# Perturbative Quantum Monte Carlo Method for Nuclear Physics

Bing-Nan Lü[1]

**吕炳楠**

Nuclear Lattice EFT Collaboration

[1]Graduate School of China Academy of Engineering Physics, Beijing

中国工程物理研究院研究生院
GRADUATE SCHOOL OF CHINA ACADEMY OF ENGINEERING PHYSICS

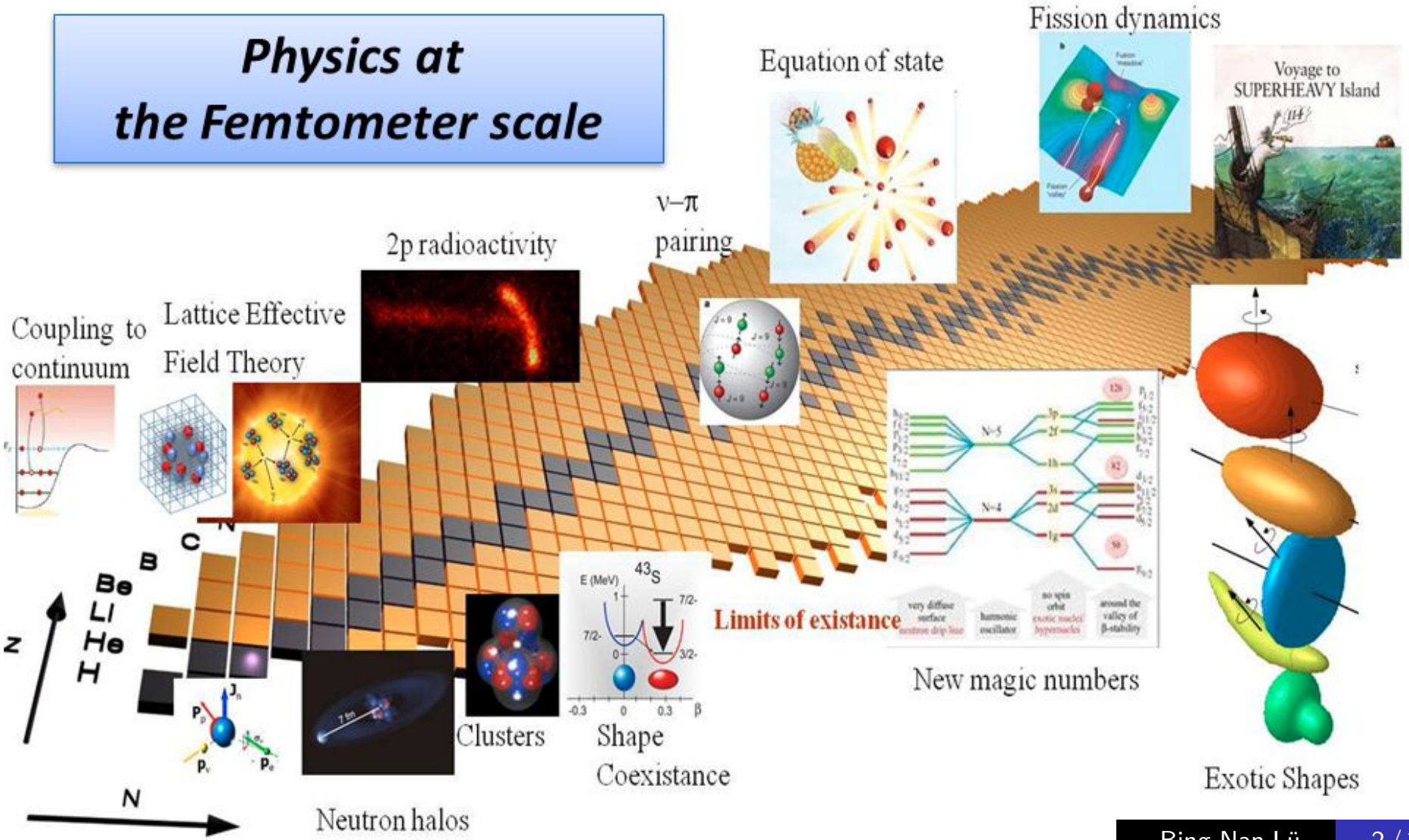

MICHIGAN STATE UNIVERSITY

中山大學
SUN YAT-SEN UNIVERSITY



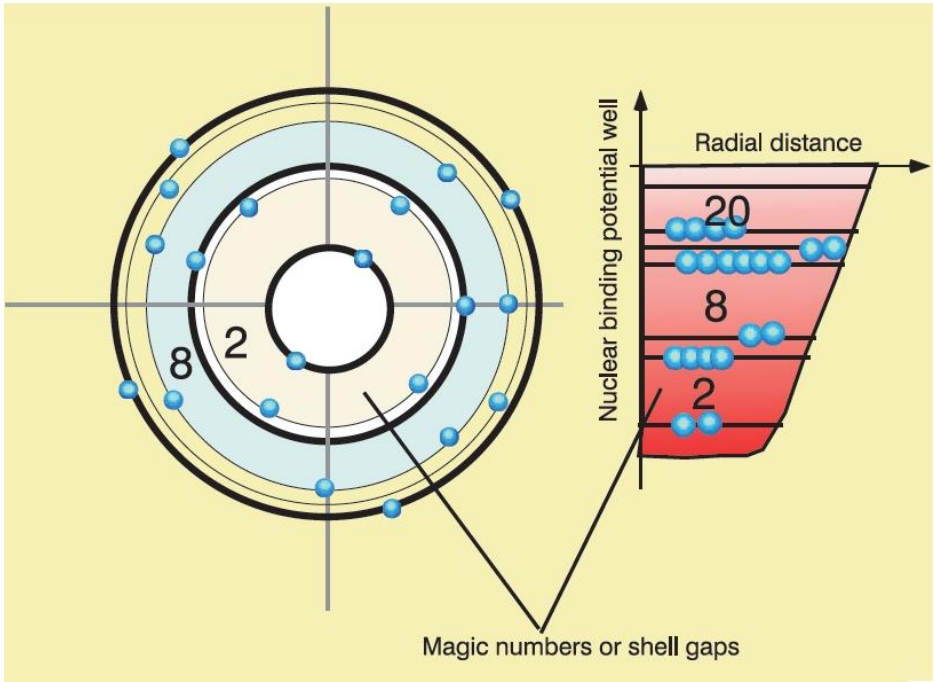

Sun Yat-sen University, School of Physics and Astronomy Sep-16-2022

# Hot Topics in Nuclear Physics

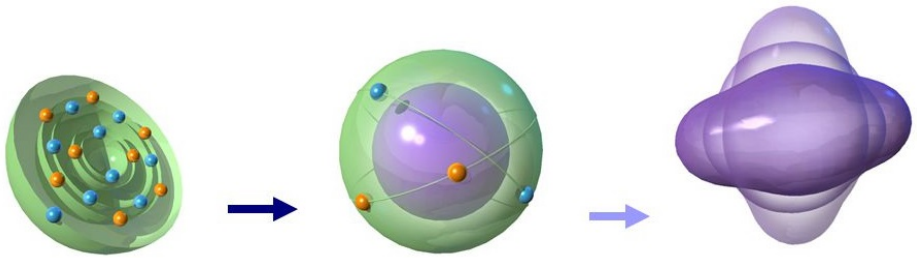


# Introduction: Standard model of nuclear physics

- Shell model: mean field, shell structure, no central force (M. Mayer, J. Jensen, 1963 Nobel Prize)




- Collective motions: rotation and vibration, particle-vibration coupling (A. Bohr, B. Mottelson, J. Rainwater, 1975 Nobel Prize)



**Road map** - Towards a comprehensive description of the nucleus

- ***Ab initio* methods**:

  Microscopic interactions

  Lattice QCD (A = 0, 1, 2, ...)

  NCSM, F-Y, GFMC (A = 3-16)

  Coupled cluster, IMSRG (A = 16-100)

- **Configuration-interaction theories**:

  Phenomenological interactions

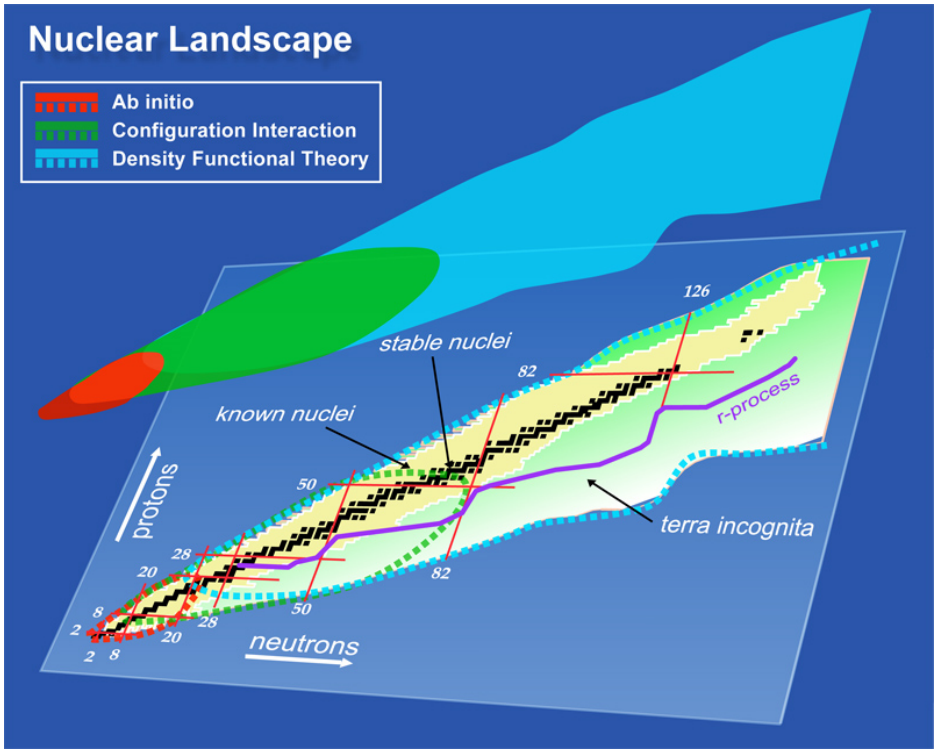
  Shell model

- **Density functional theories**:

  Phenomenological interactions

  mean field approximation

  Skyrme, Gogny, RMF, ...



