Lattice computations of atomic nuclei with NuLattice

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Nuclear Hamiltonians for Advancing Nuclear Physics and Beyond

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Acknowledgments

Collaboration

- Chenyi Gu, Ben Johnson-Toth, Maxwell Rothman (University of Tennessee)
- Francesca Bonaiti, Vivek Booshan, Matthias Heinz, Gaute Hagen (ORNL)
- Oriel Kiss (CERN)

Benchmarking

- Serdar Elhatisari (Gaziantep)

Challenges / opportunities

Chiral EFT is where it is

- Overcoming its problems requires new ideas / approaches

Ab initio computations of nuclei

- Limitations from the spherical normal-ordered two-body approximation is the obstacle to rare-earth nuclei and actinides

Classical computers now allow us to address beyond-mean-field dynamics

- Study of equilibration / chaos in nuclear dynamics → Francesca Bonaiti's talk
- Ab initio computations of fission and fusion

Quantum computers are here and are becoming more powerful

- Nuclear structure and dynamics

Challenges / opportunities

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Classical computers now allow us to address beyond-mean-field dynamics

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Computing nuclei on lattices

Quantum computers are here and are becoming more … ul

- Nuclear structure and dynamics

Why work on lattices?

- Exploit short range of interaction
  - For $n = 4L^3$ states, number of two-body matrix elements is $O(n) \cdots O(n^2)$ and not $O(n^3)$
- Makes Hamiltonian more suitable for quantum computing (Baroni, Carlson, Roggero, Stetcu; Watson, Childs, Davoudi; ...)
- Scrutinize Nuclear Lattice EFT (Elhatisari, Epelbaum, Lähde, Lee, Lu, Ma, Meissner, ...)
- Study nuclear dynamics (and go beyond time-dependent mean field)

😎 Make movies of collisions, fusion, and fission (Bulgac, Godbey, Rios, Schunck, Sekizawa, Simenel, Stevenson, Umar, Yabana, ...)

- Get insights
  - "Exactness of the normal-ordered two-body truncation of three-nucleon forces," arXiv:2508.01507; Phys. Rev. C 112, L051301 (2025)
  - Saturation by dominance of kinetic over potential energy

😩 Loss of rotational invariance

😩 Loss of shell-model phenomenology

https://github.com/NuLattice

PHYSICAL REVIEW C **113**, 034321 (2026)

Editors' Suggestion

Toward scalable quantum computations of atomic nuclei

Chenyi Gu,[1] Matthias Heinz,[2,3,*] Oriel Kiss,[4,5] and Thomas Papenbrock[1,3]

PHYSICAL REVIEW C **112**, L051301 (2025)

Letter

Exactness of the normal-ordered two-body truncation of three-nucleon forces

Maxwell Rothman,[1] Ben Johnson-Toth,[1] Francesca Bonaiti,[2,3] Gaute Hagen,[3,1]
Matthias Heinz,[4,3] and Thomas Papenbrock[1,3]

prototyping, research,
instruction,

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https://doi.org/10.1140/epja/s10050-025-01764-6

THE EUROPEAN PHYSICAL JOURNAL A

Check for updates

Code Paper

NuLattice: *Ab initio* computations of atomic nuclei on lattices

M. Rothman[1,a], B. Johnson-Toth[1,b], G. Hagen[1,2,c], M. Heinz[2,3,d], T. Papenbrock[1,2,e]

https://github.com/NuLattice

Maxwell Rothman, Ben Johnson-Toth, G. Hagen, M. Heinz, TP, Eur. Phys. J. A 62, 28 (2026); arXiv:2509.08771

What's in `NuLattice`?

- So far: only interactions from pionless EFT at leading order
  - Soon: One-pion exchange, Coulomb, smeared contact potentials from Elhatisari et al., Phys. Rev. Lett. 119, 222505 (2017); Phys. Rev. Lett. 117, 132501 (2016); Bing-Nam Lu et al., Phys. Lett. B 797, 134863 (2019)
- Full Configuration Interaction for $A = 2,3,4$ nuclei (benchmarking); ^{4}He runs with $L \leq 4$ on laptops
- Hartree-Fock ($L = 10$ is possible) for nuclei (nuclear matter and neutron matter soon)
- Coupled cluster method (CCSD); ^{16}O runs with $L \leq 6$ on laptops (storage of T_2 is limiting factor, 20 GB)
- IMSRG(2): runs on laptops for $L \leq 3$ (because sparsity of cluster operator not exploited)

Quantum simulations of nuclei on lattices

Nucleons on a cubic lattice (L^3 sites, spacing $a = 2$ fm) with periodic boundaries

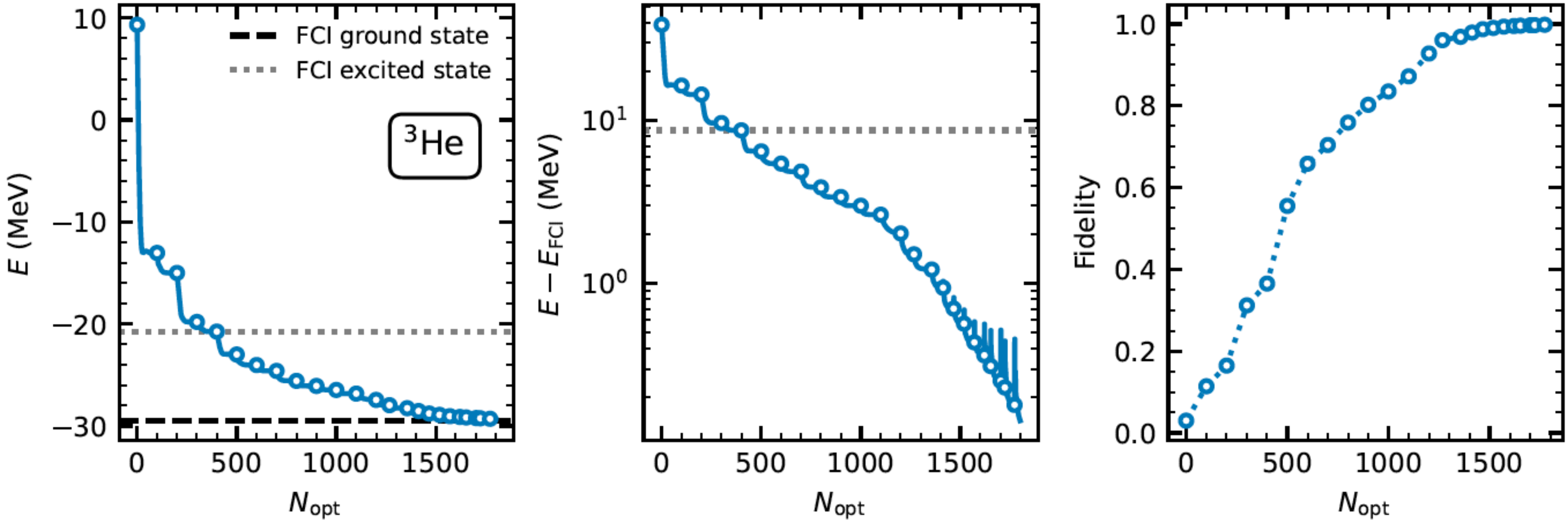
Hamiltonian: leading-order pion-less effective field theory [Bedaque, van Kolck 2002]

$$\hat{H} = \sum_{\langle \mathbf{l},\mathbf{l}'\rangle} \sum_{\tau s} T^{\mathbf{l}}_{\mathbf{l}'} \hat{a}^\dagger_{\mathbf{l}\tau s} \hat{a}_{\mathbf{l}'\tau s} + \frac{V}{2} \sum_{\mathbf{l}} \sum_{s s' \tau \tau'} \hat{a}^\dagger_{\mathbf{l}\tau s} \hat{a}^\dagger_{\mathbf{l}\tau' s'} \hat{a}_{\mathbf{l}\tau' s'} \hat{a}_{\mathbf{l}\tau s} + W \sum_{\mathbf{l}} \sum_{\tau s} \hat{a}^\dagger_{\mathbf{l}\tau\uparrow} \hat{a}^\dagger_{\mathbf{l}\tau\downarrow} \hat{a}^\dagger_{\mathbf{l}-\tau s} \hat{a}_{\mathbf{l}-\tau s} \hat{a}_{\mathbf{l}\tau\downarrow} \hat{a}_{\mathbf{l}\tau\uparrow}$$

