



<https://github.com/NuLattice/NuLattice/>

NuLattice: Computations of nuclei on lattices

Matthias Heinz, ORNL

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NUCLEI
Nuclear Computational Low-Energy Initiative

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Simulating nuclei

- Instead of quarks and gluons, we have **nucleons and pions** as degrees of freedom
- Two ingredients:
 - Effective field theory for interactions
 - Quantum many-body methods
- **Central goal: solve the Schrödinger equation**

$$H|\Psi\rangle = E|\Psi\rangle$$

- **Hartree-Fock:** variational approximation to $|\Psi\rangle$
 → robust upper bounds on E

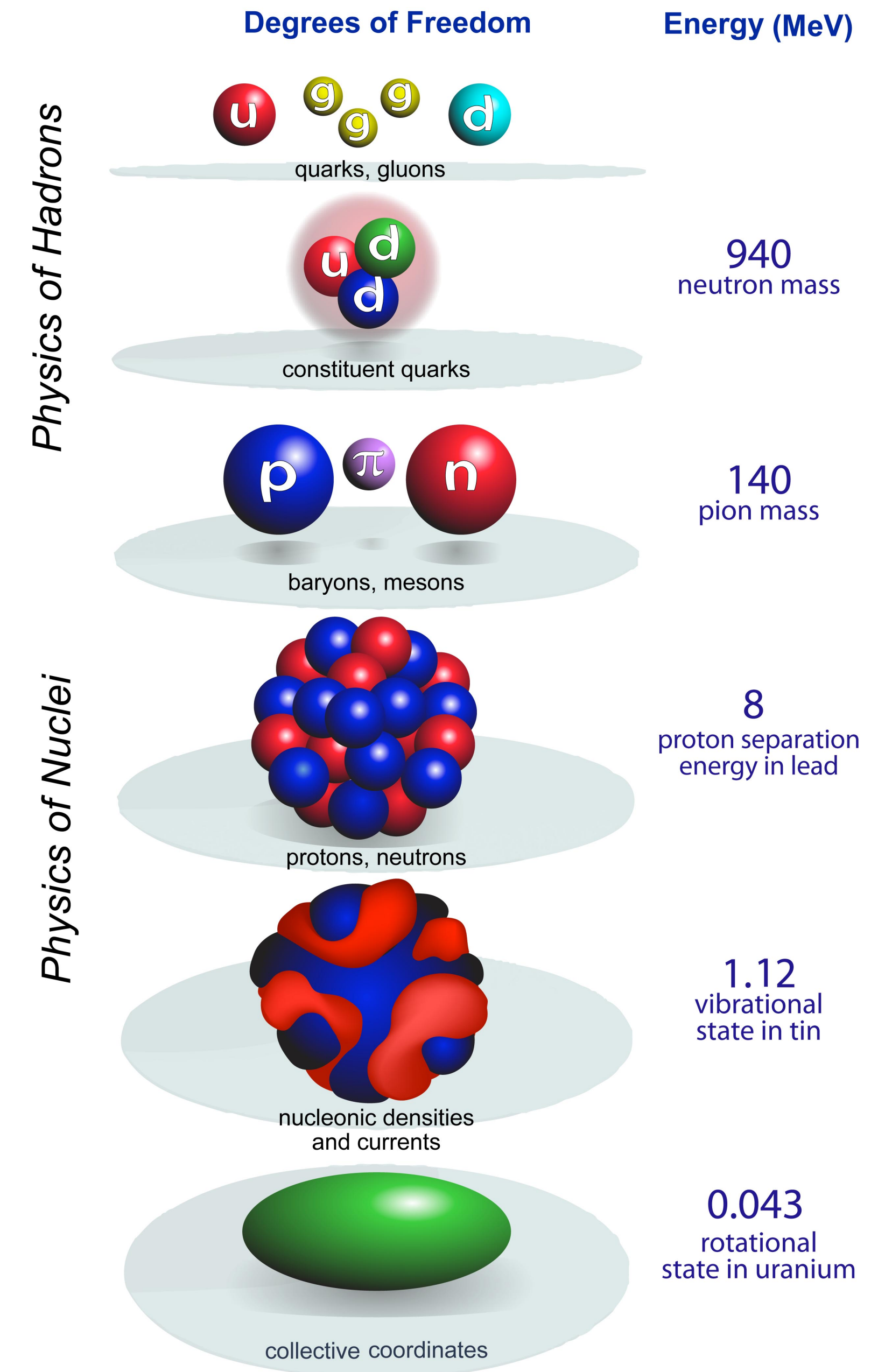
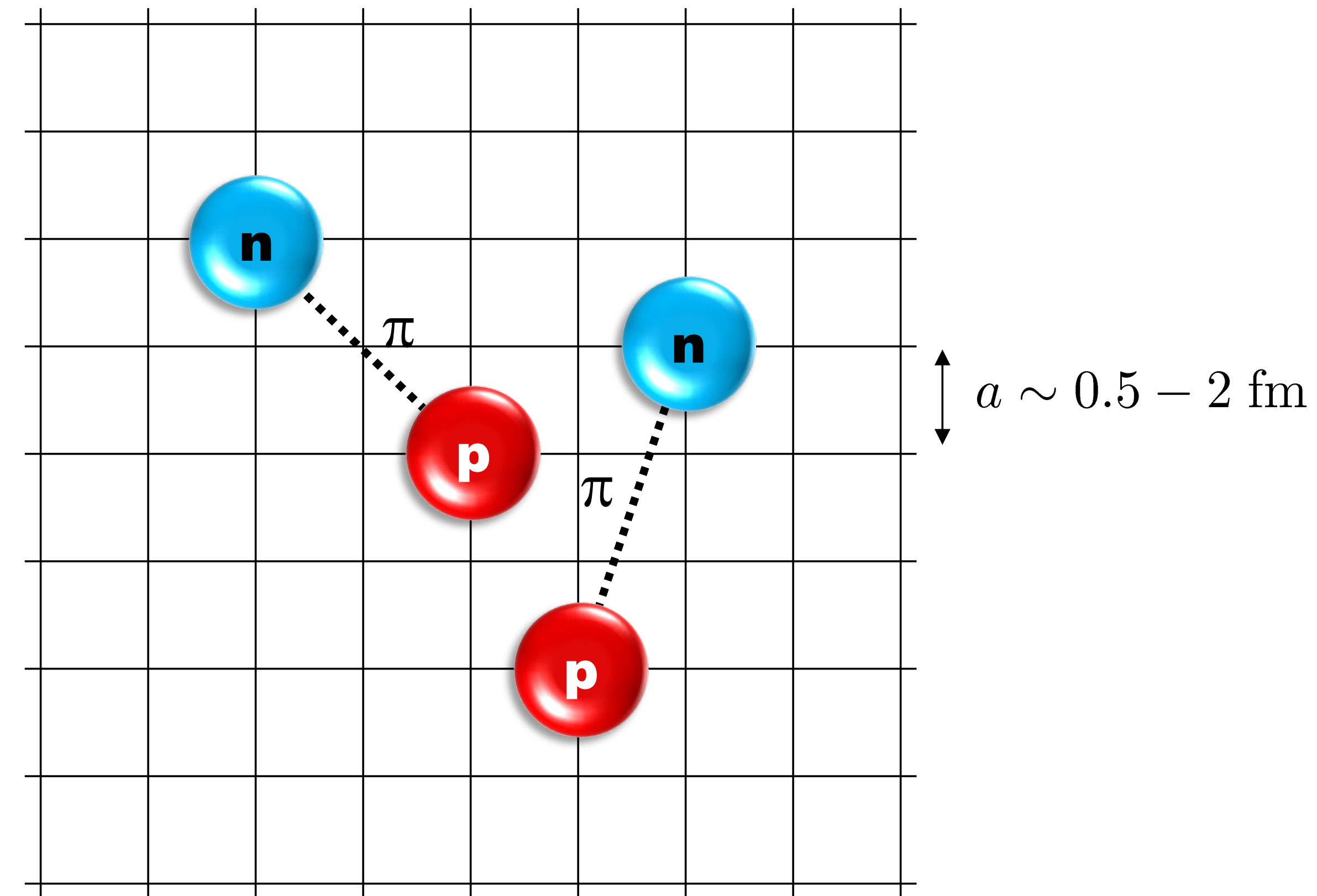


