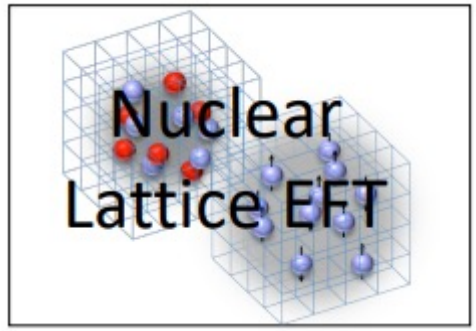
Carbon and Oxygen isotope chains in Nuclear Lattice Effective Field Theory

Young-Ho Song (IRIS, IBS)
NLEFT collaboration

Lattice QCD workshop on hadron and quark matter
(LQCDW1) 2024.01.04-06, Sejong University, Seoul
https://indico.cern.ch/event/1356314/

ibs 기초과학연구원
Institute for Basic Science

Nuclear Lattice Effective Field Theory Collaboration



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- Ulf-G. Meißner (Bonn/Juelich)
- Gautam Rupak(Mississippi State)
- Shihang Shen (Juelich)
- Gianluca Stellin(CEA Paris-Saclay)
- And More…

Effective field theories and energy scales

Lattice quantum chromodynamics

Chiral effective field theory

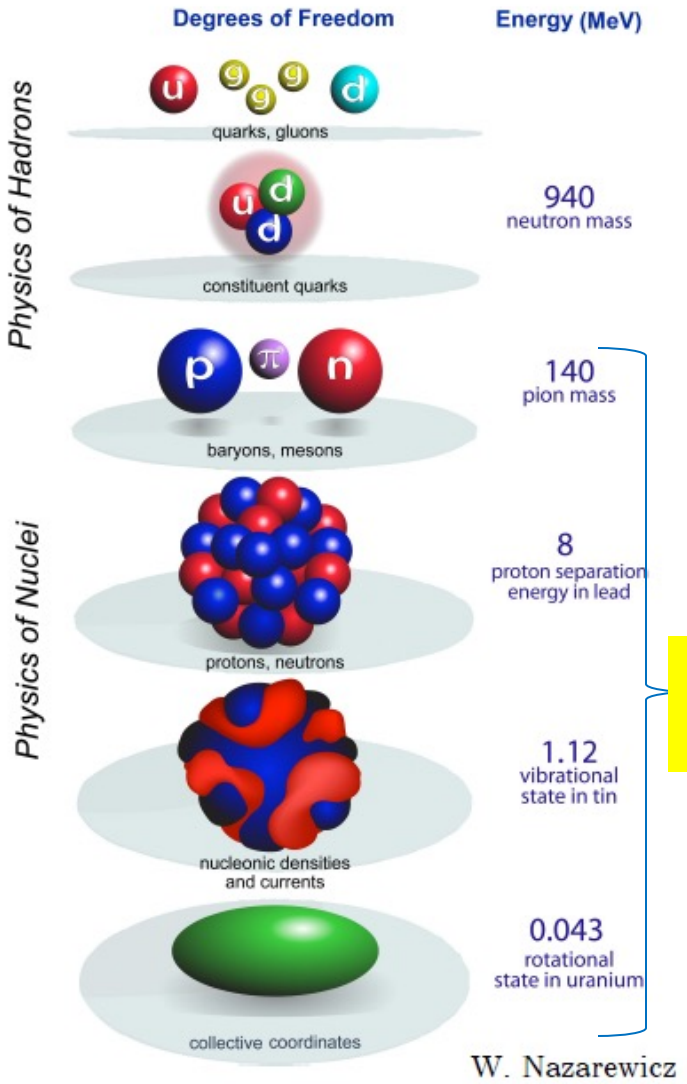
Microscopic A-body methods

Configuration interactions

Density functional methods

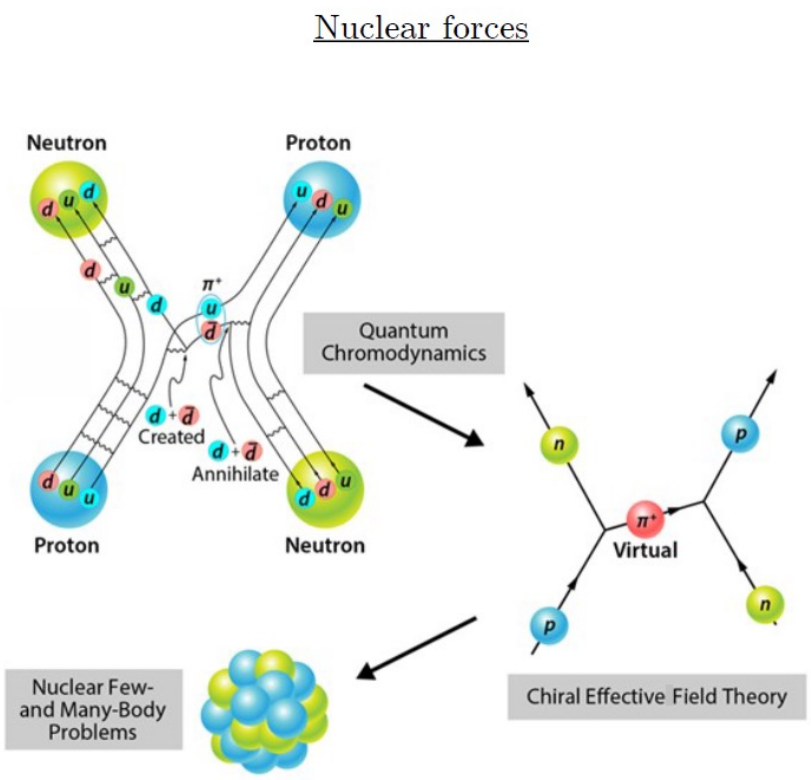
Mean field methods

Effective theory of collective modes



W. Nazarewicz

Ab-initio method



- *ab-initio* Nuclear Physics
  - (1) nucleon degrees of freedom
  - (2) nucleon-nucleon interaction

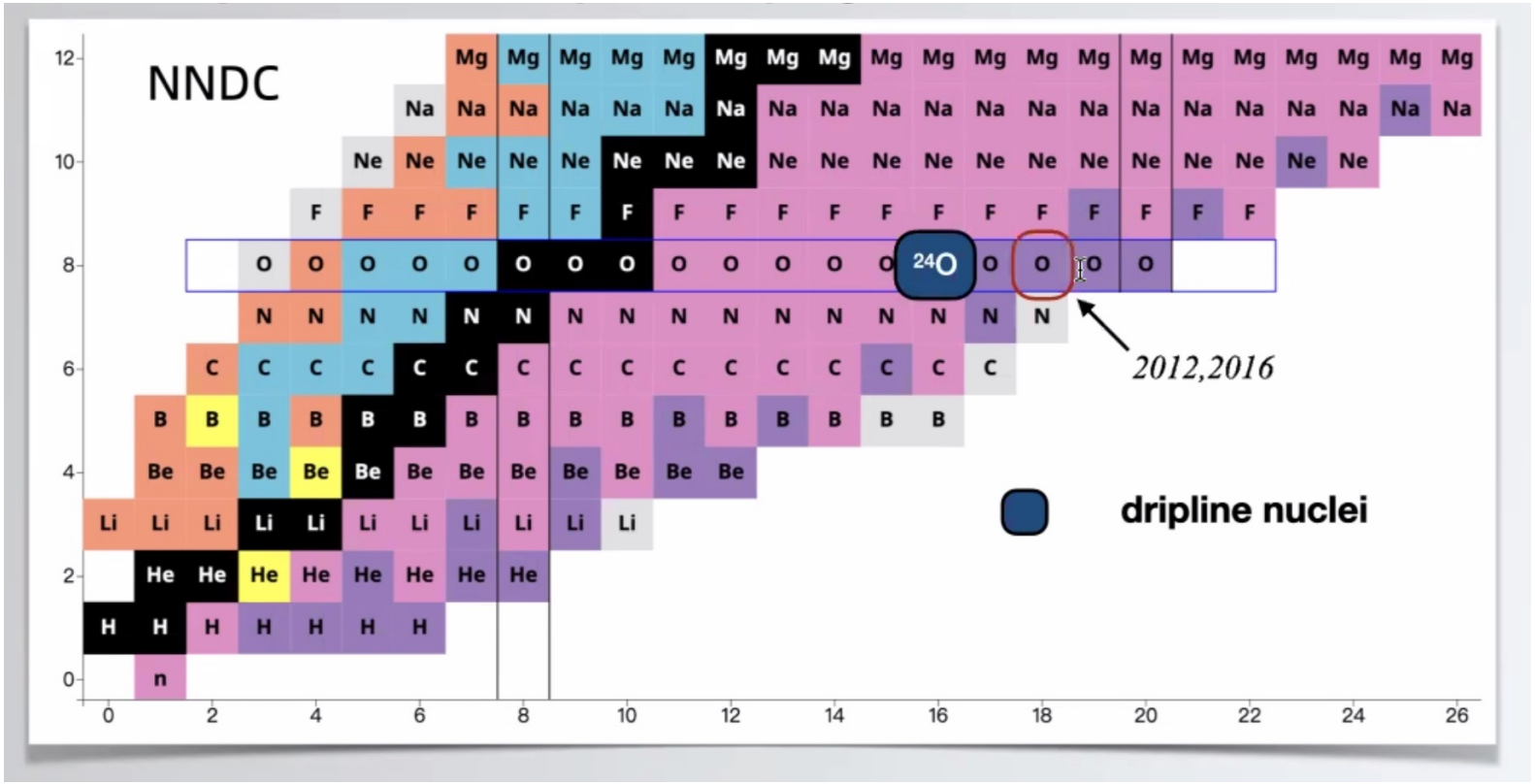
Goal: predict wide range(structure, reaction, nuclear matter) of nuclear phenomena (without parameter fitting, model assumption) from nuclear interaction (for 2-body,3-body, many-body, based on QCD)

Direct connection between
Nuclear Force ↔ Nuclear Phenomena

Ab initio Quantum many-body

- (ab initio) Nuclear physics is challenging.
  - Non-perturbative many-body problem
  - Exact Nuclear Force is not known.
- Non-perturbative many body problem
  - Ab-initio nuclear many body methods
    - Greens function Monte Carlo(GFMC)
    - No-core shell model(NCSM)
    - Coupled Cluster (CC)
    - IM-SRG, VS-SRG
    - Nuclear Lattice Effective Field Theory(NLEFT)
    - And more
  - With recent progress in ab-initio methods and chiral EFT
    - Binding energies for wide range of nuclei
    - Some reaction calculation for light nuclei.

Dripline

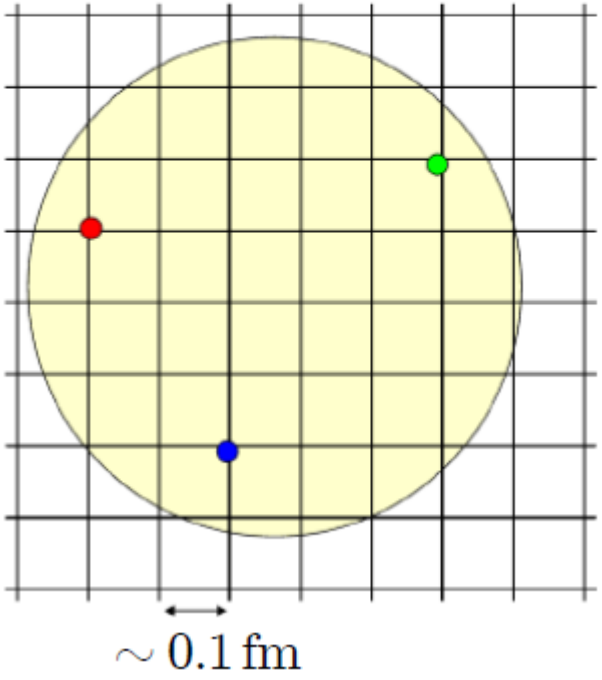


Can we explain the dripline of Carbon, Oxygen isotopes in NLEFT?
Sensitive to nuclear force ? (Role of 3-body force?)

