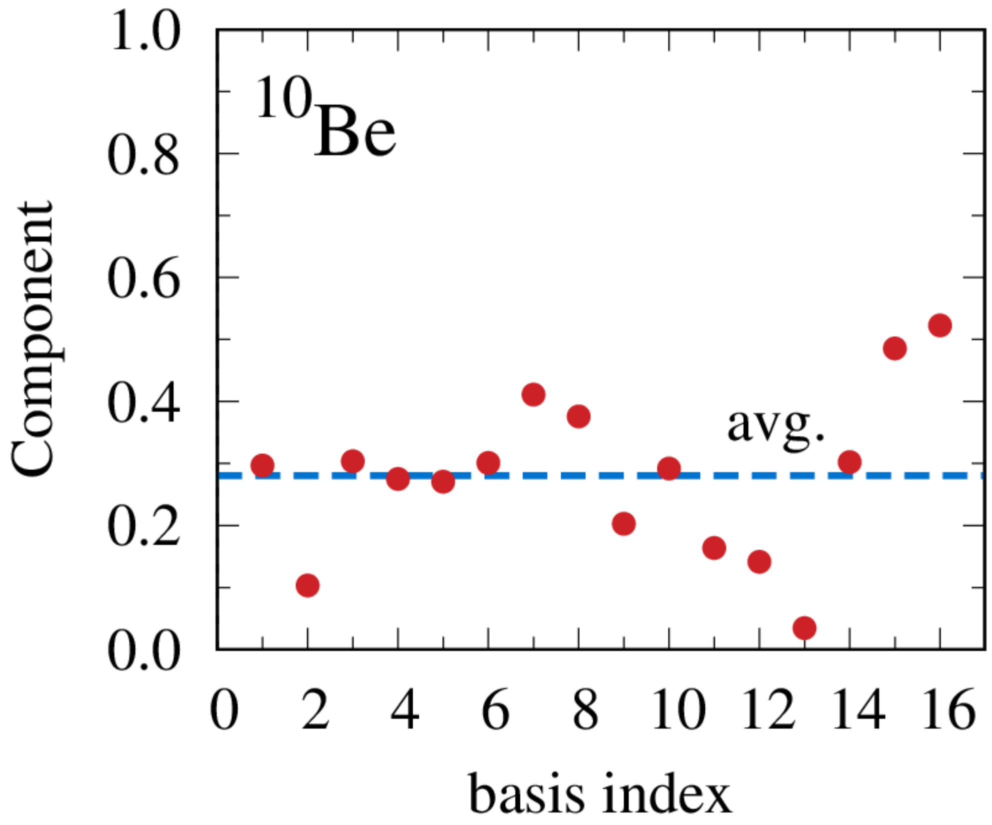
$\Phi_{\text{total}} = \sum_n^N C_n \Phi_n$

Intrinsic energies (MeV)



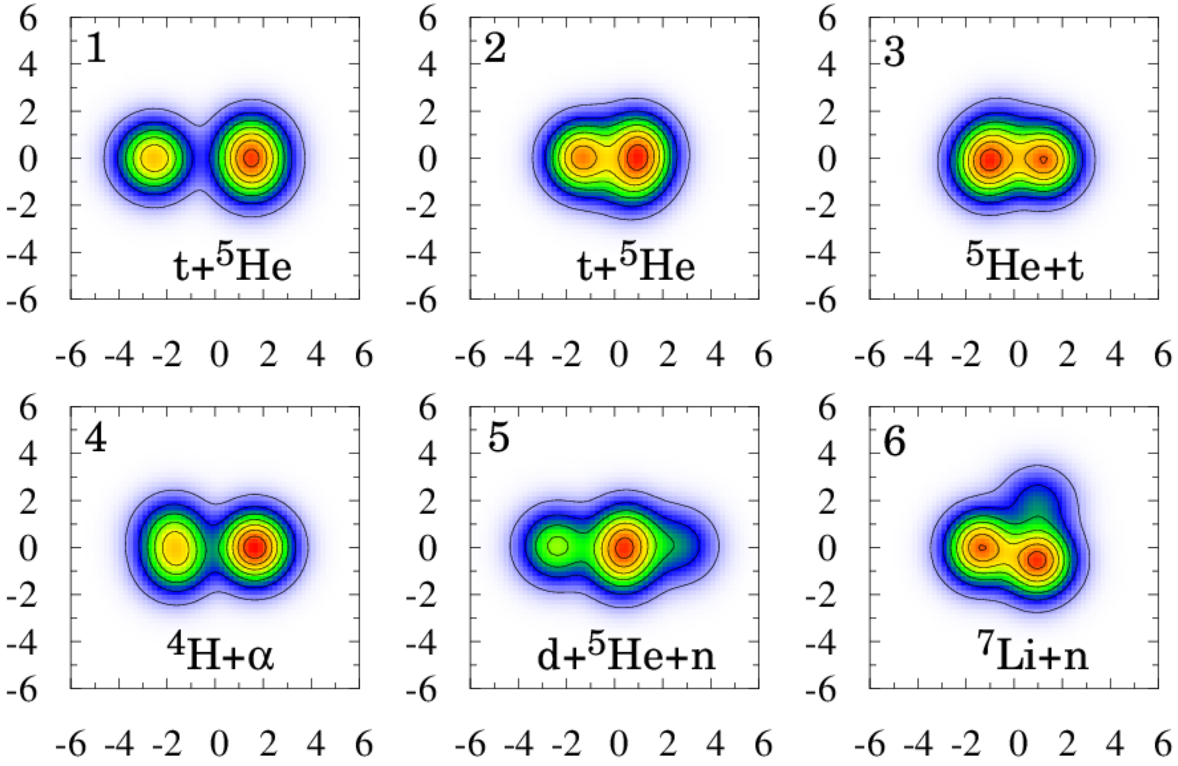
$\Delta E_{\text{GCM}} = 10$ MeV (-45 → -55)