Figure: Nazarewicz

Nuclei on a lattice

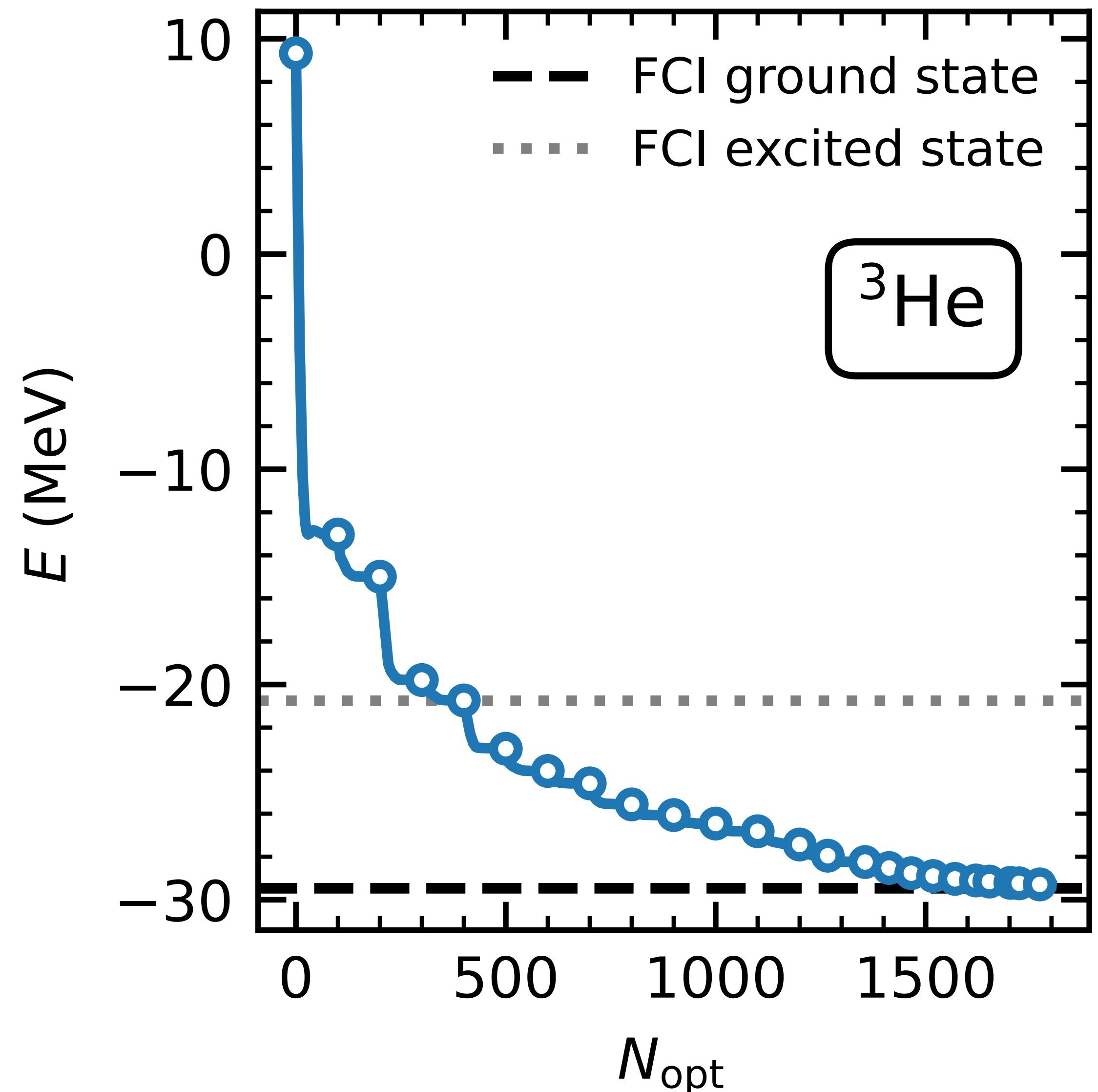
- Nuclear forces are finite-ranged
- On a spatial lattice,
Hamiltonians are very sparse
- Interactions only in finite range r_{int}
- Volume of interactions small compared to total volume
- **This can drastically simplify computations!**



