Simulations of nuclei on the lattice

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work done in collaboration with:
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Weakly Bound Systems in Atomic and Nuclear Physics

Institute for Nuclear Theory, Seattle, Washington

Outline

Effective field theory (EFT) for nucleons

Lattice effective field theory

Lattice interactions and scattering data

Ground state projection

Three-nucleon forces

Isospin breaking and Coulomb effects

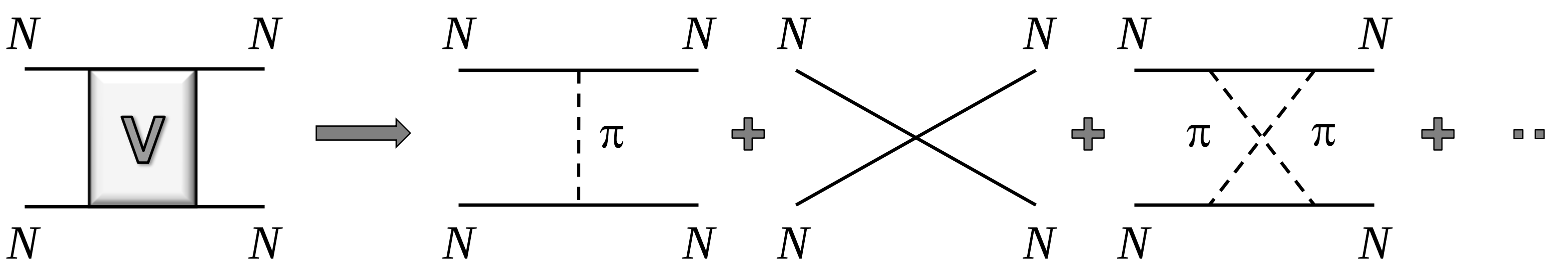
Results for $A = 3, 4, 6, 12$

Summary and future directions

Chiral EFT for low-energy nucleons

Weinberg, PLB 251 (1990) 288; NPB 363 (1991) 3

Construct the effective potential order by order



V^{OPEP} Contact interactions $1,\ \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2$ — Leading order (LO)

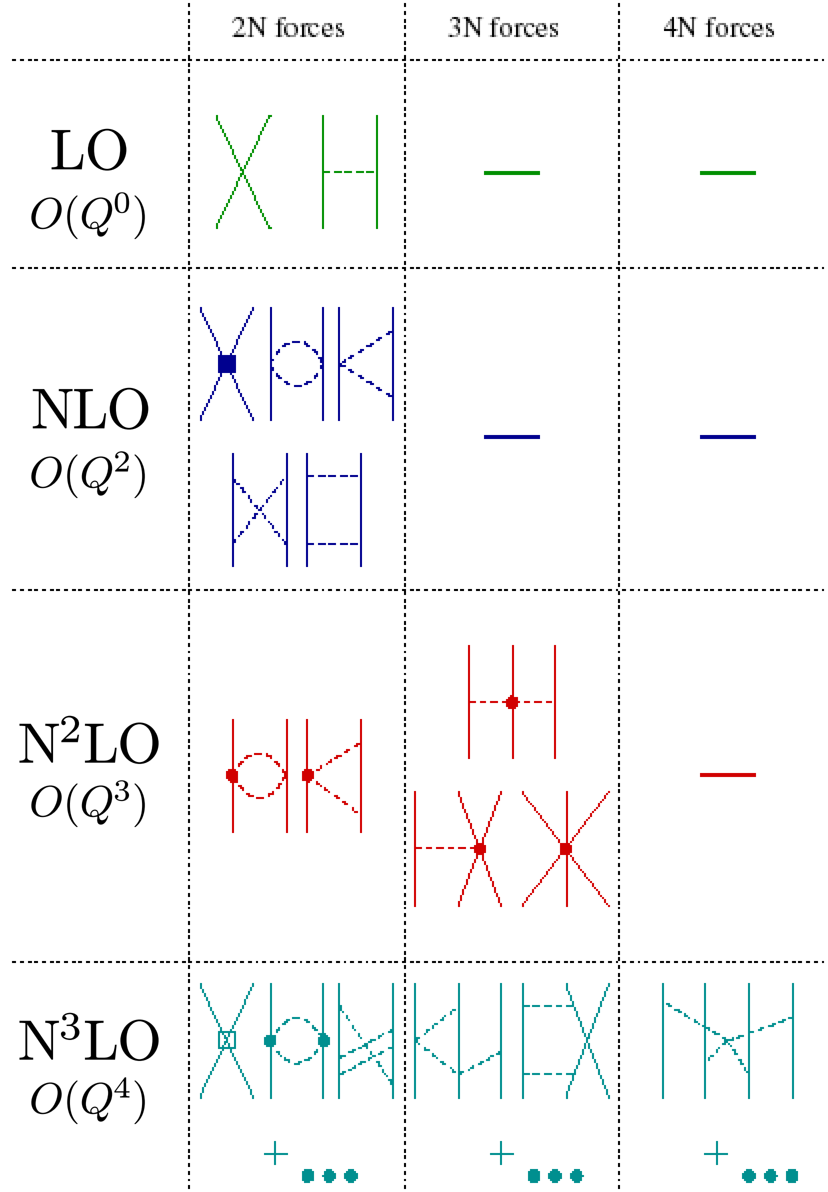
V^{TPEP} — Next-to-leading order (NLO)

Nuclear Scattering Data

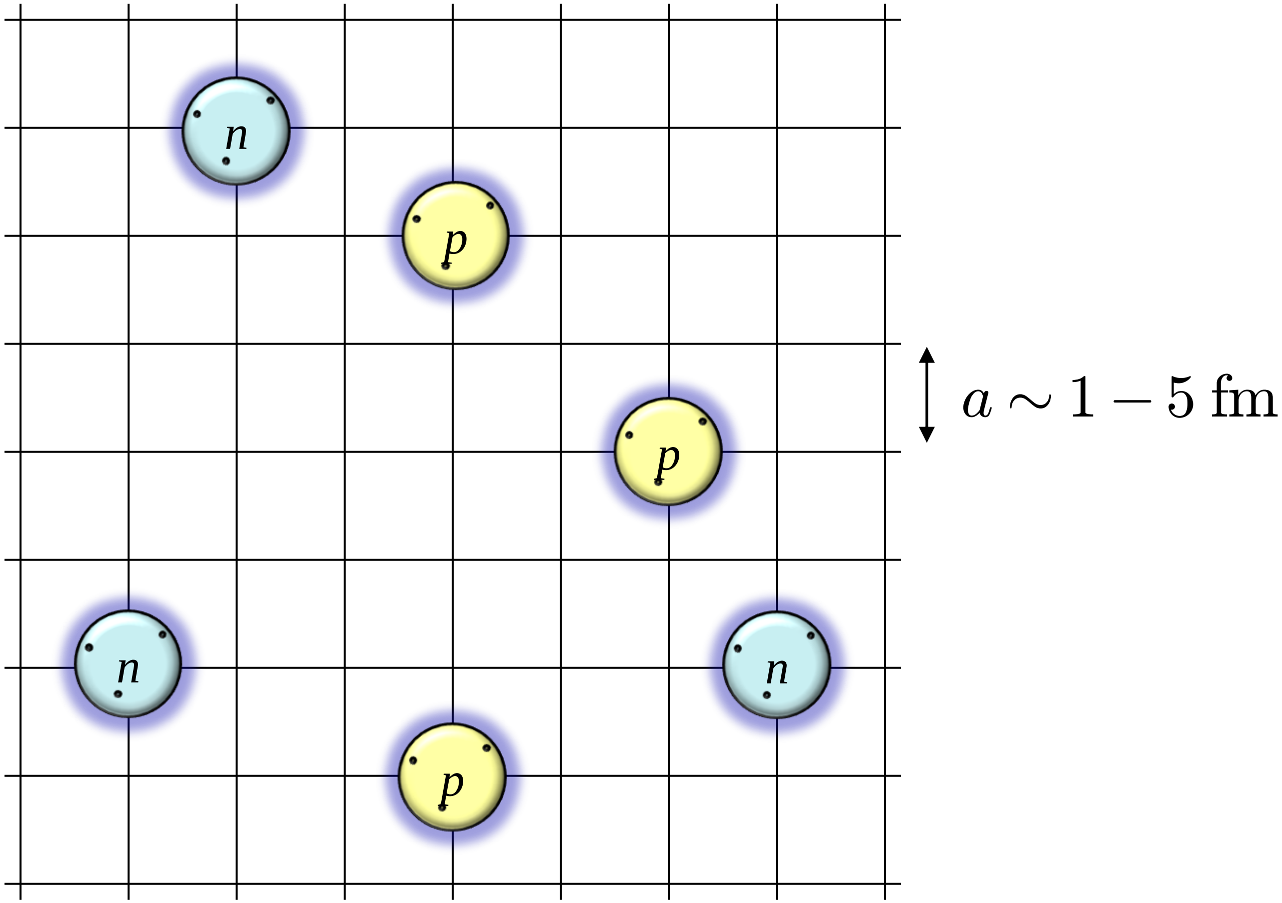
↓

Effective Field Theory

Ordonez et al. ’94; Friar & Coon ’94; Kaiser et al. ’97; Epelbaum et al. ’98, ‘03; Kaiser ’99-’01; Higa et al. ’03; …



Lattice EFT for nucleons



Early lattice EFT work

First lattice study of nuclear matter (using momentum lattice):
Brockman, Frank, PRL 68 (1992) 1830

First lattice EFT simulation of nuclear and neutron matter:
Müller, Koonin, Seki, van Kolck, PRC 61 (2000) 044320

Chiral perturbation theory using lattice regularization:
Shushpanov, Smilga, Phys. Rev. D59: 054013 (1999);
Lewis, Ouimet, PRD 64 (2001) 034005;
Borasoy, Lewis, Ouimet, hep-lat/0310054

Non-linear realization of chiral symmetry with static nucleons:
Chandrasekharan, Pepe, Steffen, Wiese, JHEP 12 (2003) 35

Pionless EFT for neutrons / Unitarity limit

Abe, Seki, 0708.2523; 0708.2524

Bulgac, Drut, Magierski, PRL 96 (2006) 090404;
PRA 78 (2008) 023625; …

Burovski, Prokofev, Svistunov, PRL 96 (2006) 160402;
New J. Phys. 8 (2006) 153; …

