Nuclear lattice simulations for *ab initio* nuclear structure

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Workshop on Precision Measurements with Radioisotopes
Texas A&M University
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Outline

Lattice effective field theory

Emergent geometry and duality of ^{12}C

Wavefunction matching

Charge radii of silicon isotopes

Properties of beryllium isotopes

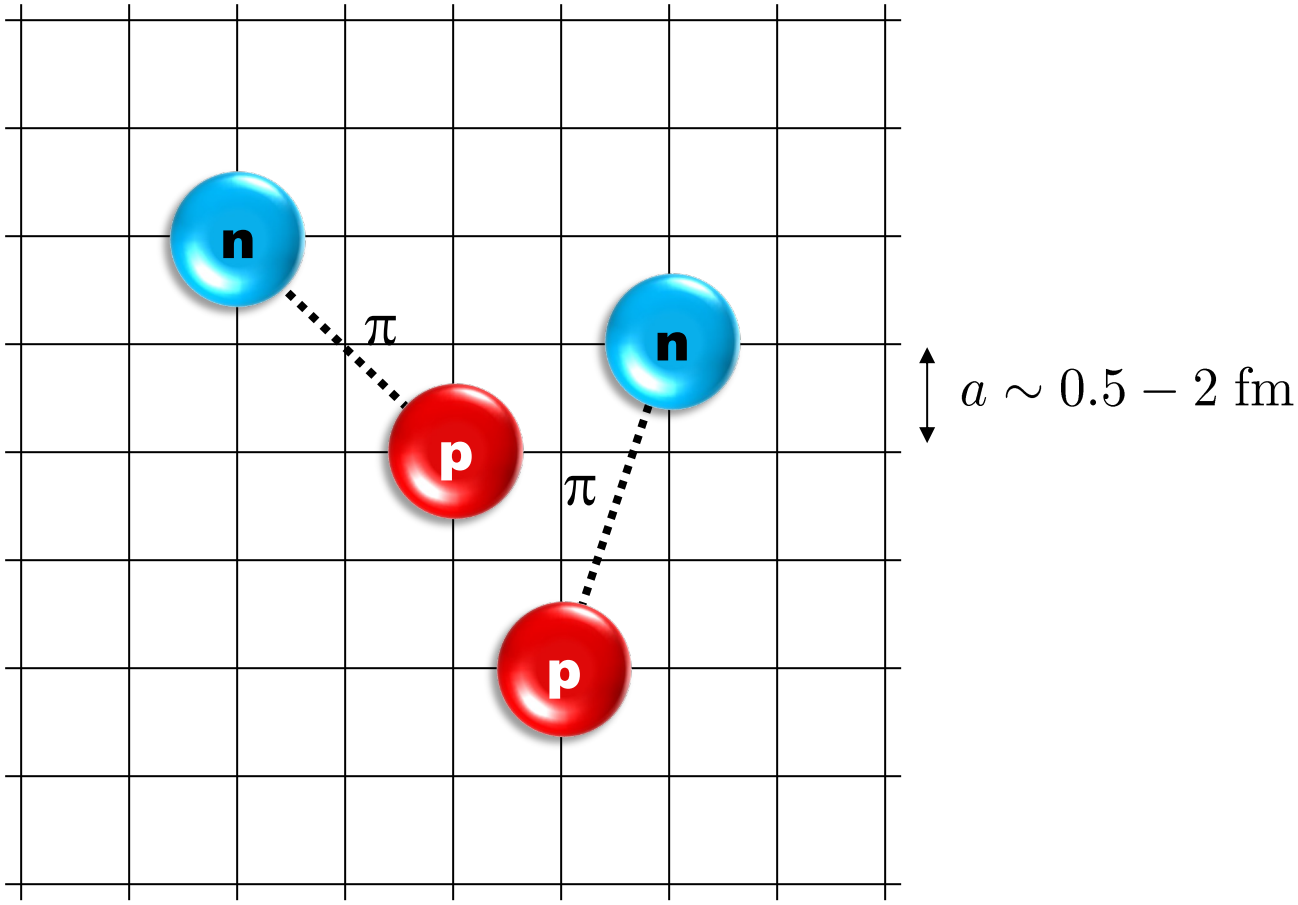
Parametric matrix models

Resummation of perturbation theory

Multimodal superfluidity of neutrons

Summary and outlook

Lattice effective field theory

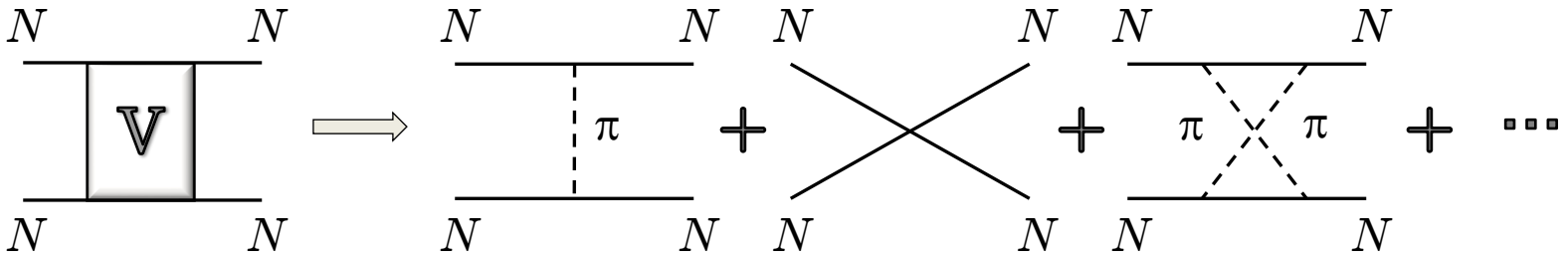


D.L, Prog. Part. Nucl. Phys. 63 117-154 (2009)

Lähde, Meißner, Nuclear Lattice Effective Field Theory (2019), Springer

Chiral effective field theory

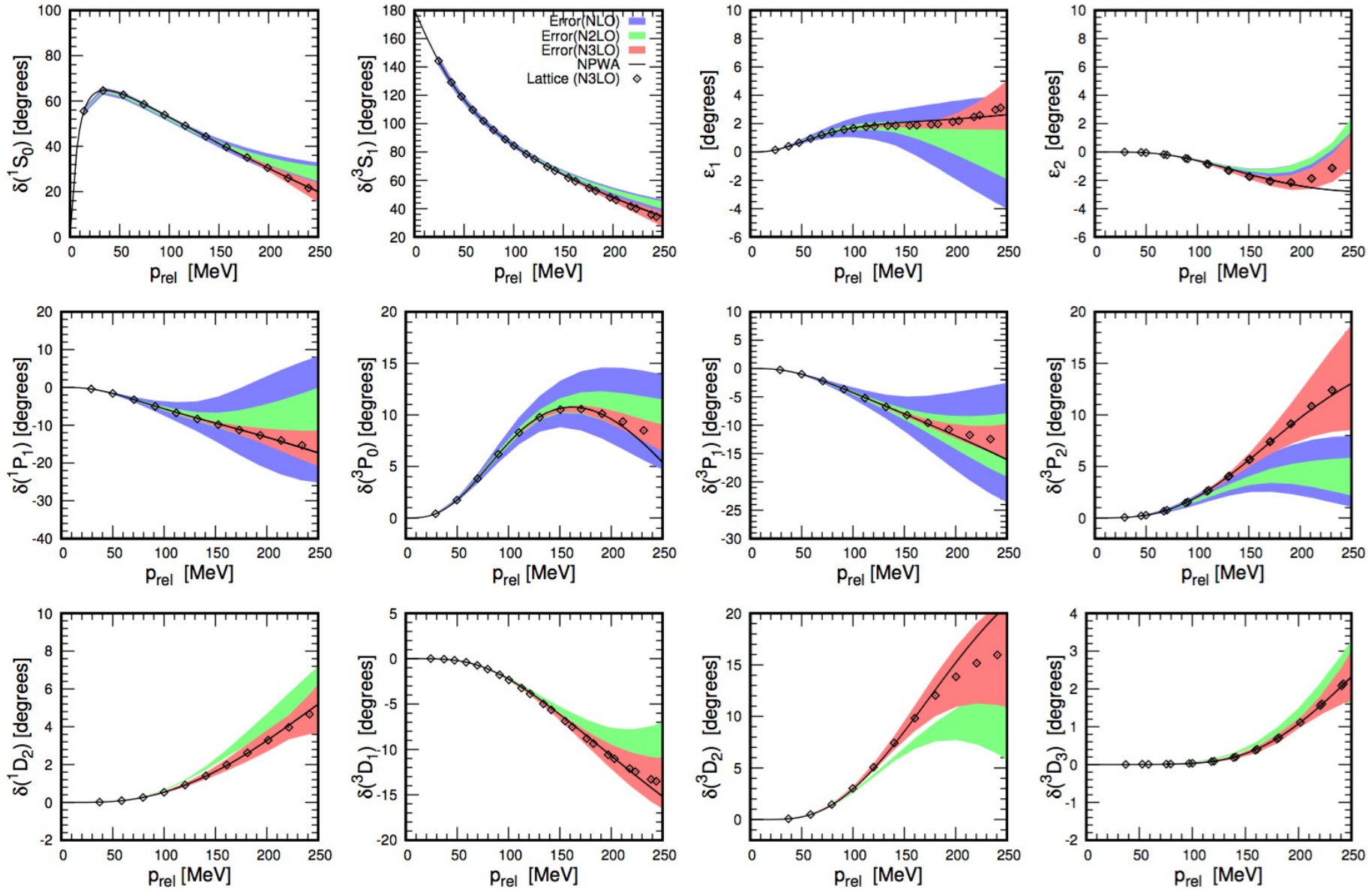
Construct the effective potential order by order



V^{OPEP} Contact interactions V^{TPEP}

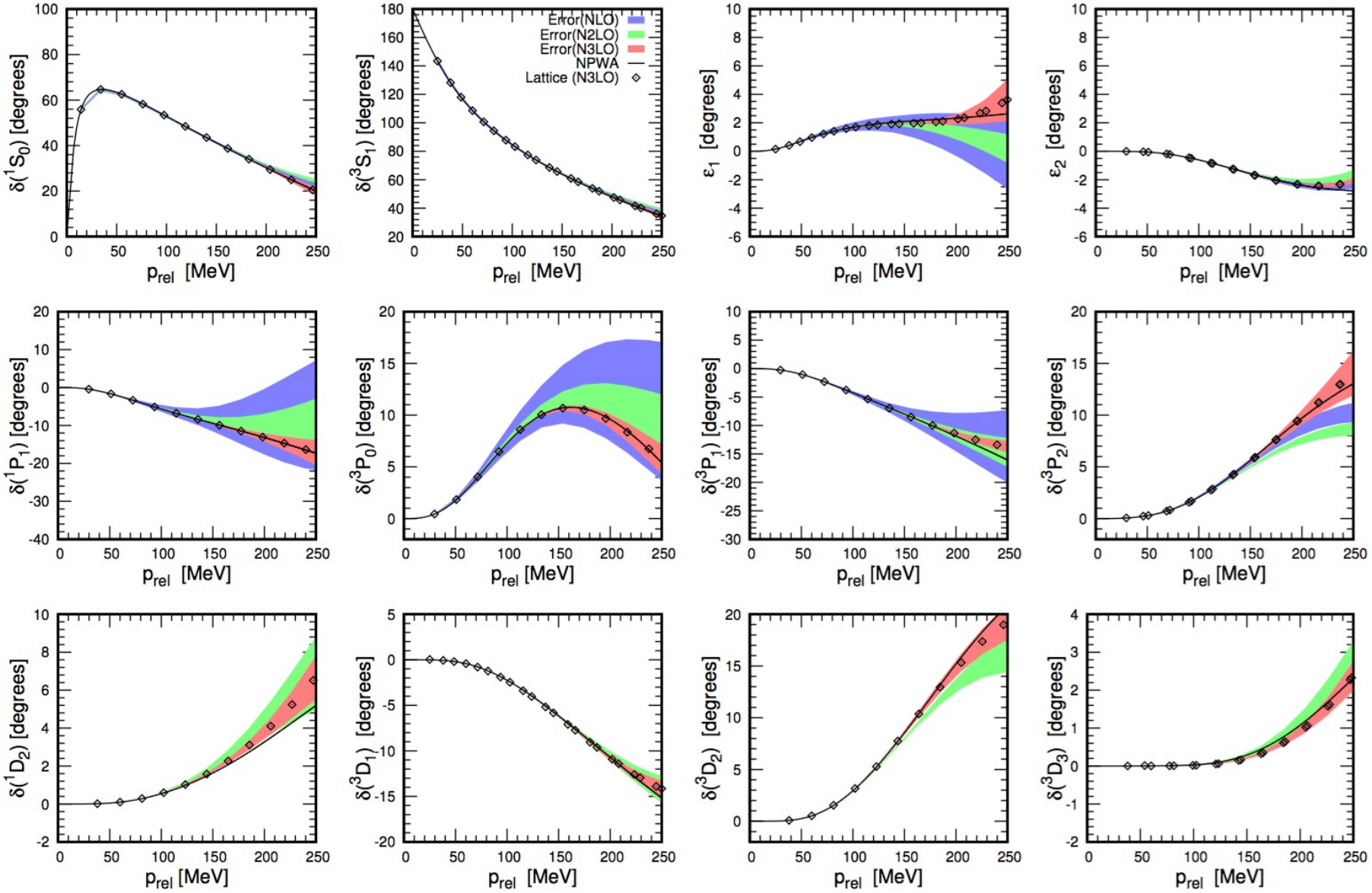
Leading order (LO) Next-to-leading order (NLO)

