Inter-species pairing and clustering in fermionic matter

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Ab initio many-body calculations:
where has the nuclear pairing gone?
CEA Paris-Saclay
May 21, 2025

Outline

Lattice effective field theory

Spectral convexity theorem

Pinhole algorithm

Emergent geometry and duality of ^{12}C

Wavefunction matching

Charge radii of silicon isotopes

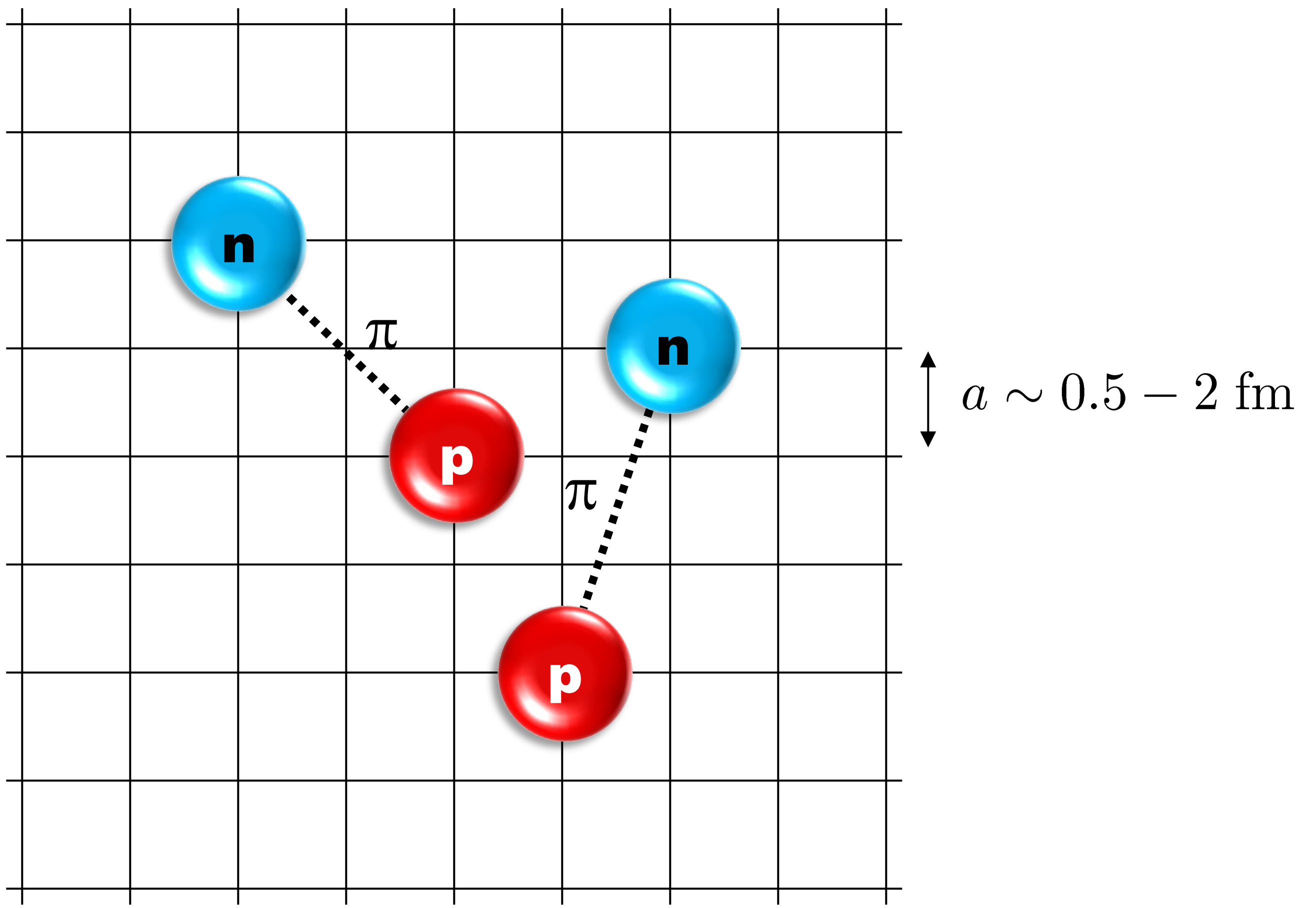
Properties of beryllium isotopes

Superfluid condensation

Multimodal superfluidity

Summary and outlook

Lattice effective field theory

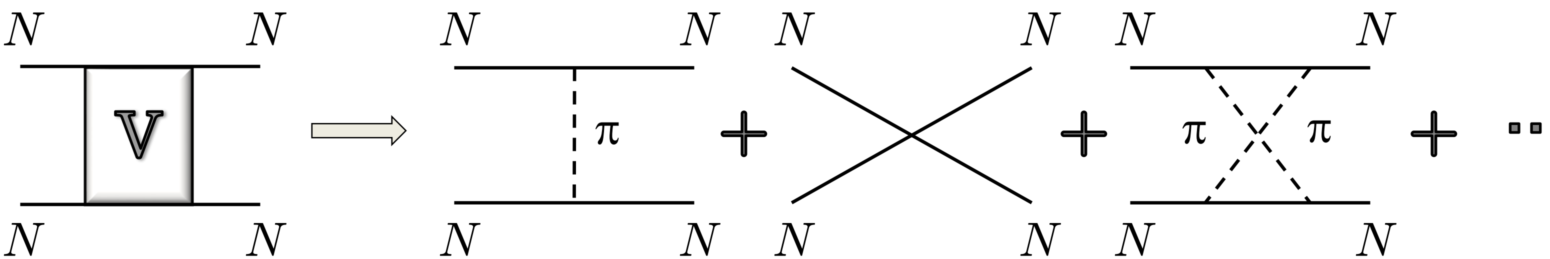


D.L, Prog. Part. Nucl. Phys. 63 117-154 (2009)

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

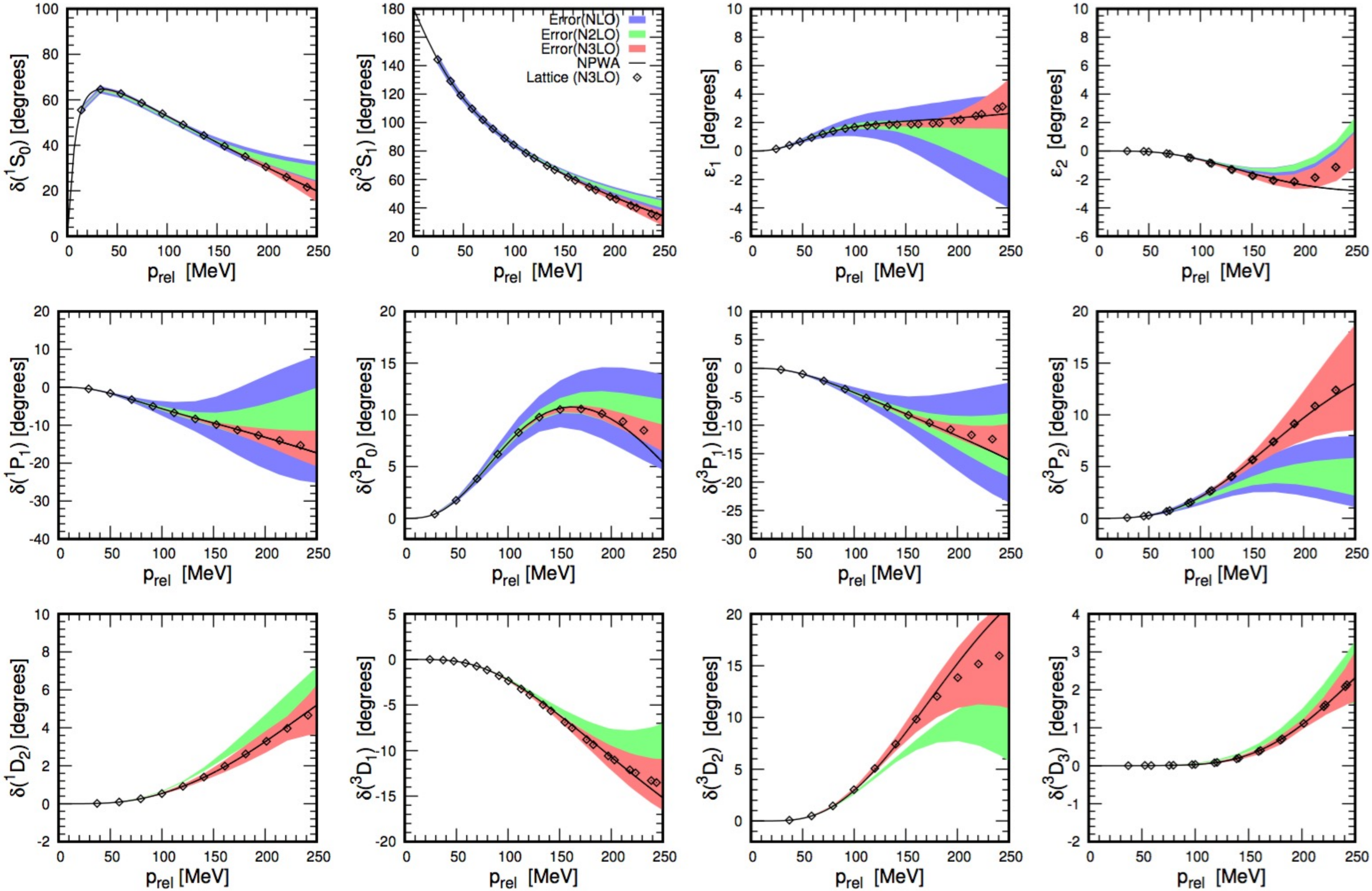
Chiral effective field theory

Construct the effective potential order by order



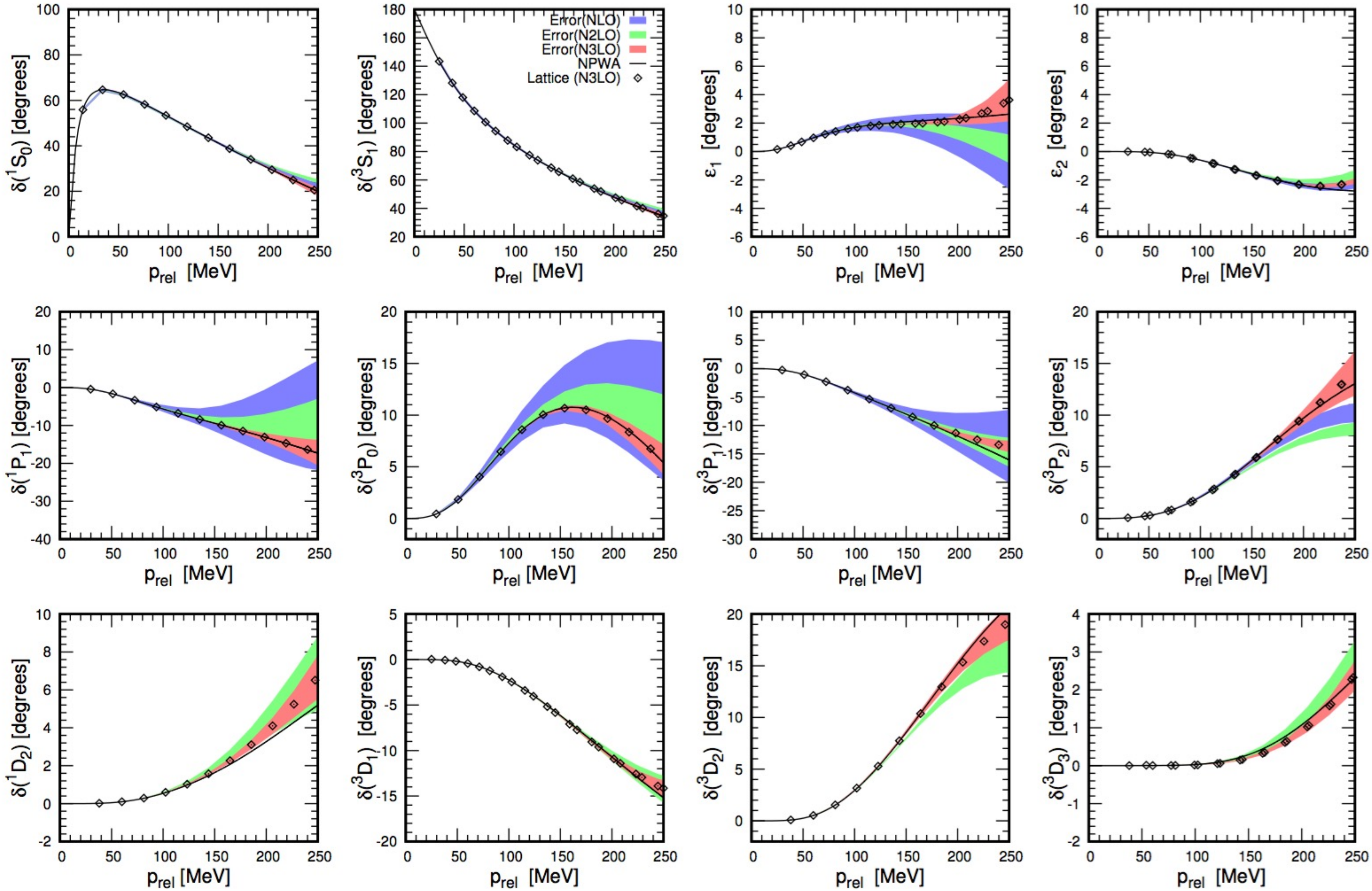
$$\underbrace{V^{\mathrm{OPEP}}\ \text{Contact interactions}}_{\text{Leading order (LO)}}\qquad\underbrace{V^{\mathrm{TPEP}}}_{\text{Next-to-leading order (NLO)}}$$

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

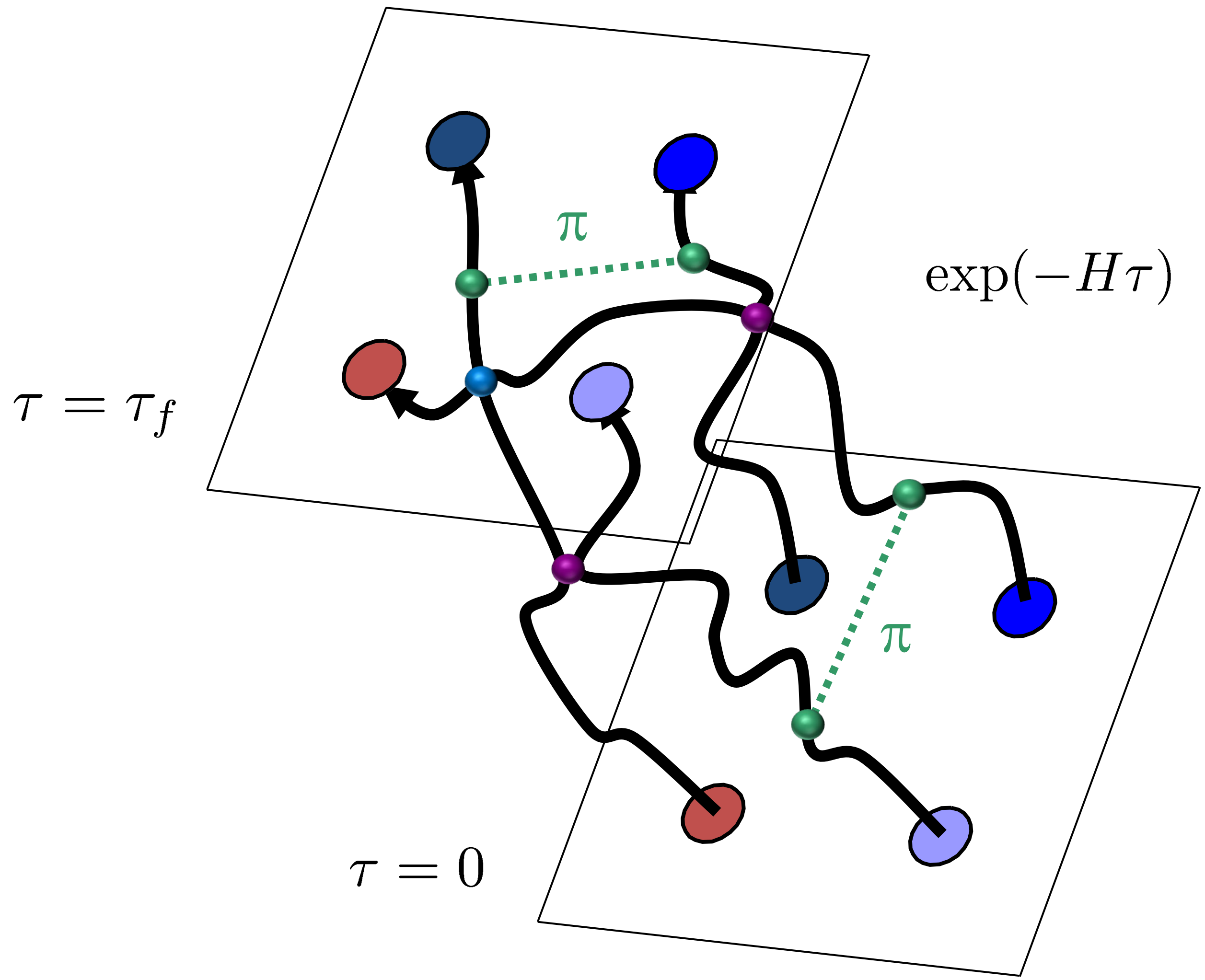


Li, Elhatisari, Epelbaum, D.L., Lu, Meißner, PRC 98, 044002 (2018)

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



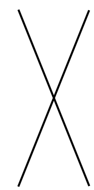
Euclidean time projection



Auxiliary field method

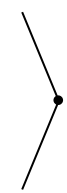
We can write exponentials of the interaction using a Gaussian integral identity