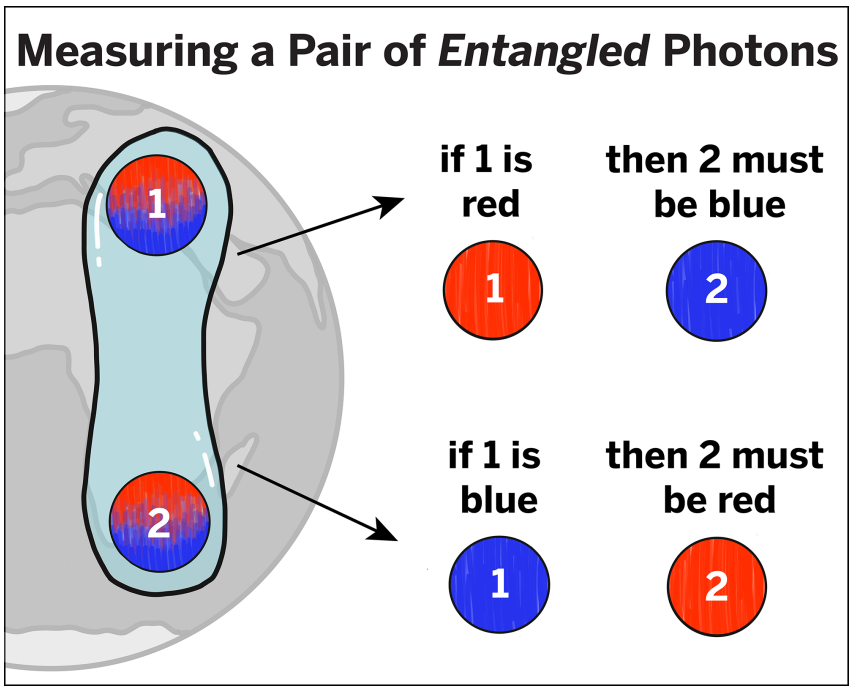

Lattice EFT: *Ab initio* method for A = 3-100

# Why need nuclear ab initio methods

Mean field models are useful

but **quantum correlations** not included

$$|\Psi\rangle = 1/\sqrt{2}\,[|0\rangle|1\rangle + |1\rangle|0\rangle]$$



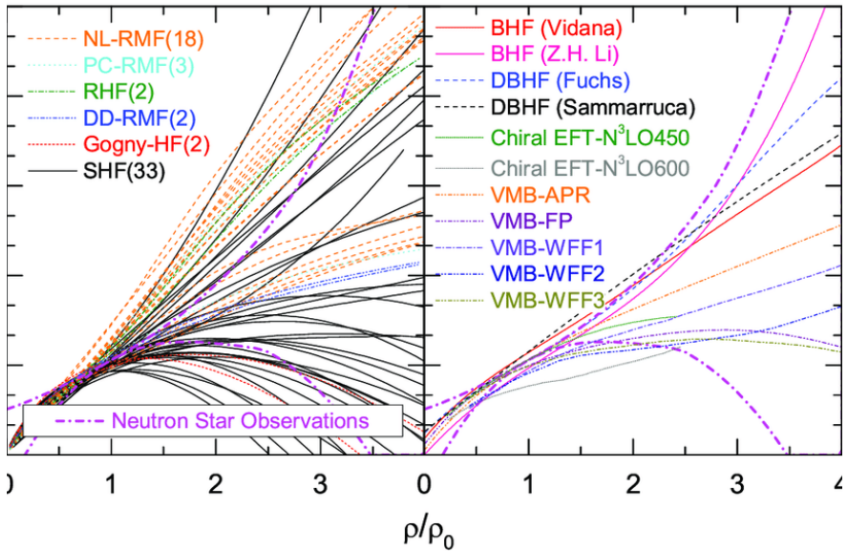

In mean field models, motion of particle 1

is independent of other particles

$$P(1,2) = P(1) \times P(2)$$

Predictions are model-dependent

Example: symmetry energy




N.-B. Zhang and B.-A. Li, EPJA 55, 39 (2019)

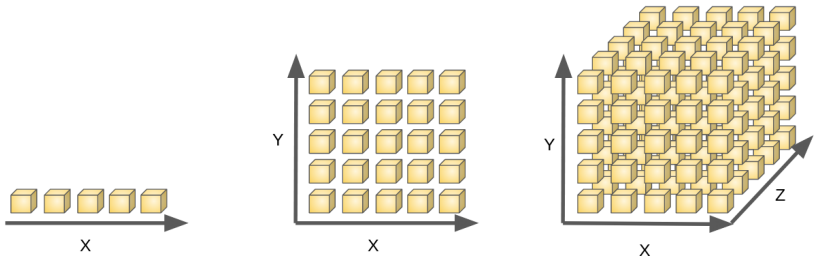
Symptom 1: Lack of quantum correlations

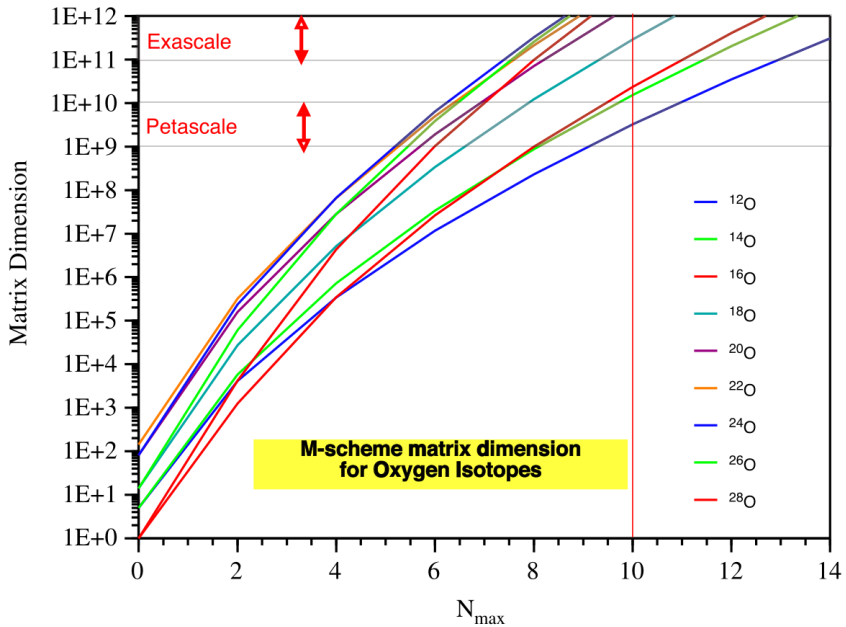
Symptom 2: Imprecise nuclear forces

Recipe: **Exactly** solve many-body Schrödinger equation with **precise** nuclear force $\Longrightarrow$ **nuclear ab initio methods**

# Dimensionality curse in nuclear many-body problems

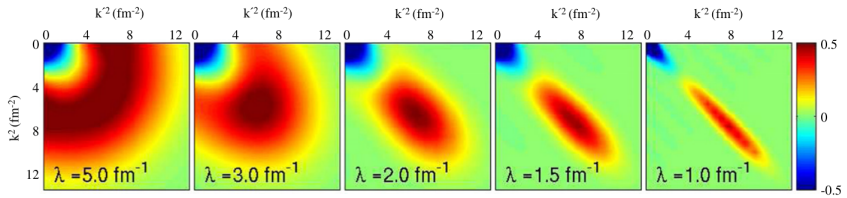
## Exponential increase of resources



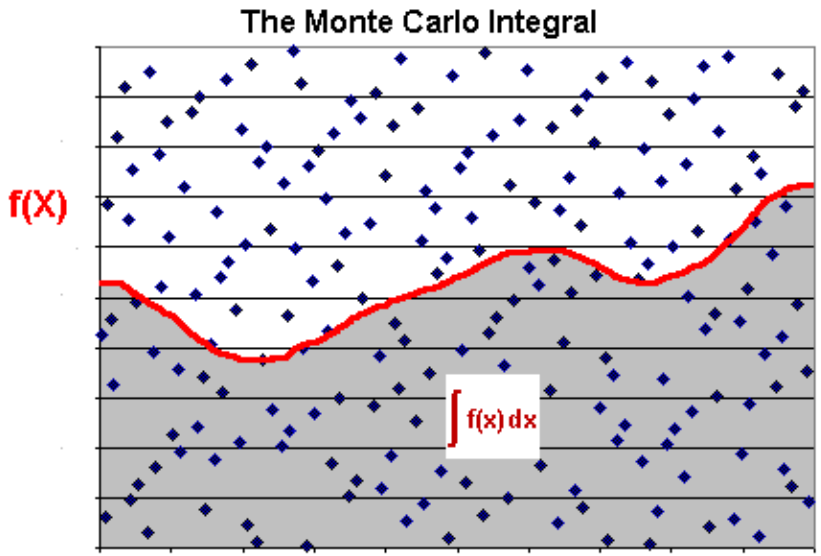




PRC 101, 014318 (2020)

## Solution 1: Reduce effective Hilbert space with SRG evolution



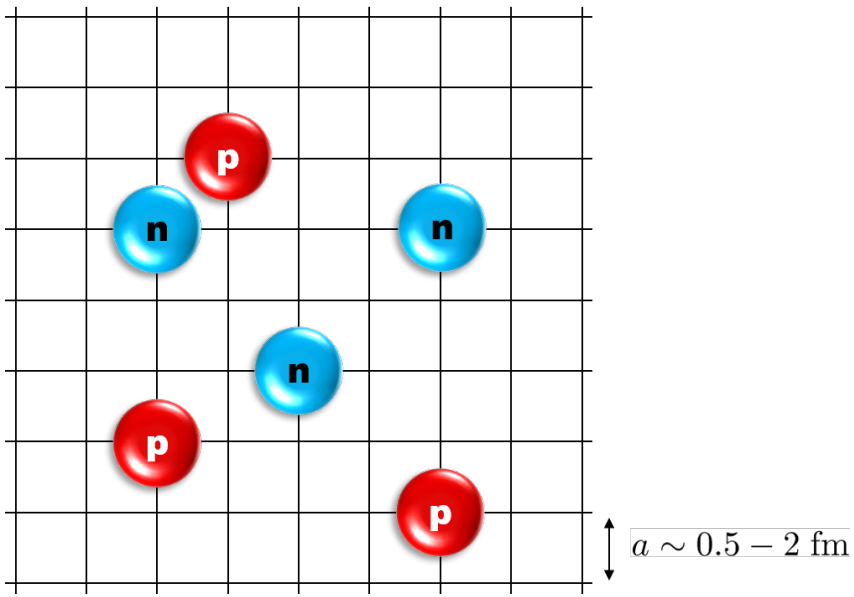

## Solution 2: Monte Carlo algorithms



**Lattice EFT = Chiral EFT + Lattice + Monte Carlo**

Review: Dean Lee, Prog. Part. Nucl. Phys. 63, 117 (2009),
Lähde, Meißner, "Nuclear Lattice Effective Field Theory", Springer (2019)

- Discretized chiral nuclear force
- Lattice spacing $a \approx 1$ fm $= 620$ MeV (∼chiral symmetry breaking scale)
- Protons & neutrons interacting via **short-range, $\delta$-like** and **long-range, pion-exchange** interactions
- Exact method, polynomial scaling ($\sim A^2$)