$a = 1.315\,\mathrm{fm}$

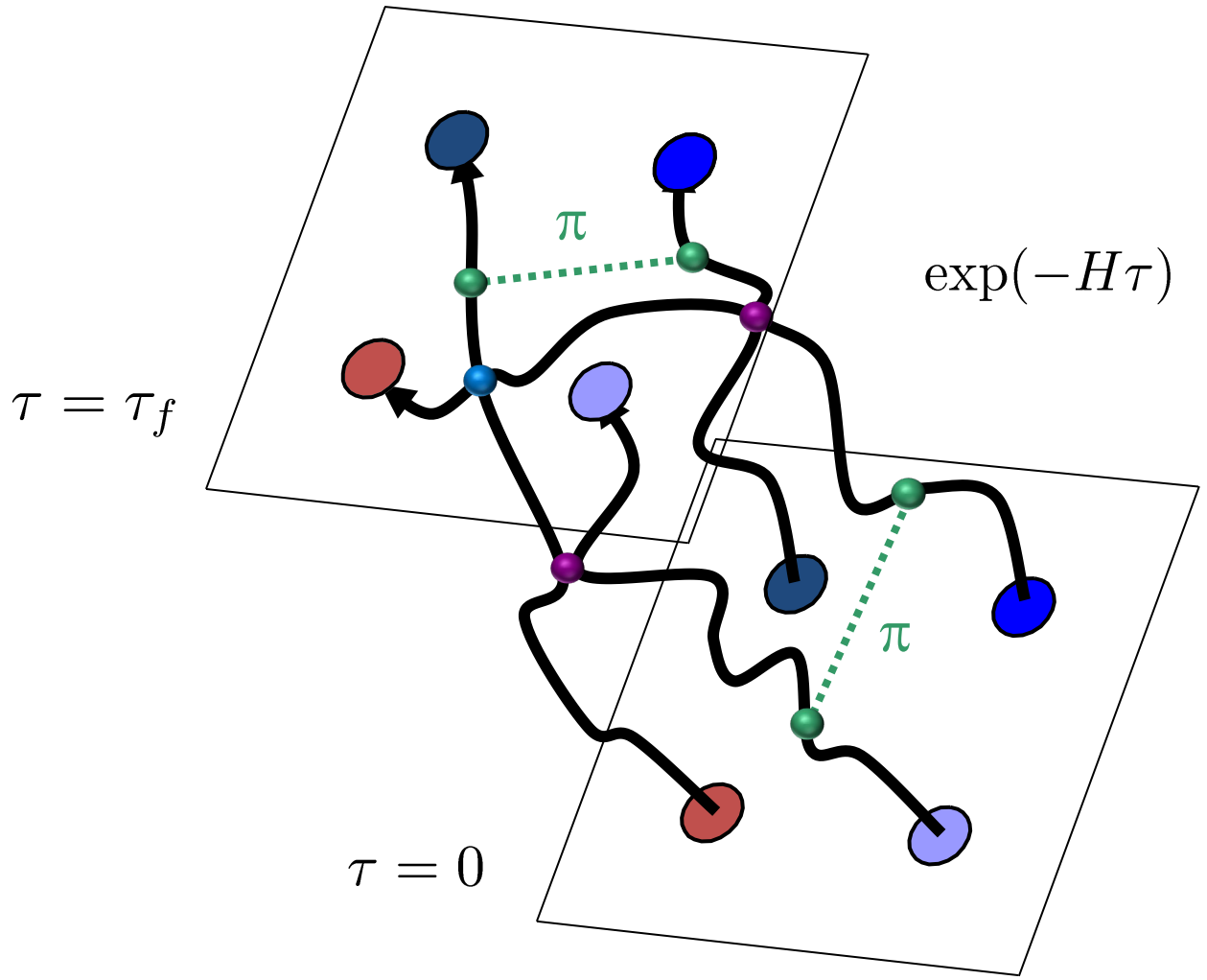


Li, Elhatisari, Epelbaum, D.L., Lu, Meißner, PRC 98, 044002 (2018)

$a = 0.987\,\mathrm{fm}$



Euclidean time projection



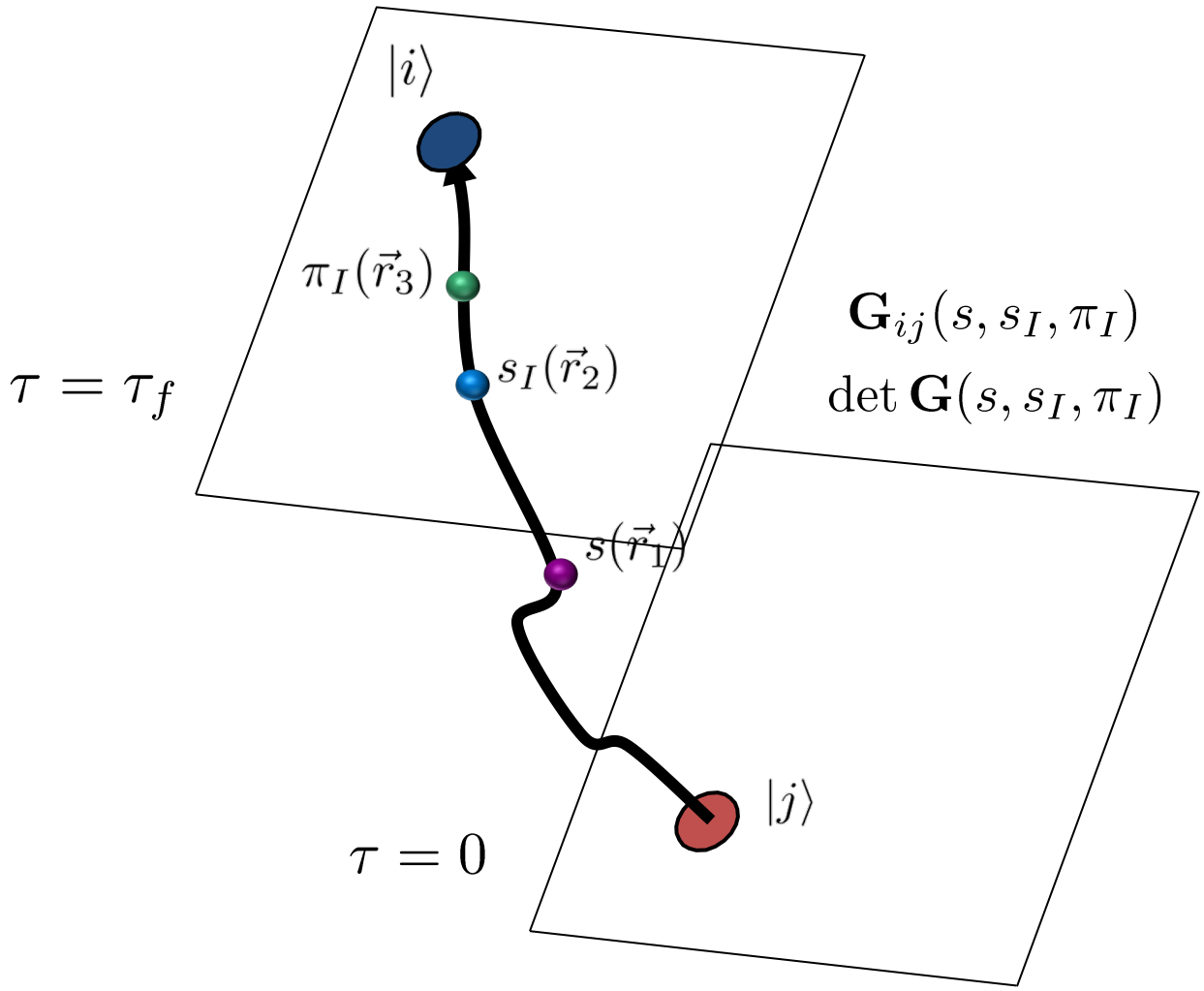
Auxiliary field method

We can write exponentials of the interaction using a Gaussian integral identity

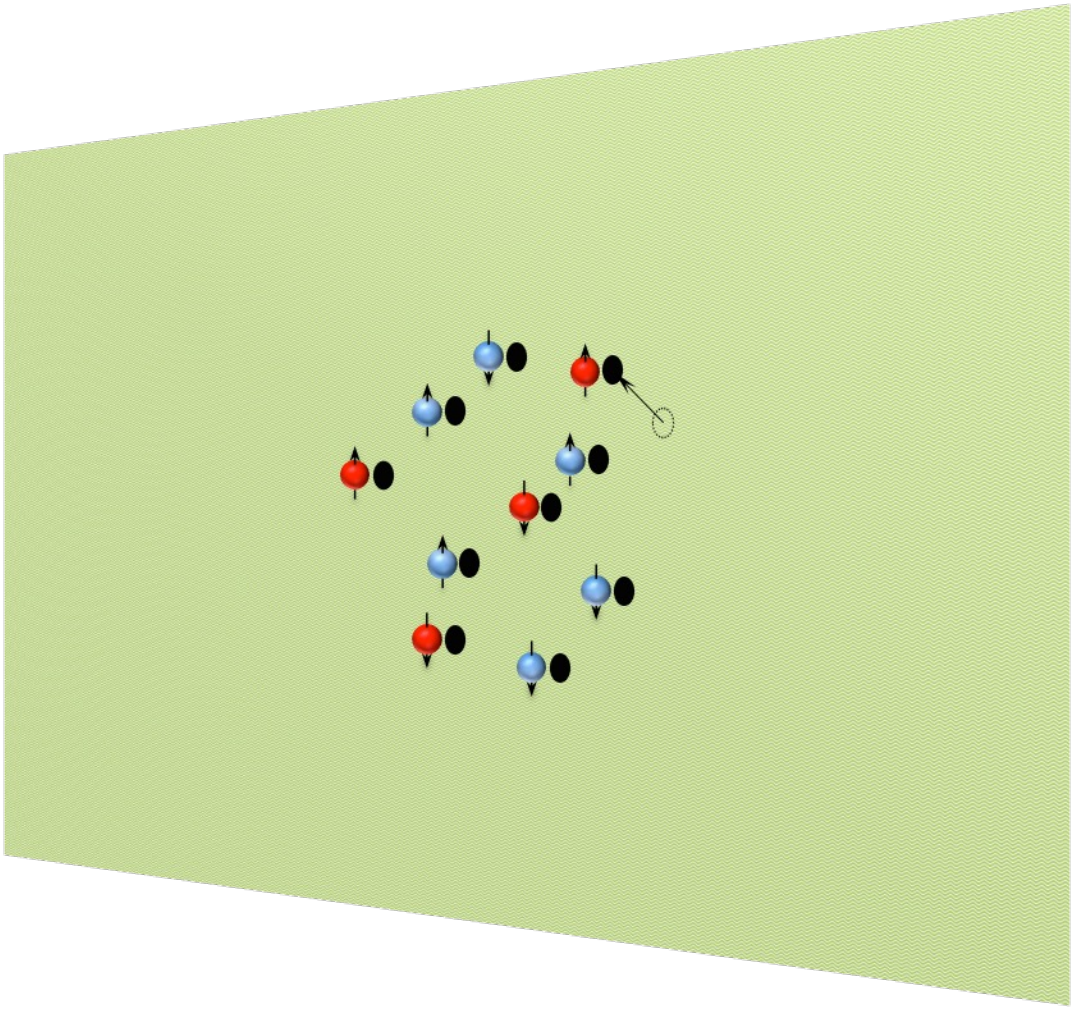
$$\exp\left[-\frac{C}{2}(N^\dagger N)^2\right] \qquad \times \quad (N^\dagger N)^2$$

$$= \sqrt{\frac{1}{2\pi}} \int_{-\infty}^{\infty} ds \exp\left[-\frac{1}{2}s^2 + \sqrt{-C}\, s(N^\dagger N)\right] \qquad \rangle \bullet \quad sN^\dagger N$$

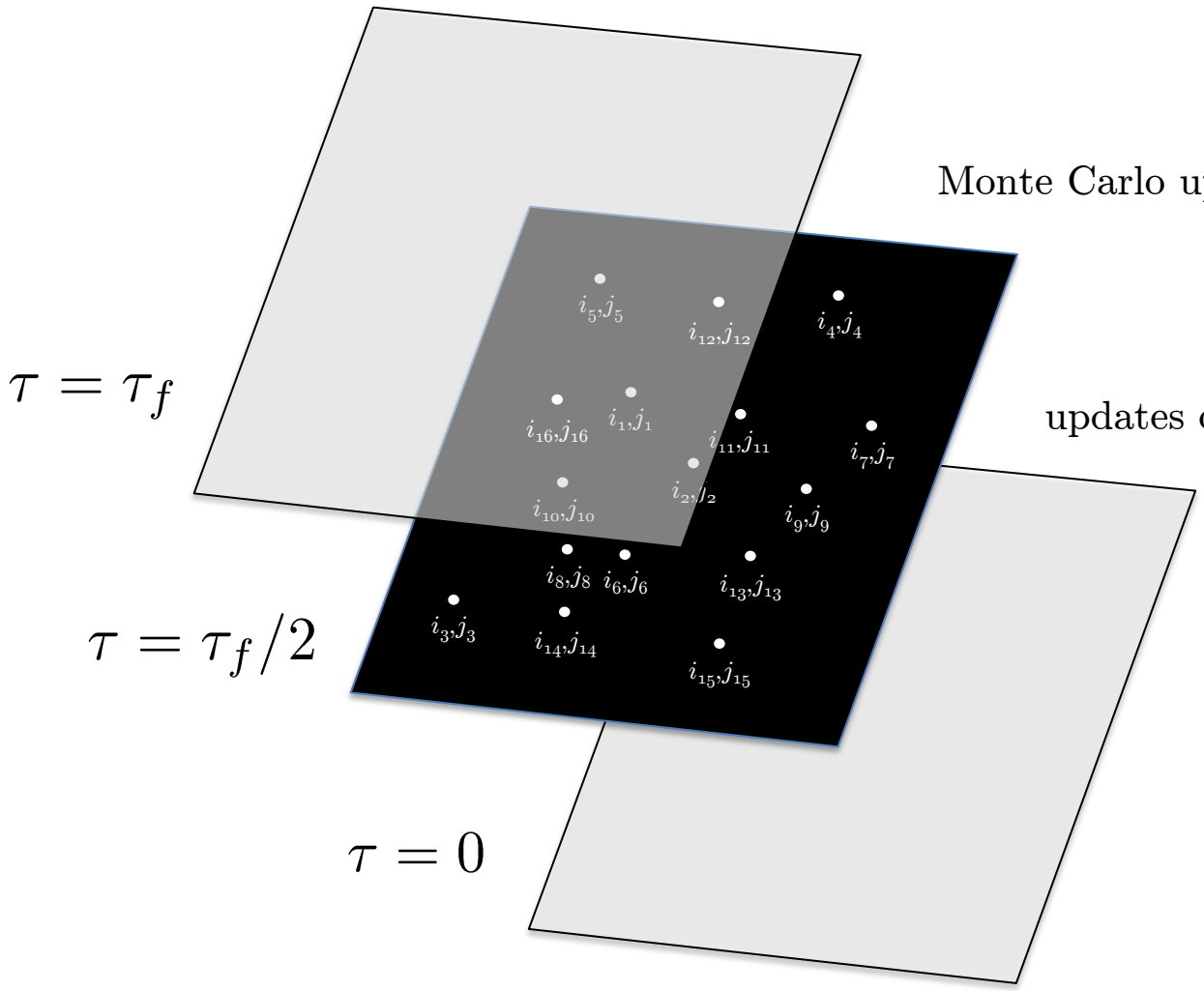
We remove the interaction between nucleons and replace it with the interactions of each nucleon with a background field.