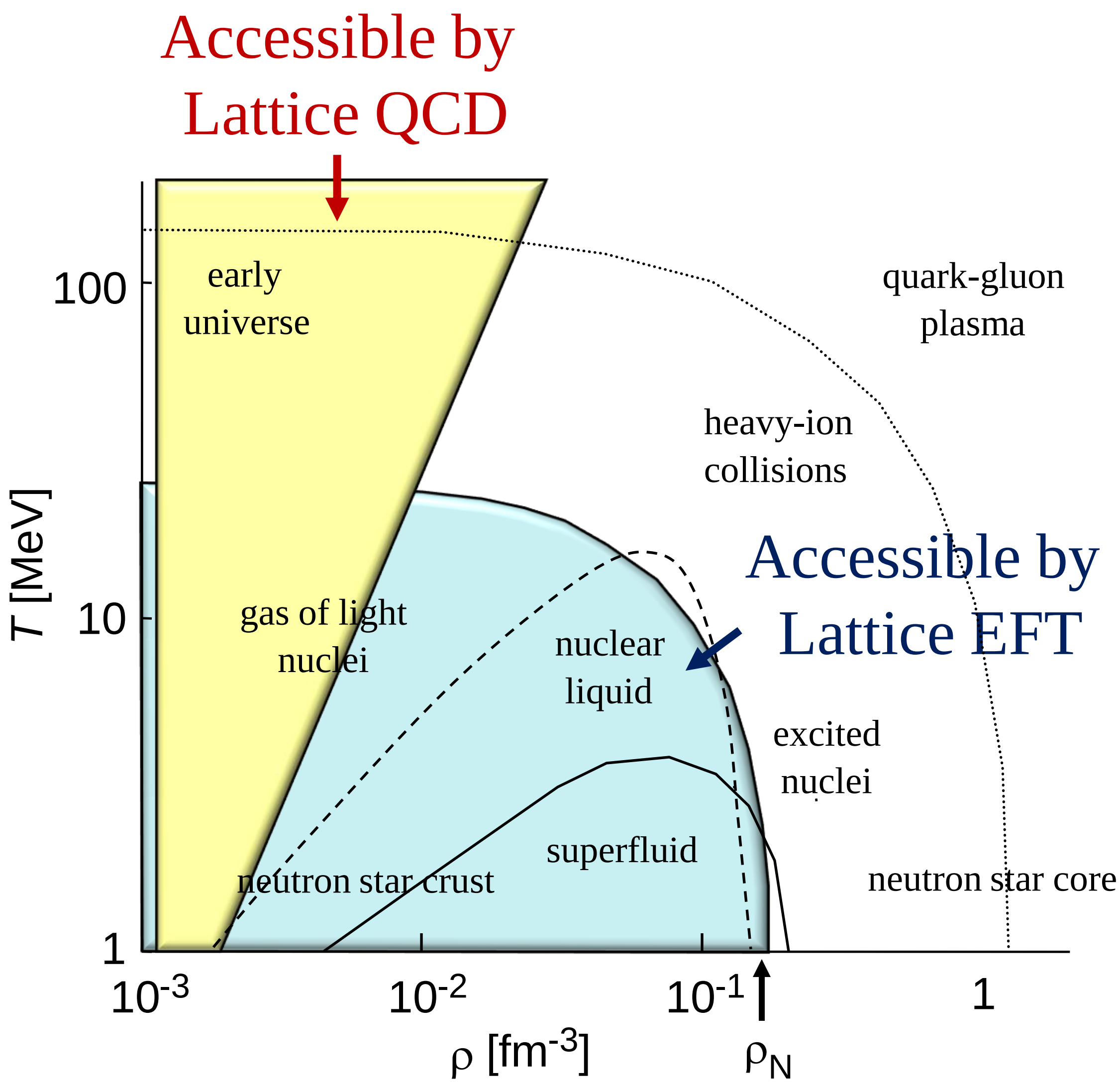
Chen, Kaplan, PRL 92 (2004) 257002

Juillet, New J. Phys. 9 (2007)163

Wingate, cond-mat/0502372

D.L., Schaefer, PRC 73 (2006) 015202; …

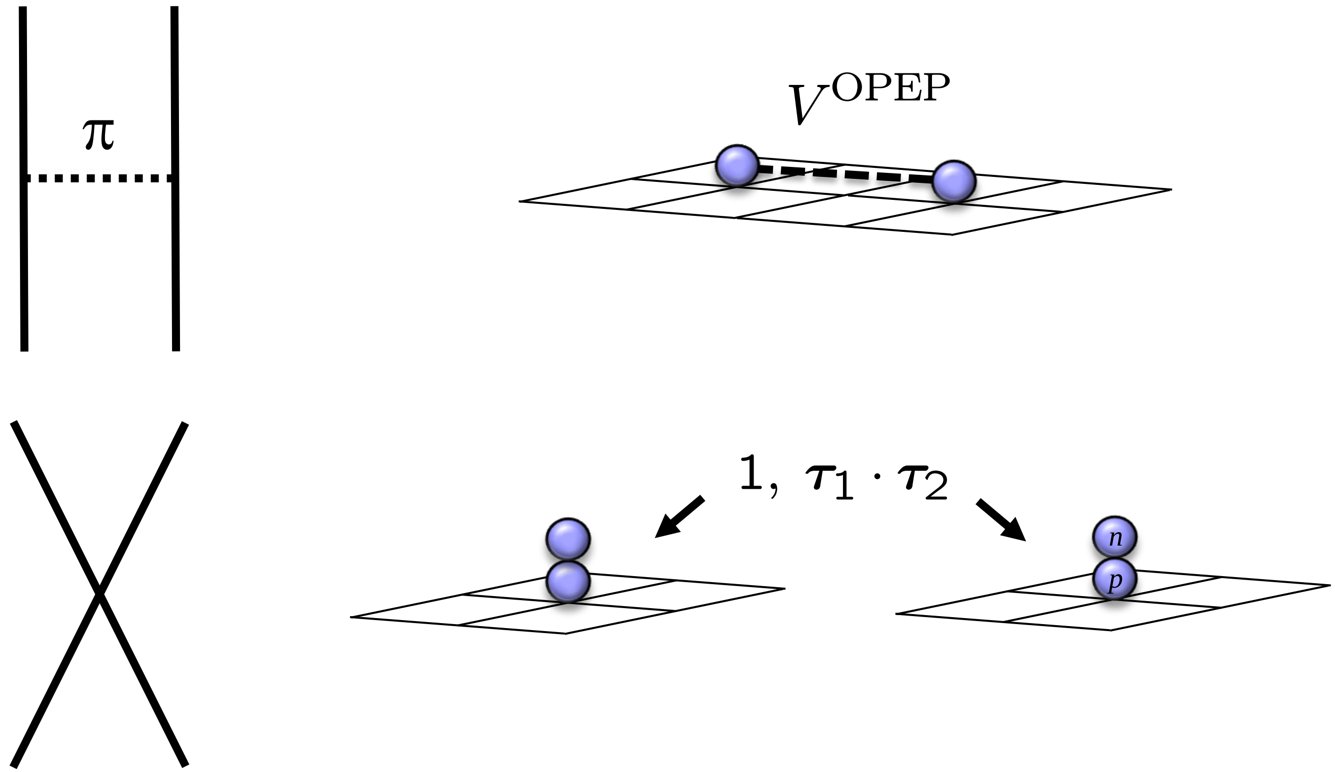
Review: *D.L., 0804.3501, PPNP 63 (2009) 117*



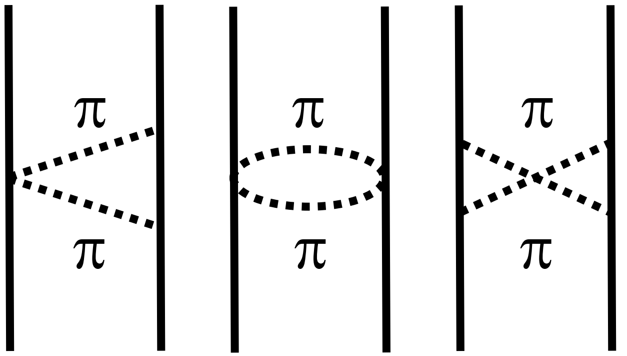
Accessible by
Lattice QCD
early
universe
quark-gluon
plasma
heavy-ion
collisions
Accessible by
Lattice EFT
gas of light
nuclei
nuclear
liquid
excited
nuclei
superfluid
neutron star crust
neutron star core
T [MeV]
100
10
1
10^{-3}
10^{-2}
10^{-1}
1
ρ [fm^{-3}]
$ρ_N$