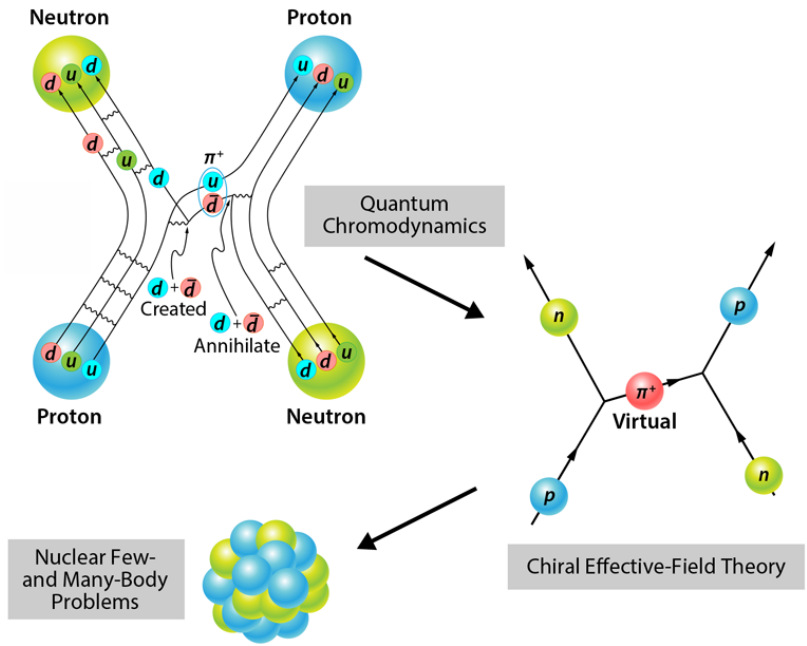

Lattice adapted for nucleus

# Introduction: Chiral effective field theory

Chiral EFT: The low-energy equivalence of the QCD

Weinberg (1979,1990,1991), Gasser, Leutwyler (1984,1985)

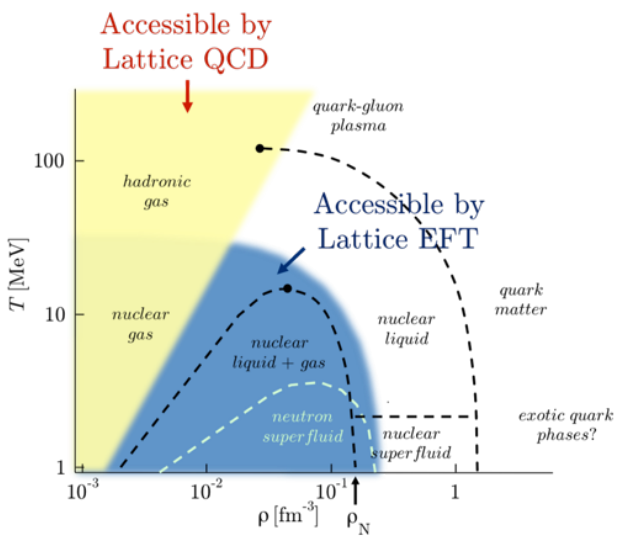
- Proton ($uud$), neutron ($udd$), pion ($u\bar{d}$)
- Spontaneously broken chiral symmetry: $SU(2)_L \times SU(2)_R \to SU(2)_V$
- Goldstone theorem implies a light pion:
  Long-range part of the nuclear force
- Contact terms:
  Short-range part of the nuclear force
- Hard scale: $\Lambda_\chi \sim 1$ GeV: Chiral EFT works for momentum $Q \ll \Lambda_\chi$

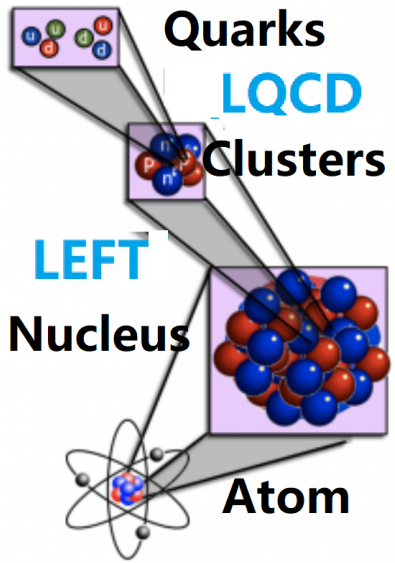



Quarks confined in nucleons and pions

# Comparison to Lattice QCD

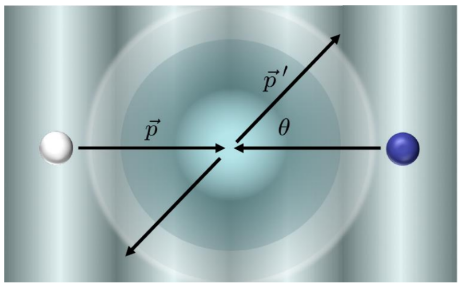
| | LQCD | LEFT |
|---|---|---|
| degree of freedom | quarks & gluons | nucleons and pions |
| lattice spacing | $\sim$0.1 fm | $\sim$1 fm |
| dispersion relation | relativistic | non-relativistic |
| renormalizability | renormalizable | effective field theory |
| continuum limit | yes | no |
| Coulomb | difficult | easy |
| accessibility | high $T$ / low $\rho$ | low $T$ / $\rho_{\rm sat}$ |
| sign problem | severe for $\mu > 0$ | moderate |

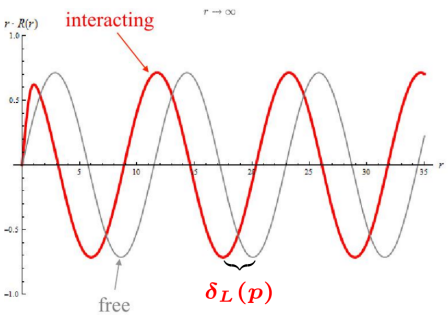


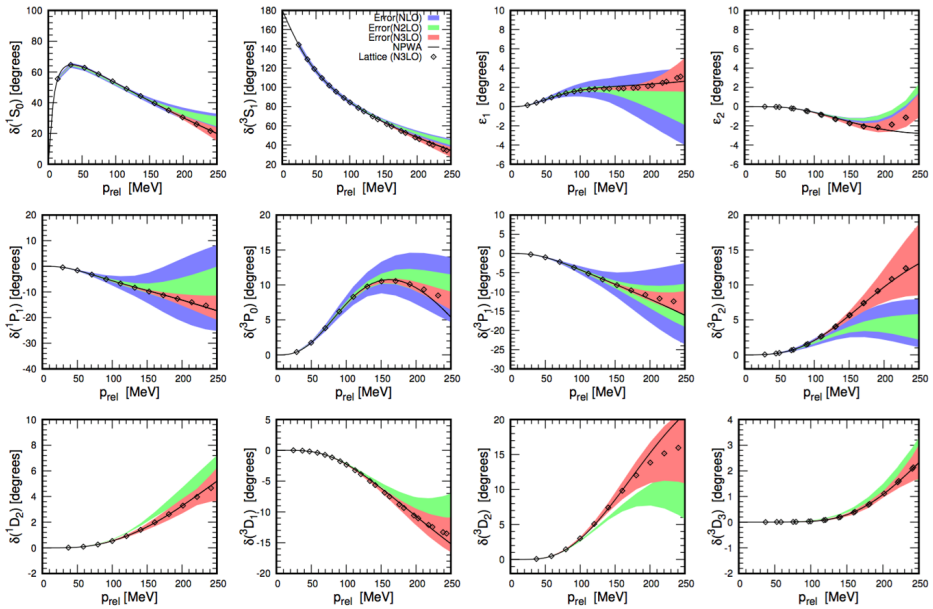



# Fit effective chiral force to N-N scattering data

- Chiral force is organized by a **power counting of** $(Q/\Lambda)^\nu$
- Fit chiral force in the **continuum** ($\Lambda \approx$ 400-500 MeV):
  - **IDAHO N$^4$LO**: Entem, Machleidt, Nosyk, PRC 96, 024004 (2017);
  - **Bochum N$^4$LO$_+$**: Reinert, Krebs, Epelbaum, EPJA 54, 86 (2018)
- Fit chiral force on the **lattice**: by Nuclear Lattice EFT group, in progress




- **Leading Order:** EPJA 31, 105 (2007)
- **Fit to NLO:** EPJA 35, 343 (2008)
- **Fit to N$^2$LO:** EPJA 53, 83 (2017)
- **Fit to N$^3$LO:** PRC 98, 044002 (2018)

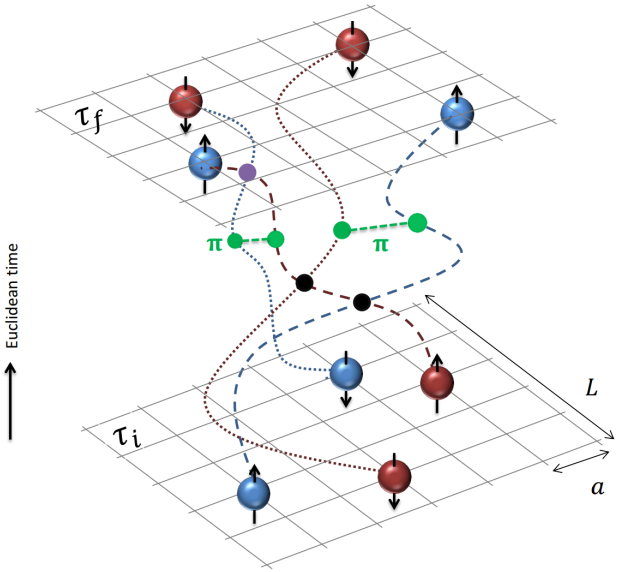
- **Restore rotational symmetry:** PRD 90, 034507 (2014)
- **Precision phase shifts on lattice:** PLB 760, 309 (2016)
- **Arbitrary coupled channels:** PRC 100, 064001 (2019)
- **Restore Galilean invariance:** PRC 99, 064001 (2019)

# Simulate many-body system in LEFT

- *g.s.* from **imaginary time projection**:

$$|\Psi_{\text{g.s.}}\rangle \propto \lim_{\tau\to\infty} \exp(-\tau H)|\Psi_A\rangle$$

with $|\Psi_A\rangle$ representing $A$ *free* nucleons.




