

Carbon and Oxygen isotope chains (And others)

Young-Ho Song (Institute for Rare Isotope Science, IBS) With NLEFT collaboration



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Nuclear Lattice Effective Field Theory Collaboration

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- And More…



Effective field theories and energy scales



Ab-initio method



Nuclear forces

- 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 2body,3-body, many-body, based on QCD)

Direct connection between Nuclear Force ↔ Nuclear Phenomena

Ab initio many-body

- (ab initio) Nuclear physics is challenging.
- 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
 - 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?)



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Nuclear Lattice Effective Field Theory

One of ab initio method for many fermion system



(Figures from Dean's presentation)

Path integral

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

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

$$\begin{split} |\Psi_A\rangle &= \sum_n c_n |n\rangle_A, \\ Z_A(t) &= \langle \Psi_A | e^{-tH} |\Psi_A\rangle = \sum_n c_n e^{-tE_n} \end{split}$$

(From Dean's presentation)

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.

Auxiliary Field Monte Carlo

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



(Figure From Dean's presentation)

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 ¹²C and ¹⁶O
 - 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)



Chiral Effective Field Theory



Sign problem in NLEFT

• However, there is a difficulty in auxiliary MC calculation

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

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

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

Improved action with non-locality

- In practical calculation, sign problem and convergence of perturbation have to be taken care of.
- To improve the non-perturbative calculation, Local and non-local smearing of contact interaction are introduced.

$$V_{0} = \frac{C_{0}}{2} : \sum_{\mathbf{n}',\mathbf{n},\mathbf{n}''} \sum_{i',j'} a_{i',j'}^{s_{\mathrm{NL}}\dagger}(\mathbf{n}') a_{i',j'}^{s_{\mathrm{NL}}}(\mathbf{n}') f_{s_{\mathrm{L}}}(\mathbf{n}'-\mathbf{n}) f_{s_{\mathrm{L}}}(\mathbf{n}-\mathbf{n}'') \\ \sum_{i'',j''} a_{i'',j''}^{s_{\mathrm{NL}}\dagger}(\mathbf{n}'') a_{i'',j''}^{s_{\mathrm{NL}}}(\mathbf{n}') :, \quad V_{0,1S_{0}}(\mathbf{n}) \text{ and } V_{0,3S_{1}}(\mathbf{n})$$

NLO

NNLO

$$\begin{aligned} a_{i,j}^{s_{\mathrm{NL}}}(\mathbf{n}) &= a_{i,j}(\mathbf{n}) + s_{\mathrm{NL}} \sum_{|\mathbf{n}'|=1} a_{i,j}(\mathbf{n} + \mathbf{n}'). \\ a_{i,j}^{s_{\mathrm{NL}}\dagger}(\mathbf{n}) &= a_{i,j}^{\dagger}(\mathbf{n}) + s_{\mathrm{NL}} \sum_{|\mathbf{n}'|=1} a_{i,j}^{\dagger}(\mathbf{n} + \mathbf{n}'). \end{aligned} \qquad \begin{array}{c} \text{non-perturbative} \\ \text{"improved" LO} \end{array} \rightarrow \end{aligned}$$



Essential elements for nuclear binding

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$$H_{\text{SU}(4)} = H_{\text{free}} + \frac{1}{2!} C_2 \sum_{\boldsymbol{n}} \tilde{\rho}(\boldsymbol{n})^2 + \frac{1}{3!} C_3 \sum_{\boldsymbol{n}} \tilde{\rho}(\boldsymbol{n})^3$$
$$\tilde{\rho}(\boldsymbol{n}) = \sum_{i} \tilde{a}_i^{\dagger}(\boldsymbol{n}) \tilde{a}_i(\boldsymbol{n}) + s_L \sum_{|\boldsymbol{n}'-\boldsymbol{n}|=1} \sum_{i} \tilde{a}_i^{\dagger}(\boldsymbol{n}') \tilde{a}_i(\boldsymbol{n}'),$$

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

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.	$R_{ m ch}$	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



Wave function matching



H and H' are fully equivalent to twobody observables

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

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

Wave function matching Hamiltonian

• N3LO Hamiltonian

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

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

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



Charge density from WFM





Charge Radius



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.

Carbon/Oxygen Isotope calculations

- WFM Hamiltonian
- Initial wave functions are prepared with HO wave functions
- No projection operator used but prepared with correct M_z



Carbon and Oxygen



Carbon isotopes





Carbon isotopes



Kinetic energy







- Some pattern observed for
 - 2N, 3N contribution
 - 1S0, 3S1 contact terms
 - p/n kinetic energies
- However, each contributions are n ot physical observable and can be model dependent