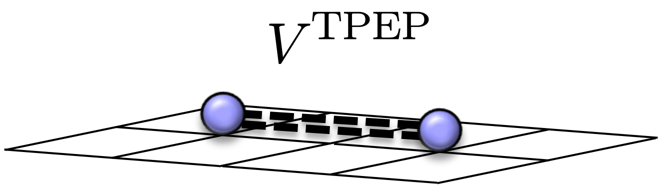
Lattice interactions

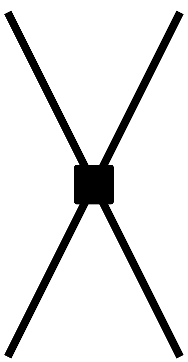
Leading order on the lattice



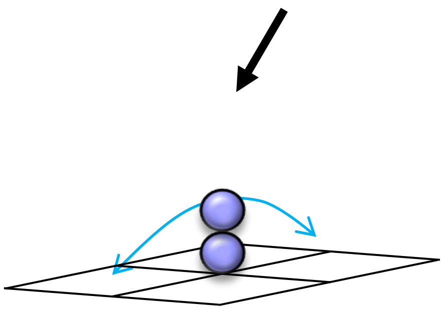
Next-to-leading order on the lattice

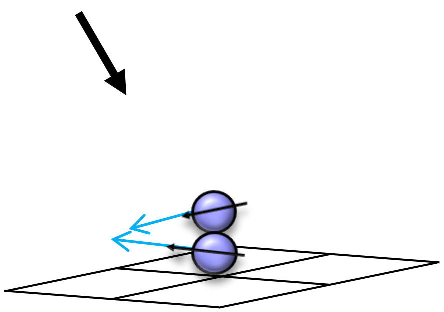




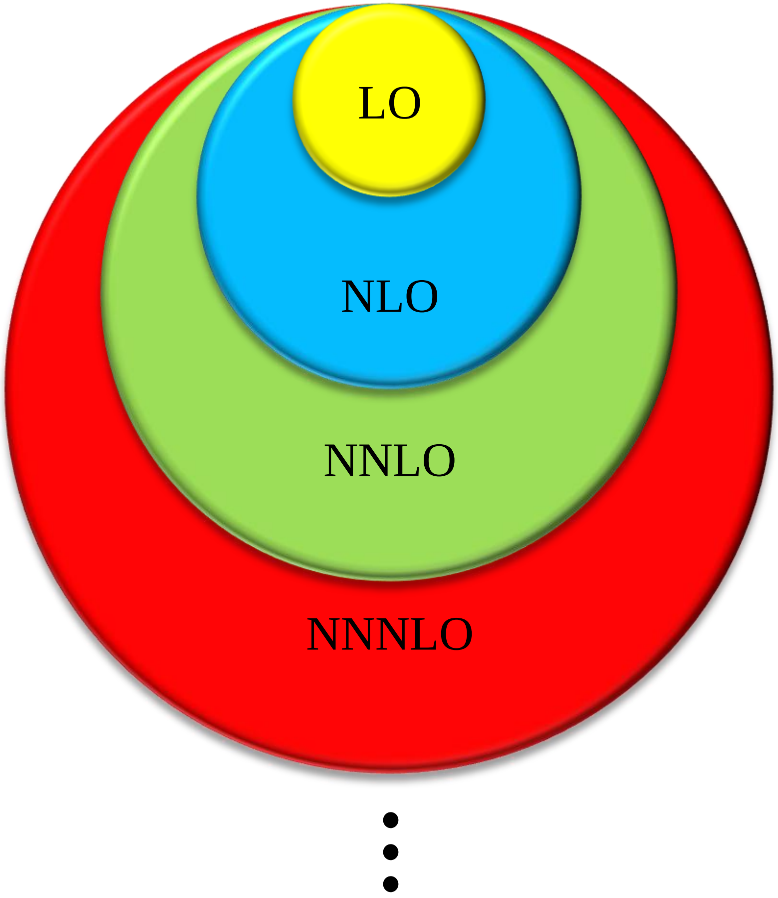


$\vec{\nabla}_1 \cdot \vec{\nabla}_2 \qquad (\vec{\sigma}_1 \cdot \vec{\nabla}_1)\,(\vec{\sigma}_2 \cdot \vec{\nabla}_2) \qquad \cdots$

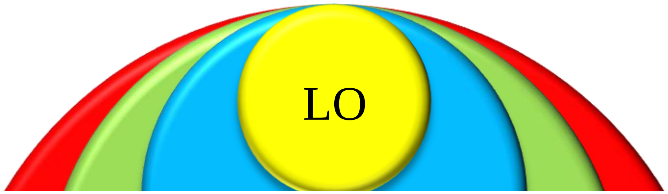




Computational strategy

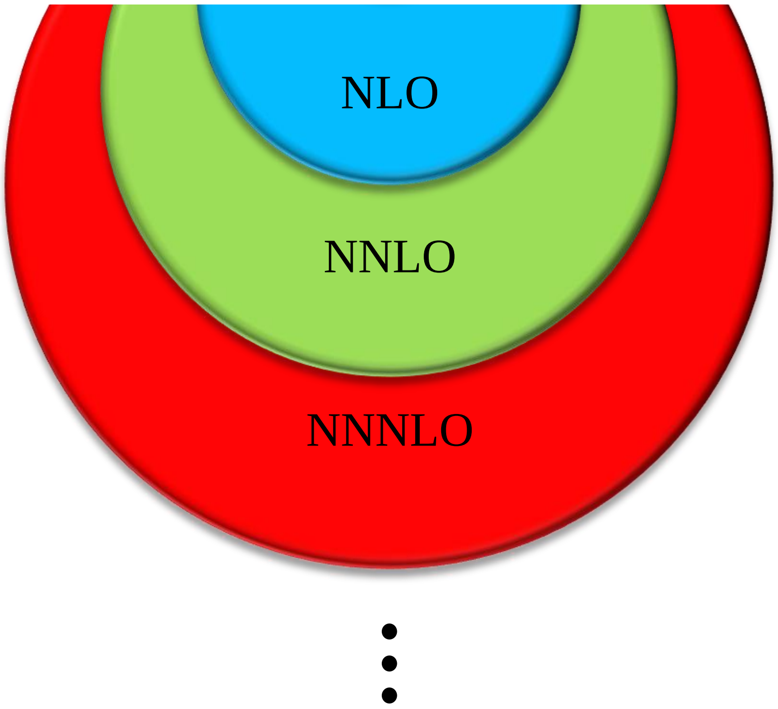


Non-perturbative – Monte Carlo



"Improved LO"

Perturbative corrections



LO_1: Pure contact interactions

$$\mathcal{A}(V_{\mathrm{LO}_1}) = C + C_I \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 + \mathcal{A}(V^{\mathrm{OPEP}})$$

LO_2: Gaussian smearing

$$\mathcal{A}(V_{\mathrm{LO}_2}) = C f(\vec{q}^{\,2}) + C_I f(\vec{q}^{\,2}) \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 + \mathcal{A}(V^{\mathrm{OPEP}})$$

LO_3: Gaussian smearing only in even partial waves

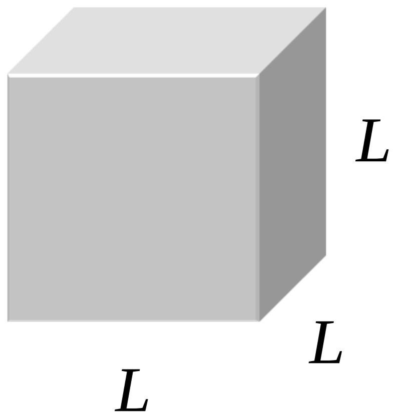
$$\begin{aligned}\mathcal{A}(V_{\mathrm{LO}_3}) = {} & C_{1S0} f(\vec{q}^{\,2}) \left(\tfrac{1}{4} - \tfrac{1}{4}\vec{\sigma}_1 \cdot \vec{\sigma}_2\right) \left(\tfrac{3}{4} + \tfrac{1}{4}\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2\right) \\ & + C_{3S1} f(\vec{q}^{\,2}) \left(\tfrac{3}{4} + \tfrac{1}{4}\vec{\sigma}_1 \cdot \vec{\sigma}_2\right) \left(\tfrac{1}{4} - \tfrac{1}{4}\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2\right) \\ & + \mathcal{A}(V^{\mathrm{OPEP}})\end{aligned}$$

Physical scattering data → Unknown operator coefficients

Lüscher's finite-volume formula

Lüscher, Comm. Math. Phys. 105 (1986) 153; NPB 354 (1991) 531

Two-particle energy levels near threshold in a periodic cube related to phase shifts



$$p \cot \delta_0(p) = \frac{1}{\pi L} S(\eta), \qquad \eta = \left(\frac{Lp}{2\pi}\right)^2$$

$$S(\eta) = \lim_{\Lambda \to \infty} \left[\sum_{\vec{n}} \frac{\theta(\Lambda^2 - \vec{n}^2)}{\vec{n}^2 - \eta} - 4\pi\Lambda \right]$$

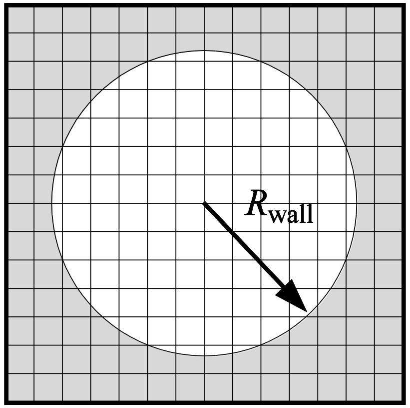
Not so useful for higher partial waves and partial wave mixing

Physical scattering data → Unknown operator coefficients

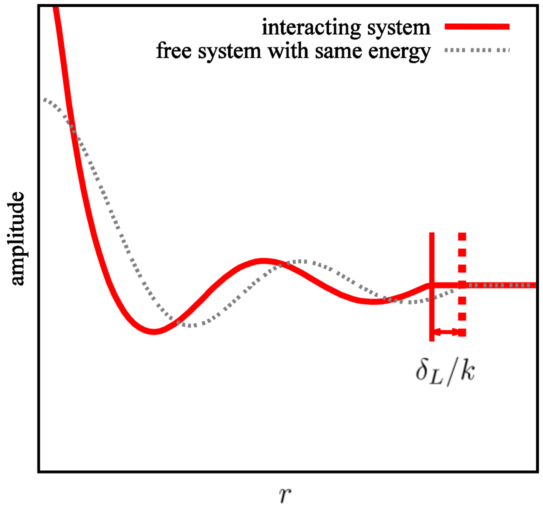
Spherical wall method

Borasoy, Epelbaum, Krebs, D.L., Meißner, EPJA 34 (2007) 185

Spherical wall imposed in the center of mass frame

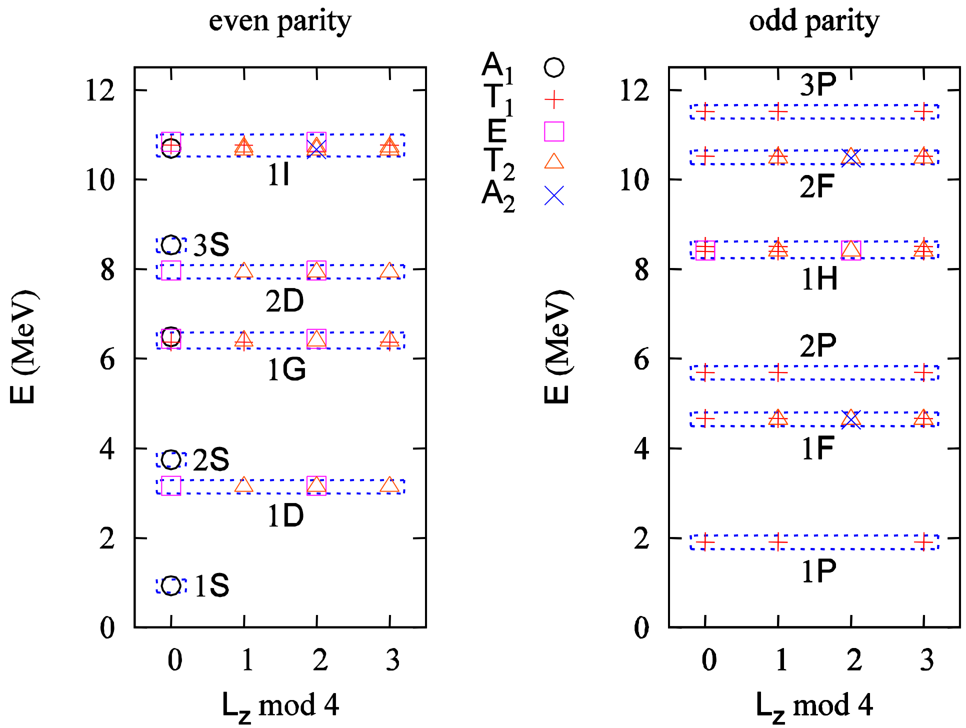


Representation	J_z	Example
A_1	$0 \bmod 4$	$Y_{0,0}$
T_1	$0,1,3 \bmod 4$	$\{Y_{1,0}, Y_{1,1}, Y_{1,-1}\}$
E	$0,2 \bmod 4$	$\left\{Y_{2,0}, \frac{Y_{2,-2}+Y_{2,2}}{\sqrt{2}}\right\}$
T_2	$1,2,3 \bmod 4$	$\left\{Y_{2,1}, \frac{Y_{2,-2}-Y_{2,2}}{\sqrt{2}}, Y_{2,-1}\right\}$
A_2	$2 \bmod 4$	$\frac{Y_{3,2}-Y_{3,-2}}{\sqrt{2}}$