$|i\rangle$
$\pi_I(\vec{r}_3)$
$s_I(\vec{r}_2)$
$s(\vec{r}_1)$
$|j\rangle$
$\tau = \tau_f$
$\tau = 0$
$\mathbf{G}_{ij}(s, s_I, \pi_I)$
$\det \mathbf{G}(s, s_I, \pi_I)$

Pinhole algorithm



Elhatisari, Epelbaum, Krebs, Lähde, D.L., Li, Lu, Meißner, Rupak, PRL 119, 222505 (2017)

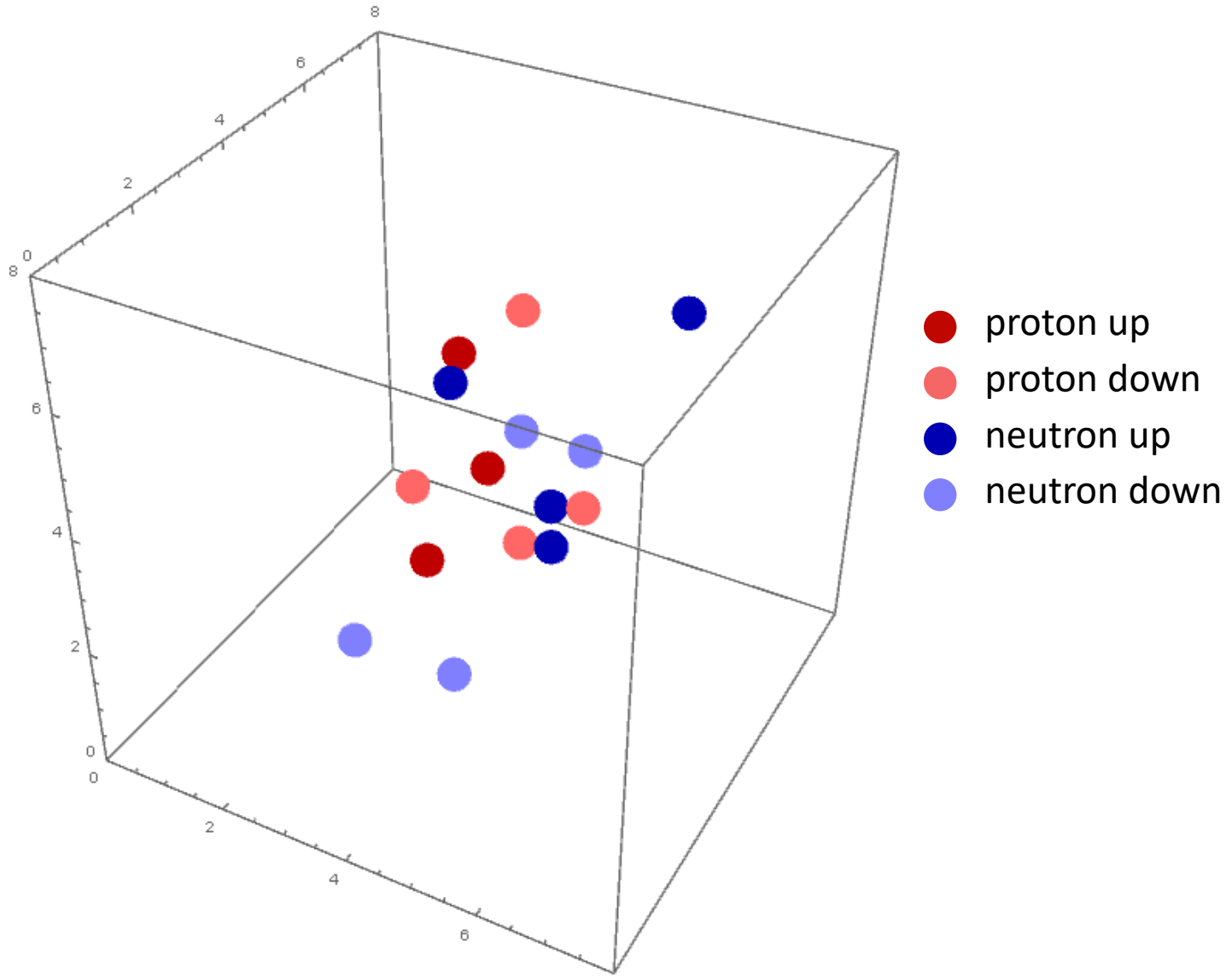


Monte Carlo updates of pinholes

Monte Carlo
updates of auxiliary/pion fields

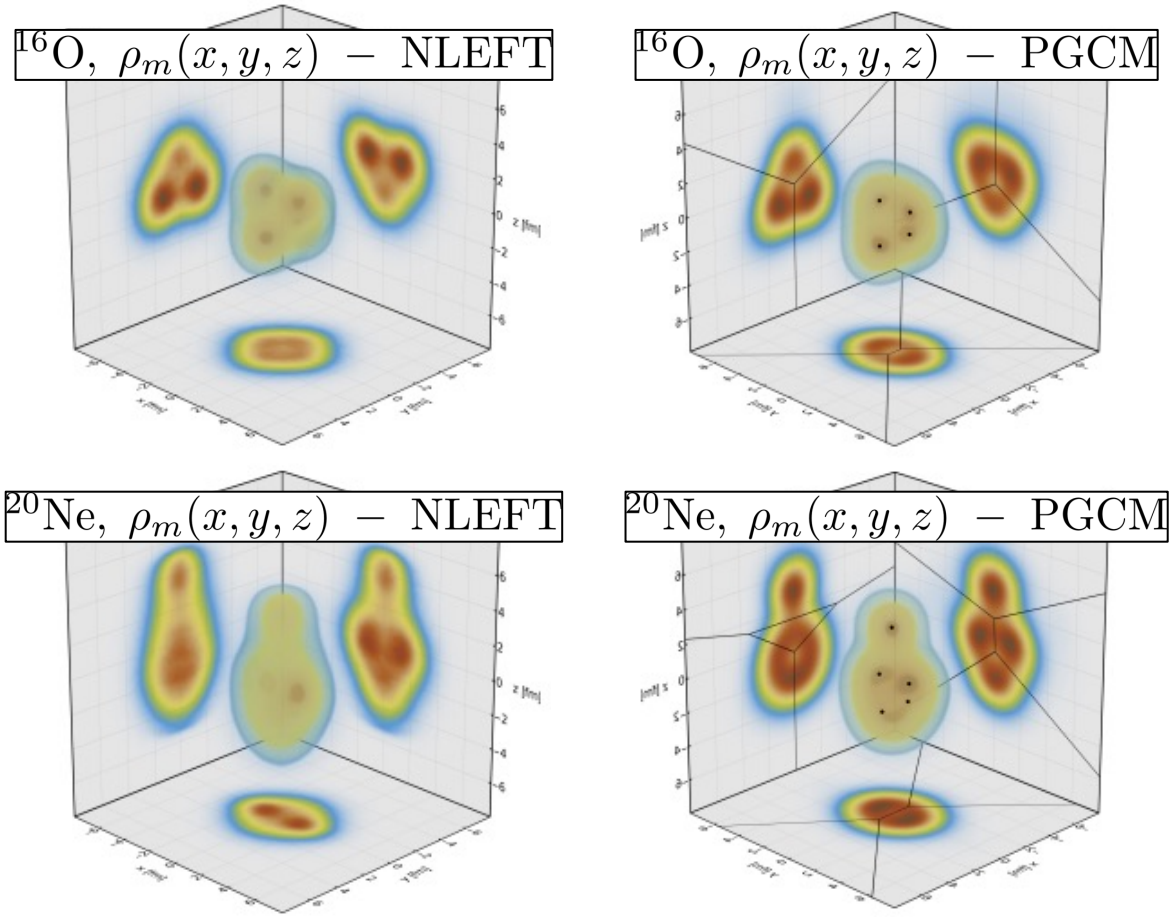
Elhatisari, Epelbaum, Krebs, Lähde, D.L., Li, Lu, Meißner, Rupak, PRL 119, 222505 (2017)

^{16}O



Summerfield, Lu, Plumberg, D.L., Noronha-Hostler, Timmins, Phys. Rev. C 104 L041901 (2021)

Structure of ^{16}O and ^{20}Ne



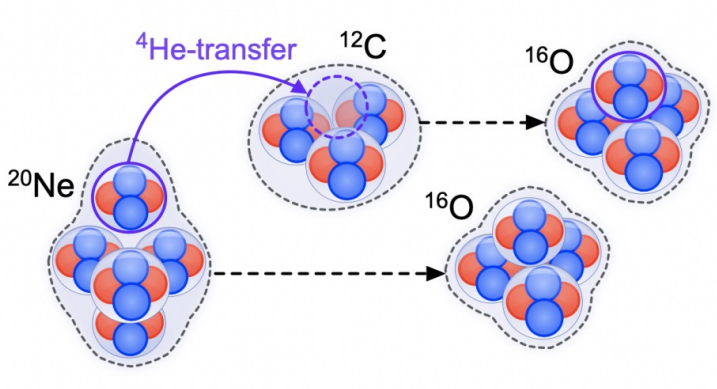
Giacalone et al., Phys. Rev. Lett. in press, arXiv:2402.05995

Giacalone et al., Phys. Rev. Lett. 134, 082301 (2025)

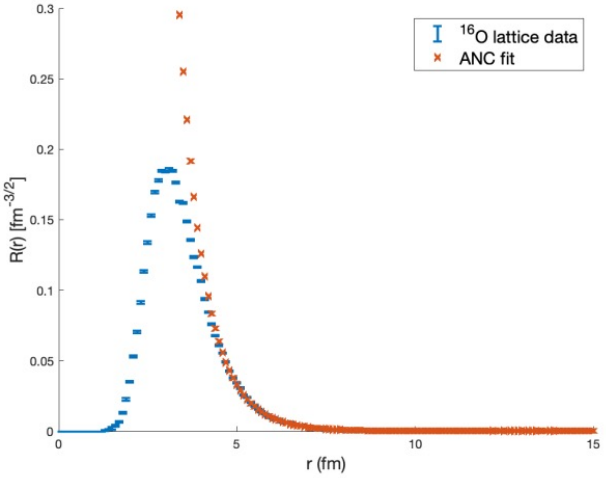
Quantifying α clustering in the ground states of ^{16}O and ^{20}Ne

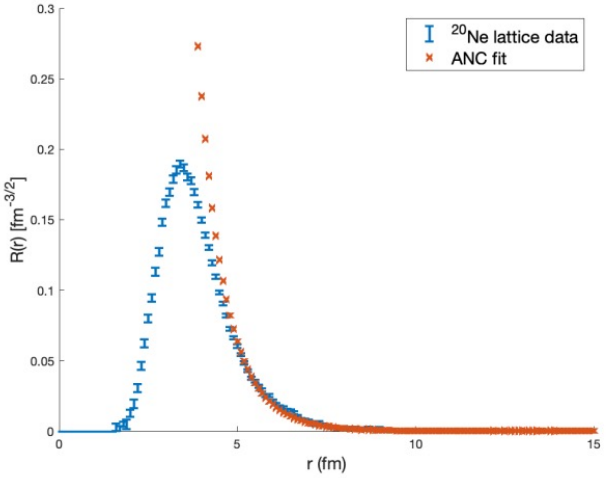
E. Harris,[1,2] M. Barbui,[2] J. Bishop,[2,*] G. Chubarian,[2] Sebastian König,[3] E. Koshchiy,[2,†] K.D. Launey,[4] Dean Lee,[5,6] Zifeng Luo,[1,2] Yuan-Zhuo Ma,[6] Ulf-G. Meißner,[7,8] C.E. Parker,[2] Zhengxue Ren,[9,10] M. Roosa,[1,2] A. Saastamoinen,[2] G. H. Sargsyan,[6] D.P. Scriven,[1,2] Shihang Shen,[9,10] A. Volya,[11] Hang Yu,[3,12] and G.V. Rogachev[1,2,13,‡]

arXiv:2507.17059

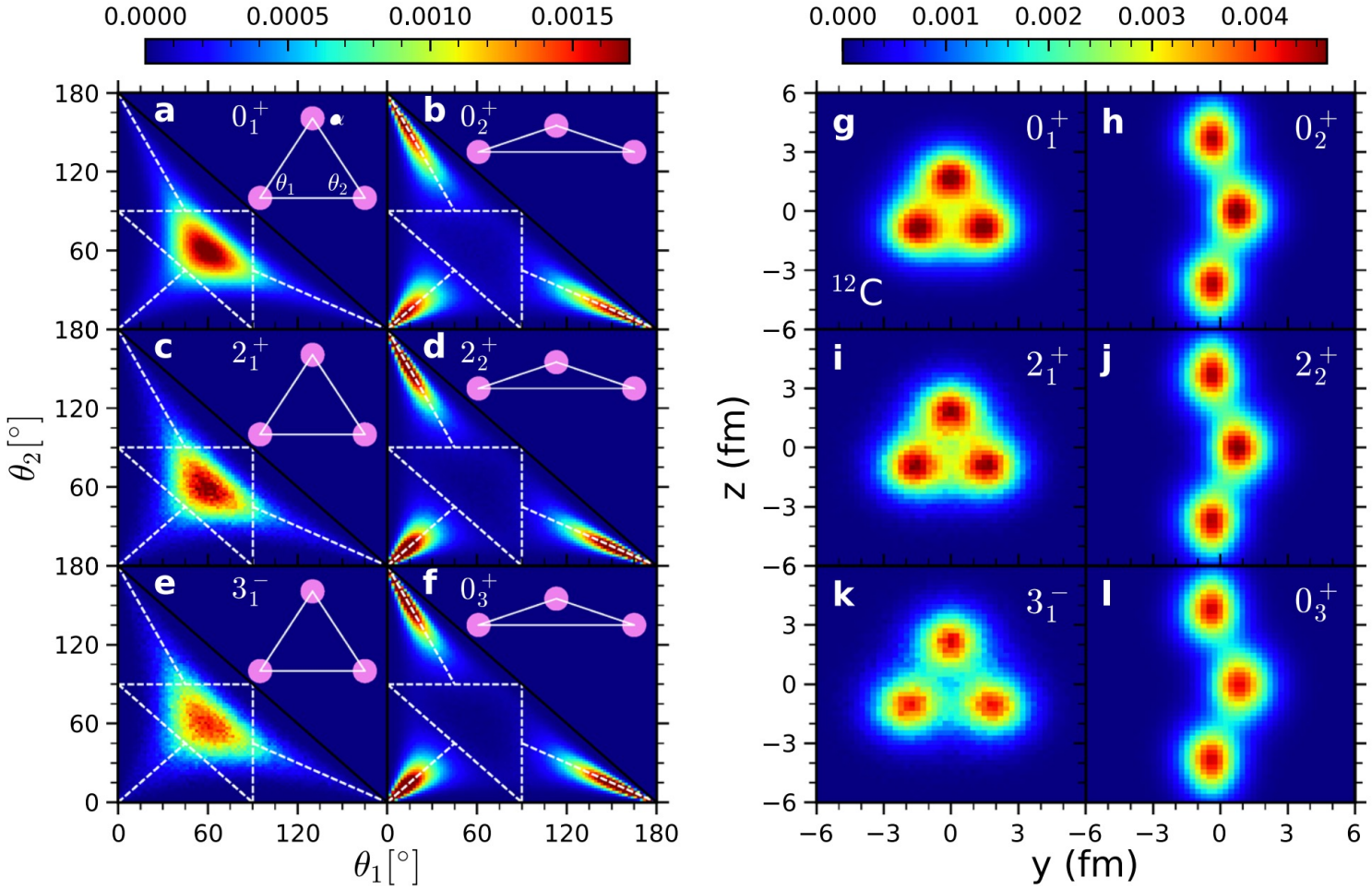


	$C^{^{16}O}_{\alpha,^{12}C}$ (fm$^{-1/2}$)	$C^{^{20}Ne}_{\alpha,^{16}O}$ (fm$^{-1/2}$)	$[(C^{^{16}O}_{\alpha,^{12}C})^2(C^{^{20}Ne}_{\alpha,^{16}O})^2]^{1/4}$ (10^3 fm$^{-1/2}$)
Experiment			1.75(7)(9)
NLEFT	380(80)	3800(950)	1.20(25)
SA-NCSM	210(30)	3760(470)	0.89(14)
CN-CI	520(30)	4500(500)	1.53(13)
Extreme CM	640	5700	1.9

