Status and perspectives of NLEFT

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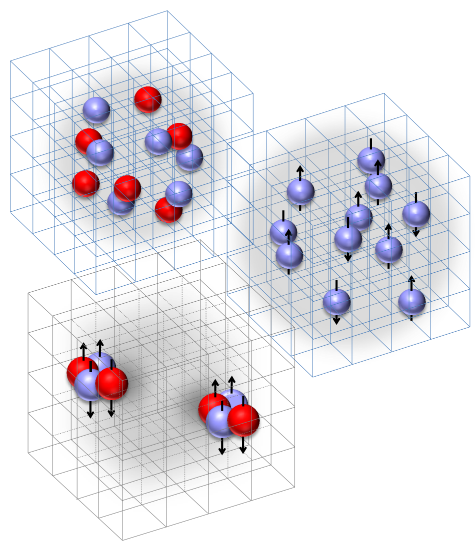
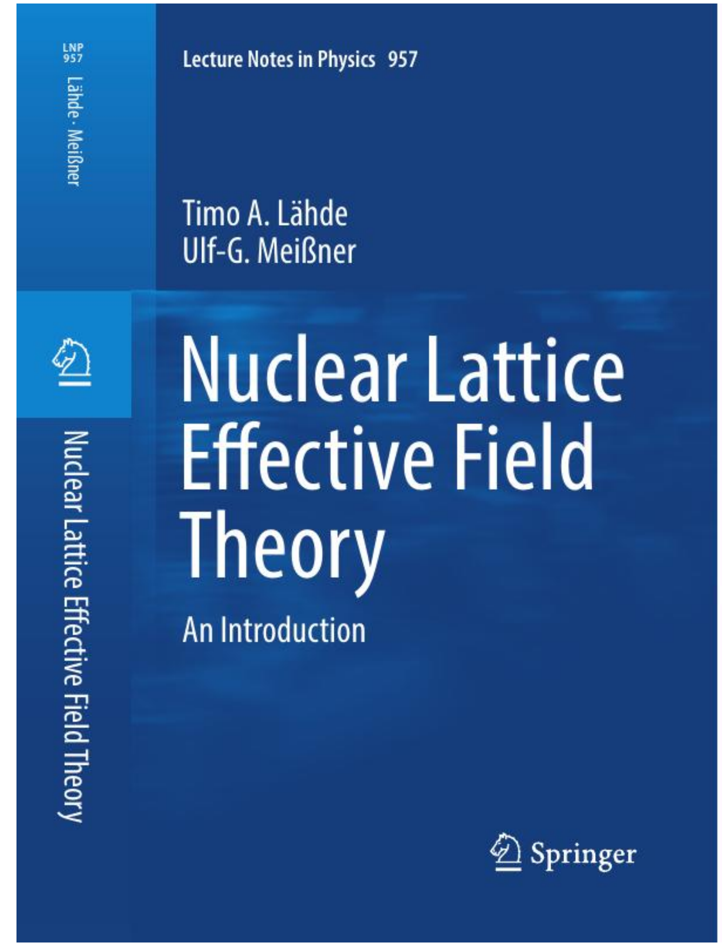
Contents

Nuclear physics on a lattice





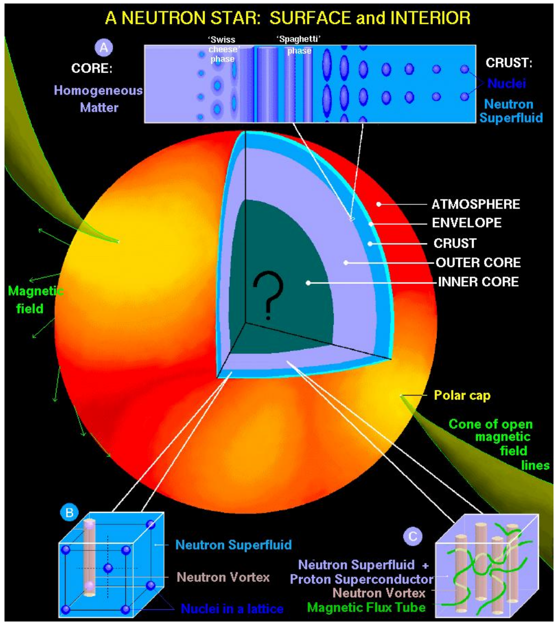
T. Lähde & UGM

Nuclear Lattice Effective Field Theory - An Introduction

Springer Lecture Notes in Physics **957** (2019) 1 - 396 [2nd edition in the works]

The nucleus as a quantum laboratory

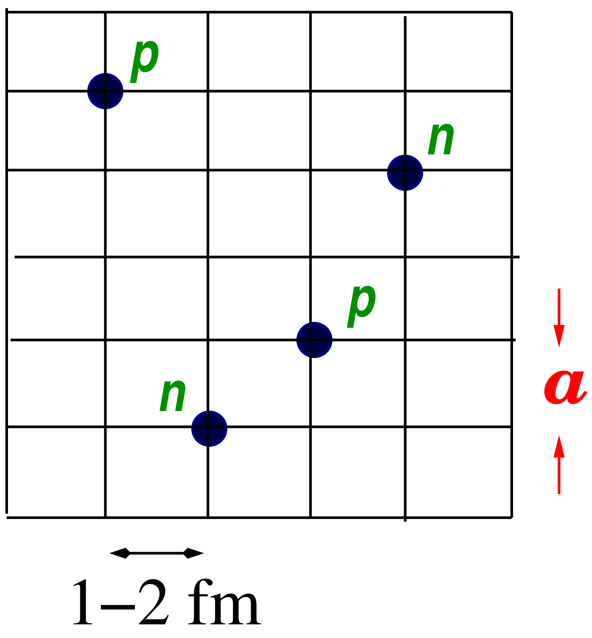
- The nucleus is a challenging and fascinating many-body system
  - ↪ non-perturbative strong interactions balanced by the Coulomb force
  - ↪ many interesting phenonema: drip lines, clustering, reactions, ...
  - ↪ a plethora of few-body/many-body methods already exists
- Macroscopic nuclear matter = neutron stars
  - ↪ gained prominence again in the multi-messenger aera
  - ↪ must be able to describe these with the same methods



- I will advocate here a new quantum many-body appraoch
  - ↪ synthezies chiral EFT w/ stochastic methods
  - ↪ allows to tackle nuclear structure *and* reactions
  - ↪ allows to access the multiverse

Foundations

Nuclear lattice effective field theory (NLEFT)



- *new method* to tackle the nuclear many-body problem

- discretize space-time $V = L_s \times L_s \times L_s \times L_t$:
  nucleons are point-like particles on the sites

- discretized chiral potential w/ pion exchanges
  and contact interactions + Coulomb

  → see Epelbaum, Hammer, UGM, Rev. Mod. Phys. **81** (2009) 1773

- EFT on the lattice, maximal momentum:

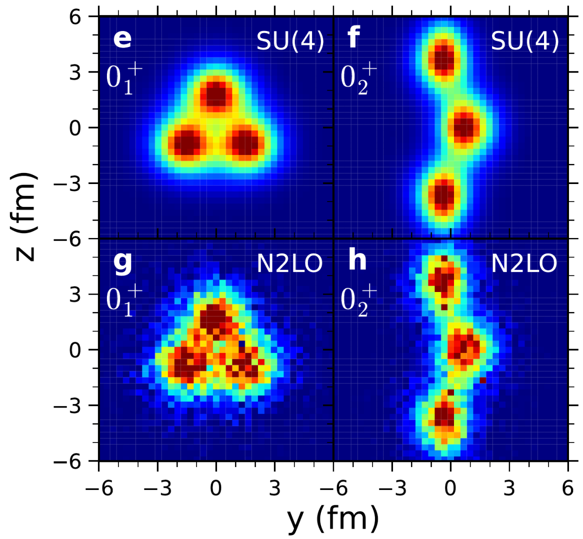
$$p_{\mathrm{max}} = \frac{\pi}{a} \simeq 315 - 630 \,\text{MeV [UV cutoff]}$$

- strong suppression of sign oscillations SU(4)
  due to approximate Wigner (spin-isospin) symmetry

  Wigner, Phys. Rev. **51** (1937) 106; Chen et al., Phys. Rev. Lett. **93** (2004) 242302

↪ works well for even-even nuclei

↪ we still need another method

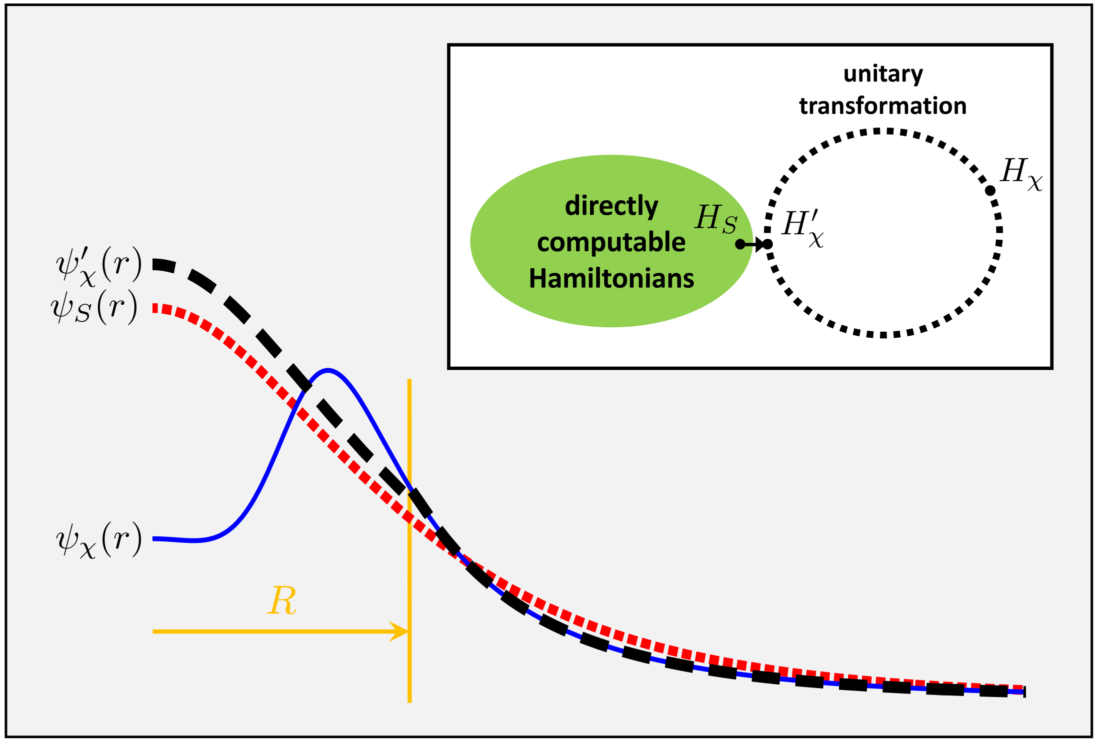


Shen et al., Nature Commun. **14** (2023) 2777

Wave function matching

Elhatisari et al., Nature **630** (2024) 59

- A new quantum many-body method: Bring a complex Hamiltonian $\boldsymbol{H_\chi}$ close to a simple one $\boldsymbol{H_S}$ (with $\boldsymbol{H_S}$ essentially free of sign oscillations)
  $\hookrightarrow$ treat $\boldsymbol{H_S}$ non-perturbatively & $\boldsymbol{H'_\chi} - \boldsymbol{H_S}$ in perturbation theory
- Graphical representation of w.f. matching



$\Rightarrow$ Efficient suppression of sign oscillations, applicable in many fields!

Pinhole algorithm

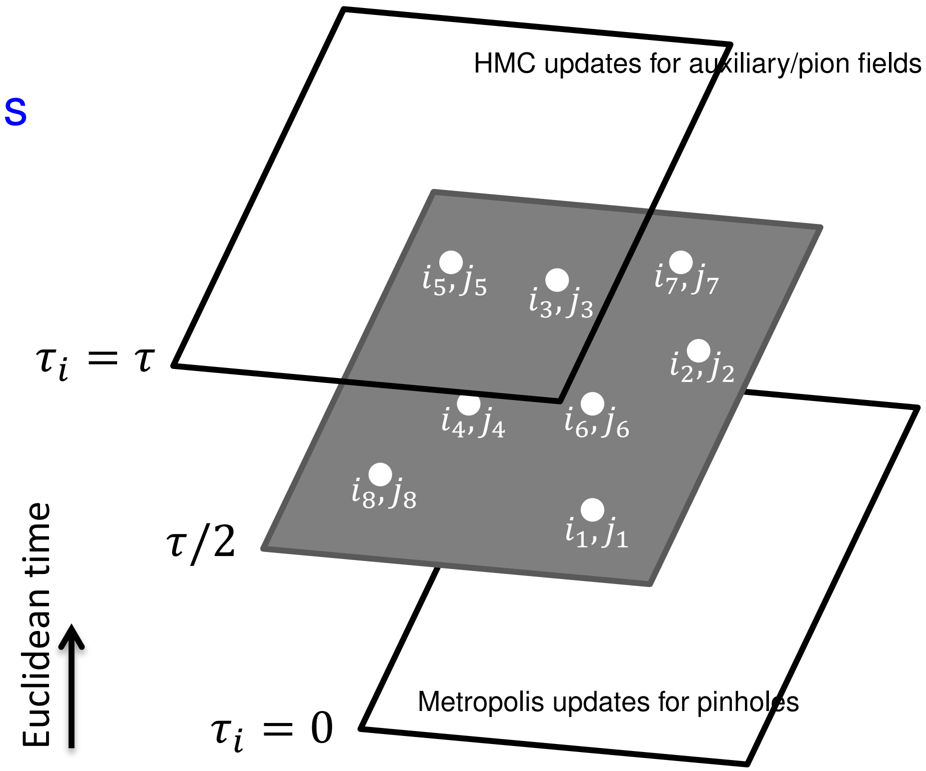
Elhatisari et al., Phys. Rev. Lett. **119** (2017) 222505

- Solution to the CM-problem:

  track the individual nucleons using the *pinhole algorithm*

- Insert a screen with pinholes with spin & isospin labels that allows nucleons with corresponding spin & isospin to pass = insertion of the A-body density op.:

$$\rho_{i_1,j_1,\cdots i_A,j_A}(\mathbf{n}_1,\cdots \mathbf{n}_A) = :\rho_{i_1,j_1}(\mathbf{n}_1)\cdots\rho_{i_A,j_A}(\mathbf{n}_A):$$



- MC sampling of the amplitude:

$$A_{i_1,j_1,\cdots i_A,j_A}(\mathbf{n}_1,\ldots,\mathbf{n}_A,L_t) = \langle\Psi_A(\tau/2)|\rho_{i_1,j_1,\cdots i_A,j_A}(\mathbf{n}_1,\ldots,\mathbf{n}_A)|\Psi_A(\tau/2)\rangle$$

- Allows to measure proton and neutron distributions & A-body correlations

- Resolution scale $\sim a/A$ as cm position $\mathbf{r}_{\rm cm}$ is an integer $\mathbf{n}_{\rm cm}$ times a/A

- Induces some sign oscillations, partiularly in p/n-rich nuclei

Partial pinhole algorithm

Ren, Elhatisari, UGM, PRL **135** (2025) 152502

- Nuclear radii can be expressed in terms of two-particle correlations G_{pp}, G_{pn}, G_{nn}

$$\langle r^2 \rangle = \sum_{c_1, c_2} \langle : \rho_{i_1 j_1}(\mathrm{n}_1) \rho_{i_2 j_2}(\mathrm{n}_2) : \rangle (\mathrm{n}_1 - \mathrm{n}_2)^2 \,, \quad c_k = (i_k, j_k, \mathrm{n}_\mathrm{k})$$

↪ the number of pinholes needed in such a calculation can be reduced:

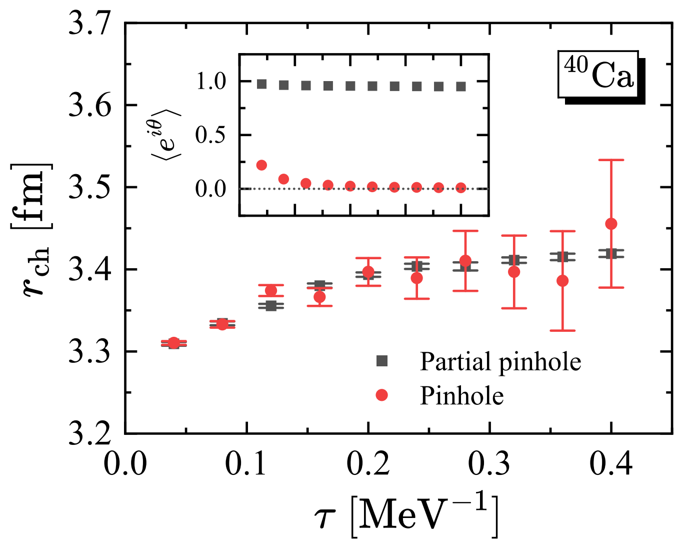
$$\rho_M(c_1, \ldots, c_M) = \frac{(A-M)!}{A!} : \rho_{i_1 j_1}(\mathrm{n}_1) \cdots \rho_{i_M j_M}(\mathrm{n}_M) : \,,$$

with $\sum_{c_1, \ldots, c_M} \rho_M = 1$

- However, $\rho_M |\Psi_A\rangle$ is not a Slater determinant, even if $|\Psi_A\rangle$ is

↪ use the rank-one operator method for ρ_M Ma et al. (2024)

$$: \rho_{i_1 j_1}(\mathrm{n}_1) \cdots \rho_{i_M j_M}(\mathrm{n}_M) :$$
$$= \lim_{\varepsilon \to \infty} \frac{1}{\varepsilon^M} : e^{\varepsilon [\rho_{i_1 j_1}(\mathrm{n}_1) + \cdots]} :$$



↪ much improved signal allows for a more precise extraction

The chiral Hamiltonian at N3LO

The chiral Hamiltonian

- Chiral Hamiltonian with **smeared** N3LO (2N) and N2LO (3N) interactions

$$H = K + V_{\rm OPE} + V_{\rm C} + V_{\rm 3N}^{\rm Q^3} + V_{\rm 2N}^{\rm Q^4} + W_{\rm 2N}^{\rm Q^4}$$

  – K – kinetic energy term with correct nucleon dispersion relation (FFT)
  – $V_{\rm OPE}$ – regulated OPE (similar to continuum case) Reinert et al. (2018)
  – $V_{\rm C}$ – Coulomb interaction
  – $V_{\rm 3N}^{\rm Q^3}$ – 3N interaction at N2LO $\to$ to be discussed later
  – $V_{\rm 2N}^{\rm Q^4}$ – 2N short-range interaction at N3LO (2π exchange absorbed) $\to$ next^2 slide
  – $W_{\rm 2N}^{\rm Q^4}$ – 2N Galilean invariance restoration (GIR) interaction at N3LO Li et al. (2019)

- Smearing explained in what follows
- Throughout, we use $a = 1.32$ fm, corresponding to the magic momentum cutoff $\Lambda \simeq 470$ MeV Lee et al. (2021)