Energy levels with hard spherical wall

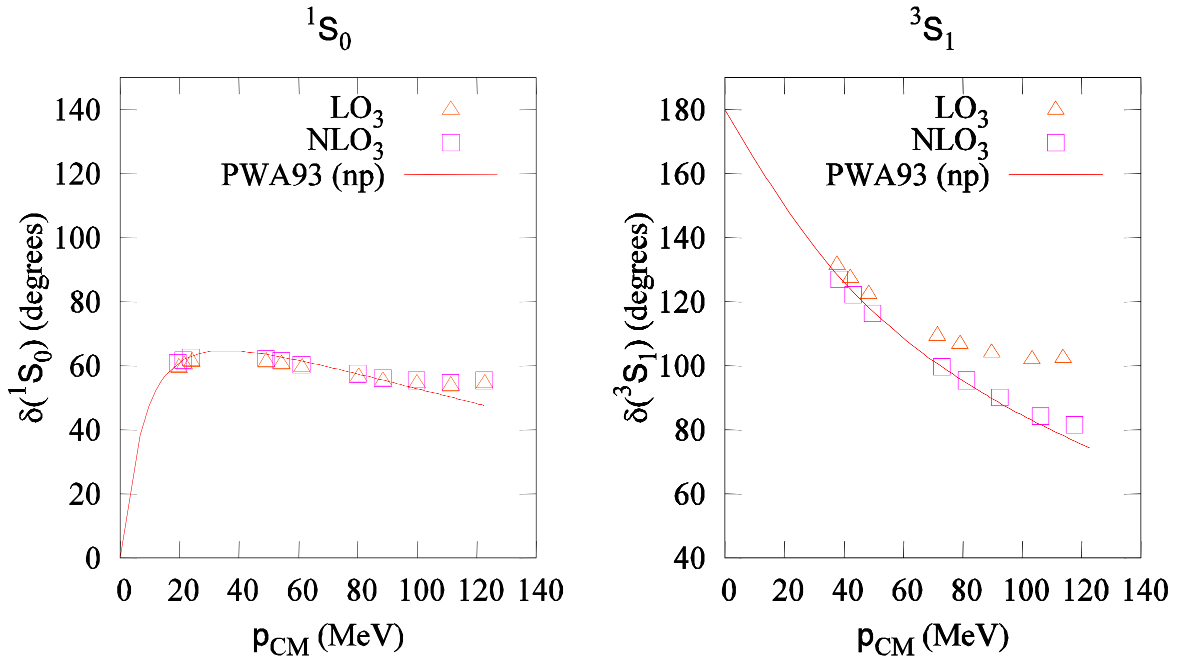
$$R_{\text{wall}} = 10a$$
$$a = 1.97\ \text{fm}$$



Energy shift from free-particle values gives the phase shift

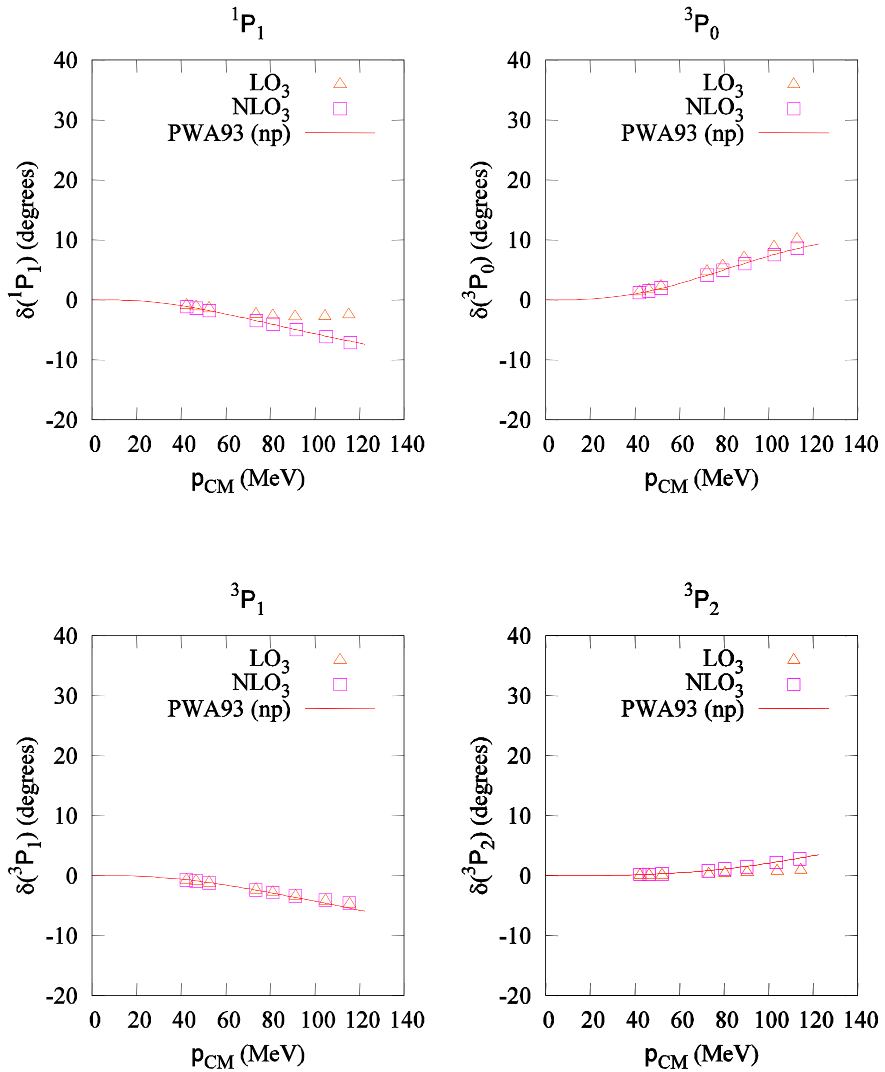
LO_3: S waves

$a = 1.97$ fm



LO_3: P waves

$$a = 1.97 \text{ fm}$$



Ground state projection

Let H be the Hamiltonian for a quantum system. We don't know the energies and energy eigenstates, but label them as

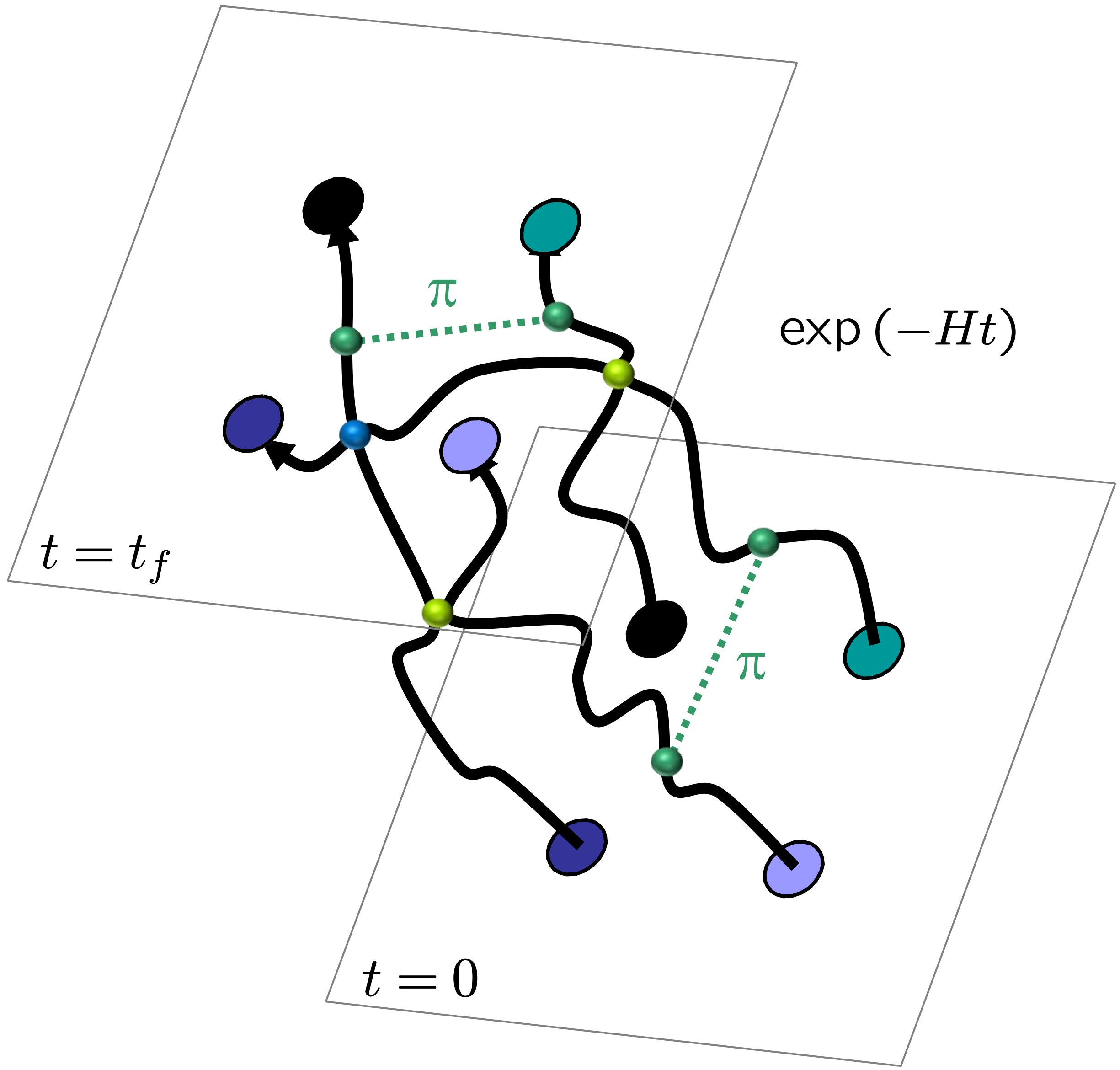
$$H\,|\psi_n\rangle = E_n\,|\psi_n\rangle$$
$$E_0 < E_1 \leq E_2 \leq \cdots$$

Convenient to work with exponentials of the Hamiltonian

$$\exp(-Ht)\,|\psi_n\rangle = \exp(-E_n t)\,|\psi_n\rangle$$

The ground state dominates as Euclidean time goes to infinity

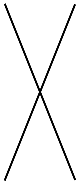
$$\exp(-Ht)\,|\phi\rangle \to \exp(-E_0 t)\,|\psi_0\rangle\,\langle\psi_0|\,\phi\rangle$$


π
π
$\exp(-Ht)$
$t = t_f$
$t = 0$

Auxiliary fields

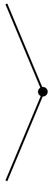
We can write exponentials of the interaction using a Gaussian integral identity

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



$(N^{\dagger}N)^{2}$

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



$sN^{\dagger}N$

We remove the interaction between nucleons and replace it with the interactions of each nucleon with a background field.

