New Algorithms in Lattice Effective Field Theory

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The 7th Symposium on "Symmetries and the emergence of Structure in QCD",
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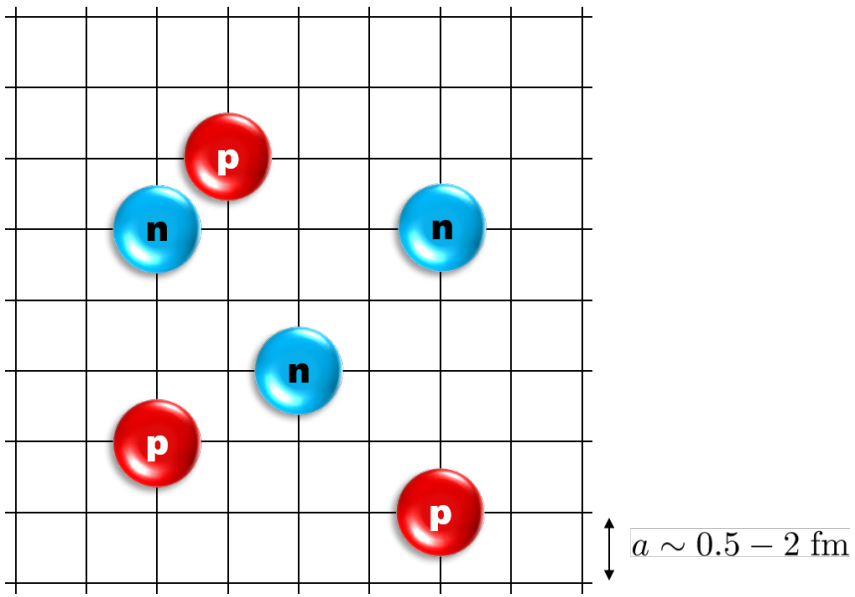
Introduction to Lattice Effective Field Theory

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, δ-like** and **long-range, pion-exchange** interactions
- Exact method, polynomial scaling ($\sim A^2$)



Lattice adapted for nucleus

Euclidean time projection

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

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

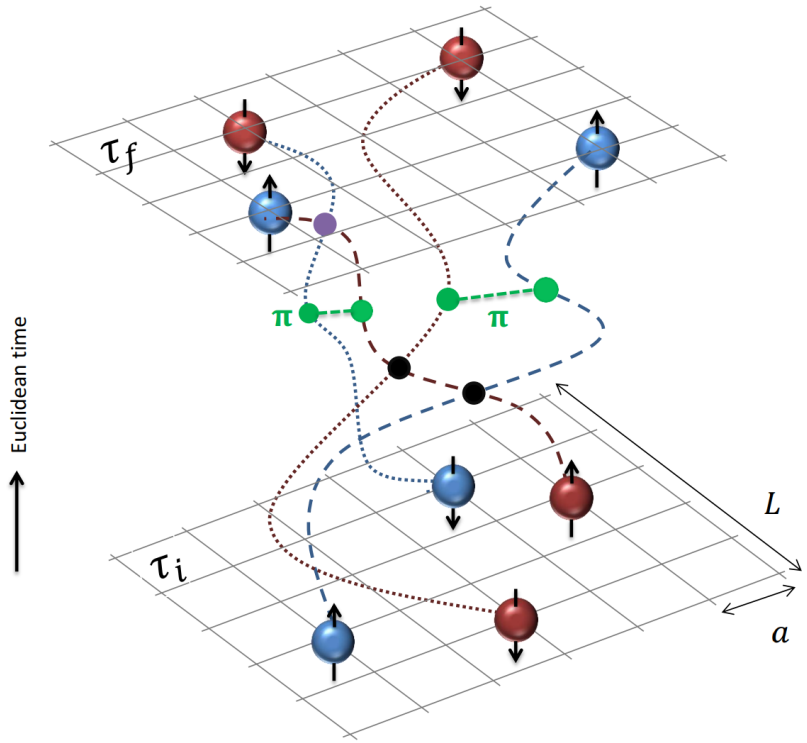
with $|\Psi_A\rangle$ representing A *free* nucleons.