- At finite temperature:

$$\langle O\rangle = \frac{\text{Tr}\left(e^{-\beta H}\hat{O}\right)}{\text{Tr}\left(e^{-\beta H}\right)}$$

For a two-body $\delta-$ function interaction on the lattice

$$H = \sum_{\boldsymbol{nn'}} -\psi^\dagger_{\boldsymbol{n}} \frac{\nabla^2_{\boldsymbol{nn'}}}{2M} \psi_{\boldsymbol{n'}} + C\sum_{\boldsymbol{n}} :(\psi^\dagger_{\boldsymbol{n}}\psi_{\boldsymbol{n}})^2:$$

$\psi^\dagger_{\boldsymbol{n}}(\psi_{\boldsymbol{n}})$ create (annihilate) a partice at mesh point $\boldsymbol{n}$.
N-N interactions decomposed with **Hubbard–Stratonovich transformation:**

$$:\exp(-a_t H):= \int \prod_{\boldsymbol{n}} ds_{\boldsymbol{n}} :\exp\left[\sum_{\boldsymbol{n}}\left(-\frac{s^2_{\boldsymbol{n}}}{2} + a_t\psi^\dagger_{\boldsymbol{n}}\sum_{\boldsymbol{n'}}\frac{\nabla^2_{\boldsymbol{nn'}}}{2M}\psi_{\boldsymbol{n'}} + \sqrt{-a_t C}\, s_{\boldsymbol{n}}\psi^\dagger_{\boldsymbol{n}}\psi_{\boldsymbol{n}}\right)\right]:$$

# Imaginary time extrapolation to find ground state

Samples are generated by

**Markov Chain Monte Carlo**

Observables calculated as $\langle O \rangle = (1/N) \sum_{i=1}^{N} O_i$

Error scales as $\varepsilon \sim \mathscr{O}(1/\sqrt{N})$

Number of samples $N \sim 10^3 \sim 10^6$

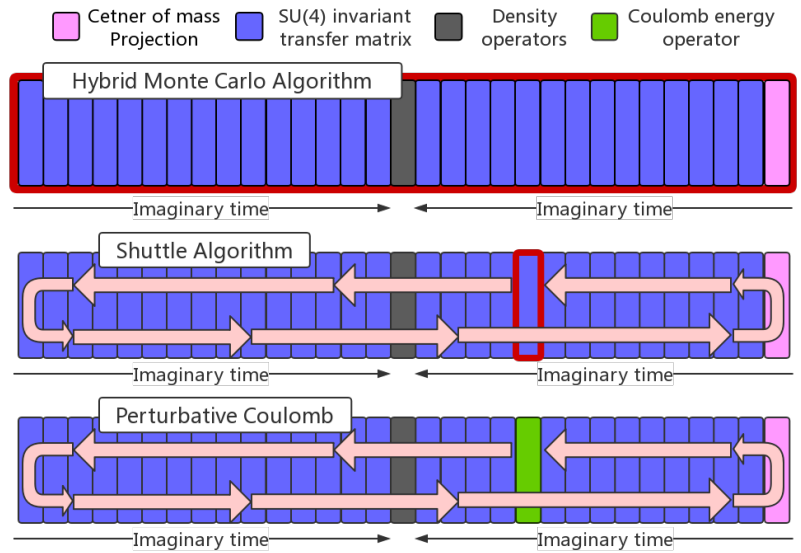
Total energies at large $t$ follow

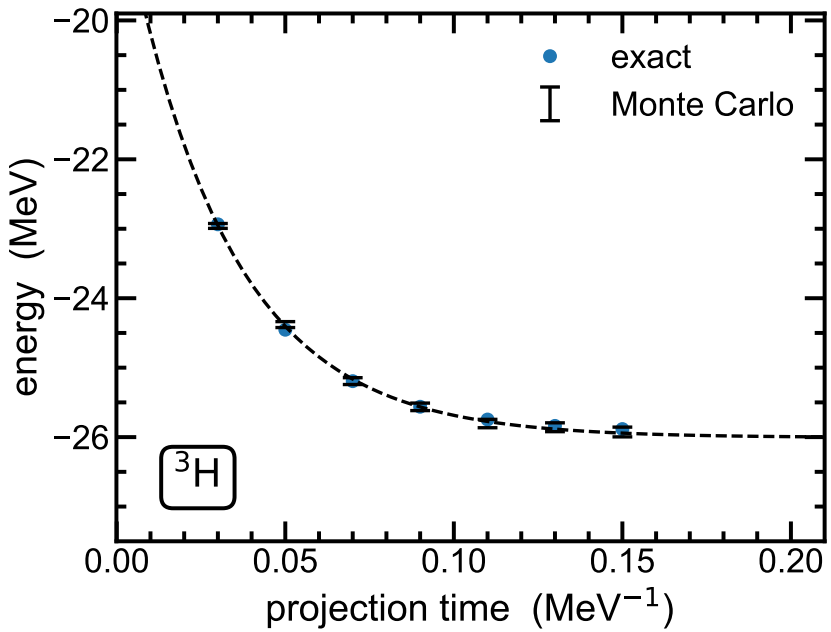
$$E_A(t) = E_A(\infty) + c \exp[-\Delta E \tau] .$$

For any inserted operator $\mathscr{O}$,

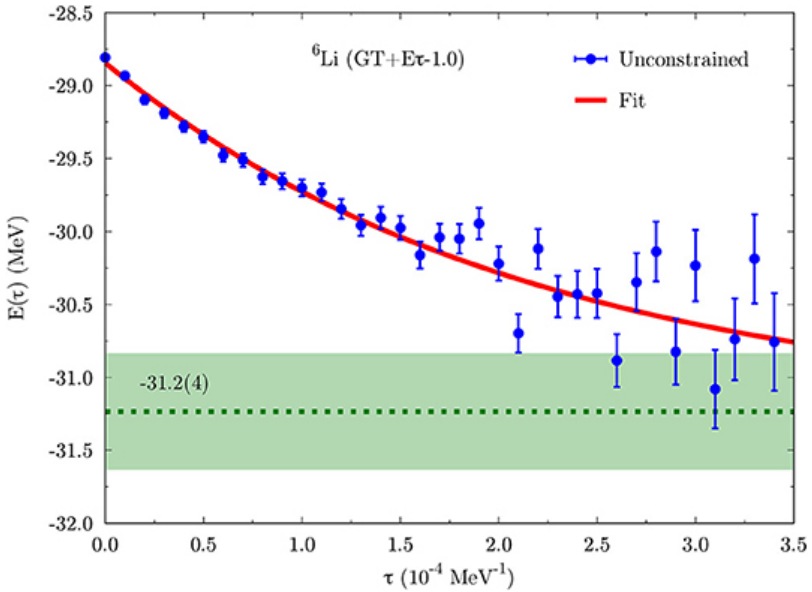
$$\mathscr{O}_A(\tau) = \mathscr{O}_A(\infty) + c' \exp[-\Delta E \tau/2] ,$$

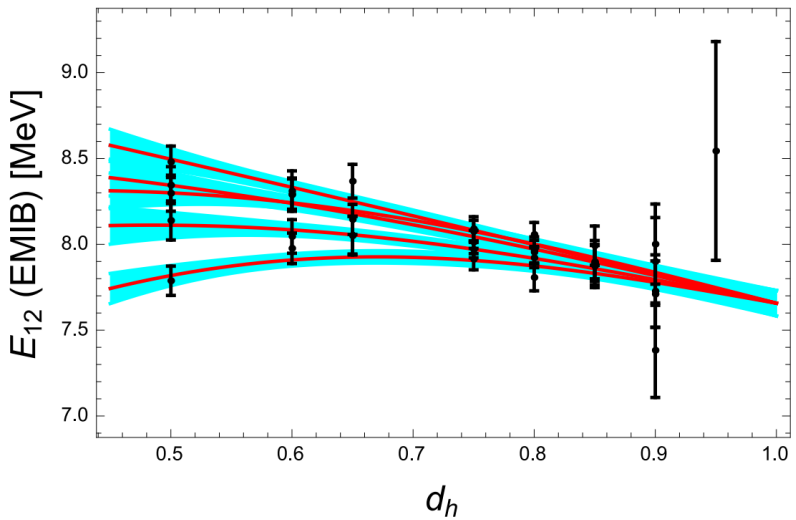
$c$, $c'$, $\Delta E$ are fitting parameters.

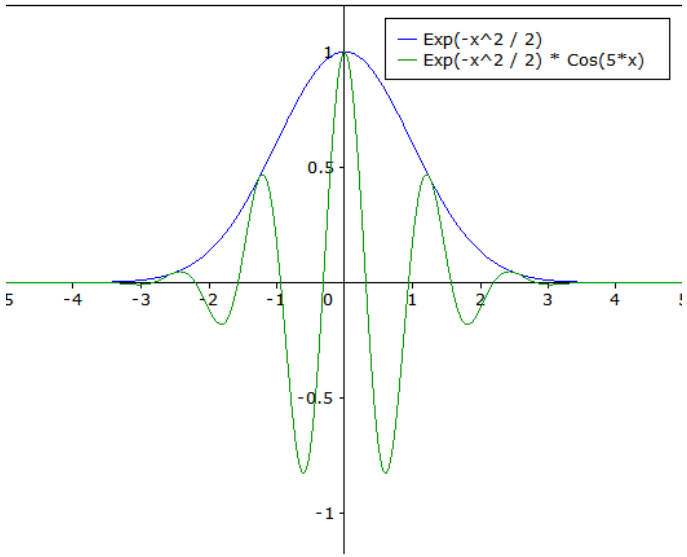


# Monte Carlo sign problem




- Sign problem: Monte Carlo works well for well-behaved functions, however, sometimes the integral becomes highly oscillating.
- QMC sign problem comes from the fermion anti-symmetrization.
- Split $H = H_0 + \lambda V_C$. $H_0$: w/o sign problem; $V_C$: w/ sign problem.
- **Solution 1**: numerical extrapolation from $\lambda = 0$ to $\lambda = 1$.
- **Solution 2**: perturbative calculation near $\lambda = 0$.

# Monte Carlo sign problem

Monte Carlo methods are powerful, but limited by sign problem
Fortunately, there are sign-problem-free systems with specific symmetries

"For example, the **nuclear systems** can be simulated with a SU(4) symmetric interaction in lattice EFT[18], or with simplified interactions such as AV8' with Green's function Monte Carlo method[44]. In **condensed matter physics**, the square-lattice Heisenberg model can be free from sign problem for specific parametrizations[45], and unified principles for designing sign-problem-free actions for lattice fermionic models are proposed[46-48]. In these works it was revealed that the sign problem can be avoided by imposing certain symmetries, such as time-reversal symmetry[46], Majorana positivity[47] or Majorana-time-reveral symmetry[48]. For **ultracold atoms**, spin- 3/2 fermionic system with exact SO(5) symmetry can be sign-problem-free[49] and more general rules for finding such systems are discussed[50]. The **unitary Fermi gas** with equal number of spin-up and spin-down particles provides another important system that can be simulated with QMC without the sign problem[51, 52]. In **quantum chemistry**, it is shown that the sign problem can be alleviated by optimizing the wave functions[53], or introducing efficiently computable basis changes[54]."