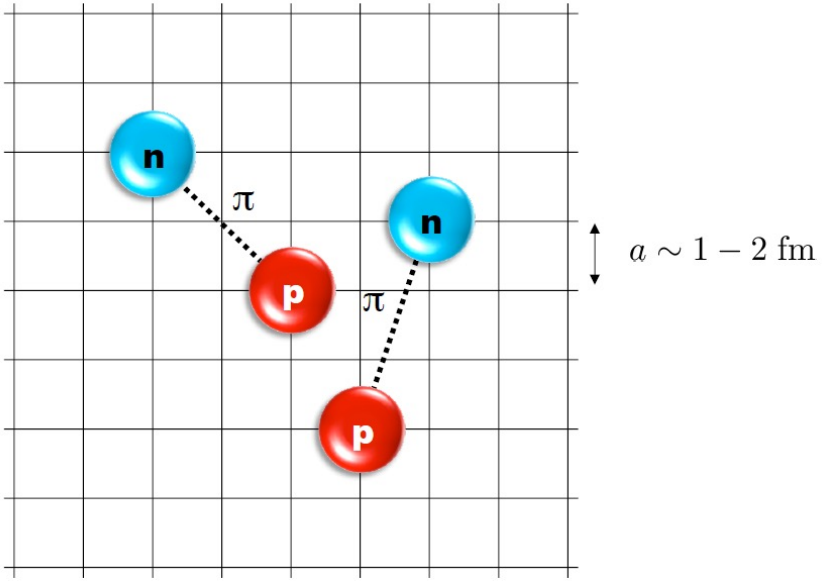
Nuclear Lattice Effective Field Theory

- One of ab initio method for many fermion system

Nucleon in LQCD



Nucleons as point particles on the lattice



Path integral

Correlator function for A Nucleons $\quad Z_A(t) = \langle \Psi_A | \exp(-tH) | \Psi_A \rangle$

Slater Determinants for A free Nucleons

Ground state energy by time derivative of the correlator

$$E(t) = -\frac{d}{dt} \ln Z_A(t)$$

At large time only ground states survive

$$E_A^0 = \lim_{t \to \infty} E_A(t)$$

$$|\Psi_A\rangle = \sum_n c_n |n\rangle_A,$$

$$Z_A(t) = \langle \Psi_A | e^{-tH} | \Psi_A \rangle = \sum_n c_n e^{-tE_n}$$

Transfer matrix

Transfer matrix operator formalism $\hat{M} =: \exp(-H_{\mathrm{LO}}\, a_t) :$

$$Z(L_t) = \langle \psi_I \,|\hat{M}(L_t-1)\,\hat{M}(L_t-2)\,\ldots\hat{M}(1)\,\hat{M}(0)\,|\,\psi_I\rangle$$

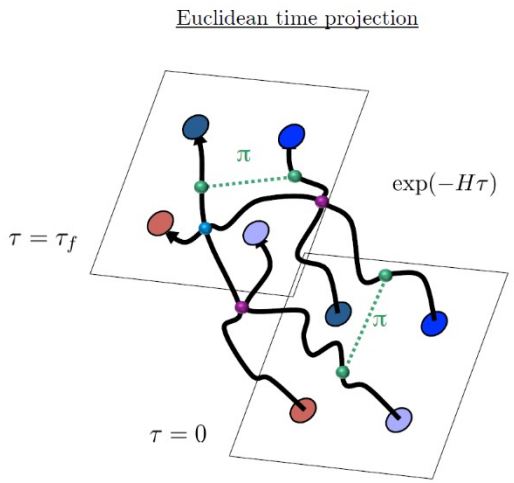
$$\lim_{L_t\to\infty} \frac{Z(L_t+1)}{Z(L_t)} = e^{-E_0\, a_t}$$

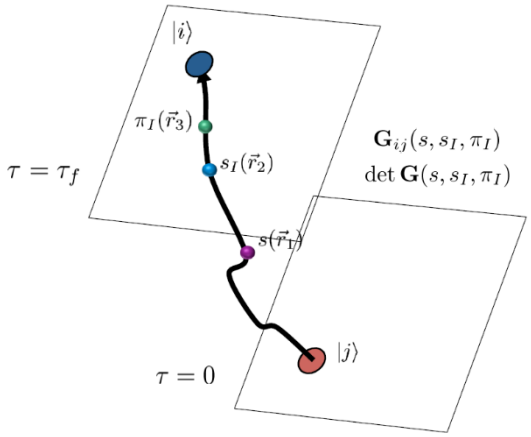
$$\lim_{L_t\to\infty} \frac{\langle\psi_I|\,\hat{M}^{L_t/2}\,H_{\mathrm{LO}}\,\hat{M}^{L_t/2}\,|\psi_I\rangle}{\langle\psi_I|\,\hat{M}^{L_t}\,|\psi_I\rangle} = E_0$$

Auxiliary Field Monte Carlo

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

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





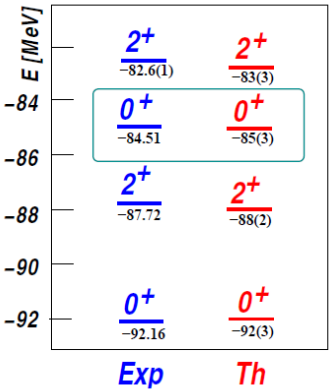
Interacting nucleons
→ Nucleons interacts with auxiliary fields
(no direct interaction betw een nucleons)

computing fermion Correlator amplitude
→ Integration over auxiliary fields
→ M.C. integral (sampling auxiliary field)

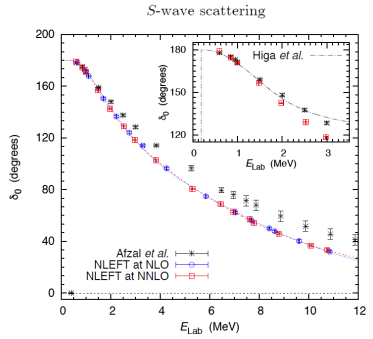
Applications of NLEFT

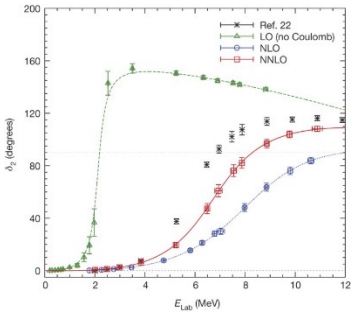
- Has been successfully applied to
  - Nuclear matter, Cold atom, dilute fermion system
  - Finite nuclei (A<=50)
  - First ab-initio calculation of Hoyle state
  - Cluster structure of ^{12}C and ^{16}O
  - NN scattering, N-D scattering
  - Alpha-alpha scattering
  - radiative capture, fusion
  - Etc.

The first ab-initio calculation of Hoyle state



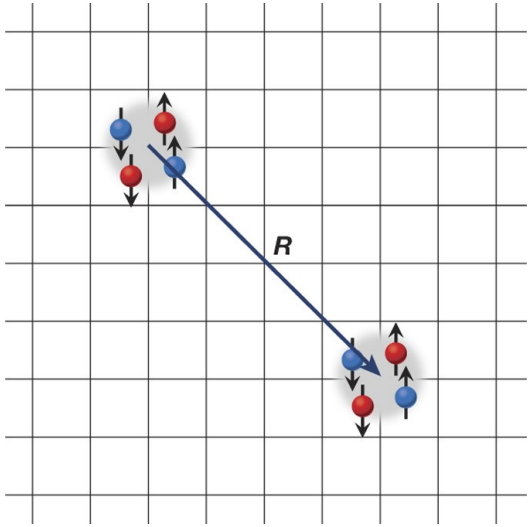
Epelbaum, Krebs, Lähde, Lee, Meißner: Phys. Rev. Lett. 109, 252501 (2012)





Ab initio alpha-alpha scattering
(Nature 528, 111-114(2015))

Adiabatic projection method



Construction of effective Hamiltonian between two clusters

$$|\vec{R}\rangle = \sum_{\vec{r}} |\vec{r}+\vec{R}\rangle_1 \otimes |\vec{r}\rangle_2$$

$$|\vec{R}\rangle_\tau = \exp(-H\tau)|\vec{R}\rangle$$

$$[H_\tau]_{\vec{R},\vec{R}'} = {}_\tau\langle\vec{R}|H|\vec{R}'\rangle_\tau \qquad [N_\tau]_{\vec{R},\vec{R}'} = {}_\tau\langle\vec{R}|\vec{R}'\rangle_\tau$$

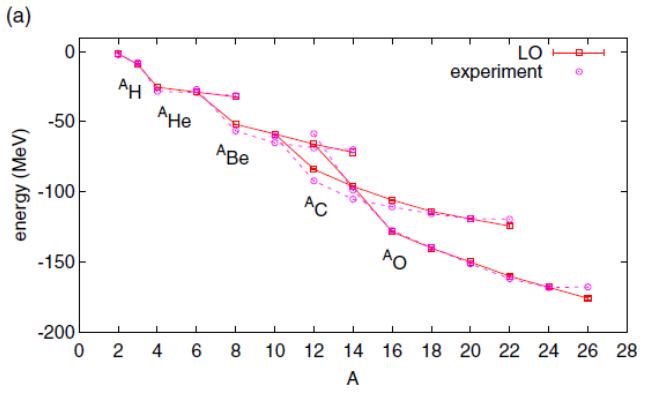
The adiabatic Hamiltonian is defined by the matrix product

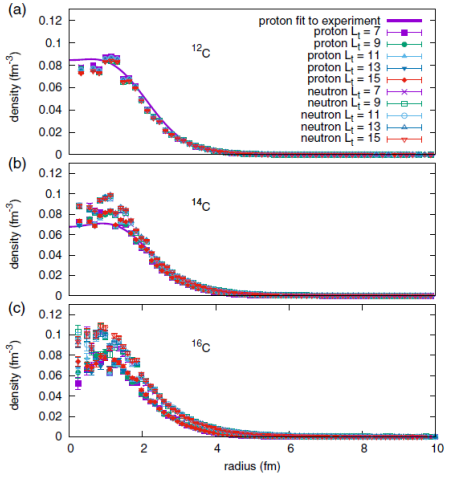
$$[H^a_\tau]_{\vec{R},\vec{R}'} = \left[N_\tau^{-1/2} H_\tau N_\tau^{-1/2}\right]_{\vec{R},\vec{R}'}$$

PRL 119, 222505 (2017) PHYSICAL REVIEW LETTERS week ending 1 DECEMBER 2017

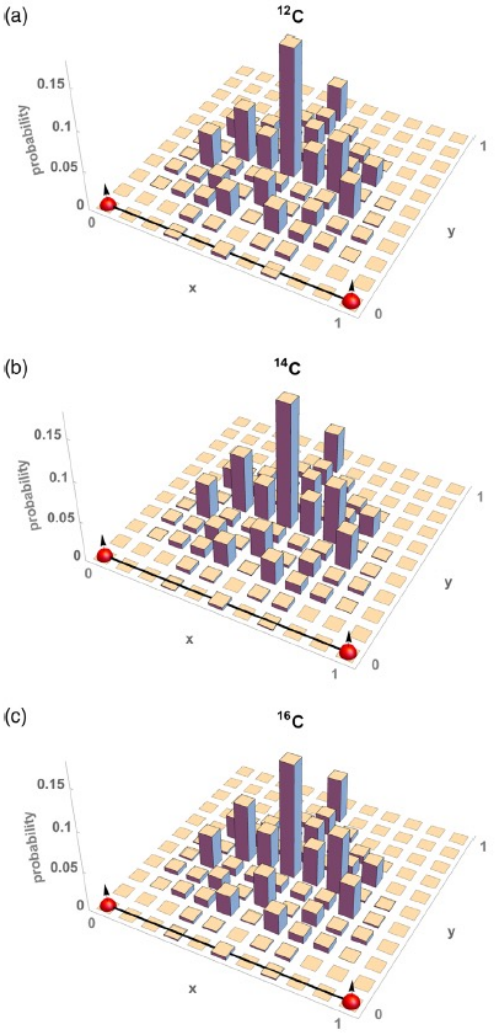
Ab initio Calculations of the Isotopic Dependence of Nuclear Clustering