- Expectation value of any operator $\mathscr{O}$:

$$\langle O\rangle = \lim_{\tau\to\infty} \frac{\langle\Psi_A|\exp(-\tau H/2)\mathscr{O}\exp(-\tau H/2)|\Psi_A\rangle}{\langle\Psi_A|\exp(-\tau H)|\Psi_A\rangle}$$

- τ is discretized into time slices:

$$\exp(-\tau H) \simeq \left[:\exp(-\frac{\tau}{L_t}H):\right]^{L_t}$$



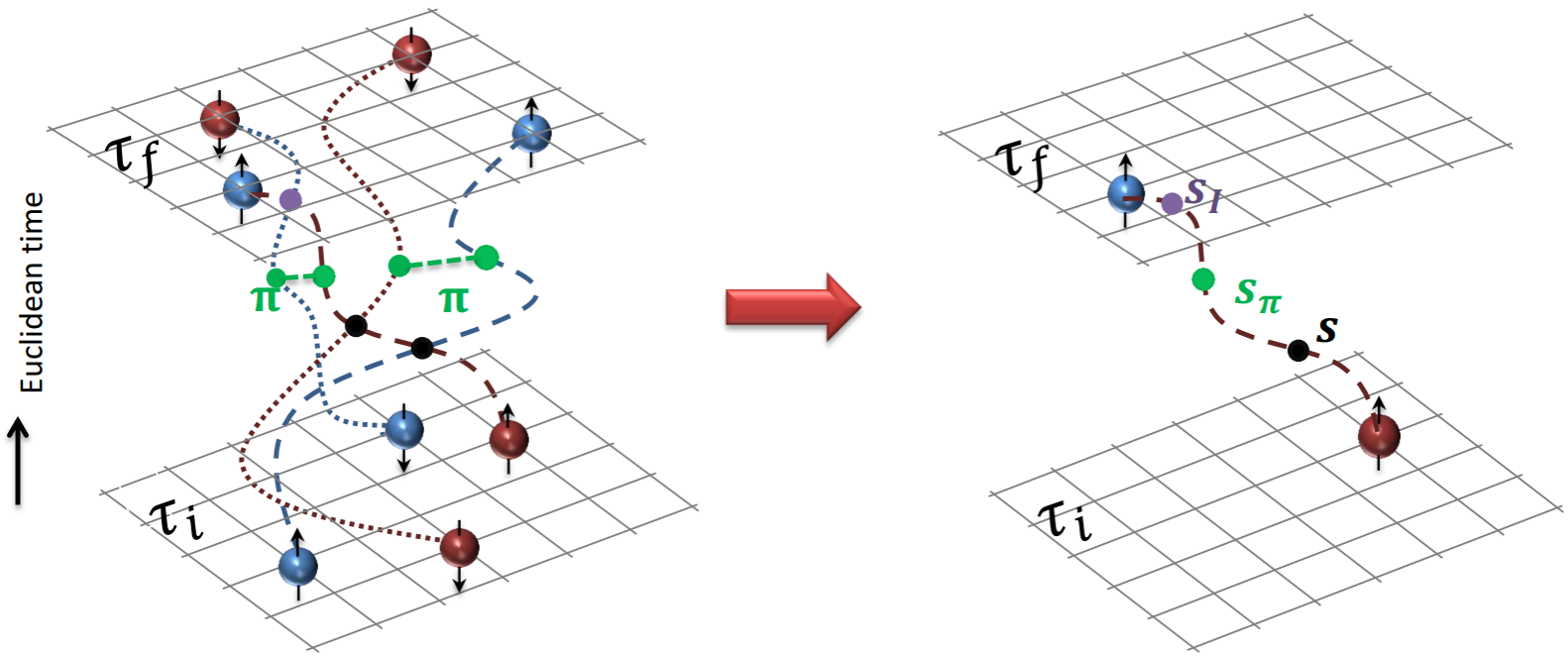
All possible configurations in $\tau \in [\tau_i, \quad \tau_f]$ are sampled.
Complex structures like nucleon clustering emerges naturally.

Auxiliary field transformation

Quantum correlations between nucleons are represented by fluctuations of the auxiliary fields.

$$:\exp\left[-\frac{C}{2}(N^\dagger N)^2\right] := \frac{1}{\sqrt{2\pi}}\int ds :\exp\left[-\frac{s^2}{2}+\sqrt{C}s(N^\dagger N)\right] :\Longrightarrow$$

$$Z=\int \mathscr{D}s \exp(-\sum\frac{s^2}{2}) \begin{vmatrix} \langle\psi_1|\phi_1\rangle & \langle\psi_1|\phi_2\rangle & \cdots & \langle\psi_1|\phi_A\rangle \\ \langle\psi_2|\phi_1\rangle & \langle\psi_2|\phi_2\rangle & \cdots & \langle\psi_2|\phi_A\rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle\psi_A|\phi_1\rangle & \langle\psi_A|\phi_2\rangle & \cdots & \langle\psi_A|\phi_A\rangle \end{vmatrix}$$