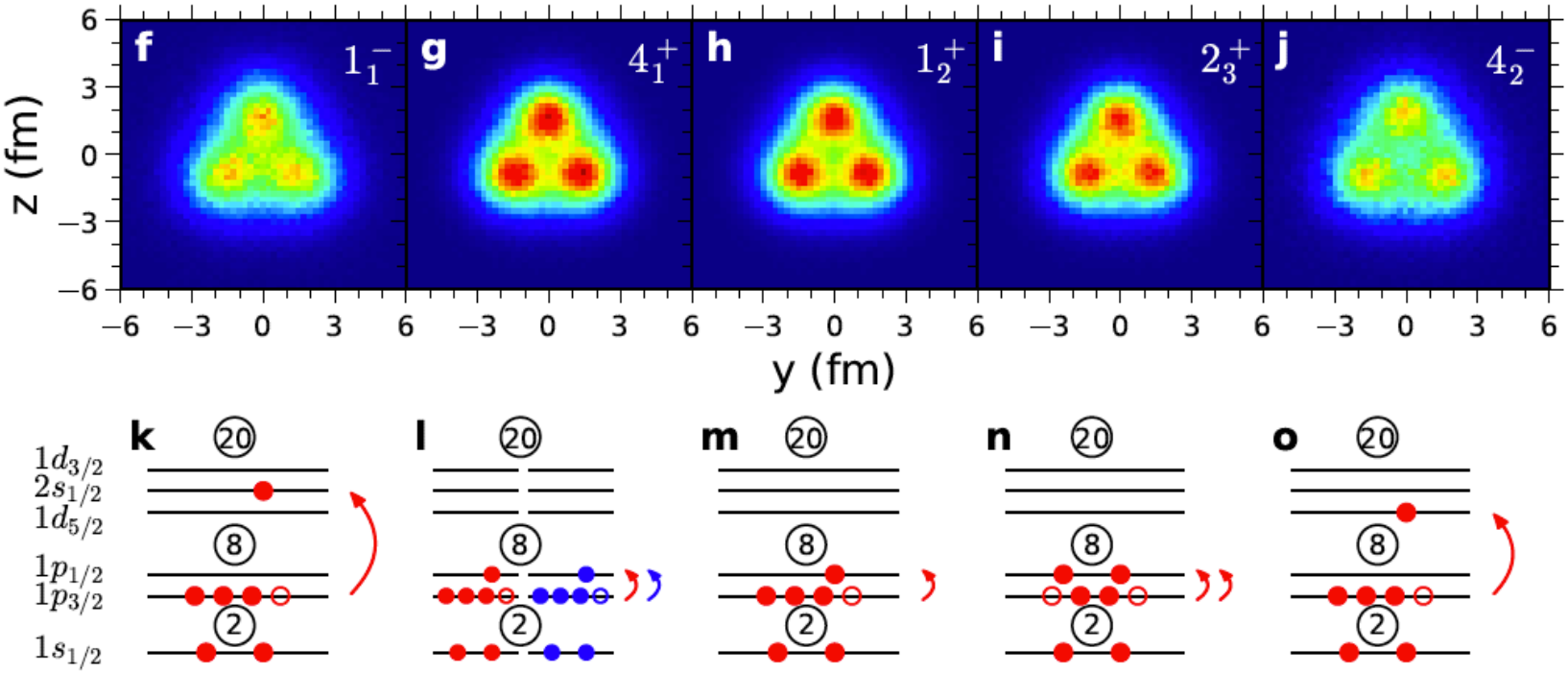


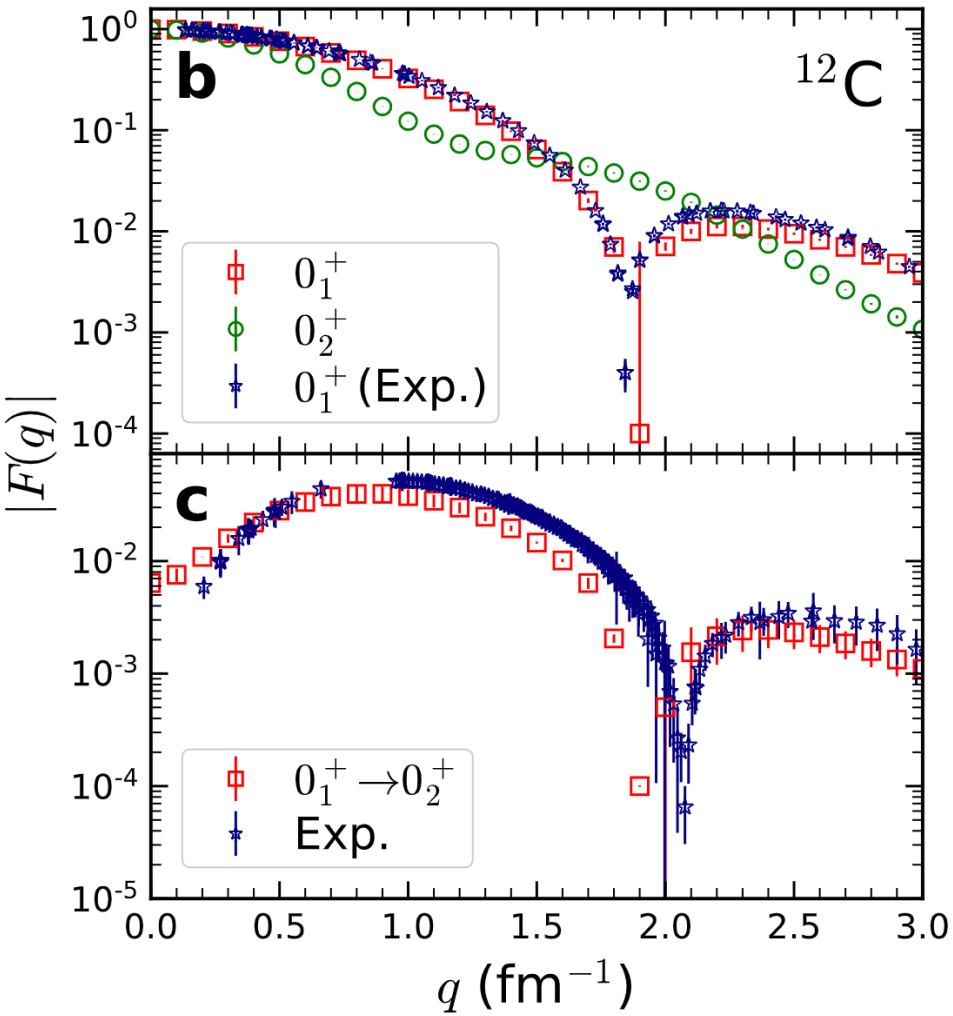


Emergent geometry and duality of ^{12}C

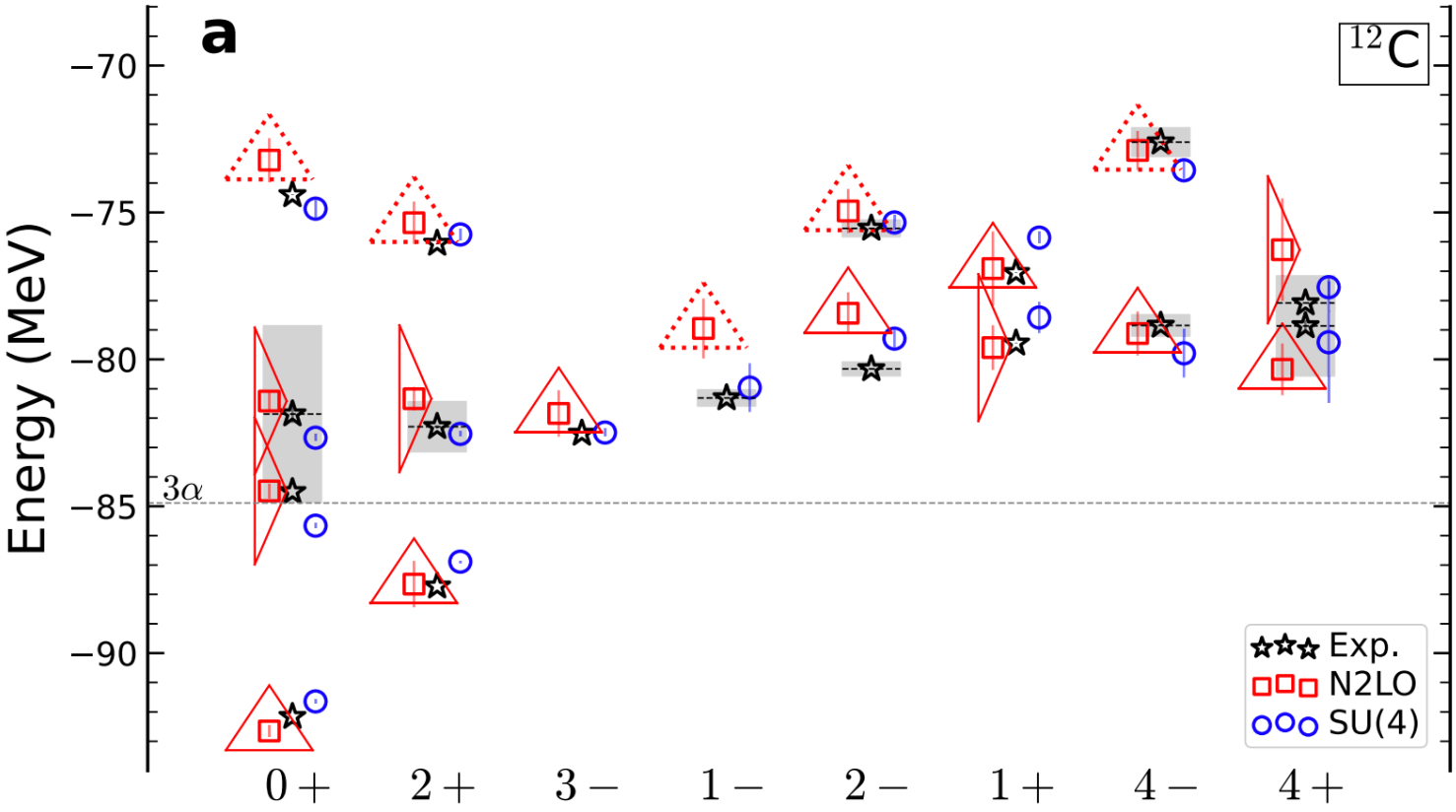


Shen, Elhatisari, Lähde, D.L., Lu, Meißner, Nature Commun. 14, 2777 (2023)


f
1^-_1
g
4^+_1
h
1^+_2
i
2^+_3
j
4^-_2
z (fm)
y (fm)
6
3
0
−3
−6
k
l
m
n
o
20
8
2
$1d_{3/2}$
$2s_{1/2}$
$1d_{5/2}$
$1p_{1/2}$
$1p_{3/2}$
$1s_{1/2}$

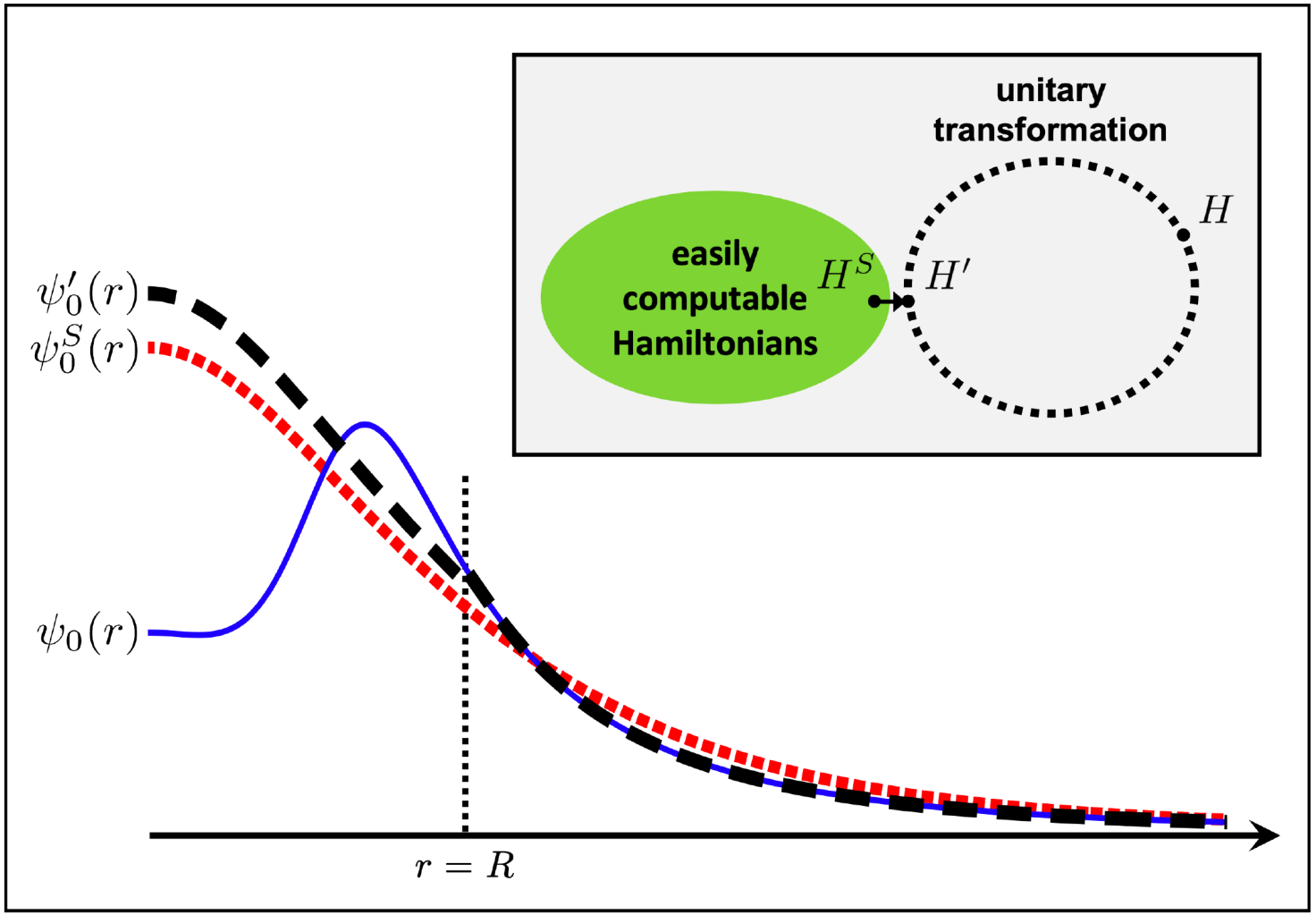


Shen, Elhatisari, Lähde, D.L., Lu, Meißner, Nature Commun. 14, 2777 (2023)