Serdar Elhatisari,[1,2] Evgeny Epelbaum,[3,4] Hermann Krebs,[3,4] Timo A. Lähde,[5] Dean Lee,[6,7,4] Ning Li,[5] Bing-nan Lu,[5] Ulf-G. Meißner,[1,5,8] and Gautam Rupak[9]



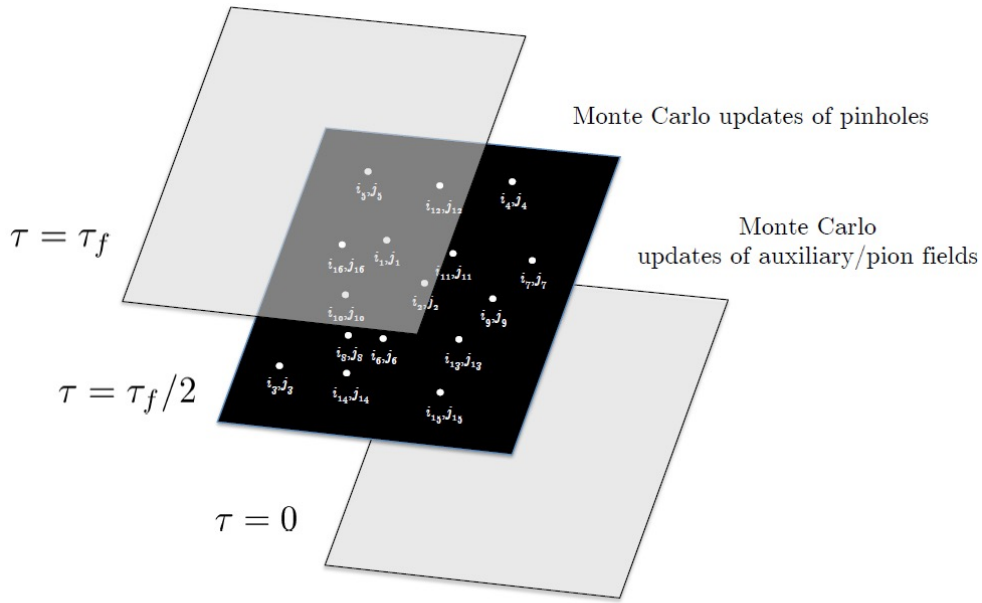


Pinhole algorithm

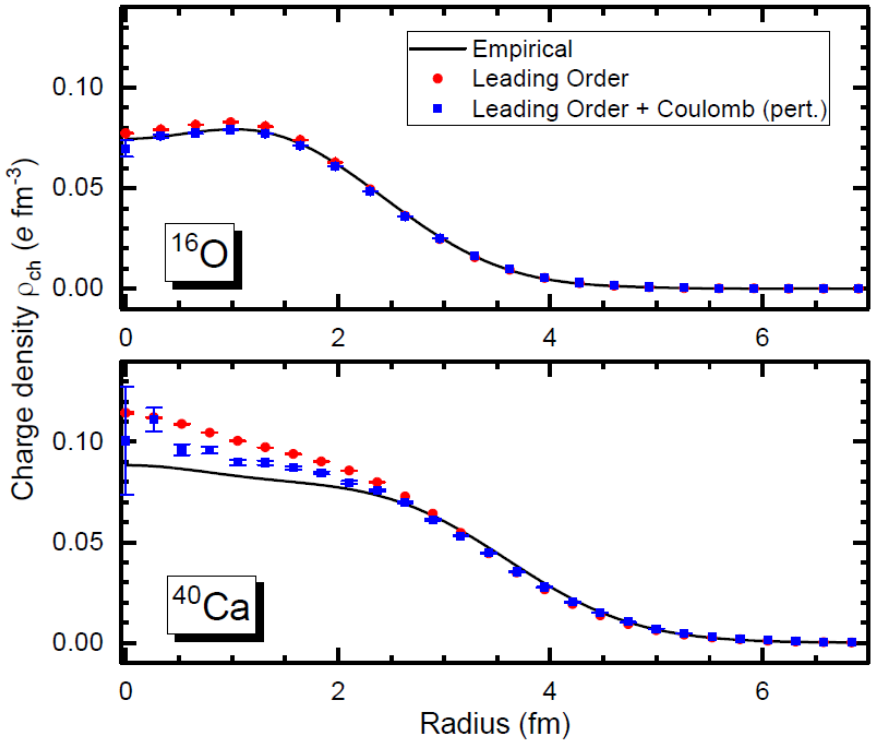


$$H_{\rm B} = H_{\rm free} + V_0 + V_{\rm OPE},$$

Pinhole Algorithm



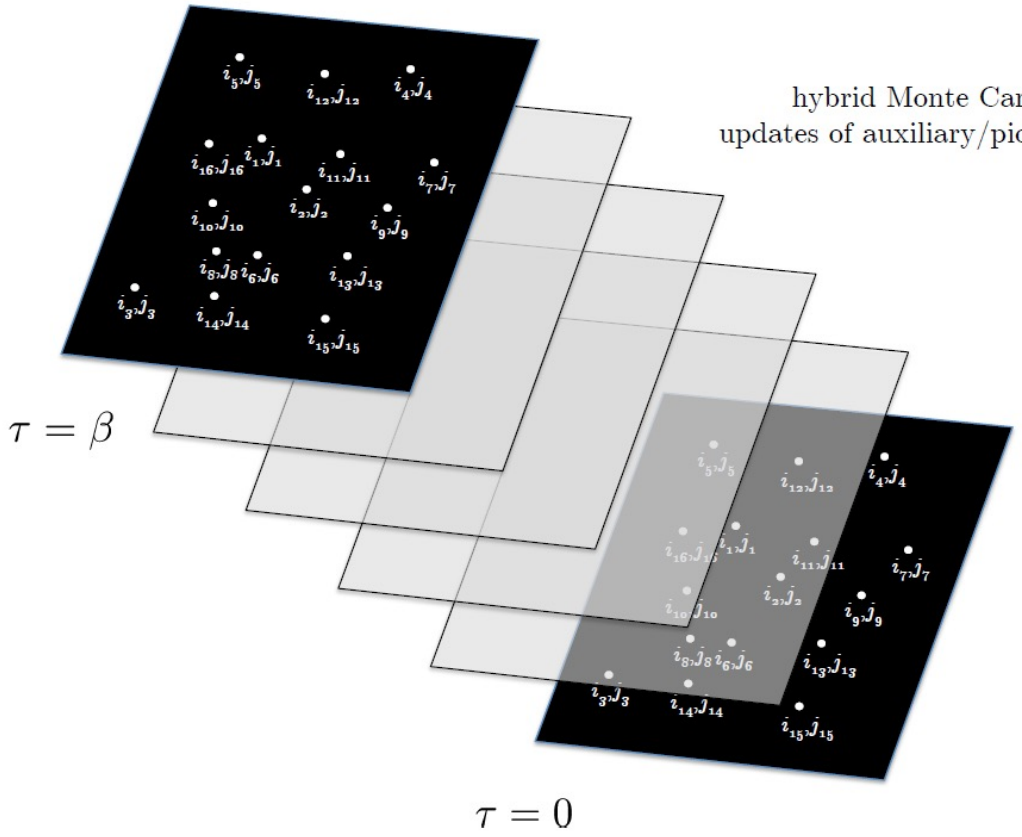
Elhatisari, Epelbaum, Krebs, Lähde, D.L., Li, Lu, Meißner, Rupak, PRL 119, 222505 (2017)



Pinhole trace algorithm

$$\mathrm{Tr}\exp(-\beta H)$$

Metropolis updates of pinholes

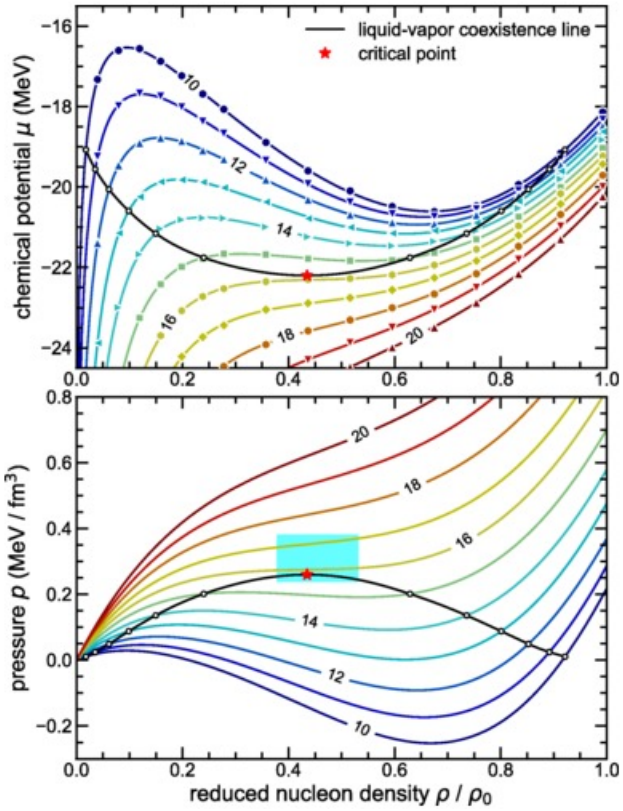


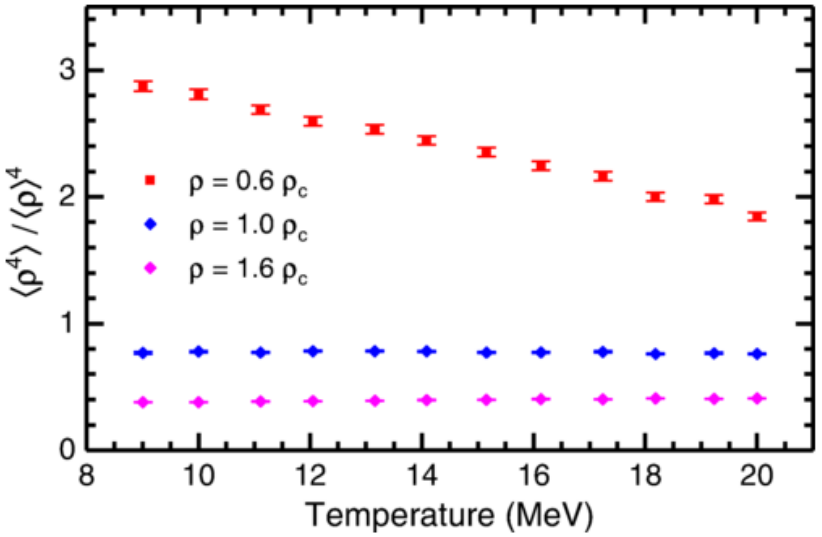
hybrid Monte Carlo
updates of auxiliary/pion fields

PHYSICAL REVIEW LETTERS **125,** 192502 (2020)

Ab Initio Nuclear Thermodynamics

Bing-Nan Lu,[1] Ning Li,[1] Serdar Elhatisari,[2] Dean Lee,[1] Joaquín E. Drut,[3] Timo A. Lähde,[4] Evgeny Epelbaum,[5] and Ulf-G. Meißner[6,4,7]



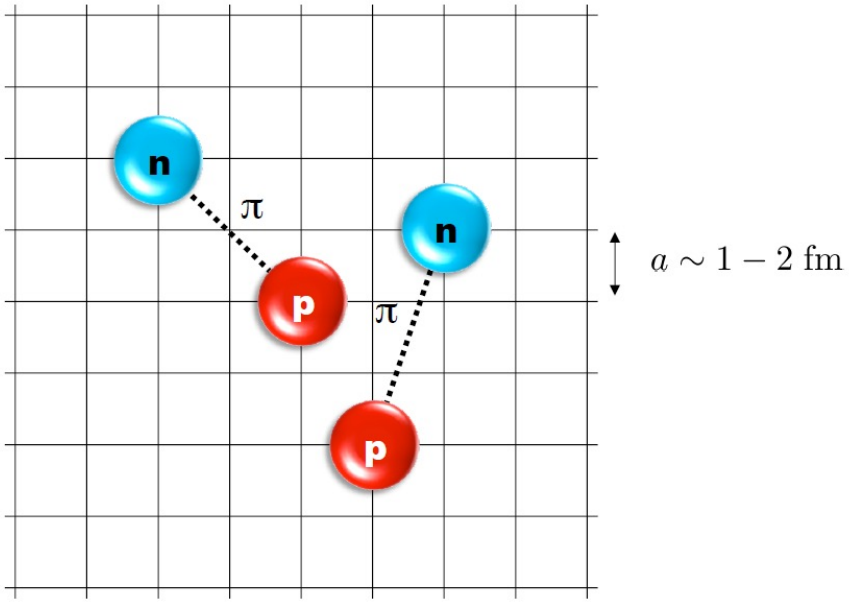


- determine the location of the critical point and the liquid-vapor coexistence line for symmetric nuclear matter with equal numbers of protons and neutrons.