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 $N \sim 10^3 \sim 10^6$

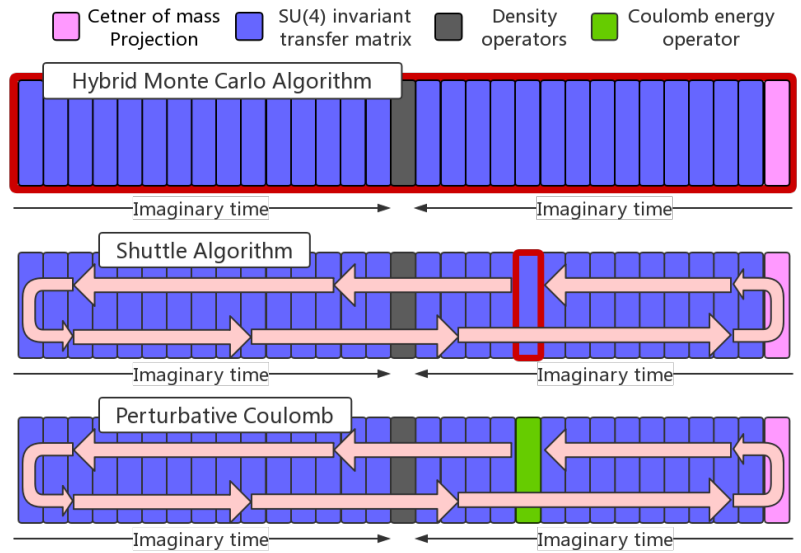
Total energies at large t follow

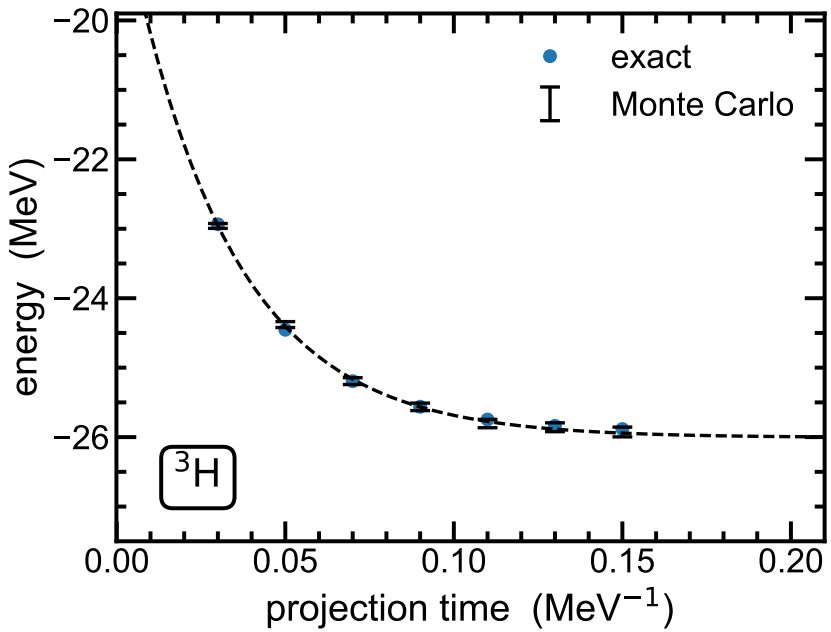
$$E_A(t) = E_A(\infty) + c \exp[-\Delta E \tau] .$$

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

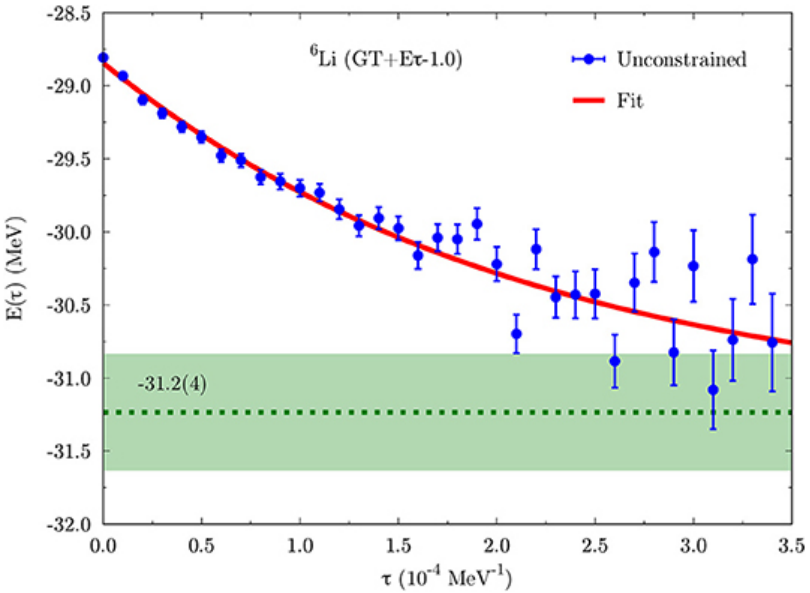
$$\mathscr{O}_A(\tau) = \mathscr{O}_A(\infty) + c' \exp[-\Delta E \tau/2] ,$$