Charge Radius

Exp			Lattice Calculation				
Carbon	Exp E/A	Exp E	charge R	E(MeV)		R_pp	R_ch
12	7680.145	92.16174	2.4702	97.72(45)		2.4141(204)	2.5426(204)
13	7469.850	97.10805	2.4614	97.46(25)		2.5252(441)	2.6450(441)
14	7520.320	105.28448	2.5025	106.21(32)		2.4622(314)	2.5815(314)
15	7100.17	106.50255		107.77(46)		2.5788(400)	2.6897(400)
16	6922.05	110.7528		112.34(65)		2.5974(508)	2.7043(508)
17	6558.0	111.486		113.15(27)		2.6854(416)	2.7858(416)
18	6426.1	115.6698		118.82(92)		2.6622(410)	2.7603(410)
19	6118	116.242		118.05(78)		2.7087(157)	2.8020(157)
20	5961	119.22		124.17(104)		2.7704(752)	2.8587(752)
21	5674#	119.154		119.27(65)		2.7736(845)	2.8587(845)
22	5421	119.262		124.88(34)		2.7682(1679)	2.8504(1679)
23	5080#	116.840		119.58(53)		-	

From Yuanzhuo Ma

$$\begin{split} \langle r_{\rm ch}^2 \rangle &= \langle r_{\rm pp}^2 \rangle + R_{\rm p}^2 + \frac{N}{Z} R_{\rm n}^2 + \frac{3 \hbar^2}{4 m_{\rm p}^2 c^2}, \quad {\rm Rn} \wedge 2 = -0.105 \\ \\ 0.\overline{7056} \quad 0.0\overline{33172} \end{split}$$

	Exp			Lattice Calculation			
Oxygen	Exp E/A	Exp E	charge R	E(MeV)		R_pp	R_ch
16	7976.207	127.619312	2.6991	130.12(39)		2.7134(702)	2.8283(702)
17	7750.729	131.762393	2.6932	132.31(15)		2.6955(171)	2.8088(171)
18	7767.098	139.807764	2.7726	140.84(32)		2.8329(469)	2.9387(469)
19	7566.50	143.7635		143.27(20)		2.7702(88)	2.8760(88)
20	7568.57	151.3714		151.68(42)		2.7236(383)	2.8288(383)
21	7389.4	155.1774		154.28(29)		2.7768(796)	2.8778(796)
22	7364.9	162.0278		162.04(60)		2.9162(761)	3.0104(761)
23	7163	164.749		162.80(70)		2.7575(471)	2.8546(471)
24	7040	168.96		168.72(27)		2.9159(748)	3.0057(748)
25	6728	168.2		166.61(49)		2.9115(565)	2.9993(565)
26	6497	168.922		168.77(44)		2.9674(543)	3.0514(543)
27	6185#	166.995		166.45(15)		2.9737(408)	3.0554(408)
28	5988#	167.664					

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.

Others 1

(Only preliminary results)

G.T. transition amplitude

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Letter | Published: 11 March 2019

Discrepancy between experimental and theoretical β -decay rates resolved from first principles

P. Gysbers, G. Hagen [™], J. D. Holt, G. R. Jansen, T. D. Morris, P. Navrátil, T. Papenbrock, S. Quaglioni, A. Schwenk, S. R. Stroberg & K. A. Wendt

Nature Physics 15, 428-431 (2019) Cite this article





G.T. transition amplitude

$$Z_{ij} = \langle i | M^{L_t} | j \rangle = \int ds e^{-V(s)} \det \boldsymbol{X}_{ij}(s)$$

$$[\boldsymbol{X}_{ij}(s, L_t)]_{lm} = \langle \phi_l^{(i)} | M(s)^{L_t} | \phi_m^{(j)} \rangle$$

- 1. Needs to compute two nuclei at the same time
- 2. For orthogonal states, $Z_{12} = 0$. (Sampling channels one at a time is not suitable.)
- 3. How should we sample auxiliary fields for Z_{12} ?

As a starter,

- WFM wave function(at LO)
- only 1-body operator are used. (no 2BC contributions)

Trial: Re-weighting method

$$\begin{split} \langle O \rangle_{ij} &= \frac{\langle i | M^{L_t/2} O M^{L_t/2} | j \rangle}{\langle i | M^{L_t} | j \rangle} \\ &= \frac{\int ds e^{-V(s)} \det \mathbf{X}^O_{ij}(s)}{\int ds e^{-V(s)} \det \mathbf{X}_{ij}(s)} \\ &= \frac{\frac{1}{N} \sum_s e^{-V(s)} \det \mathbf{X}^O_{ij}(s) / P_1(s)}{\frac{1}{N} \sum_s e^{-V(s)} \det \mathbf{X}_{ij}(s) / P_2(s)} \end{split}$$

Compute A nuclei (A wave vectors)

- \rightarrow Select A-1 or A-2 s.p. waves to construct trial wave functions
- \rightarrow Use the same auxiliary fields sampling for A nuclei
- \rightarrow Reweight probability for A-1 or A-2 nuclei