Terms in the exponential of the Hamiltonian

$$\exp\left(-H\Delta t\right)$$

Free nucleons:

$$\exp\left[\frac{1}{2m}N^{\dagger}\vec{\nabla}^{2}N\Delta t\right]$$

Free pions:

$$\exp\left[-\frac{1}{2}\left(\vec{\nabla}\boldsymbol{\pi}\right)^{2}\Delta t-\frac{m_{\pi}^{2}}{2}\boldsymbol{\pi}^{2}\Delta t\right]$$

Pion-nucleon coupling:

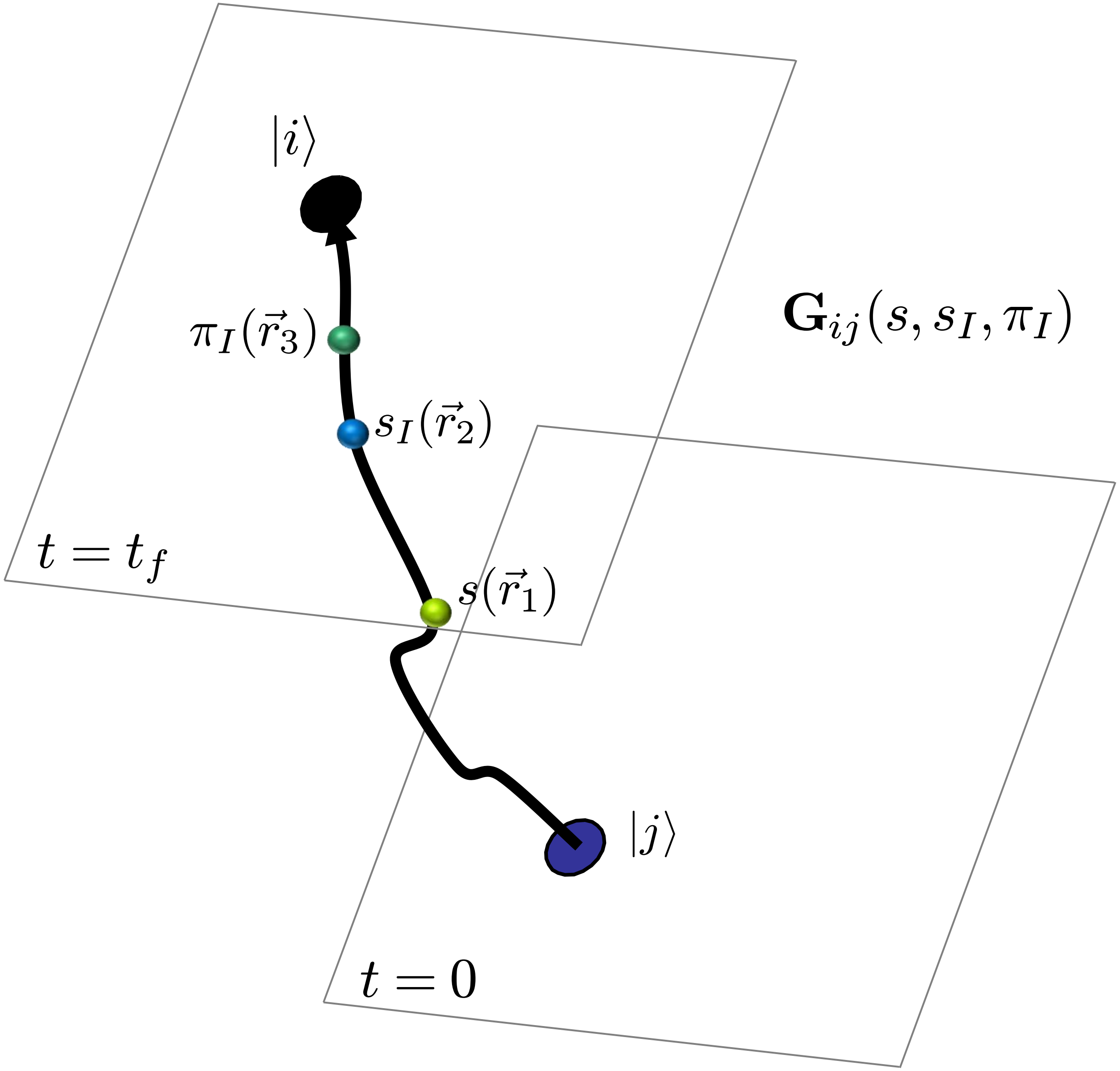
$$\exp\left[-\frac{g_{A}}{2f_{\pi}}N^{\dagger}\boldsymbol{\tau}\vec{\sigma}N\cdot\cdot\vec{\nabla}\boldsymbol{\pi}\Delta t\right]$$

C contact interaction:

$$\exp\left[-\frac{1}{2}CN^{\dagger}NN^{\dagger}N\Delta t\right] \quad (C<0)$$
$$= \frac{1}{\sqrt{2\pi}}\int ds\,\exp\left[-\frac{1}{2}s^{2}+sN^{\dagger}N\sqrt{-C\Delta t}\right]$$

C_I contact interaction:

$$\exp\left[-\frac{1}{2}C_{I}N^{\dagger}\boldsymbol{\tau}N\cdot N^{\dagger}\boldsymbol{\tau}N\Delta t\right] \quad (C_{I}>0)$$
$$= \frac{1}{\sqrt{2\pi}}\int d\boldsymbol{s}_{I}\,\exp\left[-\frac{1}{2}\boldsymbol{s}_{I}\cdot\boldsymbol{s}_{I}+i\boldsymbol{s}_{I}\cdot N^{\dagger}\boldsymbol{\tau}N\sqrt{C_{I}\Delta t}\right]$$


$|i\rangle$
$\pi_I(\vec{r}_3)$
$s_I(\vec{r}_2)$
$s(\vec{r}_1)$
$t = t_f$
$\mathbf{G}_{ij}(s, s_I, \pi_I)$
$|j\rangle$
$t = 0$

Take any initial state with the desired quantum numbers and which is an antisymmetric product of *A* single nucleon states (i.e., a Slater determinant)

$$|\psi_{\rm init}\rangle = |1\rangle \wedge |2\rangle \wedge \cdots \wedge |A\rangle$$

For any configuration of the auxiliary and pion fields,

$$\langle\psi_{\rm init}|\exp\left[-H(s,s_I,\pi_I)t\right]|\psi_{\rm init}\rangle = \det\mathbf{G}(s,s_I,\pi_I)$$

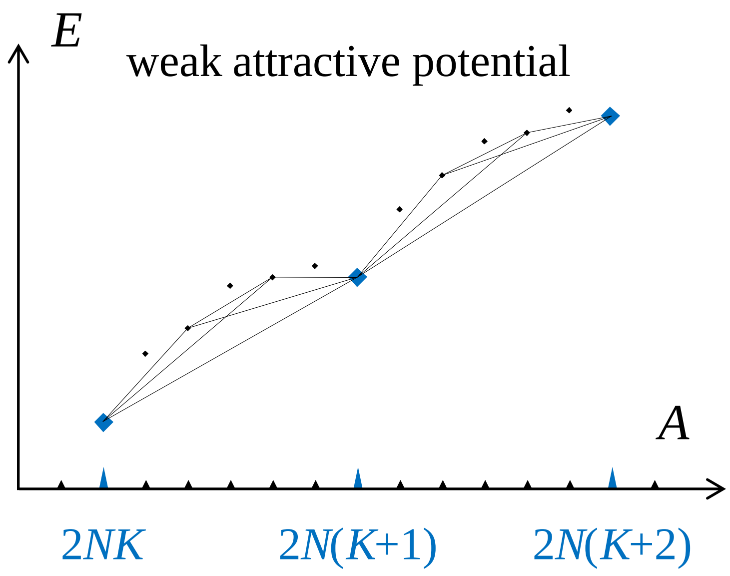
$$\mathbf{G}_{ij}(s,s_I,\pi_I) = \langle i|\exp\left[-H(s,s_I,\pi_I)t\right]|j\rangle$$

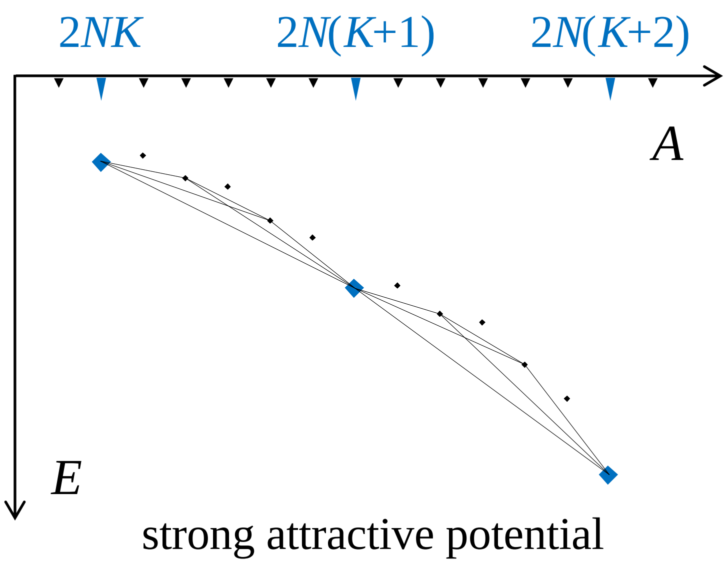
For *A* nucleons, the matrix is *A* by *A*. We use Monte Carlo to integrate over all possible configurations of the auxiliary and pion fields.