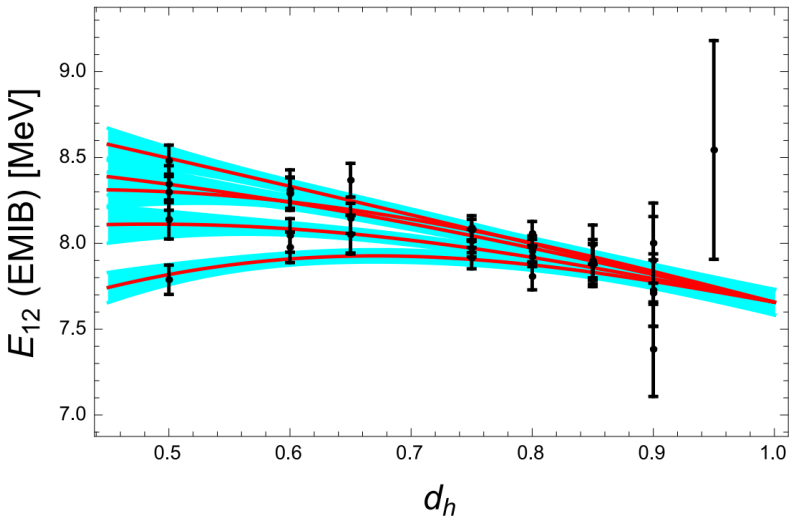
c, c', ΔE are fitting parameters.

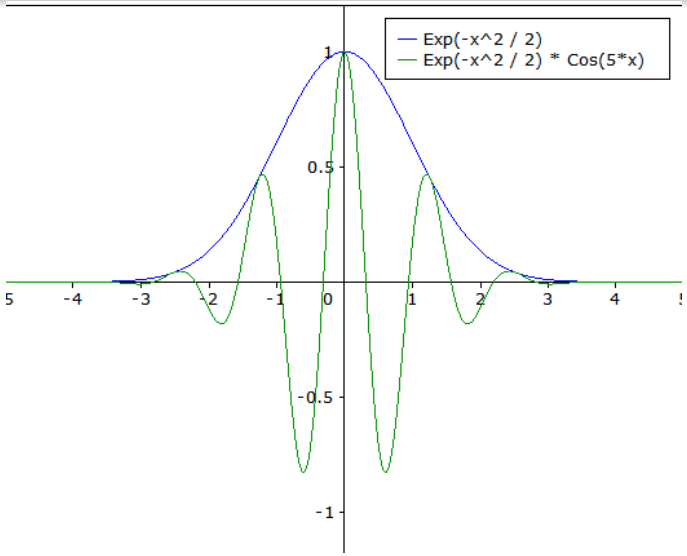




Monte Carlo sign problem







- 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.
- Sign problem as difficult as P=NP.
- 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 $\lambda = 0$.

Approximate symmetry of the nuclear force

- Construct a N^{2}LO chiral force on the $a = 1.32$ fm ($\Lambda \approx 471$ MeV) lattice.
- $H_{\mathrm{N^2LO}}$ gives good description of symmetric nuclear matter and finite nuclei:

	$\rho_{\mathrm{sat}}(\mathrm{fm}^{-3})$	E_{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				