Nuclear force has an approximate SU(4) symmetry
In this SU(4) limit the nuclear force is independent of spin-isospin and can be simulated without sign problem $\Longleftarrow$ **How good is this approximation?**

# N-N interaction in large-$N_C$

- General form of the non-relativisitc N-N potential:

$$V_{NN} = V_C + V_S \vec{\sigma}_1 \cdot \vec{\sigma}_2 + V_{LS} \vec{L} \cdot \vec{S} + V_T S_{12} + V_Q Q_{12}$$
$$+ \left( W_C + W_S \vec{\sigma}_1 \cdot \vec{\sigma}_2 + W_{LS} \vec{L} \cdot \vec{S} + W_T S_{12} + W_Q Q_{12} \right) \vec{\tau}_1 \cdot \vec{\tau}_2$$
$$S_{12} = 3 \vec{\sigma}_1 \cdot \hat{r} \vec{\sigma}_2 \cdot \hat{r} - \vec{\sigma}_1 \cdot \vec{\sigma}_2$$
$$Q_{12} = \frac{1}{2} \left\{ (\vec{\sigma}_1 \cdot \vec{L}), (\vec{\sigma}_2 \cdot \vec{L}) \right\}$$

$\Longrightarrow$Standard decomposition in central ($V_C$, $W_C$, $V_S$, $W_S$), tensor ($V_T$, $W_T$), spin-orbit ($V_{LS}$, $W_{LS}$) and quadratic spin-orbit ($V_Q$, $W_Q$) terms

- Consider the limit $N_C \to \infty$ **with** $g^2 N_C =$**constant**
  t 'Hooft, Nucl. Phys. B 72, 461(1974)
  - **Central potentials:** $V_C(r)$, $W_S(r) \sim N_C$, $W_C(r)$, $V_S(r) \sim 1/N_C$
    $\Longrightarrow$Wigner SU(4) symmetry arises Kaplan, Savage, PLB 365 (1996) 244
  - **Spin-orbit potentials:** $V_{LS}(r)$, $W_{LS}(r) \sim 1/N_C$
  - **Tensor potentials:** $V_T(r) \sim 1/N_C$, $W_T(r) \sim N_C$
  - **Quadratic spin-orbit potentials:** $V_Q(r) \sim 1/N_C^3$, $W_Q(r) \sim 1/N_C$

| Isospin | $C$ | $S$ | $LS$ | $T$ | $Q$ |
|---|---|---|---|---|---|
| $V(r)$ | $N_C$ | $1/N_C$ | $1/N_C$ | $1/N_C$ | $1/N_C^3$ |
| $W(r)\vec{\tau}_1 \cdot \vec{\tau}_2$ | $1/N_C$ | $N_C$ | $1/N_C$ | $N_C$ | $1/N_C$ |

"Hidden spin-isospin exchange symmetry", Phys. Rev. Lett. 127, 062501 (2021)

# Evidence of hidden symmetry in nucleus

- Construct a N$^2$LO chiral force on the $a = 1.32$ fm ($\Lambda \approx 471$ MeV) lattice:

$$H_{\mathrm{N^2LO}} = -\frac{\nabla^2}{2M} + V_{2N} + V_{3N} + V_{1\mathrm{pion}} + V_{\mathrm{Coulomb}}$$

  $V_{1\mathrm{pion}}$ given by (broken) chiral symmetry. $V_{2N}$ fixed by N-N scattering data.

- $H_{\mathrm{N^2LO}}$ gives good description of symmetric nuclear matter and finite nuclei:

| | $\rho_{\mathrm{sat}}(\mathrm{fm}^{-3})$ | $E_{\mathrm{sat}}/A$ (MeV) | $K$ (MeV) | $E(^{16}\mathrm{O})$ (MeV) |
|---|---|---|---|---|
| LEFT | 0.165(1) | −15.9(0) | 263(8) | −117.1(1) |
| exp. | 0.16(1) | −16(1) | 240(20) | −127.6(0) |

- Contribution of various contact terms in $V_{2N}$ to $E(^{16}\mathrm{O})$ (perturbatively):

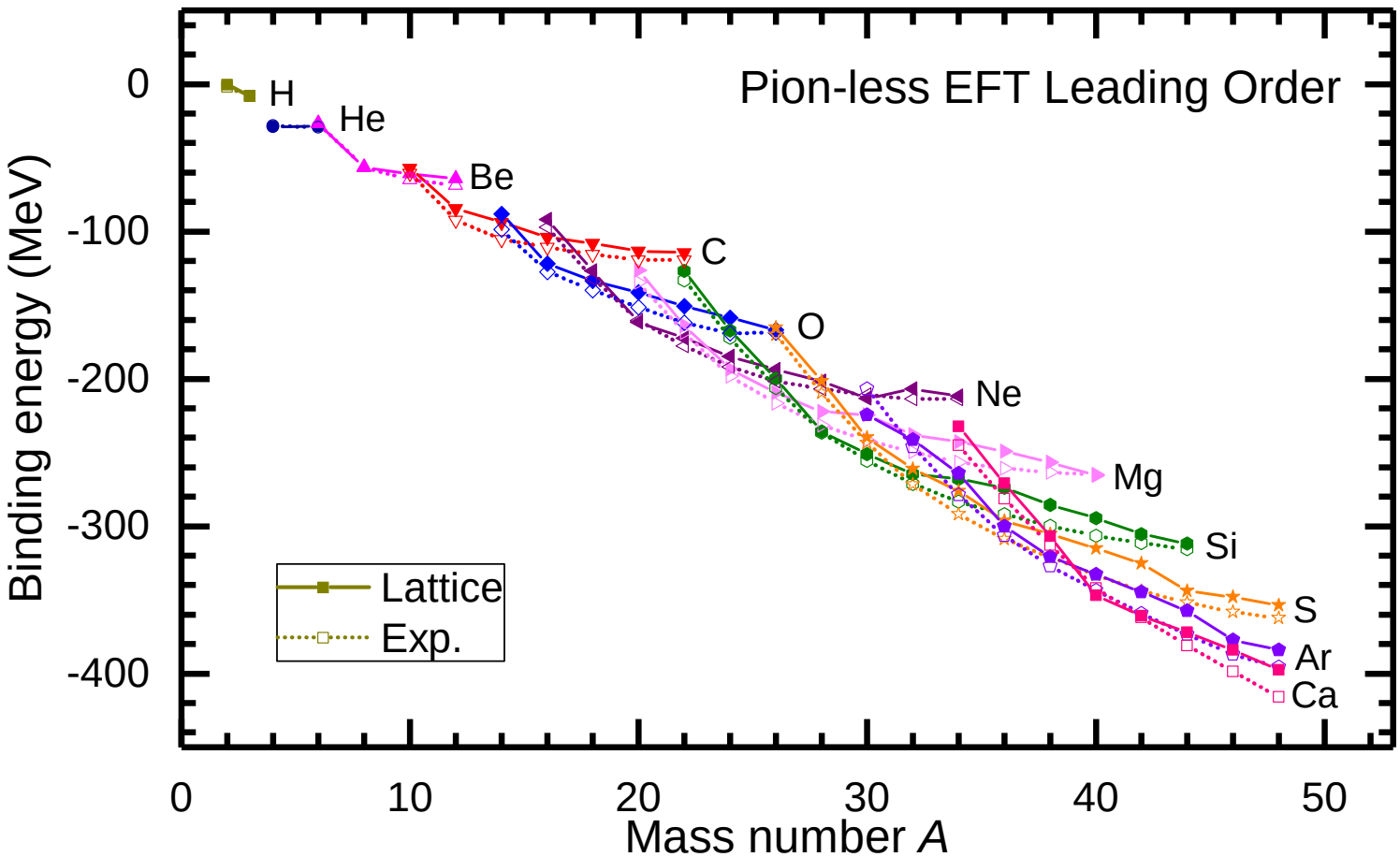
| operator | $N_C$ pow. | $Q$ pow. | $E$ (MeV) | operator | $N_C$ pow. | $Q$ pow. | $E$ (MeV) |
|---|---|---|---|---|---|---|---|
| 1 | $N_C$ | 1 | −430.4 | $q^2\vec{\sigma}_1\cdot\vec{\sigma}_2\vec{\tau}_1\cdot\vec{\tau}_2$ | $N_C$ | $(Q/\Lambda)^2$ | 24.2 |
| $\vec{\sigma}_1\cdot\vec{\sigma}_2$ | $1/N_C$ | 1 | 33.0 | $\frac{i}{2}(q\times k)\cdot(\vec{\sigma}_1+\vec{\sigma}_2)$ | $1/N_C$ | $(Q/\Lambda)^2$ | 0.0 |
| $q^2$ | $N_C$ | $(Q/\Lambda)^2$ | 22.8 | $(\vec{\sigma}_1\cdot q)(\vec{\sigma}_2\cdot q)$ | $1/N_C$ | $(Q/\Lambda)^2$ | 0.4 |
| $q^2\vec{\tau}_1\cdot\vec{\tau}_2$ | $1/N_C$ | $(Q/\Lambda)^2$ | 6.0 | $(\vec{\sigma}_1\cdot q)(\vec{\sigma}_2\cdot q)\vec{\tau}_1\cdot\vec{\tau}_2$ | $N_C$ | $(Q/\Lambda)^2$ | 30.5 |
| $q^2\vec{\sigma}_1\cdot\vec{\sigma}_2$ | $1/N_C$ | $(Q/\Lambda)^2$ | 0.6 | | | | |

- Note that $1/N_C^2 \approx 0.1$, $(Q/\Lambda)^2 \approx 0.2$ in $^{16}$O. **Red:** suppressed by $1/N_C^2$ or $(Q/\Lambda)^2$. **Blue:** suppressed by both factors.$\Longleftarrow$**very clear hierachy**
- SU(4) symmetric term dominate$\Longleftarrow$**No sign problem, good for MC**

# Nuclear binding from a SU(4) nuclear force

Ab initio calculation = **precise nuclear force** + **exactly solving Schrödinger equations**

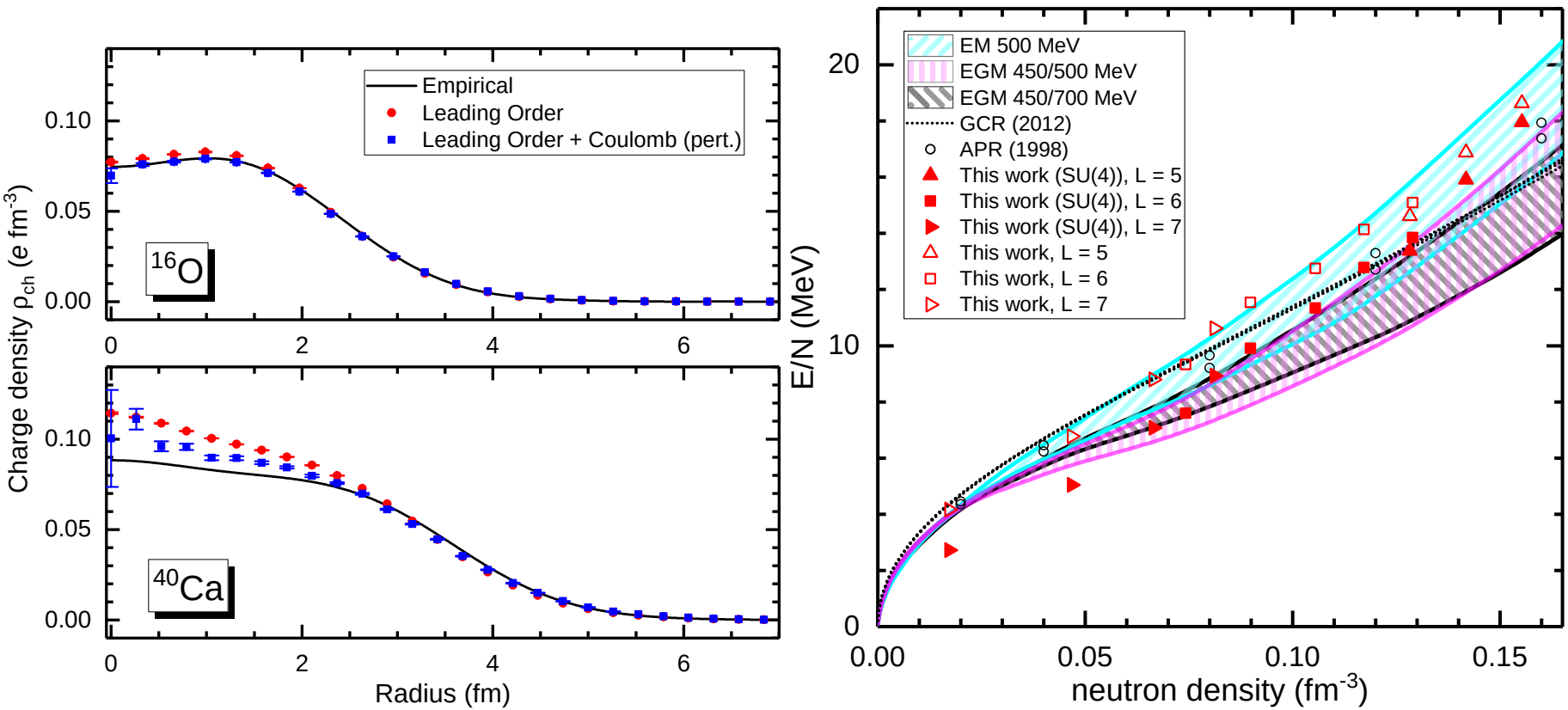
In full quantum Monte Carlo simulations, **equations are solved exactly**
**A simple SU(4) interaction** (central force only!) can describe the nuclear binding