Theorem: Any fermionic theory with SU(2N) symmetry and two-body potential with negative semi-definite Fourier transform $\tilde{V}(\vec{p}) \leq 0$ obeys SU(2N) convexity bounds.

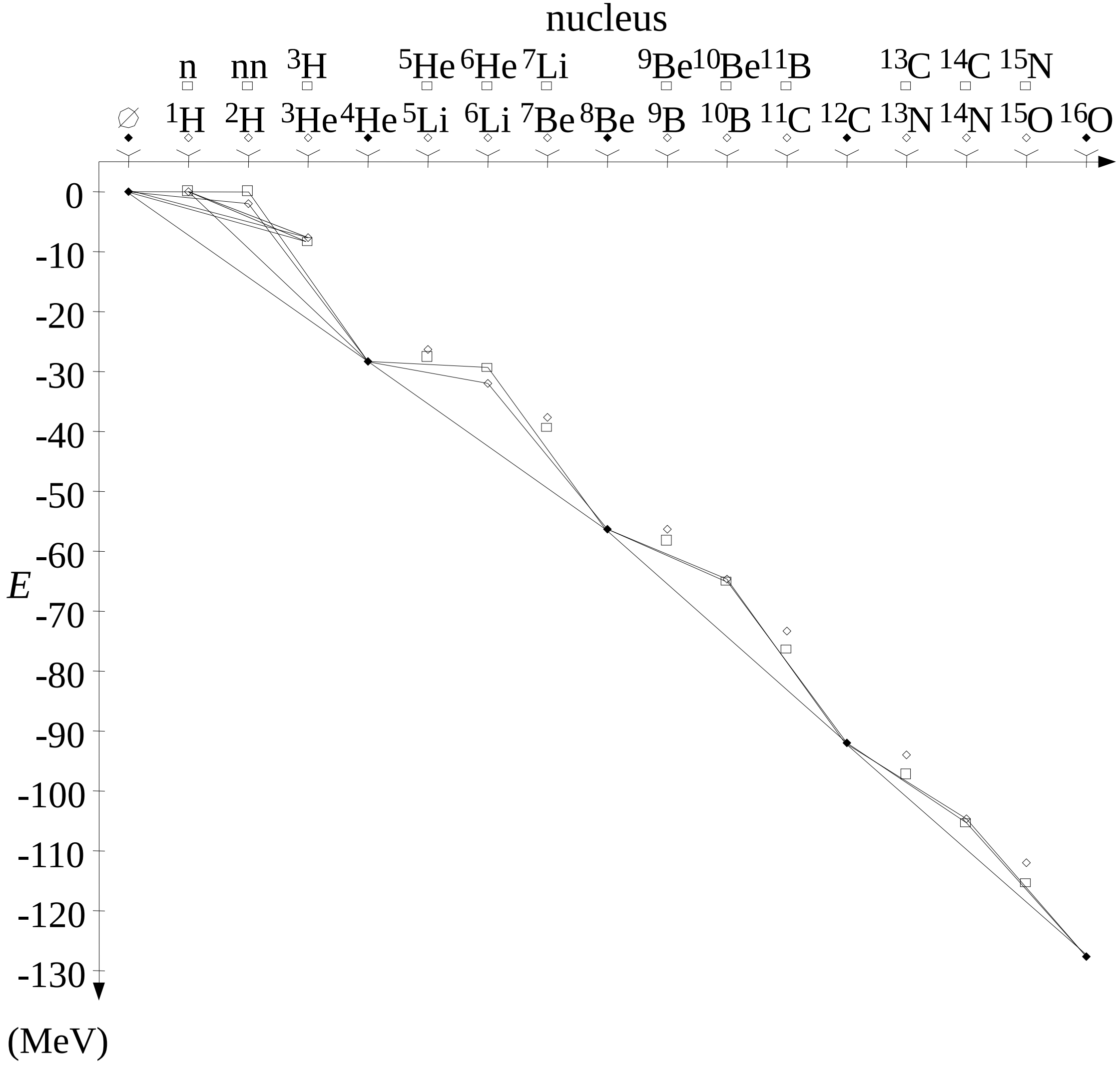
Corollary: System can be simulated without sign oscillations

Chen, D.L. Schäfer, PRL 93 (2004) 242302;
D.L., PRL 98 (2007) 182501

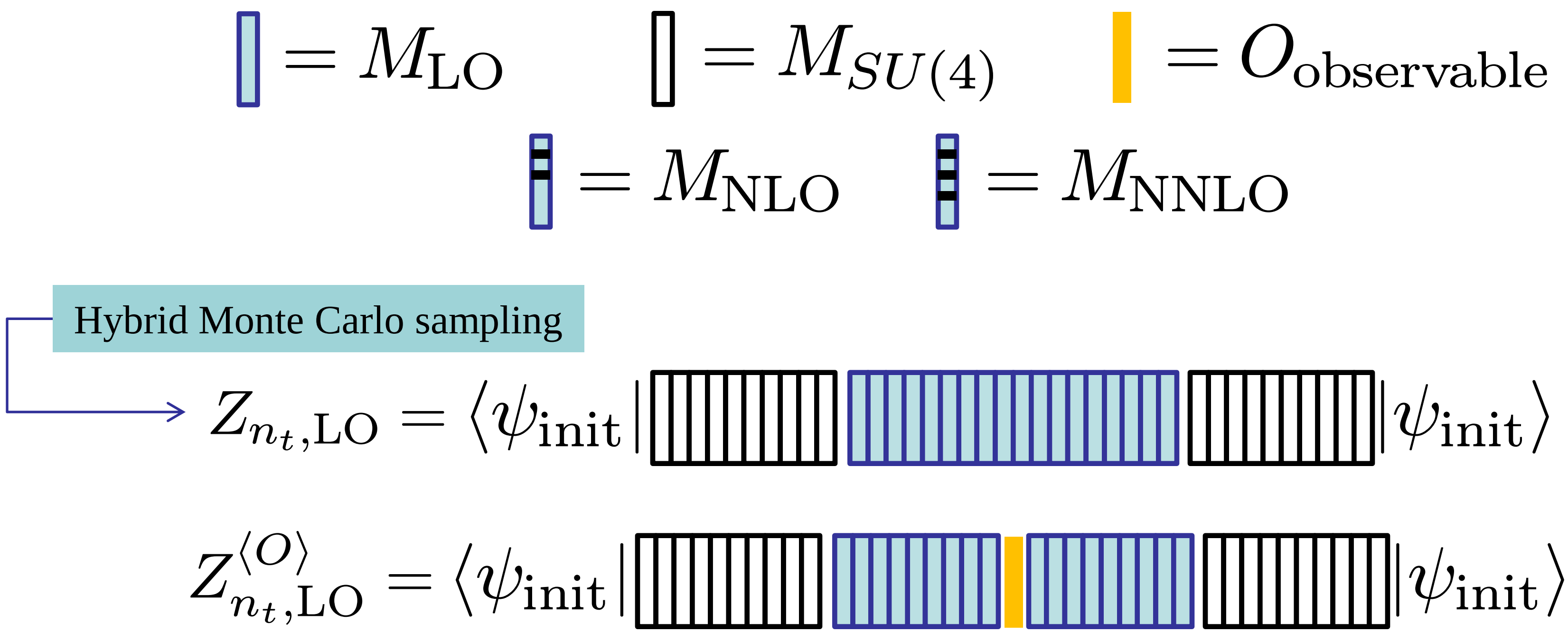




SU(4) convexity bounds

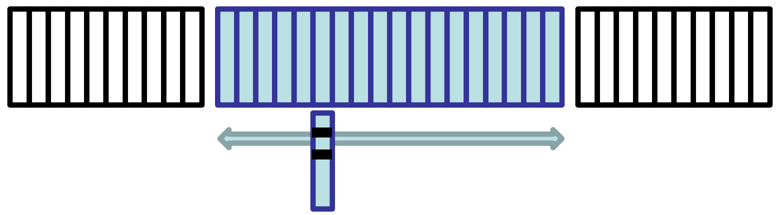


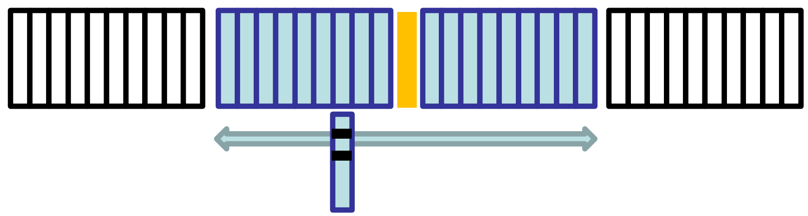
Schematic of calculations



$$e^{-E_{0,\mathrm{LO}} a_t} = \lim_{n_t \to \infty} Z_{n_t+1,\mathrm{LO}} / Z_{n_t,\mathrm{LO}}$$

$$\langle O \rangle_{0,\mathrm{LO}} = \lim_{n_t \to \infty} Z_{n_t,\mathrm{LO}}^{\langle O \rangle} / Z_{n_t,\mathrm{LO}}$$

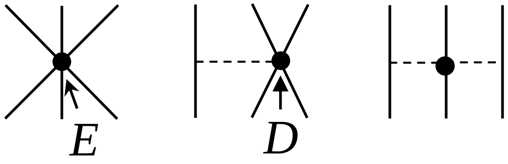
$Z_{n_t,\mathrm{NLO}} = \langle \psi_{\mathrm{init}} |$  $| \psi_{\mathrm{init}} \rangle$

$Z^{\langle O \rangle}_{n_t,\mathrm{NLO}} = \langle \psi_{\mathrm{init}} |$  $| \psi_{\mathrm{init}} \rangle$