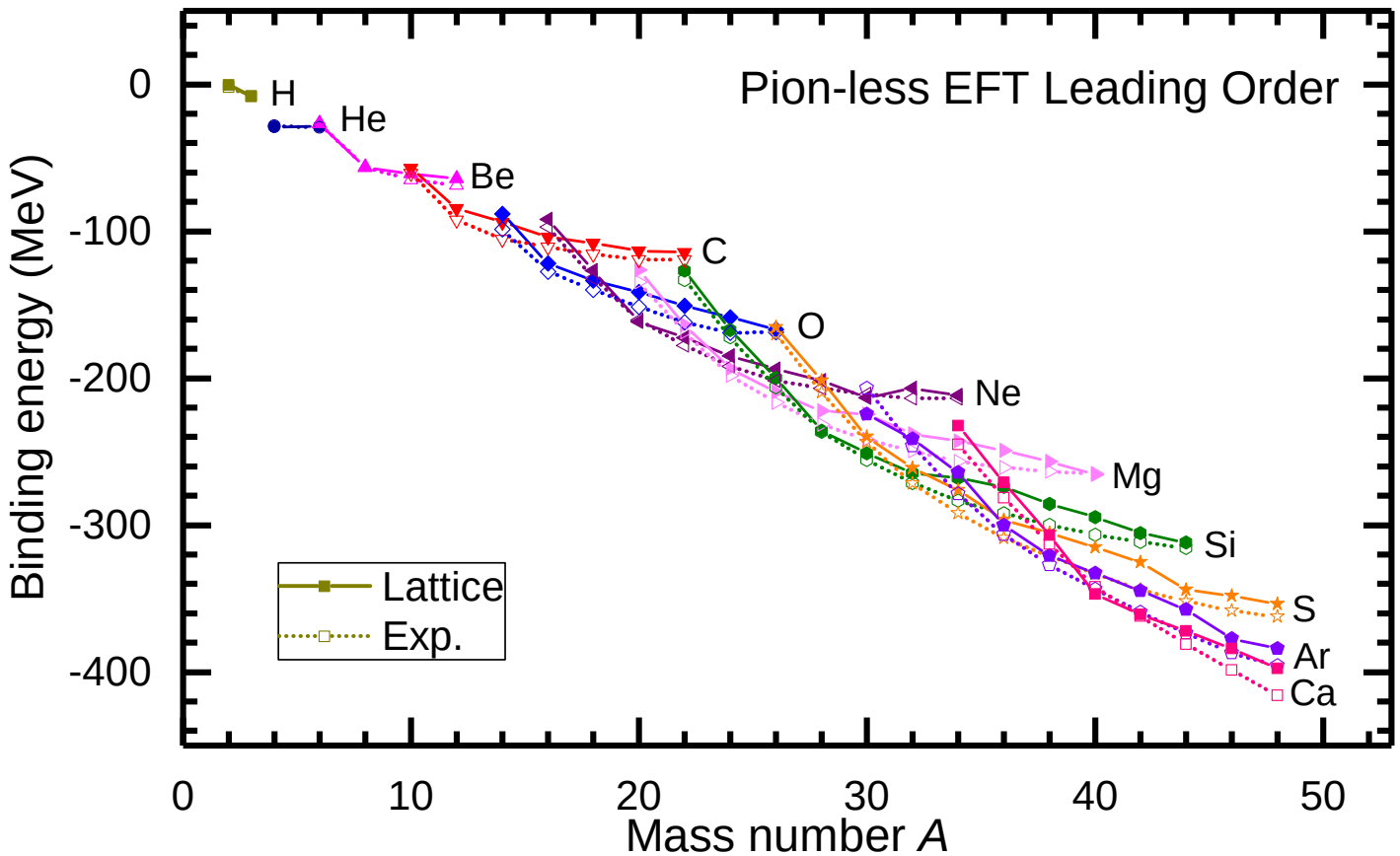
- Note that $1/N_C^2 \approx 0.1$, $(Q/\Lambda)^2 \approx 0.2$ in ^{16}O. **Red:** suppressed by $1/N_C^2$ or $(Q/\Lambda)^2$. **Blue:** suppressed by both factors.$\Longleftarrow$**very clear hierachy**
- SU(4) symmetric term dominate$\Longleftarrow$**No sign problem, good for MC**

Dean Lee, Scott Bogner, B. Alex Brown, Serdar Elhatisari, Evgeny Epelbaum, Heiko Hergert, Morten Hjorth-Jensen, Hermann Krebs, Ning Li, Bing-Nan Lu, Ulf-G. Meißner, Phys. Rev. Lett. 127, 062501 (2021)

Nuclear binding from a SU(4) nuclear force

In full quantum Monte Carlo simulations, **equations are solved exactly**

$$Z = \int \mathscr{D}s \exp(-\sum \frac{s^2}{2}) \begin{vmatrix} \langle\psi_1|\phi_1\rangle & \langle\psi_1|\phi_2\rangle & & \\ \langle\psi_2|\phi_1\rangle & \langle\psi_2|\phi_2\rangle & & \\ & & \langle\psi_1|\phi_1\rangle & \langle\psi_1|\phi_2\rangle \\ & & \langle\psi_2|\phi_1\rangle & \langle\psi_2|\phi_2\rangle \end{vmatrix}$$