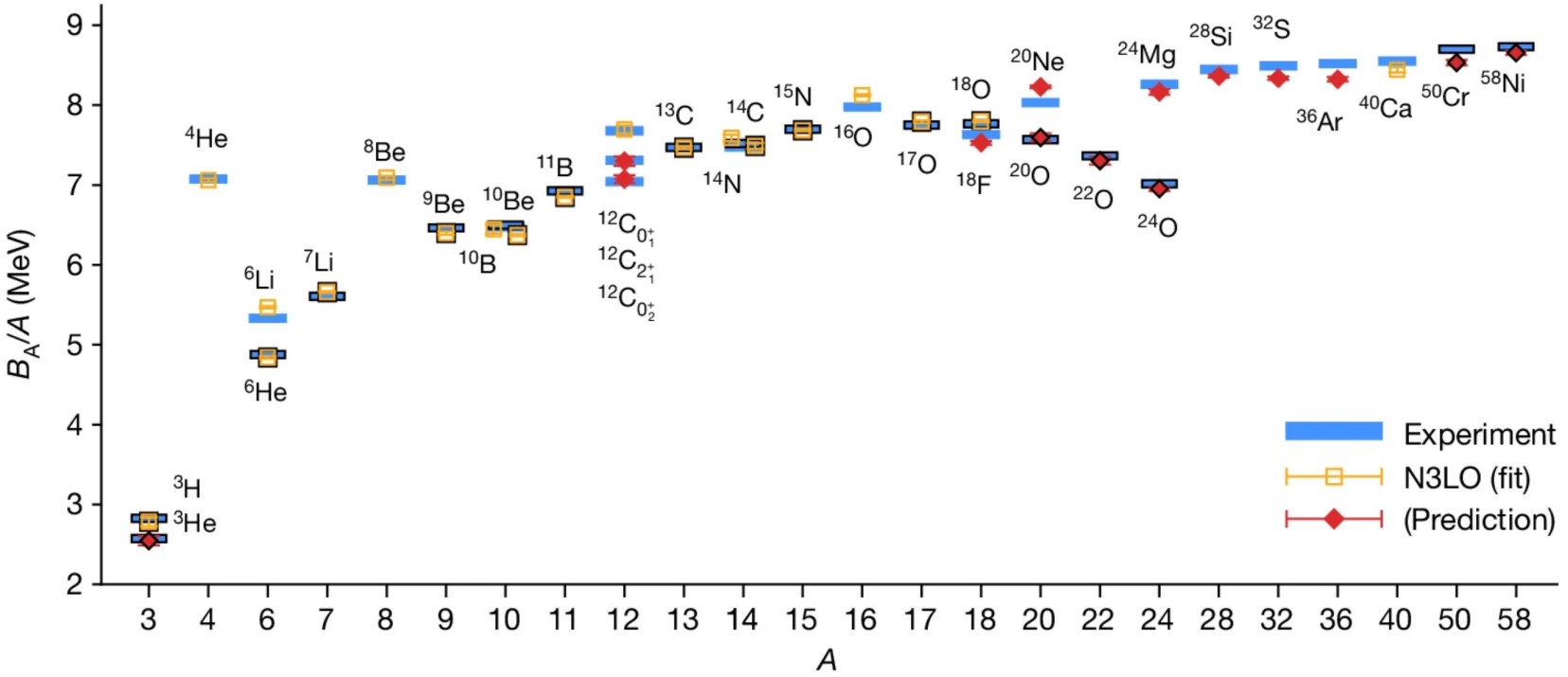
Shen, Elhatisari, Lähde, D.L., Lu, Meißner, Nature Commun. 14, 2777 (2023)

Wavefunction matching



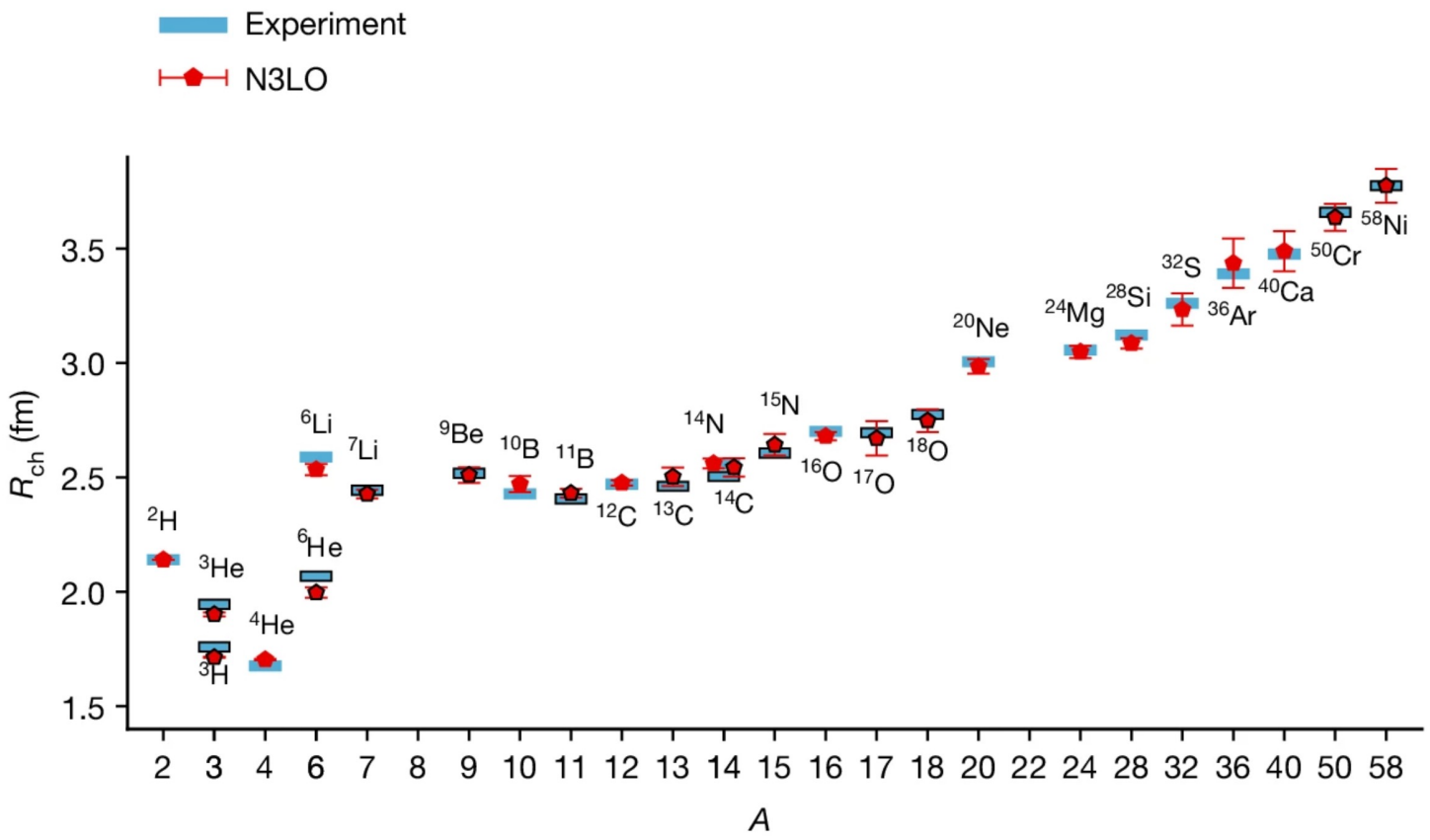
Elhatisari, Bovermann, Ma, Epelbaum, Frame, Hildenbrand, Krebs, Lähde, D.L., Li, Lu, M. Kim, Y. Kim, Meißner, Rupak, Shen, Song, Stellin, Nature 630, 59 (2024)

Binding energies



Elhatisari, Bovermann, Ma, Epelbaum, Frame, Hildenbrand, Krebs, Lähde, D.L., Li, Lu, M. Kim, Y. Kim, Meißner, Rupak, Shen, Song, Stellin, Nature 630, 59 (2024)

Charge radii



Elhatisari, Bovermann, Ma, Epelbaum, Frame, Hildenbrand, Krebs, Lähde, D.L., Li, Lu, M. Kim, Y. Kim, Meißner, Rupak, Shen, Song, Stellin, Nature 630, 59 (2024)

Neutron and nuclear matter

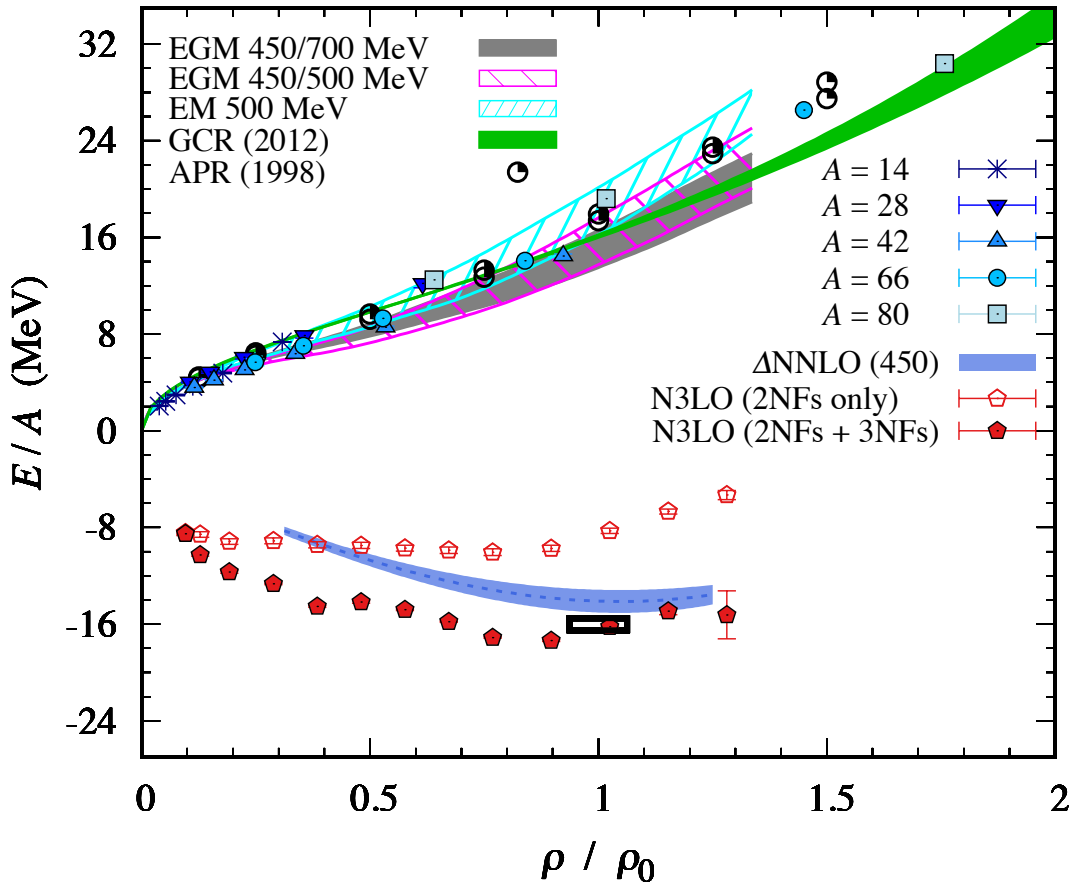
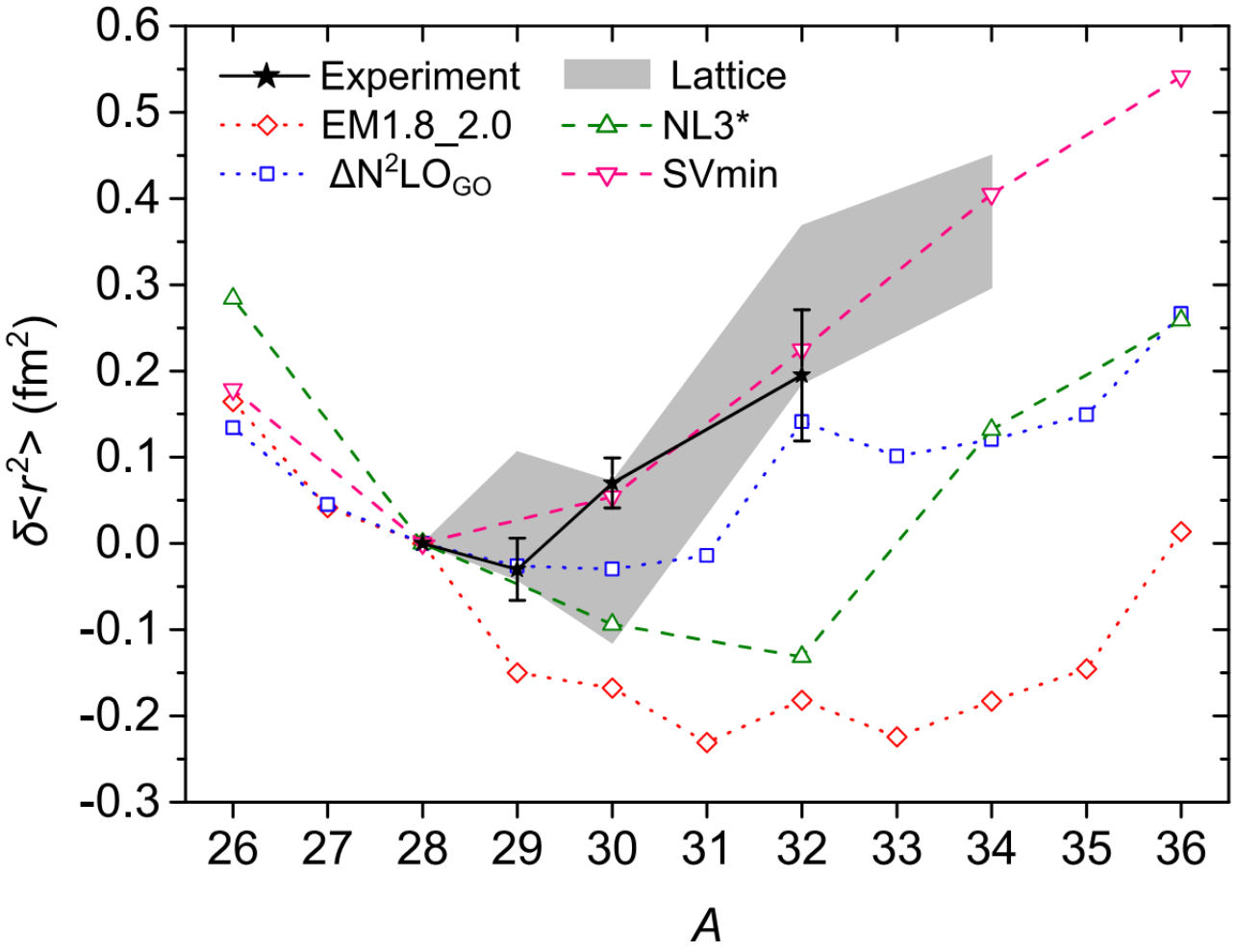


Figure adapted from Tews, Krüger, Hebeler, Schwenk, Phys. Rev. Lett. 110, 032504 (2013)