- the first *ab initio* study of the density and temperature dependence of nuclear clustering.

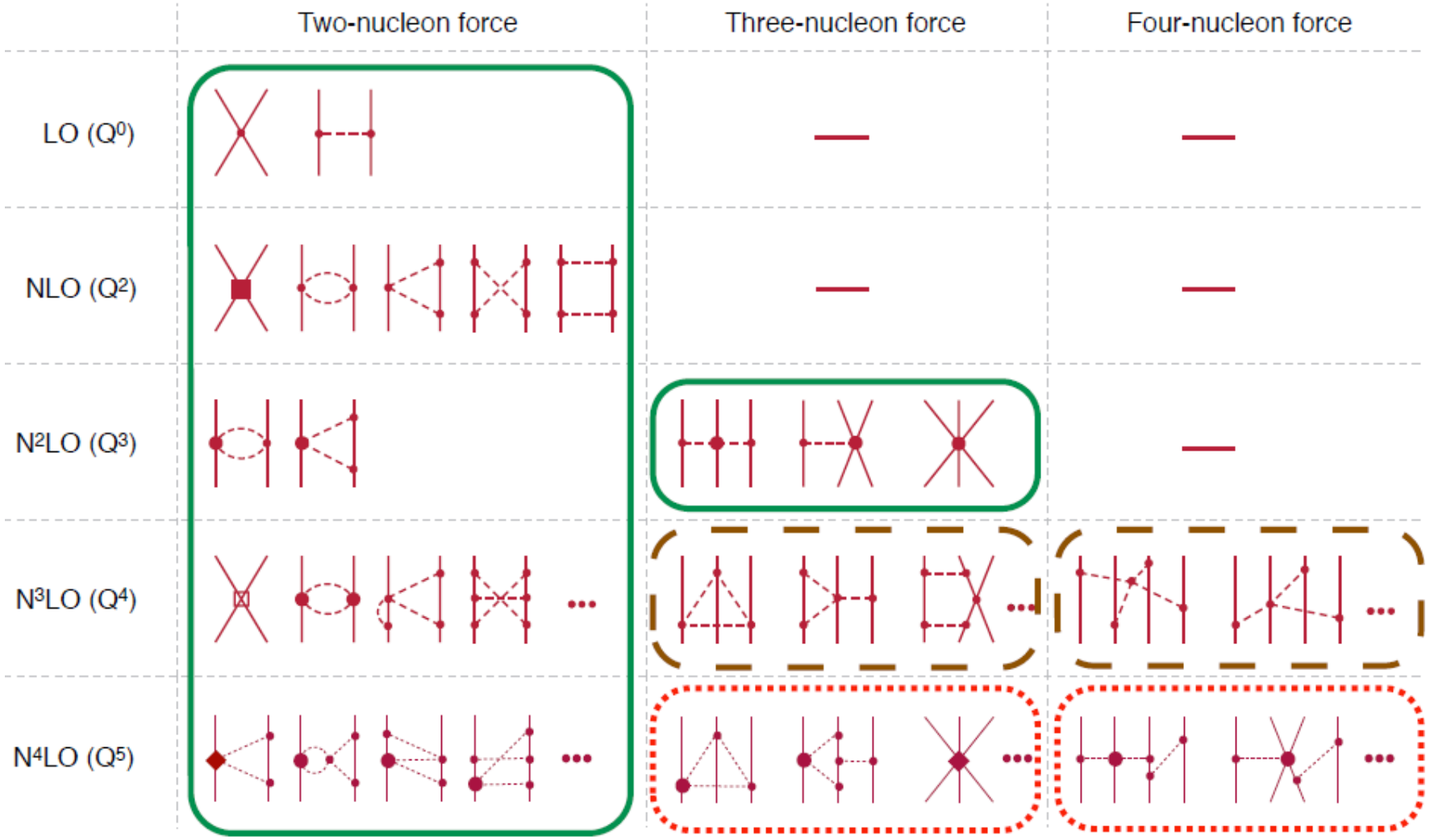
Pinhole trace algorithm

Lattice Hamiltonian



- We need to introduce a lattice scale in space and time:
- momentum space cutoff ~ 150 MeV → lattice size a= 1.316 fm
- Time cutoff ~ 1000 MeV
- We need to determine coefficients of interaction for the lattice size. (regularization scale.)
- Two-body interaction coefficients can be determined from phase shifts of np scattering.
- Three-body interaction can be fixed from binding energy of A>=3.

Chiral Effective Field Theory



Lattice chiral Hamiltonian at Leading order

- At Leading order, kinetic energy + contact interaction + one pion exchange

$$H = H_{\rm free} + V_{\rm 2N}^{\rm short} + V_{\rm 2N}^{\rm long}.$$

$$H_{\rm free} = \frac{49}{12m}\sum_{\mathbf{n}} a^\dagger(\mathbf{n})a(\mathbf{n}) - \frac{3}{4m}\sum_{\mathbf{n},i}\sum_{\langle \mathbf{n}'\,\mathbf{n}\rangle_i} a^\dagger(\mathbf{n}')a(\mathbf{n}) + \frac{3}{40m}\sum_{\mathbf{n},i}\sum_{\langle\langle \mathbf{n}'\,\mathbf{n}\rangle\rangle_i} a^\dagger(\mathbf{n}')a(\mathbf{n}) - \frac{1}{180m}\sum_{\mathbf{n},i}\sum_{\langle\langle\langle \mathbf{n}'\,\mathbf{n}\rangle\rangle\rangle_i} a^\dagger(\mathbf{n}')a(\mathbf{n}).$$

- Kinetic

$$V_{\rm OPE} = -\frac{g_A^2}{8F_\pi^2}\sum_{\mathbf{n}',\mathbf{n},S',S,I} :\rho_{S',I}(\mathbf{n}')f_{S'S}(\mathbf{n}'-\mathbf{n})\rho_{S,I}(\mathbf{n}):,$$

- Long range OPE

$$V = \frac{C}{2}\int d^3\boldsymbol{r} :[\rho(\boldsymbol{r})]^2:,$$

$$V_{I^2} = \frac{C_{I^2}}{2}\sum_{I=1,2,3}\int d^3\boldsymbol{r} :[\rho_I(\boldsymbol{r})]^2:,$$

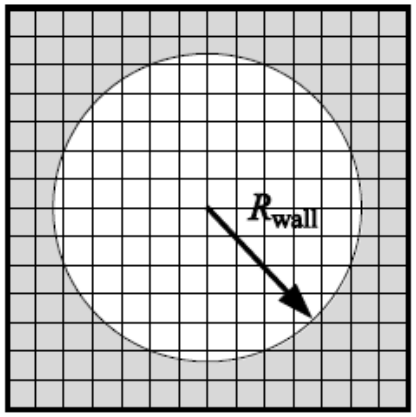
- Contact

Low energy constants in lattice EFT

- All LECs(parameters in the Hamiltonian) needs to be fixed
- (They have to be fixed for given lattice regularization)
- N-P scattering phase shifts, Deuteron binding energy
- Scattering phase shifts on the Lattice: Wall method.

Phase shift can be obtained from
The energy spectrum of E(or k) in lattice and imposed Wall size.

Spherical wall imposed in the center-of-mass frame



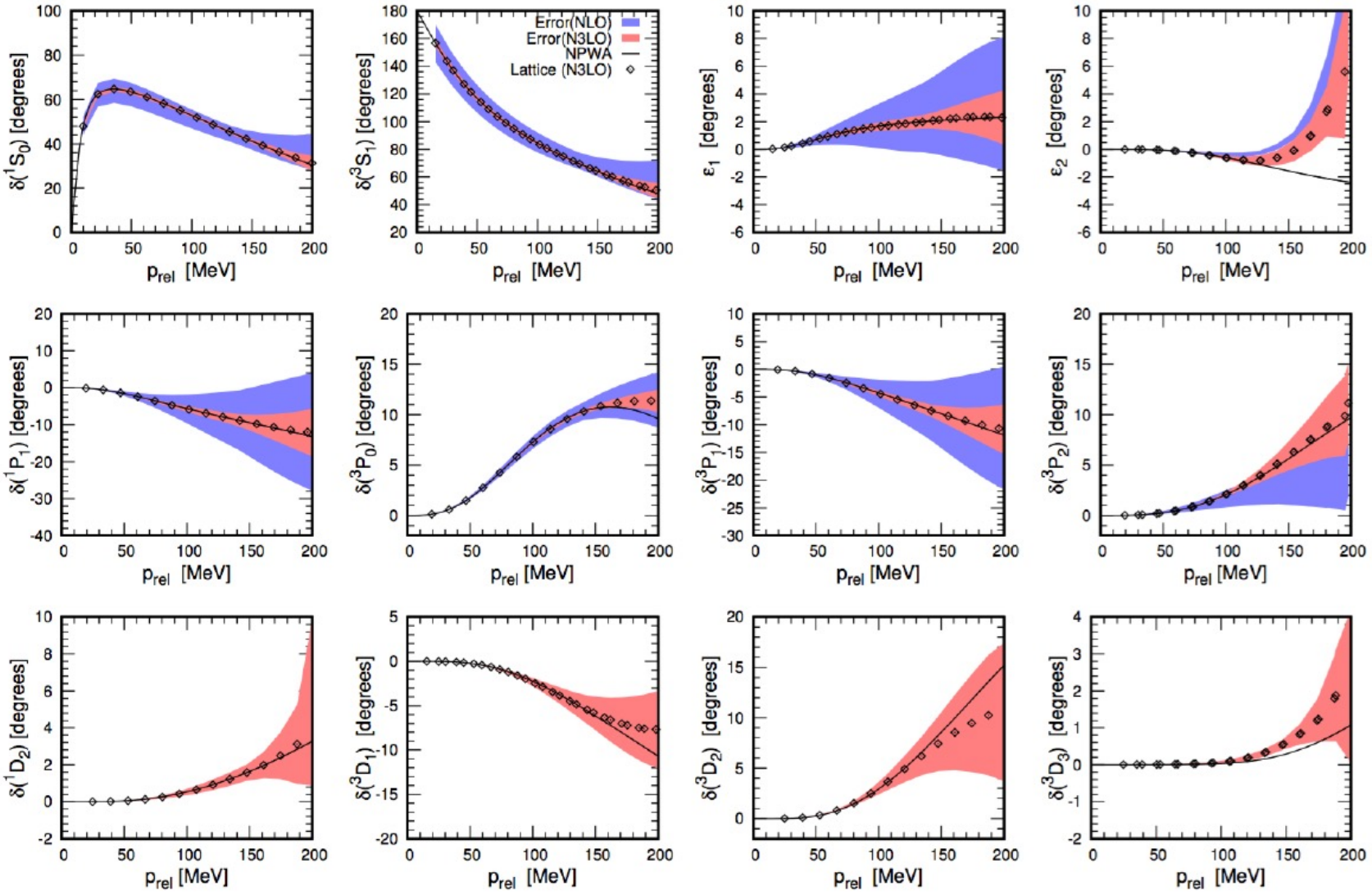
$$\Psi(\vec{r}) = [\cos\delta_L j_L(kr) - \sin\delta_L y_L(kr)]Y_{L,m}(\theta,\phi)$$