Bing-Nan Lu, Ning Li, Serdar Elhatisari, Dean Lee, Evgeny Epelbaum, Ulf-G. Meißner, Phys. Lett. B 797, 134863 (2019)

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

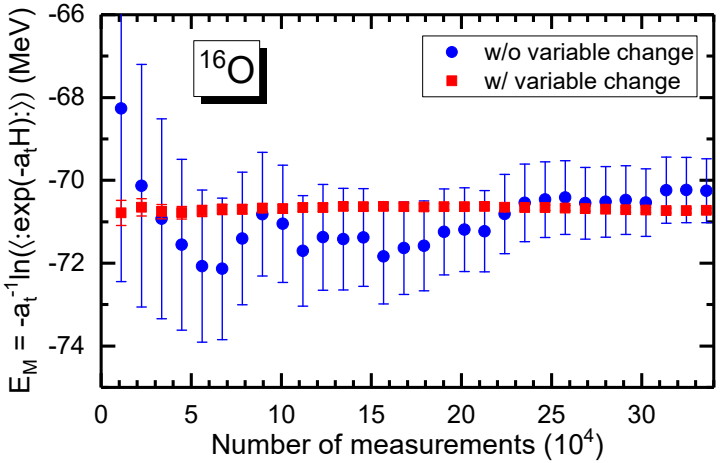
$$\begin{aligned} E_0 &= \langle\Psi_0|(K+V)|\Psi_0\rangle/\langle\Psi_0|\Psi_0\rangle, \\ \delta E_1 &= \langle\Psi_0|V_C|\Psi_0\rangle/\langle\Psi_0|\Psi_0\rangle, \\ \delta E_2 &= \left(\langle\Psi_0|V_C|\delta\Psi_1\rangle - \delta E_1 \mathrm{Re}\langle\delta\Psi_1|\Psi_0\rangle\right)/\langle\Psi_0|\Psi_0\rangle,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

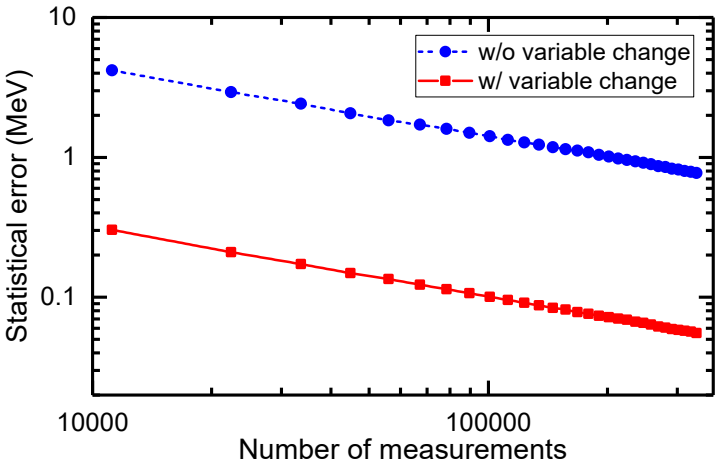
in which all matrix elements and overlaps can be expressed with,

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

Bing-Nan Lu, Ning Li, Serdar Elhatisari, Yuan-Zhuo Ma, Dean Lee, Ulf-G. Meißner, Phys. Rev. Lett. 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 $E = -\ln\langle:\exp(-a_tH):\rangle/a_t$
Bing-Nan Lu, Ning Li, Serdar Elhatisari, Yuan-Zhuo Ma, Dean Lee, Ulf-G. Meißner, Phys. Rev. Lett. 128, 242501 (2022)

