New insights into strongly interacting fermionic systems

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by NRW-FAIR

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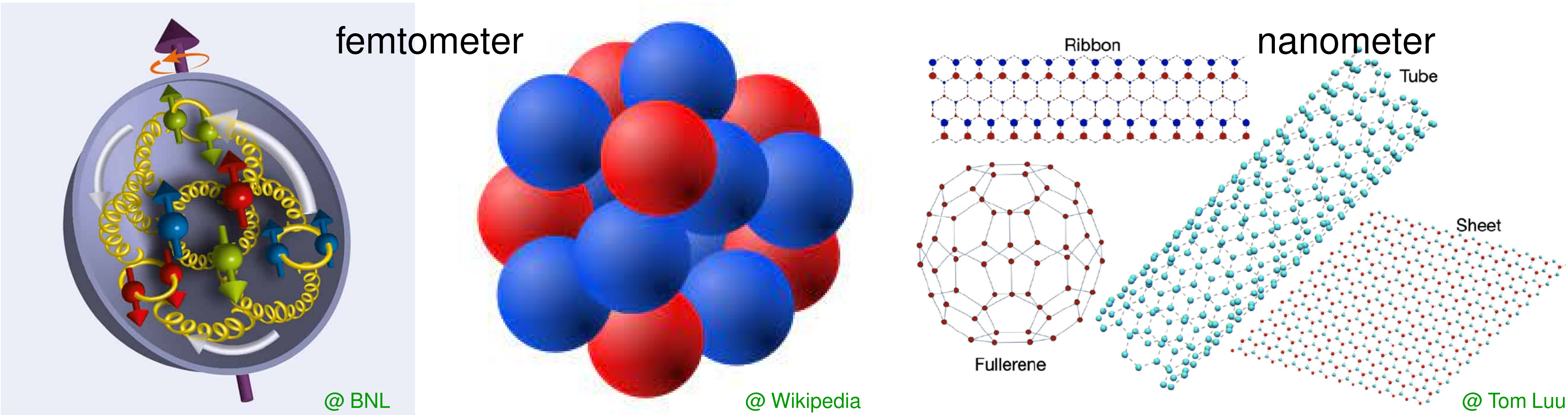
Introduction:
Why and how

Strongly correlated fermionic systems

- Strongly correlated fermionic systems come in different forms, shapes and sizes



- ... and are a challenge in particle & nuclear & condensed matter physics
  as well as material science, quantum chemistry, ...

↪ the Pauli principle combined with strong interactions / correlations makes
such systems difficult to compute / calculate / investigate theoretically

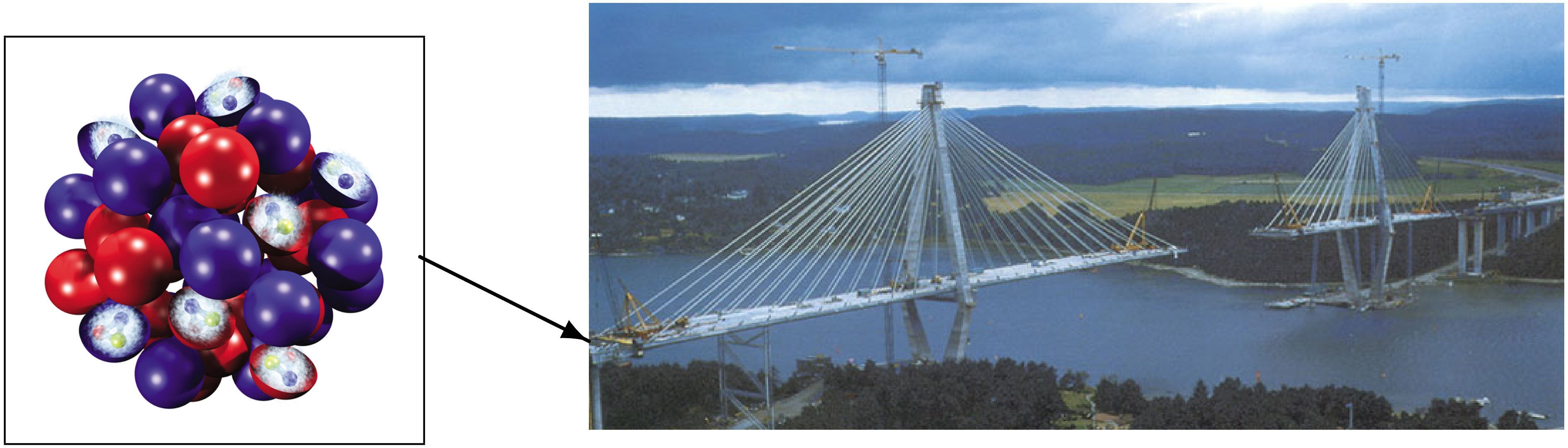
↪ I propose here the marriage of Effective Field Theories w/ Monte Carlo simulations

Intro to EFTS: Resolution matters

- Dynamics at long distances does not depend on what goes on at short distances

- Equivalently, low-energy interactions do not care about the details of high-energy interactions

- Or: you don't need to understand nuclear physics to build a bridge



Intro to EFTS: Organisation

- This is quite true, but how to make the idea precise and quantitative?
- necessary & sufficient ingredients to construct an **E**ffective **F**ield **T**heory:

  ⋆ *scale separation* – what is low, what is high?

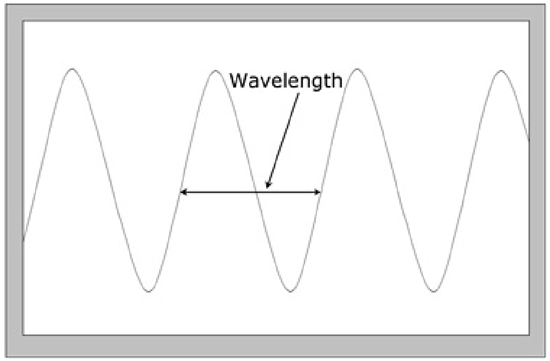
  ⋆ *active degrees of freedom* – what are the building blocks?

  ⋆ *symmetries* – how are the interactions constrained by symmetries?

  ⋆ *power counting* – how to organize the expansion in low over high?

- a note on units for a quantum particle ($\hbar = c = 1$)

$$p \sim \frac{1}{\lambda}, \quad E = p \quad \text{or} \quad E = \frac{p^2}{2m}$$



→ long wavelength ↔ low momentum

↪ In a modern view, all QFTs are EFTs Georgi, Weinberg, ...

Intro to Monte Carlo simulations: Basics

- Just outline schematically the basic steps:

$Z = \mathrm{Tr}\, e^{-\beta H}$ → discretize space $V = L^3$ (or a lattice is already there)

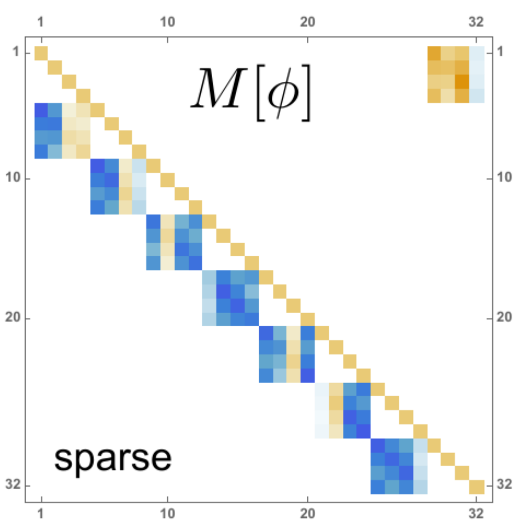
discretize time, $\delta = \beta / N_t$

introduce auxiliary fields

Integrate out Grassmann variables → fermion determinant $\det M[\phi]$

... and so on ...

$$\underbrace{\int \mathcal{D}[\phi] \det M[\phi] \exp\left(-\frac{1}{2V_{\rm int}\delta}\sum_{x,t}\phi^2(x,t)\right)}_{\int \mathcal{D}[\phi]\exp(-S[\phi])}$$



Intro to Monte Carlo simulations: The sign problem

- At finite chemical potential (density) or doping, **det$M$ is no longer positive definite**

$\hookrightarrow$ the basic assumption of a probability distribution no longer holds, the method fails

$\hookrightarrow$ this is an **NP hard** problem Troyer, Wiese, Phys. Rev. Lett. **94** (2005) 170201

$\hookrightarrow$ must tailor problem-dependent solutions to mitigate this

- discuss three methods here:

    $*$ Wigner's SU(4) symmetry in nuclear physics

    Wigner, Phys. Rev. **51** (1937) 106

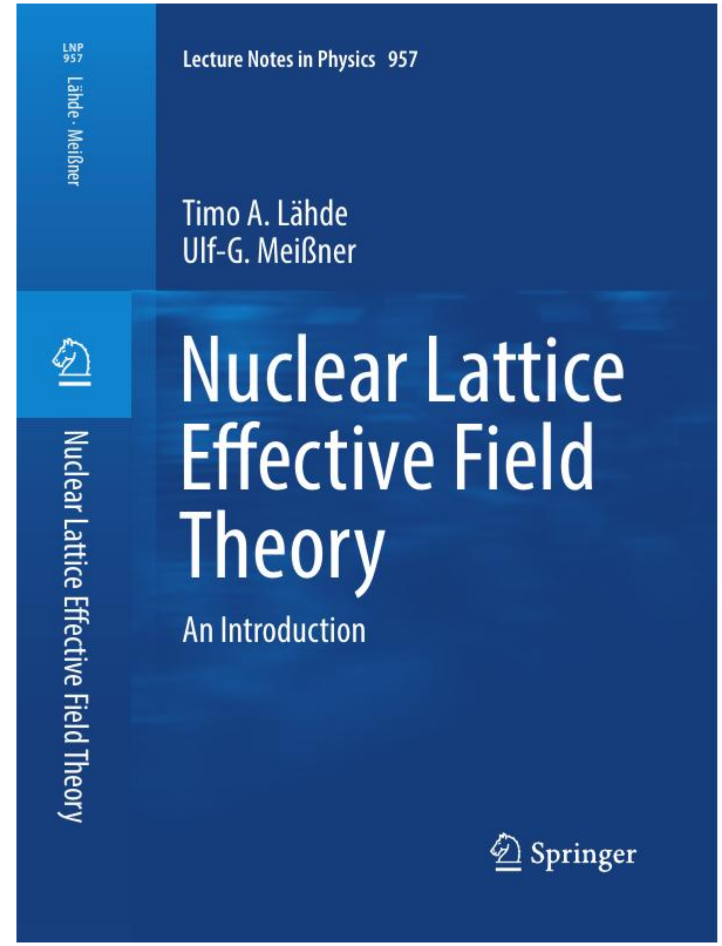
    $*$ Wave function matching (applied to nucl. phys. here but more general)

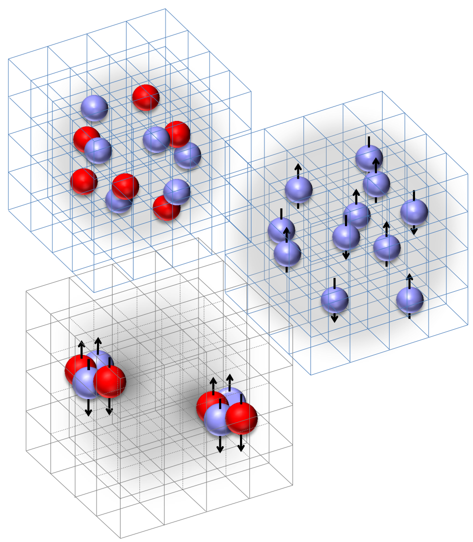
    Elhatisari et al., Nature **630** (2024) 8015, 59

    $*$ Lefschetz thimbles (contour deformations) (applied to low-d materials here)

    Cristoforetti et al., Phys. Rev. D **88** (2013) 051501(R)

Nuclear physics on a lattice





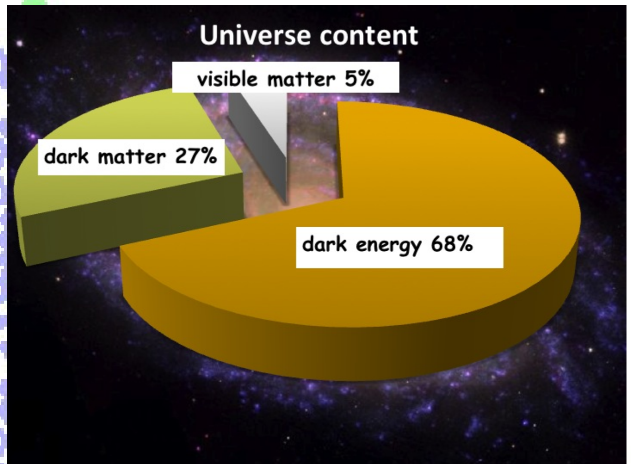
T. Lähde & UGM

Nuclear Lattice Effective Field Theory - An Introduction

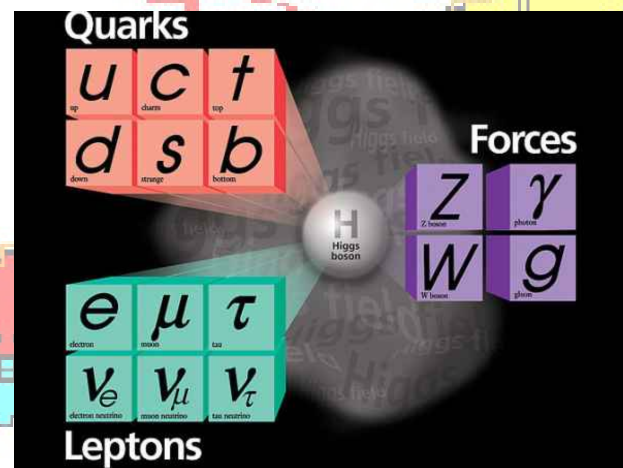
Springer Lecture Notes in Physics **957** (2019) 1 - 396

Why nuclear physics?