Lee, PPNP (2009)

Quantum computing

- **Sparse Hamiltonian reduces number of 2-qubit gates**
- 2- and 3-body forces from EFT
- Simulations of ^2H , ^3He
- Exact benchmarks met
- **Mild scaling of computational resources suggests this approach is scalable**



NuLattice

<https://github.com/NuLattice>

- **Python computations of nuclei**
- Many quantum many-body methods implemented
- Educational tool
- But also new science insights:
 - Validation of standard approximation for 3-body forces
 - Hartree Fock is pretty good for short-ranged forces
- GPU acceleration and multi-node scaling with JAX



Maxwell Rothman @ UTK



Ben Johnson-Toth @ UTK



Vivek Booshan @ ORNL

Lattice Hamiltonians

- Basis: $|p\rangle = |\mathbf{n} = (x, y, z), i = (t_z, s_z)\rangle$ w/ lattice spacing a and extent L

$$H = T + V_{\text{NN}} (+ W_{3\text{N}})$$

- LO pionless EFT: 0-range $V_{\text{NN}}, W_{3\text{N}} \rightarrow$ **does not bind alpha particles**
- Smearing gives interactions a range

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

$$\tilde{\rho}(\mathbf{n}) = \sum_i \left[\tilde{a}_i^\dagger(\mathbf{n}) \tilde{a}_i(\mathbf{n}) + s_L \sum_{|\mathbf{n}-\mathbf{n}'|=1} \tilde{a}_i^\dagger(\mathbf{n}') \tilde{a}_i(\mathbf{n}') \right]$$