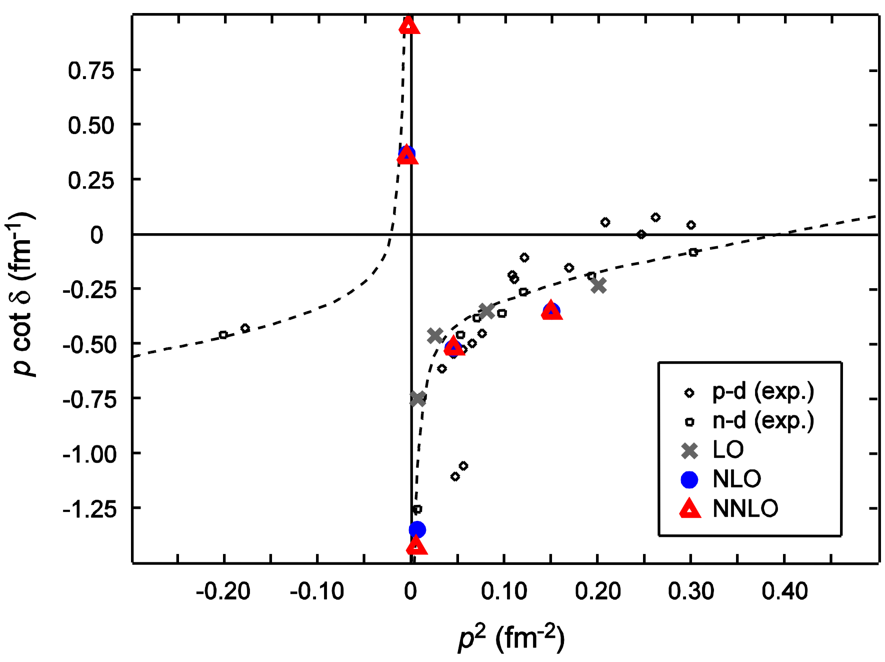
$$\langle O \rangle_{0,\mathrm{NLO}} = \lim_{n_t \to \infty} Z^{\langle O \rangle}_{n_t,\mathrm{NLO}} / Z_{n_t,\mathrm{NLO}}$$

Three-nucleon forces

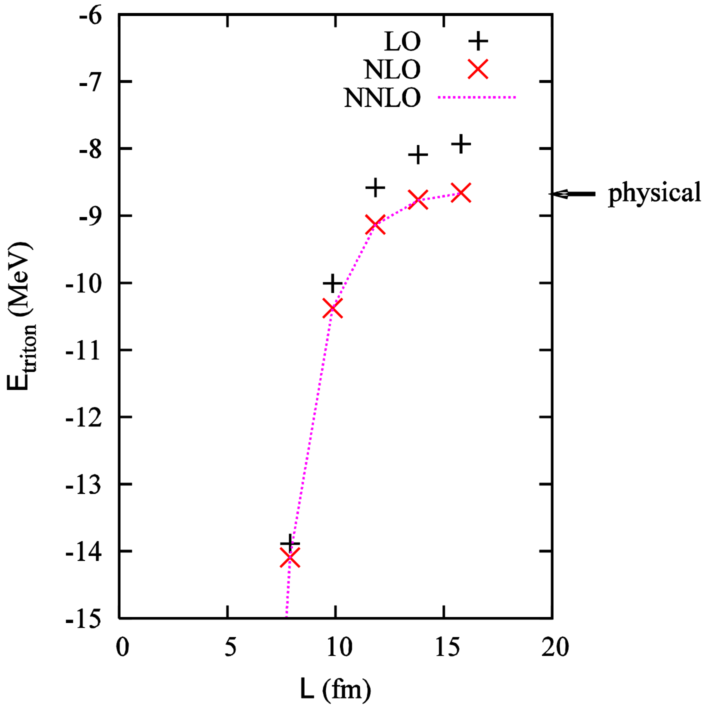
Fit c_D and c_E to spin-1/2 nucleon-deuteron scattering and ^{3}H binding energy



Spin-1/2 nucleon-deuteron



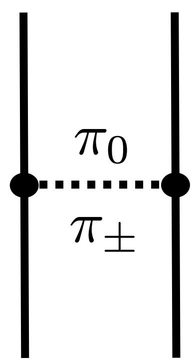
^{3}H binding energy



Isospin breaking and Coulomb effects

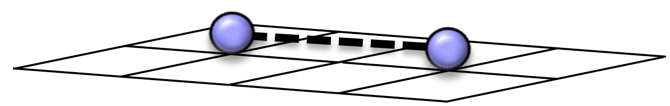
Isospin-breaking and power counting *[Friar , van Kolck, PRC 60 (1999) 034006; Walzl, Meißner, Epelbaum NPA 693 (2001) 663; Friar, van Kolck, Payne, Coon, PRC 68 (2003) 024003; Epelbaum, Meißner, PRC72 (2005) 044001…]*