Only $O(L^3)$ Pauli terms

Adjusted V, W such to the deuteron and ^{3}He binding energies on large lattices

Quantum simulation of ^{3}He on a 2×2×2 lattice



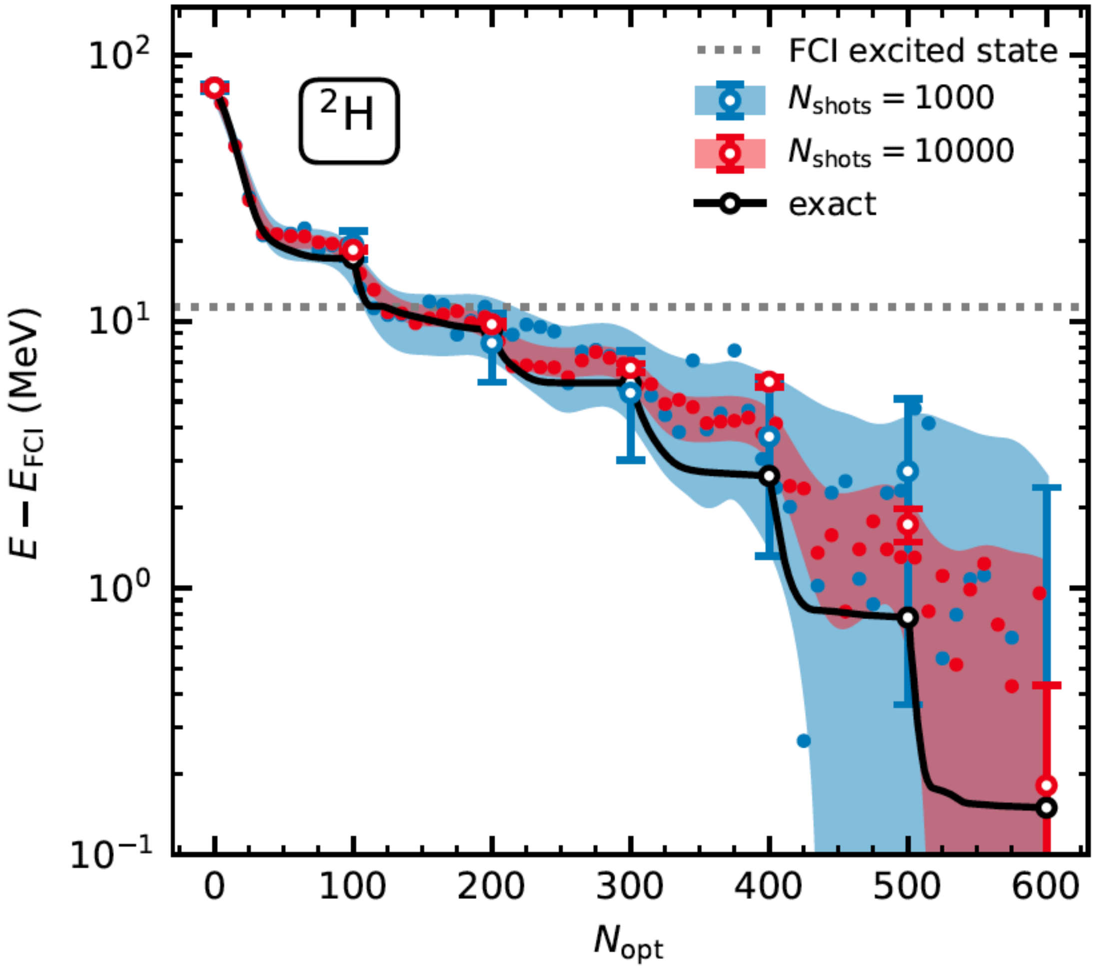
10 operators per epoch
100 optimization steps per epoch
20+ epochs used

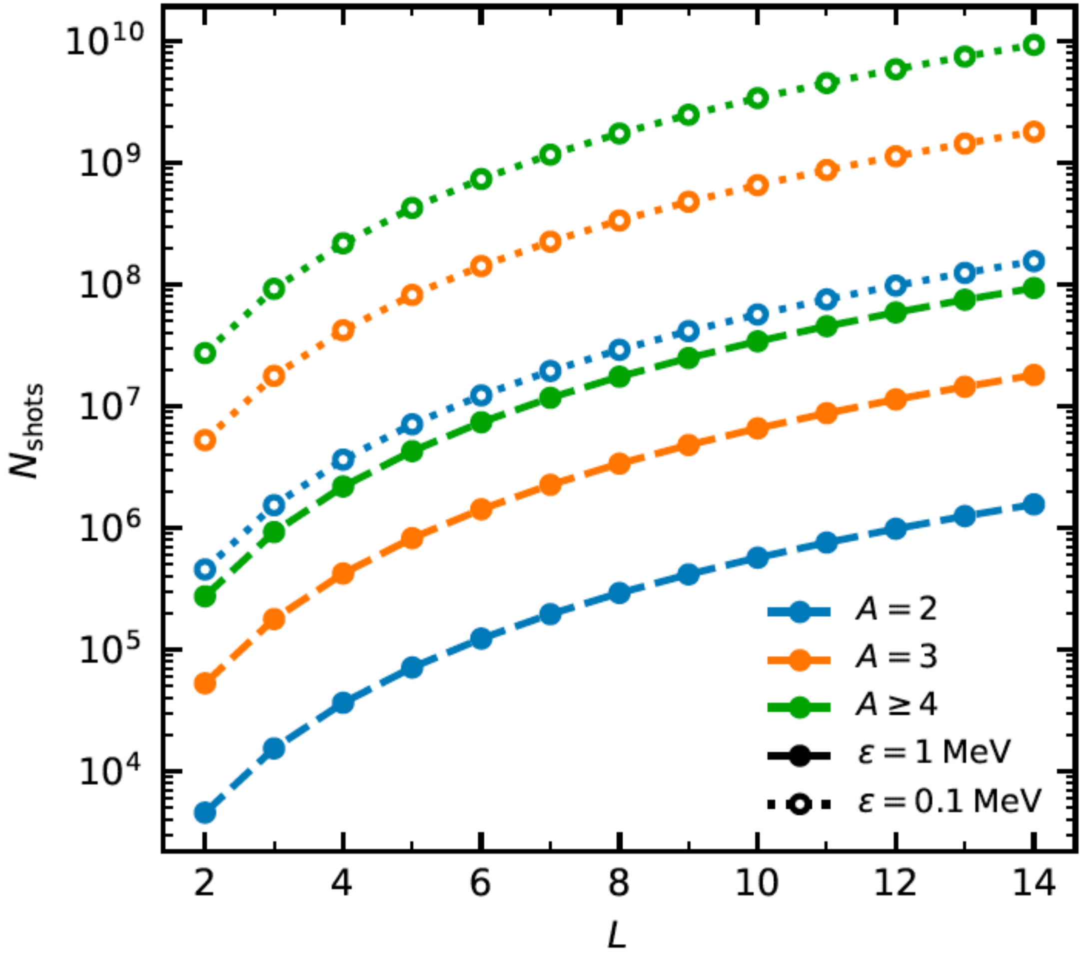
$$|\vec{\theta}\rangle = \prod_{\alpha=1}^{N_e} \exp\left(\sum_{\beta=1}^{N_p} \theta_{\alpha\beta} \hat{A}_{\alpha\beta}\right) |\phi_0\rangle$$

Fidelity:
$$|\langle\vec{\theta}|\psi_{\text{exact}}\rangle|^2$$

Chenyi Gu, Matthias Heinz, Oriel Kiss, TP, Phys. Rev. C 113, 034321 (2026)