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



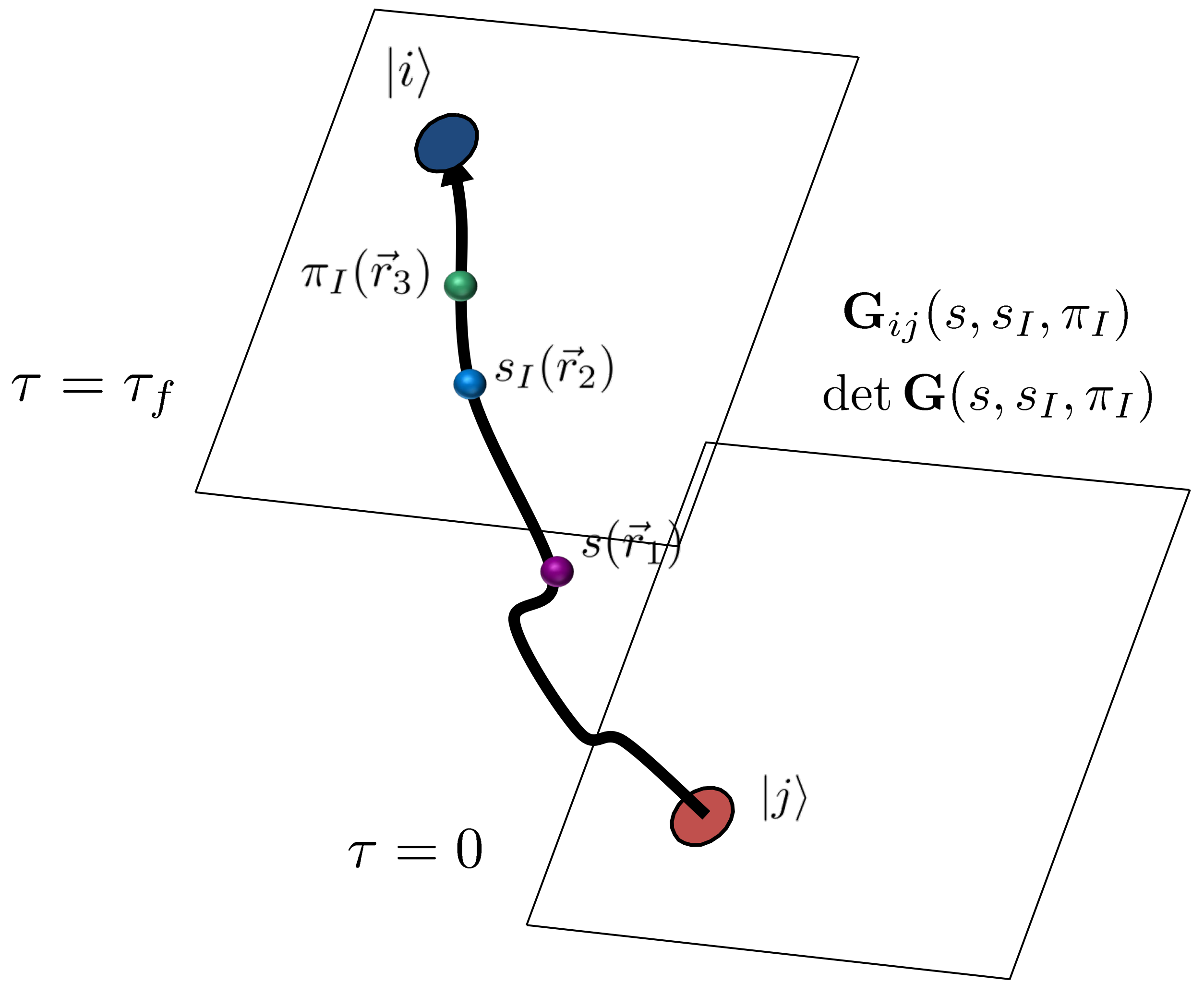
$(N^\dagger N)^2$

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



$sN^\dagger N$

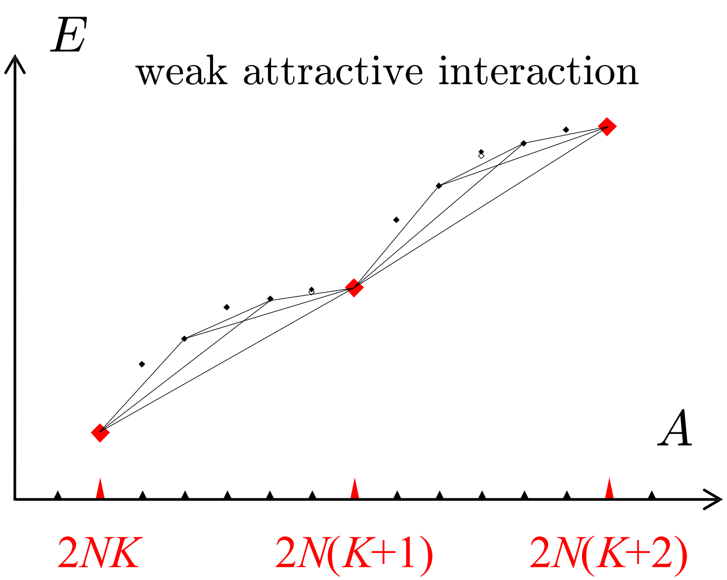
We remove the interaction between nucleons and replace it with the interactions of each nucleon with a background field.

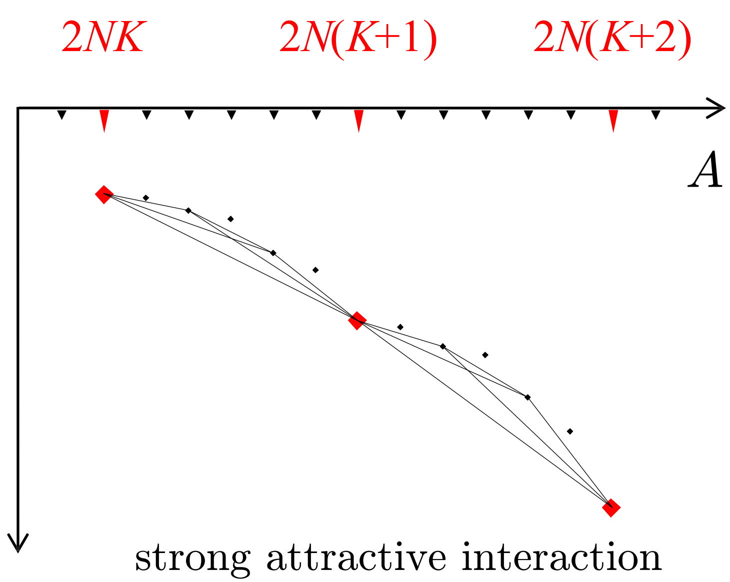

$|i\rangle$
$\pi_I(\vec{r}_3)$
$s_I(\vec{r}_2)$
$\tau = \tau_f$
$\mathbf{G}_{ij}(s, s_I, \pi_I)$
$\det \mathbf{G}(s, s_I, \pi_I)$
$s(\vec{r}_1)$
$|j\rangle$
$\tau = 0$

Spectral convexity theorem

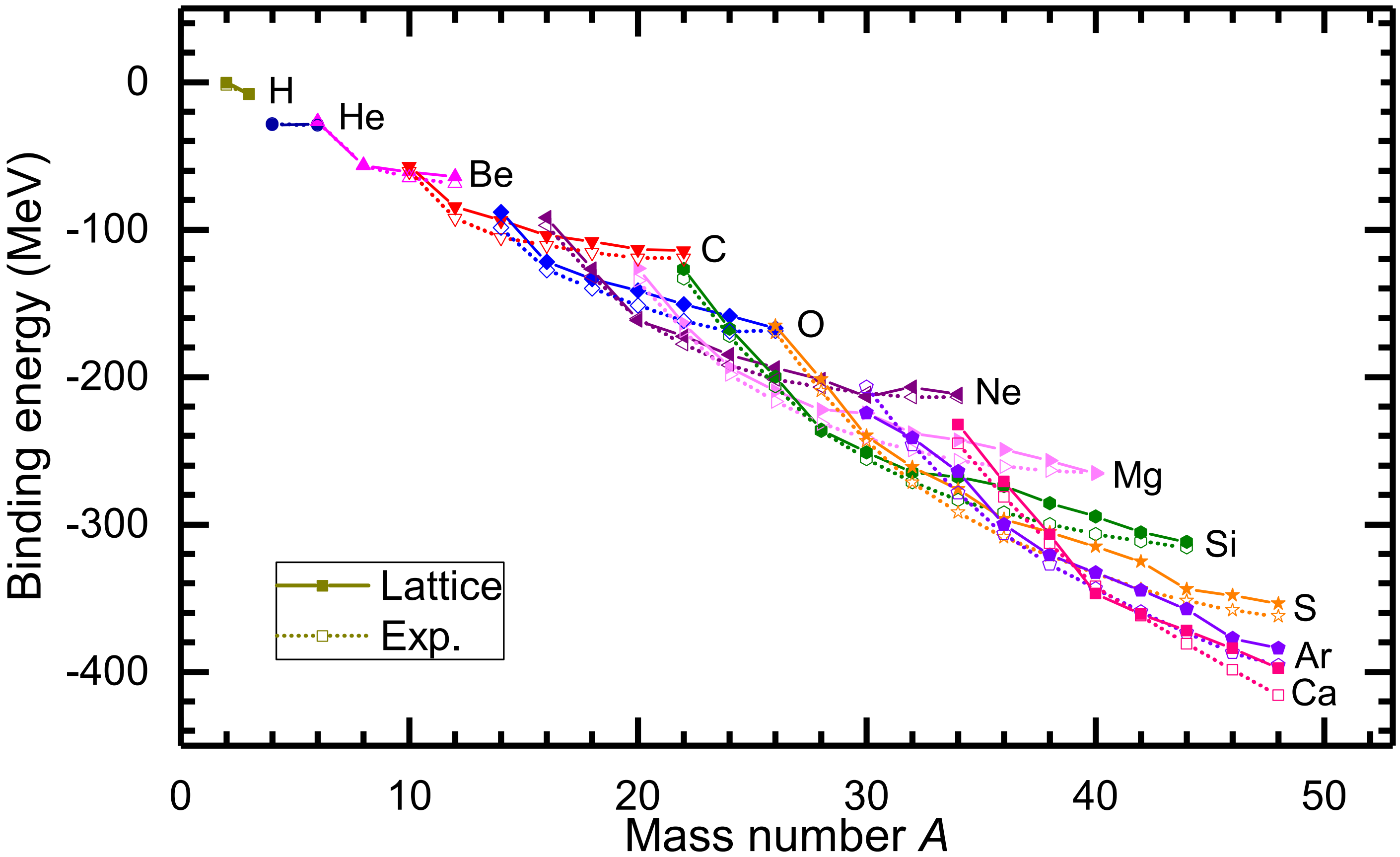
Any fermionic theory with SU($2N$) symmetry that can be simulated without any sign oscillations using auxiliary field Monte Carlo simulations must obey the SU($2N$) convexity bounds illustrated below.

Chen, D.L. Schäfer, Phys. Rev. Lett. 93, 242302 (2004)
D.L., Phys. Rev. Lett. 98, 182501 (2007)



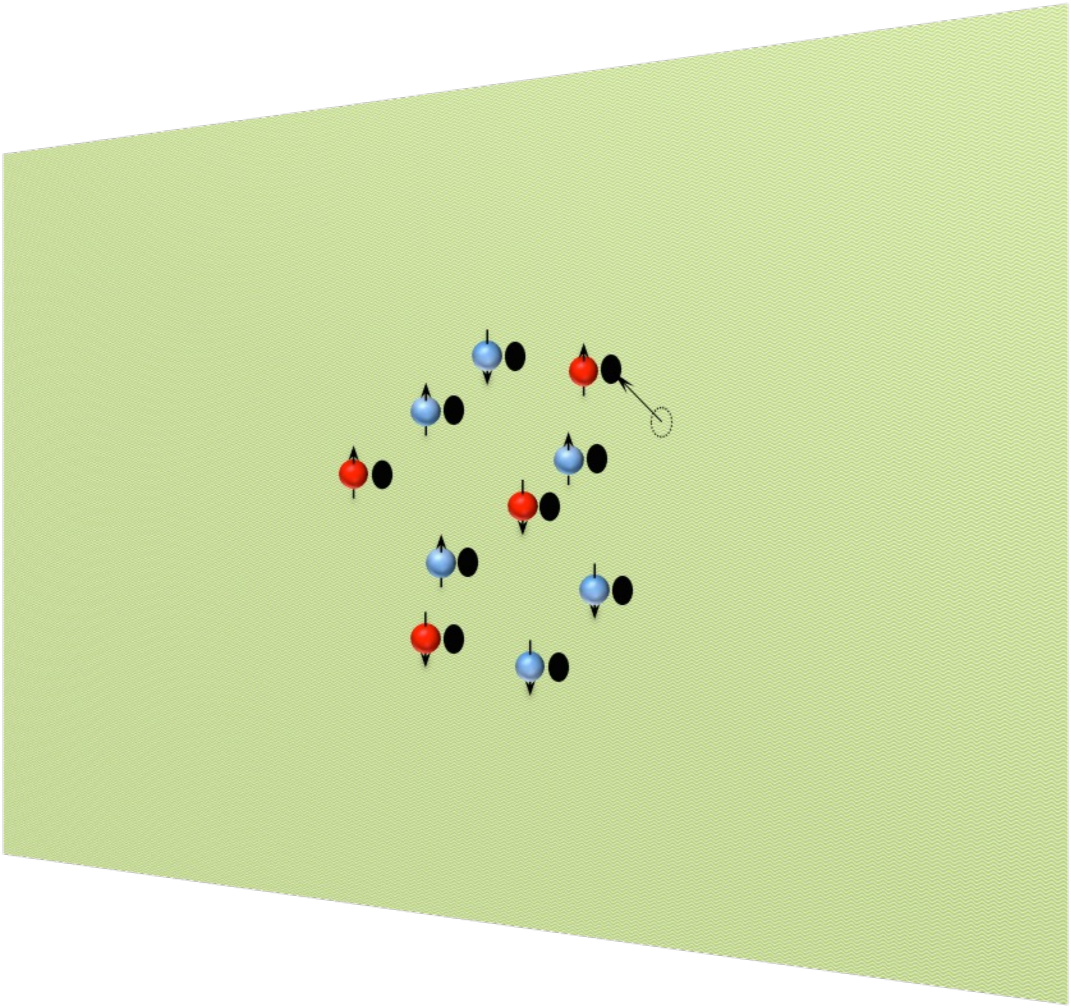


$$H = H_{\text{free}} + \frac{1}{2!} C_2 \sum_{\mathbf{n}} \tilde{\rho}(\mathbf{n})^2 + \frac{1}{3!} C_3 \sum_{\mathbf{n}} \tilde{\rho}(\mathbf{n})^3 + V_{\text{Coulomb}}$$

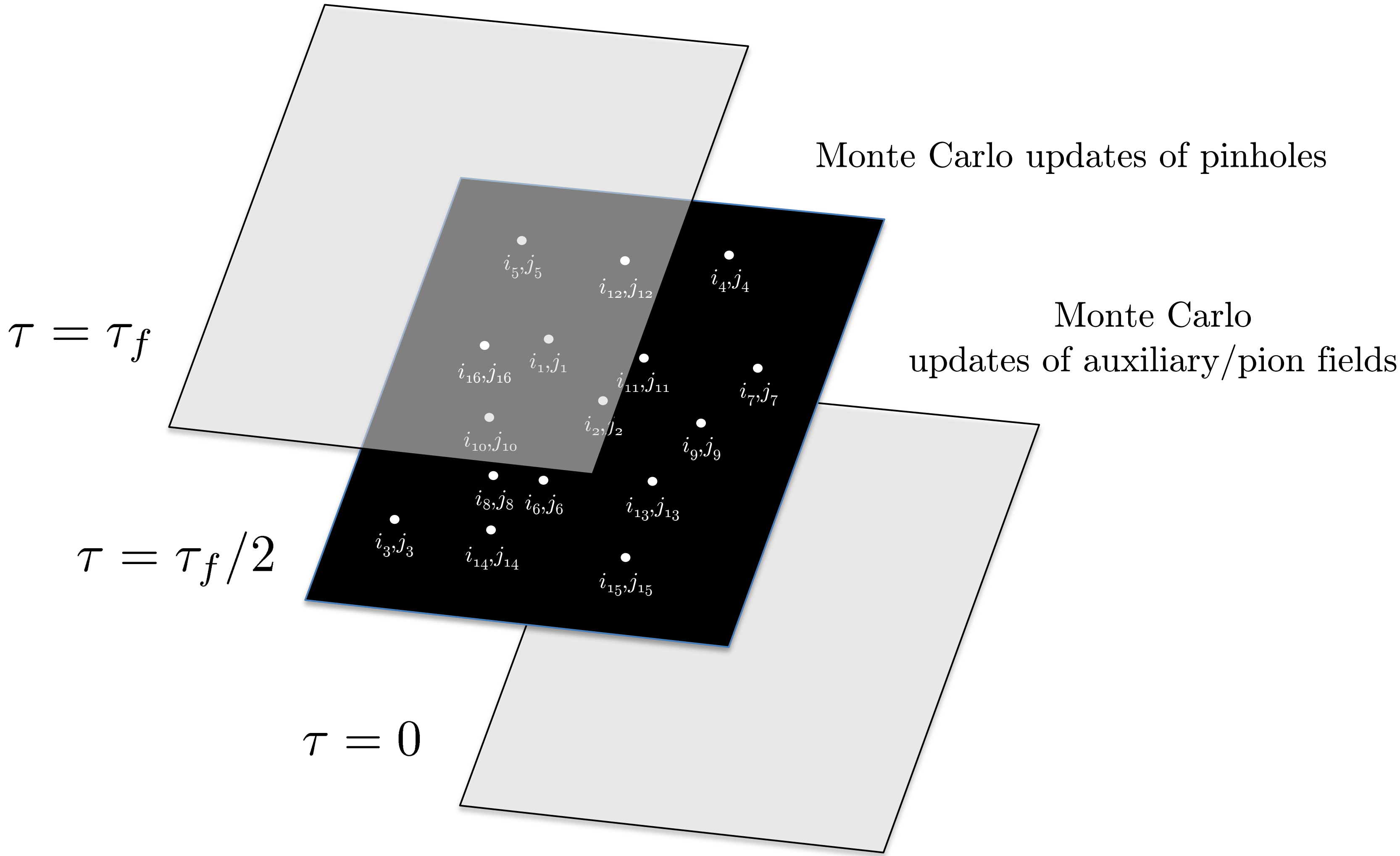


Lu, Li, Elhatisari, D.L., Epelbaum, Meißner, Phys. Lett. B 797, 134863 (2019)