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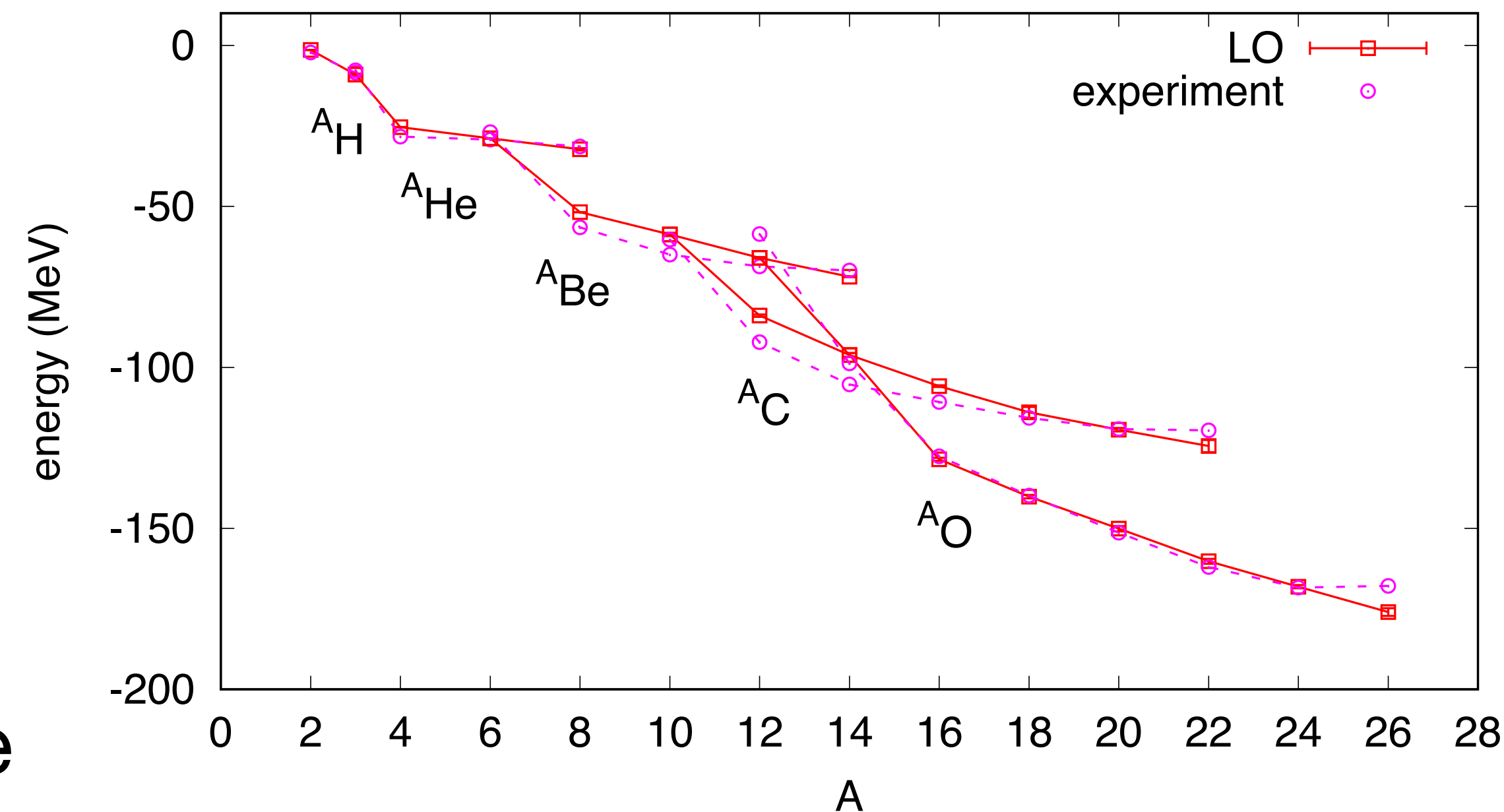
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Key features: lattice spacing a , nonlocal smearing s_{NL} , local smearing s_L

How simple is too simple?

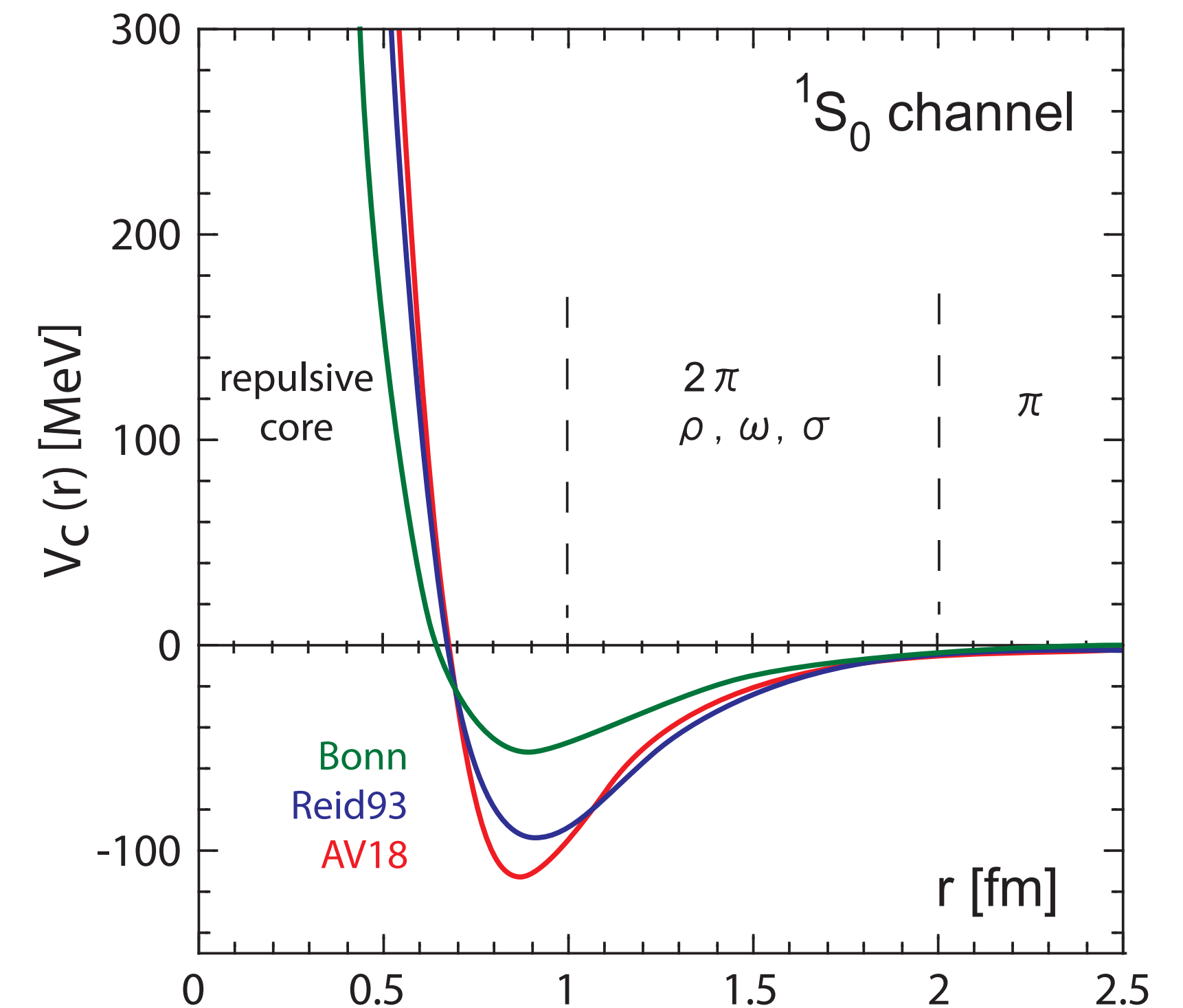
- Chiral EFT: 23 parameters at $N^3\text{LO}$
- Complicated, scale-dependent balance between many terms
- LO pionless EFT:
too simple, doesn't bind α clusters
- But some NLEFT Hamiltonians propose to be simple, yet accurate
- 2017: Attractive contact + one-pion exchange
→ weak smearing: $s_{NL} = 0.08$, $s_L = 0.08$
→ lattice spacing: $a = 1.97$ fm
→ single coupling: $c_0 = -18.5$ MeV