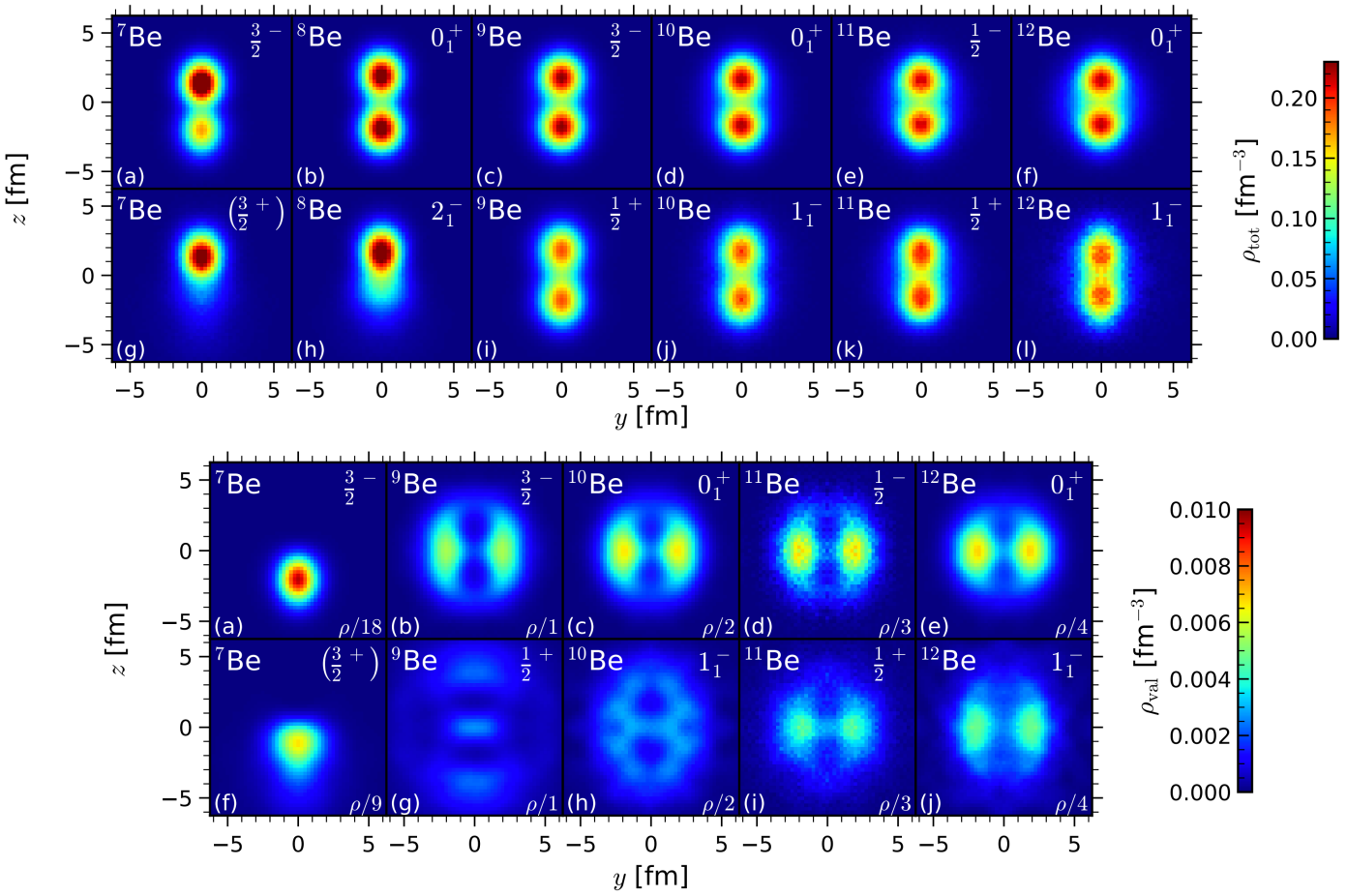
Elhatisari, Bovermann, Ma, Epelbaum, Frame, Hildenbrand, Krebs, Lähde, D.L., Li, Lu, M. Kim, Y. Kim, Meißner, Rupak, Shen, Song, Stellin, Nature 630, 59 (2024)

Charge radii of silicon isotopes



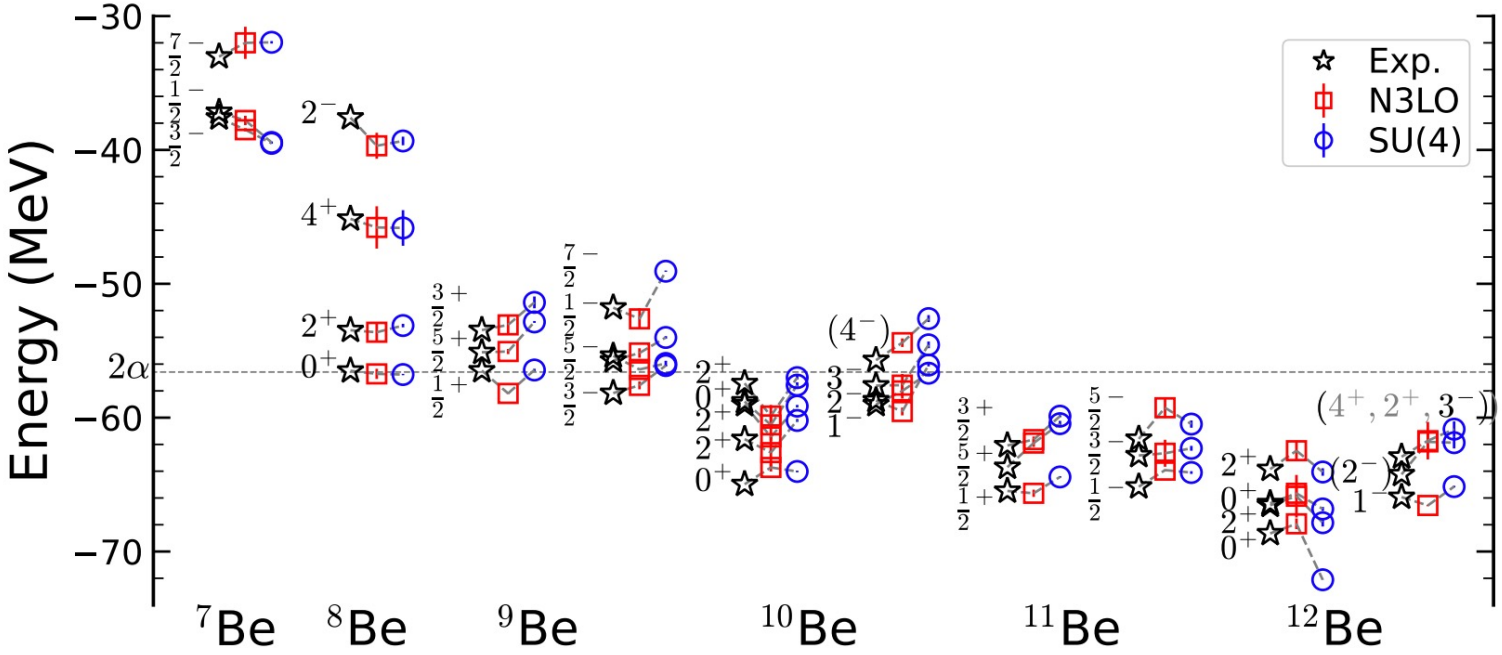
K. König et al., Phys. Rev. Lett. 132, 162502 (2024)

Properties of the beryllium isotopes



Shen, Elhatisari, D.L. Meißner, Ren, PRL 134, 162503 (2025)

Properties of the beryllium isotopes



Shen, Elhatisari, D.L. Meißner, Ren, PRL 134, 162503 (2025)

Parametric Matrix Models

Consider the one-parameter affine problem

$$H(c) = H_0 + cH_1$$

We now do eigenvector continuation with d training vectors. This corresponds to solving the eigenvalue problem for the new one-parameter affine system,

$$M(c) = M_0 + cM_1$$

where the matrices are d by d.

Frame, He, Ipsen, Da. Lee, D.L., Rrapaj, Phys. Rev. Lett. 121, 032501 (2018)

Duguet, Ekström, Furnstahl, König, D.L., Rev. Mod. Phys. 96, 031002 (2024)

Cook, Jammooa, Hjorth-Jensen, Da. Lee, D.L., Nat. Commun. 16, 5929 (2025)

Note that the eigenvalues will be roots of the characteristic polynomial

$$P[E(c)] = \det\left[E(c)I - M(c)\right] = \det\left[E(c)I - M_0 - cM_1\right]$$

The polynomial P will be degree d in with respect to $E(c)$ and degree d with respect to c.

In contrast with polynomial interpolation or rational interpolation (Padé approximants), eigenvector continuation is performing algebraic interpolation using roots of polynomials.

Suppose that we don't have access to the training vectors. We can still make a matrix model

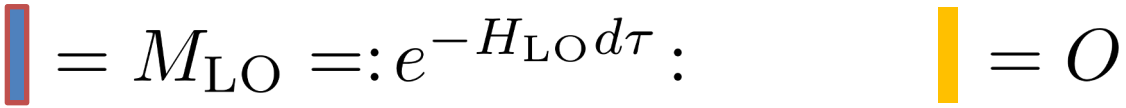
$$M(c) = M_0 + cM_1$$

The unknown elements of these matrices are learned using the training data for the eigenvalues $E(c)$. This is a simple example of a general technique called parametric matrix models (PMM).

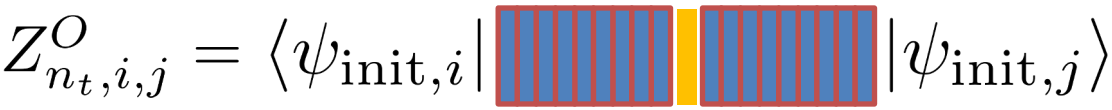
Instead trying to directly fit some output functions, we try to learn the set of matrix equations whose solutions produce the output functions. This is similar to how we usually solve physics problems. We start from the equations.

Cook, Jammooa, Hjorth-Jensen, Da. Lee, D.L., Nat. Commun. 16, 5929 (2025)

Resummation of perturbation theory



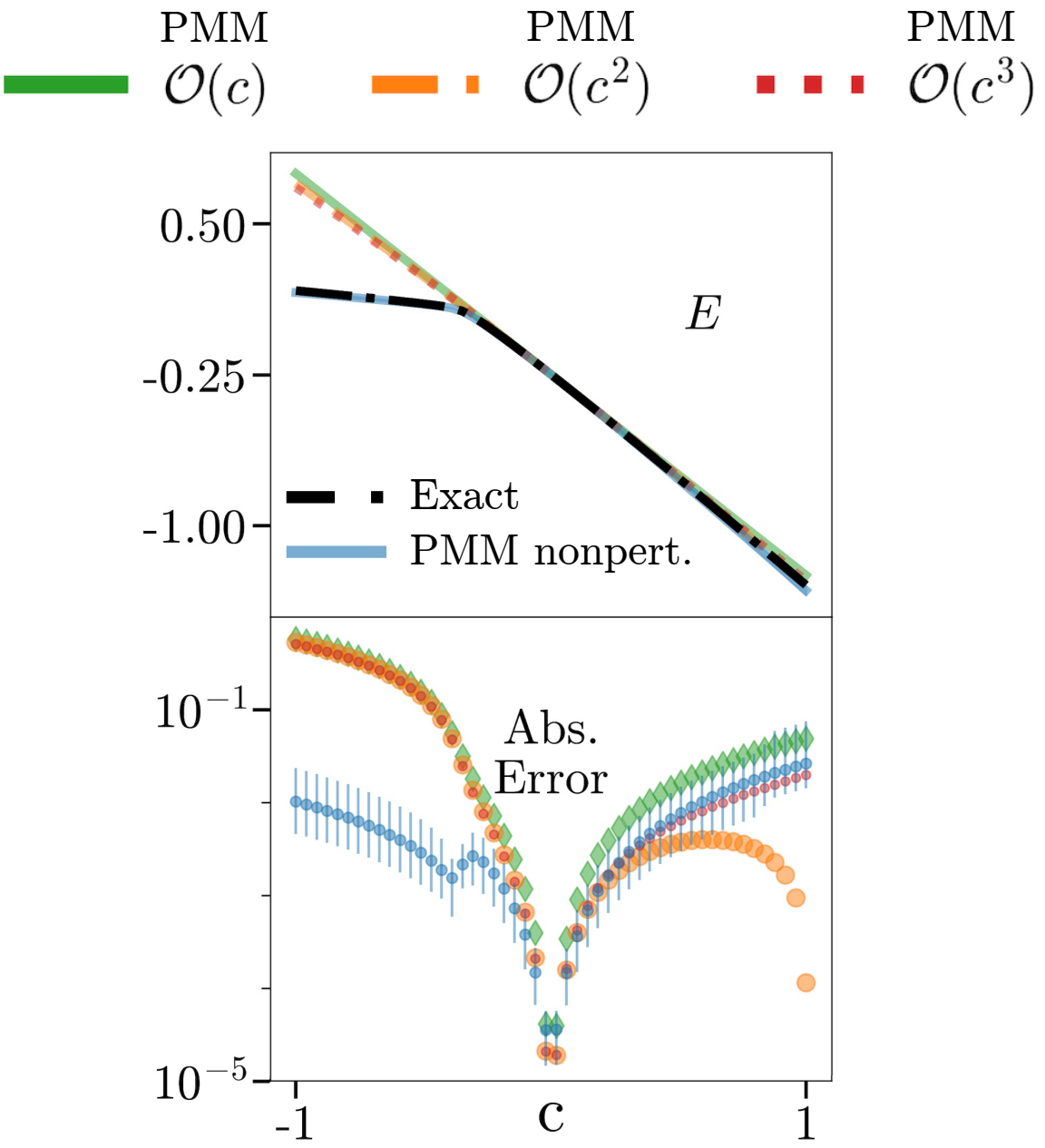




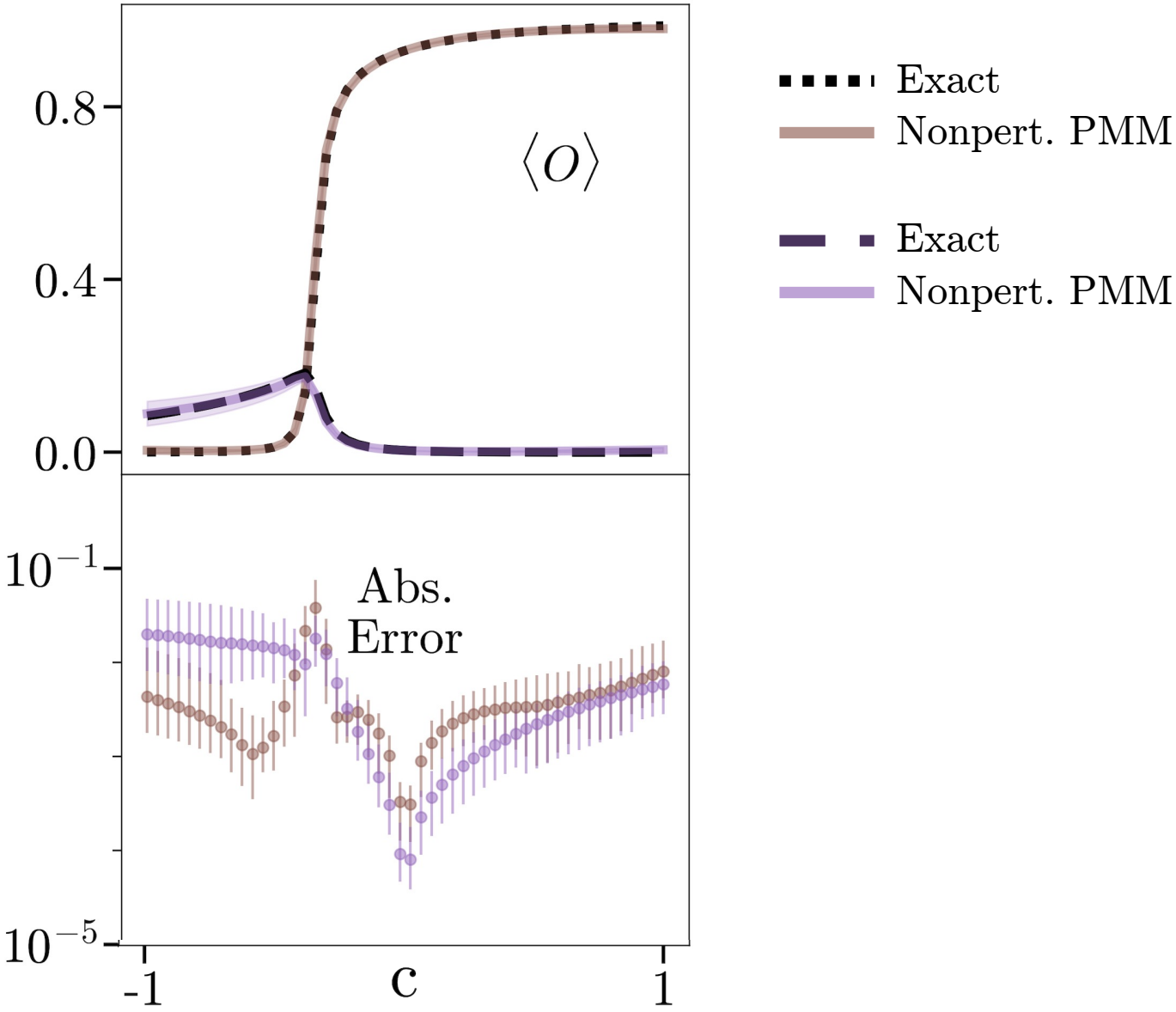
$$O = H_{\mathrm{NLO}}, H_{\mathrm{N^2LO}}, H_{\mathrm{N^3LO}}, \cdots, F[\rho(\vec{r})], \cdots$$

Make a low-dimensional parametric matrix model to represent vectors and matrices in the subspace of low-energy states of H_{LO}. Then diagonalize to get nonperturbative eigenvectors. Extrapolate in the dimensions of the parametric model to eliminate systematic errors.