Pinhole algorithm

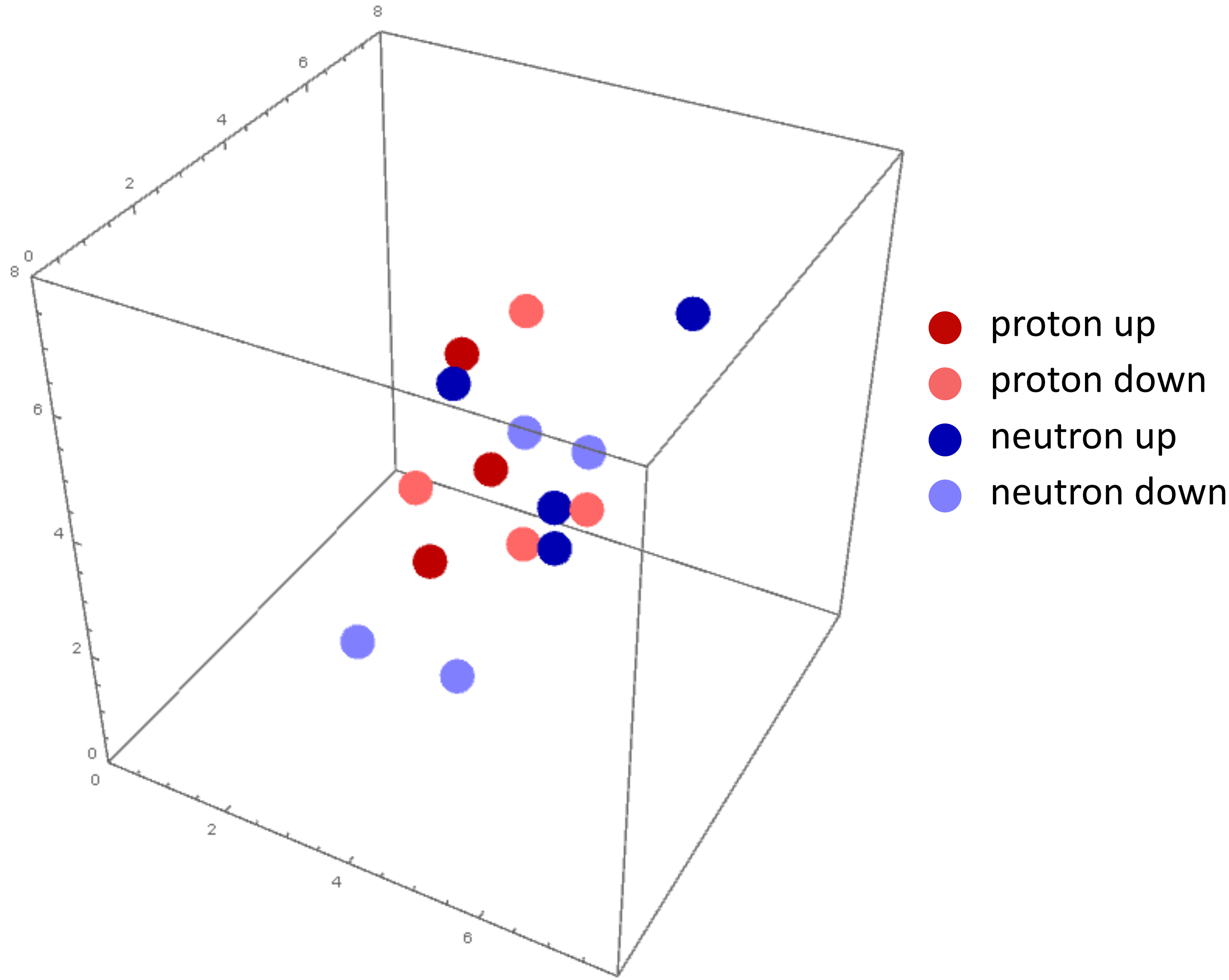


Elhatisari, Epelbaum, Krebs, Lähde, D.L., Li, Lu, Meißner, Rupak, PRL 119, 222505 (2017)



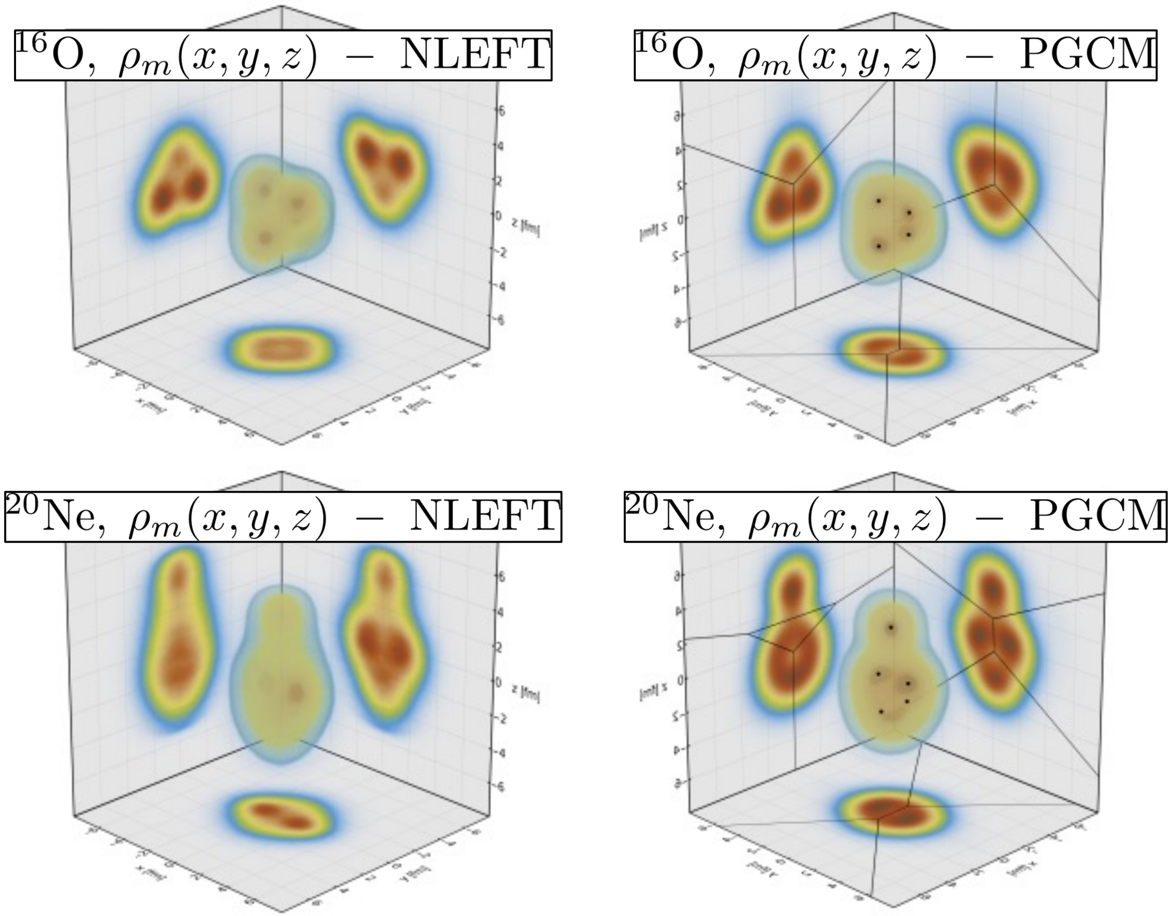
Elhatisari, Epelbaum, Krebs, Lähde, D.L., Li, Lu, Meißner, Rupak, PRL 119, 222505 (2017)