Elhatisari et al., PRL (2017)

Nuclear saturation

- Nuclei are incompressible
 - $E/A \sim 8 \text{ MeV/nucleon}$
 - $R_{\text{ch}} \propto A^{1/3}$
- Central density of nuclei saturates
- Old view: Short-range repulsion in NN force gives saturation
- EFT/RG view: Repulsive three-nucleon interactions give saturation
- **How does a Hamiltonian with a purely attractive NN interaction give saturation?**

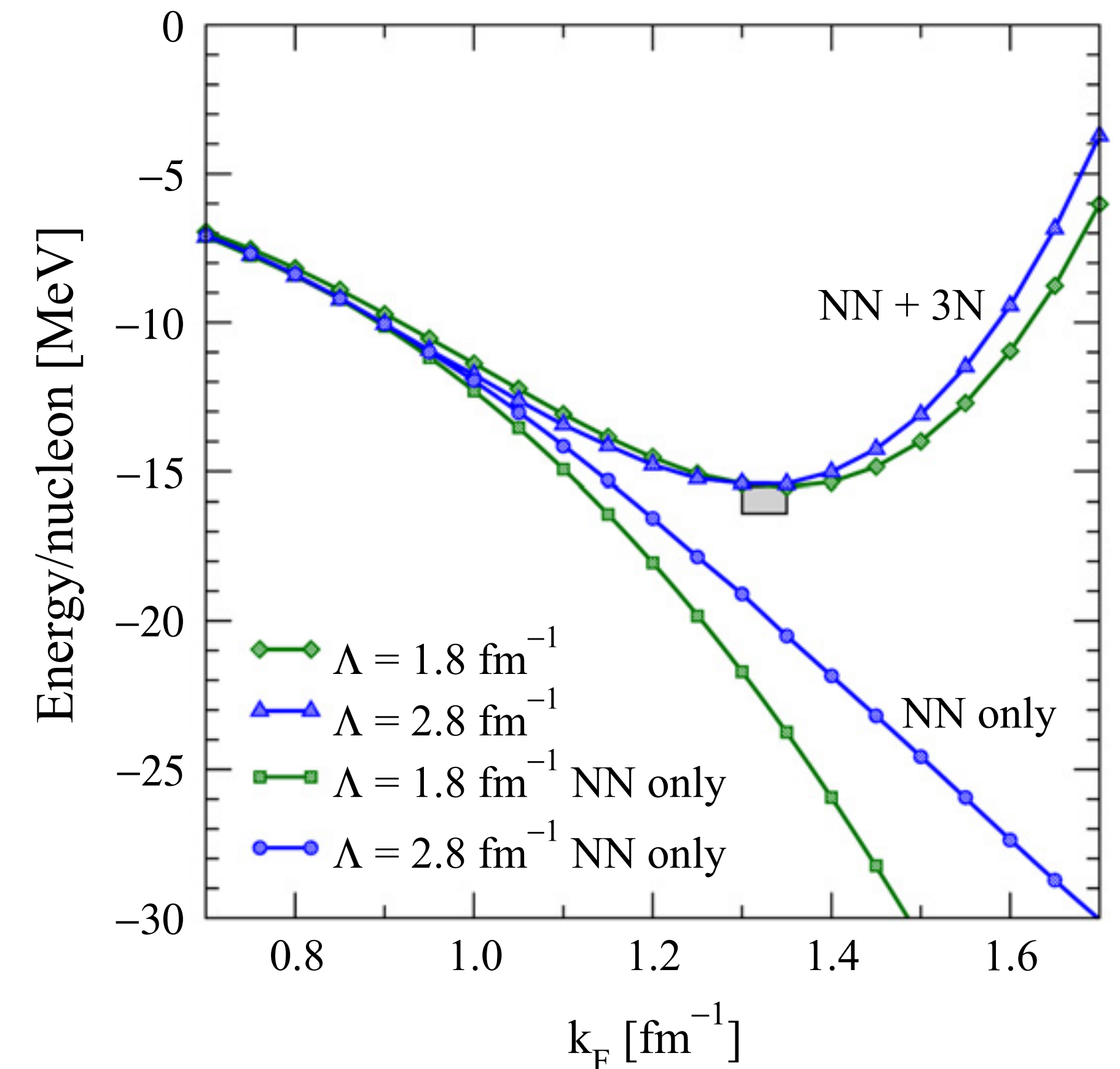


Aoki et al., Comp. Sci. Dis. (2008)