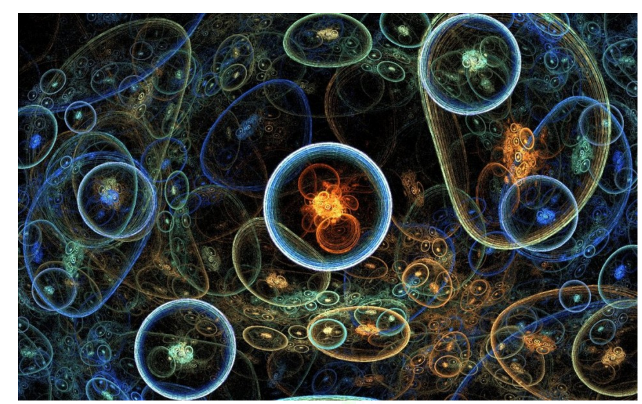
- The matter we are made off



- The last frontier of the SM



- Access to the Multiverse



Proton Number Z

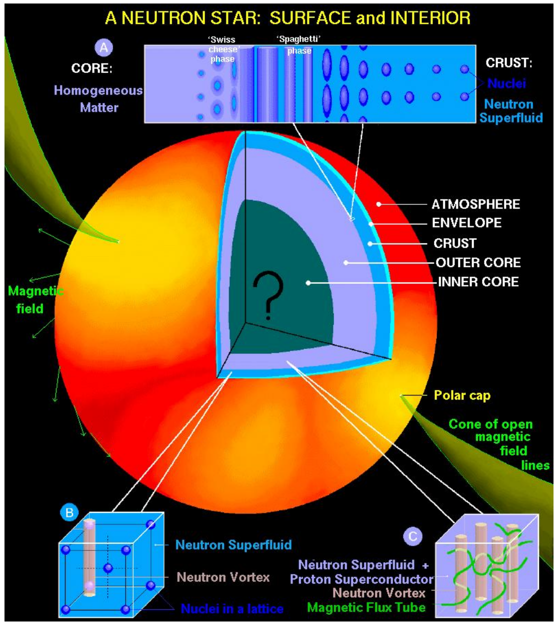
Neutron Number N

⇒ **Precision mandatory**

The nucleus as a quantum laboratory

- The nucleus is a challenging and fascinating many-body system
  - $\hookrightarrow$ non-perturbative strong interactions balanced by the Coulomb force
  - $\hookrightarrow$ many interesting phenonema: drip lines, clustering, reactions, ...
  - $\hookrightarrow$ a plethora of few-body/many-body methods already exists

- Macroscopic nuclear matter = neutron stars
  - $\hookrightarrow$ gained prominence again in the multi-messenger aera
  - $\hookrightarrow$ must be able to describe these with the same methods



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

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

$\longrightarrow$ see Epelbaum, Hammer, UGM, Rev. Mod. Phys. **81** (2009) 1773

- EFT on the lattice, maximal momentum:

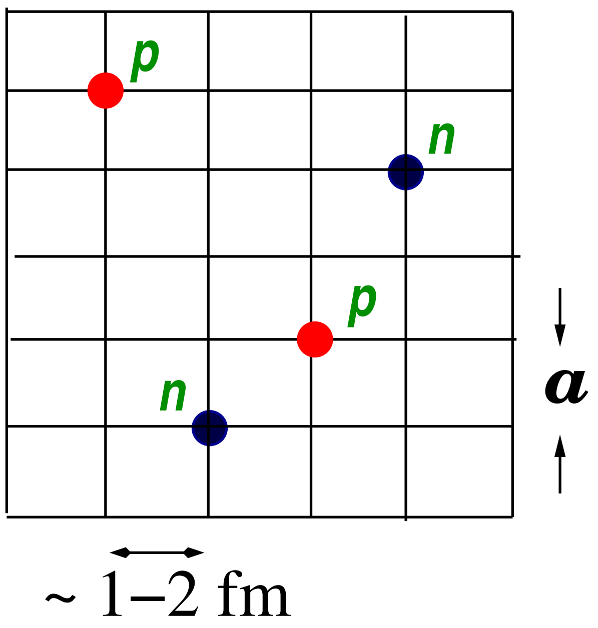
$$p_{\max} = \frac{\pi}{a} \simeq 315 - 630 \,\text{MeV [UV cutoff]}$$

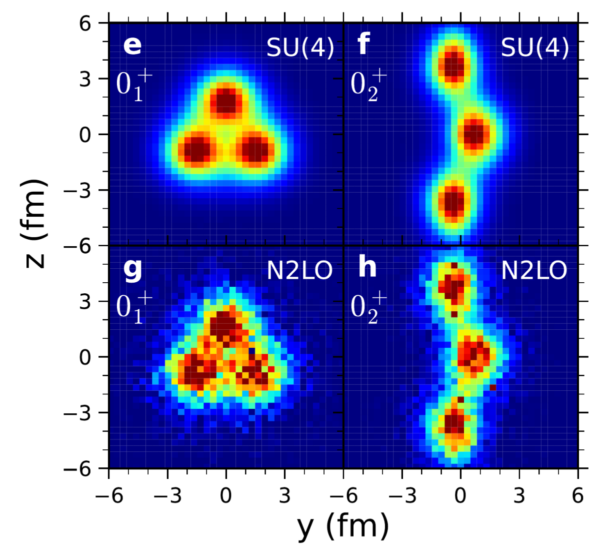
- strong suppression of sign oscillations SU(4)
  due to approximate Wigner (spin-isospin) symmetry

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

$\hookrightarrow$ works well for even-even nuclei

$\hookrightarrow$ we still need another method



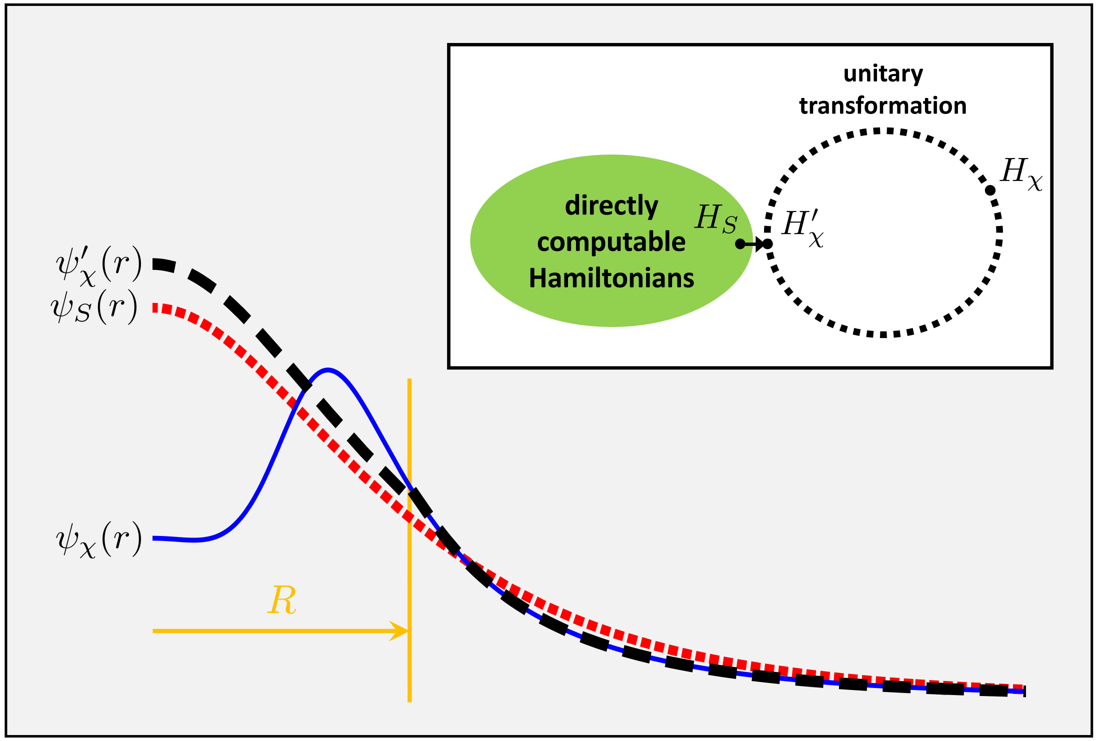


Shen et al., Nature Commun. **14** (2023) 2777

Wave function matching

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

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



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

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

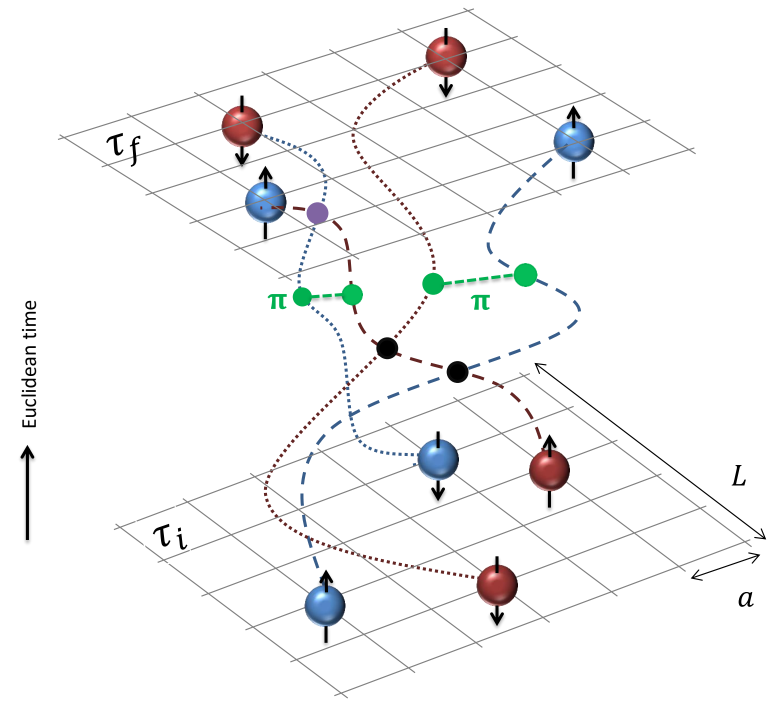
$$E_A(\tau) = -\frac{d}{d\tau} \ln Z_A(\tau)$$