Number of measurements "shots" required





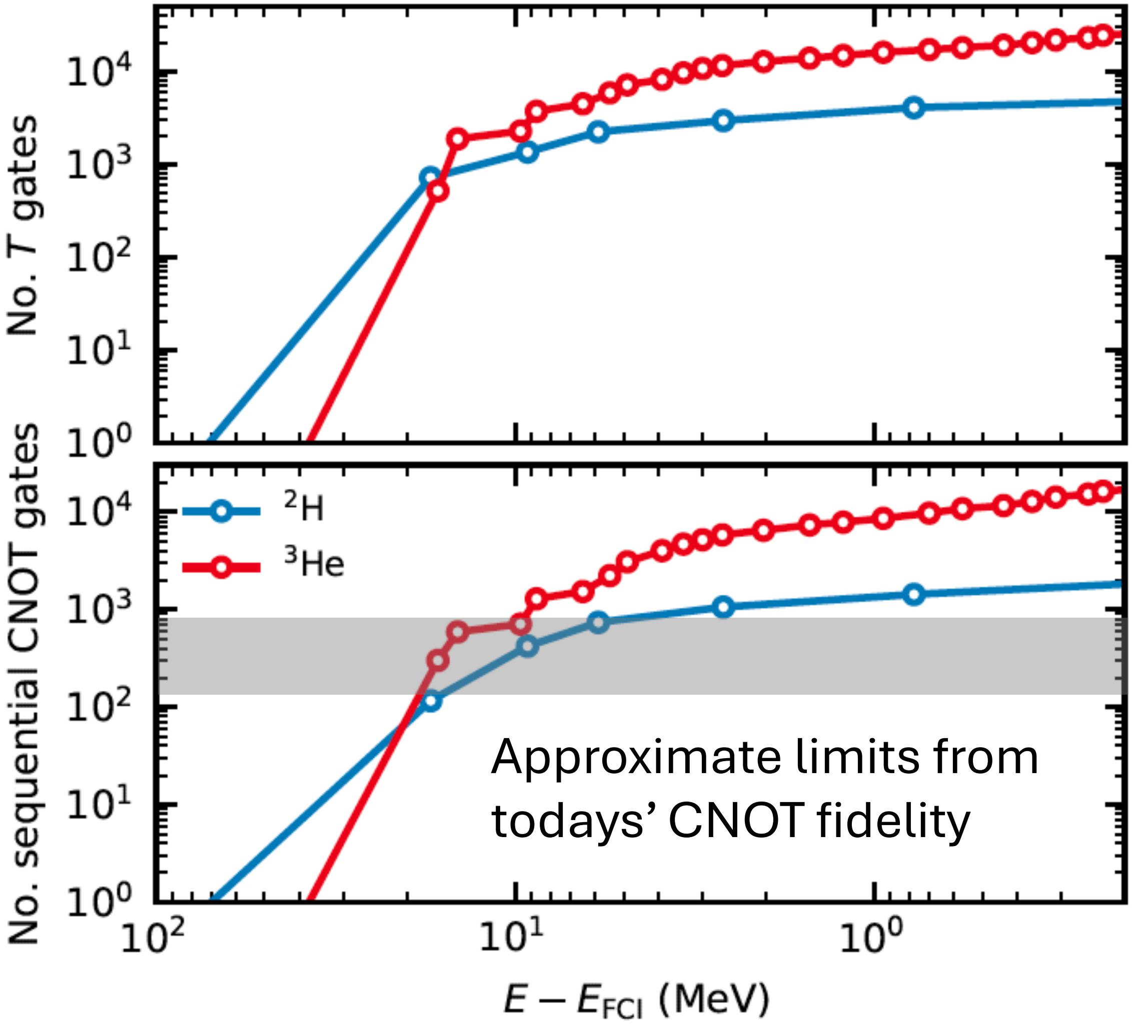
Chenyi Gu, Matthias Heinz, Oriel Kiss, TP, Phys. Rev. C 113, 034321 (2026)

Complexity of the used quantum circuits

Quantum simulations with PennyLane

[V. Bergholm et al., arXiv:1811.04968]

The complexity of circuits is reflected in the number of CNOT and T gates, $T = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\frac{\pi}{4}} \end{pmatrix}$.



Chenyi Gu, Matthias Heinz, Oriel Kiss, TP, Phys. Rev. C 113, 034321 (2026)

Reminders from the lattice

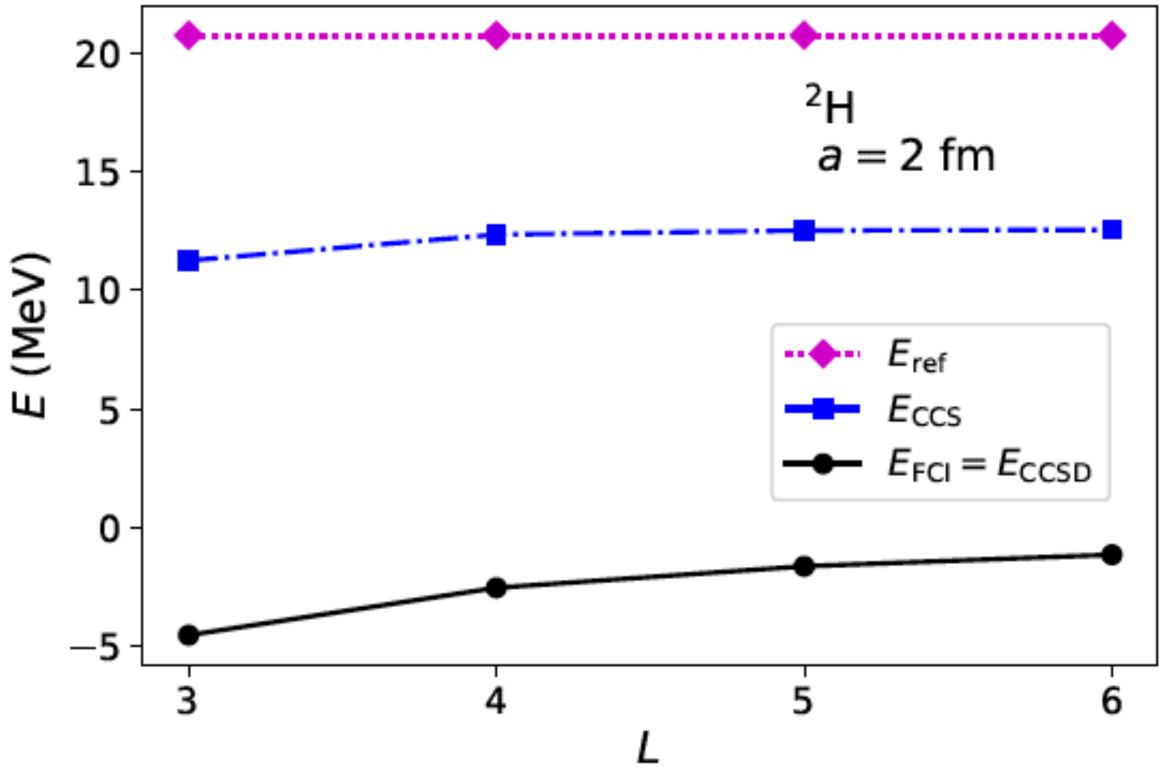
(pionless EFT at leading order)

$$H = T(a) + V_{NN}(v) + W_{NNN}(w)$$

a	v	w	^{4}He	^{3}He	^{2}H
2.5	−9.0	6.0	−29.70	−16.32	−2.48
2.0	−8.0	5.5	−29.45	−14.84	−2.53
1.7	−7.0	4.4	−28.97	−10.82	−2.33

	^{3}He			^{4}He		
a	1.7	2.0	2.5	1.7	2.0	2.5
E_{ref}	10.04	−2.59	−9.95	−2.87	−10.37	−19.91
HF	−4.62	−12.09	−15.18	−26.37	−27.65	−29.06
CCS	−4.09	−11.85	−15.08	−26.82	−28.52	−29.28
CCSD	−4.80	−12.18	−15.22	−26.41	−27.73	−29.11
FCI	−10.82	−14.84	−16.32	−28.97	−29.45	−29.70

Energies converge from below
(tunneling under periodic boundary conditions)
→ Lüscher (1980s); König et al (2010s)