$$\Psi(\vec{R}_{\rm Wall}) = 0$$

$$\tan\delta_L = \frac{j_L(kR_{\rm Wall})}{y_L(kR_{\rm Wall})}$$

Similar for Spin-triplet case

$a = 1.973\,\mathrm{fm}$



Determine LECs by fitting phase shifts of N-N scattering

Sign problem in NLEFT

- However, there is a difficulty in auxiliary MC calculation

$$Z(t) = \int \mathcal{D}s Z(s,t), \quad Z(s,t) = e^{-\frac{s^2}{2}} \det X(s,t),$$
$$= \int \mathcal{D}s e^{i\theta(s,t)} |Z(s,t)|$$

$$\langle O \rangle = \frac{\langle O e^{i\theta} \rangle_{pq}}{\langle e^{i\theta} \rangle_{pq}}, \quad \langle O \rangle_{pq} \equiv \frac{\int ds |\det X(s)| O}{\int ds |\det X(s)|}.$$

- We needs a large Euclidean time extrapolation
- If the denominator's sign oscillates rapidly
- → large uncertainty in the expectation value
- → sign problem
- SU(4) symmetric interaction in isospin symmetric system
- → No sign problem

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Essential elements for nuclear binding

Bing-Nan Lu [a], Ning Li [a], Serdar Elhatisari [b,c], Dean Lee [a,*], Evgeny Epelbaum [d], Ulf-G. Meißner [b,e,f]

$$H_{\mathrm{SU(4)}} = H_{\mathrm{free}} + \frac{1}{2!}C_2 \sum_{\boldsymbol{n}} \tilde{\rho}(\boldsymbol{n})^2 + \frac{1}{3!}C_3 \sum_{\boldsymbol{n}} \tilde{\rho}(\boldsymbol{n})^3,$$

$$\tilde{\rho}(\boldsymbol{n}) = \sum_i \tilde{a}_i^\dagger(\boldsymbol{n})\tilde{a}_i(\boldsymbol{n}) + s_L \sum_{|\boldsymbol{n}'-\boldsymbol{n}|=1} \sum_i \tilde{a}_i^\dagger(\boldsymbol{n}')\tilde{a}_i(\boldsymbol{n}'),$$

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

Minimal nuclear interaction

Which reproduce

(1) Light nuclei

(2) medium mass nuclei

(3) neutron matter

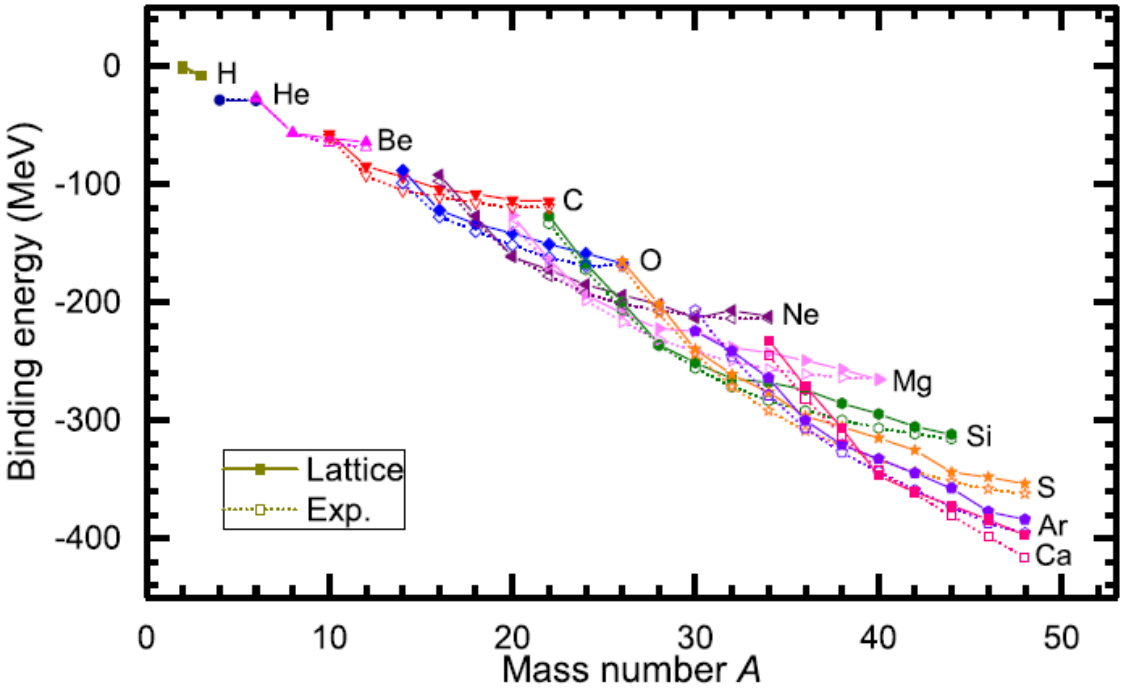
simultaneously up to few percent error in binding energy and charge radius

Only Four parameters

1. Strength of the two-nucleon S-wave interaction
2. Range of the two-nucleon S-wave interaction
3. Strength of three-nucleon contact interaction
4. Range of the local part of the two-nucleon interaction

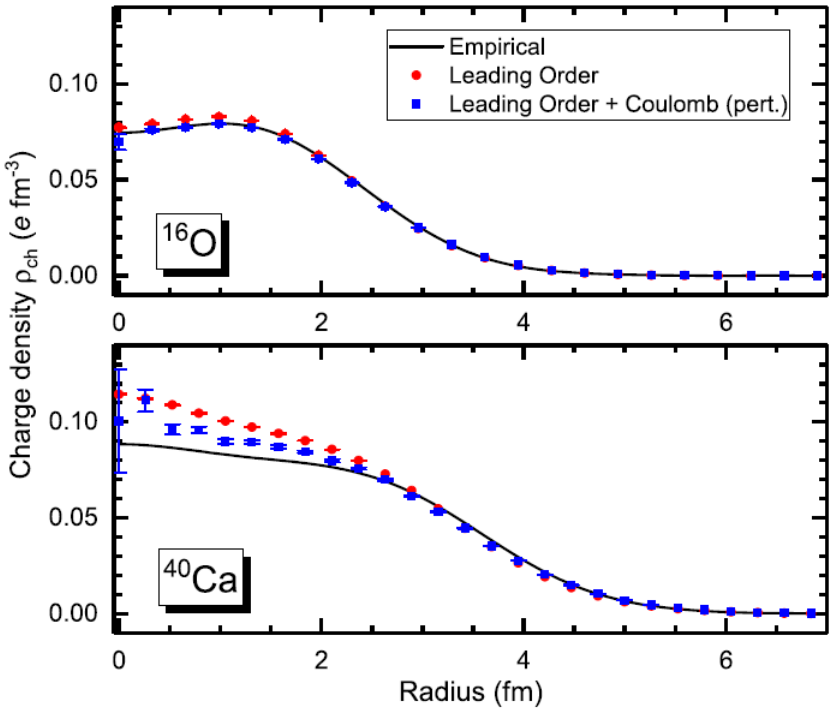
Except for the Coulomb potential, the interaction is invariant under Wigner's SU(4) symmetry.

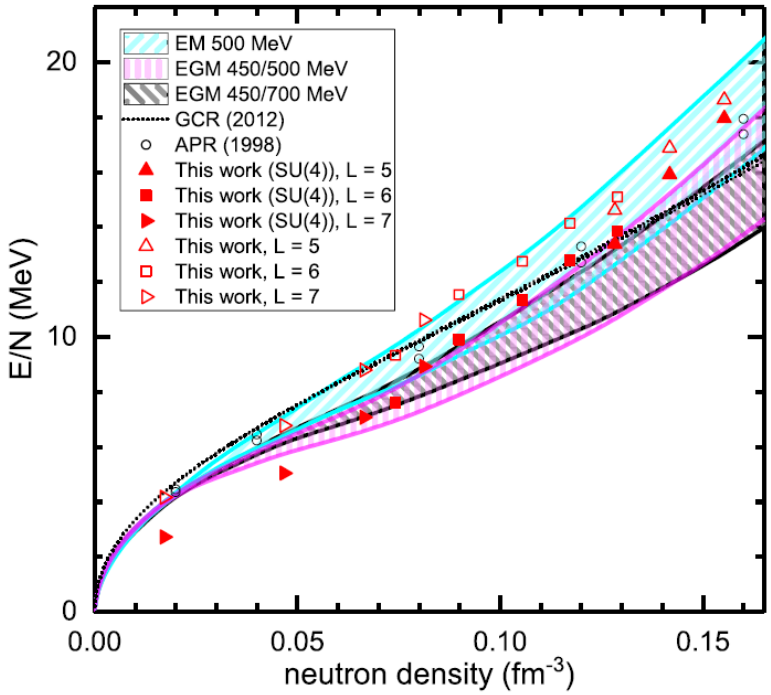
No sign problem



	B	Exp.	$R_{\rm ch}$	Exp.
^{3}H	8.48(2)(0)	8.48	1.90(1)(1)	1.76
^{3}He	7.75(2)(0)	7.72	1.99(1)(1)	1.97
^{4}He	28.89(1)(1)	28.3	1.72(1)(3)	1.68
^{16}O	121.9(1)(3)	127.6	2.74(1)(1)	2.70
^{20}Ne	161.6(1)(1)	160.6	2.95(1)(1)	3.01
^{24}Mg	193.5(02)(17)	198.3	3.13(1)(2)	3.06
^{28}Si	235.8(04)(17)	236.5	3.26(1)(1)	3.12
^{40}Ca	346.8(6)(5)	342.1	3.42(1)(3)	3.48

Can we improve the agreement by
Including higher order corrections?



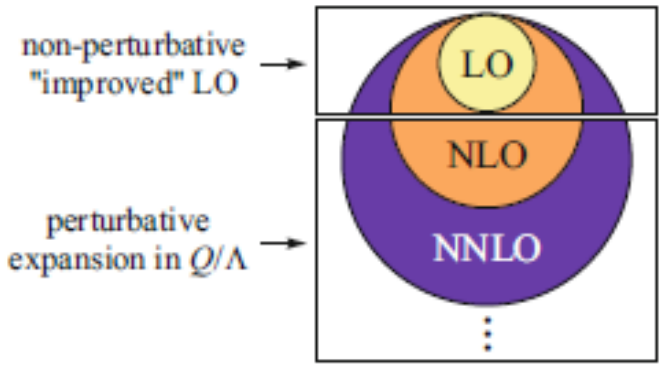


Can we improve the agreement by
Including higher order corrections?