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

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

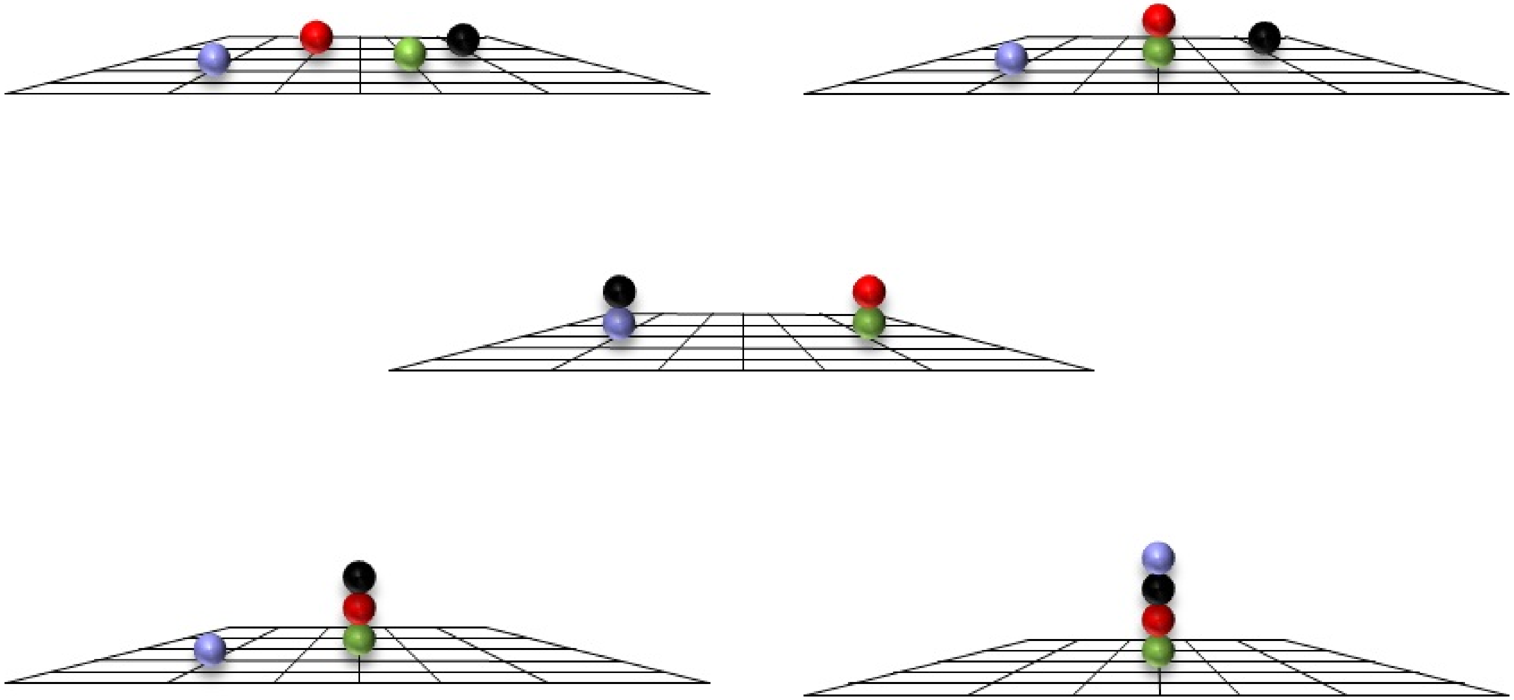
$$Z_A^{\mathcal{O}} = \langle \Psi_A | \exp(-\tau H/2)\, \mathcal{O}\, \exp(-\tau H/2)\, | \Psi_A \rangle$$

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



- 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

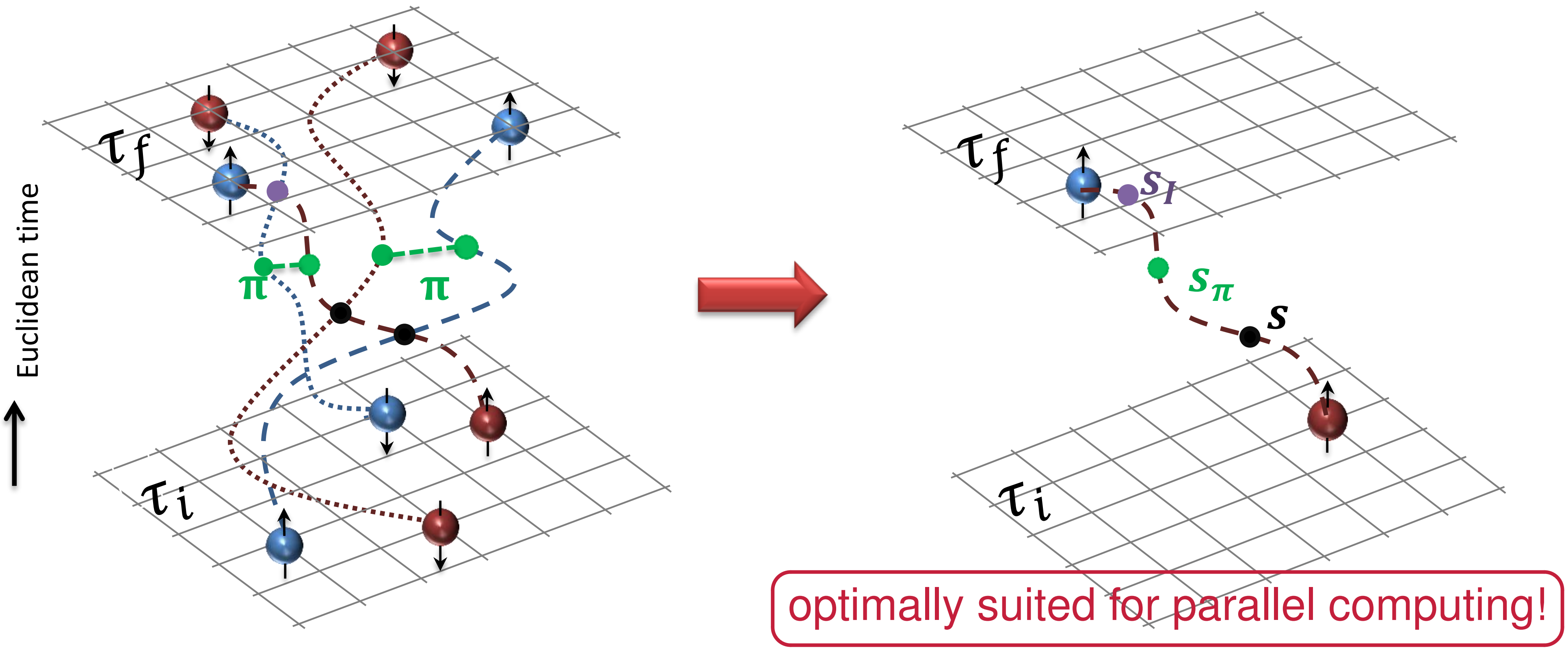
⇒ preparation of *all possible* initial/final states

⇒ *clustering* emerges *naturally*

Auxiliary field method

- Represent interactions by auxiliary fields (Gaussian completion):

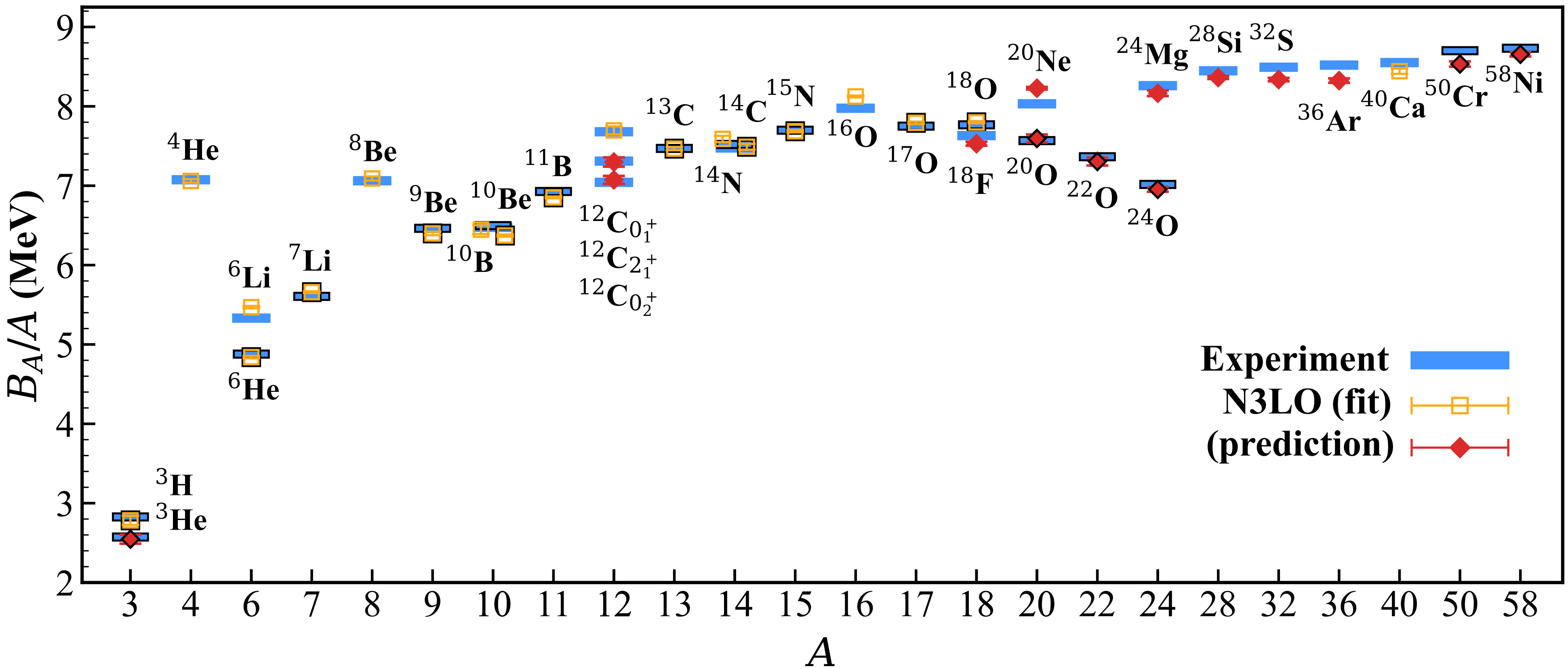
$$\exp\left[-\frac{C}{2}\left(N^\dagger N\right)^2\right] = \sqrt{\frac{1}{2\pi}}\int ds\,\exp\left[-\frac{s^2}{2}+\sqrt{C}\;s\left(N^\dagger N\right)\right]$$



Binding Energies at N3LO

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

- Need to go to next-to-next-to-next-to-leading order (N3LO) for precision
- Binding energies of nuclei for $a = 1.32$ fm: Determining the 3NF LECs