Smeared operators & densities

- Annihilation/creation operators $a_{i,j}, a^\dagger_{i,j}$, spin $i = 0,1(\uparrow,\downarrow)$ and isospin $j = 0,1(p,n)$

- Non-locally smeared annihilation and creation operators, velocity-independent:

$$\tilde{a}^{(\dagger)}_{i,j}(\vec{n}) = a^{(\dagger)}_{i,j}(\vec{n}) + s_{\rm NL} \sum_{|\vec{n}'-\vec{n}|=1} a^{(\dagger)}_{i,j}(\vec{n}')\,, \quad s_{\rm NL} = 0.1 - 0.5$$

Lu et al. (2019,2020)

- Most general form of the point-like density operators, velocity-dependent:

$$\tilde{\rho}^{(d)}(\vec{n}) = \sum_{i,j} \tilde{a}^\dagger_{i,j}(\vec{n})\,\tilde{a}_{i,j}(\vec{n}) + s_{\rm L} \sum_{|\vec{n}-\vec{n}'|^2=1}^{d} \sum_{i,j} \tilde{a}^\dagger_{i,j}(\vec{n}')\,\tilde{a}_{i,j}(\vec{n}')\,, \quad s_{\rm L} = 0.05 - 0.15$$

Elhatisari et al., (2016), Lu et al. (2019,2020)

- In the NN system, local and non-local interactions are equally valid

- However, α-α scattering is very sensitive to the degree of locality of the NN interaction

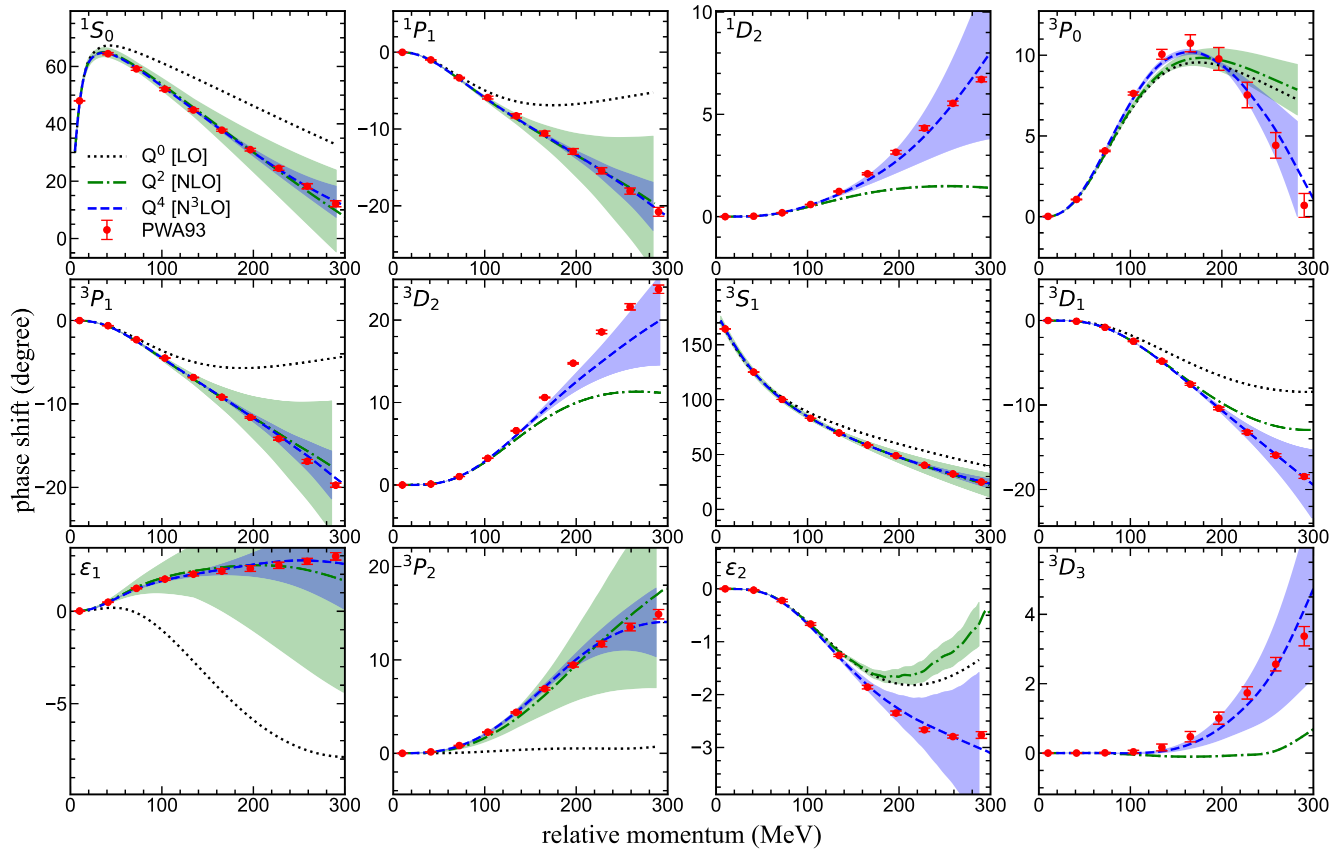
Elhatisari et al., (2016)

$\hookrightarrow$ purely nonlocal forces suppress the α-α interaction

$\hookrightarrow$ thus require stronger 3NFs in heavier nuclei to compensate for this

Two-pion exchange potential

- Here, we absorb the TPEP in the short distance LECs $\rightarrow$ works, see also Li et al. (2018)



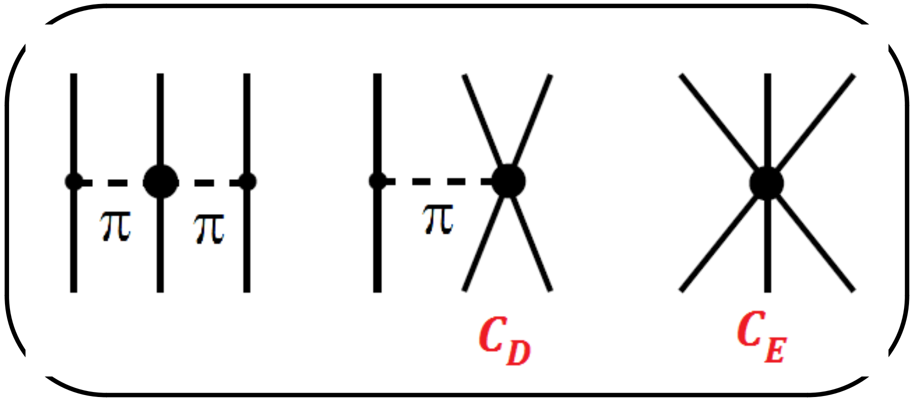
$\hookrightarrow$ needs to be improved (work underway)

$\hookrightarrow$ especially important for getting consistent currents beyond LO

Determination of 3NFs

Three-nucleon forces

- Basic topologies at N2LO:

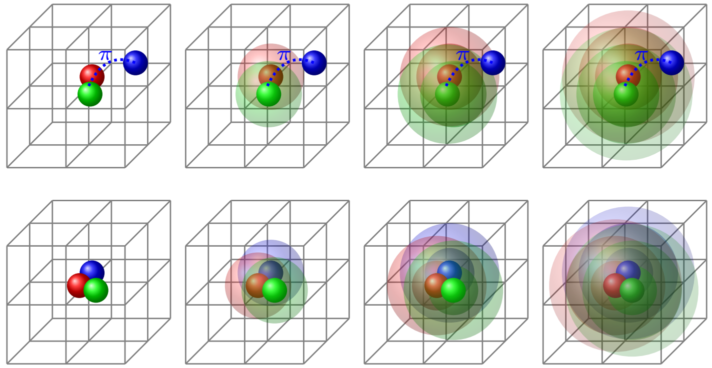


- 2-pion topology entirely fixed from πN scattering

- Smearing of the one-pion and contact term topologies

  ↪ more LECs (see below)

  ↪ effectively higher-order op's



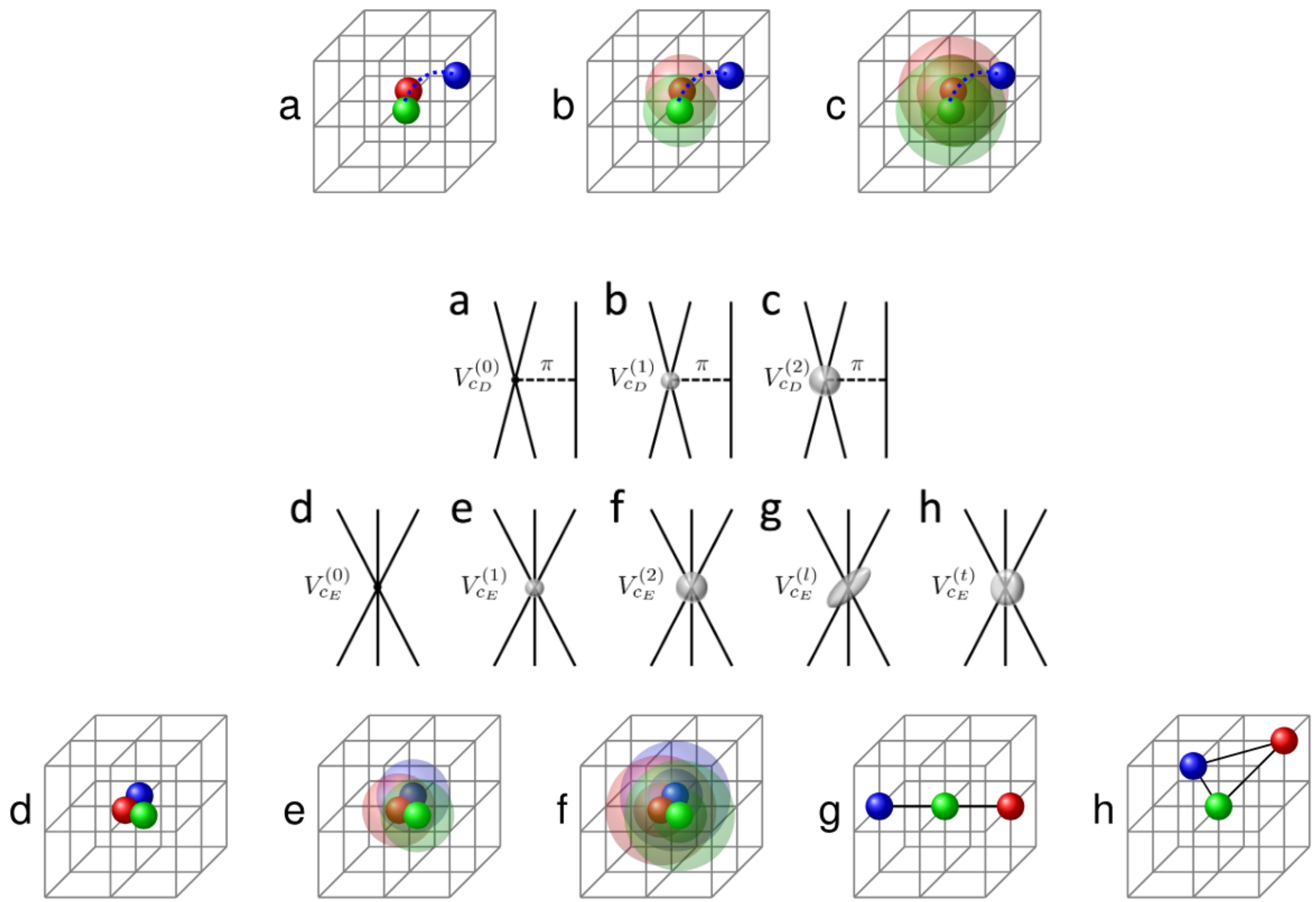
- On the market so far (more in the works!)

  ↪ $\mathcal{F}_p = 8$, only local smearings (next slide) — Elhatisari et al. (2024)

  ↪ $\mathcal{F}_p = 6$, a few non-locally smeared ops — Ren et al. (2025)

Locally smeared three-nucleon forces

- Most used set with $\mathcal{F}_p = 8$ locally smeared op's:



- Note the two additional SU(4) symmetric terms $V_{cE}^{(l,t)}$ motivated by cluster EFT

Determination of the 3NFs

- Main ingredients to fit the parameters of the 3NFs:

  – **Objective function:** Gaussian likelihood for selected binding energies

$$\mathcal{L}(\vec{\beta},\sigma^2) \propto \prod_{n\in\mathcal{S}} \exp\left\{ -\frac{1}{2\sigma_n^2}\left[z_n^{\rm exp} - z_{n,\rm NP}^{\rm th} - \sum_{k\in\mathcal{F}_p} \beta_k \frac{\partial z_n^{\rm th}}{\partial \beta_k} \right]^2 \right\}$$

  β_k = 3NF LECs, $\mathcal{S}$ = subset of nuclei, $\mathcal{F}_p$ = chosen set of $p \in \{6,7,8\}$ 3NF ops

  – **Number & sampling of observables:** to avoid bias, perform MCMC over (i) subsets $\mathcal{S}$ and (ii) operator sets $\mathcal{F}_p$ with update of $\vec{\beta}$

  – **Choice-of-observables uncert.:** sensitivity to chosen set of energies & subset of 3NFs

  – **Expected N3LO accuracy:** EFT truncation uncertainties either using history matching or the EKM procedure with $Q \simeq 0.3 - 0.4$

HM: Vernon et al. (2018), Hu et al. (2022), Elhatisari et al. (2024)

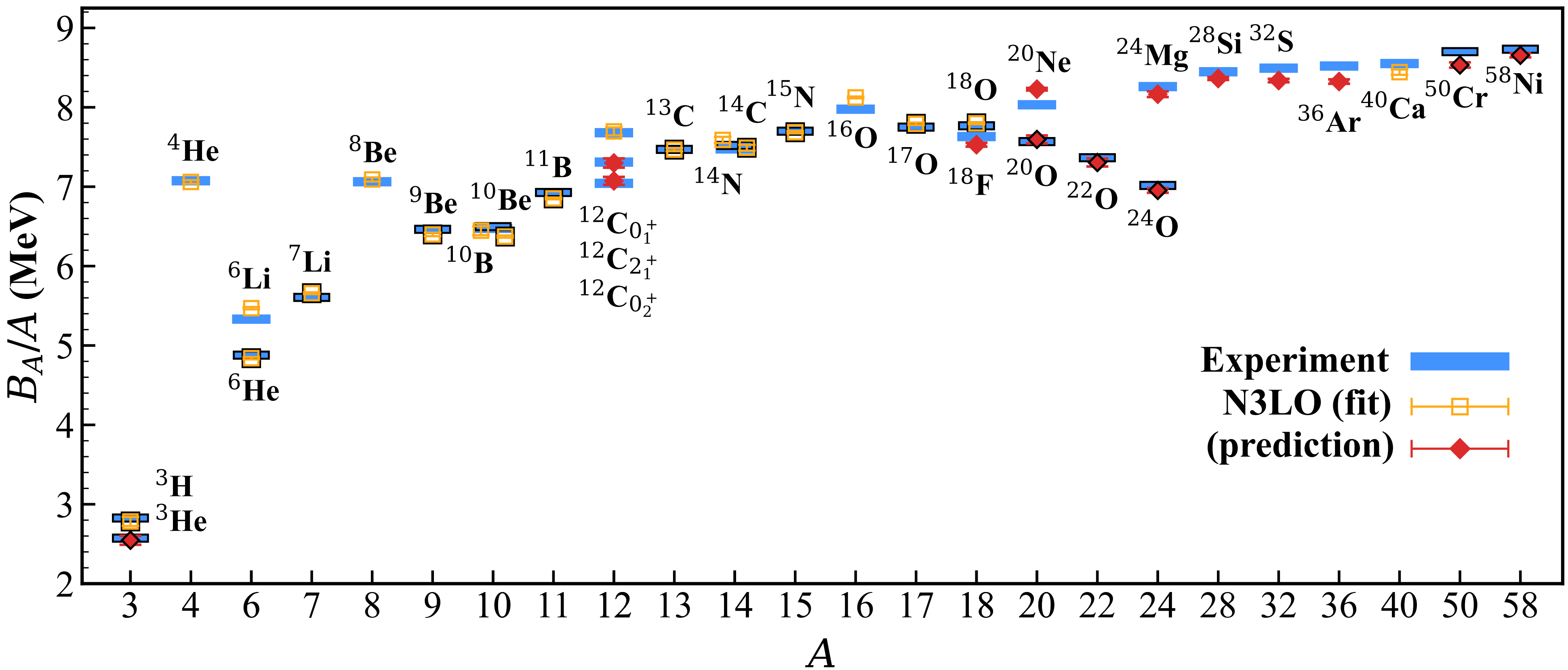
EKM: Epelbaum et al. (2015)

Fixing the 3NF LECs: Binding Energies at N3LO

Elhatisari et al., Nature **630** (2024) 59

- Quality of the fit: $\mathrm{RMSD}(\mathcal{S}) = \sqrt{\frac{1}{M_\mathcal{S}} \sum_{i\in\mathcal{S}} \left(\frac{E_i - E_i^{\exp}}{A_i} \right)^2}$ with size $M_\mathcal{S}$

$\hookrightarrow$ here, $\mathbf{RMSD = 0.079\ MeV}$ = 1.11% of the average BE per nucleon