Jammooa, Cook, Ma, et al., work in progress

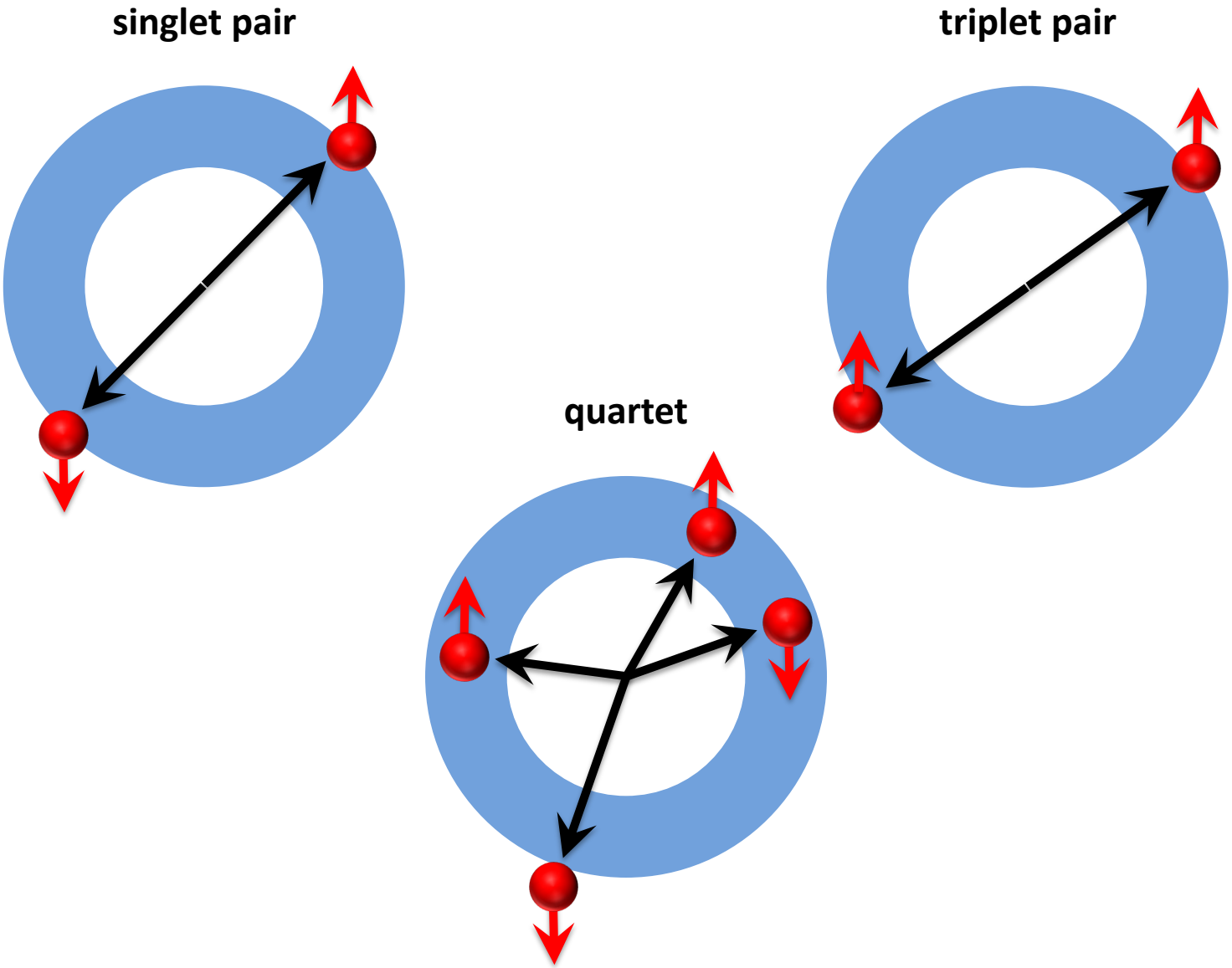


Jammooa, Cook, Ma, et al., work in progress



Jammooa, Cook, Ma, et al., work in progress

Multimodal superfluidity



Multimodal superfluidity of neutrons

$$N_\uparrow = 19, N_\downarrow = 19$$
$$N_\uparrow = 20, N_\downarrow = 19$$
$$N_\uparrow = 21, N_\downarrow = 19$$
$$N_\uparrow = 20, N_\downarrow = 20$$

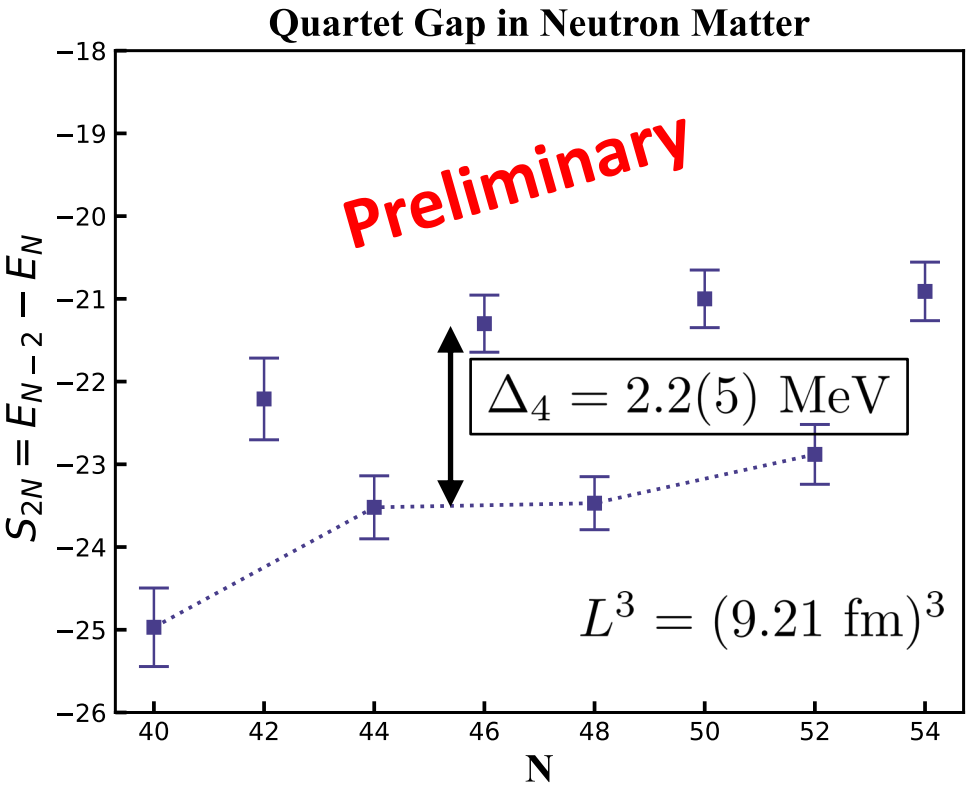
$$L^3 = (9.21 \text{ fm})^3$$
$$k_F = 190 \text{ MeV}$$
$$E_F = 19 \text{ MeV}$$

$$\Delta_{^1S_0} = 3.4(6) \text{ MeV}$$
$$\Delta_{^3P_0} = 1.0(5) \text{ MeV}$$
$$\Delta_{^3P_1} = -0.1(7) \text{ MeV}$$
$$\Delta_{^3P_2} = 1.1(6) \text{ MeV}$$

Preliminary

Ma, Palkanoglou, Carlson, Gandolfi, Gezerlis,
D.L., Schmidt, Reddy, Yu, in progress

Multimodal superfluidity of neutrons



Ma, Palkanoglou, Carlson, Gandolfi, Gezerlis,
D.L., Schmidt, Reddy, Yu, in progress

Experimental evidence for spin-triplet pairing?

$^{18}\mathrm{O}\ (1^+)$ at 8.817 MeV excitation energy and width 0.070 MeV

$$B(^{17}\mathrm{O}, \tfrac{5}{2}^+) - B(^{16}\mathrm{O}, 0^+) = 4.143 \text{ MeV}$$
$$B(^{19}\mathrm{O}, \tfrac{5}{2}^+) - B(^{18}\mathrm{O}, 0^+) = 3.956 \text{ MeV}$$
$$B(^{17}\mathrm{O}, \tfrac{3}{2}^+) - B(^{16}\mathrm{O}, 0^+) = -0.944 \text{ MeV}$$
$$B(^{18}\mathrm{O}, (1^+)) - B(^{16}\mathrm{O}, 0^+) = 3.371 \text{ MeV}$$

$$3.371 - [\tfrac{1}{2}(4.143 + 3.956) + -0.944] = 0.266 \text{ MeV}$$

Ma, Palkanoglou, Carlson, Gandolfi, Gezerlis,
D.L., Schmidt, Reddy, Yu, in progress

Experimental evidence for spin-triplet pairing?

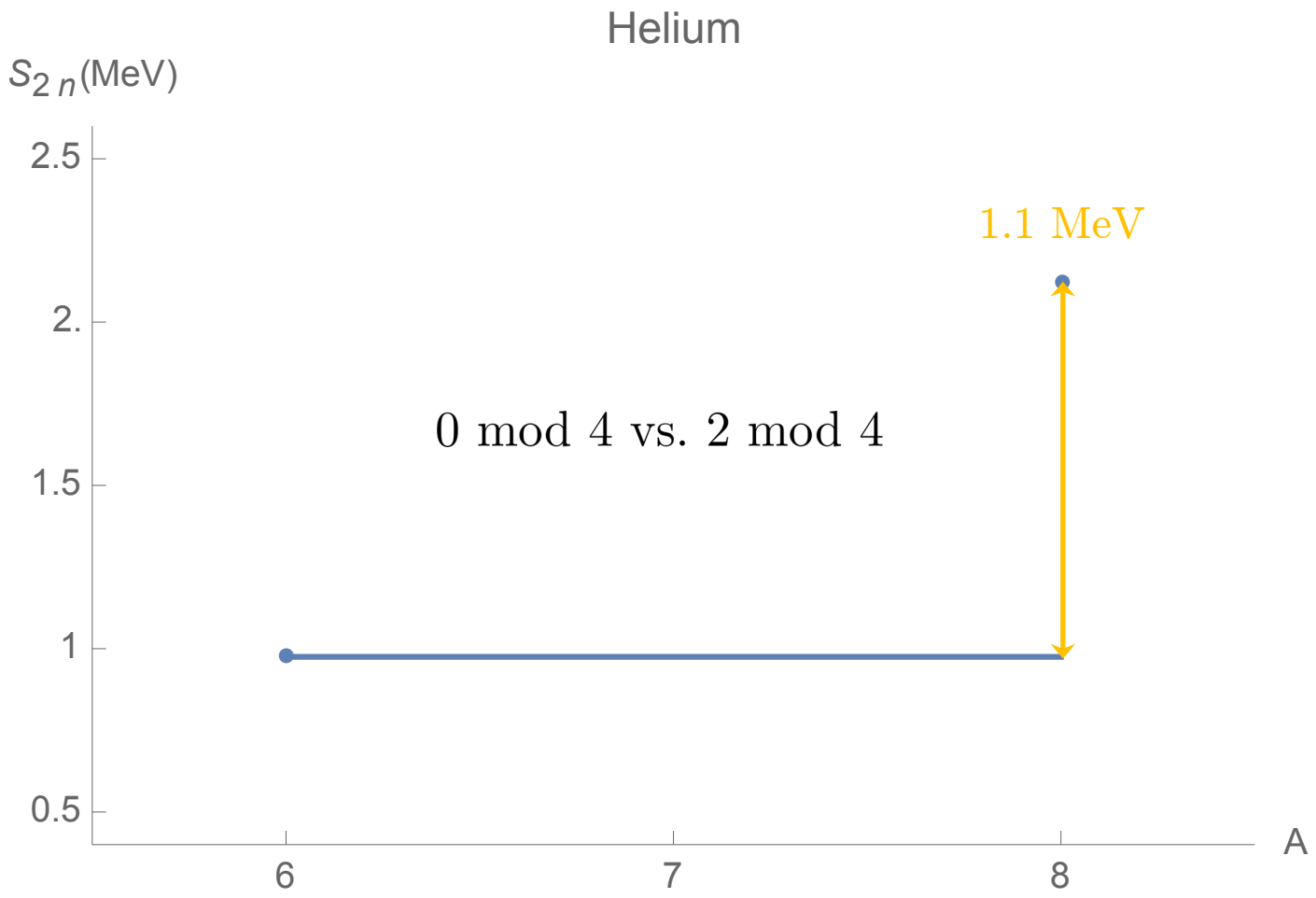
^{58}Ni 1^+ at 2.902 MeV excitation energy

$$B(^{57}\mathrm{O}, \tfrac{3}{2}^-) - B(^{56}\mathrm{O}, 0^+) = 10.248 \text{ MeV}$$
$$B(^{59}\mathrm{O}, \tfrac{3}{2}^-) - B(^{58}\mathrm{O}, 0^+) = 8.999 \text{ MeV}$$
$$B(^{57}\mathrm{O}, \tfrac{5}{2}^-) - B(^{56}\mathrm{O}, 0^+) = 9.479 \text{ MeV}$$
$$B(^{58}\mathrm{O}, 1^+) - B(^{56}\mathrm{O}, 0^+) = 19.562 \text{ MeV}$$