^{16}O



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

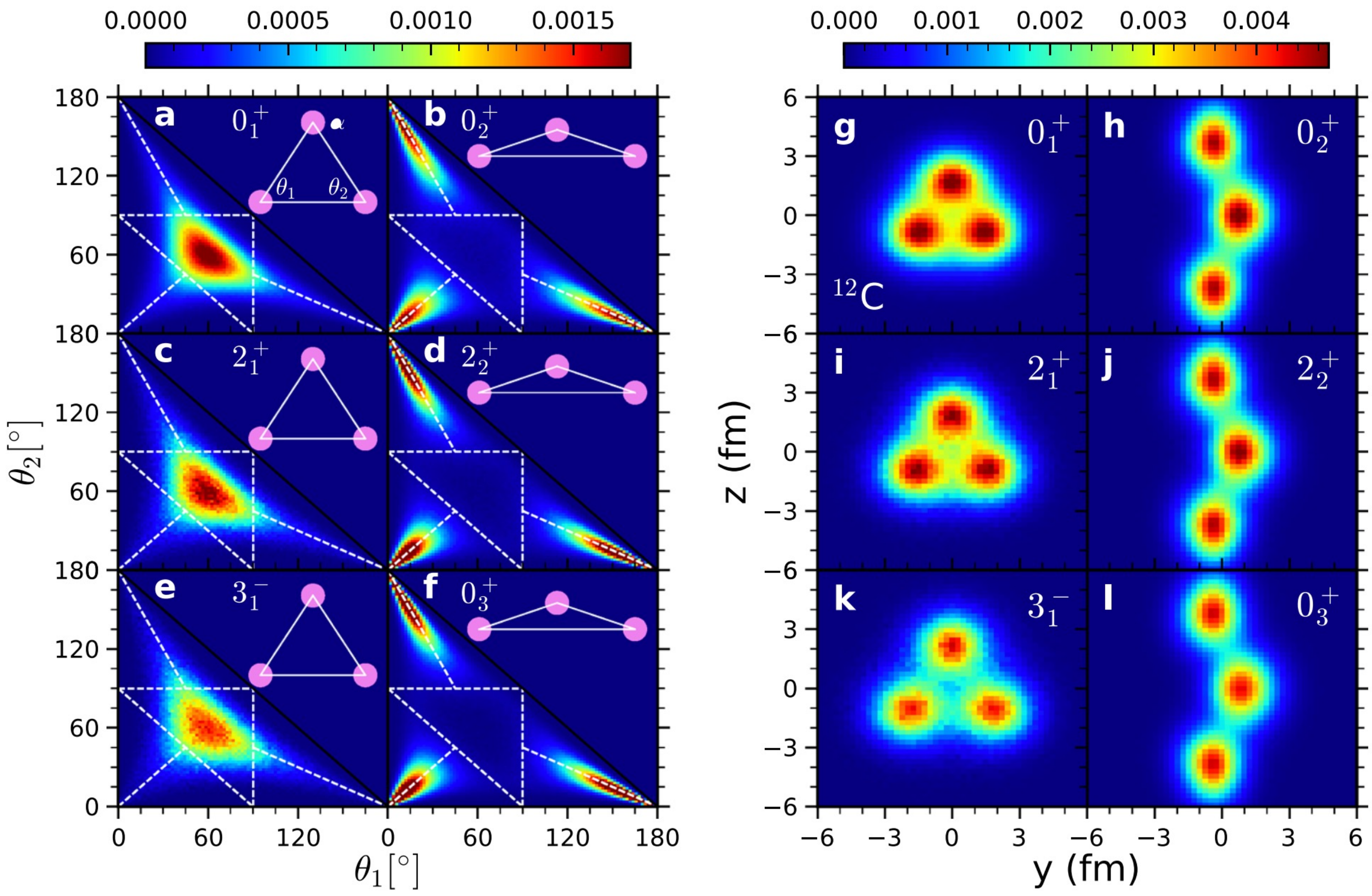
Structure of ^{16}O and ^{20}Ne



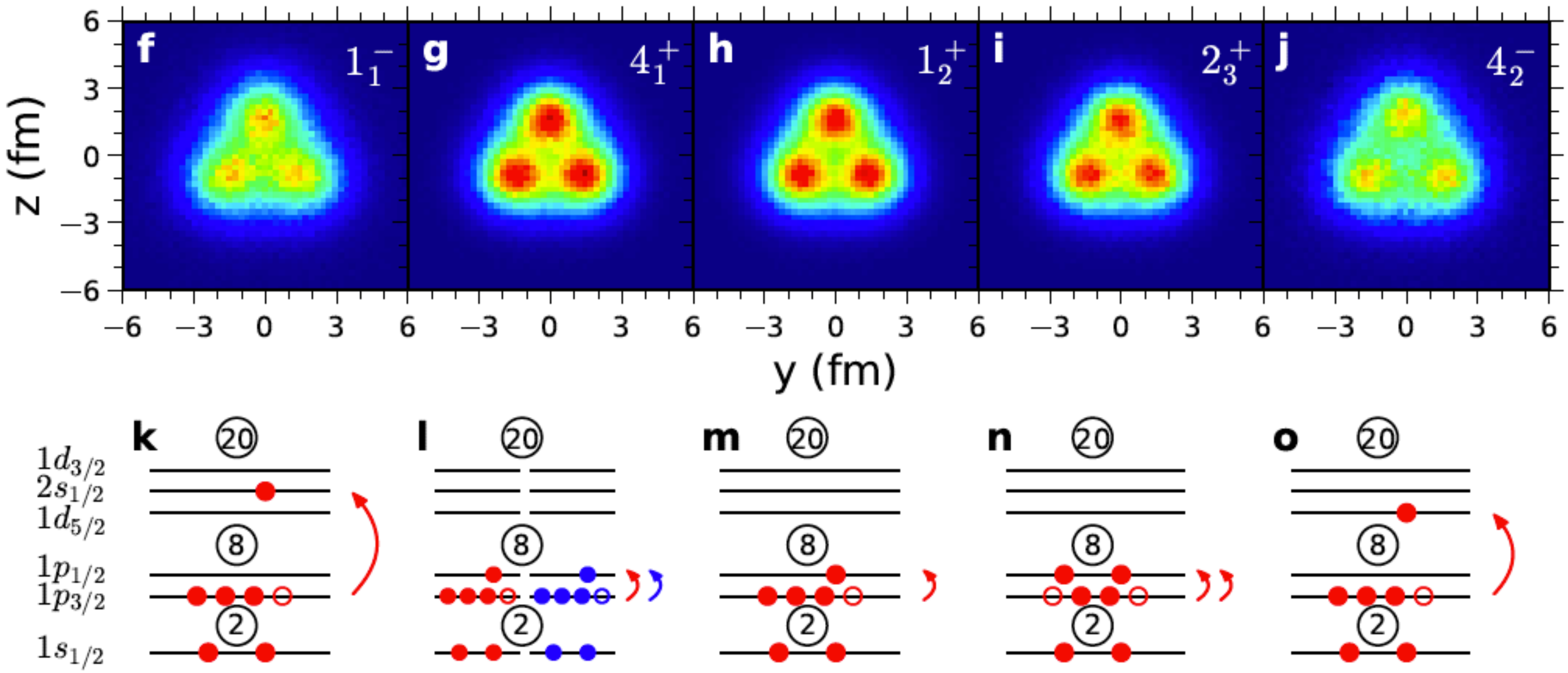
Giacalone et al., arXiv:2402.05995

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

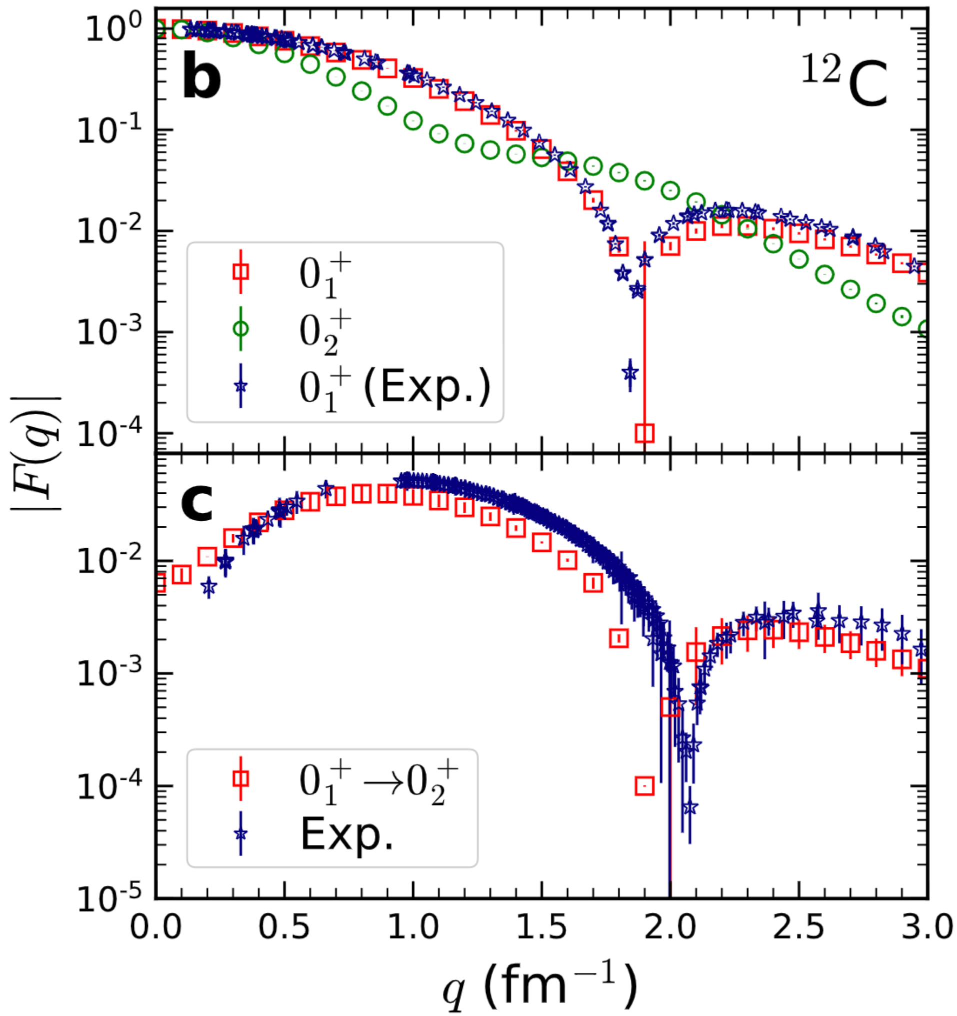
Emergent geometry and duality of ^{12}C



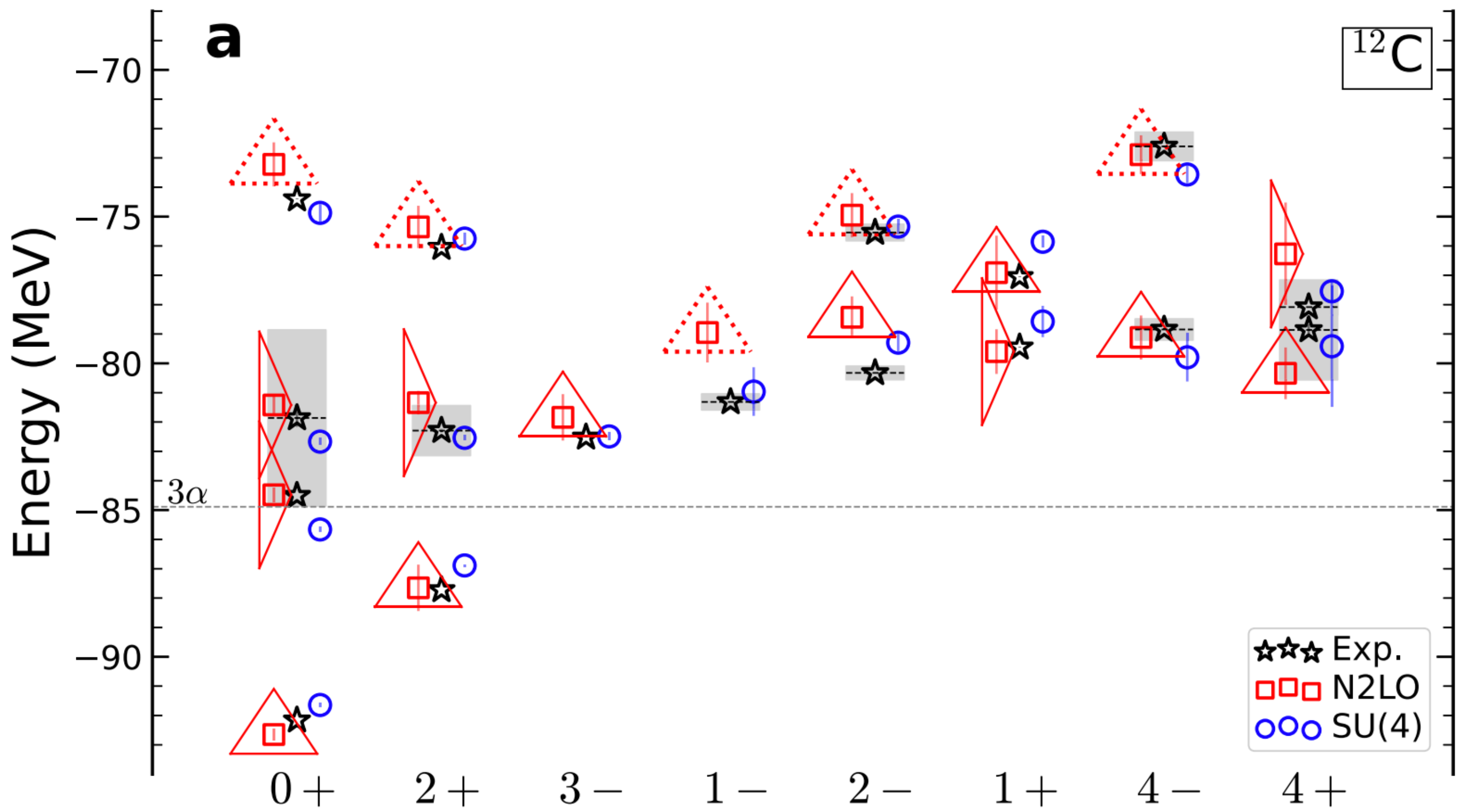
Shen, Elhatisari, Lähde, D.L., Lu, Meißner, Nature Commun. 14, 2777 (2023)



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

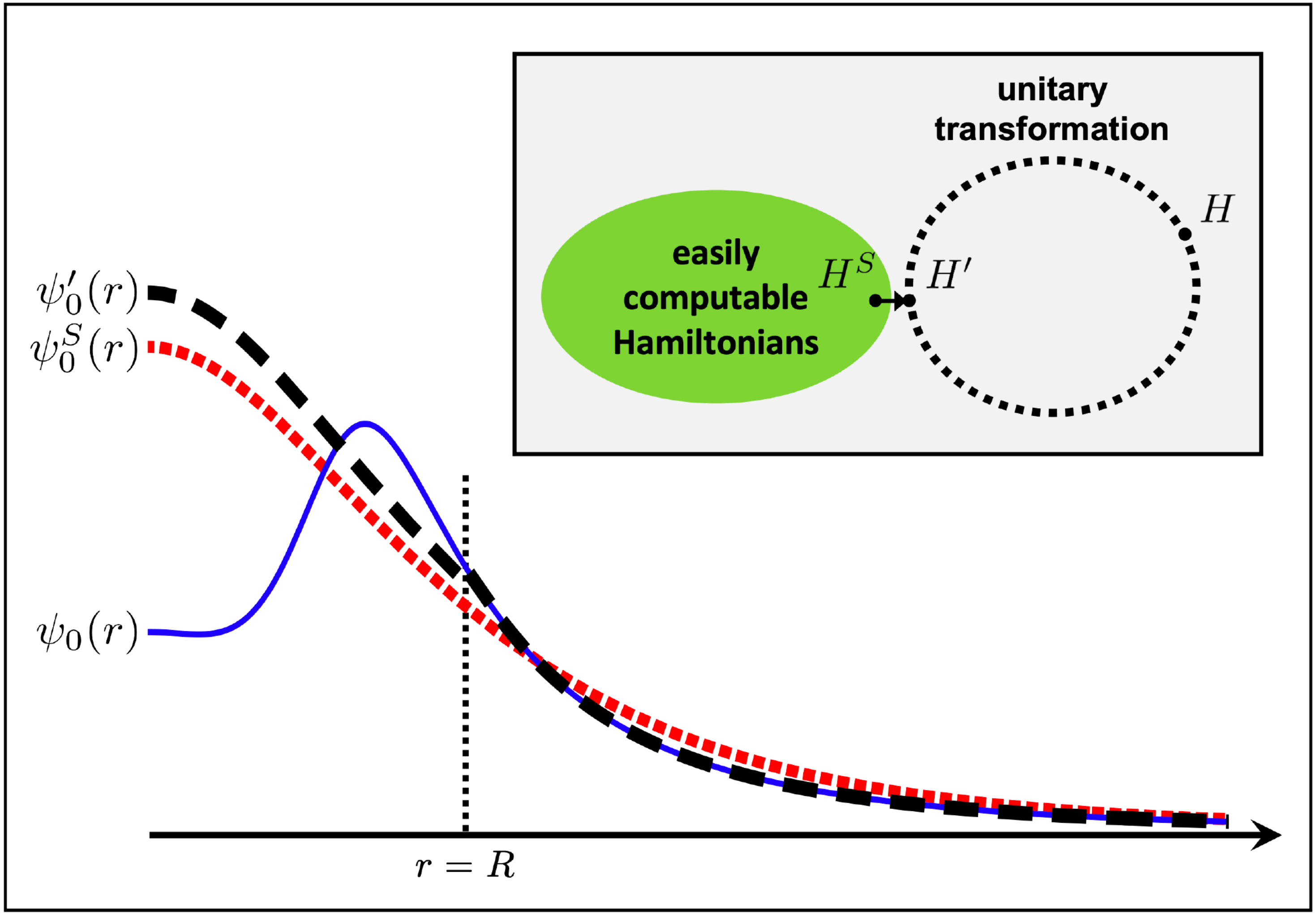


Shen, Elhatisari, Lähde, D.L., Lu, Meißner, Nature Commun. 14, 2777 (2023)



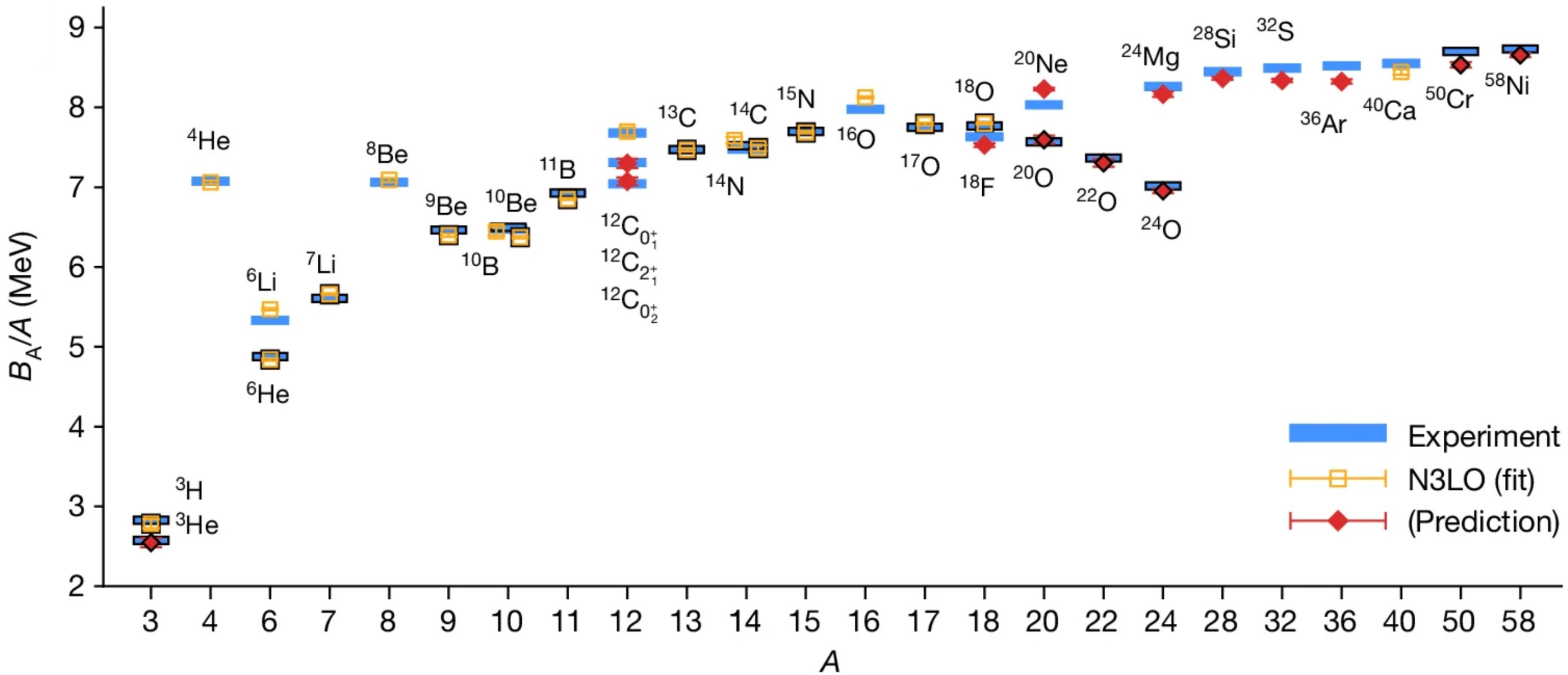
Shen, Elhatisari, Lähde, D.L., Lu, Meißner, Nature Commun. 14, 2777 (2023)

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



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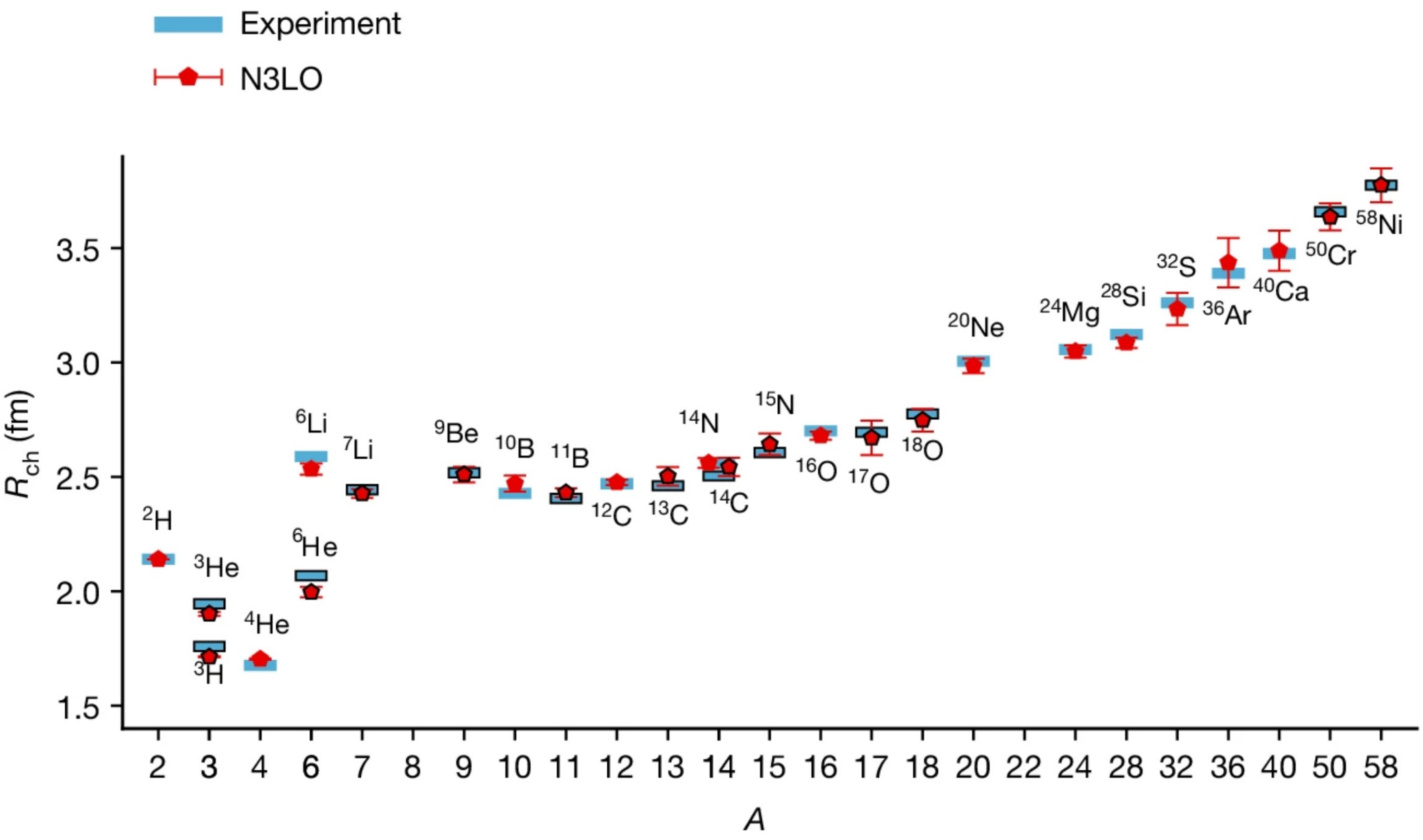
Charge radii