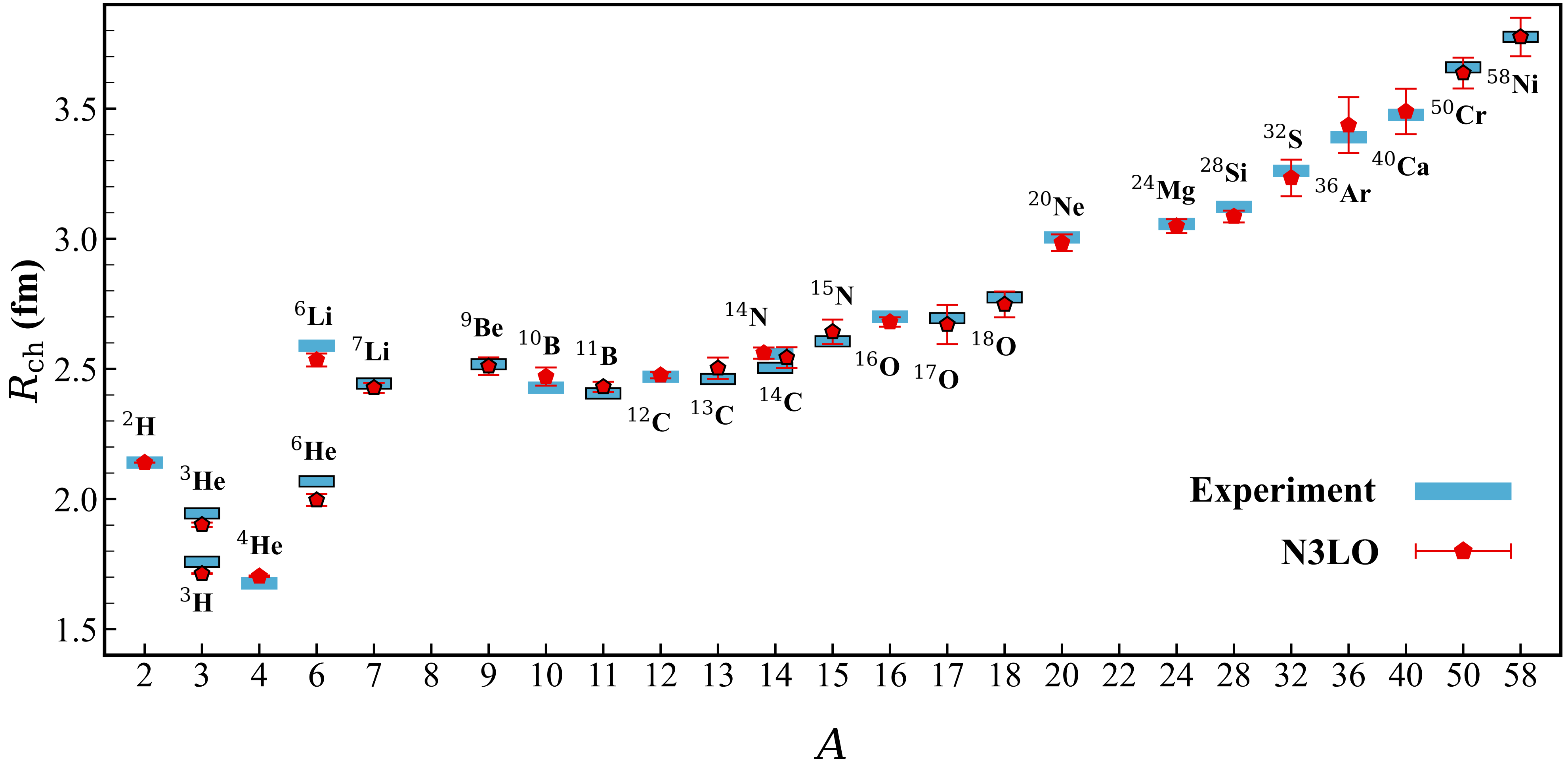


$\rightarrow$ excellent starting point for precision studies

Prediction: Charge radii at N3LO

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

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

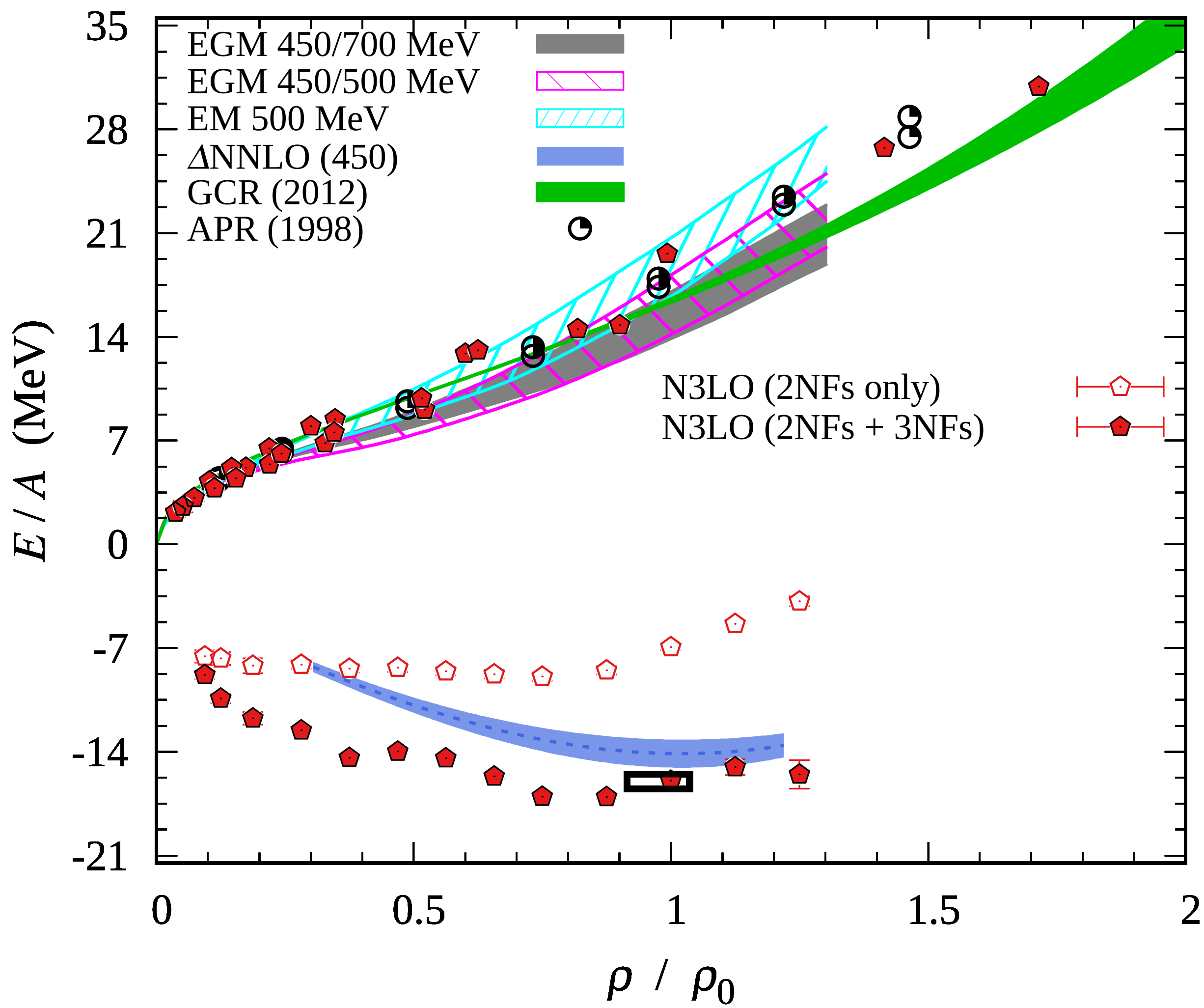


$\hookrightarrow$ no radius problem!

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)

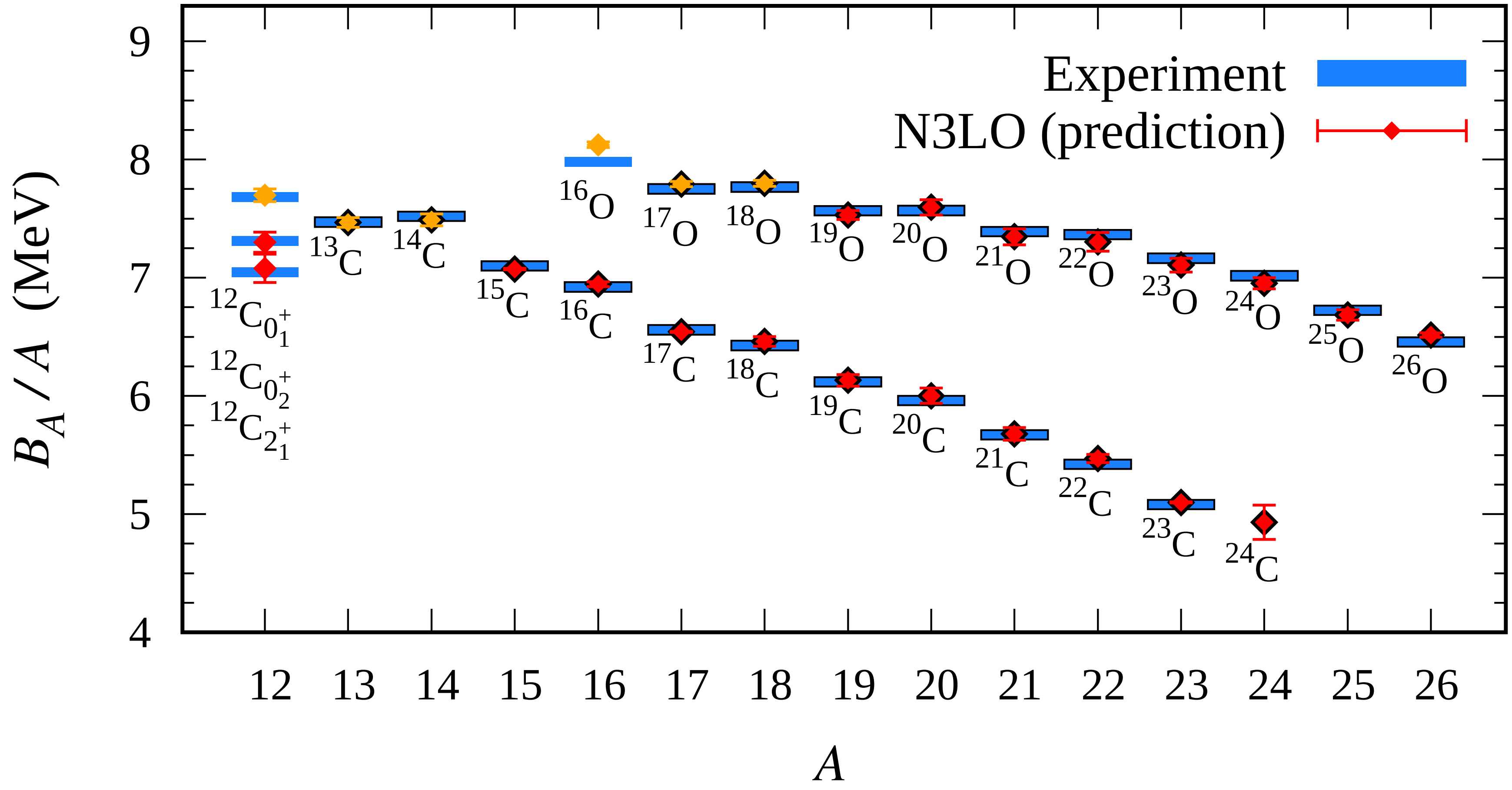


$\hookrightarrow$ can be improved using twisted b.c.'s

Prediction: Isotope chains of carbon & oxyen

Song et al., 2502.18722 [nucl-th]

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



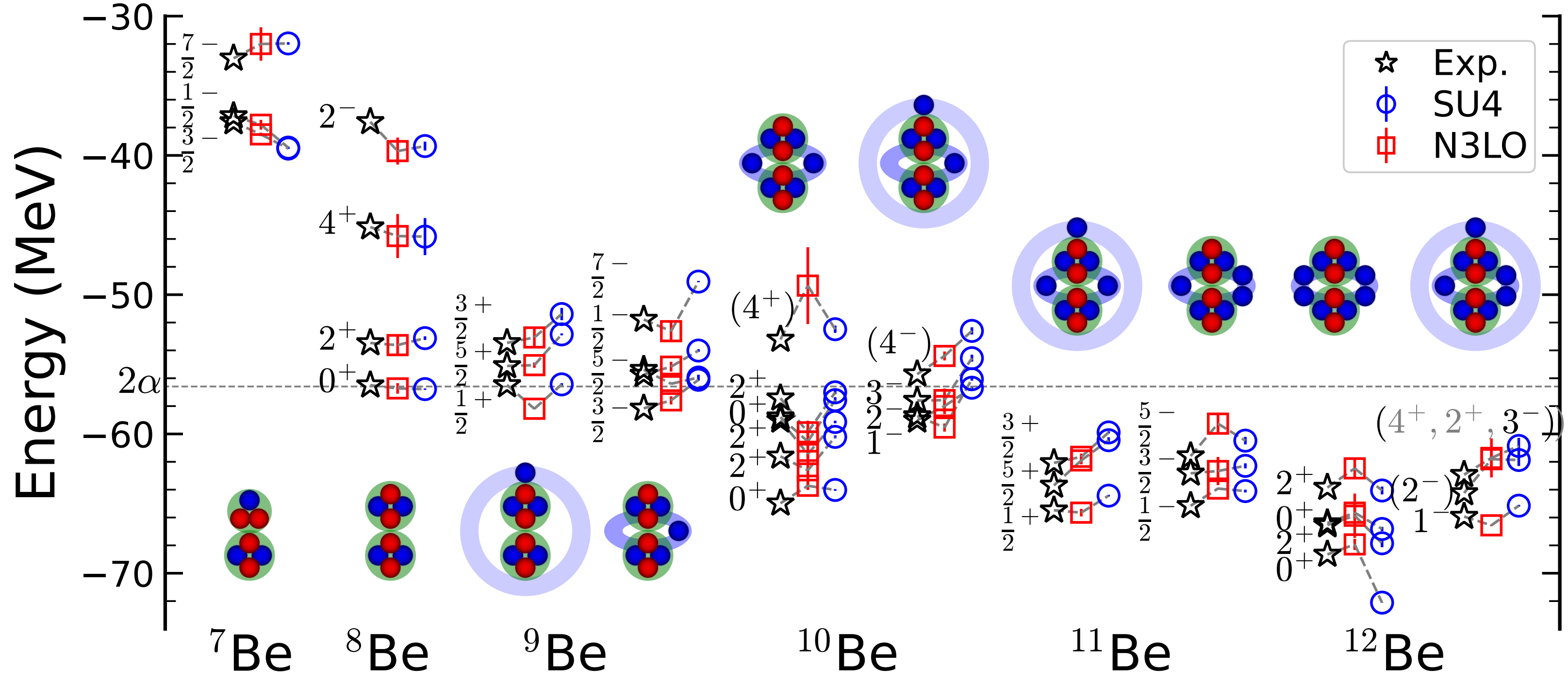
$\hookrightarrow$ 3NFs of utmost importance for the n-rich isotopes!