Trial : Re-weighting method

• 4He within 5He

	5He		4He	
Lt=100	-0.25592E+02	0.12145E+00	-0.28048E+02	0.22358E+00
Lt=200	-0.26400E+02	0.21669E+00	-0.28407E+02	0.25195E+00
Lt=300	-0.26458E+02	0.18151E+00	-0.28794E+02	0.28754E+00
Lt=400	-0.26647E+02	0.15672E+00	-0.27967E+02	0.33789E+00
Fit	26.62 +/- 0.12		28.43 +/- 0.42	2
Exp.	27.5605		28.2956	

- It may be used for the Separation energy calculation
- \rightarrow Correlated error estimation of separation energy

Trial : Re-weighting method

- Preliminary calculation of $3H \rightarrow 3He$ by using 4He sampling
 - |<3He| tau_{+}|3H >|~1 and |<3He|sigma_z tau_{+}|3H>|~1
 - Significant increase of BE error compared to independent calculations

- Preliminary calculation of $6He(0+) \rightarrow 6Li(1+)$ by using 7Li(3/2-) sampling
 - To fix the angular momentum, two projection operators are used.
 - However,
 - Bad convergence in binding energy of 6He, 6Li
 - Two Projection operators raises sign problem.

 $\langle A|P_B M^{L_t/2} O M^{L_t/2} P_A|B \rangle$

$$= \sum_{\theta_1,\theta_2} f_A(\theta_1) f_B(\theta_2) \langle A | R_A(\theta_1) M^{L_t/2} O M^{L_t/2} R_B(\theta_2) | B \rangle$$

Trial : Mixed Sampling

Working on mixed sampling approach

Preliminary

- $P(x) \simeq a |\det X_{11}(x)| + b |\det X_{22}(x)|$
- Instead of projection operator, fix the Jz of initial wave functions



- Preliminary calculation 3H->3He
 - Better convergence than reweight method
 - <3He| GT| 3H> ~ 1.0 for all Lt
 - (Only LO wave function)

BE(3He)= 7.718 (exp.) BE(3H) = 8.482 (exp.) <3He| GT| 3H> ~ 0.958 (exp.)

Trial : Mixed Sampling

Preliminary





- Mixed Sampling
- 6He(0+)→6Li(1+)
- B.E. Lt dependence changed
- <6Lil (GT) |6He> have Lt dependence

```
BE(6He) =29.27(exp.)
BE(6Li) =31.99(exp.)
<6Li| (GT) |6He> ~ 1.25 (exp)
```

Summary

- G.T. Transition amplitudes
 - Two nuclei with different Z at the same time
 - \rightarrow re-weighting method was not successful
 - \rightarrow mixed sampling seems to work
- To do :
 - 2BC correction
 - higher order wave function correction

Others 2

(Only preliminary results)

Dripline for unitary Fermions

- Unitary Fermion Gas :
 - A strongly coupled conformal system
 - Physically interesting multi-fermion system with simple interaction

$$\mathcal{A} = \frac{4\pi}{M} \frac{1}{p \cot \delta - ip} \qquad \qquad p \cot \delta = -\frac{1}{a} + \frac{1}{2} r_0 p^2 + O(p^4)$$

• $p \cot \delta = 0$: Unitary limit

→largest possible scattering amplitude. Infinite scattering length.

(Realistic nuclear force is close to unitary limit.)

Universality of unitary limit of many fermion system → Bertsch Parameter

$$r_e \ll n^{-\frac{1}{3}} \ll a_s,$$

$$E_0 = \xi E_{FG},$$

Bertsch parameter

Unitary limit Hamiltonian



1S0 NN scattering phase shift is fitted for unitary limit .
→ Very large scattering length.
In cubic and BCC lattice

N=66 neutrons (33 spin up, 33 spin down) L = 4,..., 10

$$\xi = E_0 / E_{\rm FG}$$

 $\xi_{33,33}^{\text{thermo}} = 0.369(2) \text{ and } \xi_{33,33}^{\text{finite}} = 0.372(2).$ Cubic lattice $\xi^{\text{therm}} = 0.369(2).$ $\xi^{\text{few}} = 0.371(2).$ BCC lattice

Unitary Fermions under trap

- Unitary Fermion itself does not form a bound nuclei
 → Introduce an external spherical well potential
 Can we find a relation between trap shape and dripline?
- Separation energy have to be calculated accurately

 → Use an re-weighting method to reduce error in separation energy.
 (correlated error estimation in energy difference.)
- Unfortunately, realistic mean-field potential is rather expensive. (reaching dripline in Unitary limits is difficult.)
 - → limited to shallow external potential. Try to see the dependence on parameter : $y0 = m R^2 V$

(Work in progress. Only preliminary results)

Neutrons in trap



Separation energies

Lattice spacing 100 MeV

Spherical well radius~ 4fm



Preliminary

V0=8MeV density contour





V0=8MeV density contour







Extrapolation?



- Linear Fit
- Needs More data

Preliminary

Summary

- Unitary Fermions in trap
 - One could find driplines from two neutron separation energies
 - Density distribution shows leakage of neutrons
 - y0 dependence
 - However, not enough data yet for any conclusion.
 - \rightarrow To reduce computational cost, looking at 1d case.