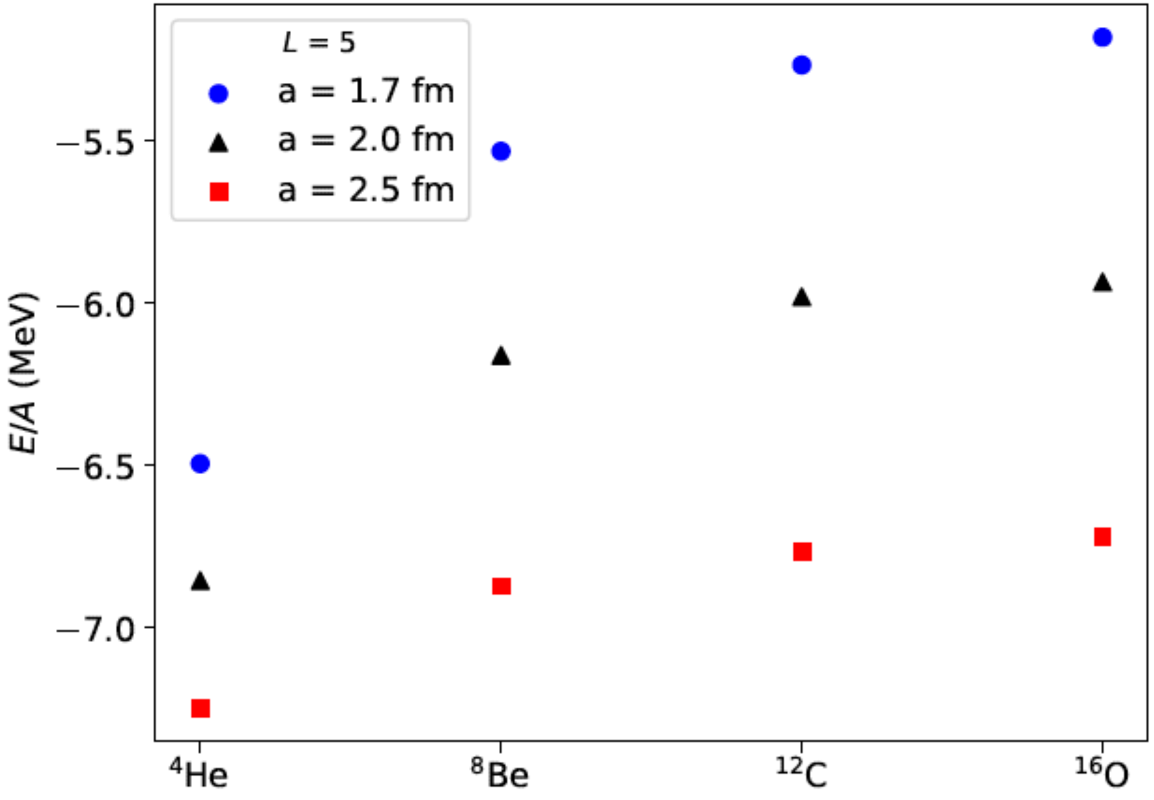


^{3}He: Center of mass important; particularly for small a

^{4}He: HF / CCS yields most of the energy (only kin. energy is off-diagonal)

Easily seen on the lattice

Pionless EFT fails to bind α particles into nuclei [Contessi et al (2017); Bazak et al (2021)]



Normal-ordered two-body approximation of three-nucleon forces becomes exact for zero-range forces.

On-site three-body contact:

$W_{ijk}^{lmn} \neq 0$ and $W_{abc}^{def} \neq 0$

Those cannot contribute to T_1 and T_2 cluster amplitudes, because

$W_{ijk}^{lmn} t_{mn}^{ab} \to \overline{H}_{ijk}^{l}$ and $W_{abc}^{def} t_{ij}^{ab} \to \overline{H}_{c}^{def}$

Rothman, Jonson-Toth, Bonaiti, Hagen, Heinz, TP, Phys. Rev. C 112, L051301 (2025); arXiv:2508.01507

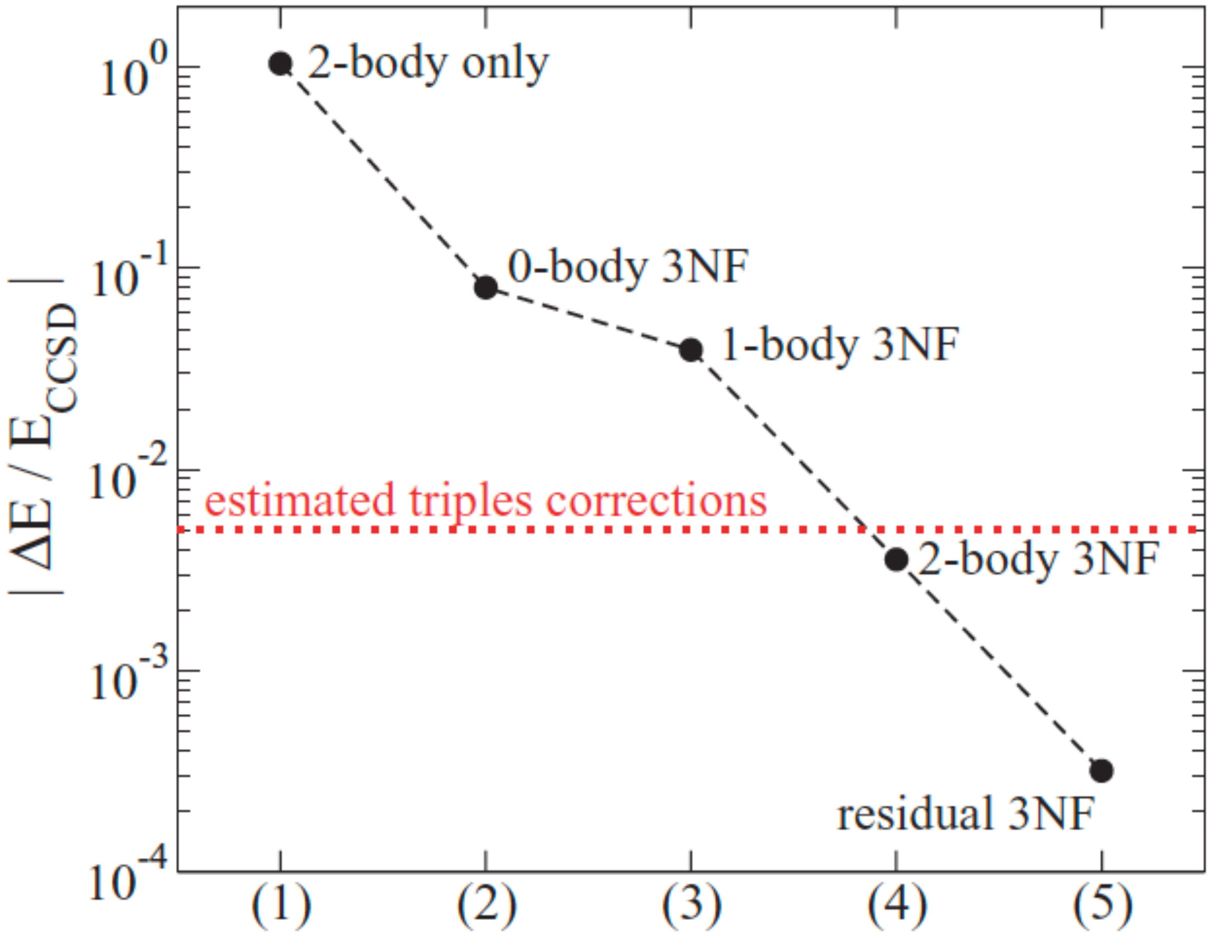
Normal-ordered two-body approximation

$$\hat{H} = E_0 + \sum_{pq} F_q^p \{\hat{a}_p^\dagger \hat{a}_q\} + \frac{1}{4} \sum_{pqrs} V_{rs}^{pq} \{\hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_s \hat{a}_r\} + \frac{1}{36} \sum_{pqrstu} W_{stu}^{pqr} \{\hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_r^\dagger \hat{a}_u \hat{a}_t \hat{a}_s\}.$$

$$E_0 = \sum_i \tau_i^i + \frac{1}{2} \sum_{ij} v_{ij}^{ij} + \frac{1}{6} \sum_{ijk} W_{ijk}^{ijk},$$

$$F_q^p = \tau_q^p + \sum_i v_{iq}^{ip} + \frac{1}{2} \sum_{ij} W_{ijq}^{ijp},$$

$$V_{rs}^{pq} = v_{rs}^{pq} + \sum_i W_{irs}^{ipq}$$



Hagen, TP, Dean, Schwenk, Nogga, Wloch, Piecuch, Phys. Rev. C 76, 034302 (2007); Roth et al (2012); Ripoche, Tichai, Duguet (2020); Miyagi et al (2022);

Nuclear saturation

Really old view:

- hard-core in nucleon-nucleon interaction, i.e. interaction is attractive at low momenta and repulsive at high

EFT/SRG view:

- Repulsive three-nucleon force yield saturation. → Hebeler, Bogner, Furnstahl, Nogga, Schwenk, Phys. Rev. C 83, 031301(R) (2011)

NLEFT:

🤔 Attractive two body alone yields accurate nuclear radii and binding energies →Elhatisari et al., Phys. Rev. Lett. 119, 222505 (2017)

🤔 Attractive two body + attractive three-body yield accurate nuclear radii and binding energies → Bing-Nan Lu et al., Phys. Lett. B 797, 134863 (2019)