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Bogner et al., PPNP (2010)



Variational bounds for nuclei

Using Hamiltonian from [Elhatisari, Epelbaum, Krebs, Lähde, Lee, Li, Lu, Meißner, Rupak, PRL \(2017\)](#)

- Hartree-Fock (HF) gives **variational upper bounds** for ground-state energy

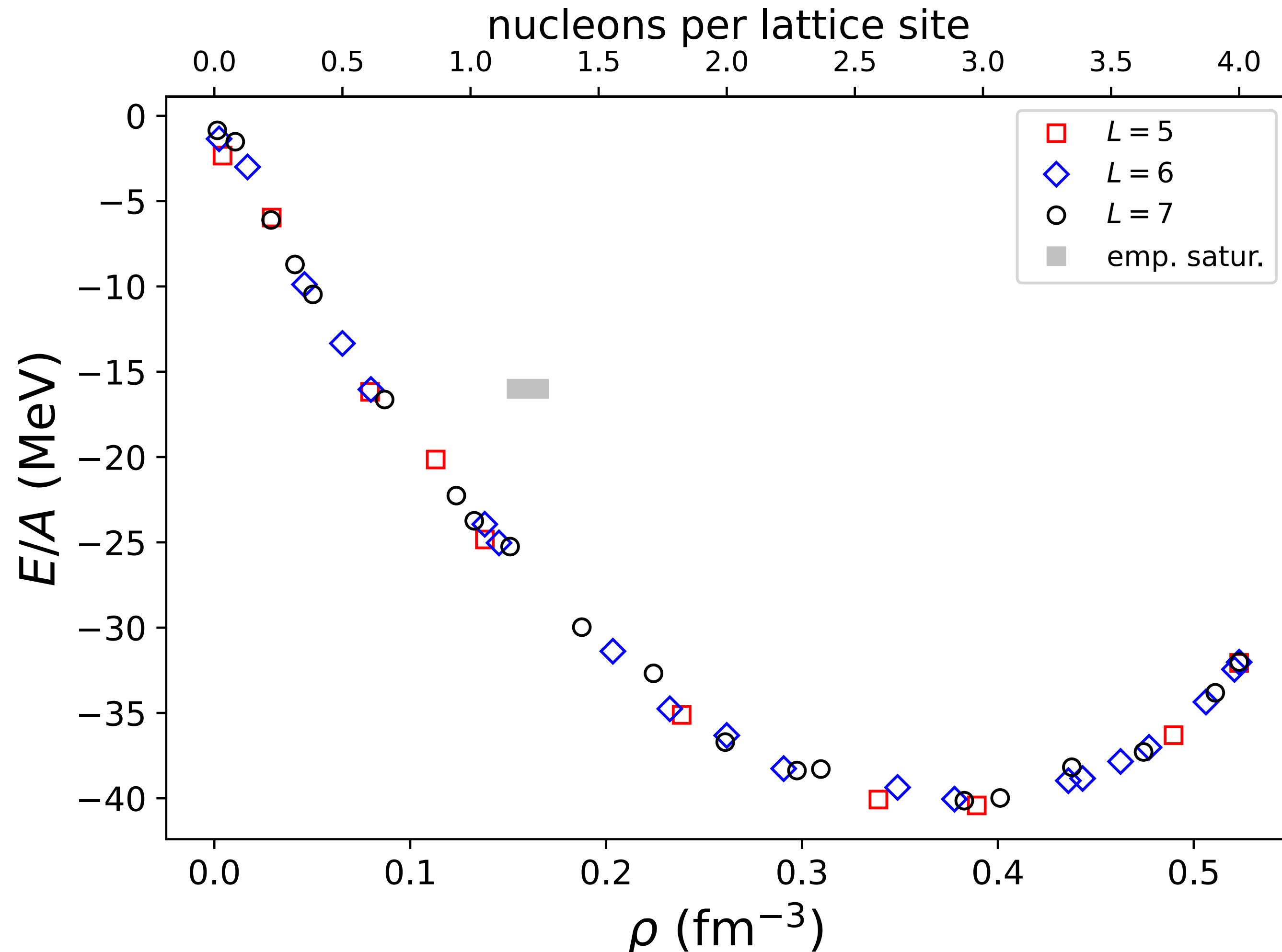
Nucl.	HF	NLEFT	Exp.
${}^4\text{He}$	-19.81	-25.4	-28.3
${}^8\text{Be}$	-63.17	-51.9	-56.5
${}^{12}\text{C}$	-137.28	-83.8	-92.2
${}^{16}\text{O}$	-213.37	-128.2	-127.6