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

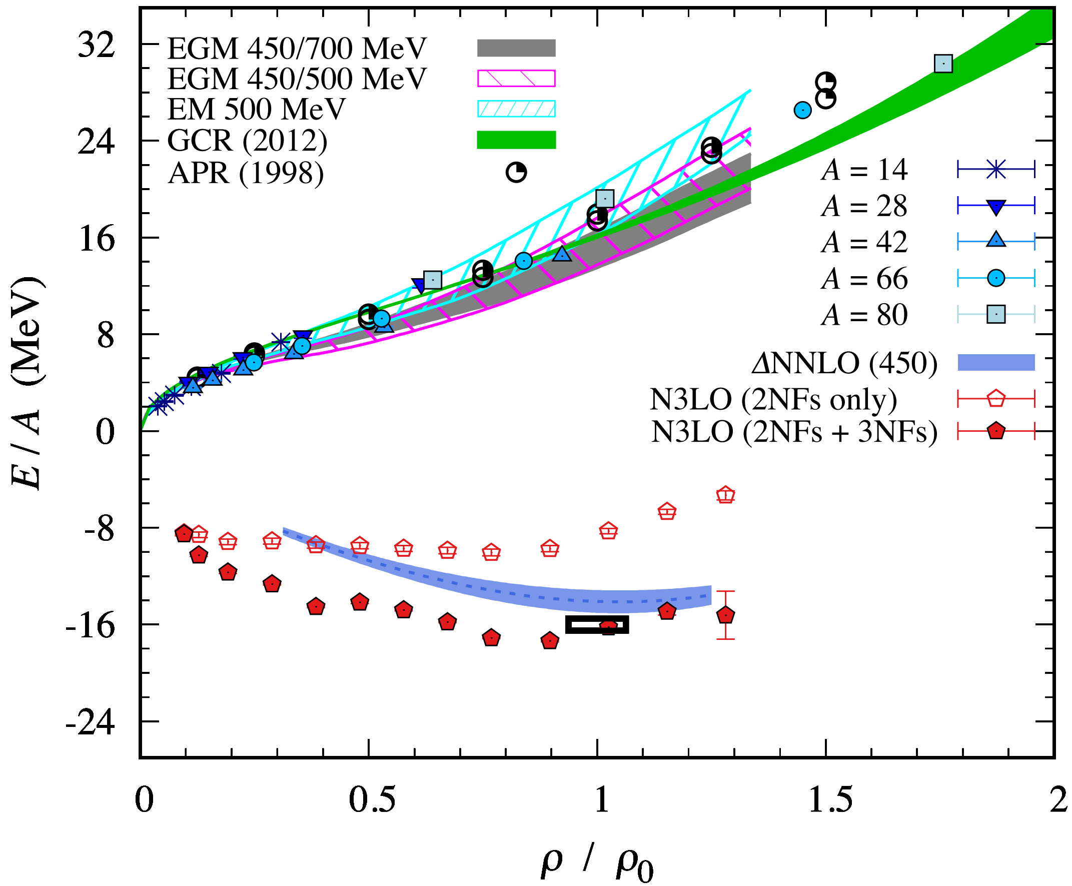
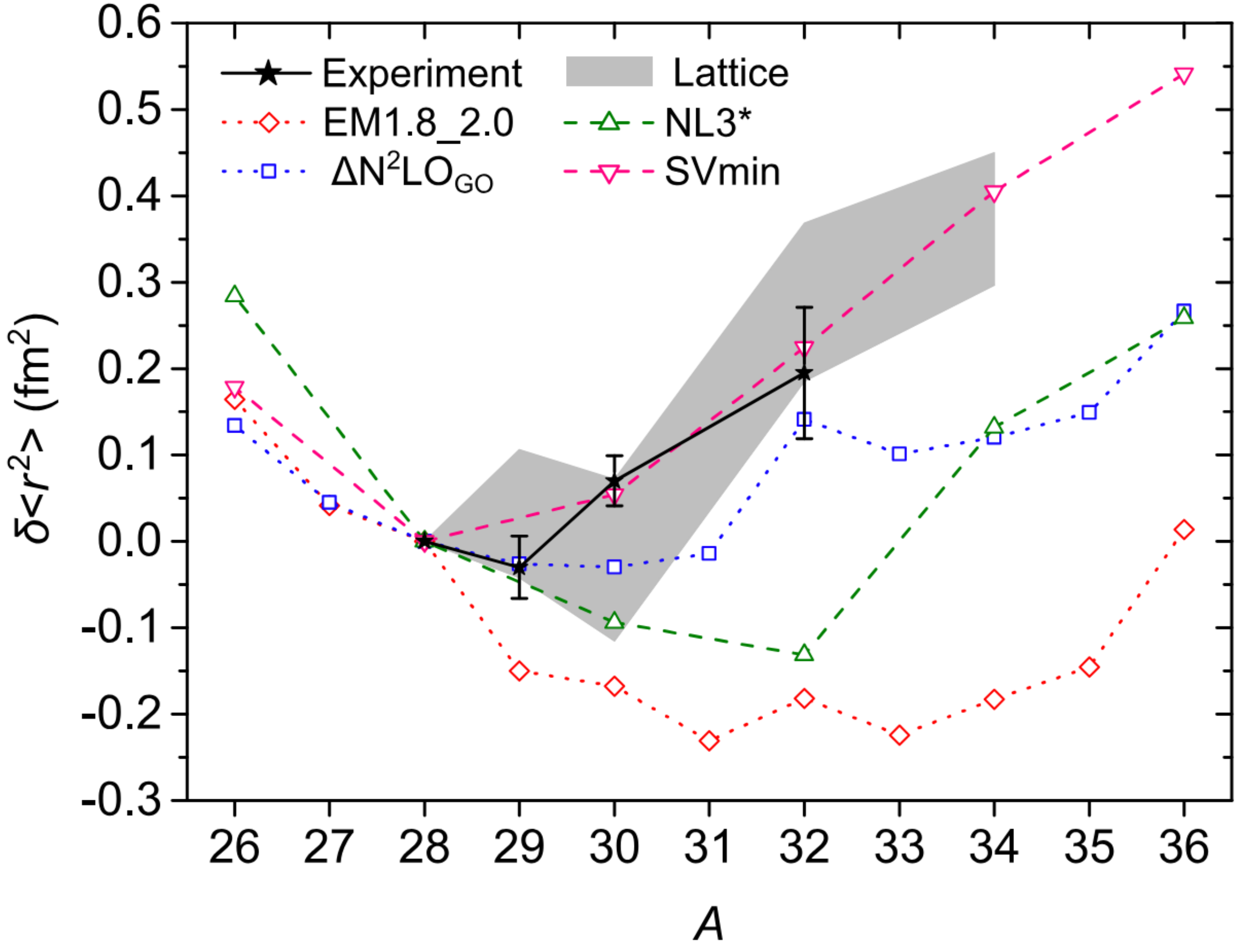


Figure adapted from Tews, Krüger, Hebeler, Schwenk, Phys. Rev. Lett. 110, 032504 (2013)

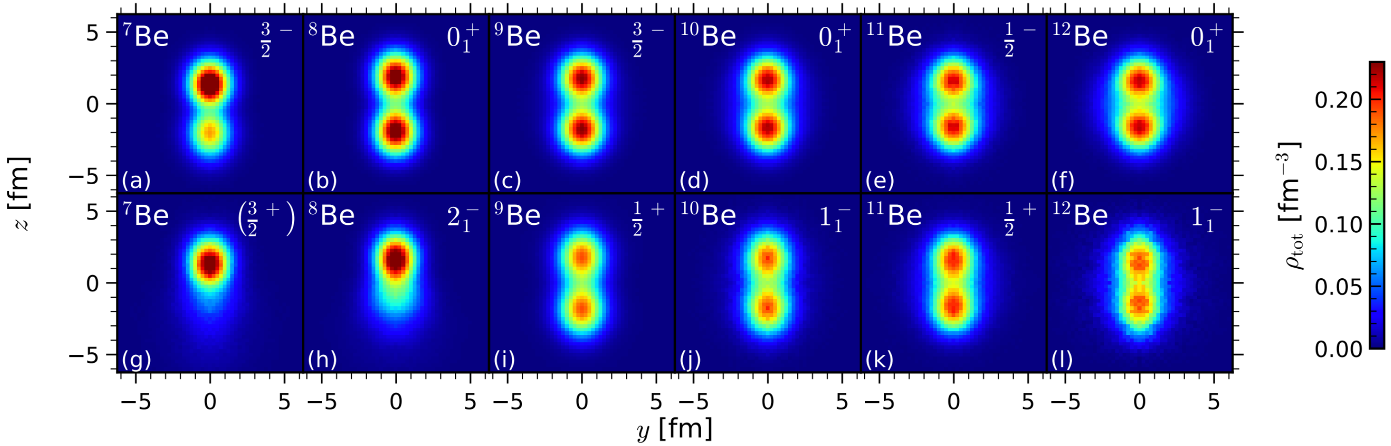
Elhatisari, Bovermann, Ma, Epelbaum, Frame, Hildenbrand, Krebs, Lähde, D.L., Li, Lu, M. Kim, Y. Kim, Meißner, Rupak, Shen, Song, Stellin, Nature 630, 59 (2024)

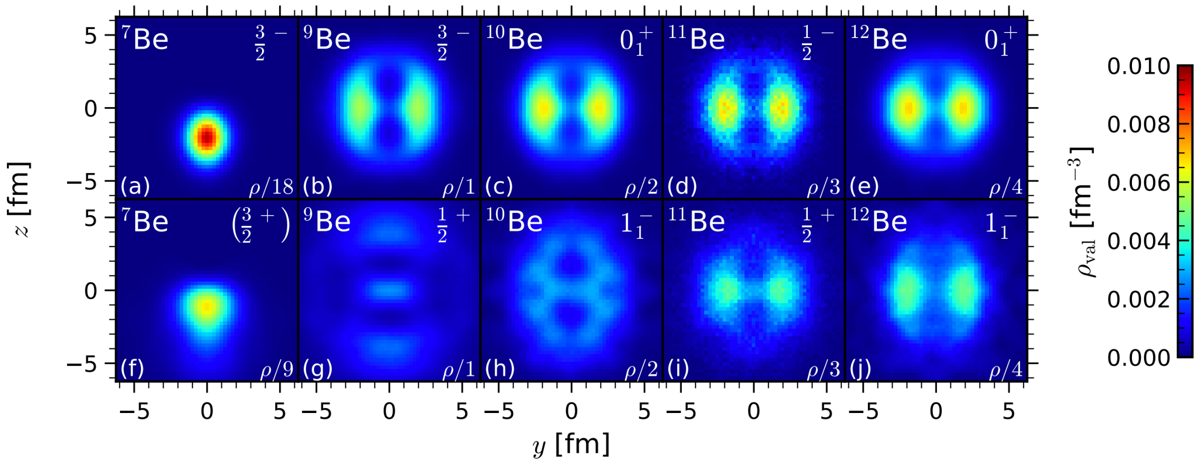
Charge radii of silicon isotopes



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

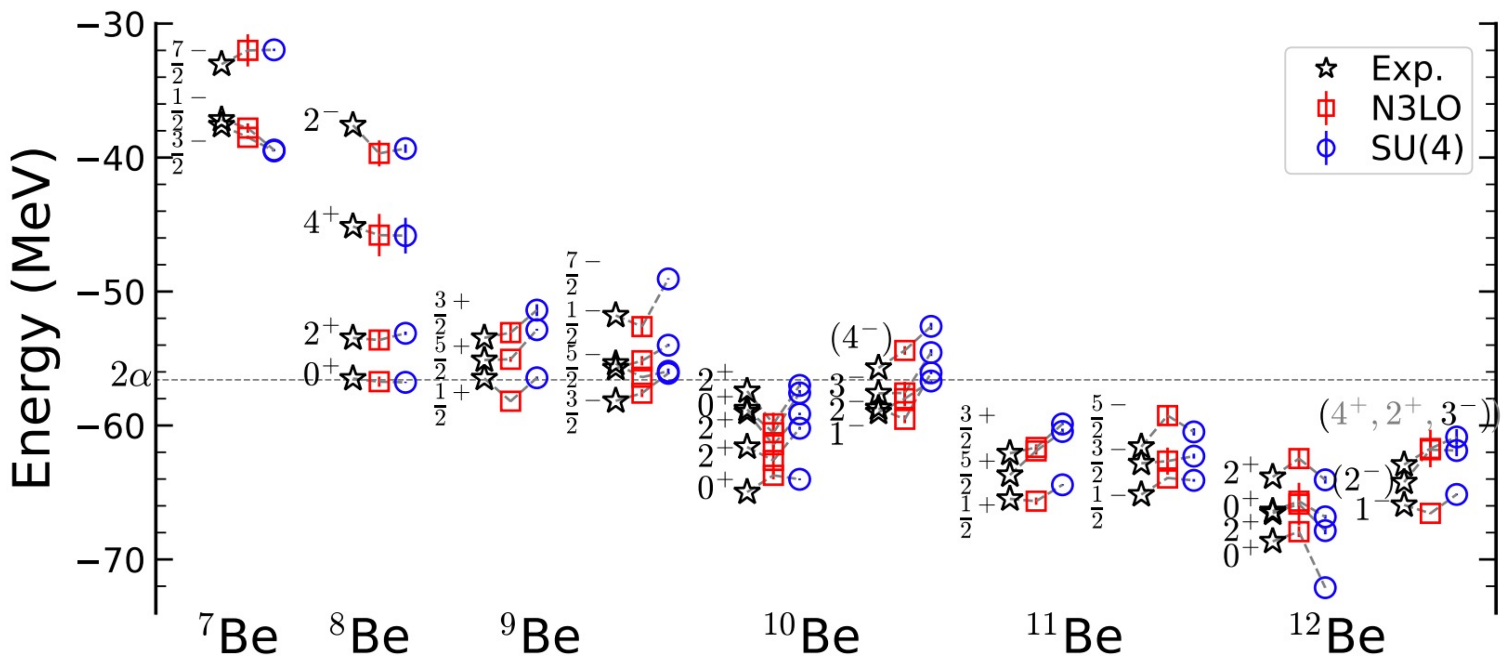
Properties of the beryllium isotopes





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

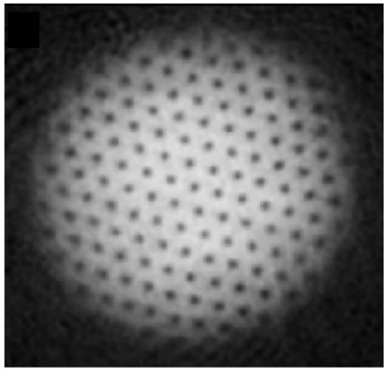
Properties of the beryllium isotopes



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

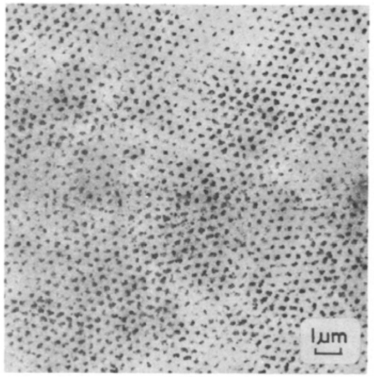
Superfluid condensation

BEC Theory



Ketterle, Zwierlein,
Ultracold Fermi Gases (2008)

BCS Theory



Essmann, Träuble,
Physics Letters A 27, 3 (1968)

Off-diagonal long-range order

Bosonic superfluidity

$$\langle \Psi_0 | a^\dagger(\mathbf{r}) a(\mathbf{0}) | \Psi_0 \rangle$$

Fermionic superfluidity (S-wave)

$$\langle \Psi_0 | a^\dagger_\downarrow(\mathbf{r}) a^\dagger_\uparrow(\mathbf{r}) a_\uparrow(\mathbf{0}) a_\downarrow(\mathbf{0}) | \Psi_0 \rangle$$

Fermionic superfluidity (P-wave)

$$\langle \Psi_0 | a^\dagger_\uparrow(\mathbf{r}) a^\dagger_\uparrow(\mathbf{r} + \Delta\mathbf{r}) a_\uparrow(\Delta\mathbf{r}) a_\uparrow(\mathbf{0}) | \Psi_0 \rangle$$

Yang, RMP **34**, 694 (1962)

Unitary limit

S-wave scattering amplitude:

$$f_0(k) = \frac{1}{k\cot\delta_0(k) - ik}$$

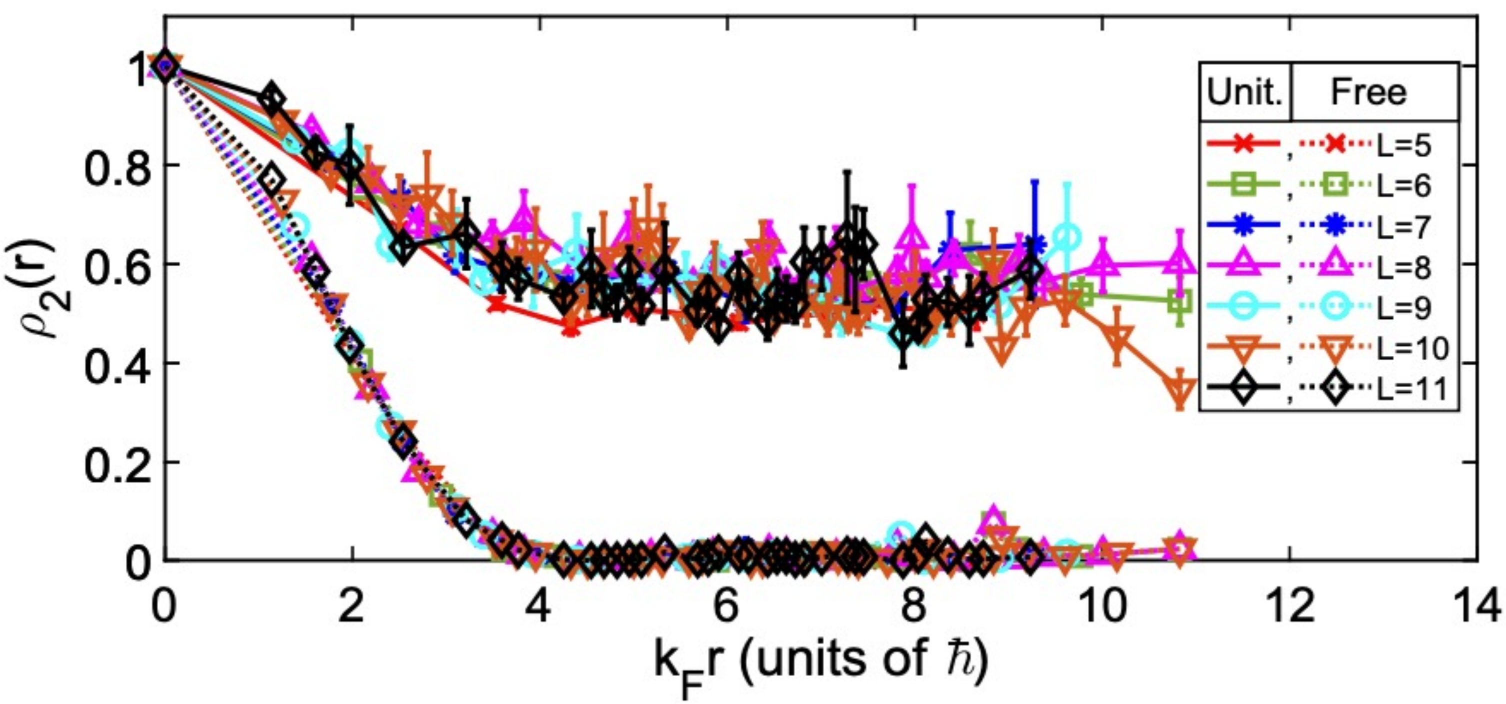
$$k\cot\delta_0(k) = -a_0^{-1} + \frac{1}{2}r_0k^2 + O(k^4)$$

The unitary limit is a scale-invariant theory where the scattering length is infinite, and the range of the interaction is negligible.