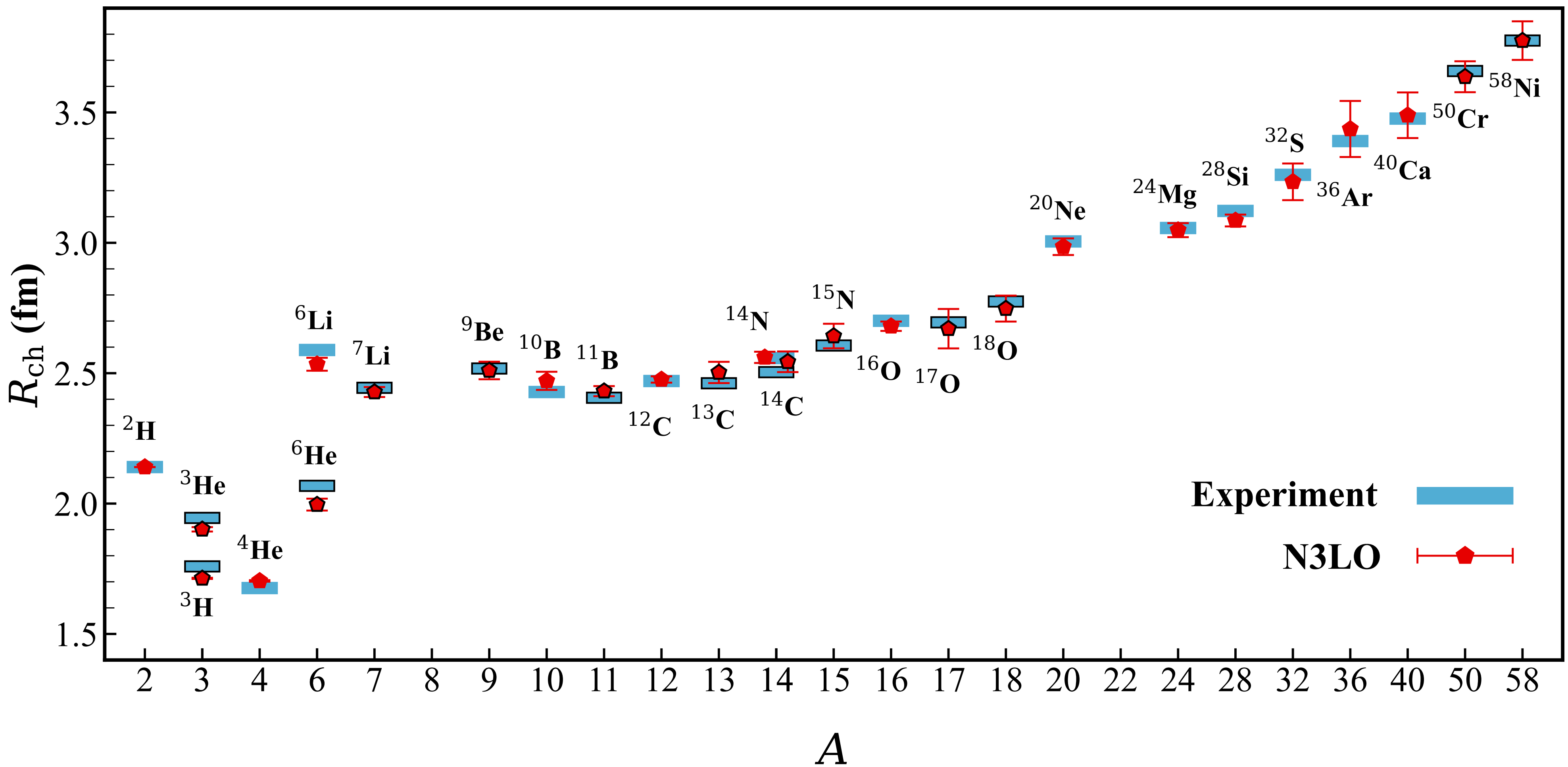


Applications to structure, reactions and matter

Prediction: Charge radii at N3LO

Elhatisari et al., Nature **630** (2024) 59

- Charge radii ($a = 1.32$ fm, statistical errors can be reduced)

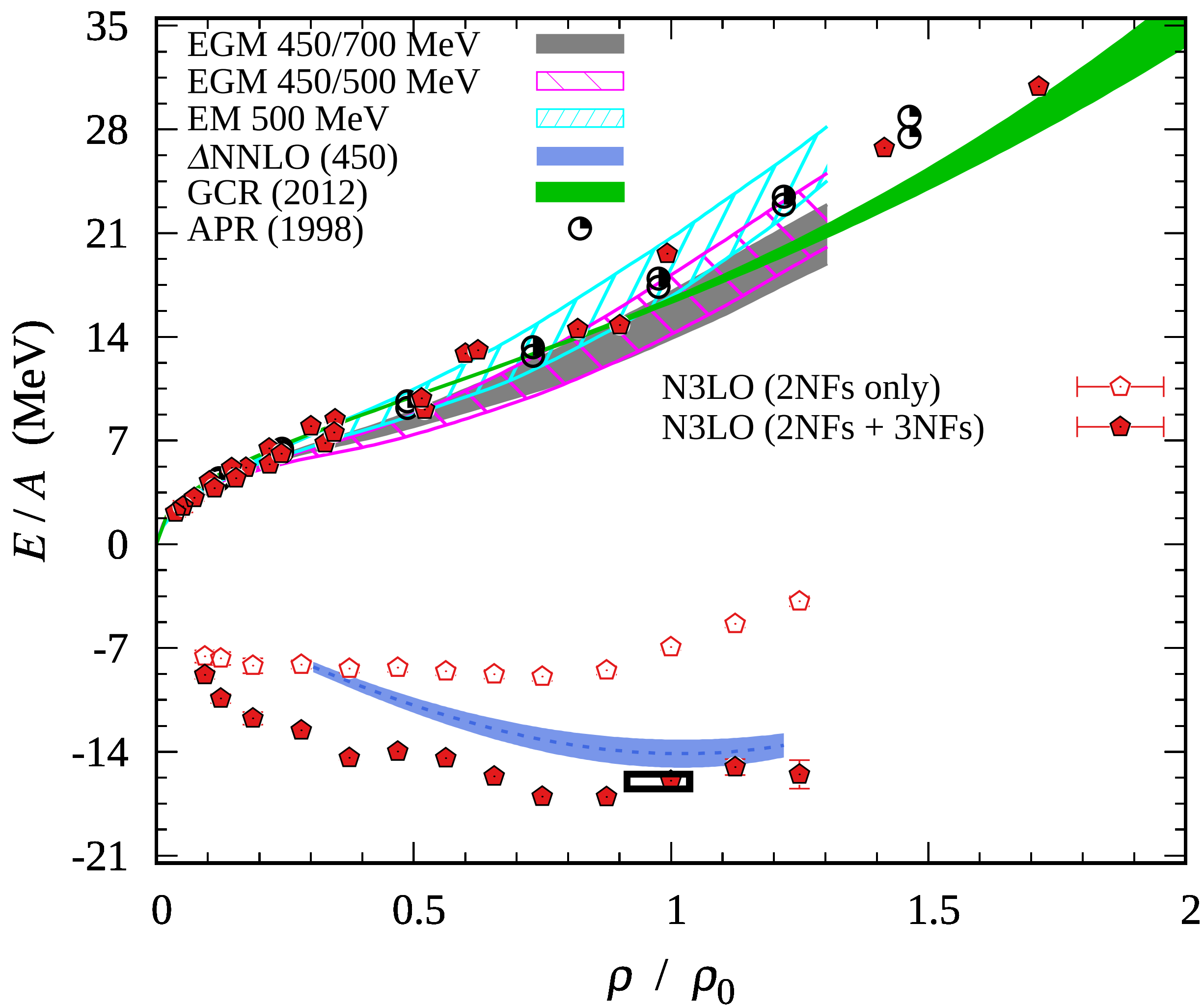


$\hookrightarrow$ no radius problem! but radii to be improved, see later

Prediction: Neutron & nuclear matter at N3LO

Elhatisari et al., Nature **630** (2024) 59

- Equation of State (EoS) of pure neutron matter & nuclear matter ($a = 1.32$ fm)



$\hookrightarrow$ can be improved using twisted b.c.'s

Some predictions based on high-fidelity forces

PHYSICAL REVIEW LETTERS **132,** 232502 (2024)

Structure Factors for Hot Neutron Matter from *Ab Initio* Lattice Simulations with High-Fidelity Chiral Interactions

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PHYSICS LETTERS B

Letter

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Lattice simulation of nucleon distribution and shell closure in the proton-rich nucleus ^{22}Si

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A R T I C L E I N F O

Editor: Dr A Schwenk

Keywords:
Effective field theory
Lattice
Silicon
Shell closure

A B S T R A C T

The proton-rich nucleus ^{22}Si is studied using Nuclear Lattice Effective Field Theory with high-fidelity chiral forces. Our results indicate that ^{22}Si is more tightly bound than ^{20}Mg, thereby excluding the possibility of two-proton emission. The $Z = 14$ shell closure in ^{22}Si is investigated through the evolution of the 2^+ state in the neighboring nuclei. We then focus on the charge radius and spatial distribution information of ^{22}Si, considering the novel phenomena that may emerge due to the small two-proton separation energy and the shell closure. We present the distribution of the 14 protons and 8 neutrons obtained from our lattice simulation, revealing insights into the spatial arrangement of the nucleons. Moreover, the spatial localization of the outermost proton and neutron suggests that ^{22}Si is a doubly magic nucleus. Furthermore, we develop the pinhole method based on the harmonic oscillator basis, which gives insight into the nuclear structure in terms of the shell model picture from lattice simulations. Our calculated occupation numbers support that $Z = 14$ and $N = 8$ are the shell closures and show that the $\pi 1s_{1/2}$ orbital component is minor in ^{22}Si.

PHYSICAL REVIEW LETTERS **134,** 162503 (2025)

***Ab Initio* Study of the Beryllium Isotopes ^7Be to ^{12}Be**

Shihang Shen,[1,2,3] Serdar Elhatisari,[4,5,6] Dean Lee,[7] Ulf-G. Meißner,[6,3,8,1,*] and Zhengxue Ren[3]

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PHYSICS LETTERS B

Letter

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***Ab initio* calculations of the carbon and oxygen isotopes: Energies, correlations, and superfluid pairing**

Young-Ho Song[a], Myungkuk Kim[b,*], Youngman Kim[b], Kihyeon Cho[c], Serdar Elhatisari[d,e], Dean Lee[f], Yuan-Zhuo Ma[f], Ulf-G Meißner[g,h,i]

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A R T I C L E I N F O

Editor: Dr. A. Schwenk

Keywords:
Nuclear lattice effective field theory
Neutron-rich isotopes
Superfluid parings
Ab initio calculation

A B S T R A C T

We perform *ab initio* nuclear lattice calculations of the neutron-rich carbon and oxygen isotopes using high-fidelity chiral interactions. We find good agreement with the observed binding energies and compute correlations associated with each two-nucleon interaction channel. For the isospin $T = 1$ channels, we show that the dependence on T_z provides a measure of the correlations among the extra neutrons in the neutron-rich nuclei. For the spin-singlet S-wave channel, we observe that any paired neutron interacts with the nuclear core as well as its neutron pair partner, while any unpaired neutron interacts primarily with only the nuclear core. For the other partial waves, the correlations among the extra neutrons grow more slowly and smoothly with the number of neutrons. These general patterns are observed in both the carbon and oxygen isotopes and may be universal features that appear in many neutron-rich nuclei.

Prediction: Tin isotopes close to the proton dripline

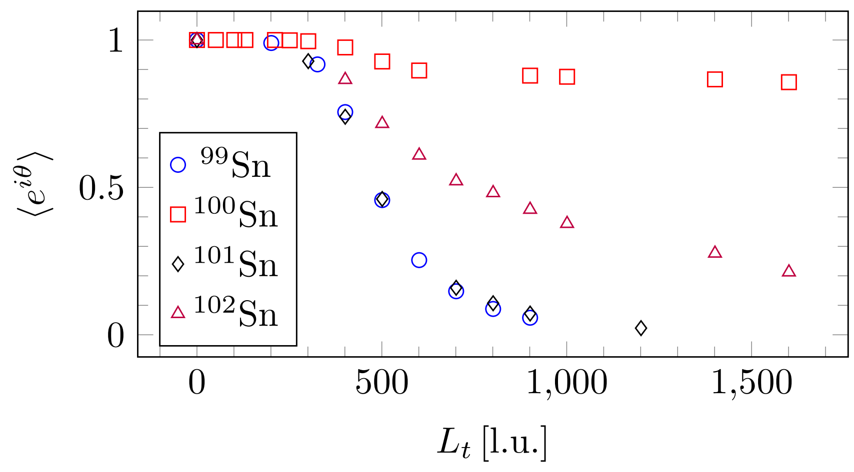
Hildenbrand et al., 2509.08579 [nucl-th]

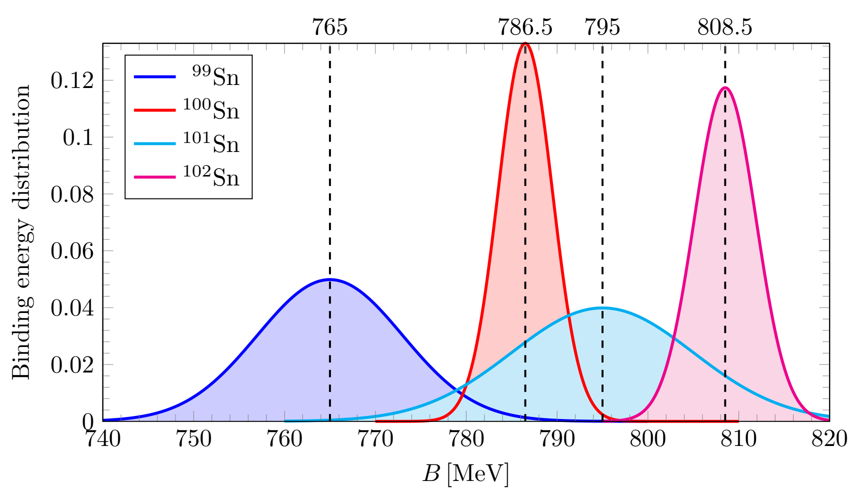
- First application using the Exascale system JUPITER @ FZJ
- Signal still strong enough for even-odd isotopes

↪ can extract the BEs of ^{99}Sn to ^{102}Sn

Nucleus	N3LO	N3LO*	Exp.
^{99}Sn	765±8	804±8	807.9± 0.6
^{100}Sn	786.5±3.0	825.2±3.0	825.16±0.24
^{101}Sn	795±10	834±10	836.39±0.30
^{102}Sn	808.5±3.4	848.1±3.4	849.09±0.10

Isotopes	N3LO	N3LO*	Exp.
102-101	13.5±10.6	14.1±10.6	12.7±0.3
102-100*	22.5±4.6	22.9±4.6	23.9±0.3
102-99	43.5±8.7	44.1±8.7	41.2±0.6
101-100	8.5±10.4	8.9±10.4	11.2±0.4
101-99*	30.0±12.8	30.1±12.8	28.5±0.7
100-99	21.5±8.6	21.2±8.6	17.3±0.7





Prediction: Multi-neutron correlations in light nuclei I

Zhang, Elhatisari, UGM, 2512.18849 [nucl-th]

- $3n$ and $4n$ clusters much thought about

$\hookrightarrow$ breakup, knockout & double charge exchange reactions

$\hookrightarrow$ investigate multi-n correlations in light nuclei

- Use 282 chiral interactions to predict:

$$E_{\rm gs}({}^6{\rm H}) = -4.94 \pm 0.14\,\text{MeV}$$

$$E_{\rm gs}({}^7{\rm H}) = -5.29 \pm 0.16\,\text{MeV}$$

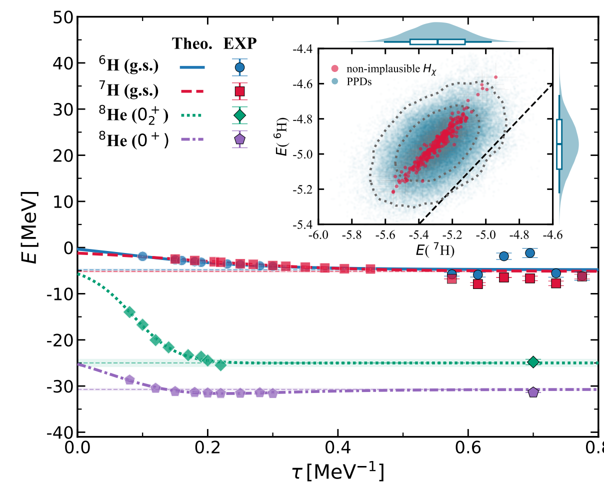
- Marginal posteriors suggest:

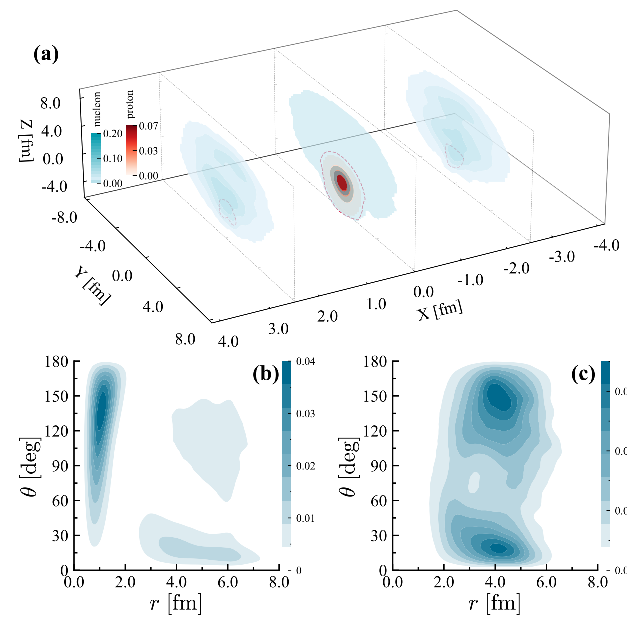
$$S_n({}^7{\rm H}) = 0.35 \pm 0.32\,\text{MeV}$$

$\hookrightarrow$ sequential ^{6}H$+n$ decay disfavored

$\hookrightarrow$ enhances the relevance of multi-n correlations

$\hookrightarrow$ two-neutron correlations clearly visible



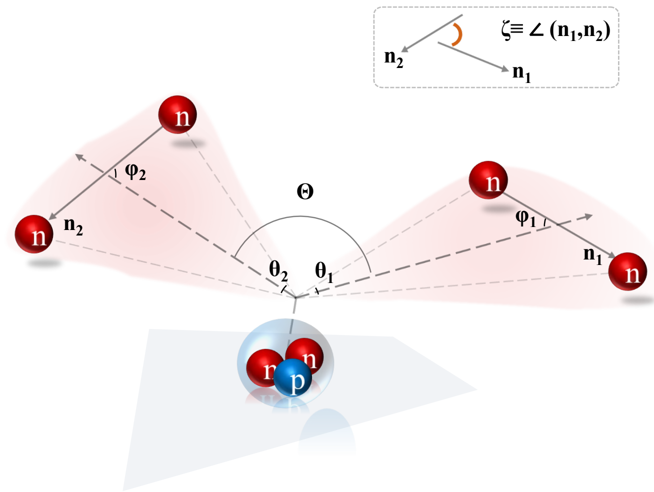


Prediction: Multi-neutron correlations in light nuclei II

Zhang, Elhatisari, UGM, 2512.18849 [nucl-th]

- Define four-neutron correlations via:

$$\rho_4(\theta_1,\varphi_1,\theta_2,\varphi_2;\Theta,\zeta) = \sum_{i<j,\,k<l}^{(ij),(kl)} \Big\langle \delta(\theta_{ij}-\theta_1)\,\delta(\varphi_{ij}-\varphi_1) \times\delta(\theta_{kl}-\theta_2)\,\delta(\varphi_{kl}-\varphi_2) \times\delta(\Theta_{ij,kl}-\Theta)\,\delta(\zeta_{ij,kl}-\zeta)\Big\rangle,$$

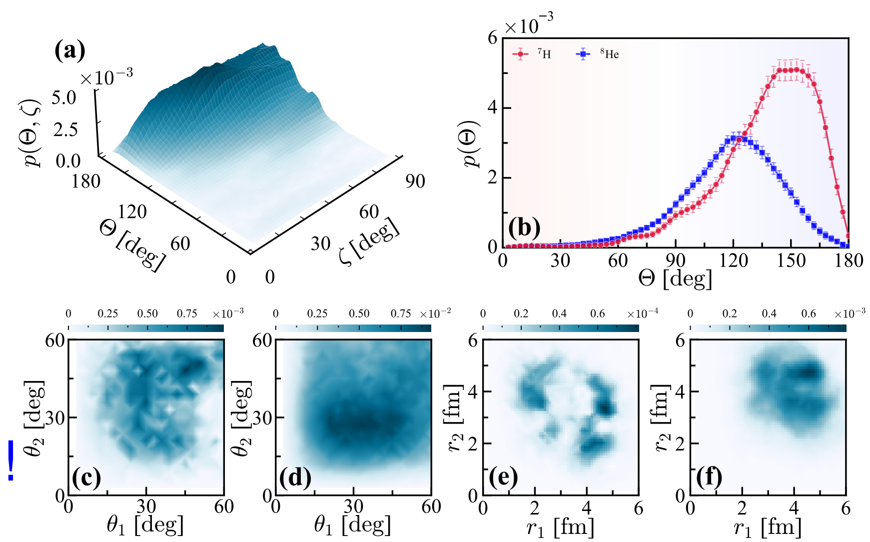


- The four-neutron correlations show:

↪ symmetric $2n$-$2n$ configuration is dominant
$(\sim 95\%,\ \ \Theta \simeq 140^\circ - 160^\circ)$

↪ compact tetraneutron configuration small
$(\sim 5\%,\ \ \Theta \simeq 60^\circ - 90^\circ)$

↪ must consider the $2n$-$2n$ config. in exp analysis!