Lattice Hamiltonian

Elhatisari, Epelbaum, Krebs, Lähde, Lee, Li, Lu, Meißner, Rupak, Phys. Rev. Lett. 119, 222505 (2017); arXiv:1702.05177

$$H = T + V_{\mathrm{OPE}} + V_0$$

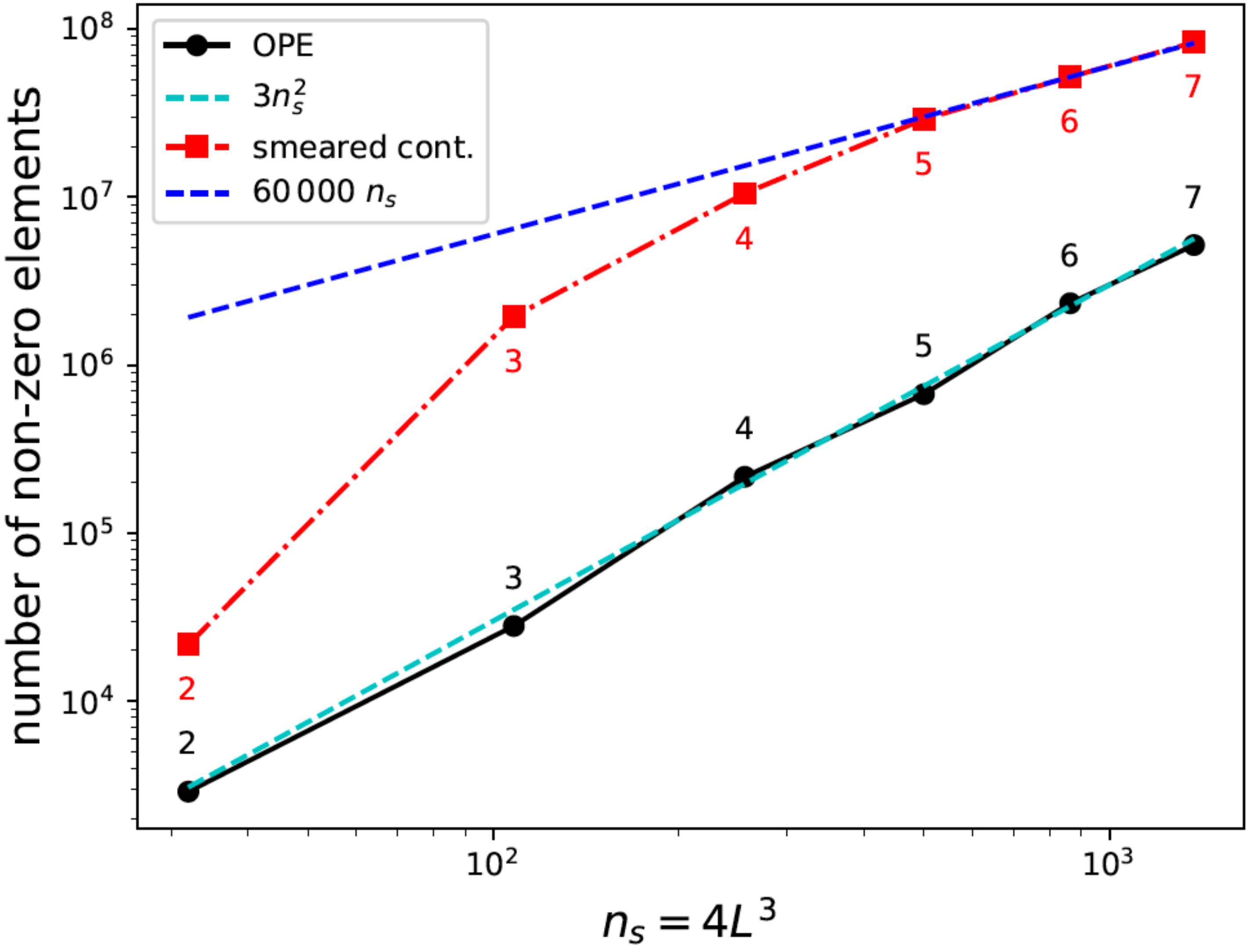
$$V_0 = \frac{c_0}{2} \sum_{n} : \widetilde{\rho}(\mathbf{n})^2 :$$

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

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

Nonlocal and local smearing are relatively small: $s_{NL} = 0.08$, $s_L = 0.08$, $c_0 = -18.5$ MeV

Number of nonzero matrix elements



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

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Energies in MeV

Nucleus	NLEFT	Exp.
^{4}He	−25.4	−28.3
^{8}Be	−51.9	−56.5
^{12}C	−83.8	−92.2
^{16}O	−128.2	−127.6

Lattice Hamiltonian

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`NuLattice` Hartree Fock

Energies in MeV

Nucleus	$L=5$	$L=6$	NLEFT	Exp.
^{4}He	-20.054	-19.797	-25.4	-28.3
^{8}Be	-63.31	-63.13	-51.9	-56.5
^{12}C	-137.75	-137.22	-83.8	-92.2
^{16}O	-214.07	-213.300	-128.2	-127.6

Rothman, Hagen, Heinz, TP, in prep.

This Hamiltonian truly yields too much binding

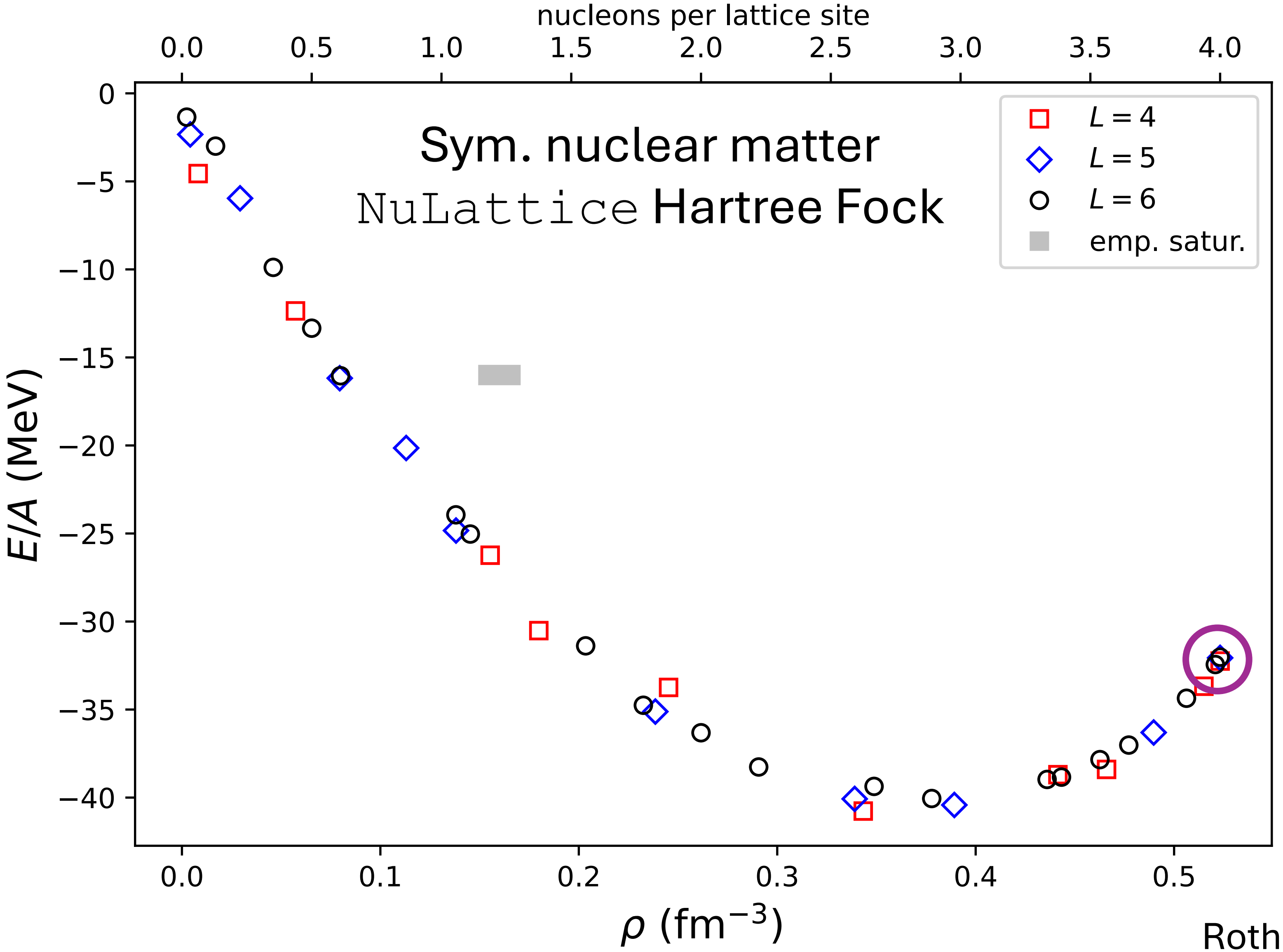
Auxiliary-field Monte Carlo with temporal time step $\tau = \frac{1}{150\text{ MeV}} = 1.32\text{fm}$ inaccurate