Components: $|\langle \Phi_{\text{n}} | \Phi \rangle|^2$

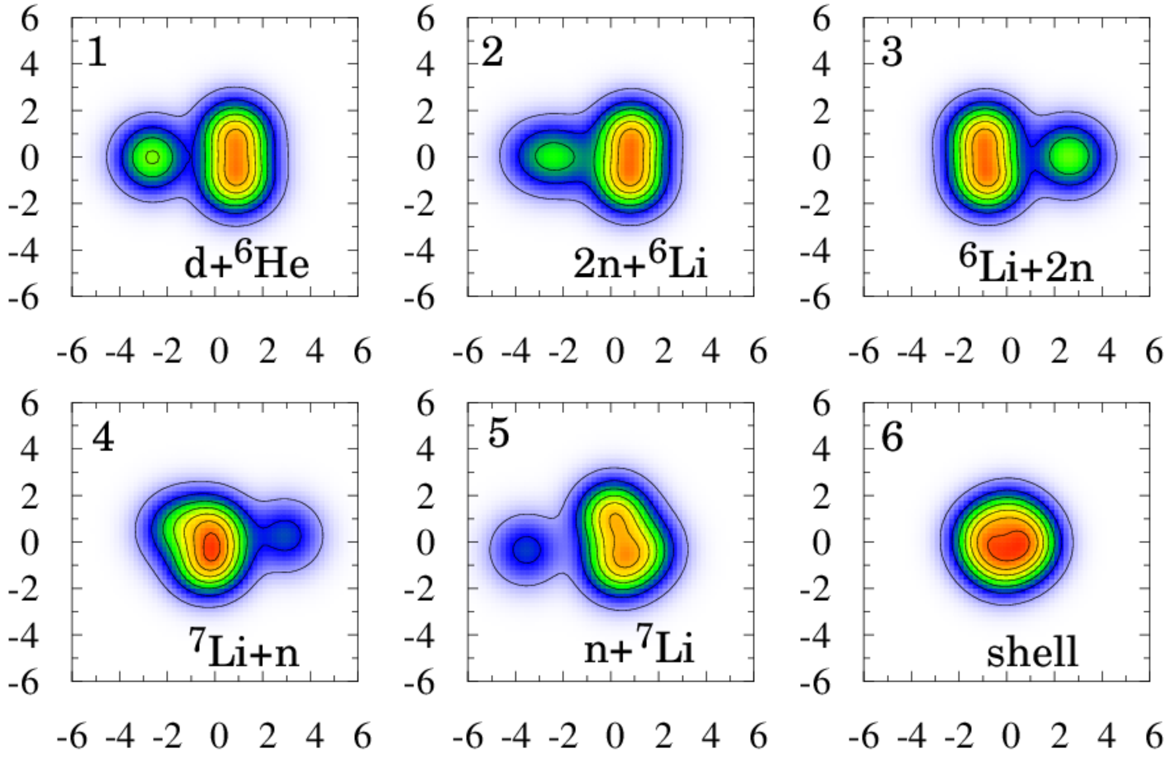


^{8}Li density

Ground State



Excited State



Experimental threshold energies: ^{7}Li+n (2.0 MeV), α+t+n (4.5 MeV), ^{6}He+d (9.8 MeV)