Prediction: Searching for the tetraneutron

Wu, Elhatisari, UGM, Shen, Geng, Kim, 2601.01801 [nucl-th]

- Latest tetraneutron sighting in ^{4}He(^{8}He,^{8}Be)$4n$

  Duer et al., Nature **606** (2022) 678

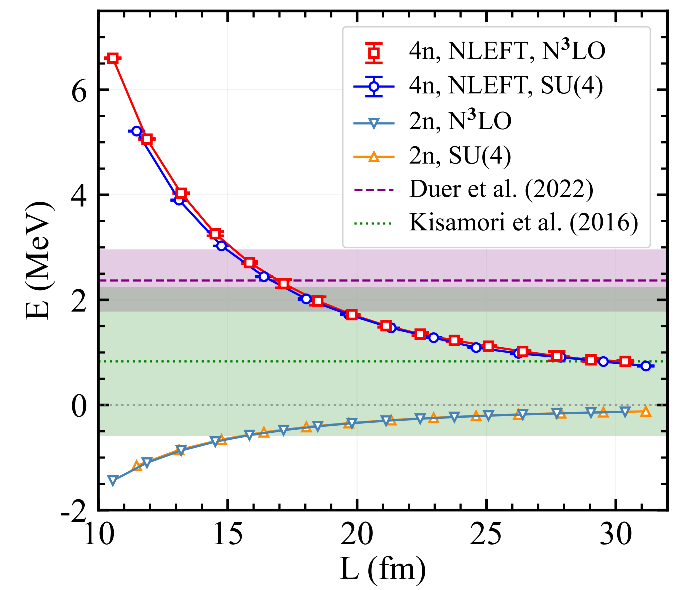
$\hookrightarrow$ analysis presumably too simplified,
various re-analyses show no resonance

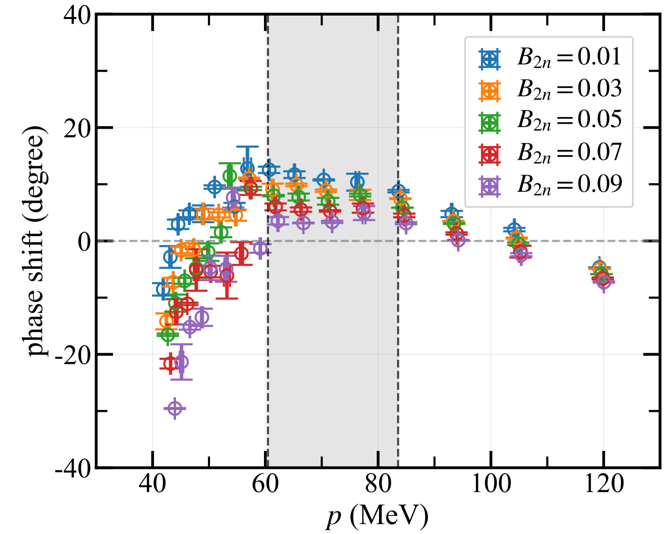
$\hookrightarrow$ most theory analyses do not give a $4n$ resonance

- Search on the lattice (SU(4) and N3LO interactions)

$\hookrightarrow$ volume-dependence shows no sign of a resonance

$\hookrightarrow$ $2n$-$2n$ scattering shows a shallow attraction
in the momentum range $p \simeq 60 - 85$ MeV
corresponds to confined $4n$ energies of $1.7 - 3.3$ MeV
similar to the $4n$ peak energies in experiment





Prediction: Neutron-alpha scattering

Elhatisari, Hildenbrand, UGM, J. Phys. **G 52** (2025) 125102

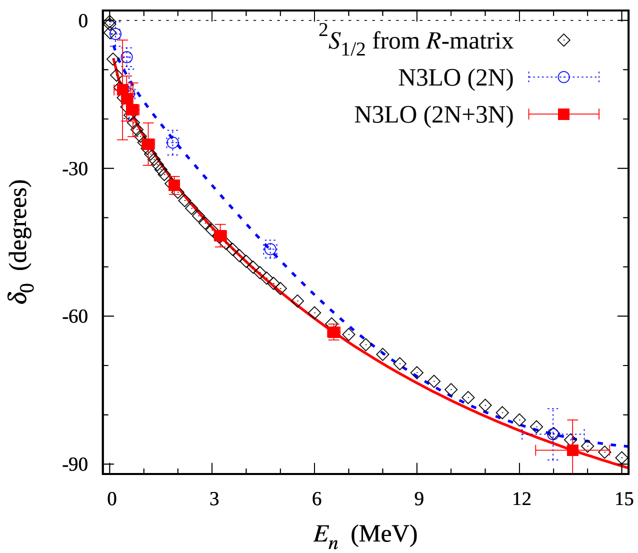
- n-α scattering know to be a good testbed of 3NFs

  Pieper, Pandharipande (1993), Quaglioni, Navratil (2008), Kravvaris et al. (2020), ...

- Use the time-honoured Lüscher approach

- Compare to R-matrix results

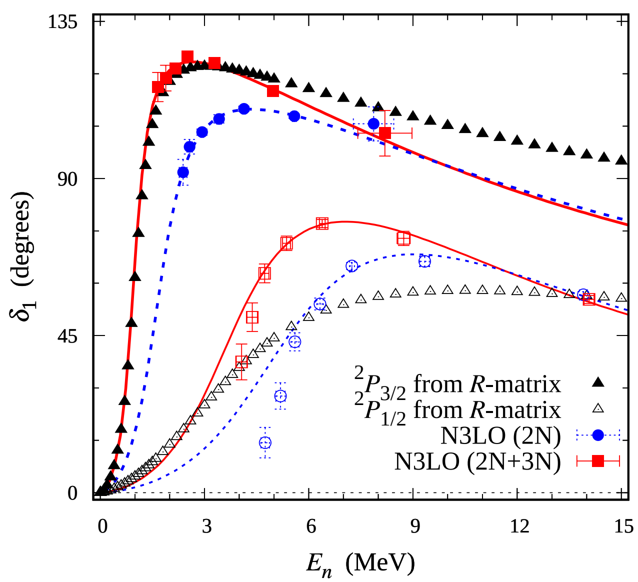
  G. M. Hale, private communication (2023)



$\hookrightarrow$ S-wave ($^2S_{1/2}$) well described when 3NFs are included

$\hookrightarrow$ Large $^2P_{3/2}$ well described when 3NFs are included

$\hookrightarrow$ Visible deviation in the $^2P_{1/2}$ wave for $E_n \geq 3$ MeV



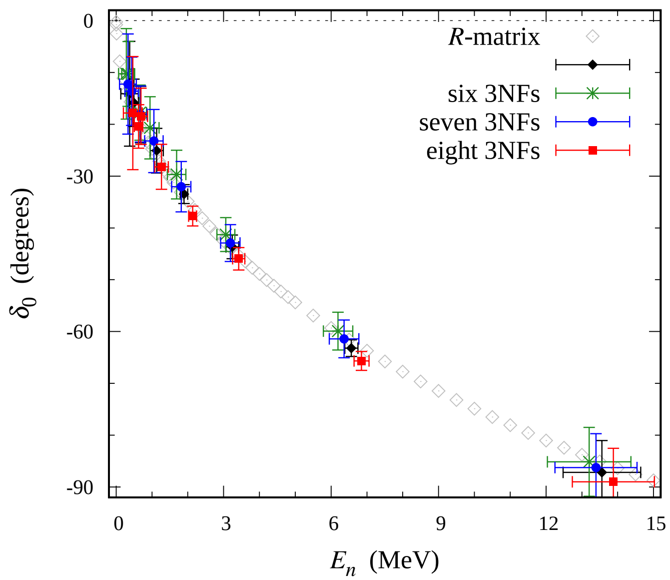
- What is the reason for the deviations in the $^2P_{3/2}$-$^2P_{1/2}$ splitting?

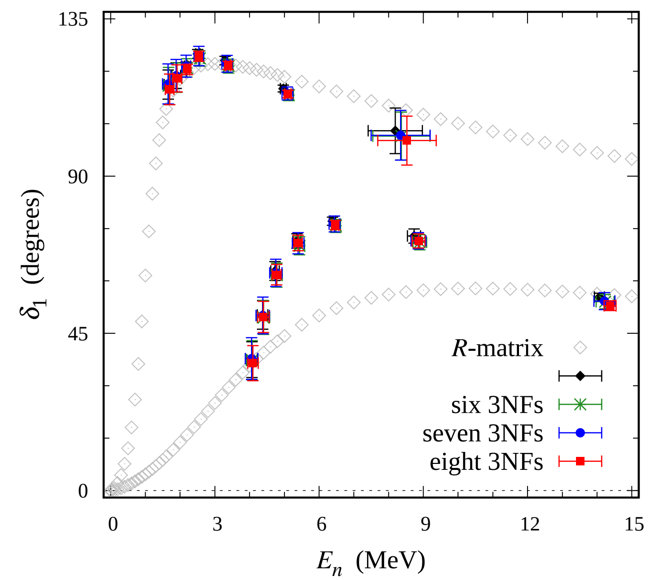
Neutron-alpha scattering revisited

Elhatisari, Hildenbrand, UGM, J. Phys. **G 52** (2025) 125102

- Investigate one possible reason: Choice of nuclei to fix the LECs?

- Perform MCMC searches to explore systematically the set of 8 3NF ops
  and also reduce to sets with 6 and 7 ops and quantify the uncertainty using RSMD





$\hookrightarrow$ clearly, this is not the source of the problem

$\hookrightarrow$ must improve the 3NFs!

Towards improved 3NFs

A minimal set of 3NFs

Ren, Elhatisari, UGM, PRL **135** (2025) 152502

- Consider sets of 6 3NF op's (called minimal set)

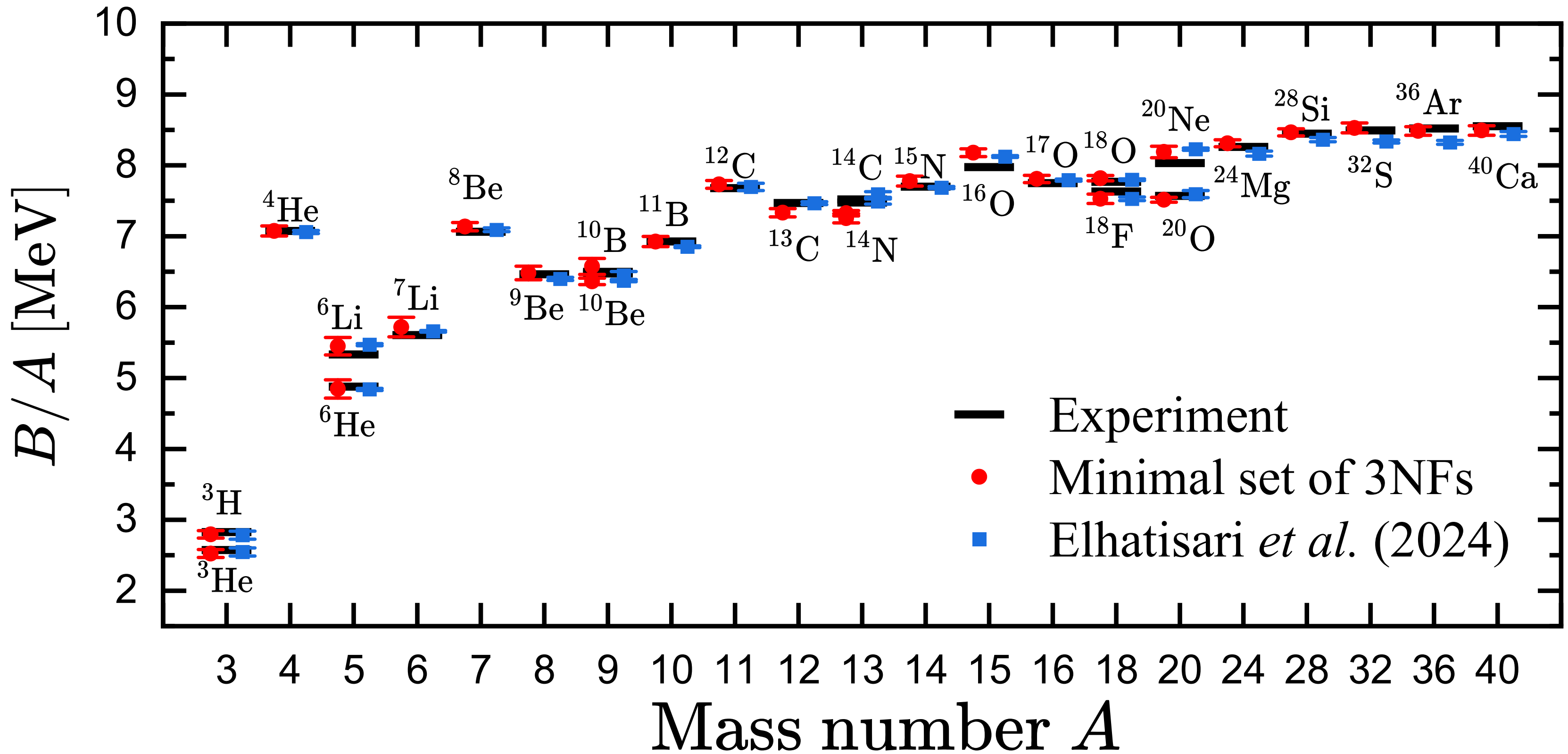
No.	V_{3N}'s
1	$V^{(0)}_{c_E,s_{NL1}}$, $V^{(3)}_{c_D}$, $[V^{(0)}_{c_E}]_{044}$, $[V^{(0)}_{c_E}]_{224}$, $[V^{(0)}_{c_E}]_{125}$, $[V^{(0)}_{c_E}]_{145}$
2	$[V^{(1)}_{c_E}]_{000}$, $V^{(3)}_{c_D}$, $[V^{(0)}_{c_E}]_{044}$, $[V^{(0)}_{c_E}]_{222}$, $[V^{(0)}_{c_E}]_{114}$, $[V_{c_E,s_L}]_{033}$
3	$V^{(0)}_{c_E,s_{NL1}}$, $V^{(3)}_{c_D}$, $[V^{(0)}_{c_E}]_{044}$, $[V^{(0)}_{c_E}]_{224}$, $[V^{(0)}_{c_E}]_{125}$, $[V^{(0)}_{c_E}]_{235}$
4	$V^{(0)}_{c_D}$, $V^{(2)}_{c_D}$, $[V^{(0)}_{c_E}]_{044}$, $[V^{(0)}_{c_E}]_{222}$, $[V^{(0)}_{c_E}]_{224}$, $[V^{(0)}_{c_E}]_{125}$
5	$V^{(1)}_{c_D}$, $V^{(3)}_{c_D}$, $[V^{(0)}_{c_E}]_{033}$, $[V^{(0)}_{c_E}]_{044}$, $[V^{(0)}_{c_E}]_{222}$, $[V^{(0)}_{c_E}]_{125}$
6	$V^{(0)}_{c_E,s_{NL1}}$, $V^{(0)}_{c_D}$, $V^{(3)}_{c_D}$, $[V^{(0)}_{c_E}]_{044}$, $[V^{(0)}_{c_E}]_{224}$, $[V^{(0)}_{c_E}]_{125}$
7	$V^{(1)}_{c_D}$, $V^{(3)}_{c_D}$, $V^{(0)}_{c_D,s_{NL2}}$, $[V^{(0)}_{c_E}]_{044}$, $[V^{(0)}_{c_E}]_{224}$, $[V^{(0)}_{c_E}]_{125}$
8	$V^{(0)}_{c_D}$, $V^{(2)}_{c_D}$, $[V^{(0)}_{c_E}]_{044}$, $[V^{(0)}_{c_E}]_{224}$, $[V^{(0)}_{c_E}]_{125}$, $[V^{(0)}_{c_E}]_{145}$
9	$[V^{(0)}_{c_E}]_{000}$, $V^{(3)}_{c_D}$, $[V^{(0)}_{c_E}]_{224}$, $[V^{(0)}_{c_E}]_{125}$, $[V_{c_E,s_L}]_{044}$, $[V^{(0)}_{c_E}]_{334}$
10	$[V^{(0)}_{c_E}]_{000}$, $V^{(0)}_{c_E,s_{NL3}}$, $V^{(1)}_{c_D}$, $V^{(0)}_{c_D,s_{NL3}}$, $[V^{(0)}_{c_E}]_{224}$, $[V^{(0)}_{c_E}]_{125}$

- contains also non-local operators (marked in blue)
- only some sets contain the SU(4) symmetric $V^{(l,t)}_{c_E}$ [here: $[V^{(0)}_{c_E}]_{144}$, $[V^{(0)}_{c_E}]_{222}$]

Determination of the 3NF LECs

Ren, Elhatisari, UGM, PRL **135** (2025) 152502

- Fit to the BE of a selected number of nuclei and also include the ^{4}He charge radius