Computing nuclear/neutron matter with `NuLattice`

1. Diagonalize kinetic energy
   - Yields translationally invariant eigenstates; good for homogeneous matter
2. Closed shells for $A = 4, 28, 76, 108, 132, \ldots$
3. Make density matrix from eigenstates at magic numbers
4. Compute energy expectation values
   - Can be done very fast; for $:\tilde{\rho}(\vec{n})^k:$ we only need a single lattice site $\vec{n}$ because $\langle \sum_{\vec{n}} :\tilde{\rho}(\vec{n})^k: \rangle = L^3 \langle :\tilde{\rho}(\vec{n}_0)^k: \rangle$ for translationally invariant densities

Lattice Hamiltonian

Elhatisari, Epelbaum, Krebs, Lähde, Lee, Li, Lu, Meißner, Rupak, Phys. Rev. Lett. 119, 222505 (2017); arXiv:1702.05177



Check: Analytical result for full lattice

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

$$\frac{\langle T\rangle}{A} = \frac{49}{12ma^2}$$

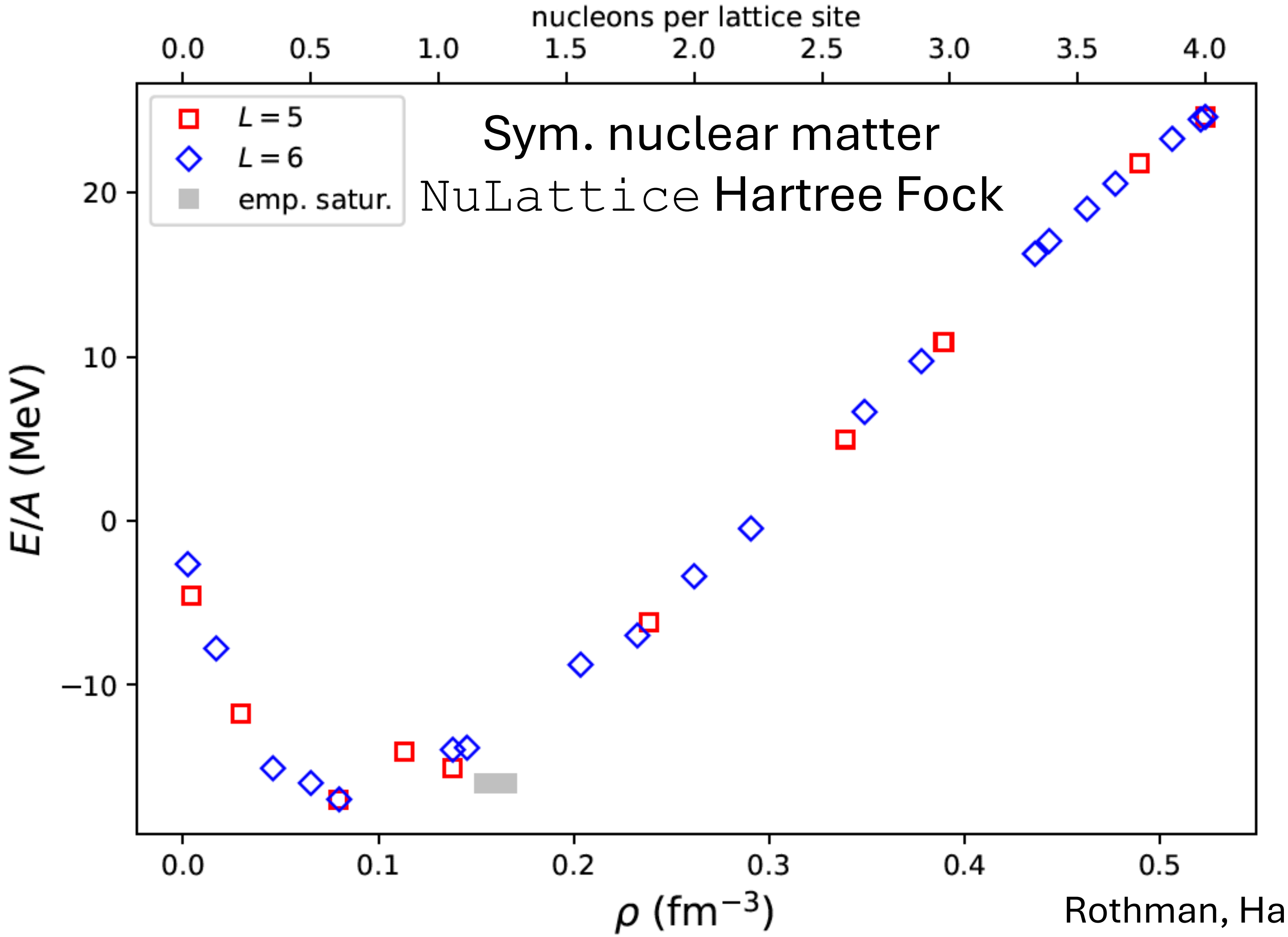
$$\frac{\langle V_0\rangle}{c_0 A} = \left[\frac{g-1}{2} + 6gs_L + 3(6g-1)s_L^2\right]\left(1+6s_{NL}^2\right)^2 - 3s_L s_{NL}^2\left(8+17s_L s_{NL}^2\right)$$

Note: One-pion exchange negligible

Rothman, Hagen, Heinz, TP, in prep.

… but the Hamiltonian does saturate (albeit at high densities)

Quick refit: $c_0 = -1.8\ \mathrm{MeV} \to -1.3\ \mathrm{MeV}$, $s_{NL} = 0.08 \to 0.4$, $s_L = 0.08$ unchanged



Saturation from kinetic energy; at filled lattice

$$\left\langle \frac{T}{A} \right\rangle = 43.49\ \mathrm{MeV}$$

Improved saturation point from larger non-local smearing.

Rothman, Hagen, Heinz, TP, in prep.

Lattice Hamiltonian with attractive 3NF

Bing-Nan Lu et al., Phys. Lett. B 797, 134863 (2019); arXiv:1812.10928

$$H = T + V_0 + W$$

$$V_0 = \frac{c_0}{2} \sum_{n} : \tilde{\rho}(\mathbf{n})^2 :$$

$$W \equiv \frac{c_3}{3!} \sum_{\mathbf{n}} : \tilde{\rho}(\mathbf{n})^3 :$$

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

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

Changes compared to previous NLEFT works

- Strong non-local smearing $s_{NL} = 0.5$, $s_L = 0.061$
- Lattice spacing $a = 1.97\ \text{fm} \rightarrow 1.32\ \text{fm}$
- Temporal spacing $\tau = \frac{1}{150\text{MeV}} \rightarrow \frac{1}{1000\text{MeV}}$