$\hookrightarrow$ universal features of neutron correlations

Prediction: Be isotopes

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

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



↪ new method to quantify nuclear shapes

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

Ab initio calculation of neutron stars

Tong, Elhatisari, UGM, Sci. Bull. **70** (2025) 825; Astrophys. J. **982**; in preparation

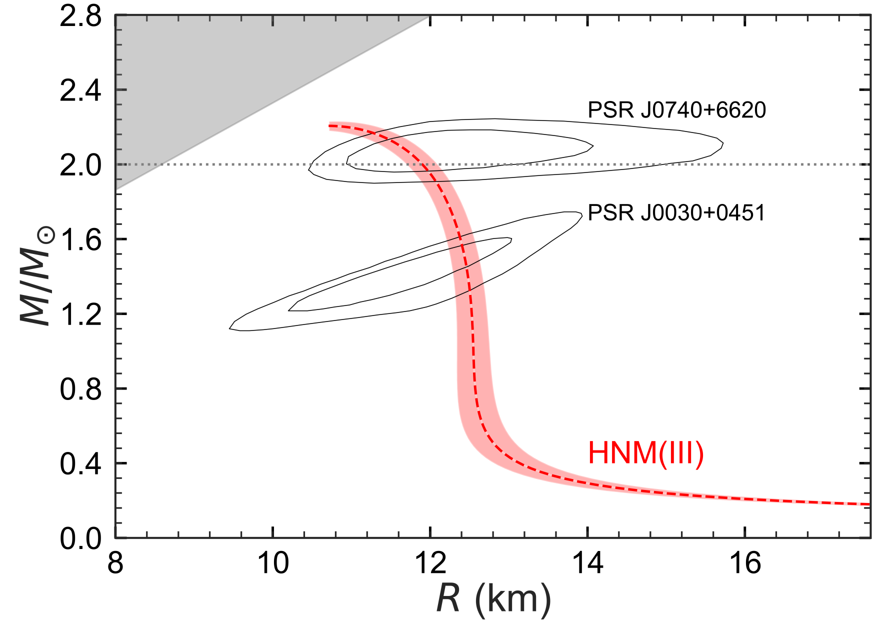
- Consider β-stable matter with neutrons, protons, $\mathbf{\Lambda}$ hyperons, electrons and muons

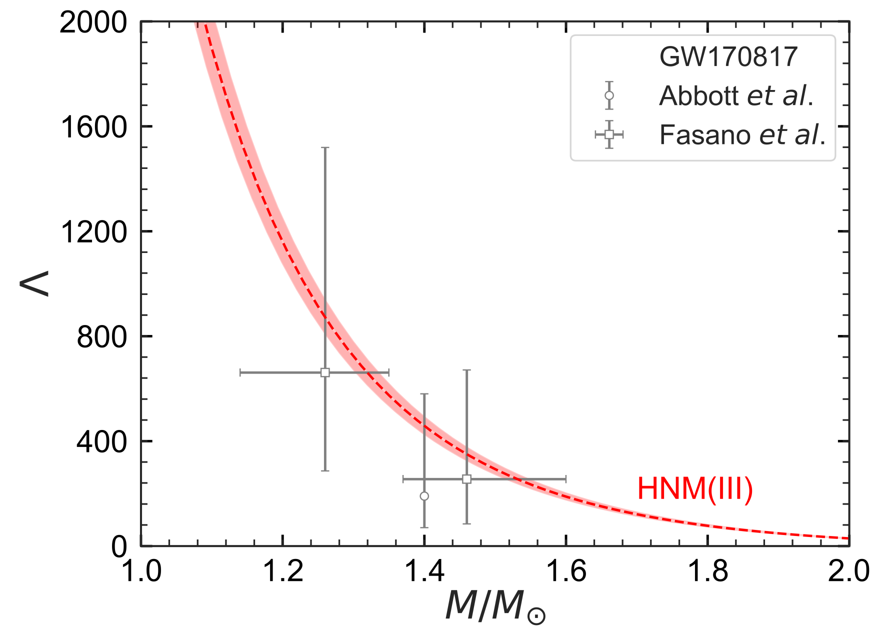
- Use a minimal model including neutrons, protons and $\mathbf{\Lambda}$ hyperons w/ two- and three-baryon forces

- Equation of state of neutron matter with up to
  - up to 232 neutrons in the box w/ $V = 288$ fm^3
  - up to 24 protons and 34 $\mathbf{\Lambda}$ hyperons

↪ first *ab initio* calculation of neutron stars consistent with all observational constraints (mass M, radius R, tidal deformability Λ, ...) and binding energies of light hypernuclei
Note: not thought to be possible!

↪ $\mathbf{\Lambda}$ hyperons present but no puzzle!





Intermediate Summary

- 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 $0\nu2\beta$ decays]

      Elhatisari, Hildenbrand, UGM, Phys. Lett. B **859** (2024) 139086
    - $\hookrightarrow$ hypernuclei are under investigation

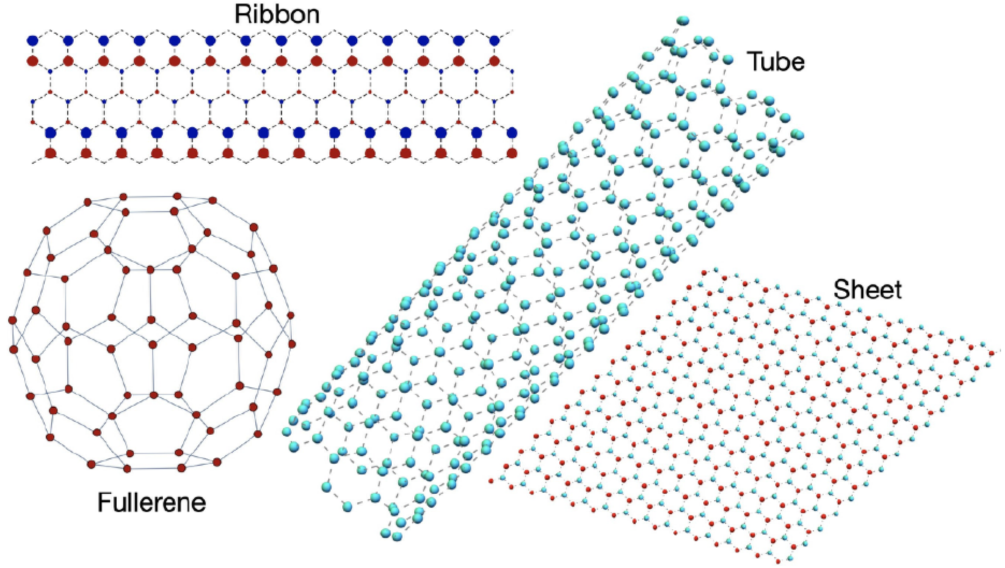
      Hildenbrand et al., Eur. Phys. J. A **60** (2024) 215

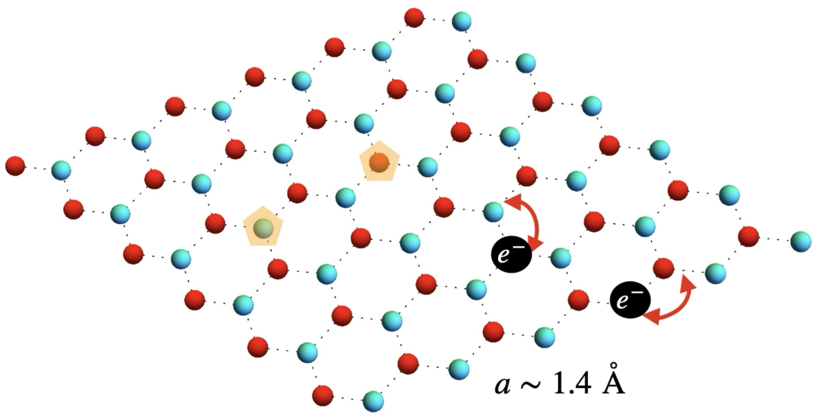
$\hookrightarrow$ stay tuned!

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

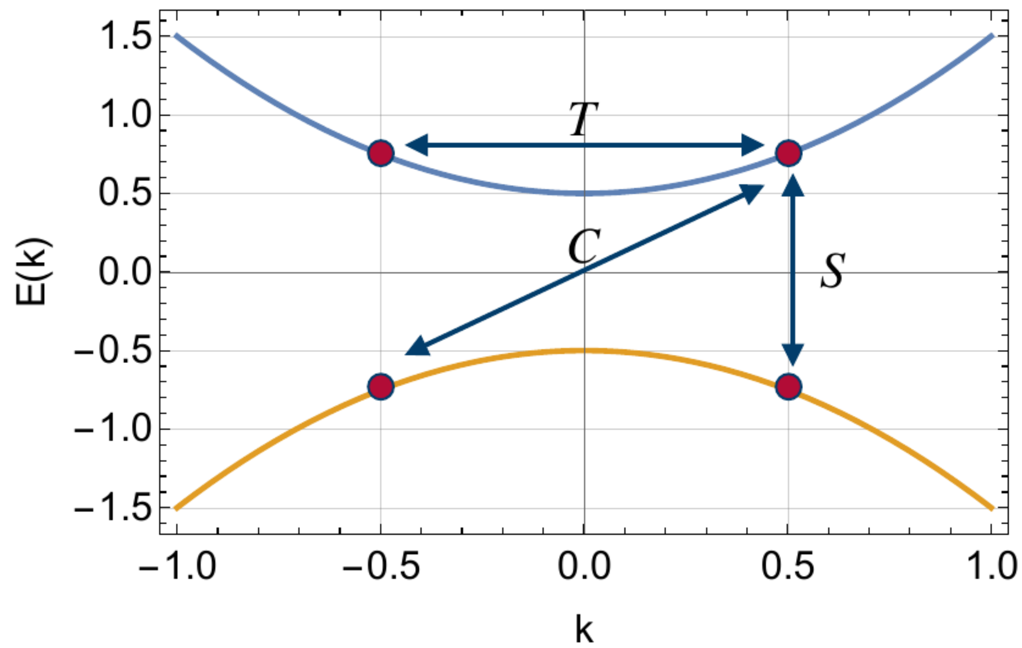
- Time-reversal symmetry T: $T^2 = \pm 1$

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

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

$\hookrightarrow$ Spectrum symmetric about zero:

$$E_+(k) = -E_-(-k)$$



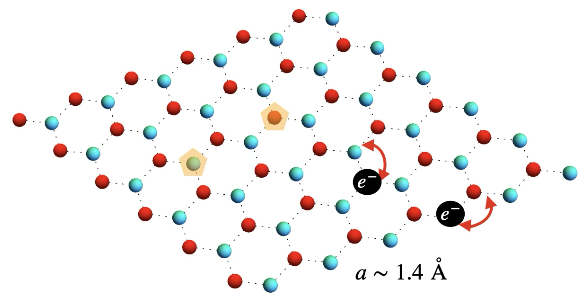
- Chiral symmetry (or *sublattice* symmetry)

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

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

$\hookrightarrow$ no Goldstone modes

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



$\Rightarrow$ Phases of matter classified topologically

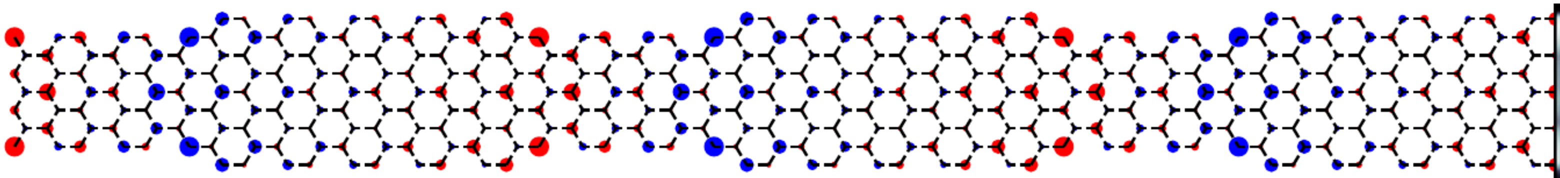
$\hookrightarrow$ all *symmetry classes* cataloged (for non-interacting systems)

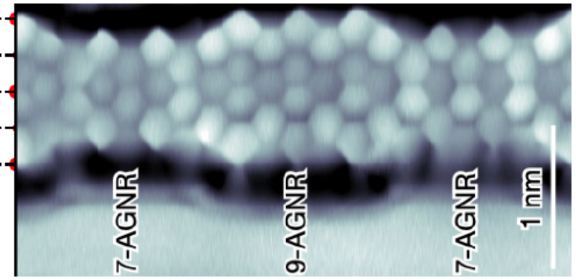
Chiu et al., Rev. Mod. Phys. **88** (2016) 035005