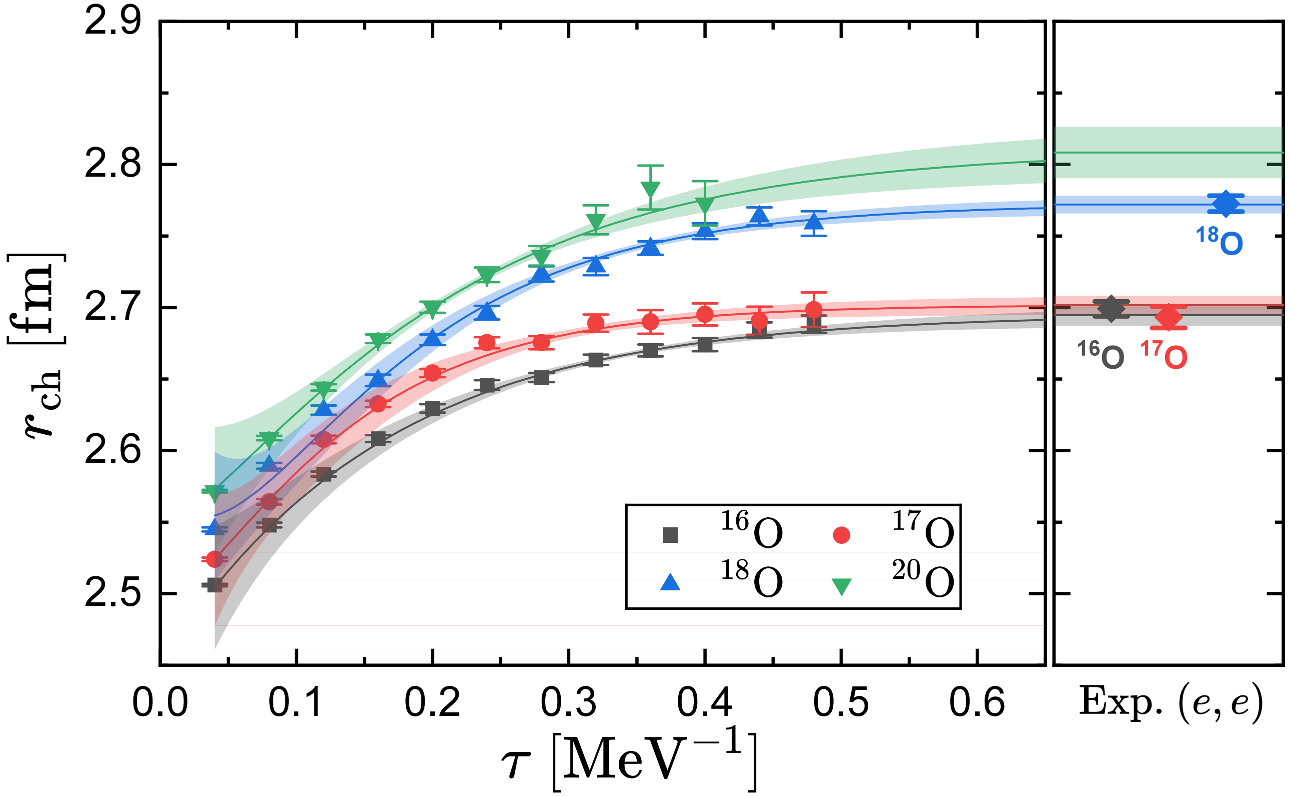
$\hookrightarrow$ Quality similar to the WFM 3NFs: RMSD = 0.101 MeV (1.4%) [0.093 MeV (1.1%)]

$\hookrightarrow$ use these now for the calculation of selected oxygen radii

Radii of selected oxygen isotopes

Ren, Elhatisari, UGM, PRL **135** (2025) 152502

- Use the partial pinhole algorithm to study the radii of ^{16,17,18,20}O with $M = 4$



Isotope	NLEFT	Exp.
^{16}O	2.704(17)	2.699(5)
^{17}O	2.709(15)	2.693(8)
^{18}O	2.768(17)	2.776(2)
^{20}O	2.810(32)	

- Trend of the data reproduced: $r_{\rm ch}(^{16}{\rm O}) \simeq r_{\rm ch}(^{17}{\rm O}) < r_{\rm ch}(^{18}{\rm O})$
- Prediction for $r_{\rm ch}(^{20}{\rm O}) \to$ nice test

Summary & outlook

- Nuclear lattice simulations: a new quantum many-body approach

  $\rightarrow$ based on the successful continuum nuclear chiral EFT

  $\rightarrow$ a number of highly visible results already obtained

- Recent developments

  $\rightarrow$ NN(N) interaction at N3LO w/ wave function matching

  $\hookrightarrow$ first promising results for nuclear structure, matter and scattering

  $\hookrightarrow$ first results for β-decays [ulitimately $0\nu 2\beta$ decays]

  Elhatisari, Hildenbrand, UGM, Phys. Lett. B **859** (2024) 139086 + PKU group

  $\hookrightarrow$ hypernuclei & neutron stars are under investigation

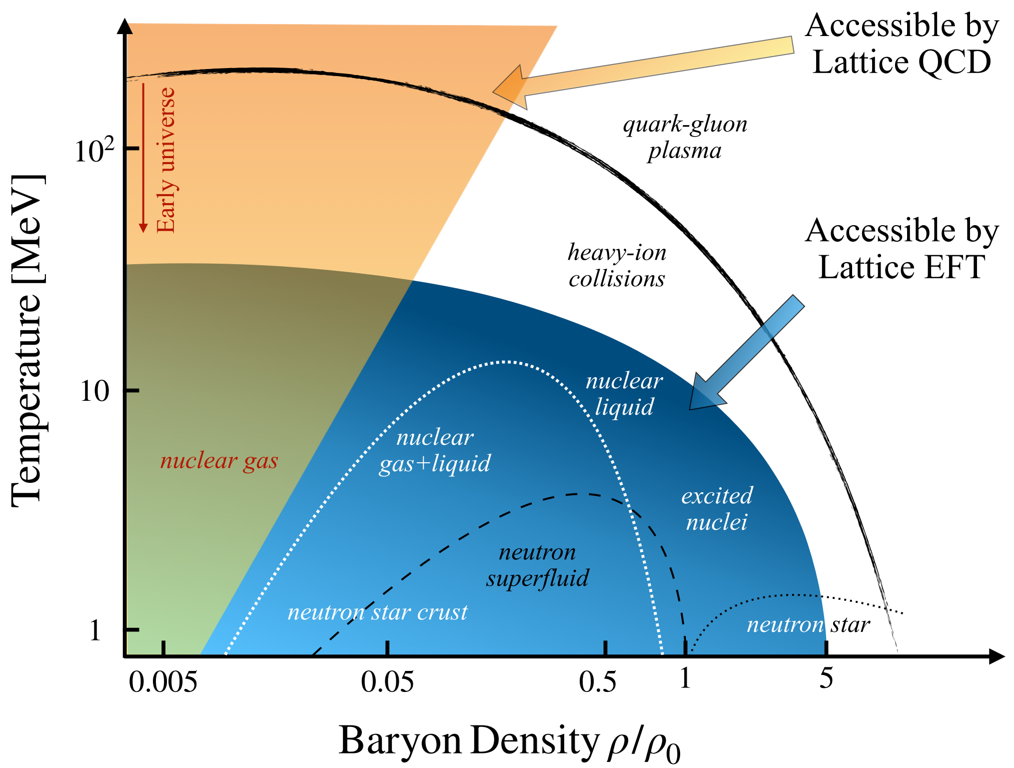
  Hildenbrand et al., Eur. Phys. J. A **60** (2024) 215; Tong et al., 2509.26148

- Improved 3NFs are being worked out $\hookrightarrow$ stay tuned!

SPARES

Comparison to lattice QCD

LQCD (quarks & gluons)	NLEFT (nucleons & pions)
relativistic fermions	non-relativistic fermions
renormalizable th'y	EFT
continuum limit	no continuum limit
(un)physical masses	physical masses
Coulomb - difficult	Coulomb - easy
high T/small ρ	small T/nuclear densities
sign problem severe	sign problem moderate



- For nuclear physics, NLEFT is the far better methodology!

Transfer matrix method

- Correlation–function for A nucleons: $Z_A(\tau) = \langle\Psi_A|\exp(-\tau H)|\Psi_A\rangle$

  with Ψ_A a Slater determinant for A free nucleons

  [or a more sophisticated (correlated) initial/final state]

Euclidean time

- Transient energy

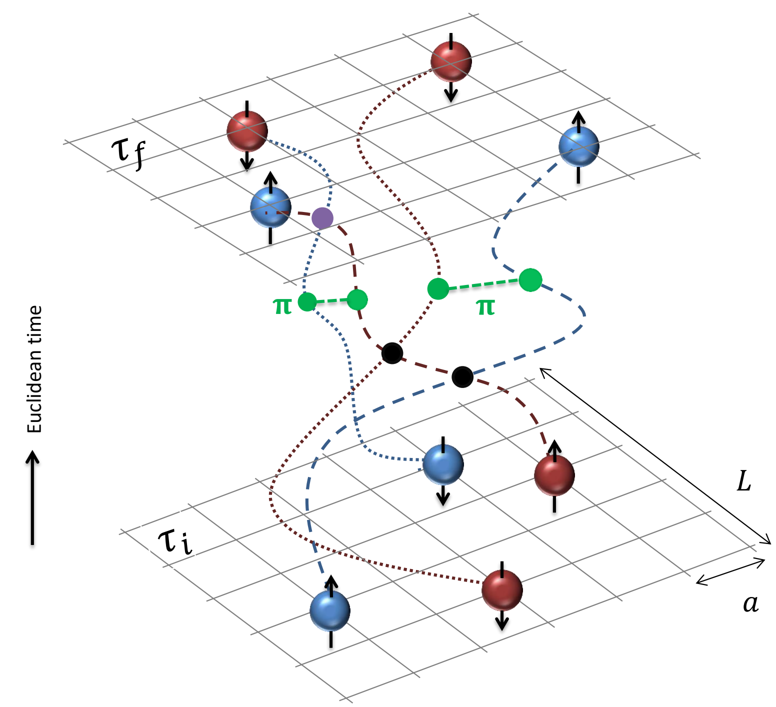
$$E_A(\tau) = -\frac{d}{d\tau}\ln Z_A(\tau)$$

$\to$ ground state: $E_A^0 = \lim_{\tau\to\infty} E_A(\tau)$

- Exp. value of any normal–ordered operator $\mathcal{O}$

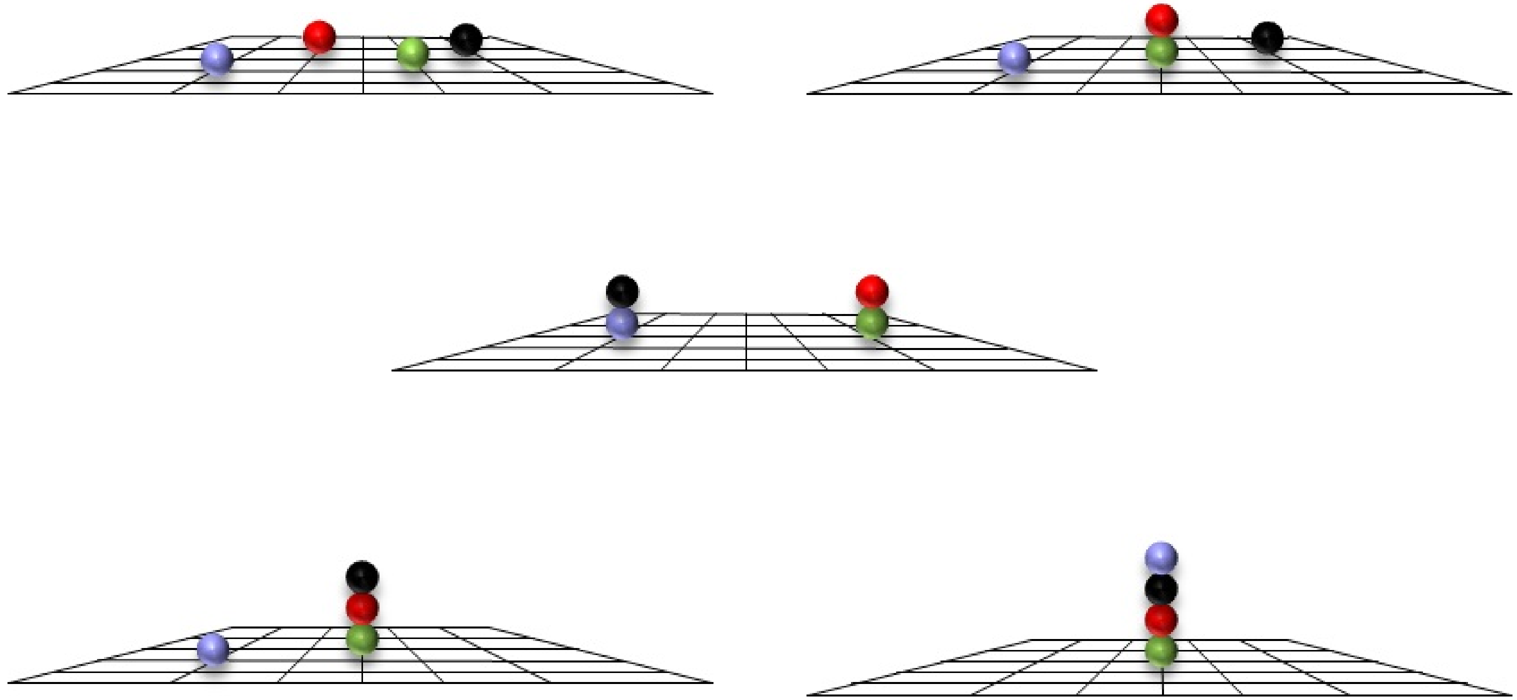
$$Z_A^{\mathcal{O}} = \langle\Psi_A|\exp(-\tau H/2)\,\mathcal{O}\,\exp(-\tau H/2)\,|\Psi_A\rangle$$

$$\lim_{\tau\to\infty}\frac{Z_A^{\mathcal{O}}(\tau)}{Z_A(\tau)} = \langle\Psi_A|\mathcal{O}\,|\Psi_A\rangle$$



- Excited states: $Z_A(\tau) \to Z_A^{ij}(\tau)$, diagonalize, e.g. $0_1^+, 0_2^+, 0_3^+, \ldots$ in ^{12}C

Configurations



⇒ all *possible* configurations are sampled

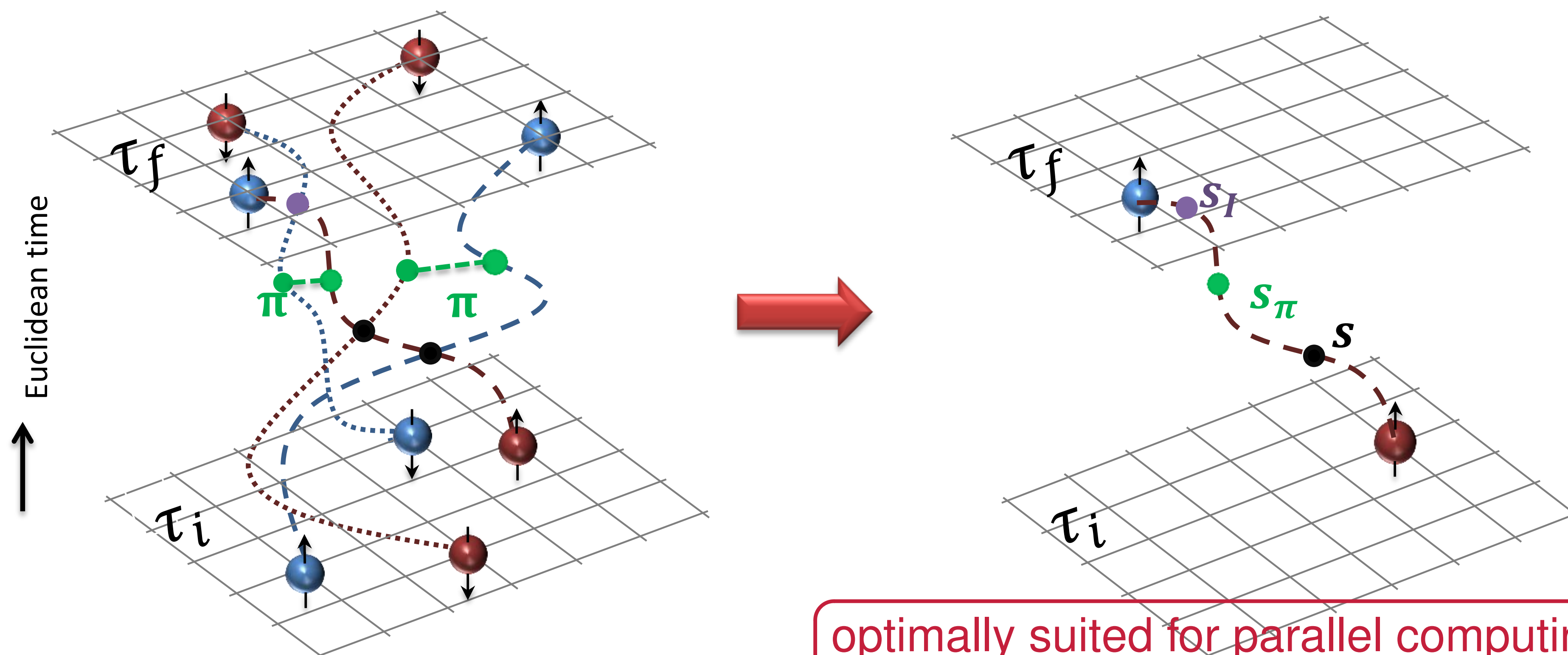
⇒ preparation of *all possible* initial/final states

⇒ *clustering* emerges *naturally*

Auxiliary field method

- Represent interactions by auxiliary fields (Gaussian completion):

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



optimally suited for parallel computing!

Computational equipment

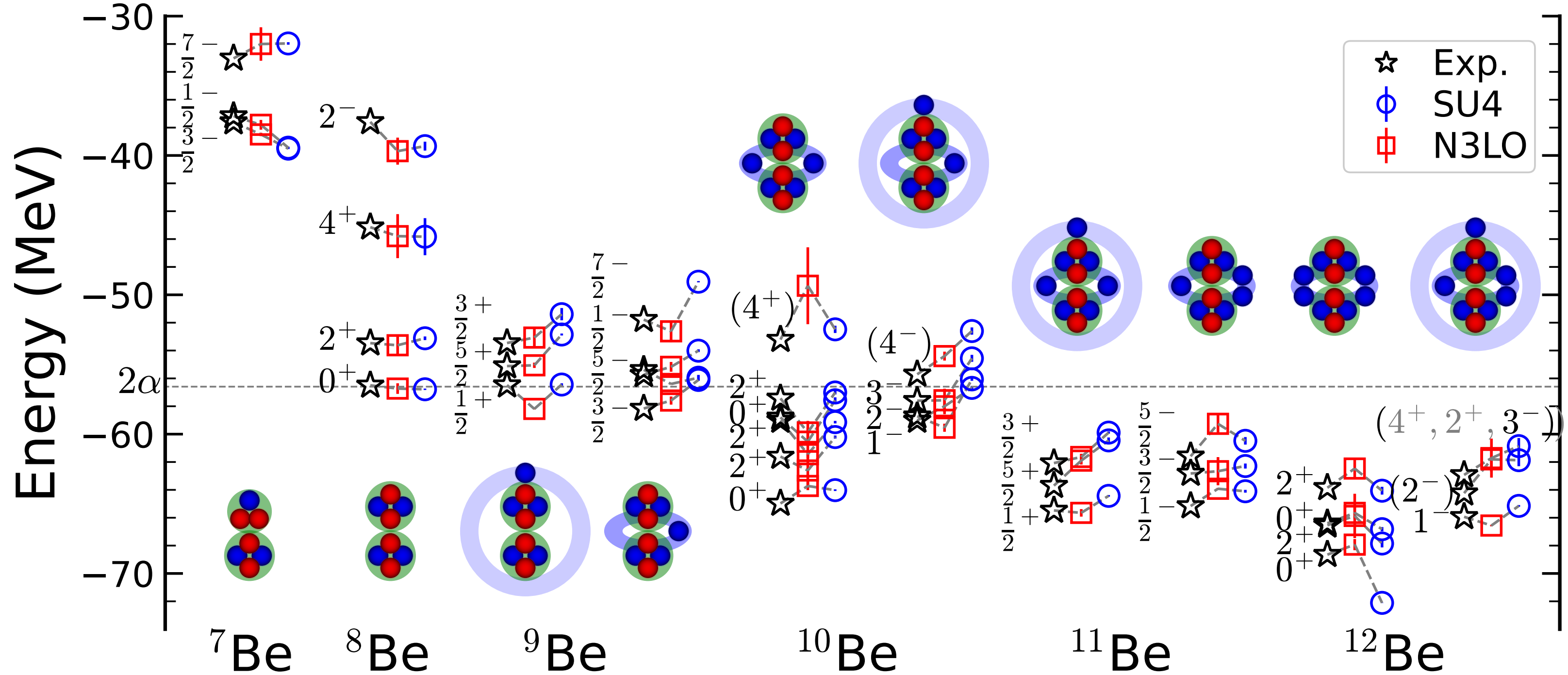
- Present = JUPITER + FRONTIER + ...