Lattice Hamiltonian with attractive 3NF

Bing-Nan Lu et al., Phys. Lett. B 797, 134863 (2019); arXiv:1812.10928

Check: Neutron matter

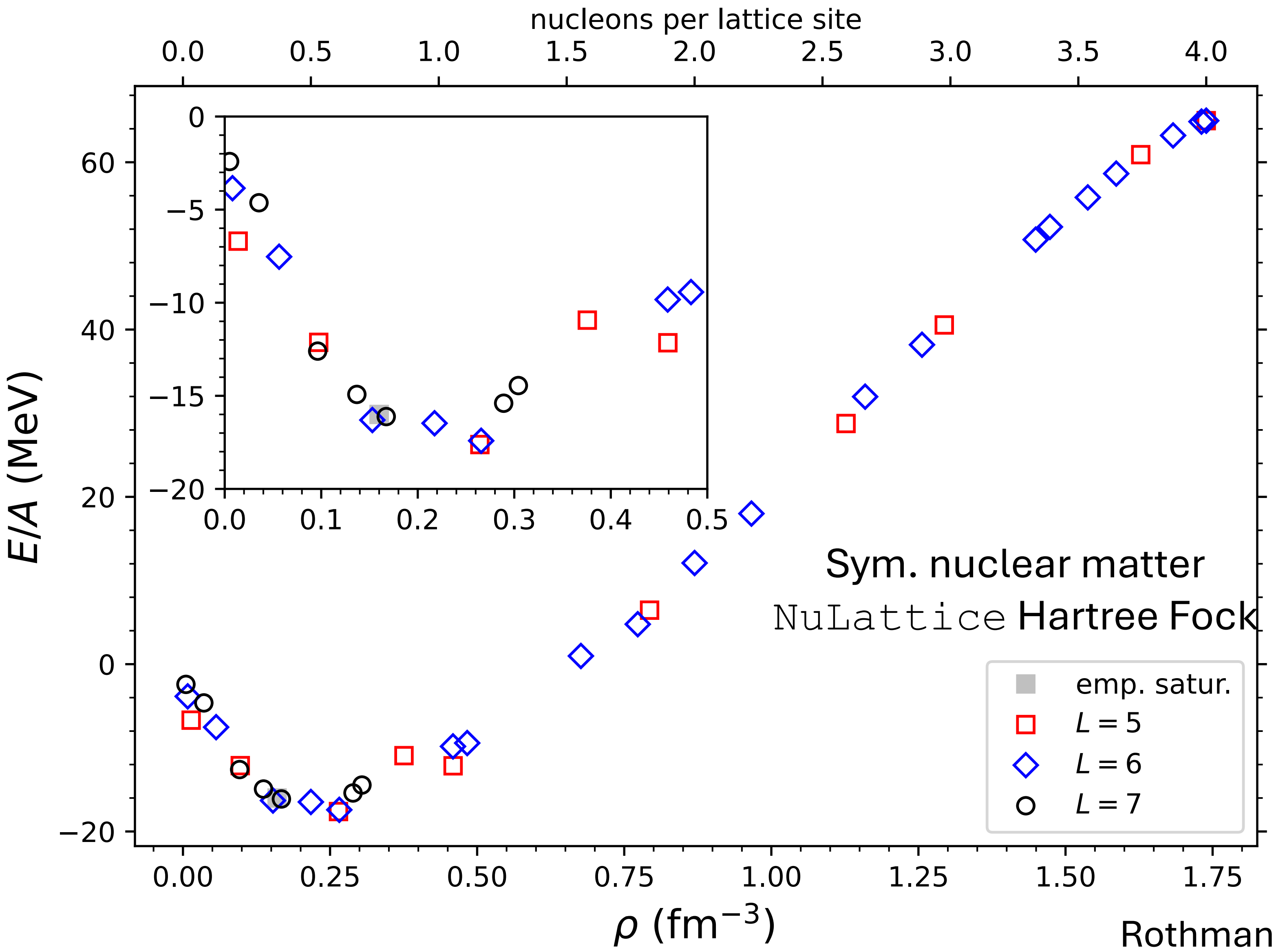
`NuLattice` Hartree Fock

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

Apparently only little correlation energy

Lattice Hamiltonian with attractive 3NF

Bing-Nan Lu et al., Phys. Lett. B 797, 134863 (2019); arXiv:1812.10928



Plausible saturation point

Analytical result for full lattice: ✅

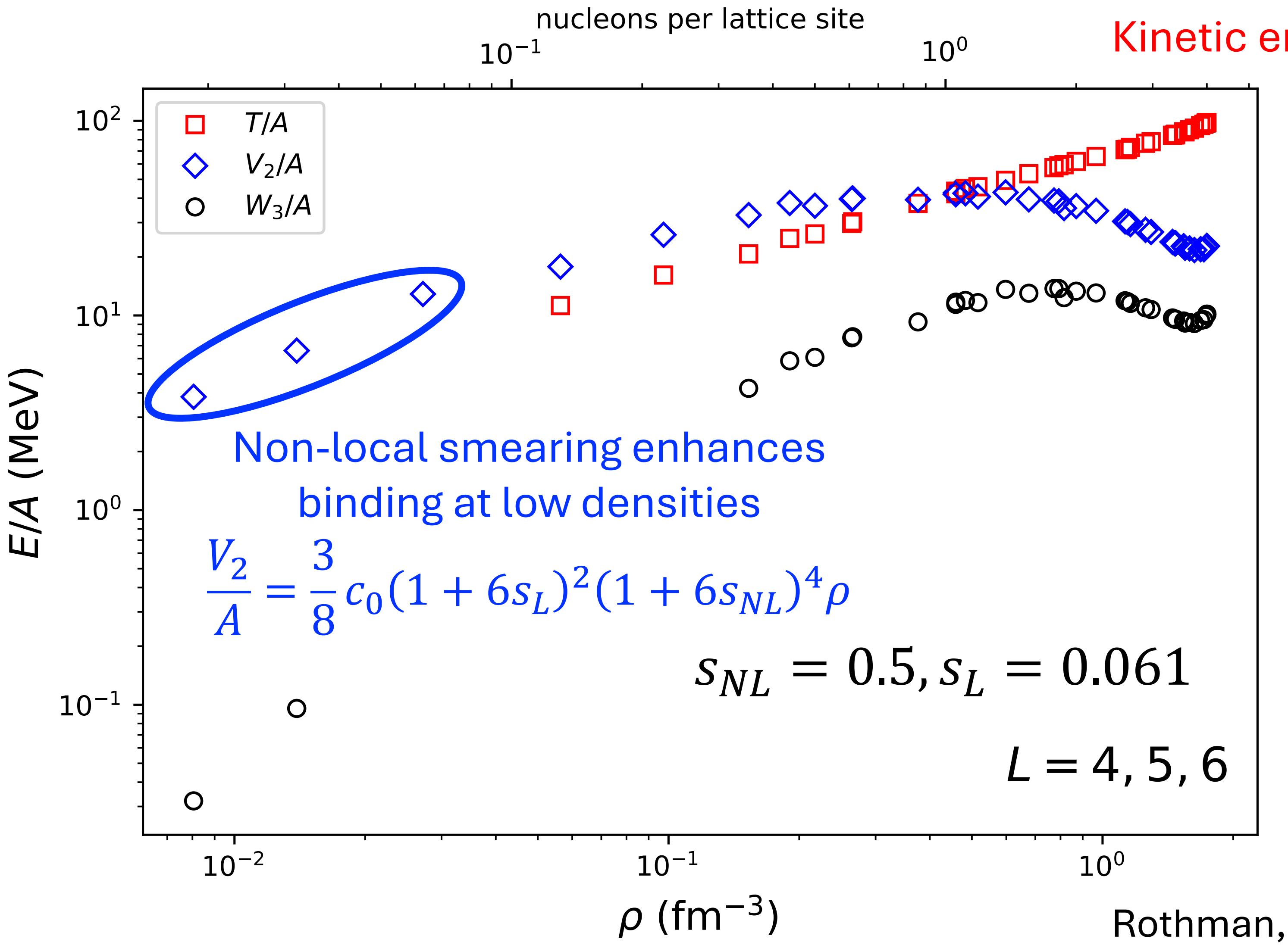
$$
\begin{aligned}
\frac{\langle W\rangle}{c_3 A} &= \left(1+6s_{NL}^2\right)^3 \left\{\tfrac{1}{6}(g-1)(g-2) + 3g(g-1)s_L \right.\\
&\left. + 3g(6g-1)s_L^2 + 2\left[1+9g(2g-1)\right] s_L^3 \right\}\\
&- \left(1+6s_{NL}^2\right) \left[24(g-1)s_L s_{NL}^2 + 24(6g-1)s_L^2 s_{NL}^2 \right.\\
&\left. + 51 g s_L^2 s_{NL}^4 + 102(3g-1)s_L^3 s_{NL}^4\right]\\
&+ 8 s_L^2 s_{NL}^4 \left(27 + 28 s_L s_{NL}\right) \ .
\end{aligned}
$$

Rothman, Hagen, Heinz, TP, in prep.

Lattice Hamiltonian with attractive 3NF

Bing-Nan Lu et al., Phys. Lett. B 797, 134863 (2019); arXiv:1812.10928

Kinetic energy $\frac{T}{A} \propto \rho^{2/3}$



Saturation comes from the kinetic energy; potential energies are negative at all densities

At high densities, crowding reduces potential energies

The non-local smearing increases binding at low densities.

Rothman, Hagen, Heinz, TP, in prep.