- Hamiltonian clearly overbinds nuclei significantly
- Aux. field Monte Carlo (NLEFT) do not solve the Hamiltonian accurately
- Culprit: temporal lattice spacing $a_t = 1.97$ fm (see [Niu et al. arxiv:2607.06044](#) for details)

*also used in previous studies since [Epelbaum et al., PRL \(2010\)](#) and earlier

Saturation in nuclear matter

Using Hamiltonian from Elhatisari, Epelbaum, Krebs, Lähde, Lee, Li, Lu, Meißner, Rupak, PRL (2017)



- Hamiltonian does not give realistic saturation in nuclear matter
- Supported by analytical results on full lattice (see [arxiv:2606.25019](https://arxiv.org/abs/2606.25019))

V	$\langle V \rangle / A$	$\langle T + V \rangle / A$
V_0	-76.80	-33.31
$V_0 + V_{\text{OPE}}$	-75.55	-32.06

- Note: one-pion exchange contribution negligible

Lattice Hamiltonian with attractive 3NF

Using Hamiltonian from [Lu et al., PLB \(2019\)](#)

- Smeared two-body and three-body contact (both attractive)
- $s_{NL} = 0.5$, $s_L = 0.061$, $a = 1.32 \text{ fm}$, $c_0 = -1.15 \text{ MeV}$ $c_3 = -0.16 \text{ MeV}$
- Note: Hartree-Fock only variational for same L and N

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Pure neutron matter

L	N	ρ	E/N	E/N (NLEFT)
7	14	0.018	3.8	2.7
7	38	0.048	5.6	5.1
7	54	0.068	7.5	7.1
6	38	0.076	8.0	7.6
7	66	0.084	9.3	8.9
6	54	0.11	11.6	11.3
5	38	0.13	13.6	13.4
6	66	0.13	14.0	13.8

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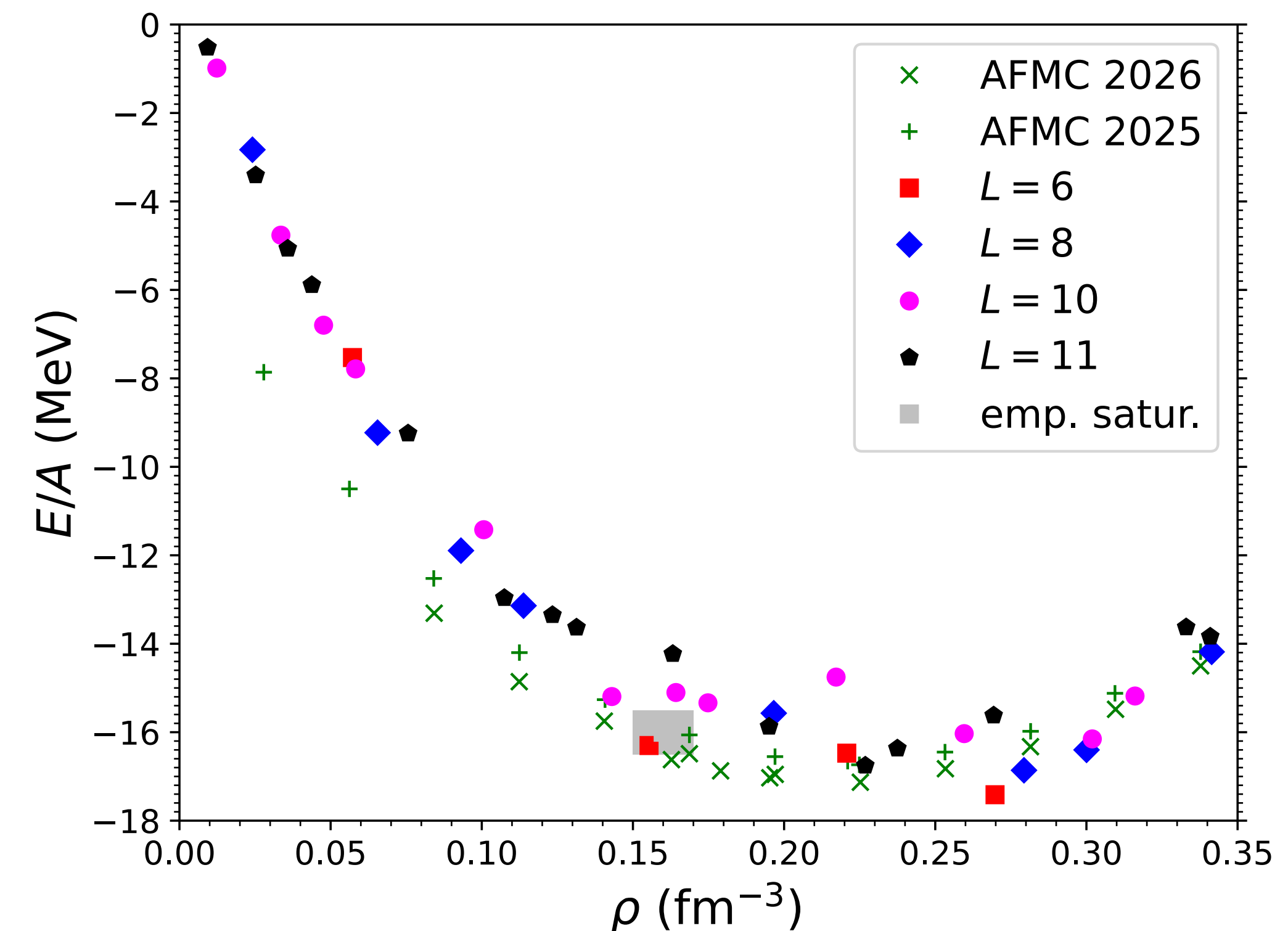
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Nuclear matter