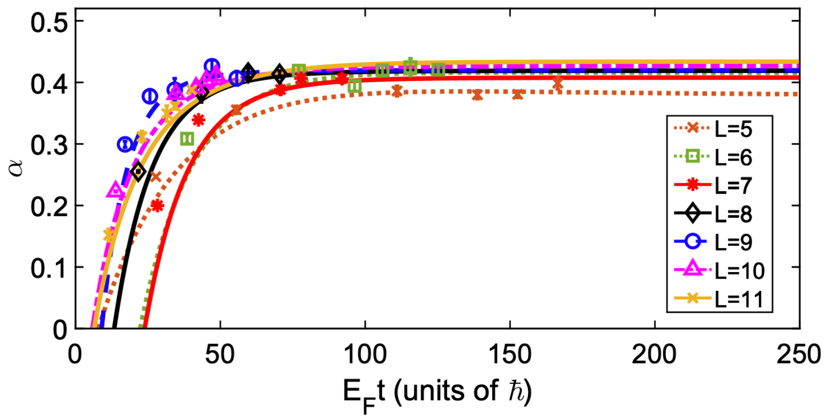
$$f_0(k) \to \frac{i}{k}$$

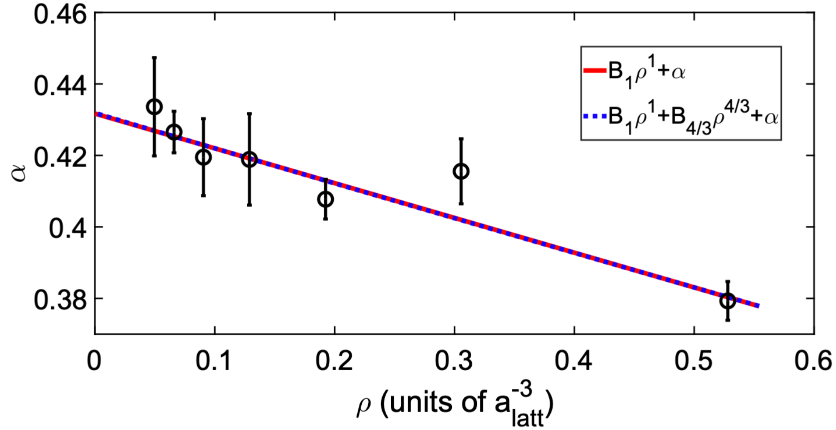
We compute the two-particle S-wave correlation function

$$\rho_2(r) = \frac{\langle\Psi_0|a_\downarrow^\dagger(\mathbf{r})a_\uparrow^\dagger(\mathbf{r})a_\uparrow(\mathbf{0})a_\downarrow(\mathbf{0})|\Psi_0\rangle}{\langle\Psi_0|a_\downarrow^\dagger(\mathbf{0})a_\uparrow^\dagger(\mathbf{0})a_\uparrow(\mathbf{0})a_\downarrow(\mathbf{0})|\Psi_0\rangle}$$



He, Li, Lu, D.L., Phys. Rev. A 101, 063615 (2020)





condensate fraction = 0.43(2)

He, Li, Lu, D.L., Phys. Rev. A 101, 063615 (2020)

^{6}Li experiments: 0.46(7) [1, 2] and 0.47(7) [3]

[1] Zwierlein, Stan, Schunck, Raupach, Kerman, Ketterle, PRL 92, 120403 (2004).
[2] Zwierlein, Schunck, Stan, Raupach, Ketterle, PRL 94, 180401 (2005).
[3] Kwon, Pace, Panza, Inguscio, Zwerger, Zaccanti, Scazza, Roati, Science 369, 84 (2020).

Attractive extended Hubbard models

See George's talk presented on Tuesday of last week

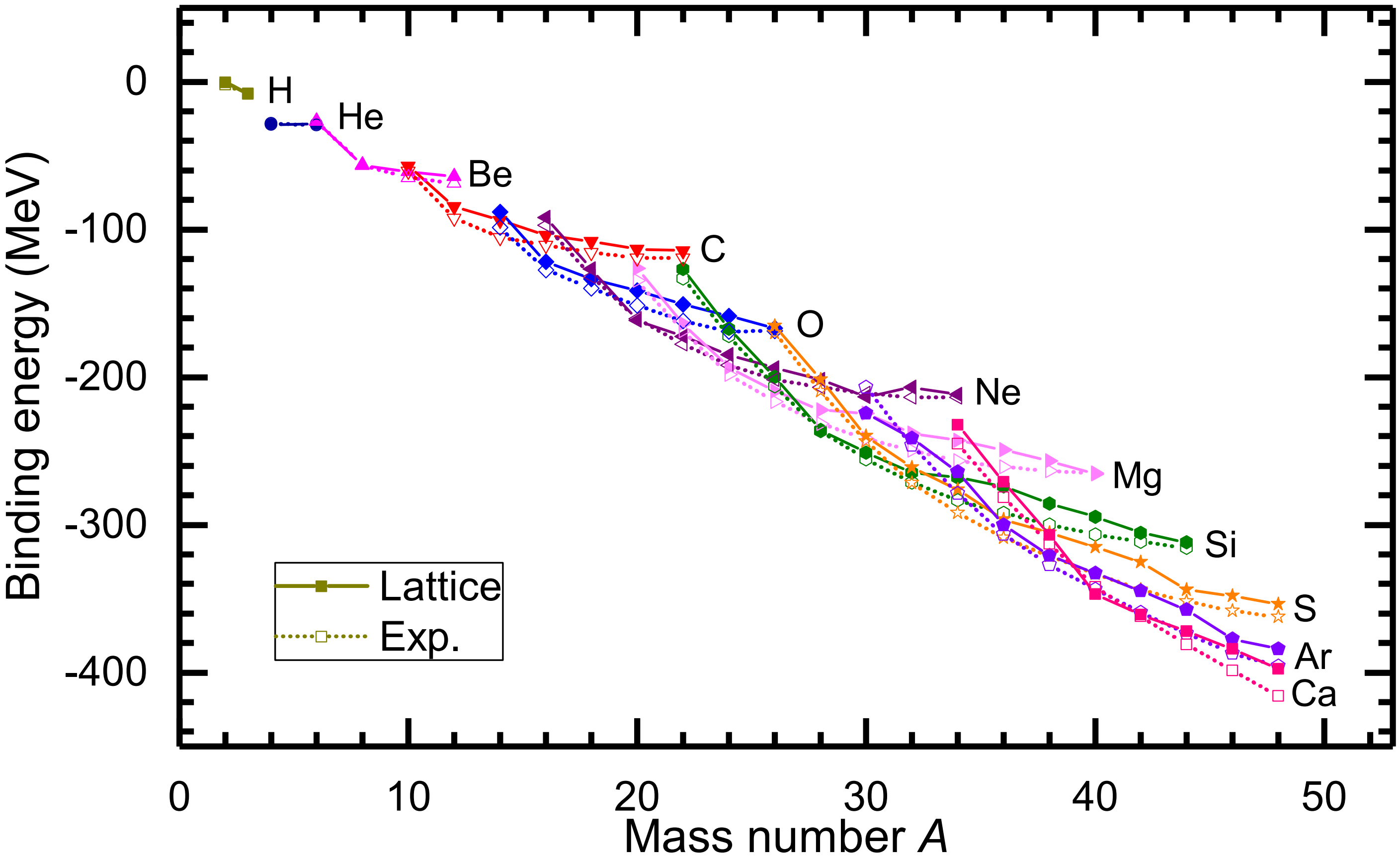
We consider attractive extended Hubbard models for two-component fermions in 1, 2, 3 dimensions

$$H = H_{\text{free}} + \tfrac{1}{2}C_2 \sum_{\mathbf{n}} \tilde{\rho}(\mathbf{n})^2$$

$$\tilde{\rho}(\mathbf{n}) = \sum_{j=\uparrow,\downarrow} \tilde{a}_j^\dagger(\mathbf{n})\tilde{a}_j(\mathbf{n}) + s_L \sum_{|\mathbf{n}-\mathbf{n}'|=1} \sum_{j=\uparrow,\downarrow} \tilde{a}_j^\dagger(\mathbf{n}')\tilde{a}_j(\mathbf{n}')$$

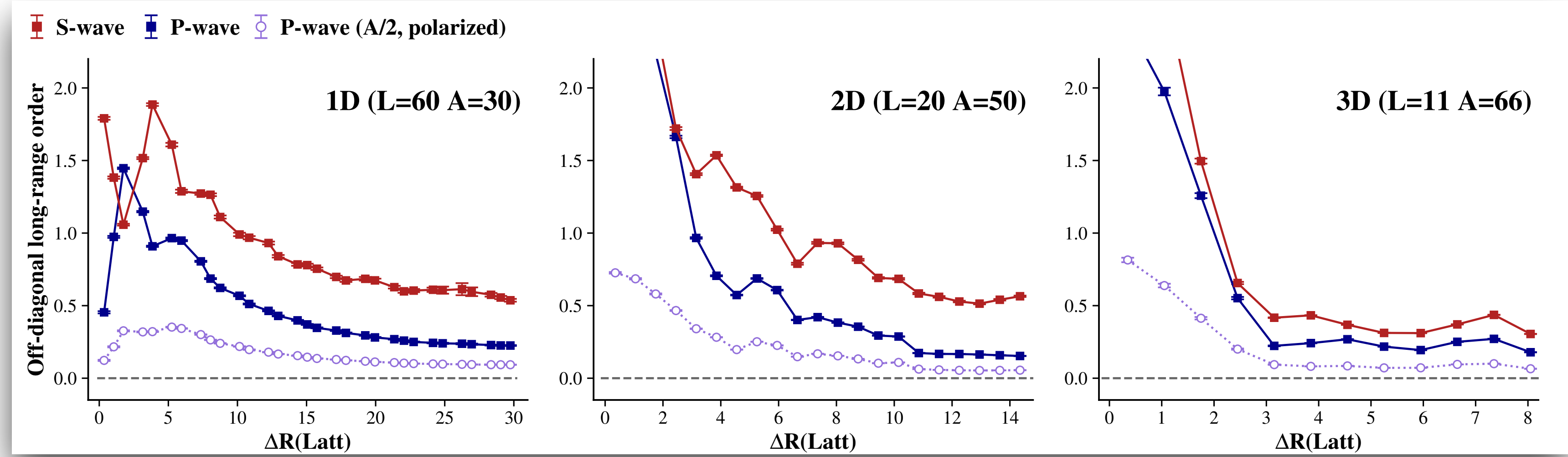
$$\tilde{a}_j(\mathbf{n}) = a_j(\mathbf{n}) + s_{NL} \sum_{|\mathbf{n}-\mathbf{n}'|=1} a_j(\mathbf{n}')$$

While just a toy model, attractive extended Hubbard models are quite useful for nuclear physics. If we include protons, a three-body interaction, and Coulomb interactions, we can reproduce the binding energies of light and medium-mass nuclei fairly well.



Lu, Li, Elhatisari, D.L., Epelbaum, Meißner, PLB 797, 134863 (2019)

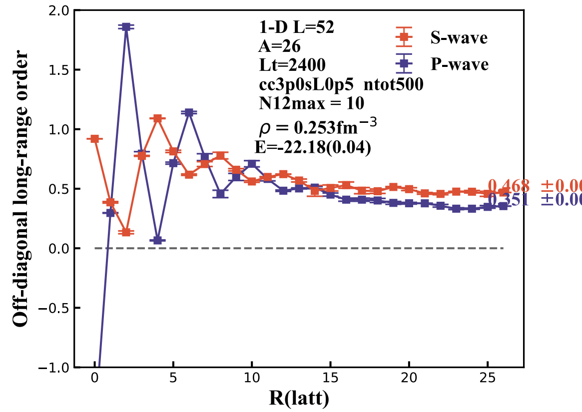
But our focus here is on pure neutron systems. The 1D system is a Luther-Emery liquid. The 1D condensate fraction decreases as a negative fractional power of the number of particles.