Lu et al., Phys. Lett. B 797, 134863 (2019)

# Charge density and neutron matter from a SU(4) force

Charge density and neutron matter equation of state
are impotant in element creation, neutron star merger, etc.




Lu et al., Phys. Lett. B 797, 134863 (2019)

# Trade-off in Monte Carlo simulations

- Simplified interactions with high symmetry $\Longrightarrow$Sign-problem-free, exactly solvable with MC
- Realistic complex interactions $\Longrightarrow$Severe sign problem, can only be approximately solved with mean field methods

**Is it possible to exactly solve a realistic interaction with MC?**

**Idea: Starting from a simplified sign-problem-free interaction add corrections with perturbation theory**

- Much weaker sign problem in perturbative calculations
- Most quantum correlations included non-perturbatively
- Systematically improvable order by order, can check convergence

Higher order perturbation theory is complicated
(e.g., exponentially increasing number of Feynman diagrams)
Adaptation to MC is even more challenging!

# Reyleigh-Schrödinger perturbation theory

For a Hamiltonian $H = H^{(0)} + \lambda V_C$,

- In conventional stationary perturbation theory:

$$E_i = E_i^{(0)} + \lambda \langle \Psi_i^{(0)} | V_C | \Psi_i^{(0)} \rangle + \lambda^2 \sum_{k \neq 0} \frac{\langle \Psi_k^{(0)} | V_C | \Psi_i^{(0)} \rangle}{E_k^{(0)} - E_i^{(0)}} + \mathcal{O}(\lambda^3)$$

$$|\Psi_i\rangle = |\Psi_i^{(0)}\rangle + \lambda \sum_{k \neq 0} \frac{\langle \Psi_k^{(0)} | V_C | \Psi_i^{(0)} \rangle}{E_k^{(0)} - E_i^{(0)}} |\Psi_k^{(0)}\rangle + \mathcal{O}(\lambda^2)$$

- However, in projection Monte Carlo algorithms,

$$E_{\text{g.s.}} = \lim_{\tau \to \infty} \exp(-\tau H) |\Psi_T\rangle$$

  targets the ground states (or low-lying states) directly.
- In projection methods, excited states are very expensive. $\leftarrow$ required for 2nd order energy or 1st order wave function!
- All projection QMC calculations use at most first order perturbation theory.

# Perturbative Monte Carlo (ptQMC) algorithm

We can expand $|\Psi\rangle$ against $V_C$,

$$|\Psi\rangle = \lim_{L_t\to\infty} M^{L_t/2}|\Psi_T\rangle = |\Psi_0\rangle + |\delta\Psi_1\rangle + \mathscr{O}(V_C^2), \tag{1}$$

with the wave functions defined as

$$|\Psi_0\rangle = \lim_{L_t\to\infty} M_0^{L_t/2}|\Psi_T\rangle, \qquad |\delta\Psi_1\rangle = \lim_{L_t\to\infty} \sum_{k=1}^{L_t/2} M_0^{L_t/2-k}(M-M_0)M_0^{k-1}|\Psi_T\rangle,$$

$$E \quad = \quad E_0 + \delta E_1 + \delta E_2 + \mathscr{O}(V_C^3),$$

where the partial energy contributions at each orders are

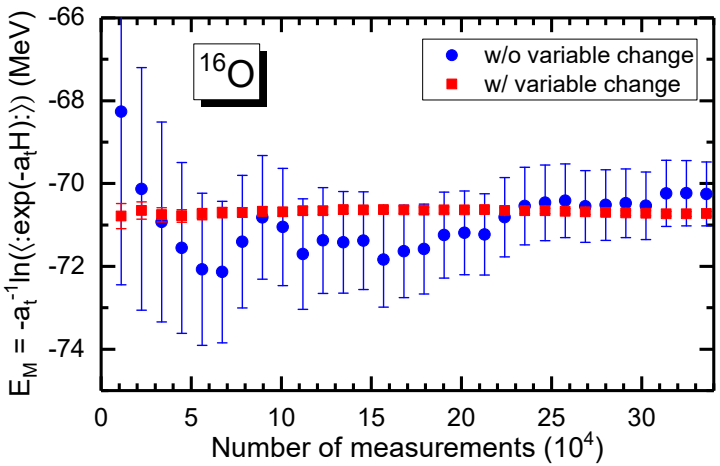
$$\begin{aligned} E_0 &= \langle\Psi_0|(K+V)|\Psi_0\rangle/\langle\Psi_0|\Psi_0\rangle, \\ \delta E_1 &= \langle\Psi_0|V_C|\Psi_0\rangle/\langle\Psi_0|\Psi_0\rangle, \\ \delta E_2 &= \left(\langle\Psi_0|V_C|\delta\Psi_1\rangle - \delta E_1 \mathrm{Re}\langle\delta\Psi_1|\Psi_0\rangle\right)/\langle\Psi_0|\Psi_0\rangle, \end{aligned} \tag{2}$$

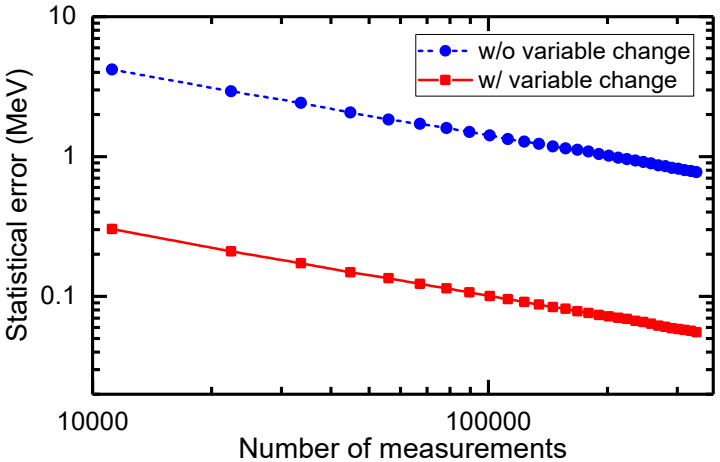
in which all matrix elements and overlaps can be expressed with,

$$\begin{aligned} \mathscr{M}(O) &= \langle\Psi_T|M_0^{L_t/2}OM_0^{L_t/2}|\Psi_T\rangle, \\ \mathscr{M}_k(O) &= \langle\Psi_T|M_0^{L_t/2}OM_0^{L_t/2-k}MM_0^{k-1}|\Psi_T\rangle. \end{aligned}$$

Lu *et al.*, PRL 128, 242501 (2022)

# ptQMC with realistic chiral interaction




Perturbed amplitude can be transformed into an approximate Gaussian integral with a variable change. Note that

$$\langle \exp(\sqrt{-a_t C}s\rho)\rangle_T \approx \exp(\sqrt{-a_t C}s\langle\rho\rangle_T)$$

$$\begin{aligned}\mathscr{M}_k(O) &= \langle\Psi_T|M_0^{L_t/2}OM_0^{L_t/2-k}MM_0^{k-1}|\Psi_T\rangle \\ &= \int \mathscr{D}c P(c+\bar{c})\langle\cdots O\cdots M(s_k,c+\bar{c})\cdots\rangle_T \\ &= \mathscr{M}(s)\exp\left(\frac{\bar{c}^2}{2}\right)\int \mathscr{D}c\exp\left(-\frac{c^2}{2}+\varepsilon\right)\end{aligned}$$

$\bar{c}(\boldsymbol{n}) = \frac{\partial}{\partial c(\boldsymbol{n})}\ln\langle\cdots M(s_k,c)\cdots\rangle_T\Big|_{c=0}$ is a constant field easy to calculate

**Integral over $c$ calculated with MC**

Left panel: Test calculation of the transfer matrix energy $E = -\ln\langle:\exp(-a_tH):\rangle/a_t$
Lu *et al.*, PRL 128, 242501 (2022)

# Benchmark Hamiltonian: N$^2$LO chiral Hamiltonian

We benchmark the ptQMC algorithm with a N$^2$LO chiral Hamiltonian
$H = K + V_{2\mathrm{N}} + V_{3\mathrm{N}} + V_{\mathrm{cou}}$

$$
\begin{aligned}
V_{2N} = & \Big[ B_1 + B_2(\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2) + C_1 q^2 + C_2 q^2 (\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2) + C_3 q^2 (\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2) + C_4 q^2 (\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2)(\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2) \\
& + C_5 \frac{i}{2} (\boldsymbol{q} \times \boldsymbol{k}) \cdot (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) + C_6 (\boldsymbol{\sigma}_1 \cdot \boldsymbol{q})(\boldsymbol{\sigma}_2 \cdot \boldsymbol{q}) + C_7 (\boldsymbol{\sigma}_1 \cdot \boldsymbol{q})(\boldsymbol{\sigma}_2 \cdot \boldsymbol{q})(\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2) \Big] e^{-\Sigma_{i=1}^{2} \left( p_i^6 + p_i'^6 \right)/\Lambda^6} \\
& - \frac{g_A^2 f_\pi(q^2)}{4F_\pi^2} \left[ \frac{(\boldsymbol{\sigma}_1 \cdot \boldsymbol{q})(\boldsymbol{\sigma}_2 \cdot \boldsymbol{q})}{q^2 + M_\pi^2} + C_\pi' \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \right] (\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2) \\
V_{3\mathrm{N}} = & \frac{c_E}{2F_\pi^4 \Lambda_\chi} e^{-\Sigma_{i=1}^{3} \left( p_i^6 + p_i'^6 \right)/\Lambda^6}
\end{aligned}
$$

with $C_{1-7}$, $g_A$, $c_E$ etc. **low energy constants** fitted to N-N scattering or $\pi$-N scattering data, $\Lambda = 340$ MeV is the **momentum cutoff**

| LEC | $B_1$ | $B_2$ | $C_1$ | $C_2$ | $C_3$ |
|---|---|---|---|---|---|
| | $-2.443$ | $-0.125$ | 0.143 | $-0.012$ | $-0.013$ |
| LEC | $C_4$ | $C_5$ | $C_6$ | $C_7$ | $c_E$ |
| | $-0.020$ | 0.273 | 0.0 | $-0.078$ | 0.712 |