Lattice chiral Hamiltonian (N3LO)

Full N3LO Hamiltonian includes

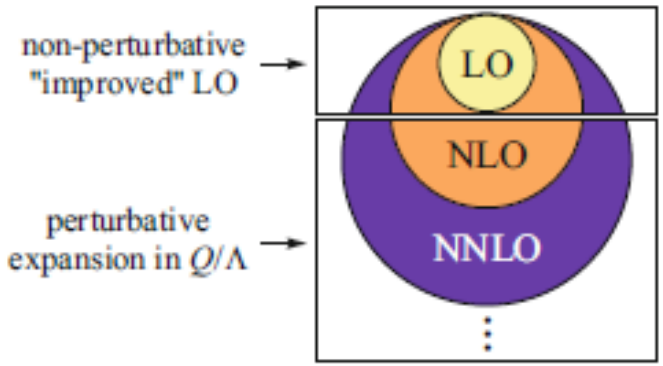
- Free Hamiltonian(Kinetic term)
- Short range (nonlocal smeared) contact interactions up to Q^4 order
- Isospin-breaking short range interactions
- One pion exchange potential
- Two pion exchange potential up to Q^4 order
- Coulomb interaction
- Long range isospin breaking interaction(isospin dependence in OPE)
- Galilean Invariance Restoration (GIR) term (because of non-local interaction.)
- Three nucleon interaction



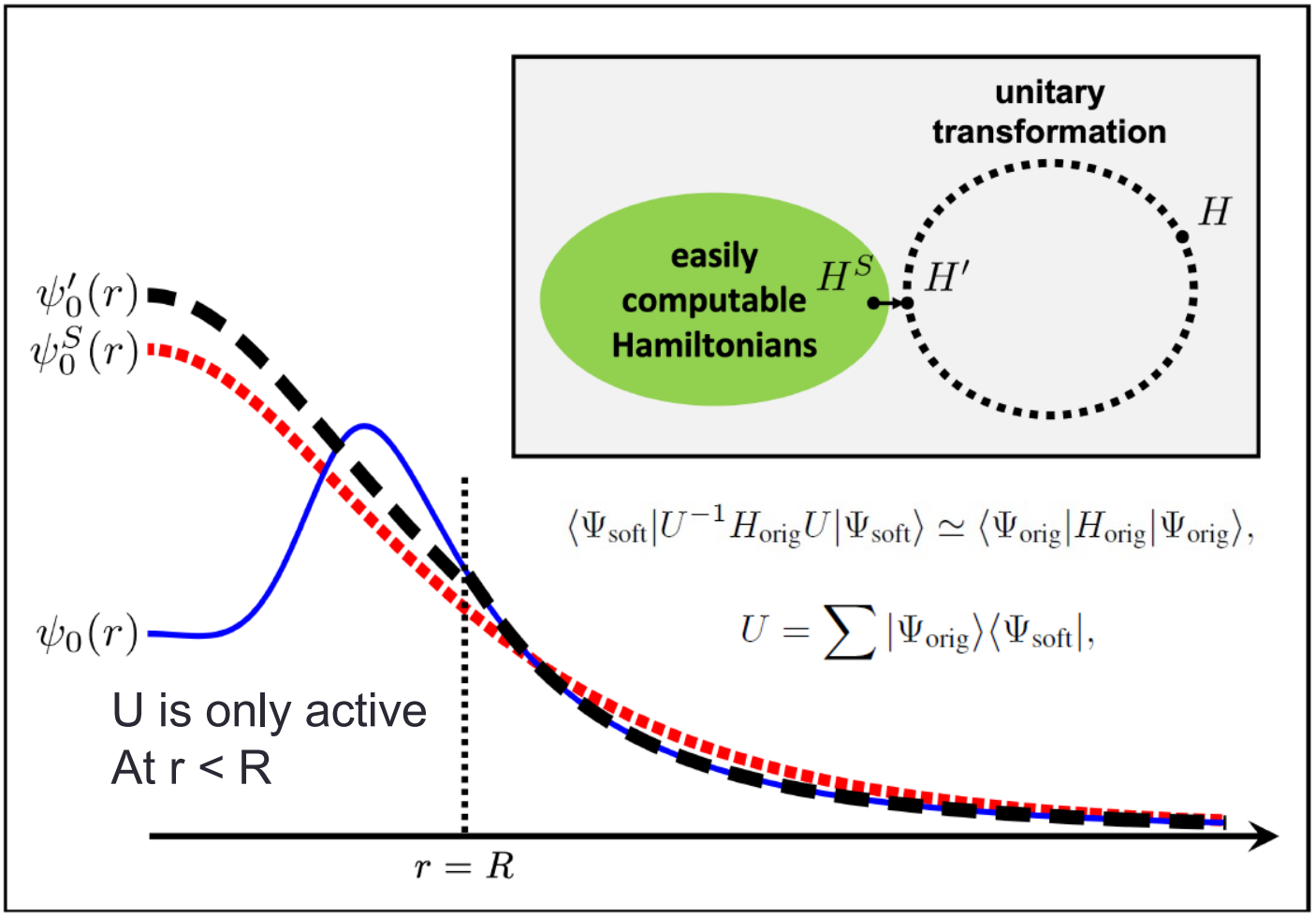
Difficulty with full chiral interaction

- Sign problem
  - NLEFT suffers sign problems at large Euclidean time limit
  - Large cancellation between positive and negative contributions→ large uncertainty.
  - SU(4) symmetric interaction does not have sign problem
  - One pion exchange and higher order chiral interaction, short range repulsion
  - Difficulty with Asymmetric nuclei
  - Needs a remedy to extend to neutron rich isotopes.

- A new approach to reduce the sign problem
- → Wave function matching Hamiltonian.



Wave function matching

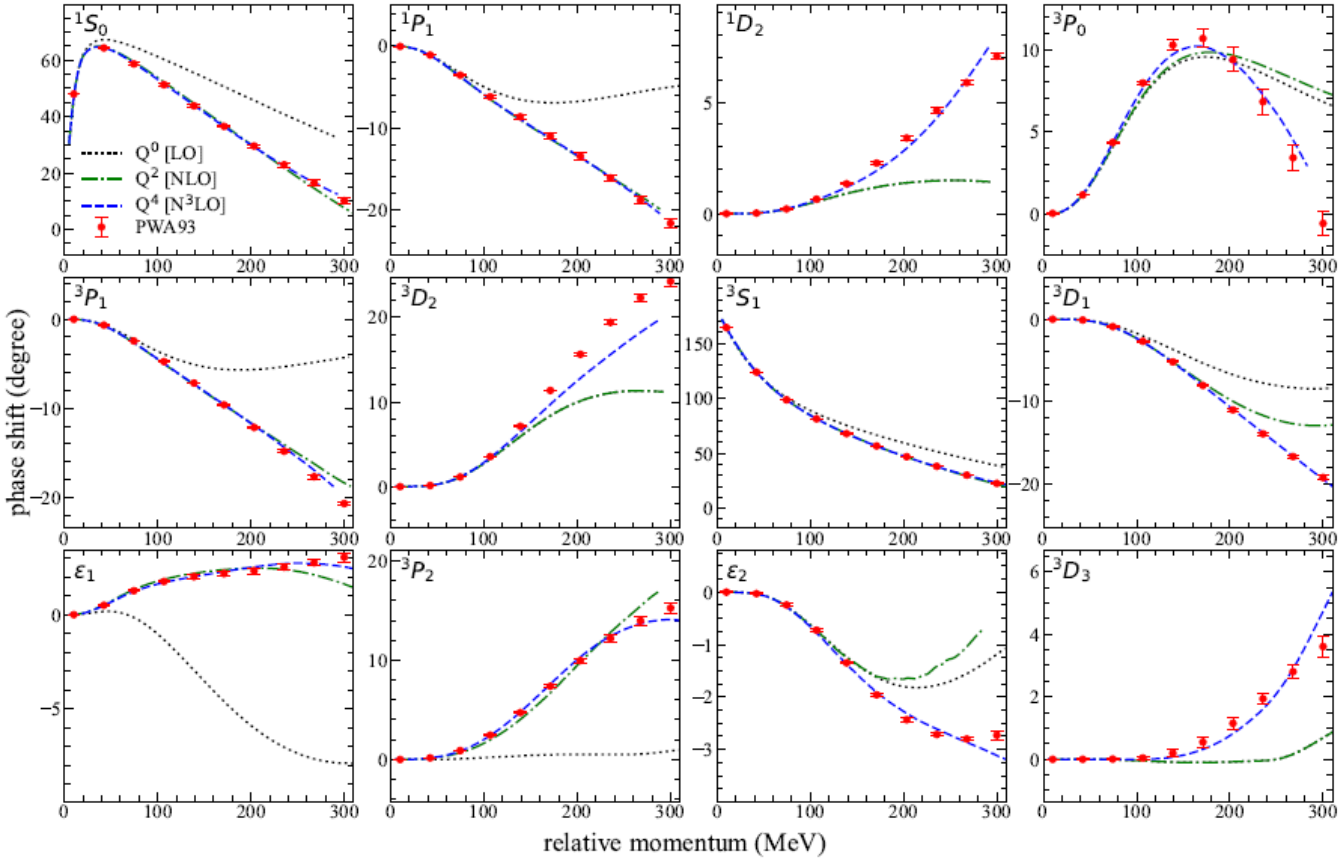


H and H' are fully equivalent to two-body observables

The goal is to make the perturbation expansion from "simple" wave function gives a good convergence

$$H_{\rm wfm} = H_{\rm soft} + (U^{-1}H_{\rm orig}U - H_{\rm soft})$$
$$= H_{\rm soft} + H_{\rm diff},$$

NN phase shifts from WFM



Original Hamiltonian is fitted to phase shifts.

H' is equivalent to original Hamiltonian.

Wave function matching Hamiltonian

- "Simple" Hamiltonian

$$H^S = K + \frac{c_{\mathrm{SU}(4)}}{2} \sum_{\vec{n}} : \left[\tilde{\rho}^{(1)}(\vec{n})\right]^2 : + \frac{c_I}{2} \sum_{I,\vec{n}} : \left[\tilde{\rho}_I^{(1)}(\vec{n})\right]^2 : + V_{\mathrm{OPE}}^{\Lambda_\pi},$$

$$\tilde{\rho}^{(d)}(\vec{n}) = \sum_{i,j=0,1} \tilde{a}_{i,j}^\dagger(\vec{n})\, \tilde{a}_{i,j}(\vec{n}) + s_{\mathrm{L}} \sum_{|\vec{n}-\vec{n}'|^2=1}^{d} \sum_{i,j=0,1} \tilde{a}_{i,j}^\dagger(\vec{n}')\, \tilde{a}_{i,j}(\vec{n}')\,,$$

$$\tilde{\rho}_I^{(d)}(\vec{n}) = \sum_{i,j,j'=0,1} \tilde{a}_{i,j}^\dagger(\vec{n})\, [\tau_I]_{j,j'}\, \tilde{a}_{i,j'}(\vec{n}) + s_{\mathrm{L}} \sum_{|\vec{n}-\vec{n}'|^2=1}^{d} \sum_{i,j,j'=0,1} \tilde{a}_{i,j}^\dagger(\vec{n}')\, [\tau_I]_{j,j'}\, \tilde{a}_{i,j'}(\vec{n}').$$

$$\tilde{a}_{i,j}(\vec{n}) = a_{i,j}(\vec{n}) + s_{\mathrm{NL}} \sum_{|\vec{n}'-\vec{n}|=1} a_{i,j}(\vec{n}').$$

(local,non-local smeared operators)