1 Exaflop

Prediction: Be isotopes

Shen et al., Phys. Rev. Lett. **134** (2025) 162503

- Systematic study of the Be isotopes & their radii & their em transitions:



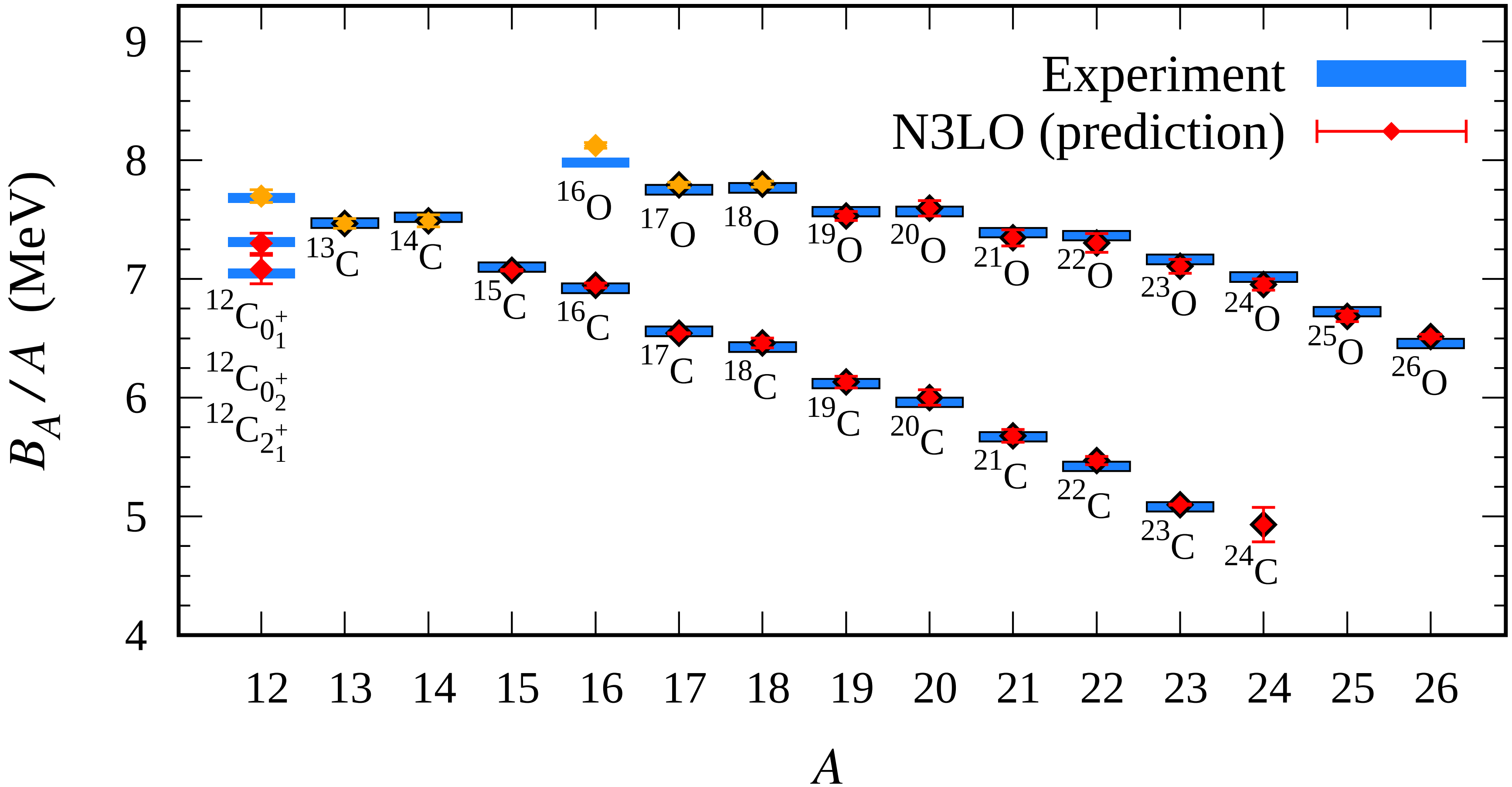
↪ new method to quantify nuclear shapes

↪ clusters, halos, molecular orbitals in **one shot**

Prediction: Isotope chains of carbon & oxyen

Song et al., Phys. Lett. **B 872** (2026) 140086

- Towards the neutron drip-line in carbon and oxygen:



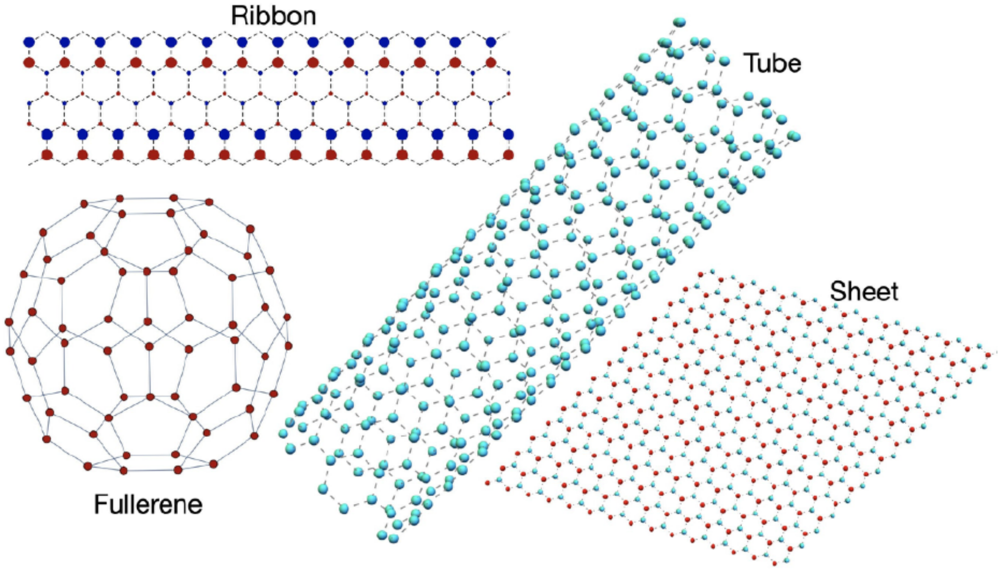
$\hookrightarrow$ 3NFs of utmost importance for the n-rich isotopes!

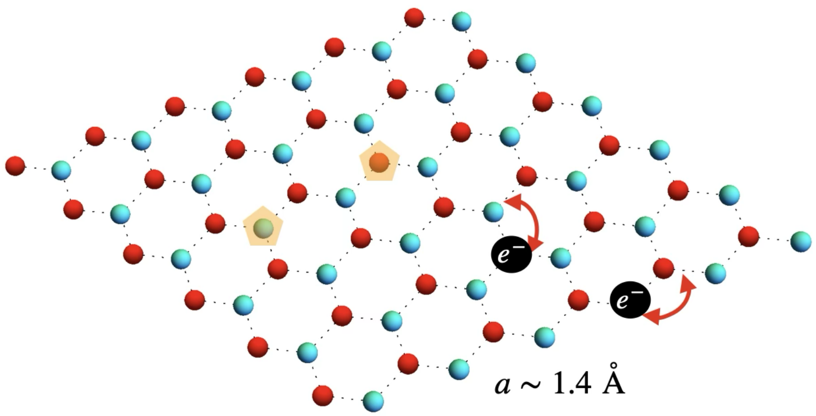
$\hookrightarrow$ universal features of neutron correlations

Strongly correlated electronic systems in low dimensions

Why low-dimensional materials?

- At least one of the dimensions of the material is small ($\sim$ nanoscale)
- Quantum effects and strong correlations induce novel phenomena (emergence)
- Novel quantum electronics
- Fault tolerant quantum computing
- Can be tackled by MC simulations & EFTs





Why strong correlations in low-d materials?

- Compare the Coulomb to the kinetic energy of an electron in a d-dimensional system:

$$\Gamma = \frac{E_C}{E_K} \approx \left(\frac{n_0}{n_d}\right)^{1/d}$$

n_d = electron density
$n_0 = (m^* e^2/\epsilon_0)^d$ = fiducial density
m^* = effective mass, ϵ_0 = dielectric constant

$\hookrightarrow$ strength of electron correlations depends on the density of electrons and the dimensionality of the system

$\hookrightarrow$ $\Gamma < 1$ perturbative , $\Gamma > 1$ non-perturbative

$\hookrightarrow$ in general, lower dimensions enhance correlations

- Graphene (2D) is a good example, linear dispersion gives for the electrons:

$$\Gamma \approx 2 - 3$$

$\hookrightarrow$ the electrons in graphene are strongly interacting

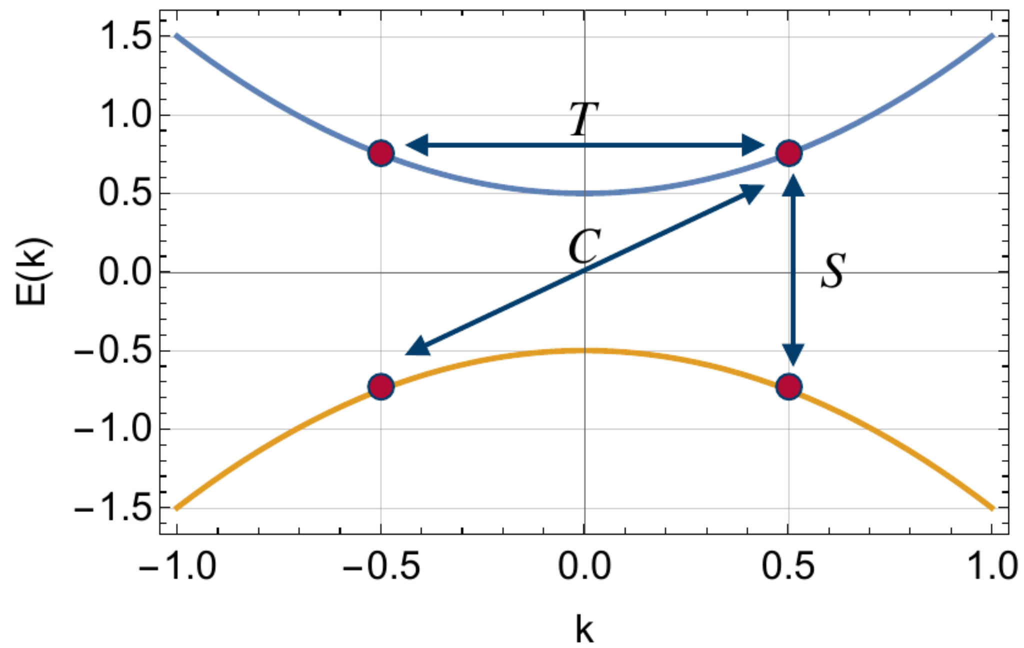
Symmetries pertinent to low-d materials

- Time-reversal symmetry T: $T^2 = \pm 1$

$$t \to -t \longrightarrow E(k) = E(-k)$$

- Charge conjugation symmetry (or *particle-hole* symmetry) C: $C^2 = \pm 1$

↪ Spectrum symmetric about zero:
$$E_+(k) = -E_-(-k)$$



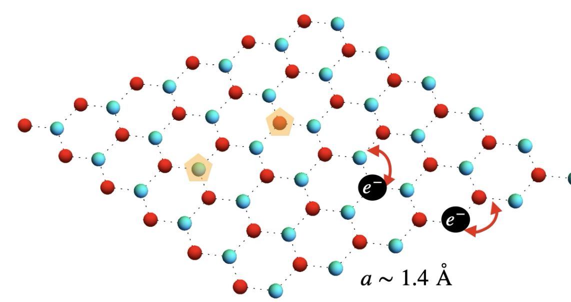
- Chiral symmetry (or *sublattice* symmetry)

$$S: \quad S^2 = S \quad E_+(k) = -E_-(k)$$

- No spontaneous symmetry breaking in $d \le 2$

↪ no Goldstone modes

Mermin, Wagner, Phys. Rev. Lett. **17** (1966) 1133



⇒ Phases of matter classified topologically

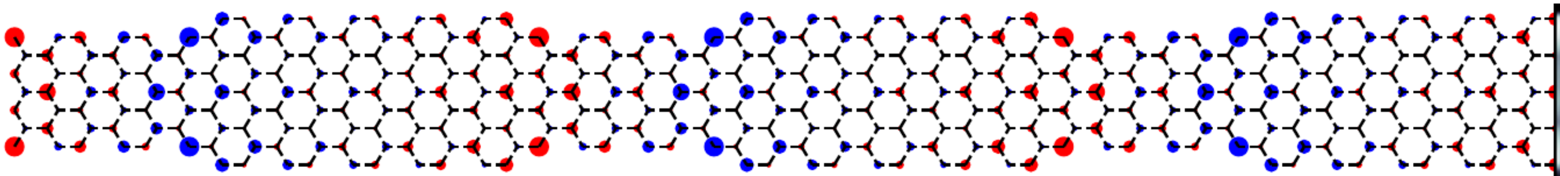
↪ all *symmetry classes* cataloged (for non-interacting systems)

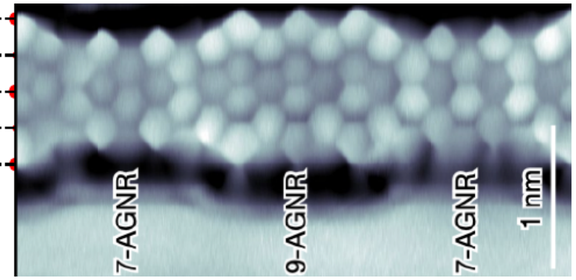
Chiu et al., Rev. Mod. Phys. **88** (2016) 035005

Localization in hybrid nanoribbons

- Consider armchair graphene nanoribbons (AGNRs), defined by the shape of their edges
- These can be fabricated!

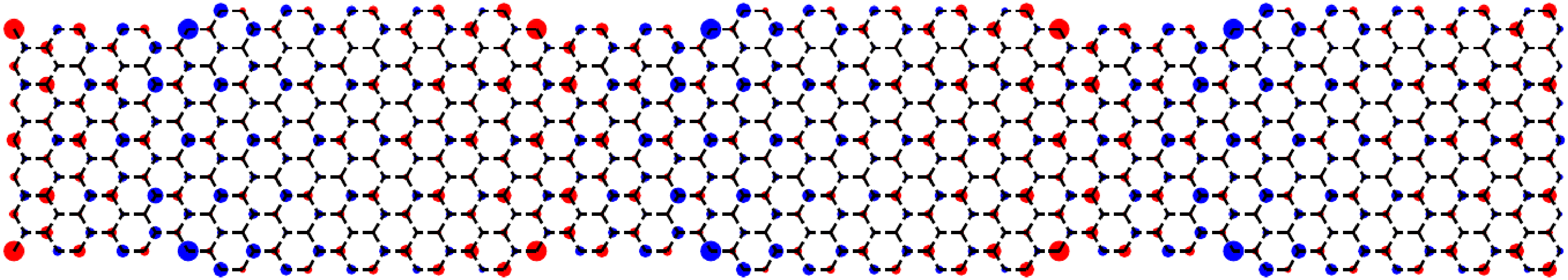
7/9 ribbon





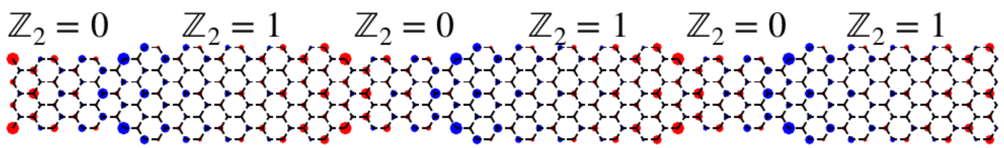
Rizzo et al. Nature **560** (2018) 204

13/15 ribbon



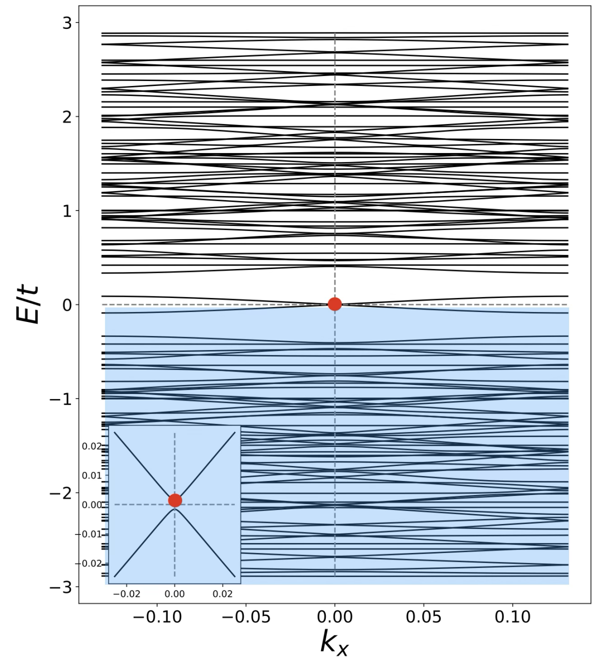
Localization in hybrid nanoribbons continued