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

1D attractive extended Hubbard model

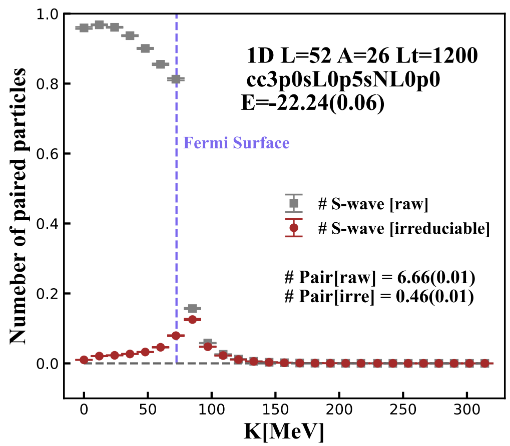
R-space



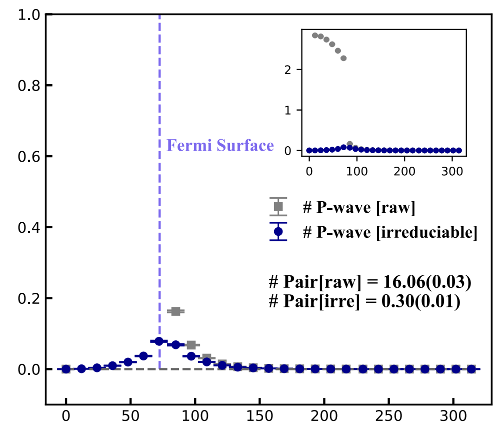
S-wave: 0.468 P-wave: 0.351

K-space

S-wave

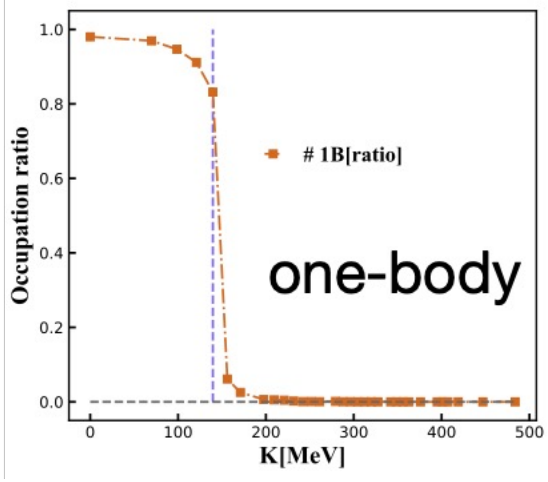


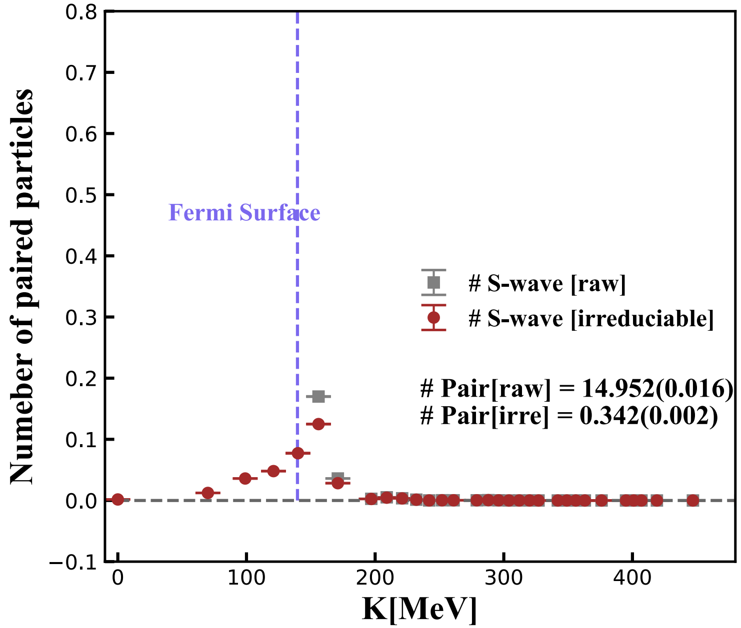
P-wave

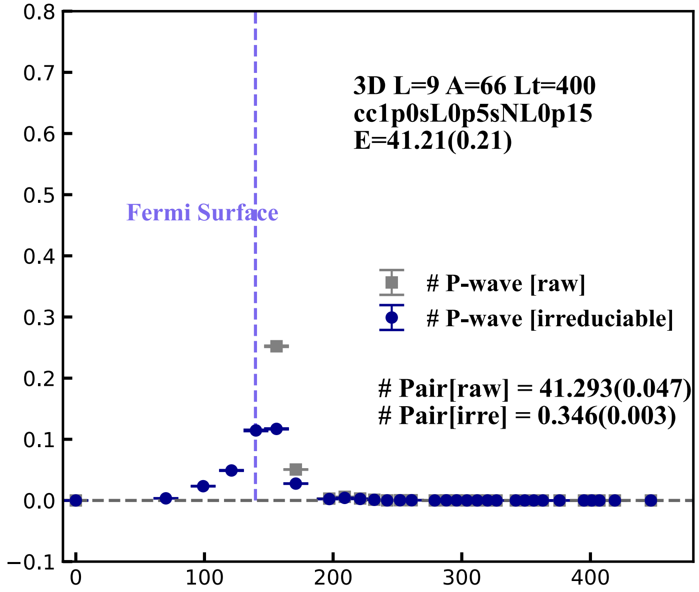


S-wave: 0.46 P-wave: 0.30

3D attractive extended Hubbard model

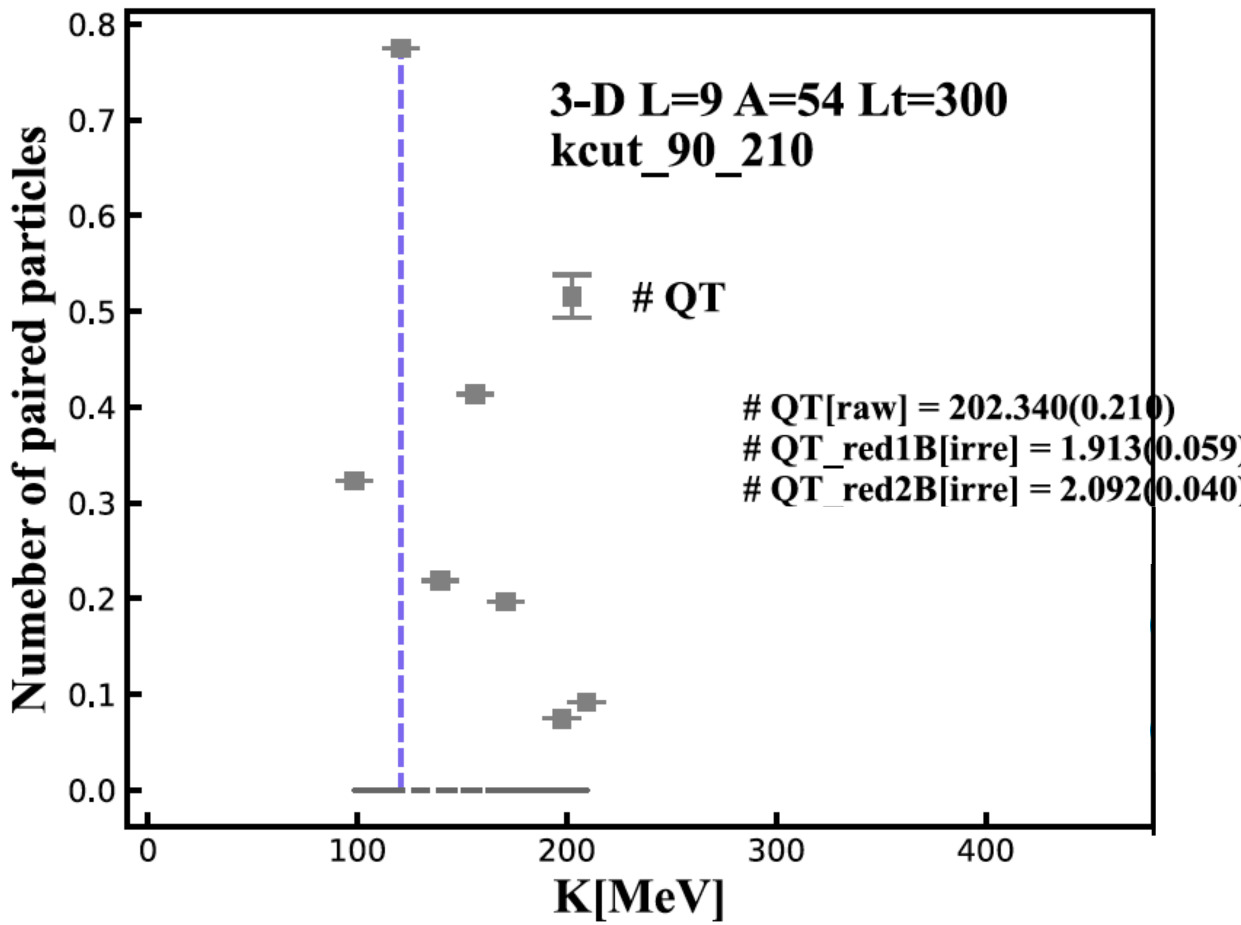




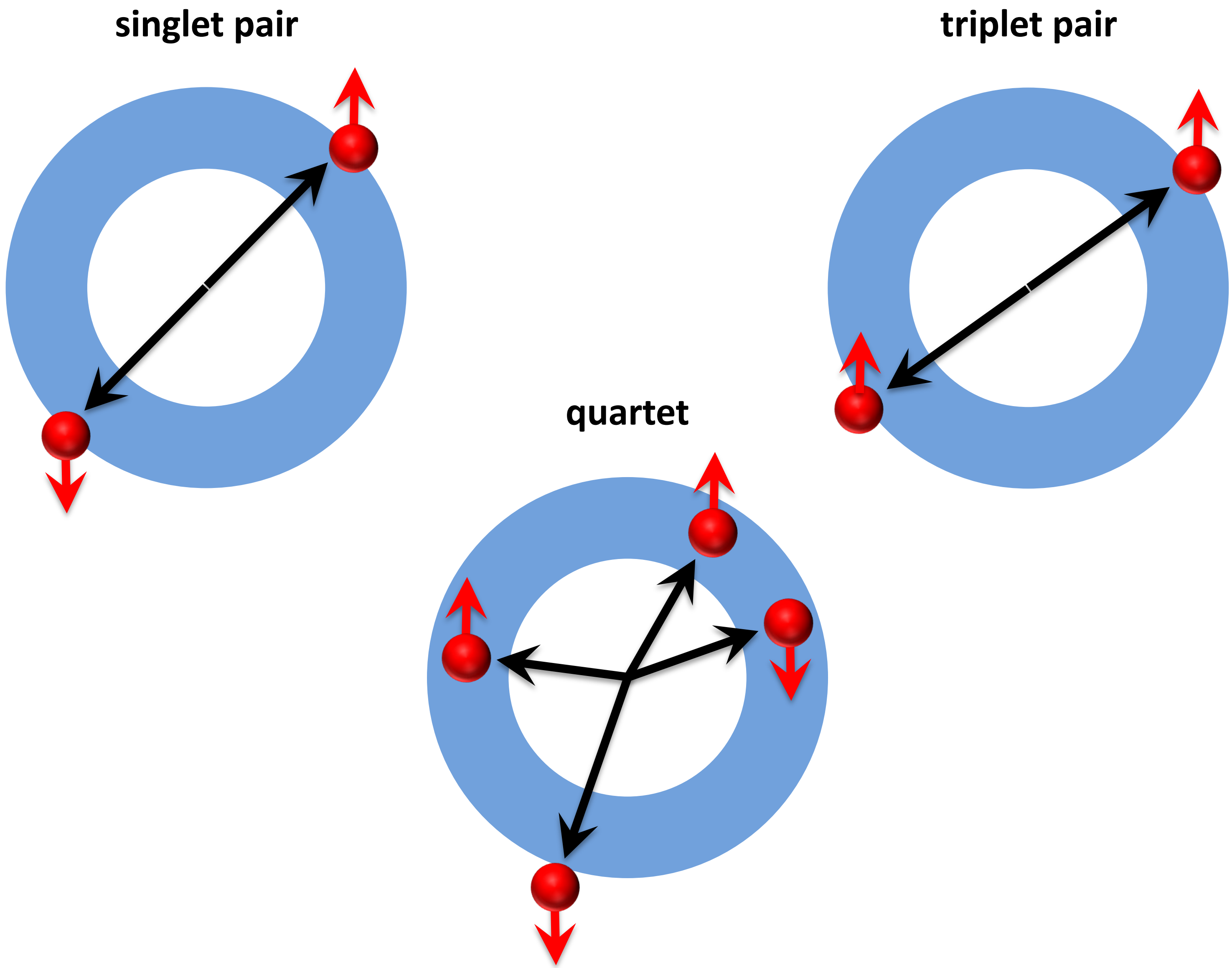


Multimodal superfluidity

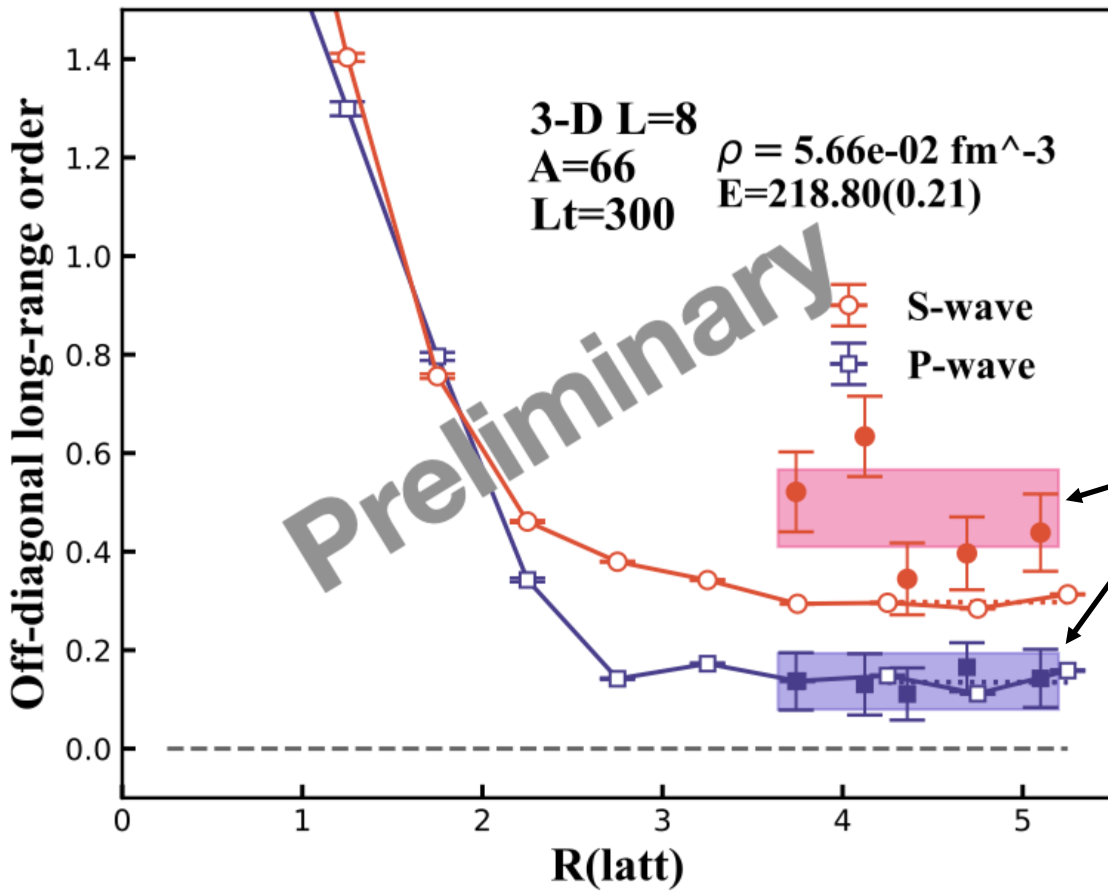
An unexpected guest: quartets



Multimodal superfluidity



Multimodal superfluidity of neutrons



N3LO chiral interactions

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

Multimodal superfluidity of neutrons

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

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

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

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

$L^3 = (9.21 \text{ fm})^3$

$k_F = 190 \text{ MeV}$

$E_F = 19 \text{ MeV}$

$$\Delta_{^1S_0} = 3.4(6) \text{ MeV}$$

$$\Delta_{^3P_0} = 1.0(5) \text{ MeV}$$

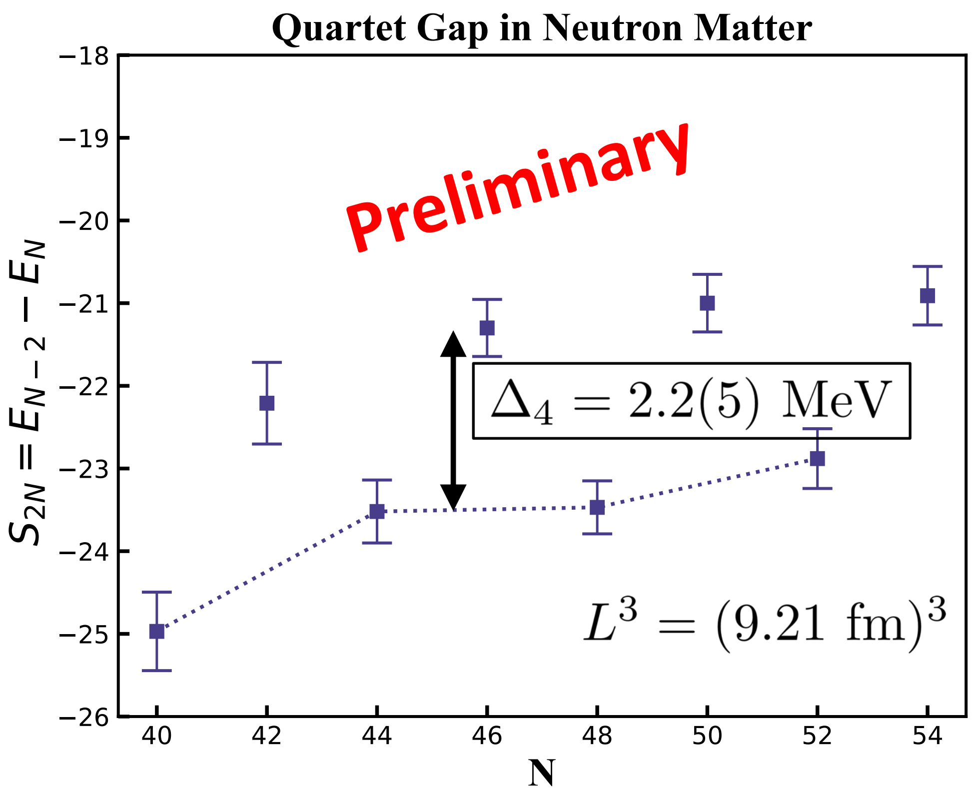
$$\Delta_{^3P_1} = -0.1(7) \text{ MeV}$$

$$\Delta_{^3P_2} = 1.1(6) \text{ MeV}$$

Preliminary

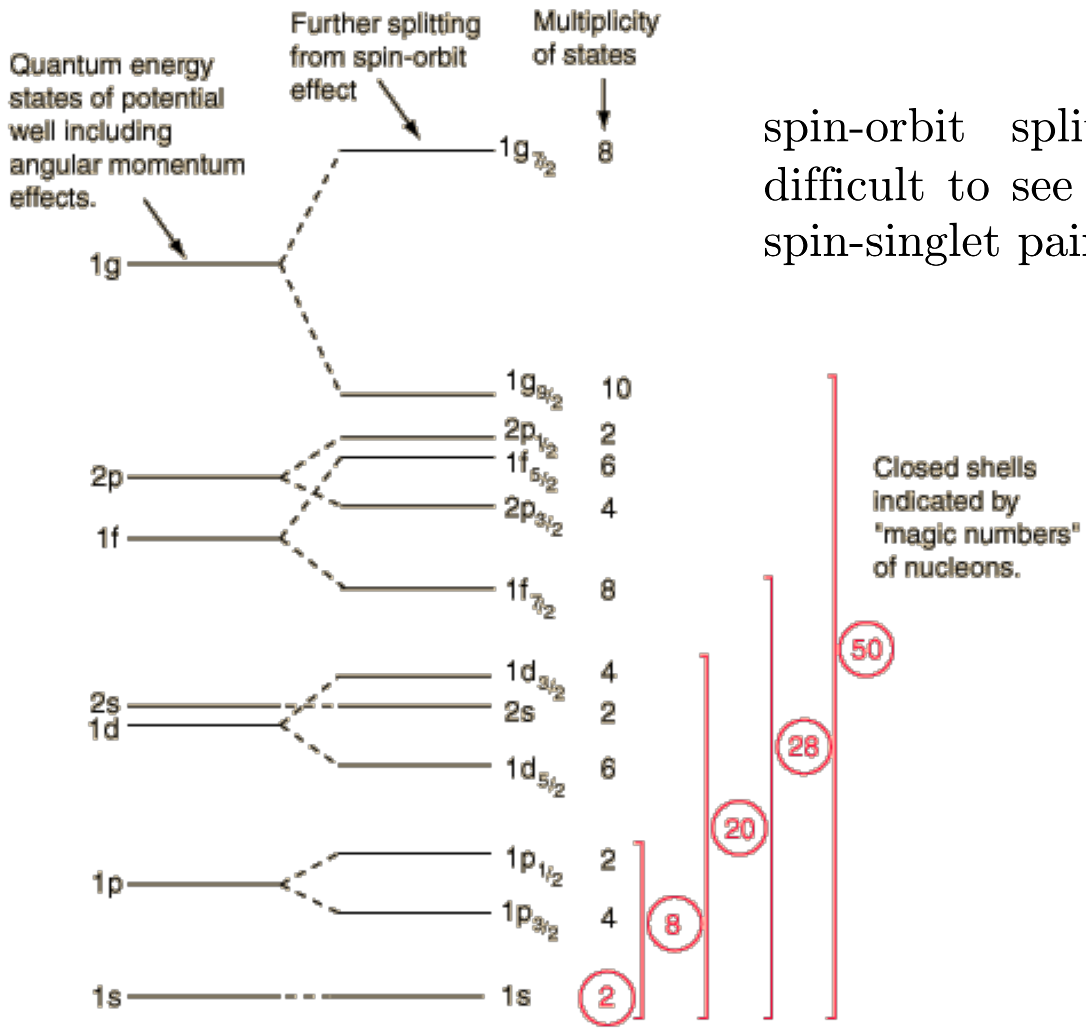
Ma, Palkanoglou, Carlson, Gandolfi, Gezerlis, Given,
D.L., Schmidt, Reddy, Yu, in progress

Multimodal superfluidity of neutrons



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

Superfluid condensates in nuclei

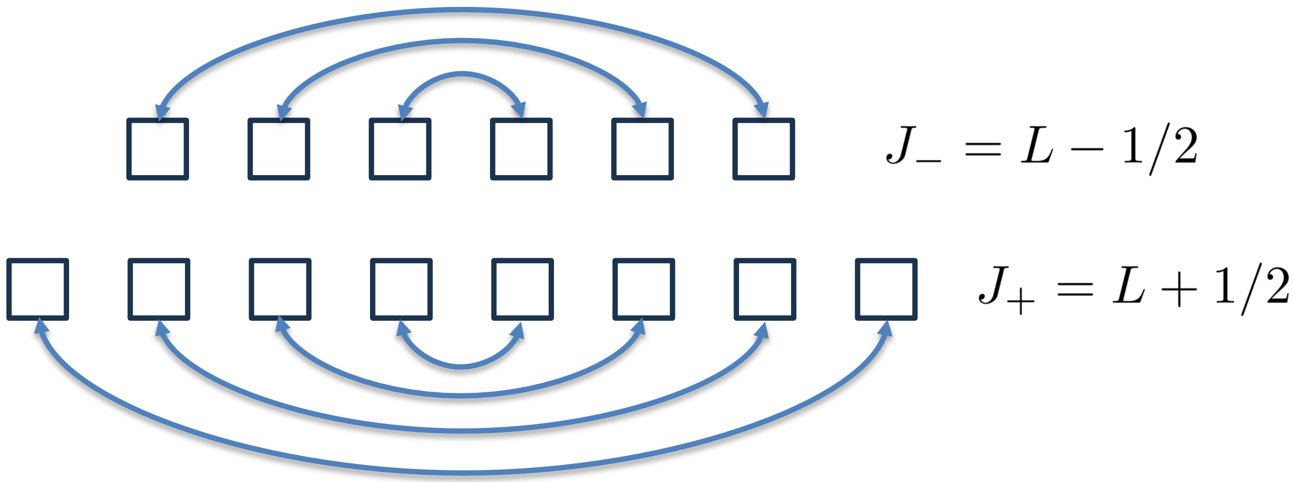


spin-orbit splitting makes it difficult to see anything except spin-singlet pairing