Wave function matching Hamiltonian

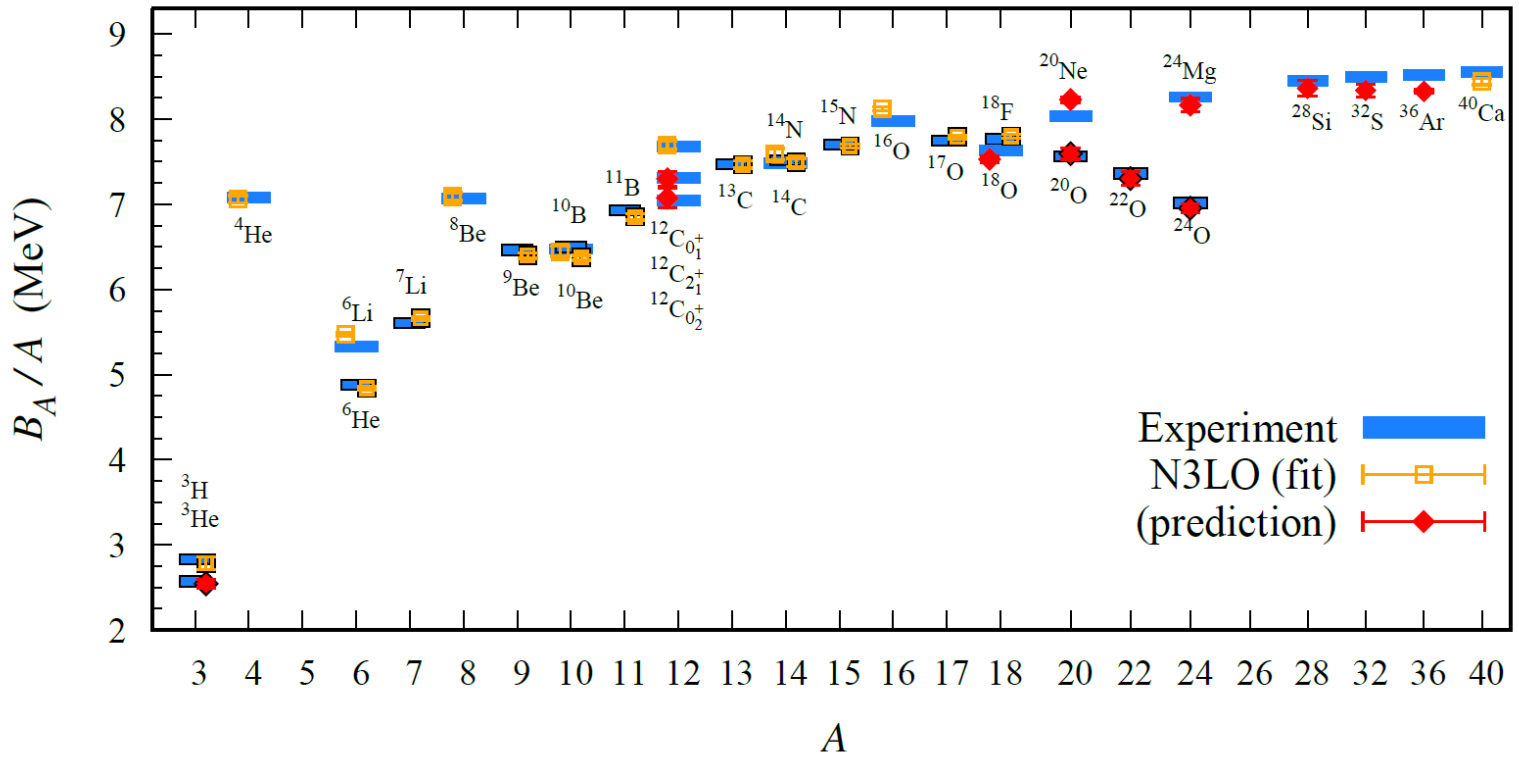
- N3LO Hamiltonian

$$H = K + V_{\mathrm{OPE}}^{\Lambda_\pi} + V_{\mathrm{C}_\pi}^{\Lambda_\pi} + V_{\mathrm{Coulomb}} + V_{\mathrm{3N}}^{\mathrm{Q}^3} + V_{\mathrm{2N}}^{\mathrm{Q}^4} + W_{\mathrm{2N}}^{\mathrm{Q}^4} + V_{\mathrm{2N,WFM}}^{\mathrm{Q}^4} + W_{\mathrm{2N,WFM}}^{\mathrm{Q}^4},$$

$$V_{\mathrm{3N}}^{\mathrm{Q}^3} = V_{c_E}^{(l)} + V_{c_E}^{(t)} + V_{c_E}^{(d)} + V_{c_D}^{(d)} + V_{\mathrm{3N}}^{(\mathrm{TPE})},$$

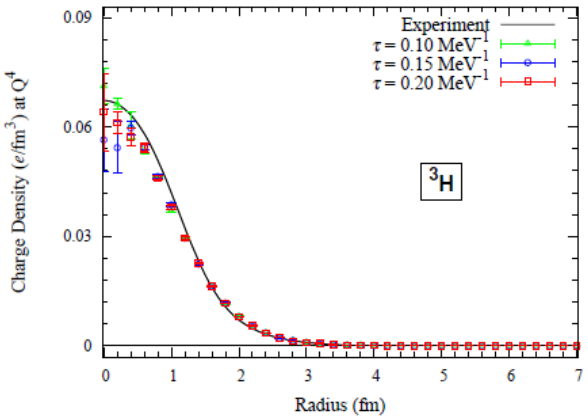
V_2N : short range NN interactions
W_2N: GIR restoration term for V_2N
V_2N,WFM : difference from H_s
W_2N,WFM: GIR restoration correction to V_2N,WFM
V_3N : contains short range 3N interaction parameters(to be fitted)
and two pion exchange correction to 3N