Lattice Hamiltonian with attractive 3NF

Bing-Nan Lu et al., Phys. Lett. B 797, 134863 (2019); arXiv:1812.10928

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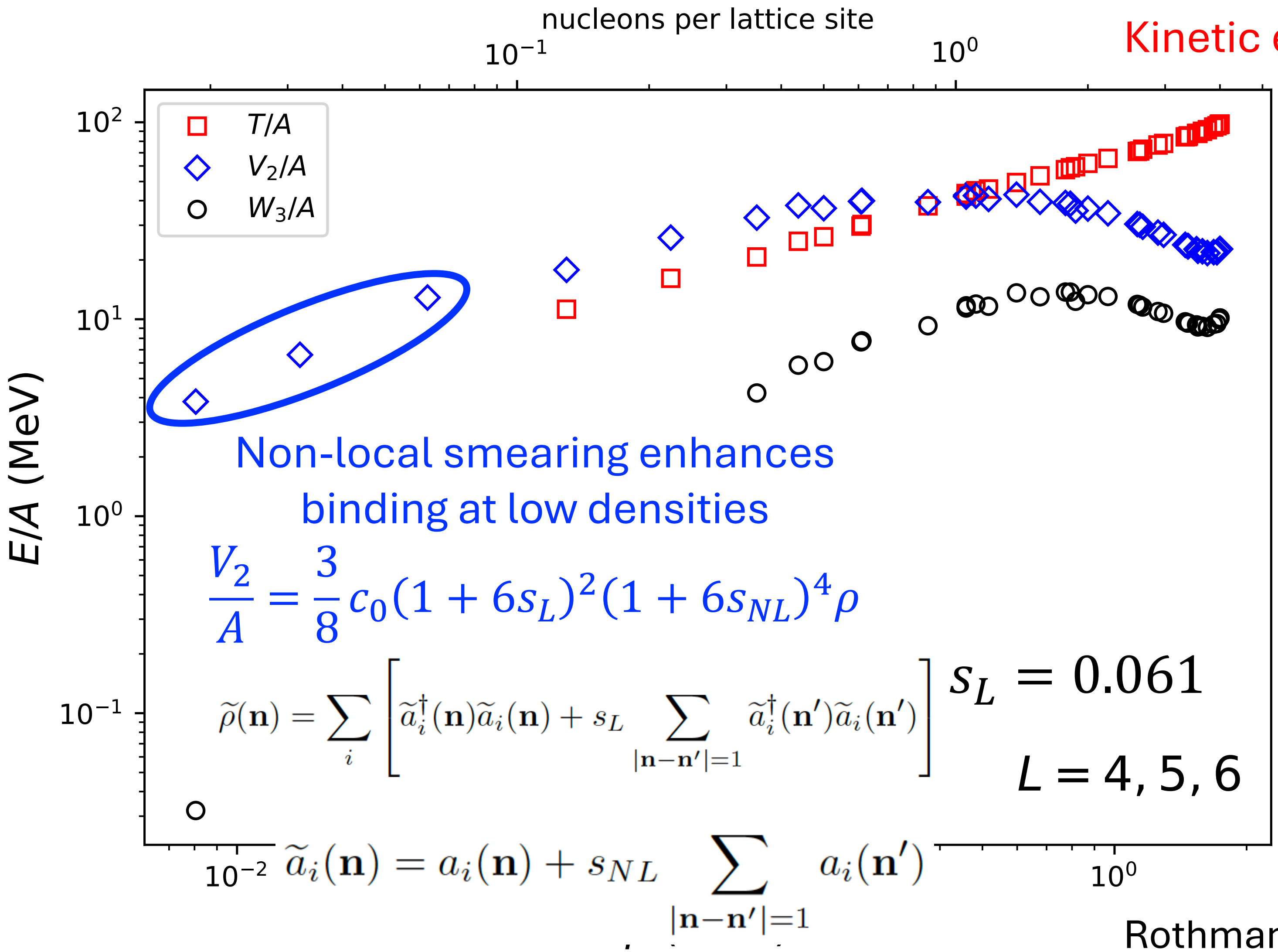

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Rothman, Hagen, Heinz, TP, in prep.

Stability of matter (atoms)

Dyson, Lieb, Teller, Thirring, … [Lieb, Rev. Mod. Phys. 48, 553 (1976)]

- Pauli principle
- Kinetic energy dominates over potential from Coulomb

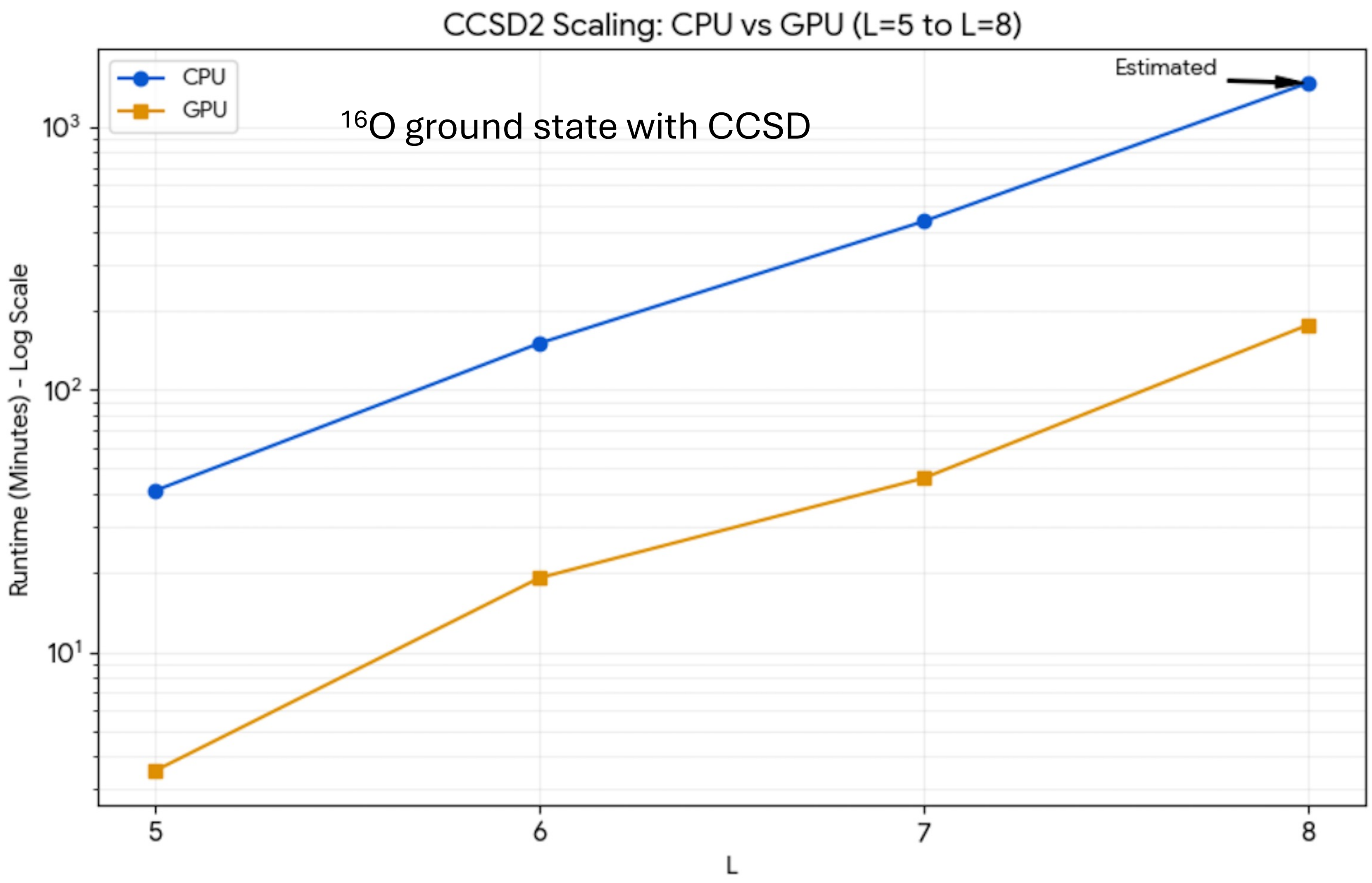
On the lattice, the lattice spacing a plays a dual role:

- Cutoff π/a
- Hard-sphere radius

→ Dominance of kinetic energy

NuLattice is going HPC

Vivek Booshan is porting NuLattice to Frontier via JAX



Scaling is roughly as $\propto L^9$ in our implementation

Summary

Computations of atomic nuclei on lattices

- Quantum simulation of ^3He via adaptive VQE using 2 & 3-body forces
- Normal-ordered 2-body approximation is exact for zero-ranged forces
- Implemented more sophisticated interactions, neutron / nuclear matter EOS
- Pointed out errors in auxiliary-field Monte Carlo simulations
- Saturation on lattices due to dominance of kinetic energy and crowding
- Physical saturation point reached with large non-local smearing
- Questions regarding ab initio alpha clustering are possibly still open

Thank you