- Lowest energy state in AGRNs exhibit localization

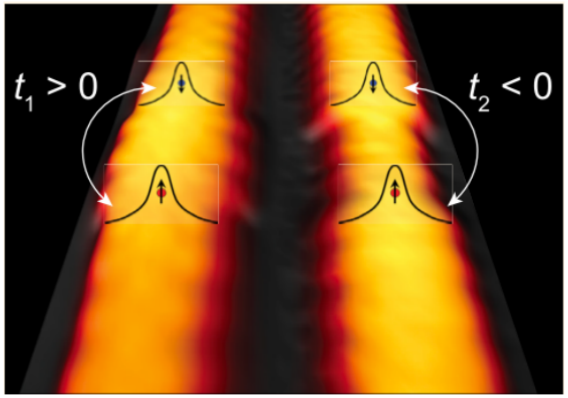


Cao et al., PRL **119** (2017) 076401

$\hookrightarrow$



- Experimental evidence



Rizzo et al., ACS Nano 2021, **15**, 12, 20633

- Potential applications: Topological quantum dots, fault-tolerant QC, ...
- But all theoretical analysis is based on *non-interacting dynamics!*

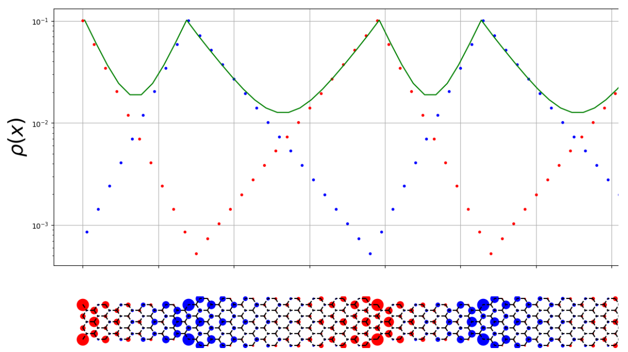
A new type of localization in hybrid nanoribbons

Ostmeyer, Razmadze, Berkowitz, Luu, UGM, Phys. Rev. B **109** (2024) 195135

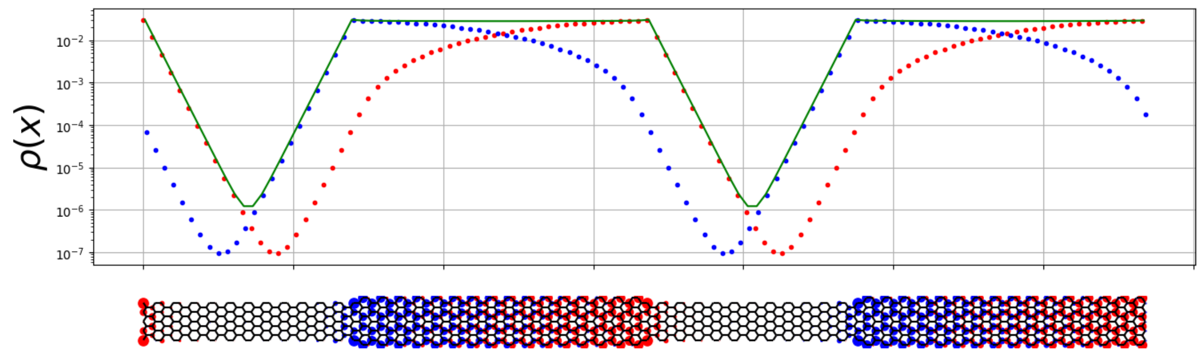
- Investigating the non-interacting model $\longrightarrow$ finding a new localization

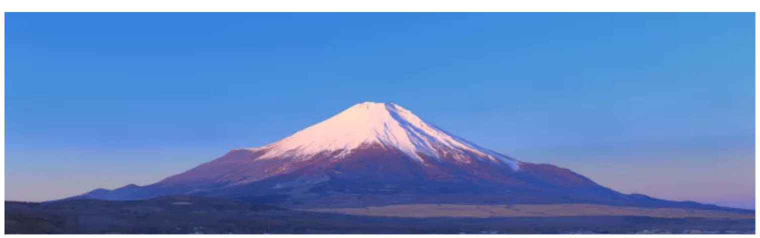
$\hookrightarrow$ standard lore: connect gapped AGNRs, but one gapped with one gapless also works!

7/9 hybrid = **Fuji** localization



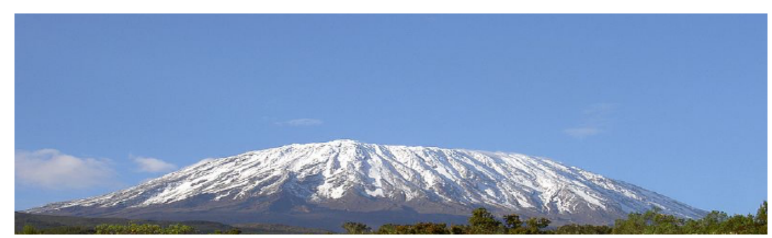
9/11 hybrid = **Kilimanjaro** localization





Predicted before

Cao et al., Rev. Lett. **119** (2017) 076401 (2017)



new form of localization!

$\hookrightarrow$ new possibilities!

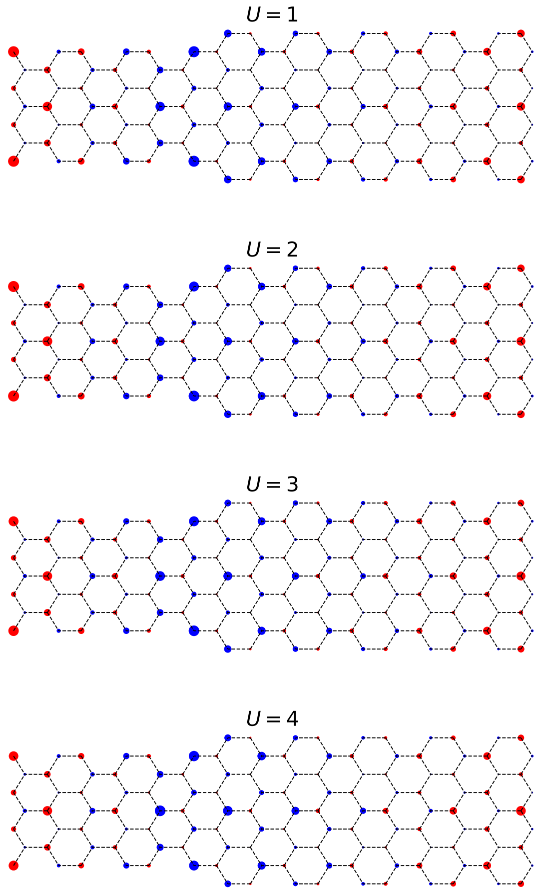
Localization in hybrid nanoribbons: Interacting systems

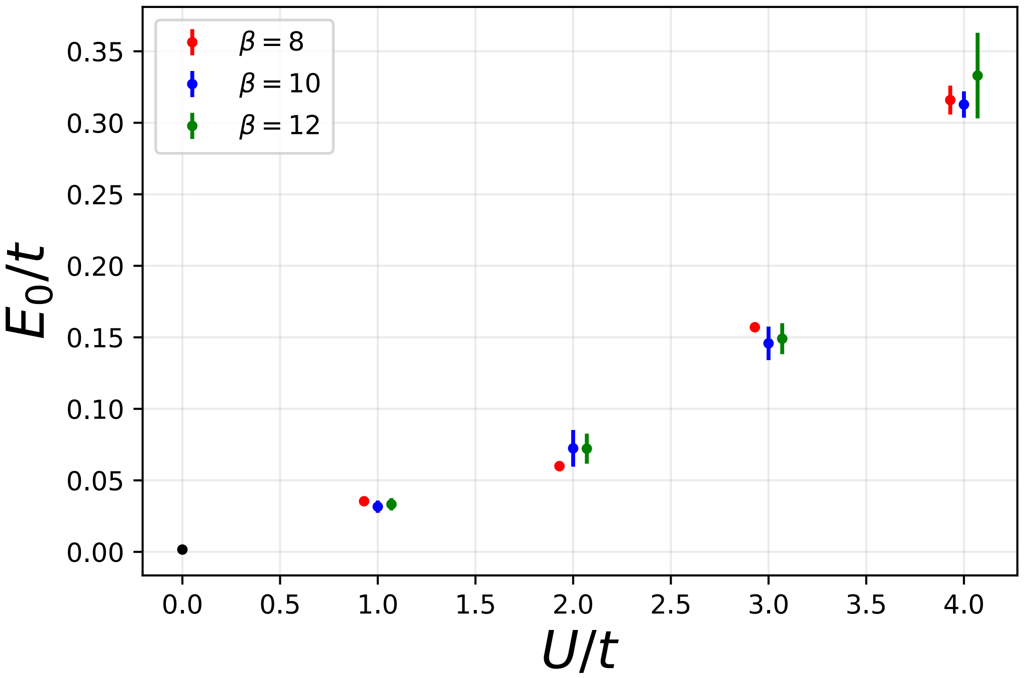
Luu, UGM, Razmadze, Phys. Rev. B **106** (2022) 195422

- Quantum MC simulations of the Hubbard model

$$H = -t \sum_{\langle i,j\rangle,\sigma=\uparrow,\downarrow} \left(a^\dagger_{i\sigma} a_{j\sigma} + h.c.\right) + U \sum_i \left(n_{i,\uparrow} - \frac{1}{2}\right)\left(n_{i,\downarrow} - \frac{1}{2}\right)$$

- Localization persists w/ strong interactions, but energy depends on U



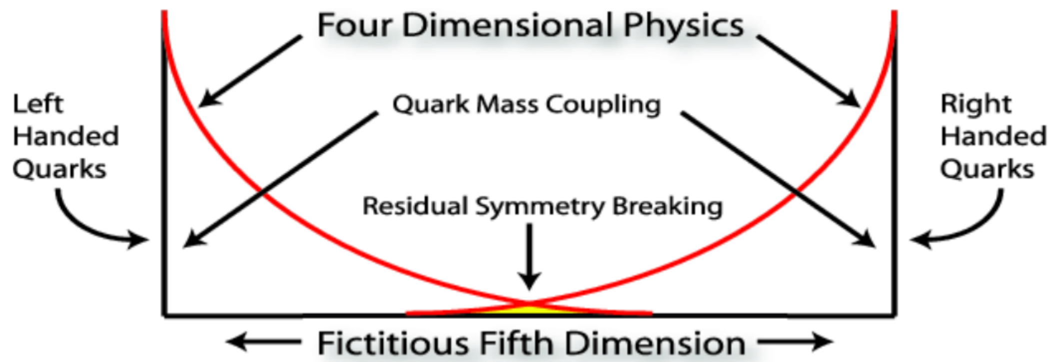


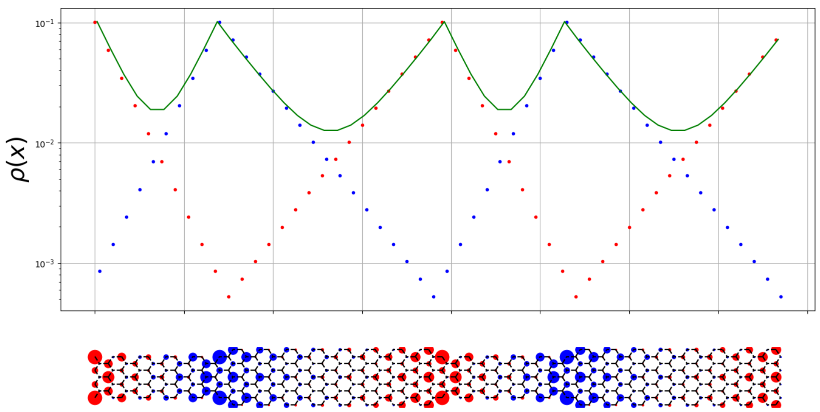
— also holds for other geometries!

Digression: Domain wall fermions

- These concepts have particle physics origins

- Domain wall fermions are allowing for representing chiral fermions on a lattice (LQCD)





Kaplan, Phys. Lett. B **288** (1992) 342

Kaplan, Phys. Rev. Lett. **132** (2024) 141603

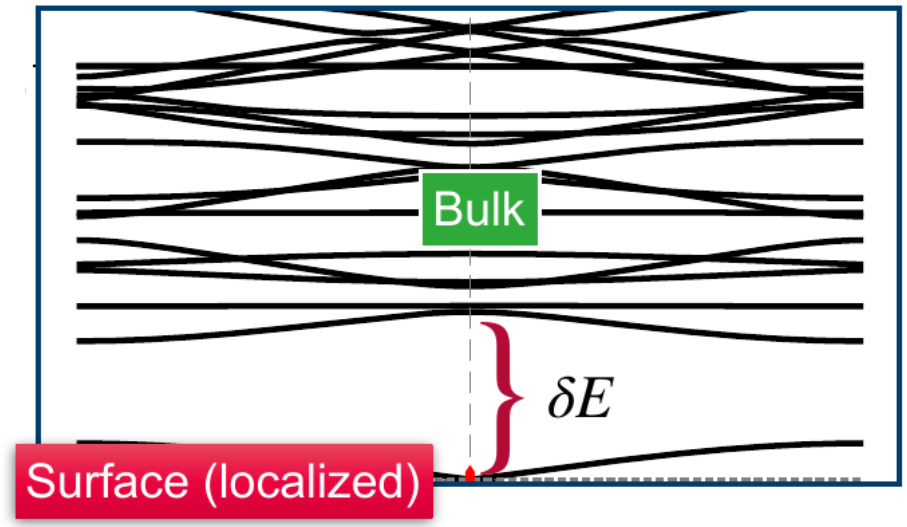
Hybrid nanoribbons provide a physical manifestation of domain wall fermions

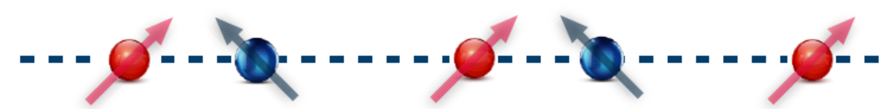
An EFT for hybrid nanoribbons

Ostmeyer, Razmadze, Berkowitz, Luu, UGM, Phys. Rev. B **109** (2024) 195135

- We have all the ingredients for an EFT:
  - Separation of scales
    i.e. energy gap to the bulk states
  - Identification of the relevant
    low-energy degrees of freedom
    i.e. the localized edge states
  - Interaction terms constrained
    by symmetries
  - Power counting
    with q some small momentum
    of the/or inpinging on the dofs

$\hookrightarrow$ let's see how that works





$$H_{1D} = -\sum_i \left(t_A a^\dagger_{2i} a_{2i-1} + t_B a^\dagger_{2i+1} a_{2i+2} + \mathrm{h.c.} \right)$$

$$\delta H^i_{T,C,S} + \mathcal{O}\left(\left(\frac{q}{\delta E} \right)^{i+1} \right)$$

Exploring the EFT: interacting case

Ostmeyer, Razmadze, Berkowitz, Luu, UGM, Phys. Rev. B **109** (2024) 195135

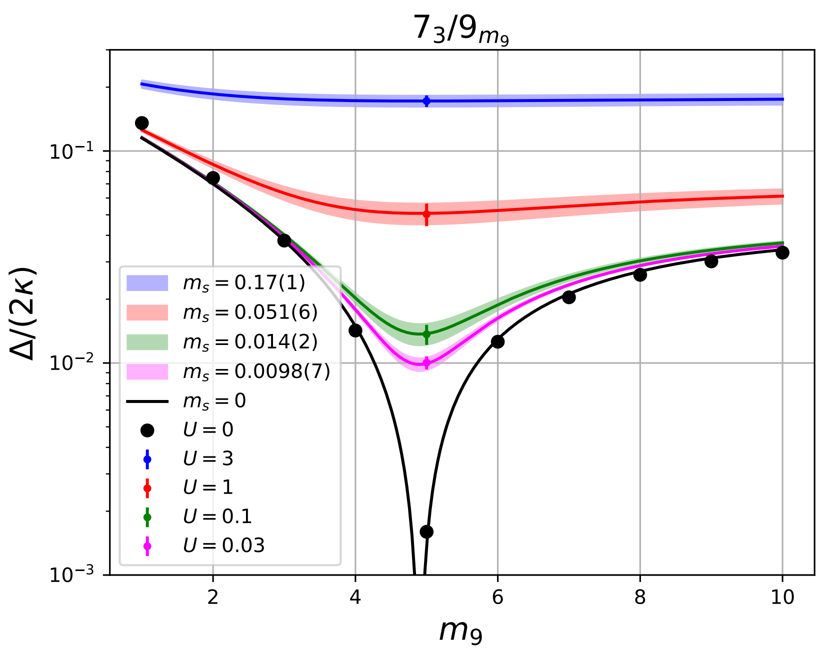
- We have a 1D EFT with the Hamiltonian with staggered mass $m_s\sigma_3$ as the energy gap is symmetric about E_F plus particle hole & chiral symmetries

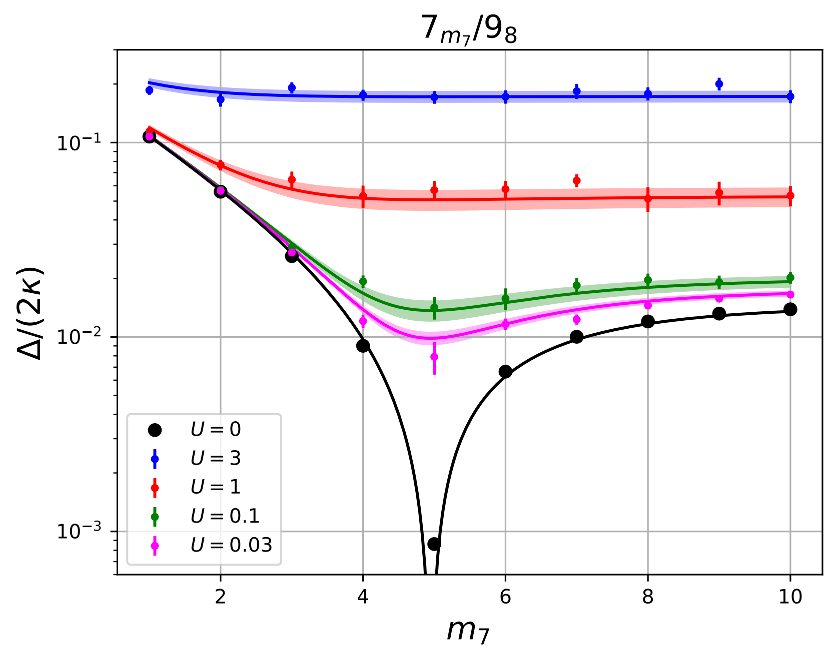
$$H_{1D} = -\sum_k a_k^\dagger \begin{pmatrix} m_s & t_A e^{ik} + t_B e^{-ik} \\ t_A e^{-ik} + t_B e^{ik} & -ms \end{pmatrix} a_k$$