Rohlf, Modern Physics

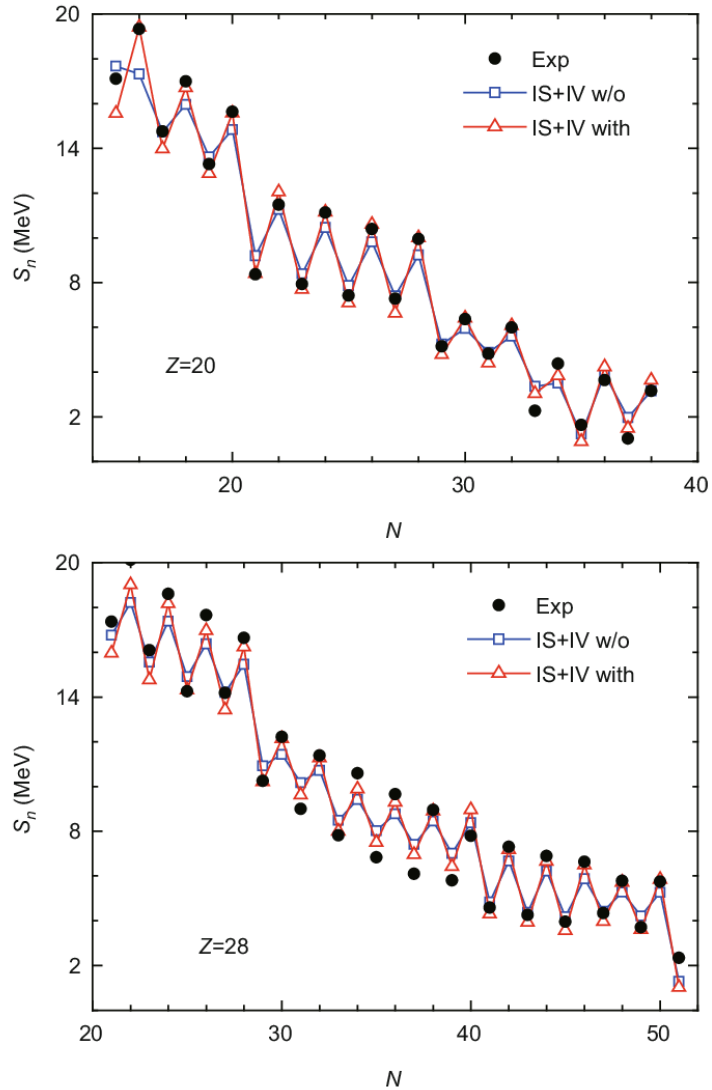
0^+

predominantly spin-singlet pairing $[{}^1S_0, {}^3P_1, {}^1D_2, \cdots]$



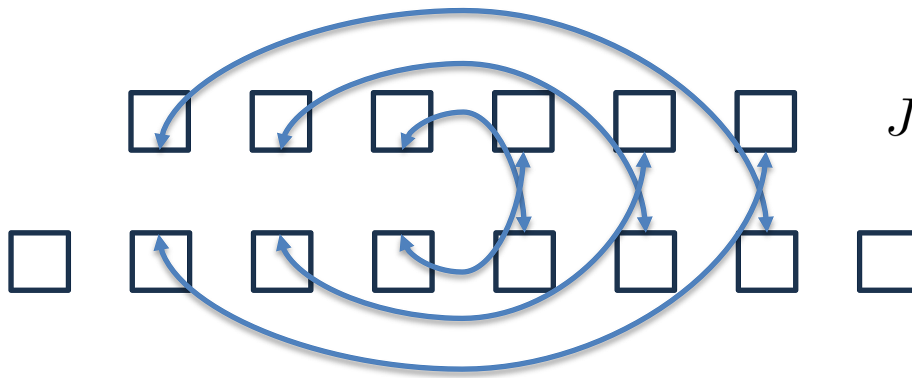
predominantly spin-singlet pairing $[{}^1S_0, {}^3P_1, {}^1D_2, \cdots]$

0^+



Yu et al., Sci. China Phys. Mech. Astron. 59, 652002 (2016)

predominantly spin-triplet pairing $[{}^3P_{0,1,2}, {}^1D_2, {}^3F_{2,3,4}, \cdots]$

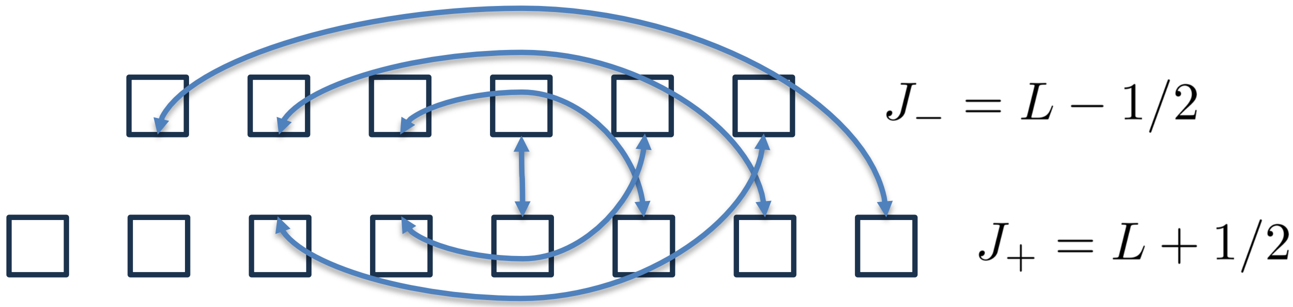


$J_- = L - 1/2$

$J_+ = L + 1/2$

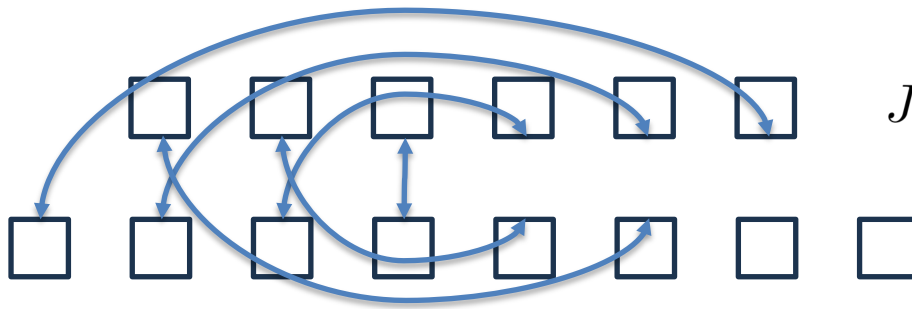
$1^+, J_z = 0$

predominantly spin-triplet pairing $[{}^3P_{0,1,2}, {}^1D_2, {}^3F_{2,3,4}, \cdots]$



$1^+, J_z = 1$

predominantly spin-triplet pairing $[{}^3P_{0,1,2}, {}^1D_2, {}^3F_{2,3,4}, \cdots]$



$J_- = L - 1/2$

$J_+ = L + 1/2$

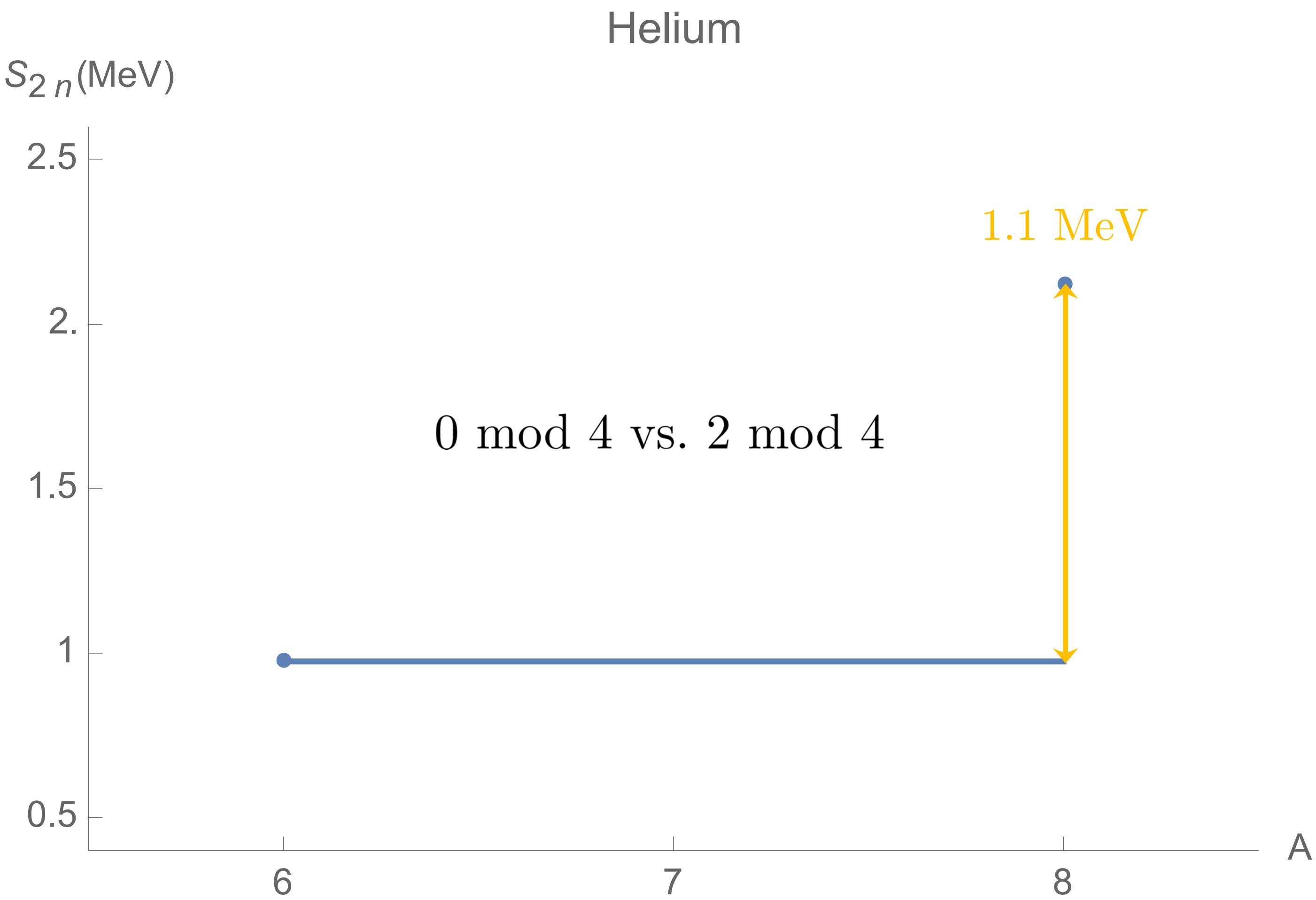
$1^+, J_z = -1$

Experimental evidence for spin-triplet pairing?

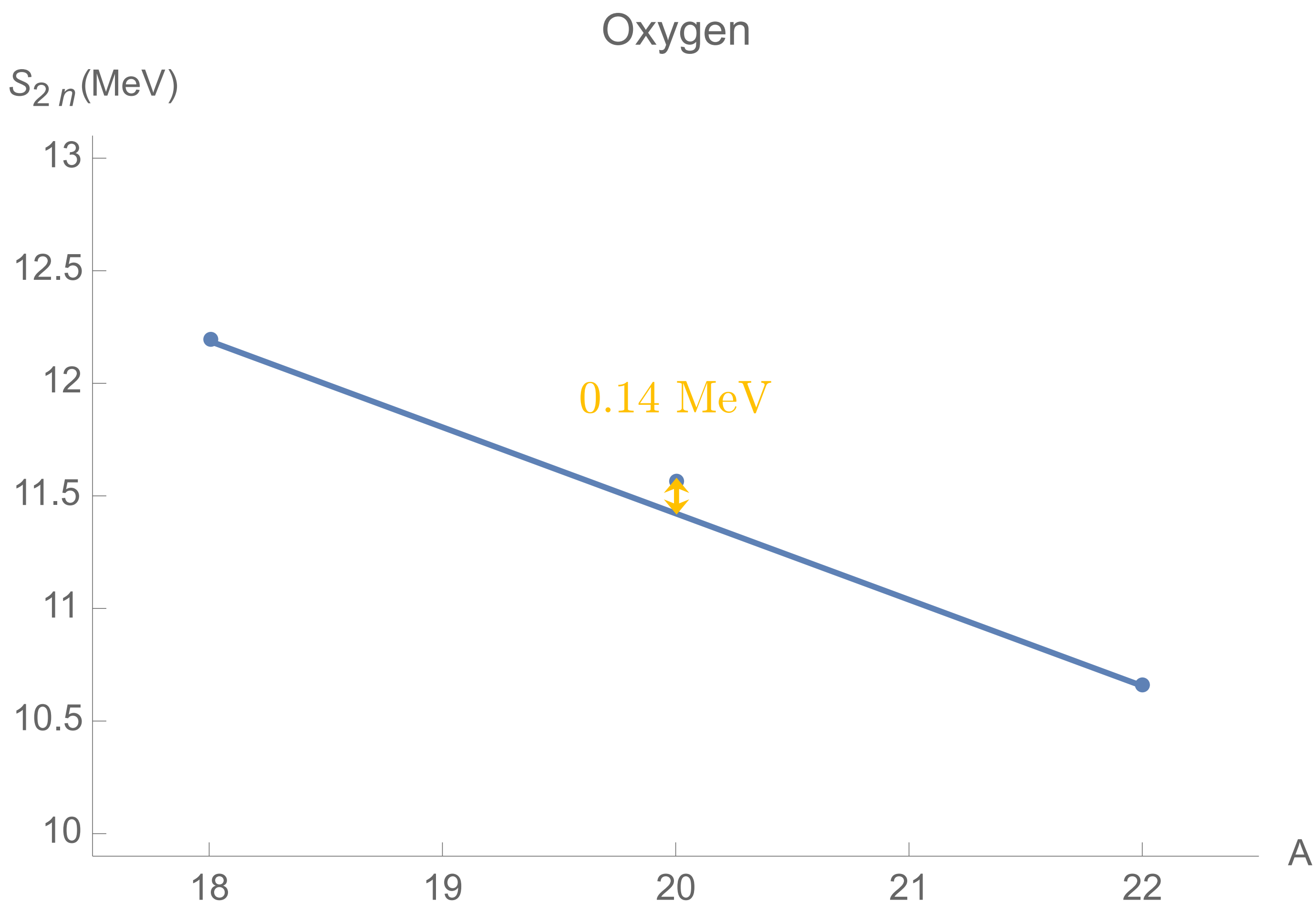
state	energy rel. to ^{16}O
$^{17}\mathrm{O}\ \frac{5}{2}^{+}$	-4.143 MeV
$^{17}\mathrm{O}\ \frac{3}{2}^{+}$	$+0.944$ MeV
$^{18}\mathrm{O}\ (1^{+})$	-3.371 MeV
extra binding	0.172 MeV

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

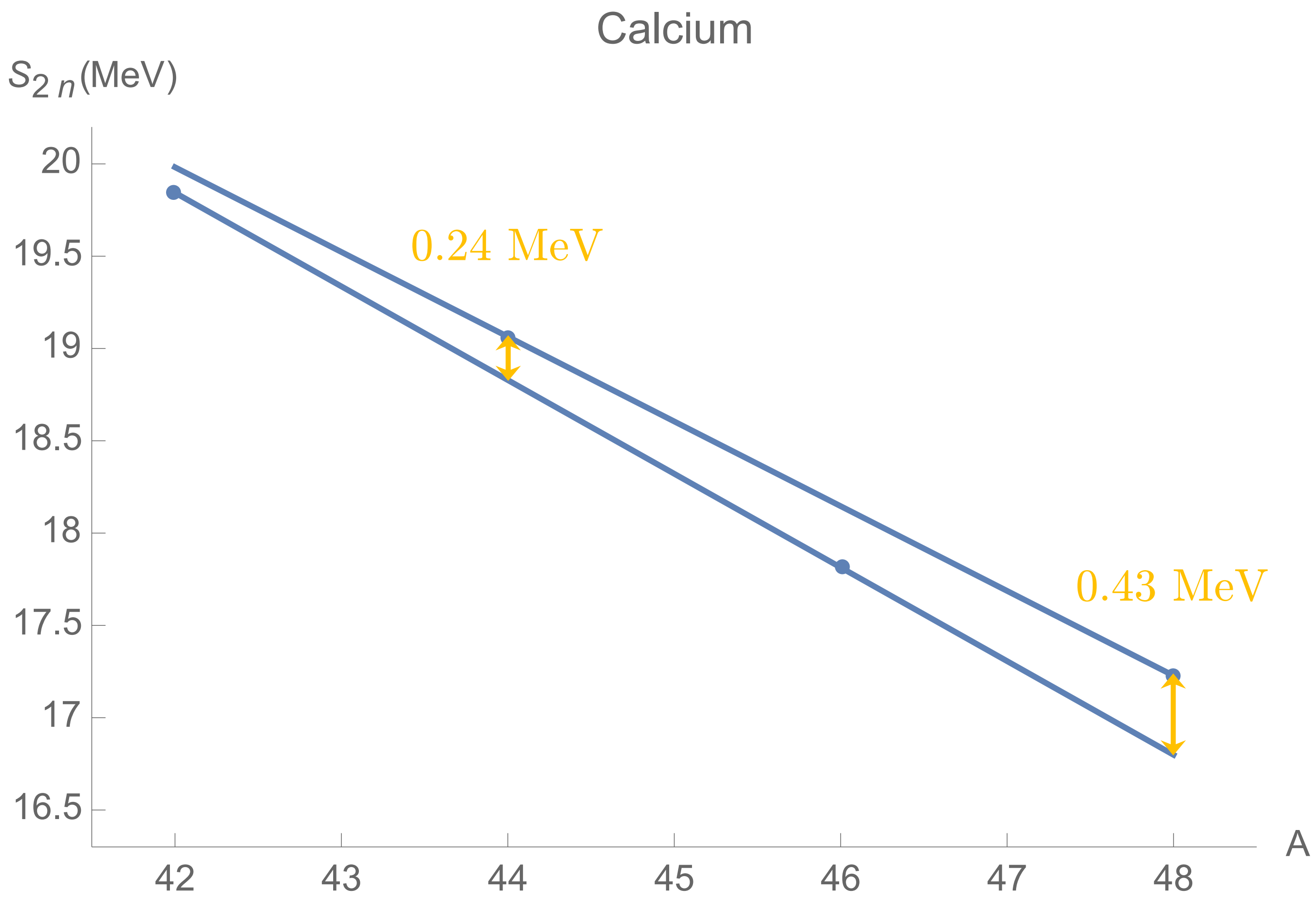
Experimental evidence for quartets?



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

Summary and outlook

We have discussed pairing and clustering in nuclear many-body systems using nuclear lattice effective field theory. We are working on *ab initio* calculations of nuclear structure, scattering, reactions, thermodynamics, and superfluidity. We have theoretical and experimental evidence for a new type of superfluidity. This multimodal superfluidity appears in neutrons and entails simultaneous S-wave, P-wave, and quartet condensation.