Table: Fitted LECs' in lattice unit

# Zeroth order Hamiltonian (perturbative order)

We use a zeroth order lattice Hamiltonian that respects the Wigner-SU(4) symmetry

$$H_0 = K + \frac{1}{2} C_{\mathrm{SU4}} \sum_{\boldsymbol{n}} : \tilde{\rho}^2(\boldsymbol{n}) :$$

The smeared density operator $\tilde{\rho}(\boldsymbol{n})$ is defined as

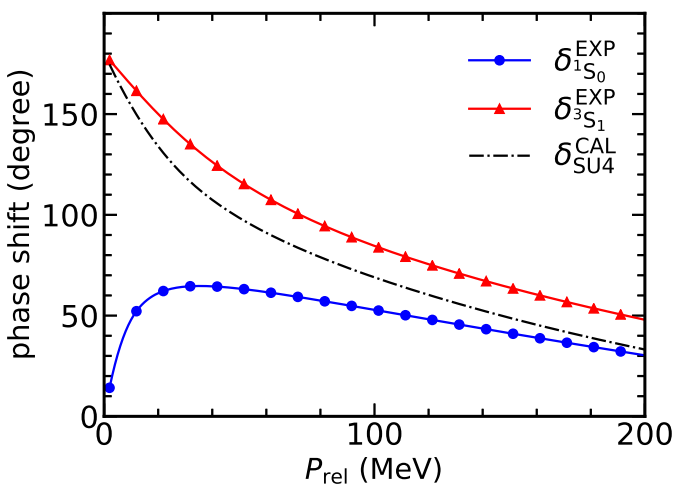
$$\tilde{\rho}(\boldsymbol{n}) = \sum_i \tilde{a}_i^\dagger(\boldsymbol{n}) \tilde{a}_i(\boldsymbol{n}) + s_L \sum_{|\boldsymbol{n}'-\boldsymbol{n}|=1} \sum_i \tilde{a}_i^\dagger(\boldsymbol{n}') \tilde{a}_i(\boldsymbol{n}'), \tag{3}$$

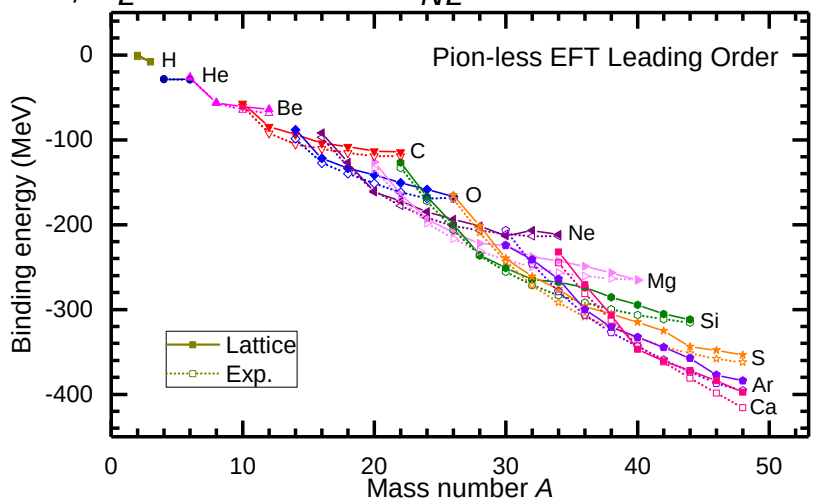
where $i$ is the joint spin-isospin index

$$\tilde{a}_i(\boldsymbol{n}) = a_i(\boldsymbol{n}) + s_{NL} \sum_{|\boldsymbol{n}'-\boldsymbol{n}|=1} a_i(\boldsymbol{n}'). \tag{4}$$

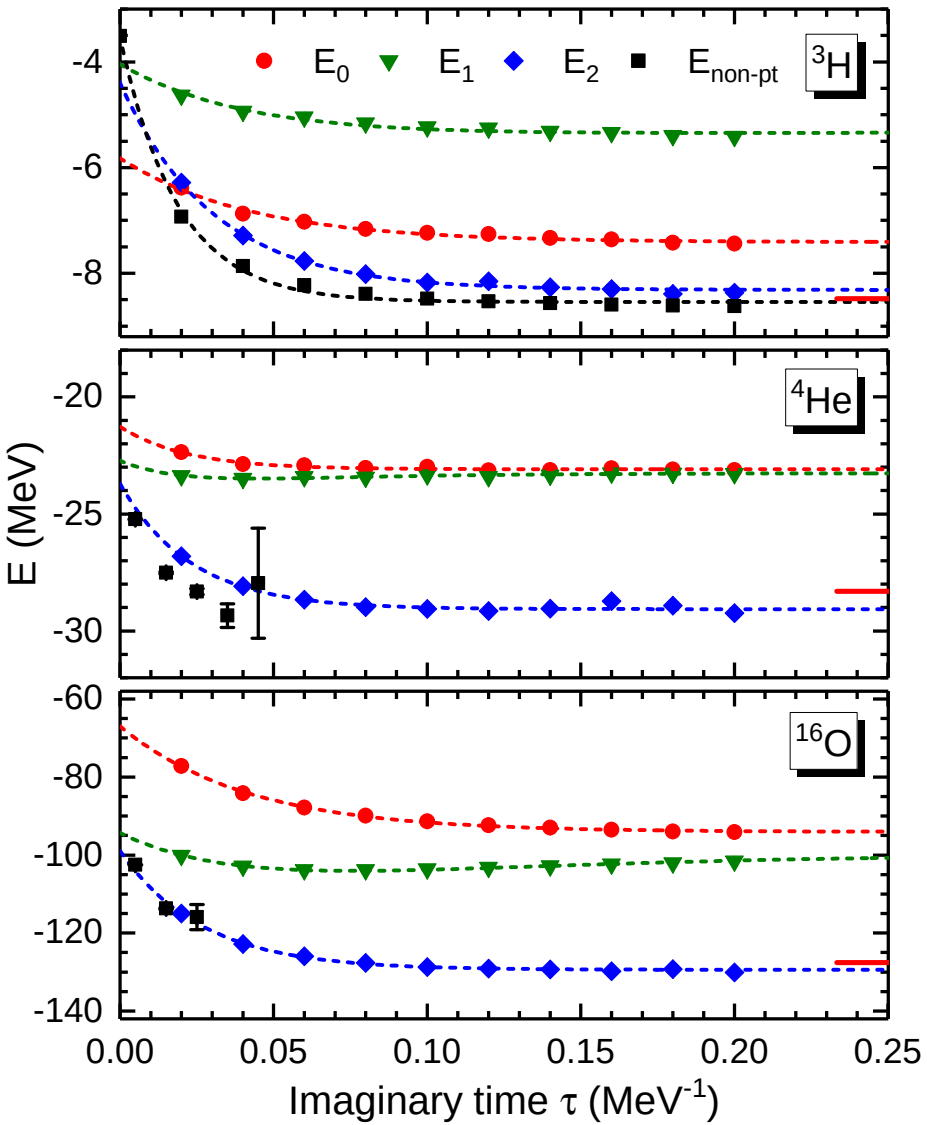
In this work we use a lattice spacing $a = 1.32$ fm and the parameter set

$C_{\mathrm{SU4}} = -3.41 \times 10^{-7}$ MeV$^{-2}$, $s_L = 0.061$ and $s_{NL} = 0.5$ .



# ptQMC with realistic chiral interaction

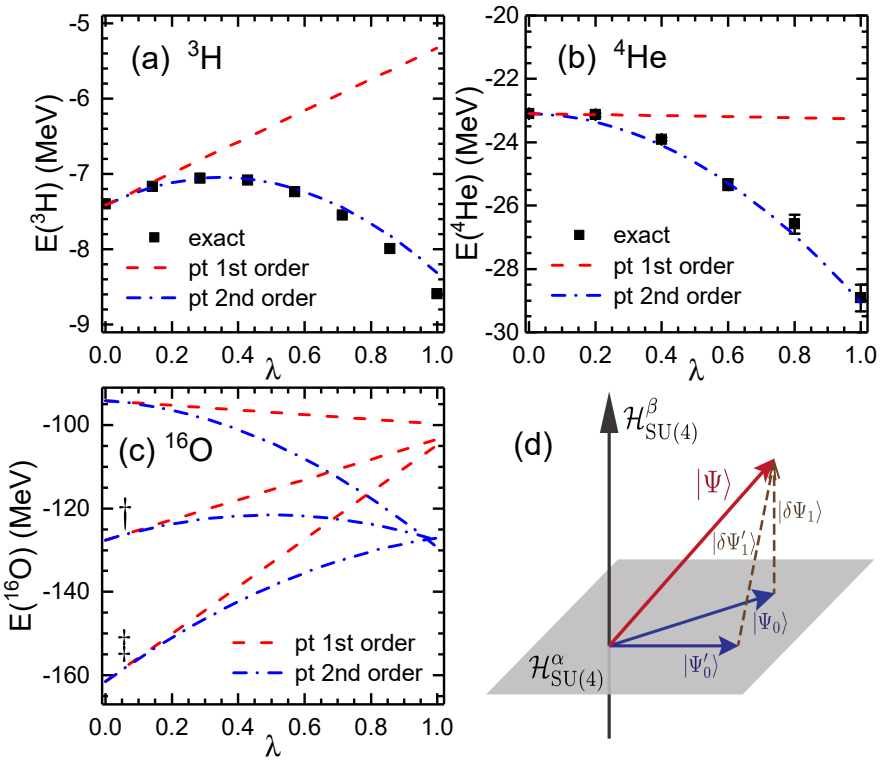



- We split $H = H_0 + (H - H_0)$ and perform perturbative calculations
- $E_0$ is the ground state of $H_0$
- $E_1 = E_0 + \delta E_1$ is the first order corrected energy
- $E_2 = E_1 + \delta E_2$ is the second order corrected energy
- $E_{\mathrm{non-pt}}$ is the exact solution (∼infinite order)
- Red bars on the right: Experiments Lu *et al.*, PRL 128, 242501 (2022)

**For $^4$He and $^{16}$O, sign problem prevent us from going to large $\tau$, resulting in large statistical errors. But no need to worry,**

**Perturbation theory can save us!**

# Abnormally large second order corrections




- Though consistent with the exact solutions, we found abnormally large second order energy corrections
- We write $H = H_0 + \lambda(H - H_0)$ and study the $\lambda$-dependence of energies $(0 \leq \lambda \leq 1)$
- $E_1 = E_0 + \lambda \delta E_1$ is a straight line
- $E_2 = E_1 + \lambda^2 \delta E_2$ is a parabola
- $E_{\text{non-pt}}$ is the exact solution
- For $^{16}$O we use three different $H_0$ Lu *et al.*, PRL 128, 242501 (2022)