- Fit t_A, t_B from the non-interacting theory

$\hookrightarrow$ Tune m_s to the underlying theory

$\Rightarrow$ Predict spectrum of new geometries

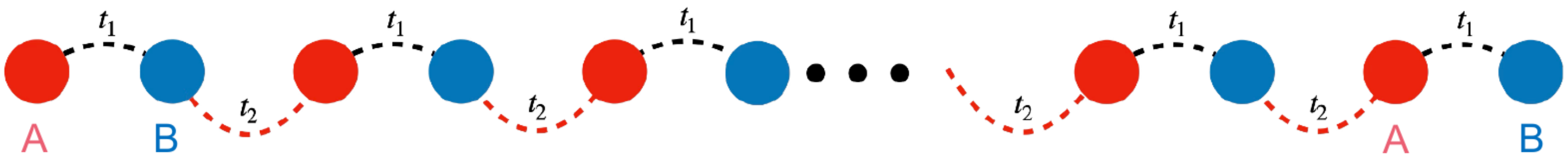




Localization in the SSH model

- Consider the renowned Su-Schrieffer-Heeger (SSH) model with even sites

Su, Schrieffer, Heeger, Phys. Rev. Lett. **42** (1979) 1698



- Localization/topology depends on the hopping parameters t_1, t_2

$$H_{\rm SSH} = \sum_i \left(t_1 c^\dagger_{i,{\rm A}} c_{i,{\rm B}} + t_2 c^\dagger_{i+1,{\rm A}} c_{i,{\rm B}} + \text{h.c.} \right)$$

- Topological $t_1 < t_2$ $E \sim 0$ due to overlap

- Trivial $t_1 > t_2$

- Gapless $t_1 = t_2$

Localization in the SSH model: Experiments

- Even site SSH model

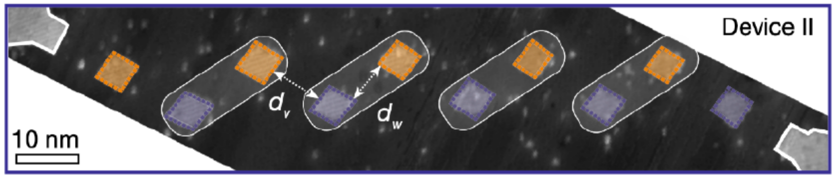
- Different types of experiments
  - Silicon quantum dots

    Kiczynski et al., Nature **606** (2022) 694
  - Artificial lattices

    Meier et al., Nature Commun. **7** (2016) 13986

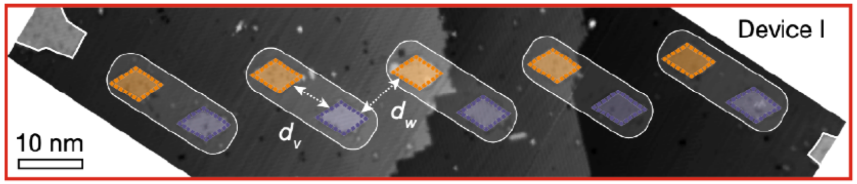
    Ligthart et al., Phys. Rev. Res. **7** (2025) 012076

- Topological $t_1 < t_2$ [t_1 =v, t_2 =w]



Topological: $v < w$, $d_v > d_w$ d_v = 9.6 nm, d_w = 7.8 nm

- Trivial $t_1 > t_2$ [t_1 =v, t_2 =w]



Trivial: $v > w$, $d_v < d_w$ d_v = 7.7 nm, d_w = 10.1 nm

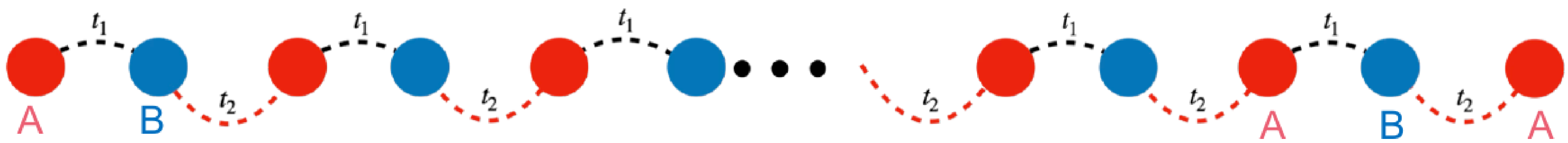
- Disadvantages:
  - Sensitive to the parameter choice, e.g., $t_1 < t_2$
  - Long enough chain to reduce wave function overlap

- Is there another/different way to generate localization in the SSH model?

Localization in the SSH model with odd sites

Wang, Luu, UGM, to be published

- Consider the SSH model with an odd number of sites



- Different types of localization for all (nonvanishing) hopping parameters t_1, t_2

- $t_1 < t_2$ $E = 0$ Chiral symmetry or sublattice symmetry

- $t_1 > t_2$ $E = 0$

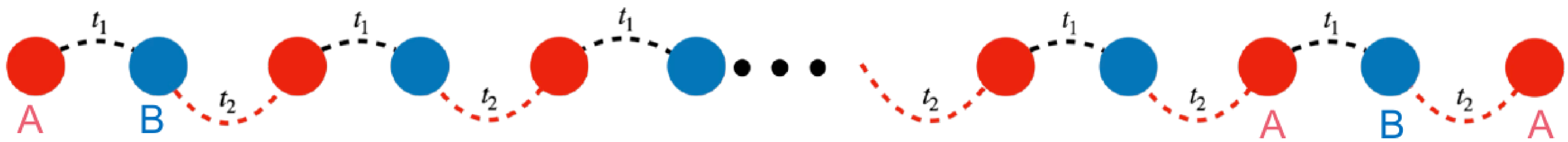
Advantages:
- Independent of parameter choice
- No length requirement but odd

- $t_1 = t_2$ $E = 0$

Defect enginnering in the SSH model with odd sites

Wang, Luu, UGM, to be published

- Consider the SSH model with an odd number of sites



- Introduce defects = $(\boldsymbol{A}, \boldsymbol{B})$ or $(\boldsymbol{B}, \boldsymbol{A})$ pairs w/ a different coupling (diff. ions)

- $t_1 < t_2$ $E = 0$ No defects

- $t_1 < t_2$ $E = 0$ With defects $t_1 \to d_1$ $t_2 \to d_2$

$\hookrightarrow$ to have control, we need interactions

The odd SSH model with interactions

Wang, Luu, UGM, to be published

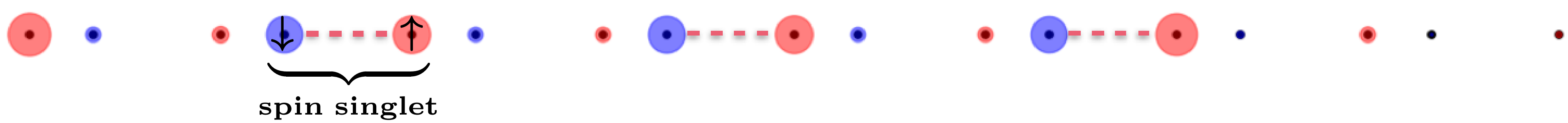
- Add an onsite Hubbard interaction

$$H_{\mathrm{SSH+U}} = H_{\mathrm{SSH}} - \frac{U}{2}\sum_x (n_{x,\uparrow} - n_{x,\downarrow})^2$$

- This generates localized spin-singlet centers (above some critical value of U):

  - $t_1 < t_2$ No interactions

  - $t_1 < t_2$ With Hubbard interactions generate localized spin-singlet centers



- With increasing coupling U, the spin centers are stronger localized
- Possible platforms:

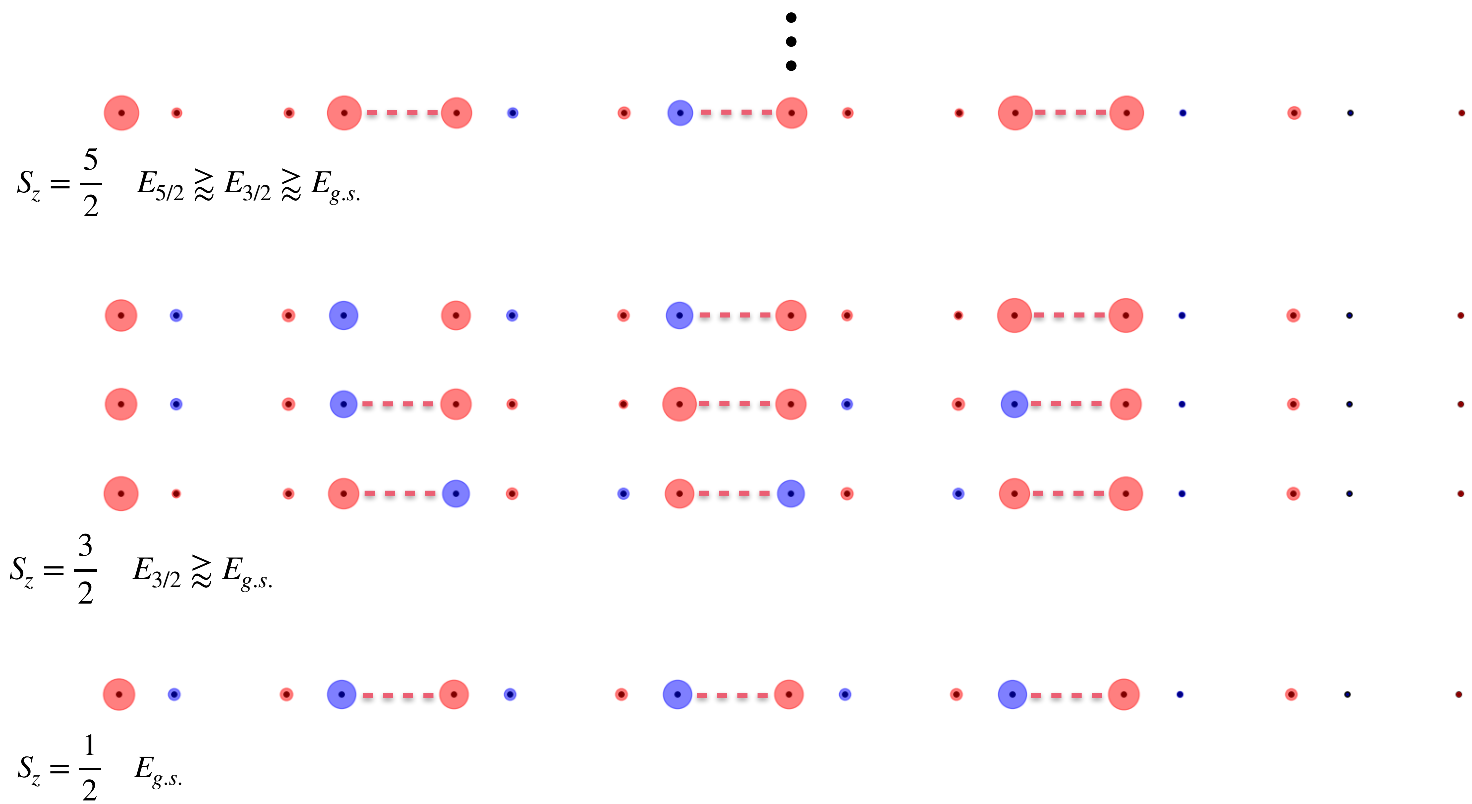
  (i) Magnetism and spintronics

  (ii) Quantum computations and simulations

Excited states in the odd SSH model with interactions

Wang, Luu, UGM, to be published

- Can engineer even more exotic forms of localization:



$\hookrightarrow$ Couple these different spin configurations (via an external magnetic field)

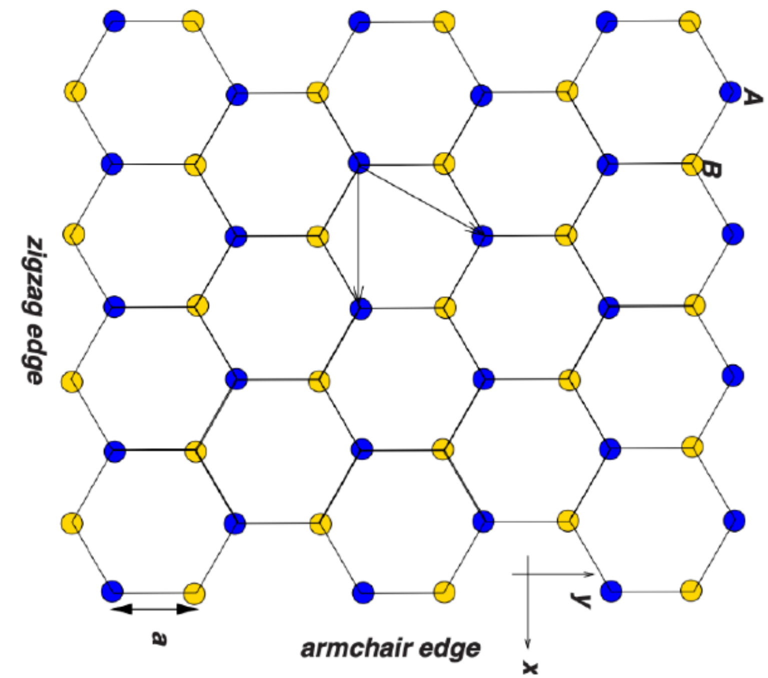
$\hookrightarrow$ engineer and/or manipulate spin qubits, other applications? $\rightarrow$ ideas welcome!

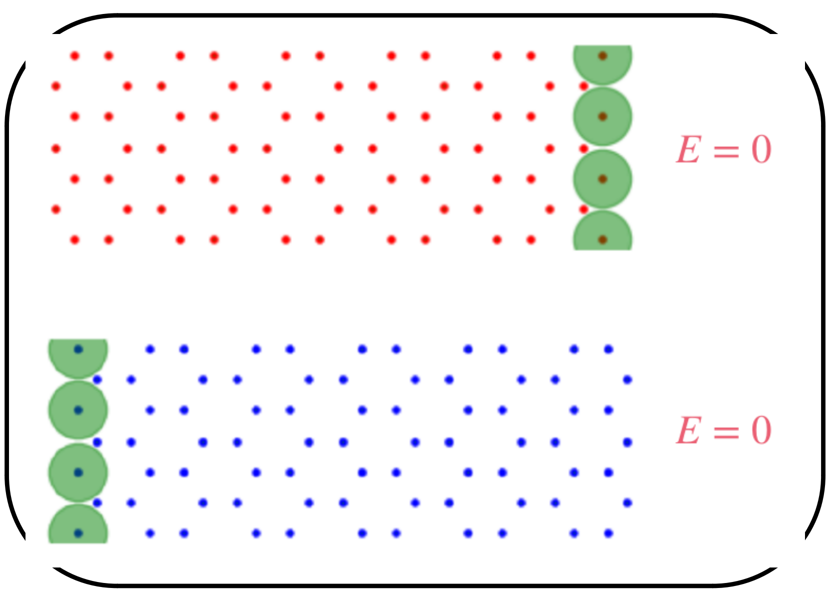
Graphene nanosystems with odd sites

Wang, Luu, UGM, to be published

- Similar to the SSH model:
  - Two sites A, B in one unit cell
  - Chiral (or sublattice) symmetry
- Consider such a systems with odd sites
  - Similar to the SSH model with equal hoppings

$\hookrightarrow$ Localized states at the edges!

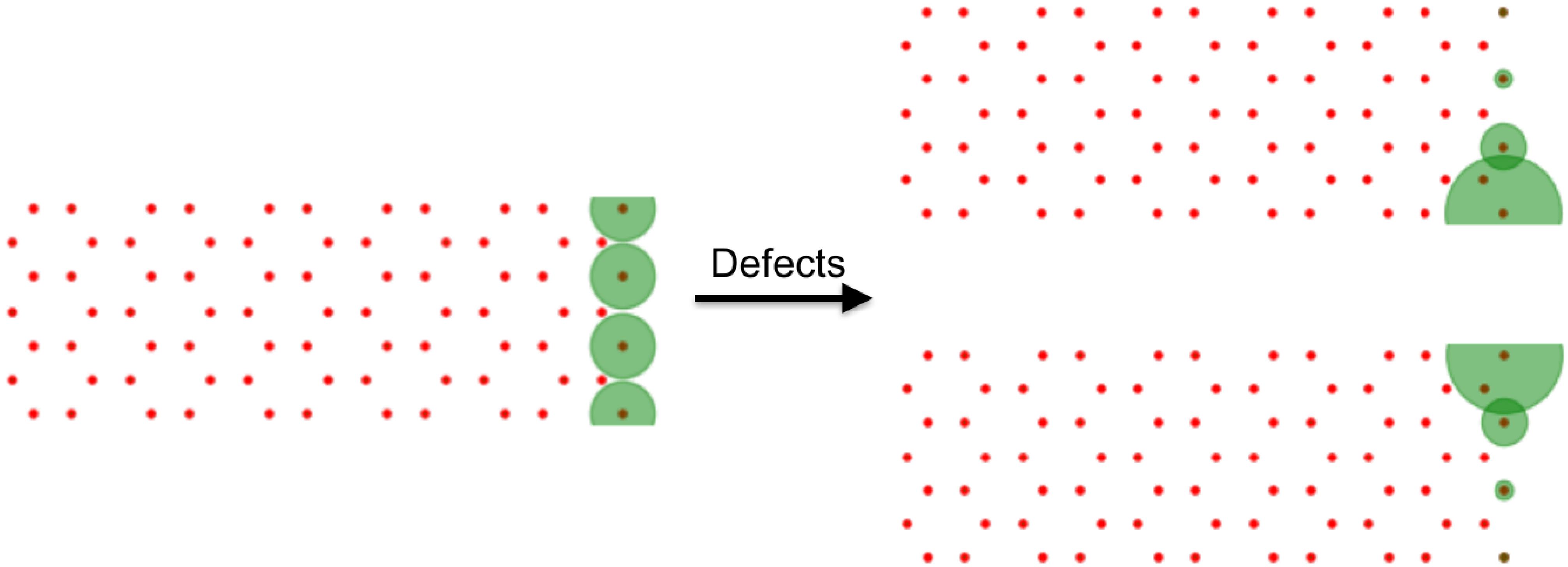




Defect engineering graphene nanosystems

Wang, Luu, UGM, to be published

- Introducing defects as before allows for a fine control of the edge states



↪ Consequences/applications need to be investigated → ideas please!

Intermediate Summary

- Low-d materials are amenable to MC simulations
  - $\rightarrow$ borrow methods from lattice field theory in QCD
  - $\rightarrow$ allows for EFTs for quicker access

- Recent developments
  - $\rightarrow$ Localization in AGNRs
    - $\hookrightarrow$ new type of localization found (Kilimanjaro)
    - $\hookrightarrow$ localization persists in the presence of strong interactions
  - $\rightarrow$ A new twist on the SSH model - odd number of sites
    - $\hookrightarrow$ localization of all values of the hopping parameters
    - $\hookrightarrow$ defects allow for new forms of localization
    - $\hookrightarrow$ control of spin centers with interactions possible
  - $\rightarrow$ Similar engineering possible in graphene nanosystems

$\hookrightarrow$ stay tuned!

Summary & outlook

- Strongly interacting fermion systems pose severe challanges
  ↪ can be tackled w/ EFT and/or MC (stochastic) methods
- Large progress made in the last few years:
  ↪ new insights into nuclear structure and nuclear matter
  ↪ new insights into toplogical matter and how to engineer it
- More interactions between fields is needed to make further progress!

Thank you for your attention!