Localization in hybrid nanoribbons

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

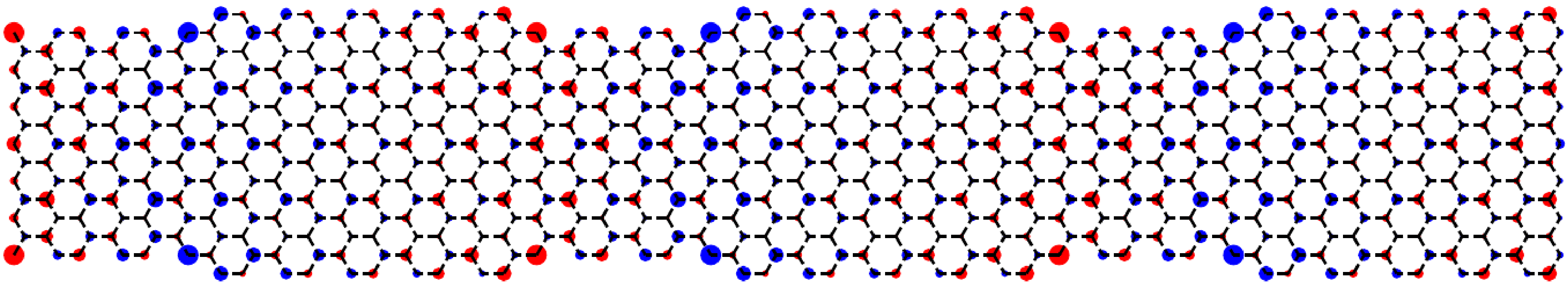
7/9 ribbon





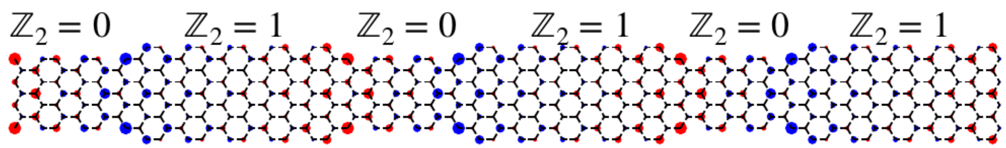
Rizzo et al. Nature **560** (2018) 204

13/15 ribbon

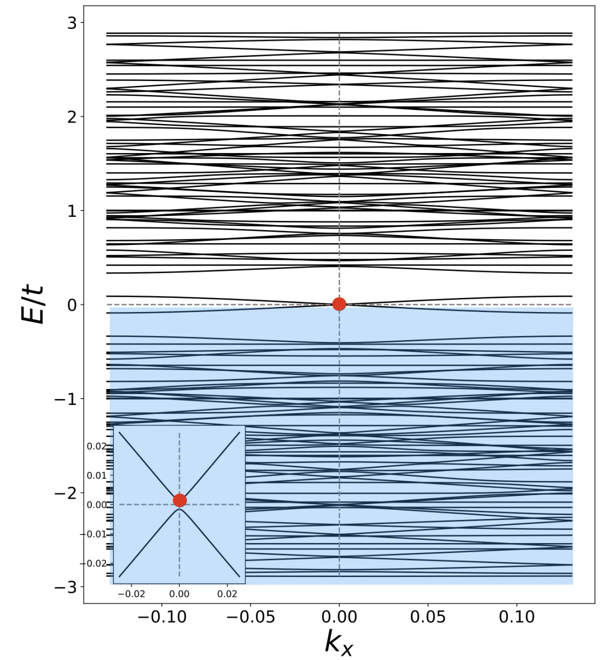


Localization in hybrid nanoribbons continued

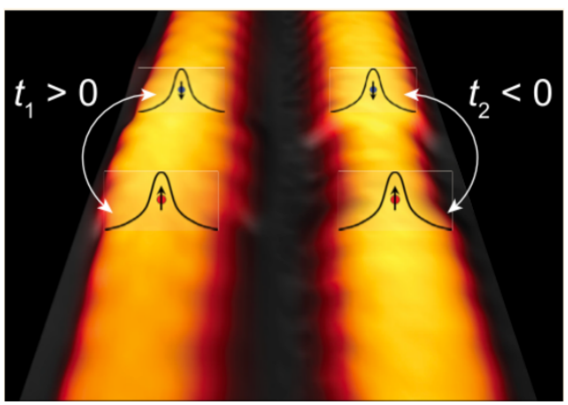
- Lowest energy state in AGRNs exhibit localization



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



- 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!*

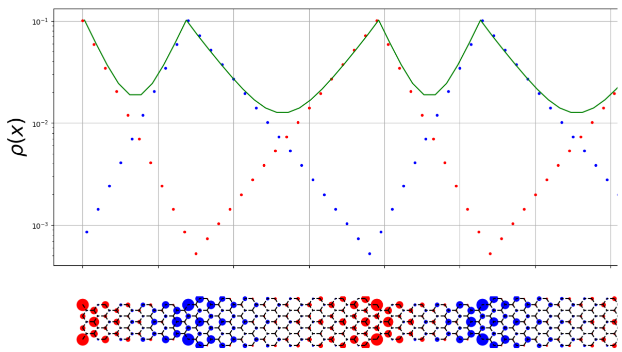
A new type of localization in hybrid nanoribbons

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

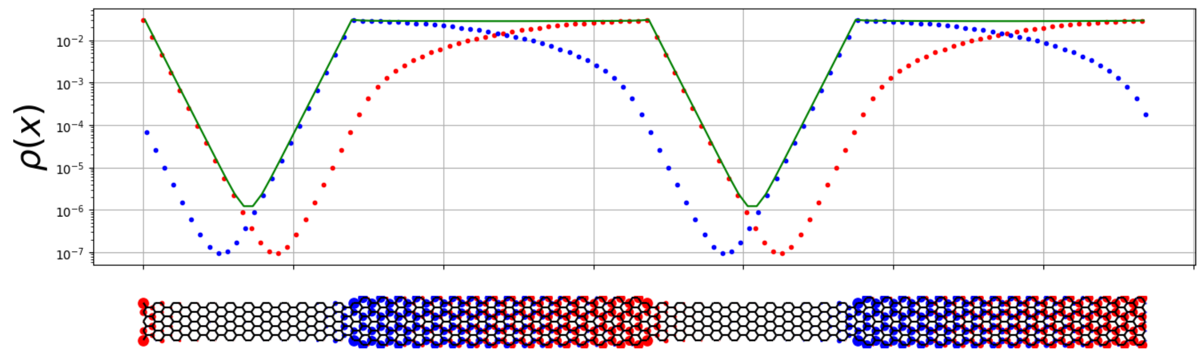
- Investigating the non-interacting model $\longrightarrow$ finding a new localization

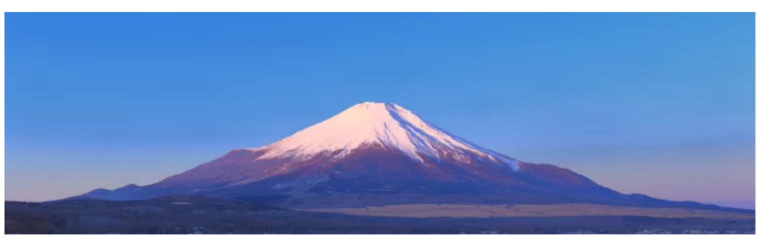
$\hookrightarrow$ standard lore: connect gapped AGNRs, but one gapped with one gapless also works!

7/9 hybrid = **Fuji** localization



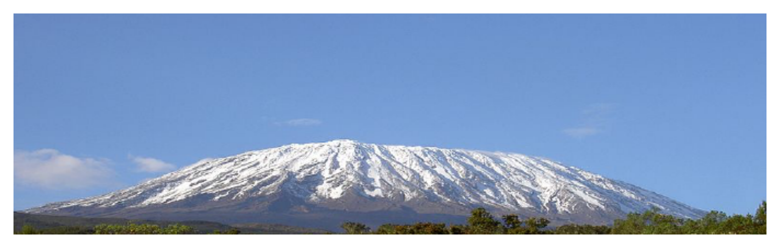
9/11 hybrid = **Kilimanjaro** localization





Predicted before

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



new form of localization!

$\hookrightarrow$ new possibilities!

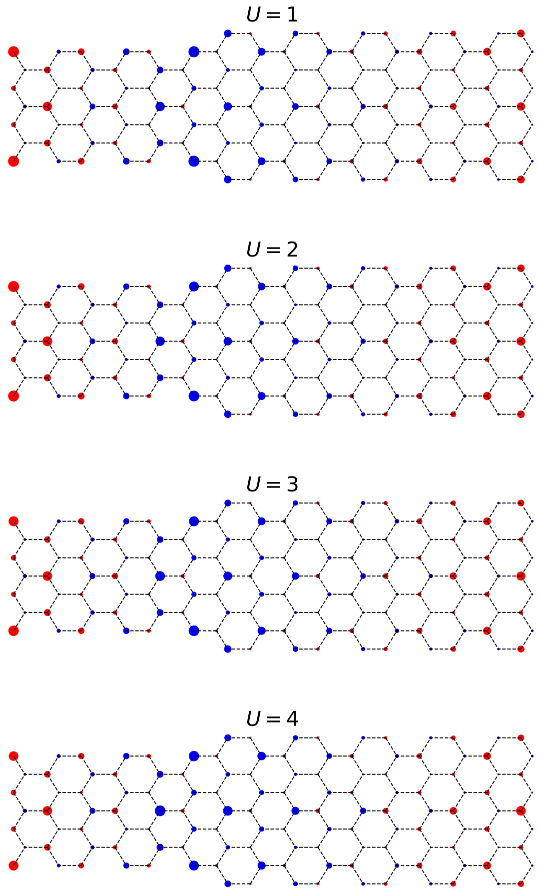
Localization in hybrid nanoribbons: Interacting systems

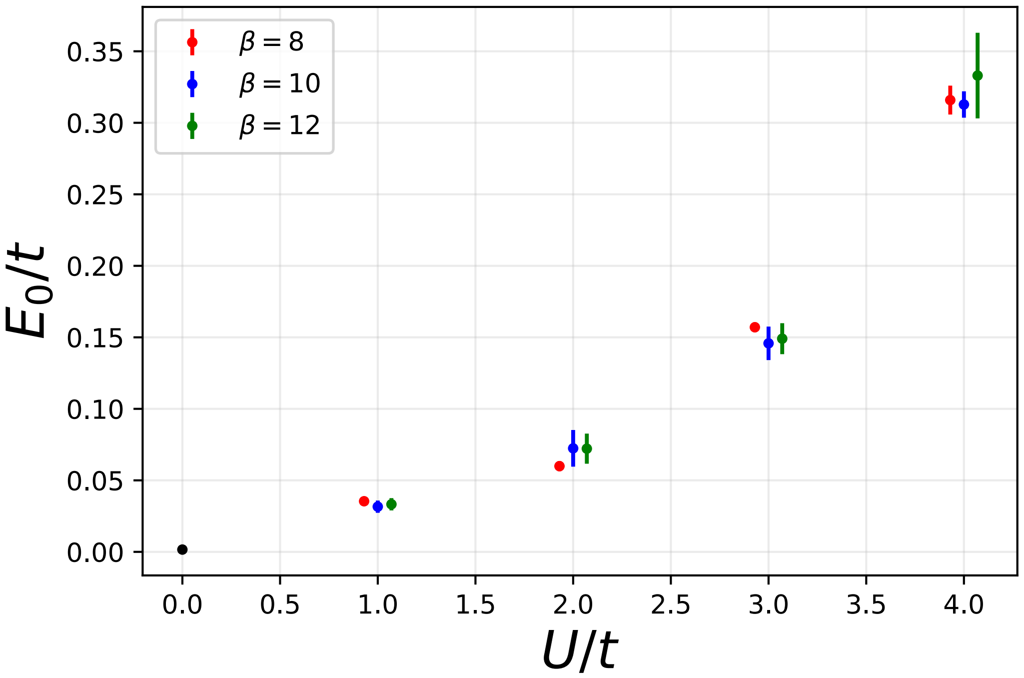
Luu, UGM, Razmadze, Phys. Rev. B **106** (2022) 195422

- 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

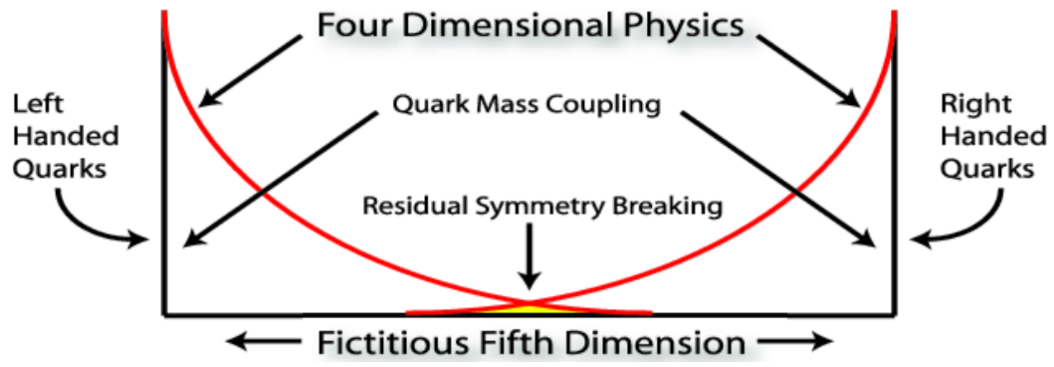


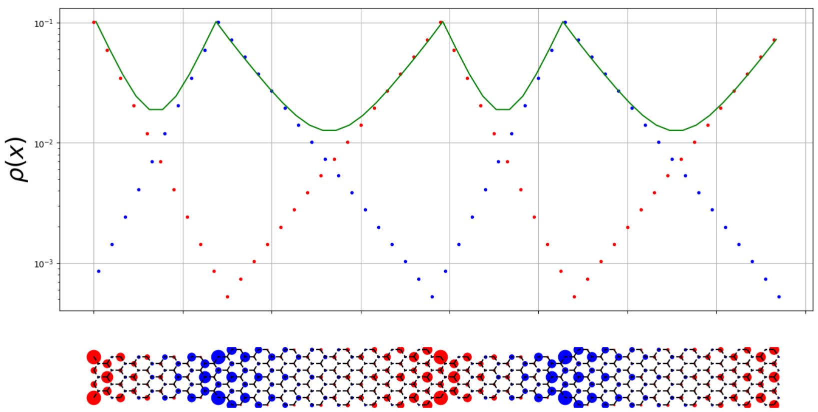


— also holds for other geometries!