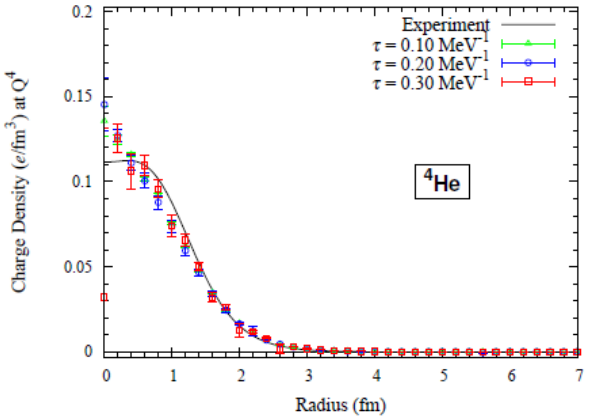
BE/A from WFM

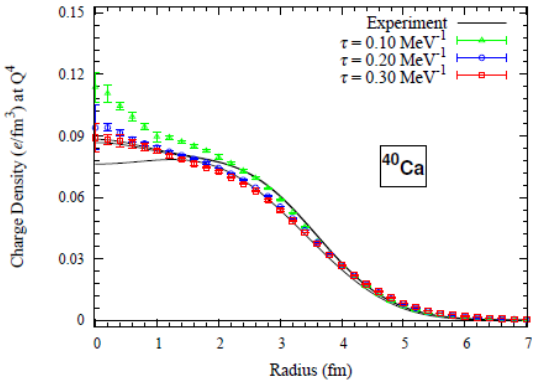


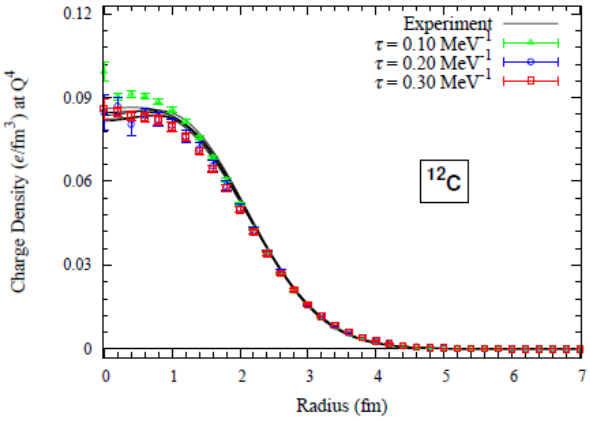
Preliminary

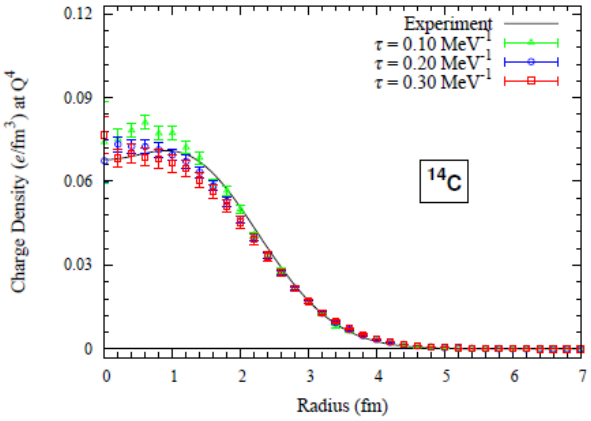
Charge density from WFM





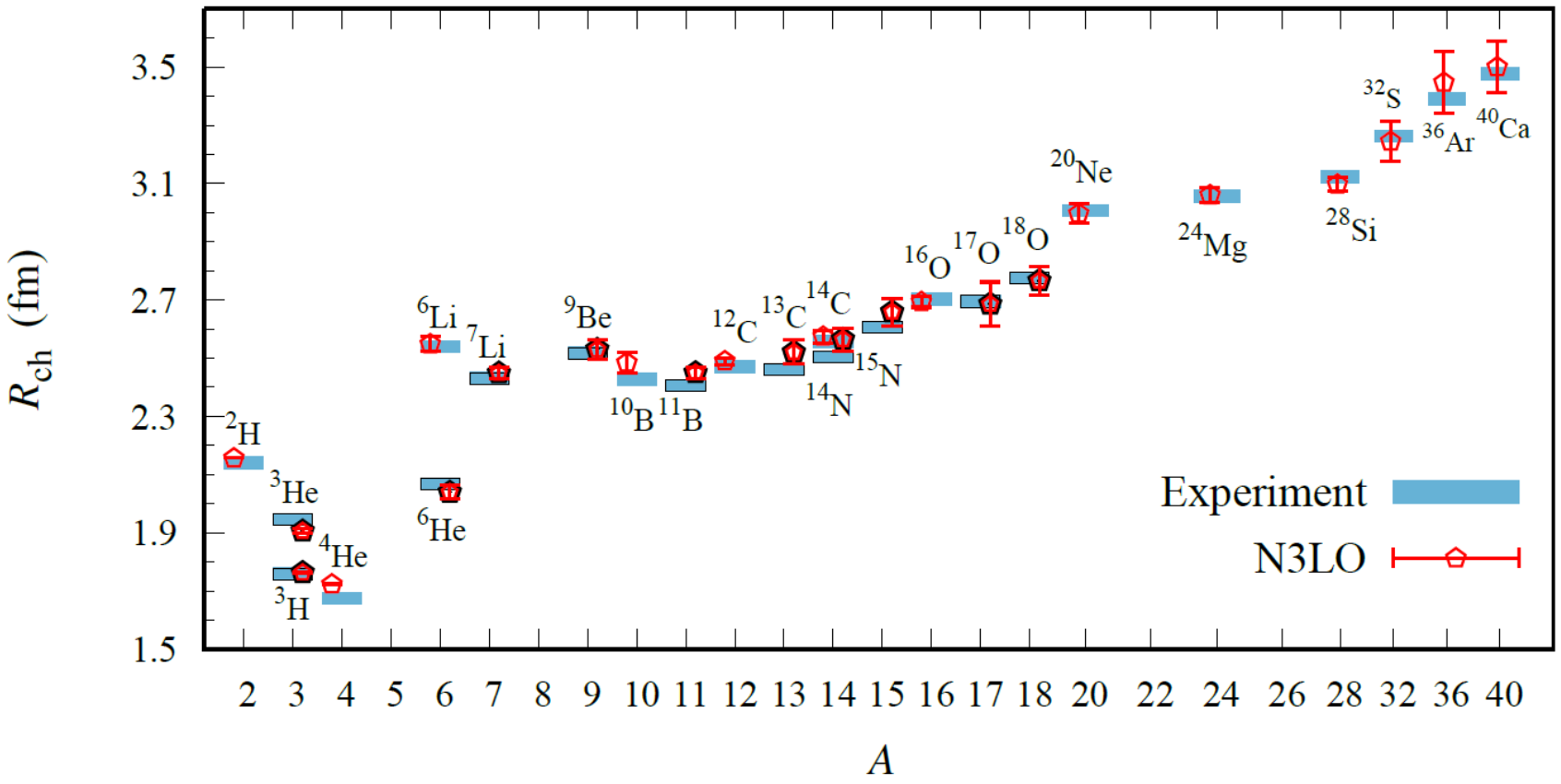






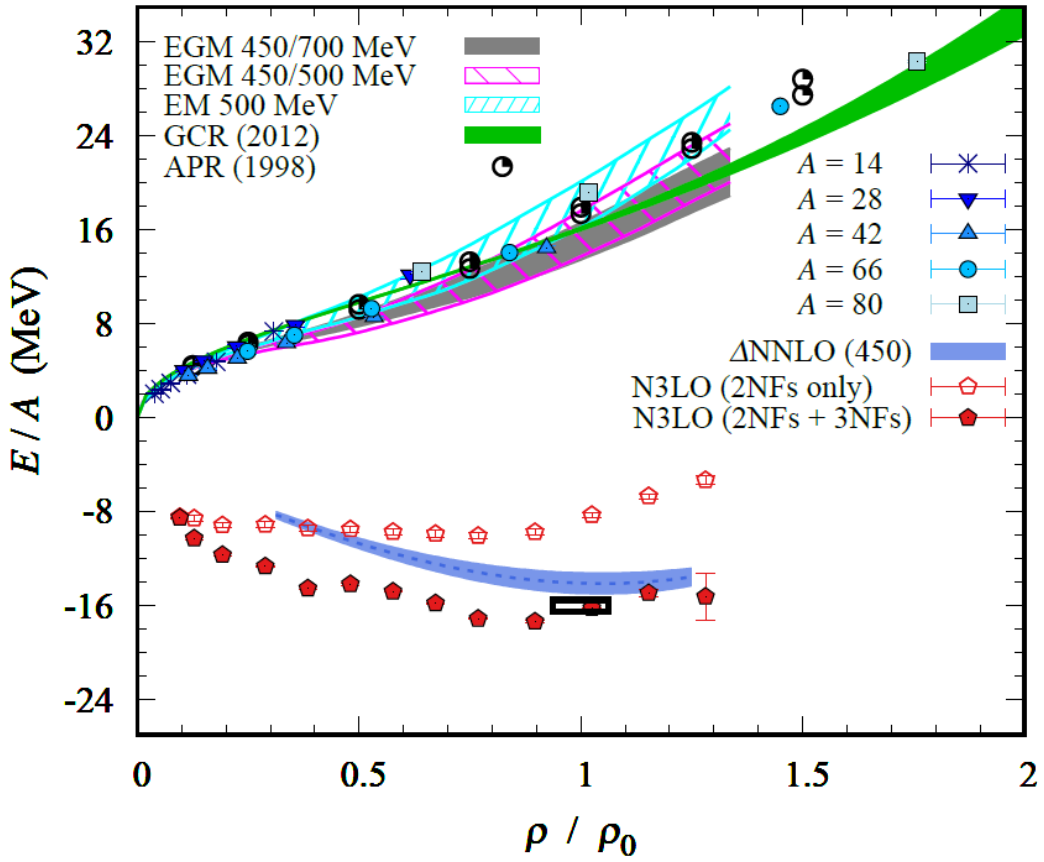
Preliminary

Charge Radius



Preliminary

Nuclear/Neutron Matter

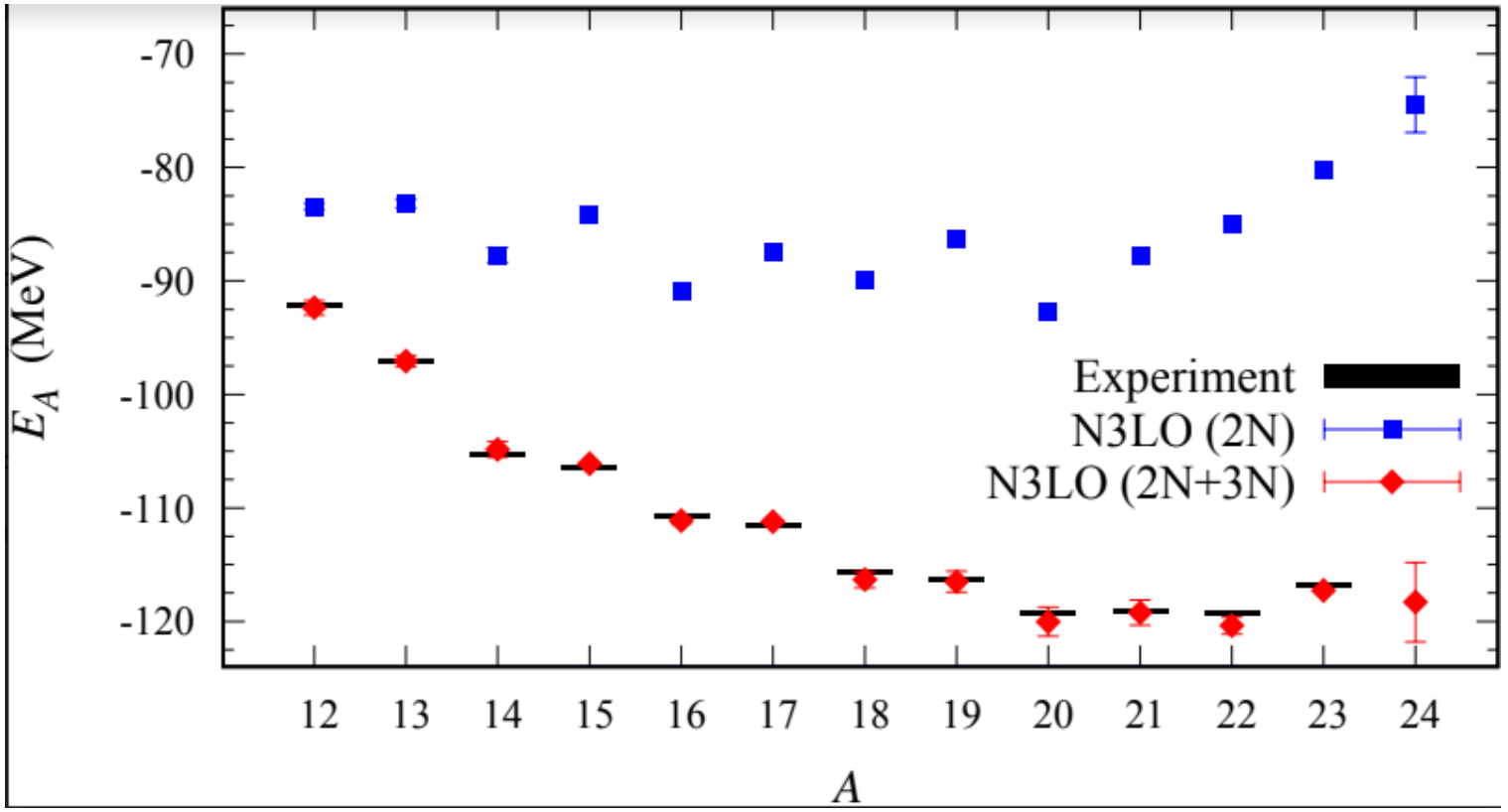


Neutron matter:
A=4~80
box size 6.6 ~ 13.2 fm.

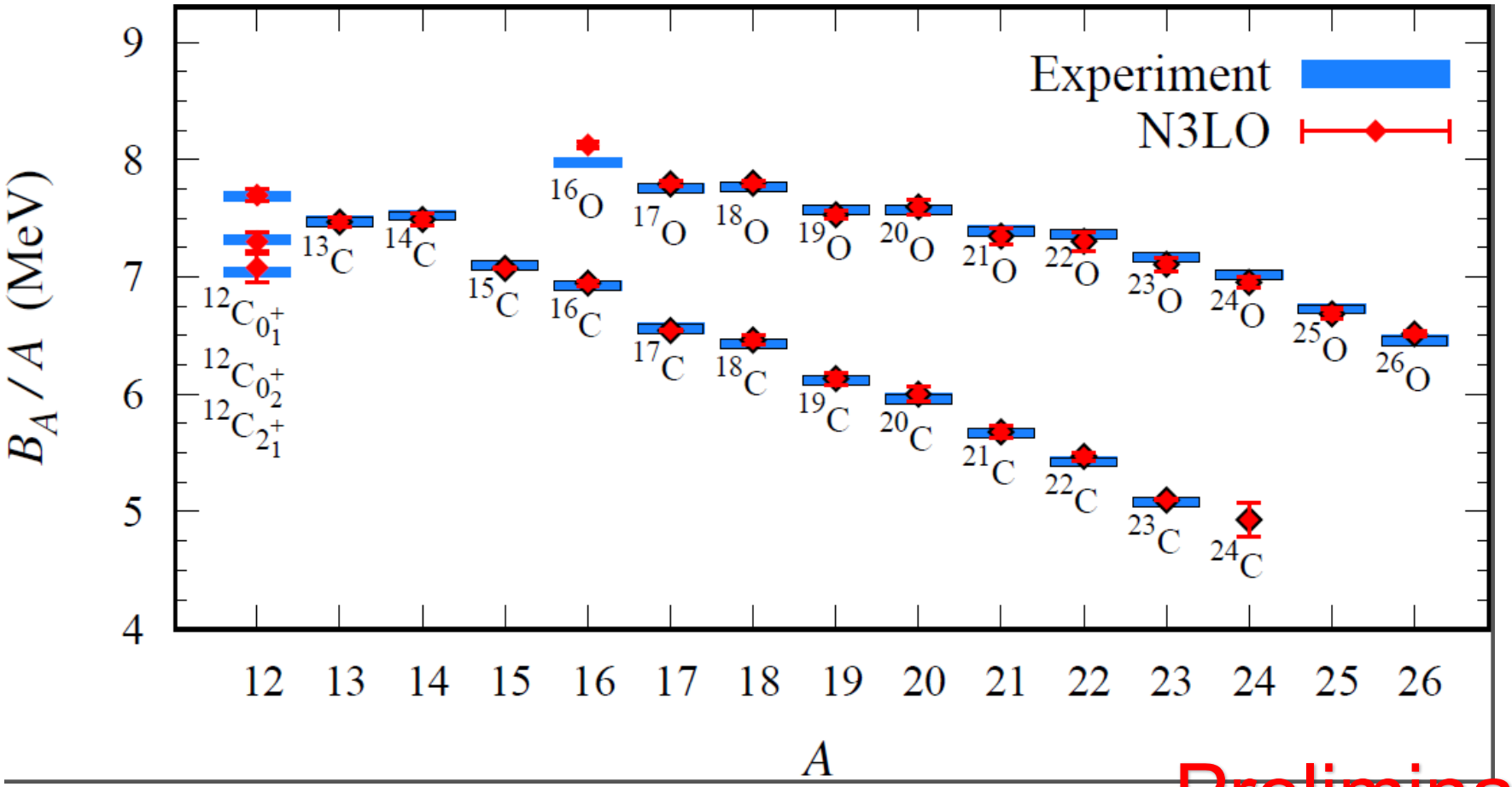
Nuclear matter:
A=4 ~ 160
Box size 7.92~9.24 fm.

Preliminary

Carbon isotopes



Carbon and Oxygen



Preliminary

Summary

- Wave function matching method seems to be promising
  - New method to improve the N3LO calculation of NLEFT
  - Preliminary study shows promising results for wide range of observables in one scheme (same interaction and many-body method)
    - NN scattering
    - Binding energy (from 3H to 40Ca)
    - Symmetric Nuclear matter
    - Neutron matter
    - Dripline of Oxygen isotope.
    - Carbon excited states
- Also, Carbon isotopes, odd Oxygen isotopes, Cluster structure, excited states will be studied.