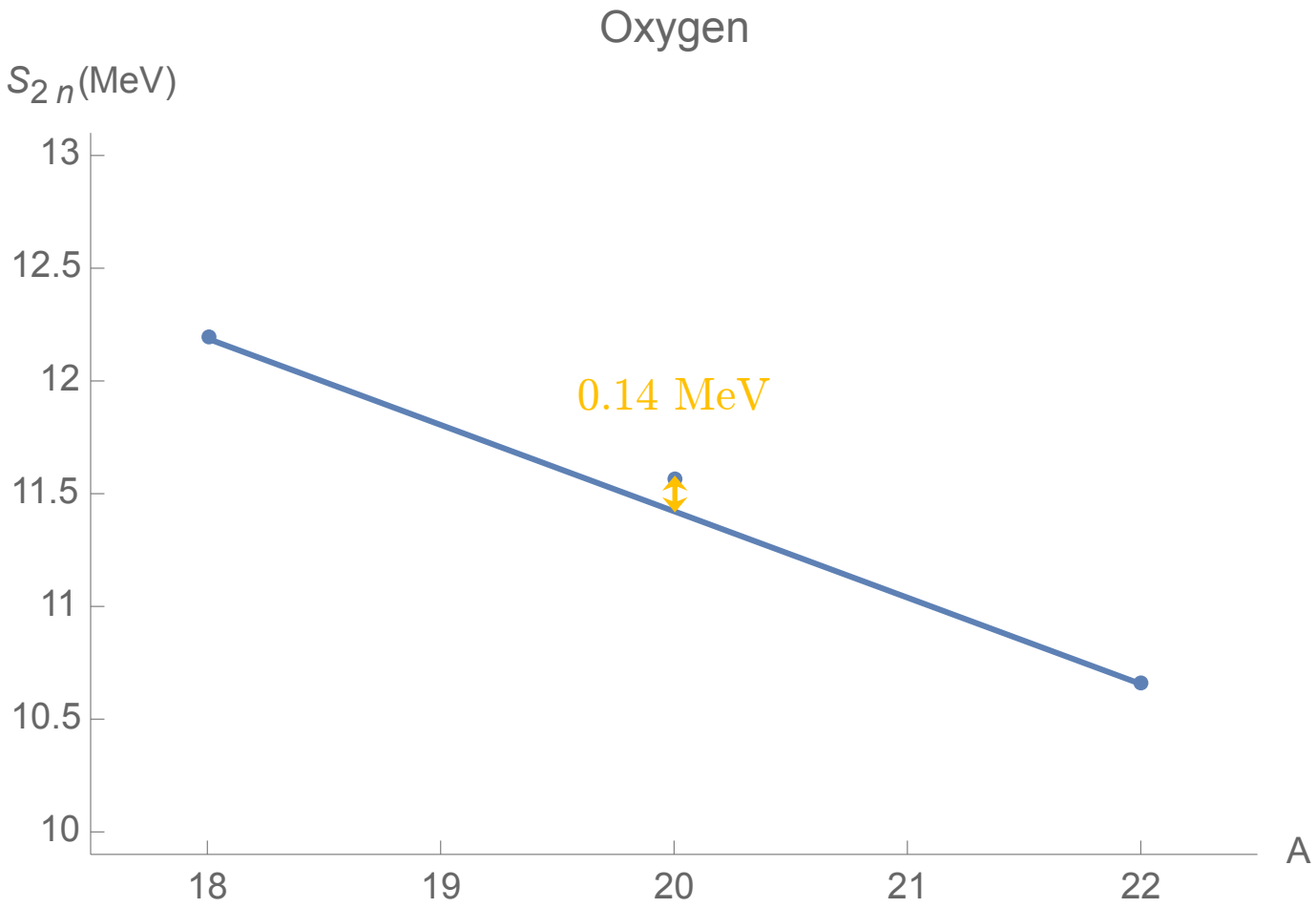
$$19.562 - [\tfrac{1}{2}(10.248 + 8.999) + 9.479] = 0.460 \text{ MeV}$$

Ma, Palkanoglou, Carlson, Gandolfi, Gezerlis,
D.L., Schmidt, Reddy, Yu, in progress

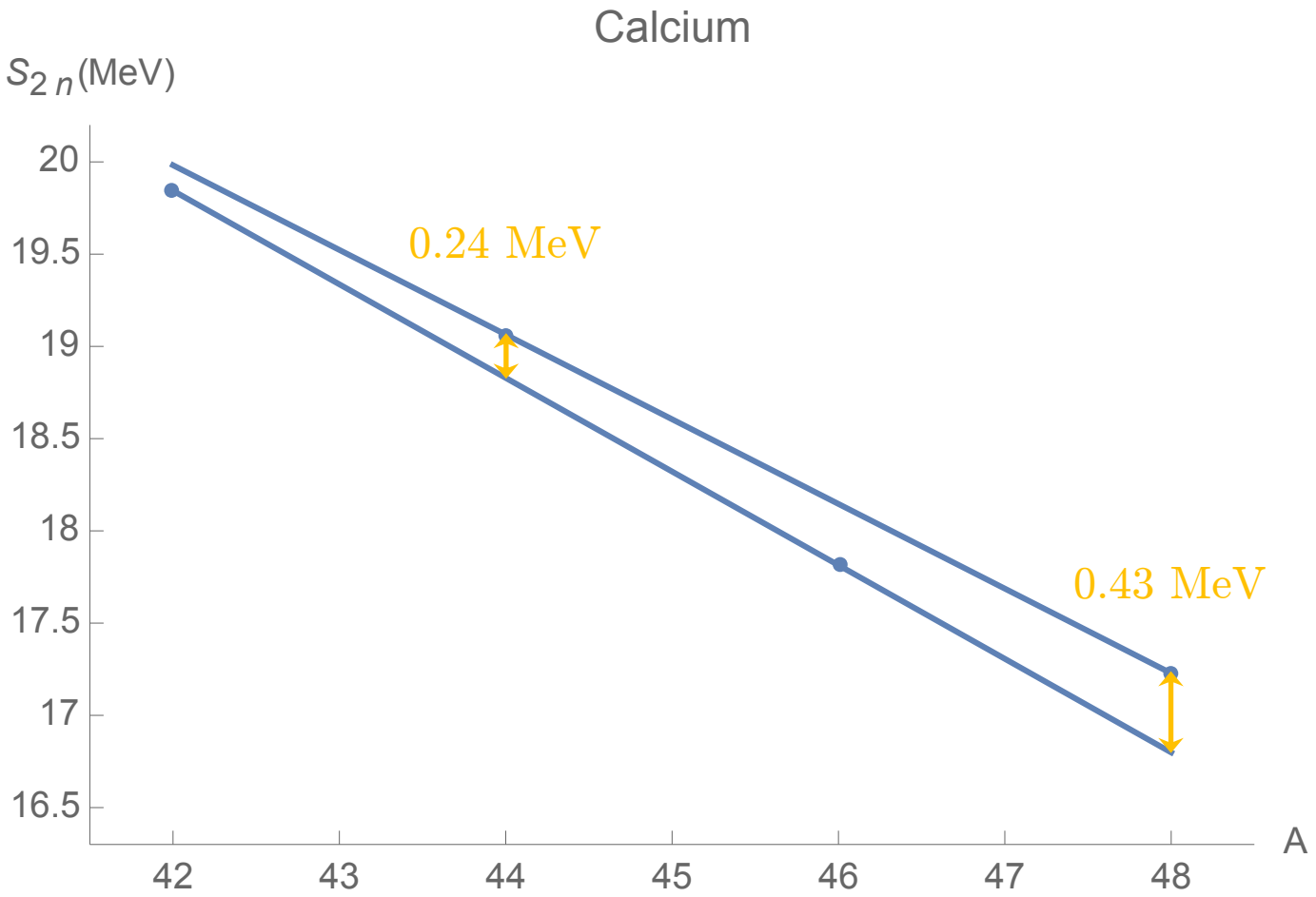
Experimental evidence for quartets?



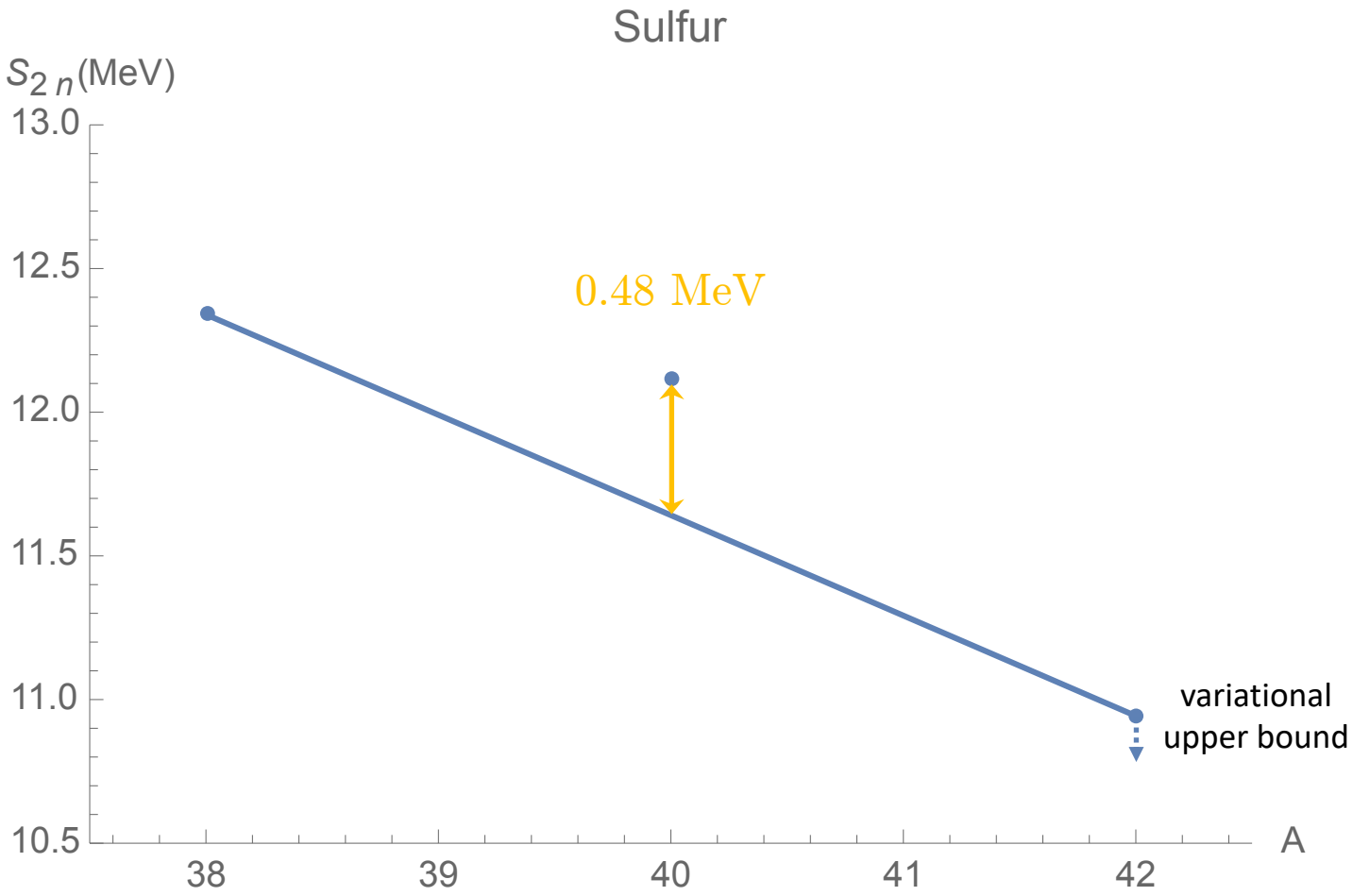
Ma, Palkanoglou, Carlson, Gandolfi, Gezerlis, Given, D.L., Schmidt, Reddy, Yu, in progress



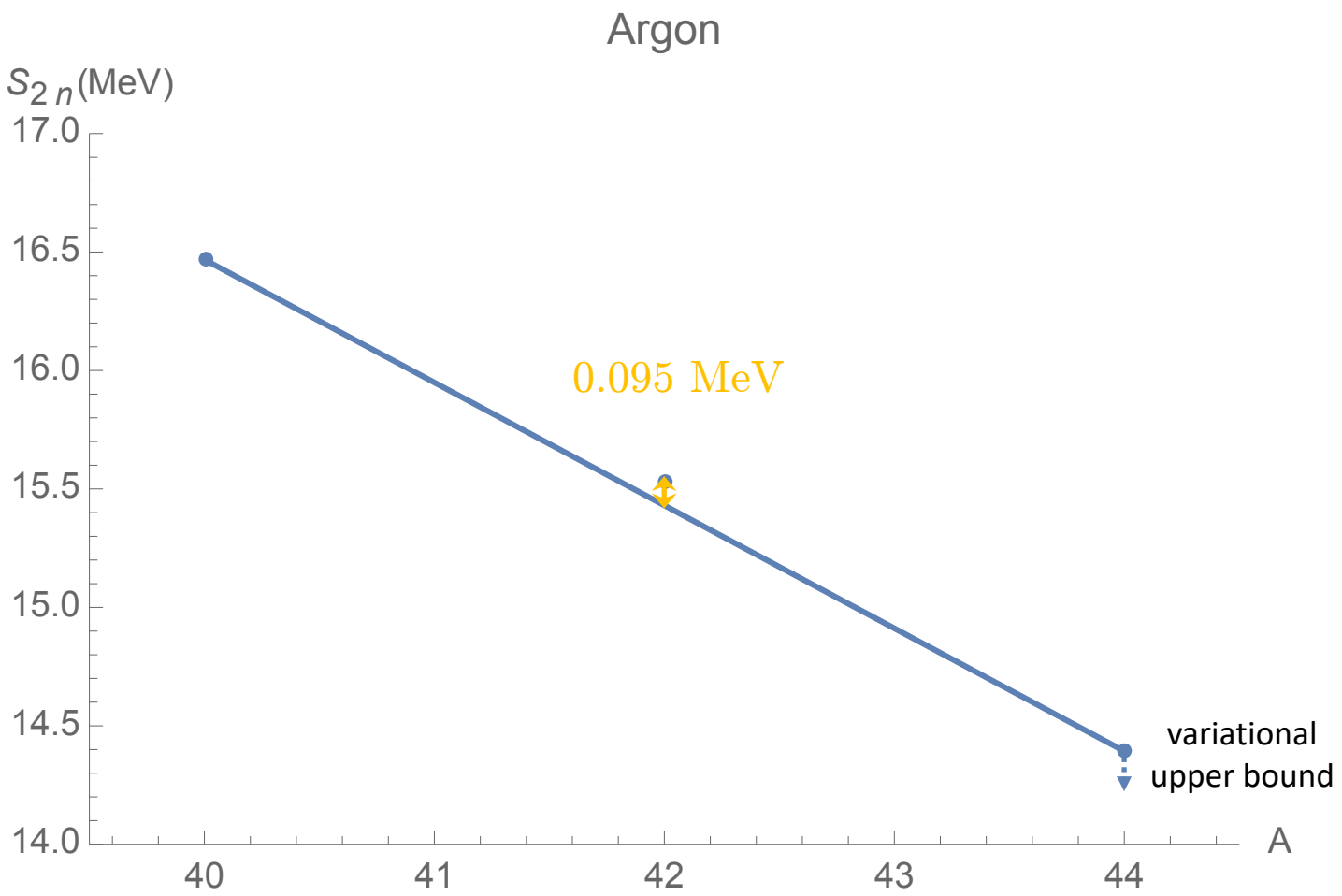
Ma, Palkanoglou, Carlson, Gandolfi, Gezerlis, Given,
D.L., Schmidt, Reddy, Yu, in progress



Ma, Palkanoglou, Carlson, Gandolfi, Gezerlis, Given,
D.L., Schmidt, Reddy, Yu, in progress



Ma, Palkanoglou, Carlson, Gandolfi, Gezerlis, Given,
D.L., Schmidt, Reddy, Yu, in progress



Ma, Palkanoglou, Carlson, Gandolfi, Gezerlis, Given,
D.L., Schmidt, Reddy, Yu, in progress

Summary

Nuclear lattice effective field theory is being used to perform *ab initio* calculations of precision nuclear structure using new approaches such as wavefunction matching, pinhole algorithms, and parametric matrix models. We are also investigating emergent many-body physics such as clustering and superfluidity. We find both theoretical and experimental evidence for multimodal superfluidity of neutrons in neutron matter as well as neutron-rich atomic nuclei.

Outlook and questions

Some topics that could motivate future studies in precision nuclear structure are the following:

What is the impact of alpha clustering on the charge radius of nuclei?

Can higher order Zemach moments be measured?

Can spin-singlet, spin-triplet, and quartet superfluid correlations be studied in low-energy reactions? In electromagnetic transitions? In multi-neutron emission?