Benchmark Hamiltonian: N^{2}LO chiral Hamiltonian

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

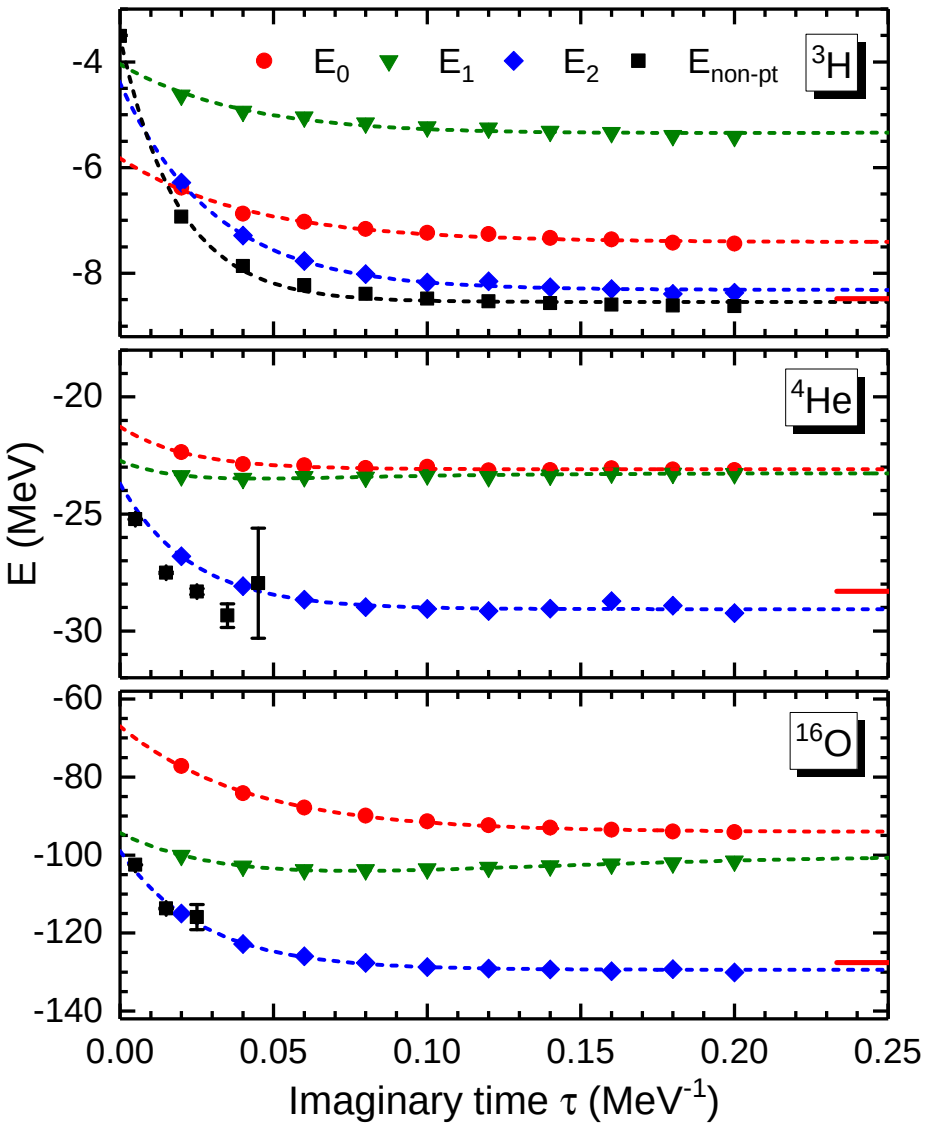
$$
\begin{aligned}
V_{2N} = & \Big[B_1 + B_2(\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2) + C_1 q^2 + C_2 q^2 (\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2) + C_3 q^2 (\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2) + C_4 q^2 (\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2)(\boldsymbol{\tau}_1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

with C_{1-7}, g_A, c_E etc. **low energy constants** fitted to N-N scattering or π-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