Saturation from lattice artifacts

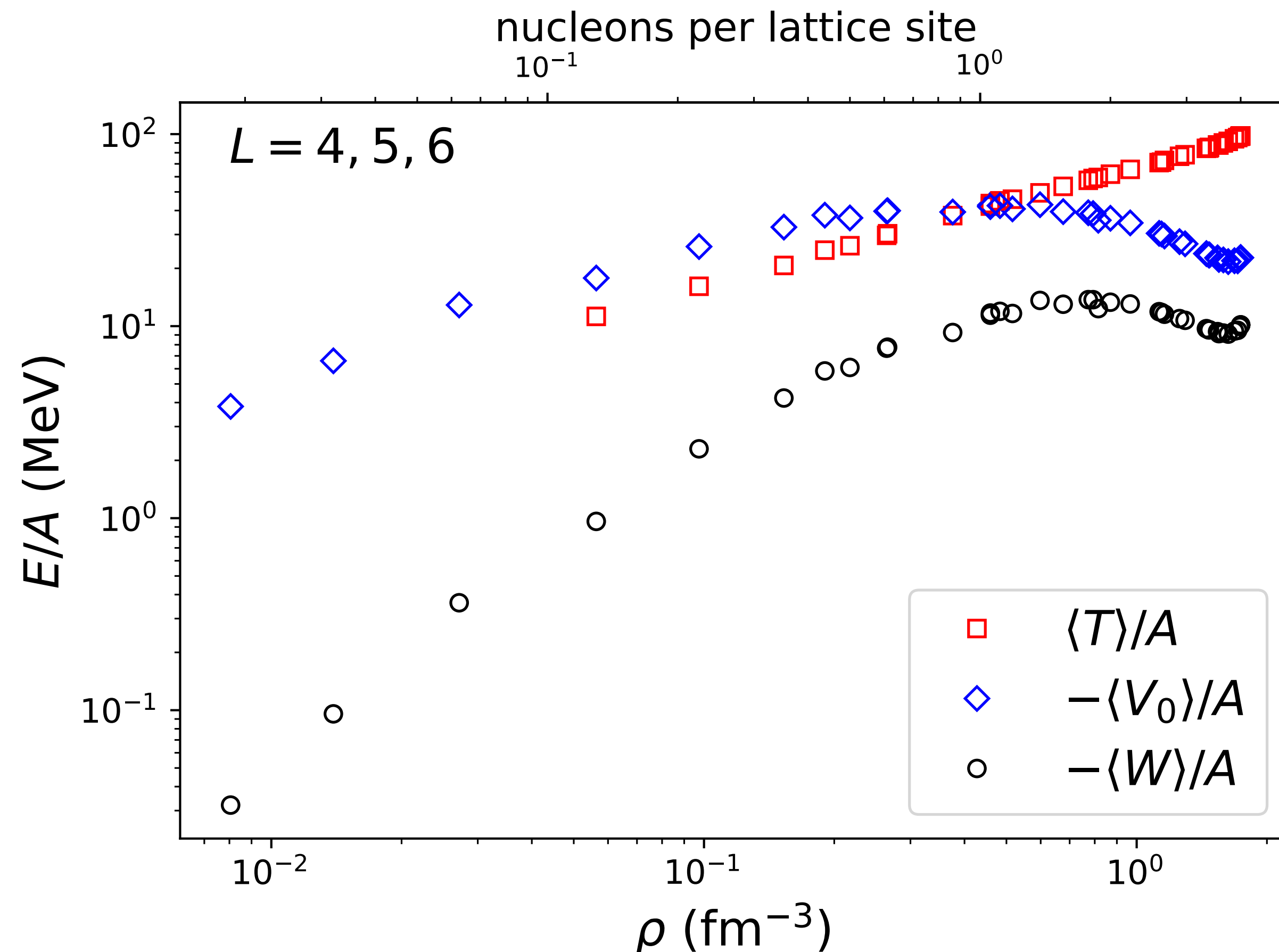
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- Saturation from kinetic energy
- At high densities, crowding of fermions on a lattice reduces potential energies
- Nonlocal smearing greatly enhances attraction at low densities
- **Saturation is a lattice artifact**

Perspectives and summary



Perspectives

- We are working on the lattice to simulate nuclear dynamics
- Time-dependent solutions to Schrödinger equation <https://github.com/NuLattice/NuLattice/> with Hartree-Fock, coupled cluster, full configuration interaction
Bonaiti et al., PRC (2026); PRL (2026), more on the way
- We want accurate lattice Hamiltonians with well-understood systematics

Summary

- NuLattice is a publicly available Python code to simulate nuclei
- Benchmarks against NLEFT results (on a laptop) show some Hamiltonians were not solved accurately
- Saturation with purely attractive interactions from lattice artifacts

Acknowledgments: Maxwell Rothman, Ben Johnson-Toth, Vivek Booshan, Francesca Bonaiti, Gaute Hagen, Thomas Papenbrock