**As $H_0$ respects the SU(4) symmetry, the wave function $|\Psi_0\rangle$ must belong to one of its irreducible representations (irreps). The full Hamiltonian $H$ breaks the SU(4) symmetry, thus its ground state $|\Psi\rangle$ is a mixture of different SU(4) irreps. The components of $|\Psi\rangle$ that mixes the SU(4) irreps can only be seen in $|\delta\Psi_1\rangle$ or $\delta E_2$**

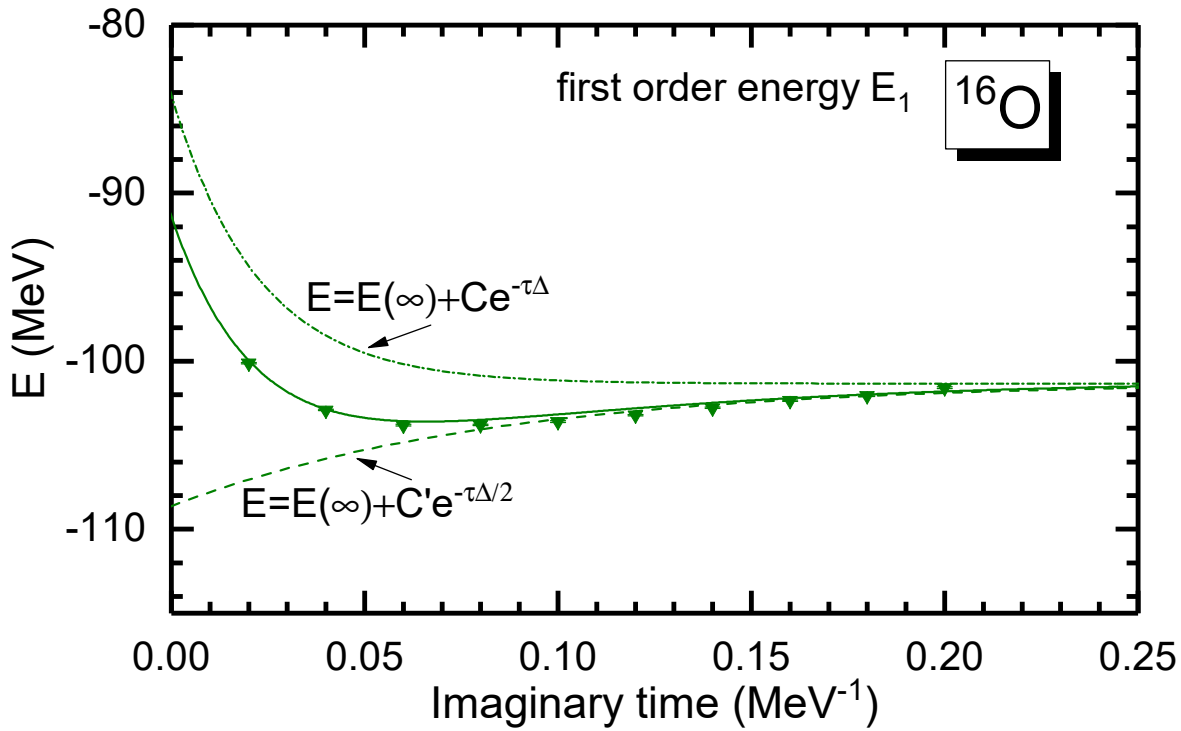
**Reminder**: A **symmetry breaking** perturbative Hamiltonian usually implies a large 2nd order energy correction!

# Asymptotic beheaviour of the first order energy $E_1$

The first order energy $E_1$ consists of components with **different decay rates**

$\Longrightarrow$ must be careful in extrapolations to $\tau \to \infty$

$$
\begin{aligned}
E_1(\tau) &= \frac{\langle \Psi_T | e^{-\tau H_0/2} (H_0 + V_C) e^{-\tau H_0/2} | \Psi_T \rangle}{\langle \Psi_T | e^{-\tau H_0} | \Psi_T \rangle} \\
&= \Big[ E_0 + e^{-\tau\Delta} |C'|^2 E_1 + \langle \Psi_0 | V_C | \Psi_0 \rangle + 2 e^{-\tau\Delta/2} \mathrm{Re} \left[ C' \langle \Psi_0' | V_C | \Psi_0 \rangle \right] \\
&\quad + |C'|^2 e^{-\tau\Delta} \langle \Psi_0' | V_C | \Psi_0' \rangle \Big] / \left( 1 + |C'|^2 e^{-\tau\Delta} \right) \\
&= E_0 + \langle \Psi_0 | V_C | \Psi_0 \rangle + e^{-\tau\Delta/2} \times 2\mathrm{Re} \left[ C' \langle \Psi_0' | V_C | \Psi_0 \rangle \right] + e^{-\tau\Delta} |C'|^2 (E_1' - E_1)
\end{aligned}
$$



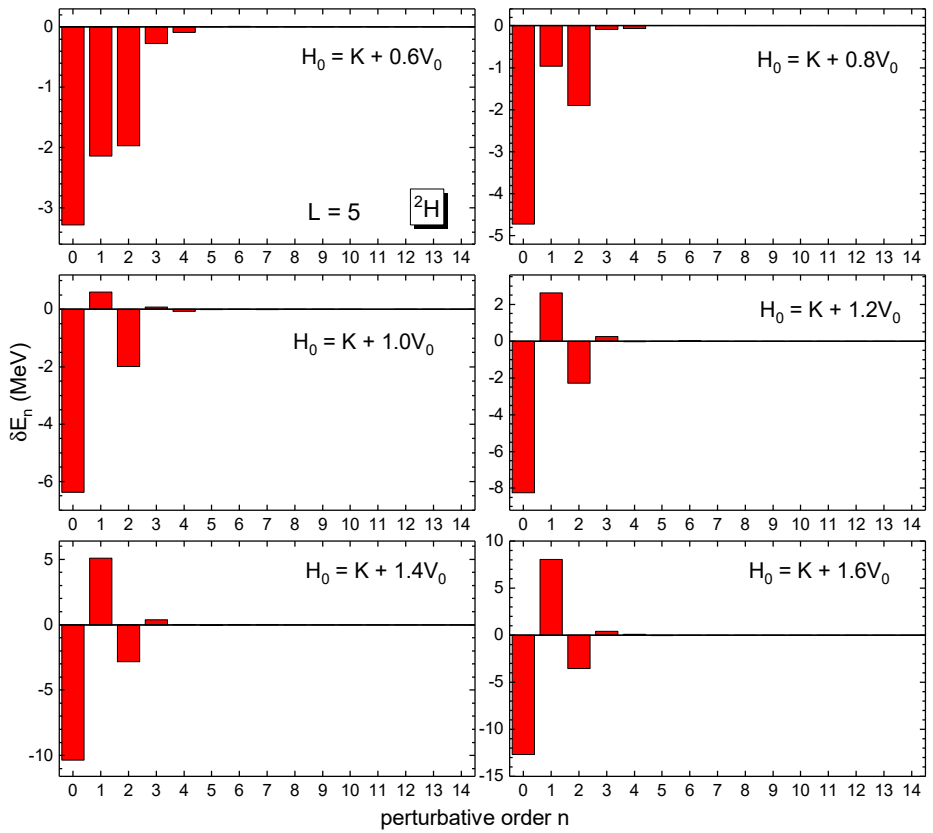
# Numerical results for several light nuclei

Table: The nuclear binding energies at different orders calculated with the ptQMC. $E_{\rm exp}$ is the experimental value. All energies are in MeV. We only show statistical errors from the MC simulations.

| | $E_0$ | $\delta E_1$ | $E_1$ | $\delta E_2$ | $E_2$ | $E_{\rm exp}$ |
|---|---|---|---|---|---|---|
| $^3$H | $-7.41(3)$ | $+2.08$ | $-5.33(3)$ | $-2.99$ | $-8.32(3)$ | $-8.48$ |
| $^4$He | $-23.1(0)$ | $-0.2$ | $-23.3(0)$ | $-5.8$ | $-29.1(1)$ | $-28.3$ |
| $^8$Be | $-44.9(4)$ | $-1.7$ | $-46.6(4)$ | $-11.1$ | $-57.7(4)$ | $-56.5$ |
| $^{12}$C | $-68.3(4)$ | $-1.8$ | $-70.1(4)$ | $-18.8$ | $-88.9(3)$ | $-92.2$ |
| $^{16}$O | $-94.1(2)$ | $-5.6$ | $-99.7(2)$ | $-29.7$ | $-129.4(2)$ | $-127.6$ |
| $^{16}$O$^\dagger$ | $-127.6(4)$ | $+24.2$ | $-103.4(4)$ | $-24.3$ | $-127.7(2)$ | $-127.6$ |
| $^{16}$O$^\ddagger$ | $-161.5(1)$ | $+56.8$ | $-104.7(2)$ | $-22.3$ | $-127.0(2)$ | $-127.6$ |

Realistic N$^2$LO chiral Hamiltonian fixed by few-body data + perturbative quantum MC simulation = nice agreement with the experiments
Excellent predicative power $\Longrightarrow$ Demonstration of both **nuclear force model** and **many-body algorithm**

# Perturbative calculations beyond the second order




Perturbative energy correction $\delta E_n$ of the deuteron at each order. For the zeroth order we show $E_0$.

- We calculated deuteron energy $E(^2\mathrm{H})$ in a small box $L = 6.6$ fm with a chiral Hamiltonian
- $H$ is split as $H = (K + \mu V_0) + (V - \mu V_0)$, $V_0$ is the SU(4) interaction and $V$ is the full chiral interaction
- $\mu = 0.6, \cdots, 1.6$ is a constant

**$E_0$, $\delta E_1$ and $\delta E_2$ are always significant. $\delta E_3$ and higher order contributions are negligible, regardless of what $H_0$ we choose as the unperturbed Hamiltonian**

**The second order correction is large due to the symmetry breaking effect. There is no such mechanism for higher-order corrections, thus the higher-order corrections follow the usual power-counting hierachy.**

# Summary & Perspective

- Ab initio nuclear physics grows rapidly in **last two decades**.
  - No core shell model, In-medium SRG, lattice EFT, Green's function Monte Carlo, Coupled cluster, ...
  - mass 4-100, ground state, excited states, finite - $T$, etc.
- Monte Carlo methods are powerful but plagued by the sign problem.
- Combining MC methods with the perturbation theory may solve the sign problem in many useful senarios.
- We developed an efficient algorithm for doing perturbative calculations in MC methods beyond the first order.
- When combined with a realistic nuclear chiral force, the results reproduce the experimental binding energies very well.
- Works in progress:
  - Efficient methods for calculating the third order corrections, or estimating the truncation errors of the perturbative series;
  - Applications to other interesting systems, e.g., bosons, finite-temperature systems, density distributions, etc.;

# Thank you for your attention