Perturbative Monte Carlo with realistic chiral interaction

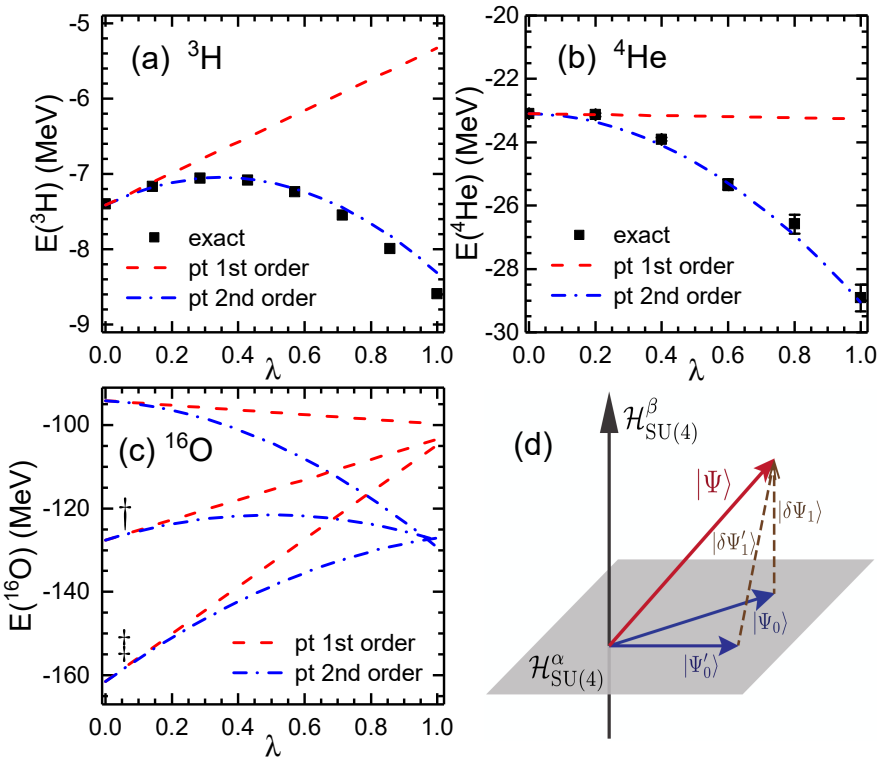


- We split $H = H_0 + (H - H_0)$ and perform perturbative calculations
- E_0 is the ground state of H_0
- $E_1 = E_0 + \delta E_1$ is the first order corrected energy
- $E_2 = E_1 + \delta E_2$ is the second order corrected energy
- $E_{\mathrm{non-pt}}$ is the exact solution (∼infinite order)
- Red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

For ^{4}He and ^{16}O, sign problem prevent us from going to large τ, 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 λ-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 Bing-Nan Lu, Ning Li, Serdar Elhatisari, Yuan-Zhuo Ma, Dean Lee, Ulf-G. Meißner, Phys. Rev. Lett. 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 δE_2

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

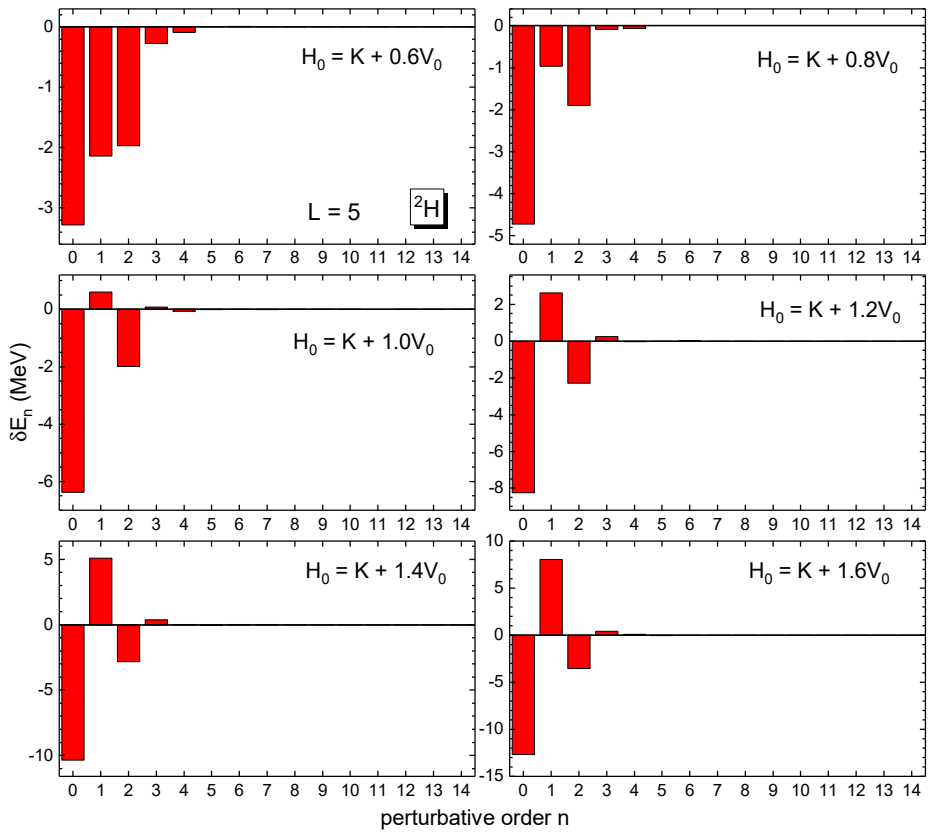
Numerical results for several light nuclei

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	δE_1	E_1	δE_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†	$-127.6(4)$	$+24.2$	$-103.4(4)$	-24.3	$-127.7(2)$	-127.6
^{16}O‡	$-161.5(1)$	$+56.8$	$-104.7(2)$	-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 δE_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, δE_1 and δE_2 are always significant. δE_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.

Thank you for your attention