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

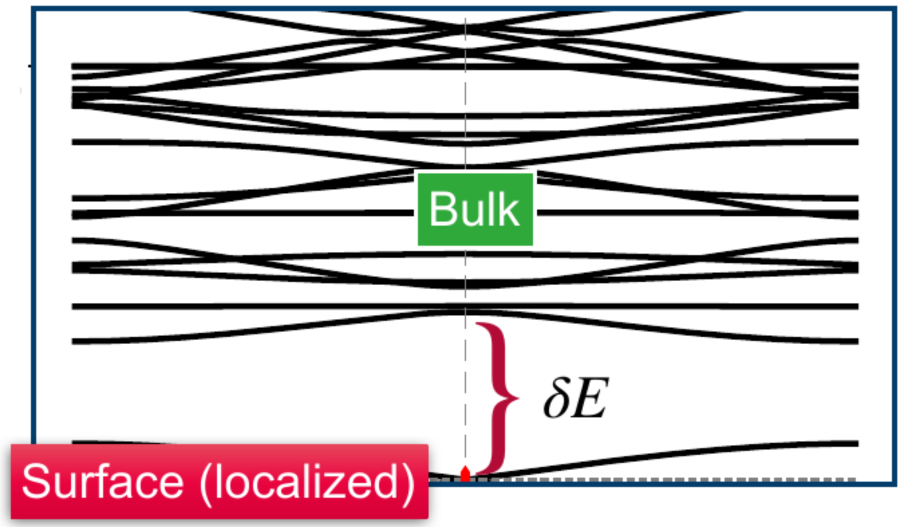
Hybrid nanoribbons provide a physical manifestation of domain wall fermions

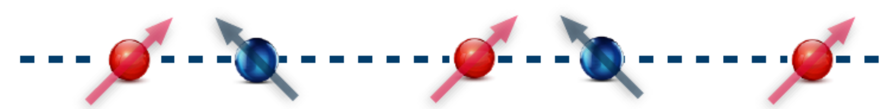
An EFT for hybrid nanoribbons

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

↪ let's see how that works





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

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

Exploring the EFT: interacting case

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

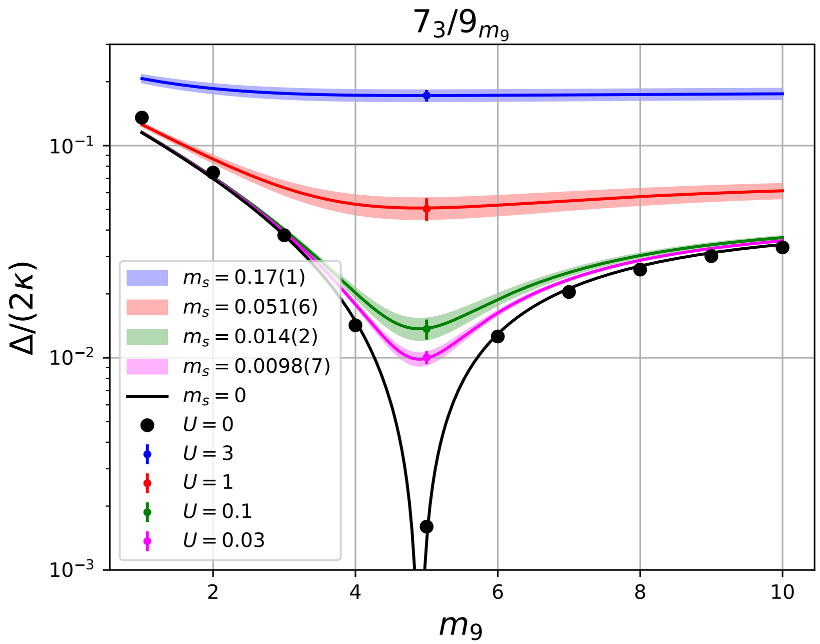
- We have a 1D EFT with the Hamiltonian with staggered mass $m_s\sigma_3$ as the energy gap is symmetric about E_F plus particle hole & chiral symmetries

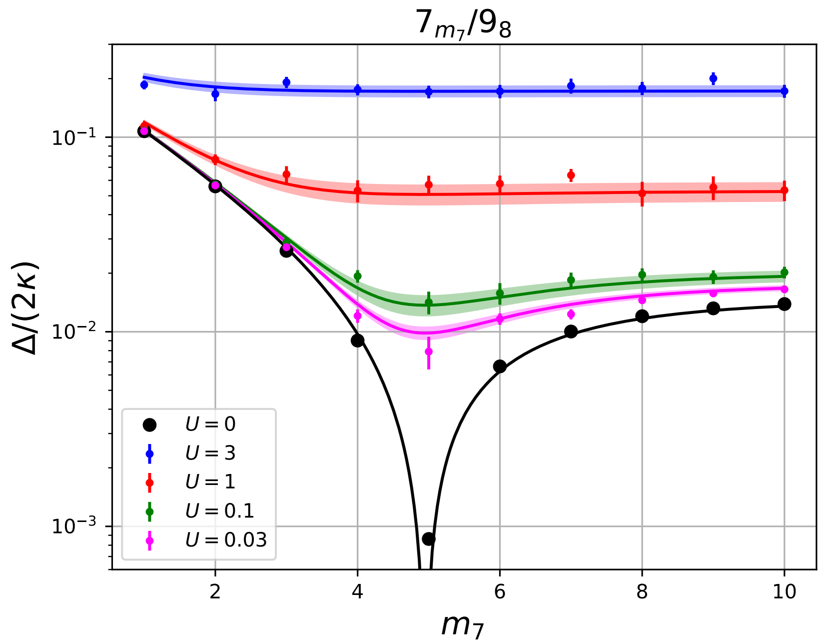
$$H_{1D} = -\sum_k a_k^\dagger \begin{pmatrix} m_s & t_A e^{ik} + t_B e^{-ik} \\ t_A e^{-ik} + t_B e^{ik} & -ms \end{pmatrix} a_k$$

- Fit t_A, t_B from the non-interacting theory

$\hookrightarrow$ Tune m_s to the underlying theory

$\Rightarrow$ Predict spectrum of new geometries

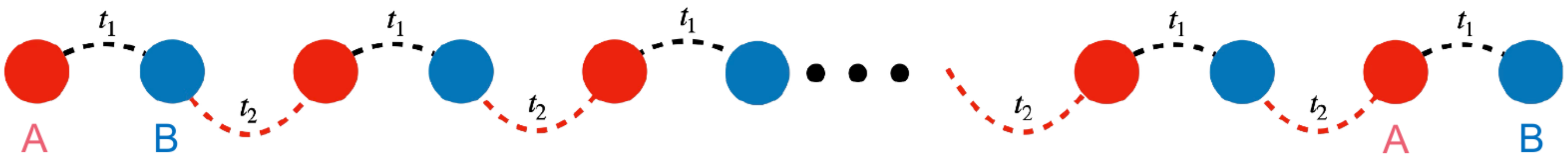




Localization in the SSH model

- 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

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

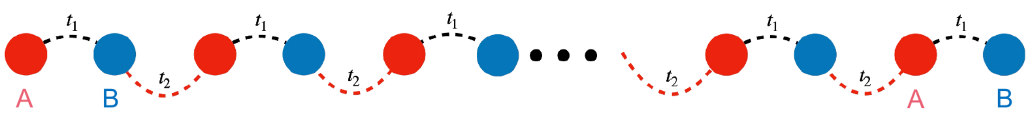
- Topological $t_1 < t_2$ $E \sim 0$ due to overlap

- Trivial $t_1 > t_2$

- Gapless $t_1 = t_2$

Localization in the SSH model: Experiments

- Even site SSH model



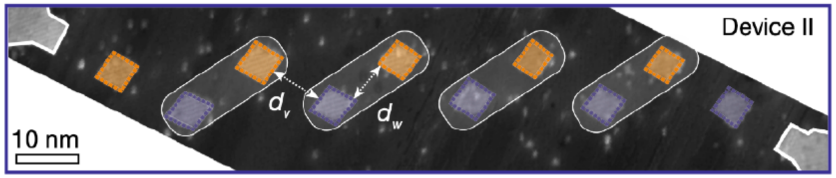
- Different types of experiments
  - Silicon quantum dots

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

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

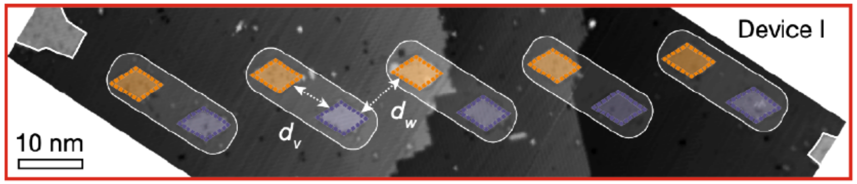
    Ligthart et al., Phys. Rev. Res. **7** (2025) 012076

- 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

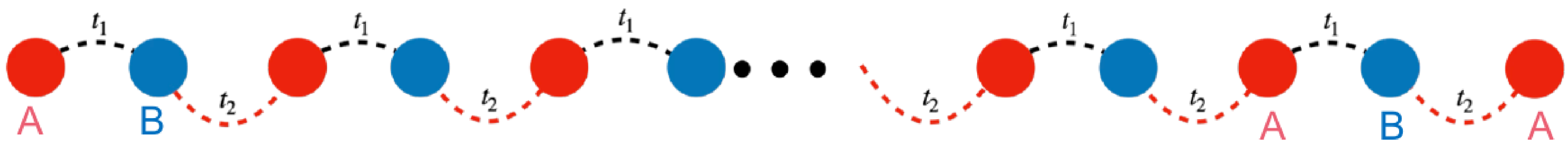
- Disadvantages:
  - Sensitive to the parameter choice, e.g., $t_1 < t_2$
  - Long enough chain to reduce wave function overlap

- 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

• $t_1 > t_2$ $E = 0$

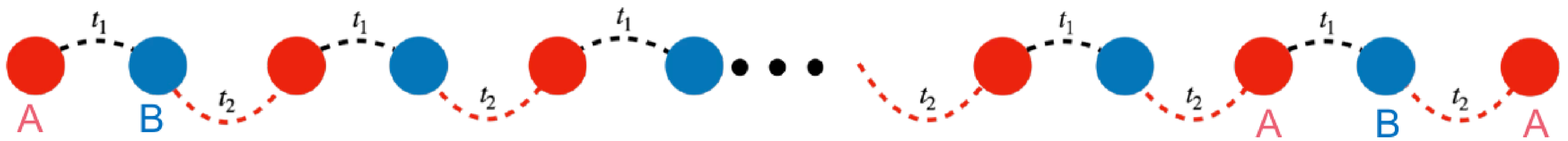
Advantages:
- Independent of parameter choice
- No length requirement but odd

• $t_1 = t_2$ $E = 0$

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

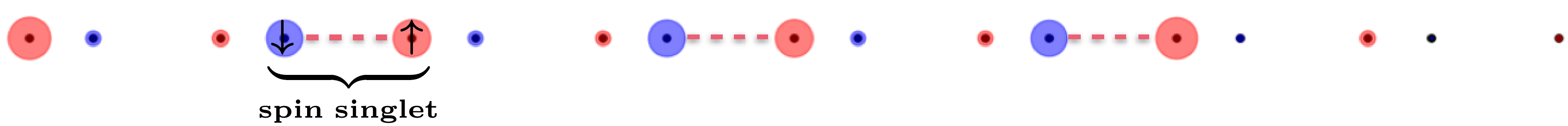
- Add an onsite Hubbard interaction

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

- 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:

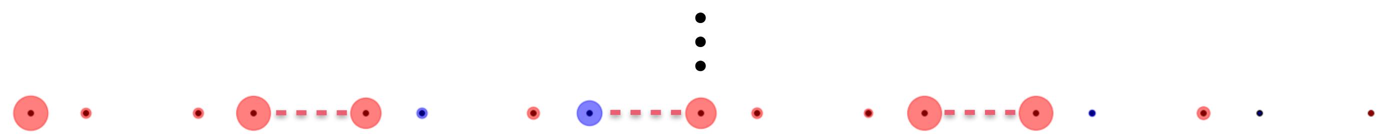
  (i) Magnetism and spintronics

  (ii) Quantum computations and simulations

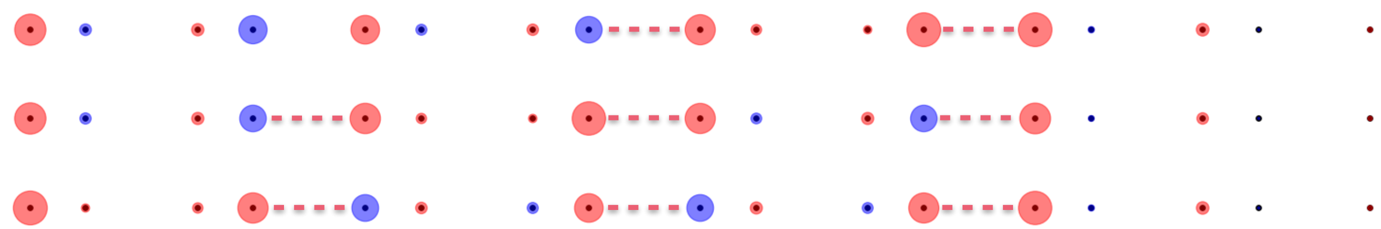
Excited states in the odd SSH model with interactions

Wang, Luu, UGM, to be published

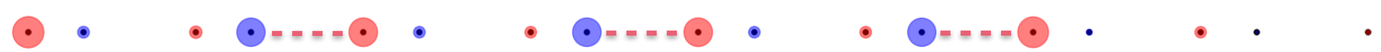
- Can engineer even more exotic forms of localization:



$S_z = \frac{5}{2}$ $E_{5/2} \gtrapprox E_{3/2} \gtrapprox E_{g.s.}$



$S_z = \frac{3}{2}$ $E_{3/2} \gtrapprox E_{g.s.}$



$S_z = \frac{1}{2}$ $E_{g.s.}$

↪ Couple these different spin configurations (via an external magnetic field)

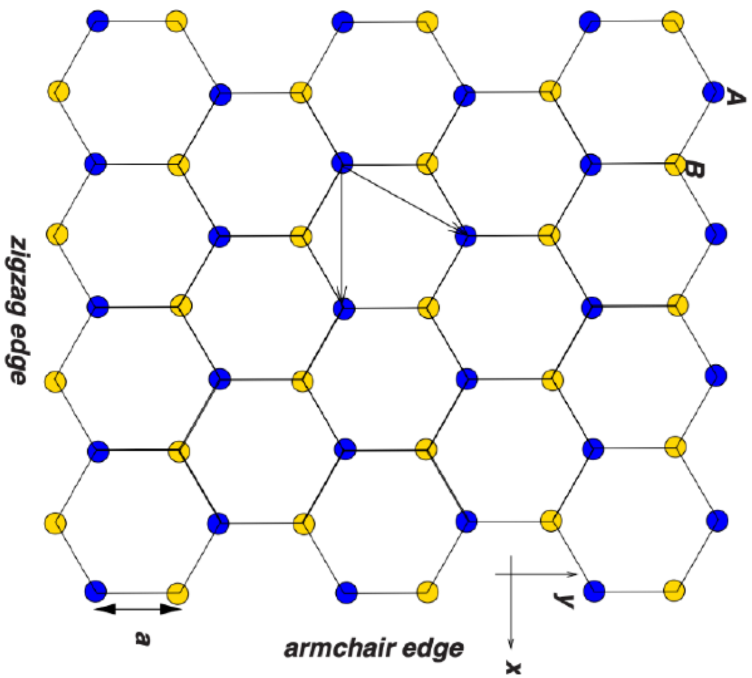
↪ engineer and/or manipulate spin qubits, other applications? → ideas welcome!

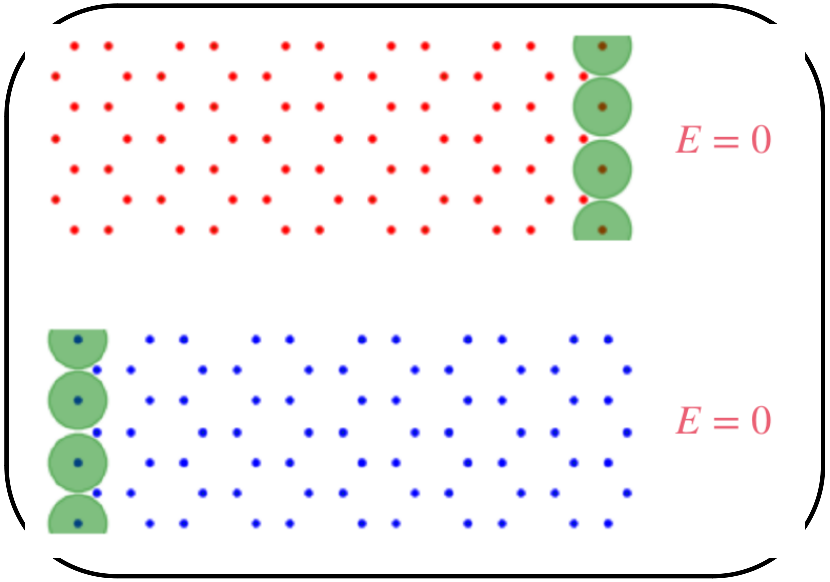
Graphene nanosystems with odd sites

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!

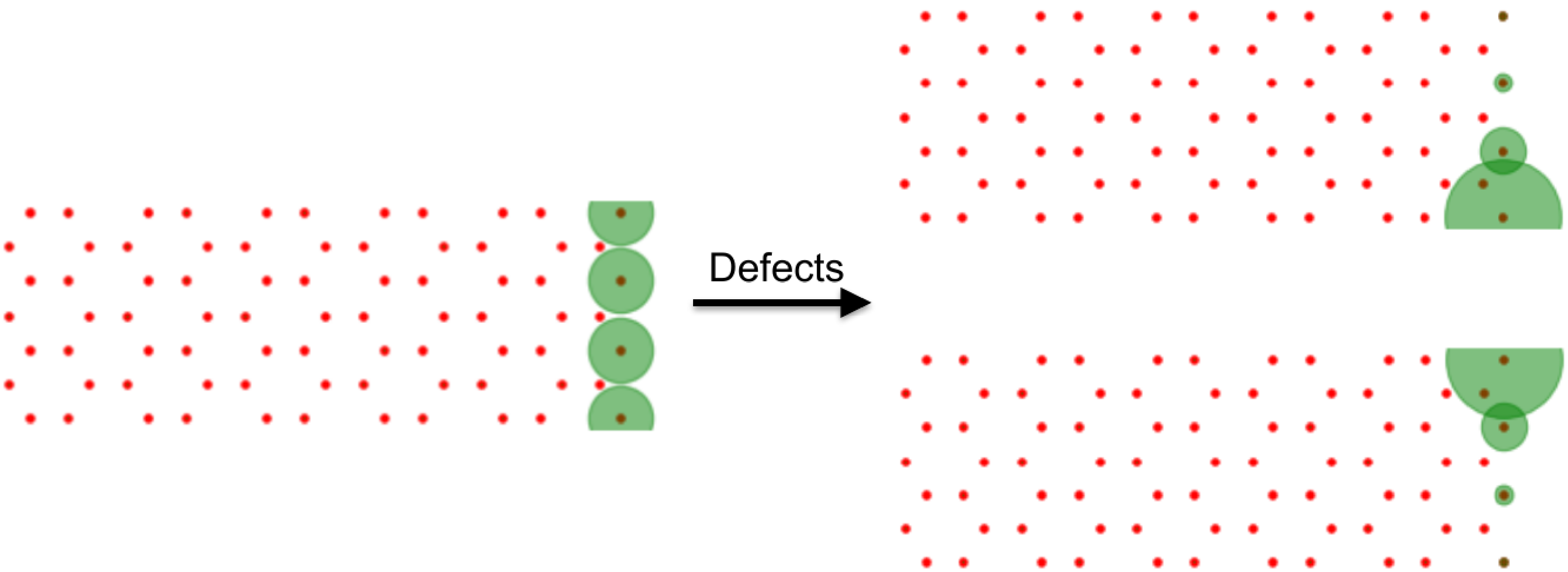




Defect engineering graphene nanosystems

Wang, Luu, UGM, to be published

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



$\hookrightarrow$ Consequences/applications need to be investigated $\rightarrow$ 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

  $\hookrightarrow$ can be tackled w/ EFT and/or MC (stochastic) methods

- Large progress made in the last few years:

  $\hookrightarrow$ new insights into nuclear structure and nuclear matter

  $\hookrightarrow$ new insights into toplogical matter and how to engineer it

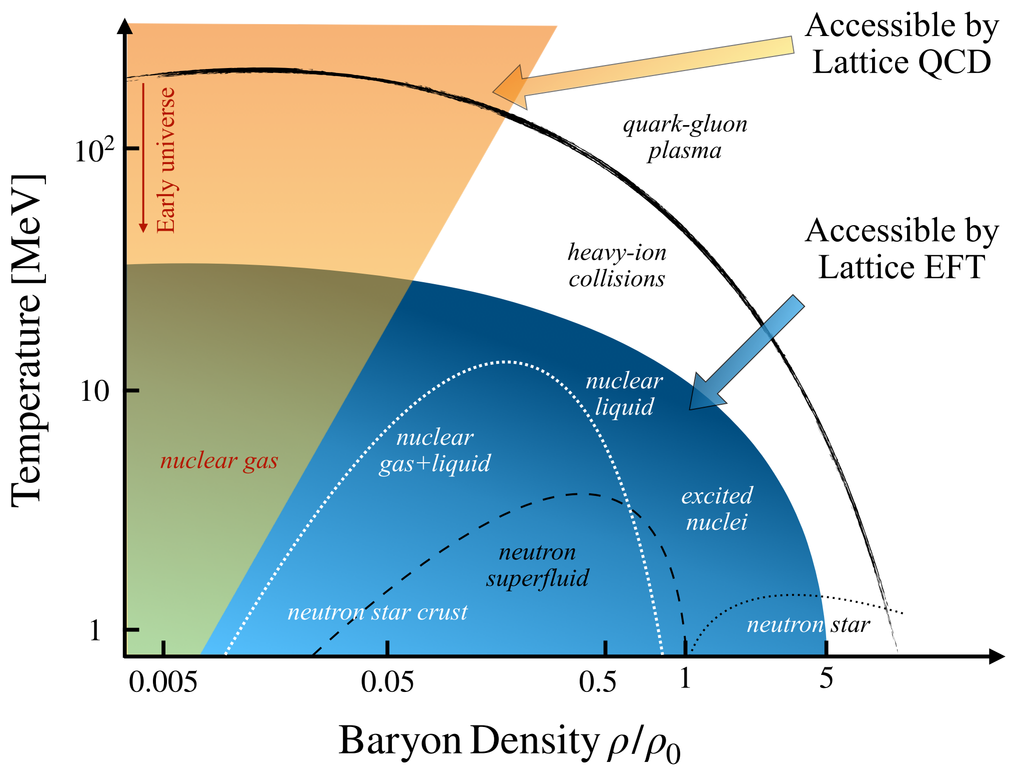
- More interactions between fields is needed to make further progress!

Thank you for your attention!

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!

Computational equipment

- Present = JUWELS (modular system) + FRONTIER + ...