<u>Pion mass difference</u>

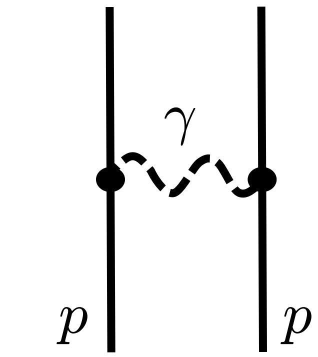


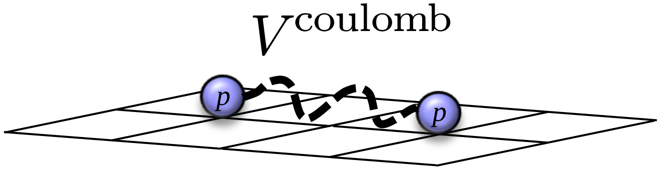
$$m_{\pi_0} \neq m_{\pi_\pm}$$

$$V_{\pi_0}^{\mathrm{OPEP}}, V_{\pi_\pm}^{\mathrm{OPEP}}$$

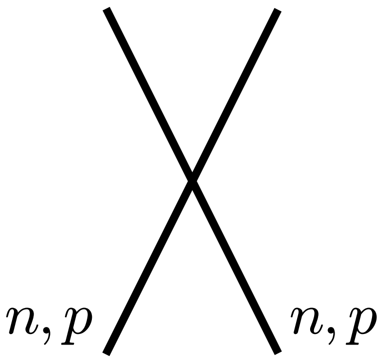


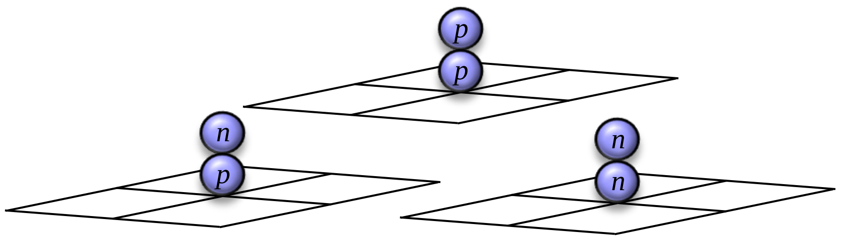
Coulomb potential



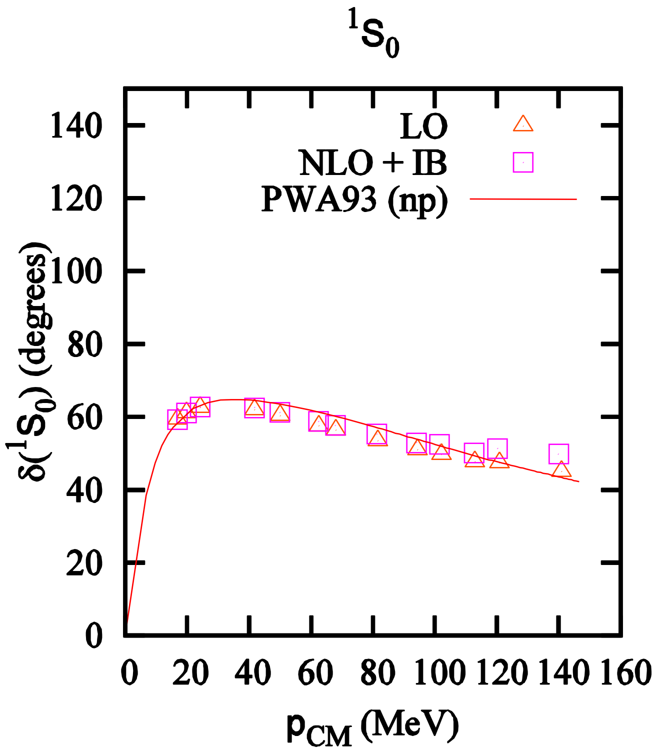


Charge symmetry breaking
Charge independence breaking

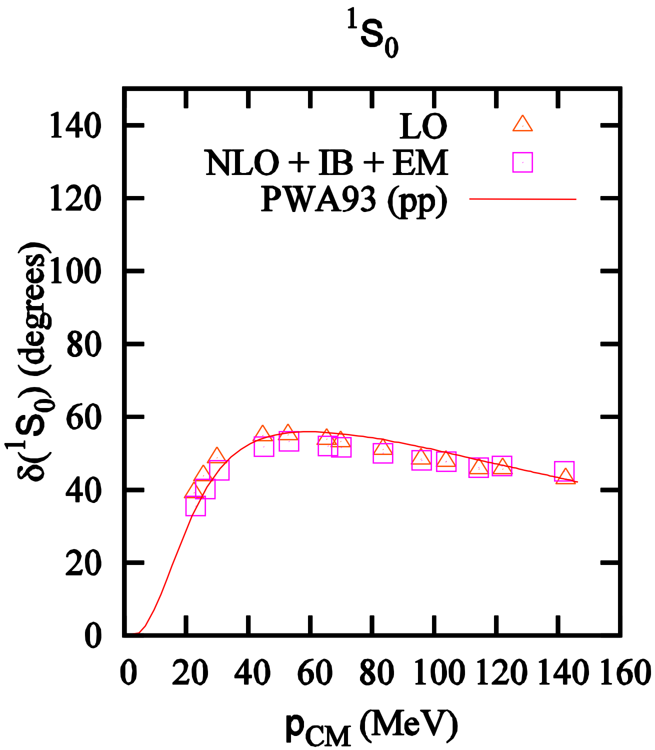




Neutron-proton



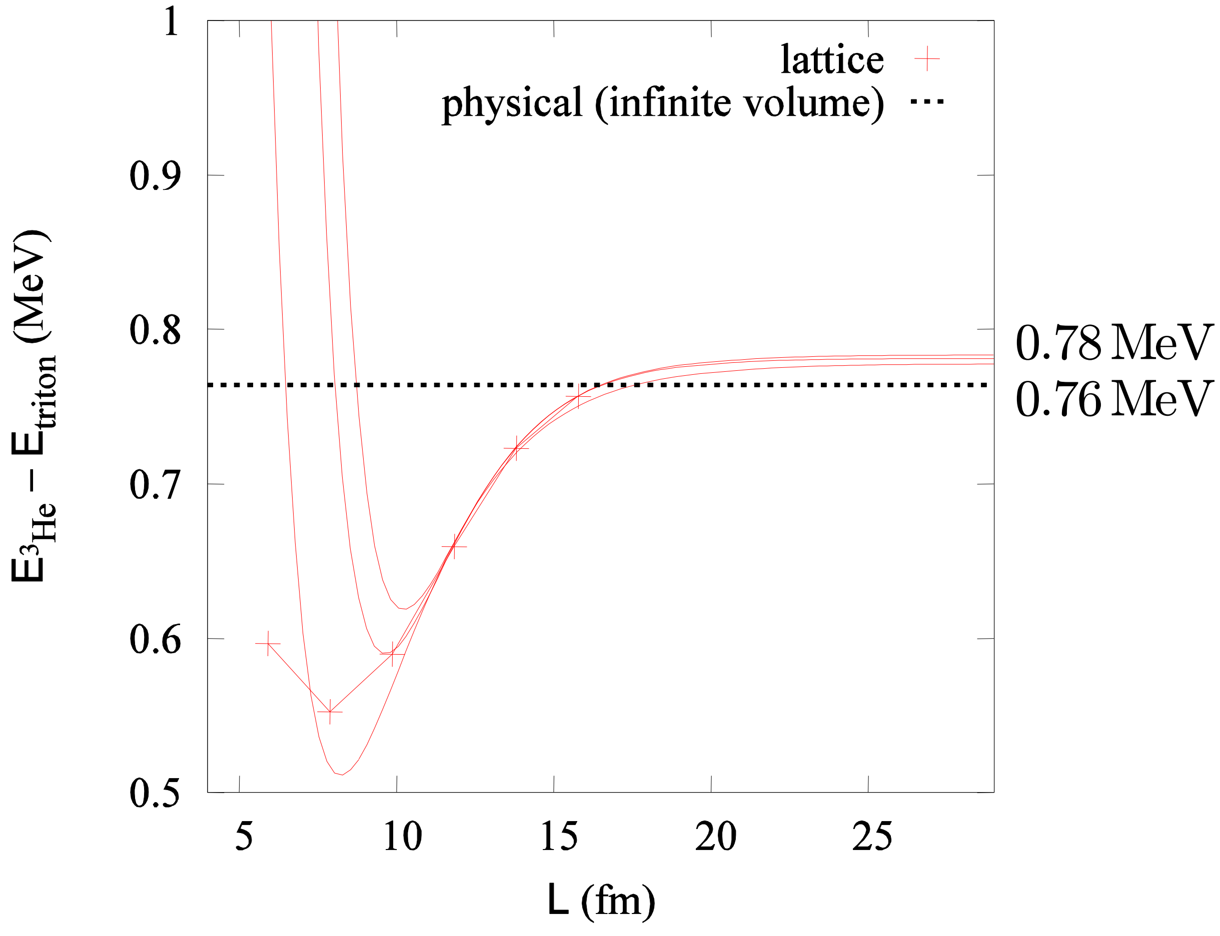
Proton-proton



Epelbaum, Krebs, D.L, Meißner, 0912.4195

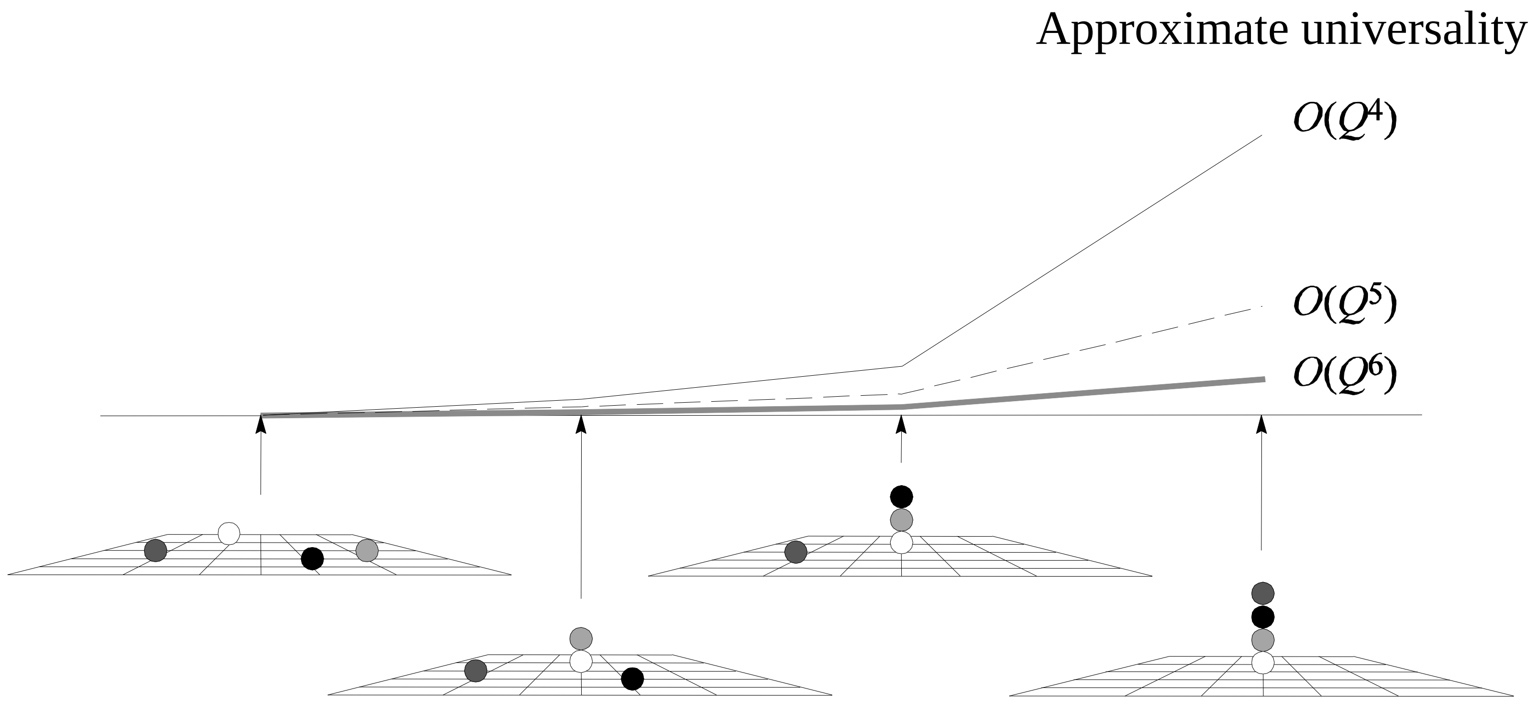
Triton and Helium-3

$$E_{^3\mathrm{He}} - E_{\mathrm{triton}} = 0.78(5)\,\mathrm{MeV}$$



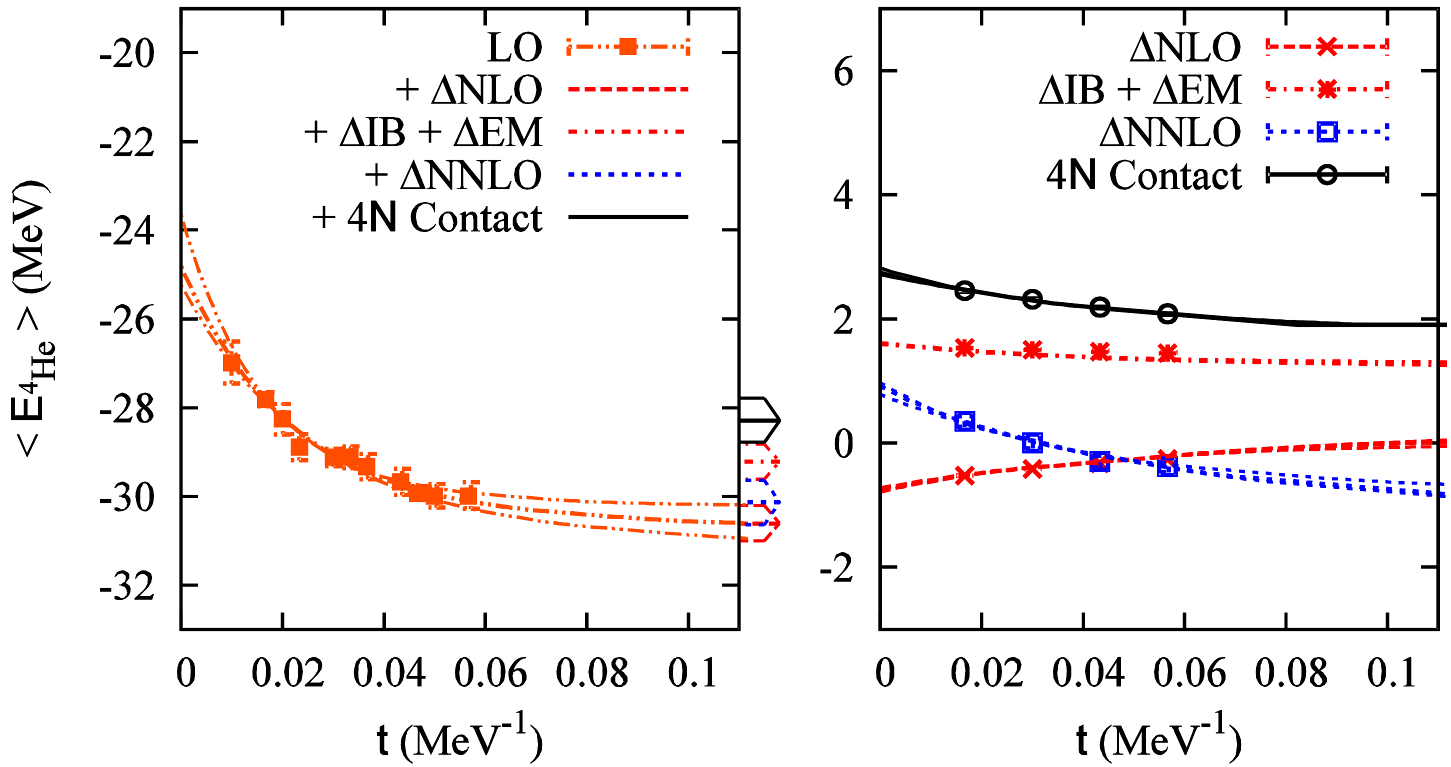
Epelbaum, Krebs, D.L, Meißner, 0912.4195

Relative contribution of omitted operators



Helium-4

$L = 9.9\,\mathrm{fm}$



Epelbaum, Krebs, D.L, Meißner, 0912.4195

Helium-4

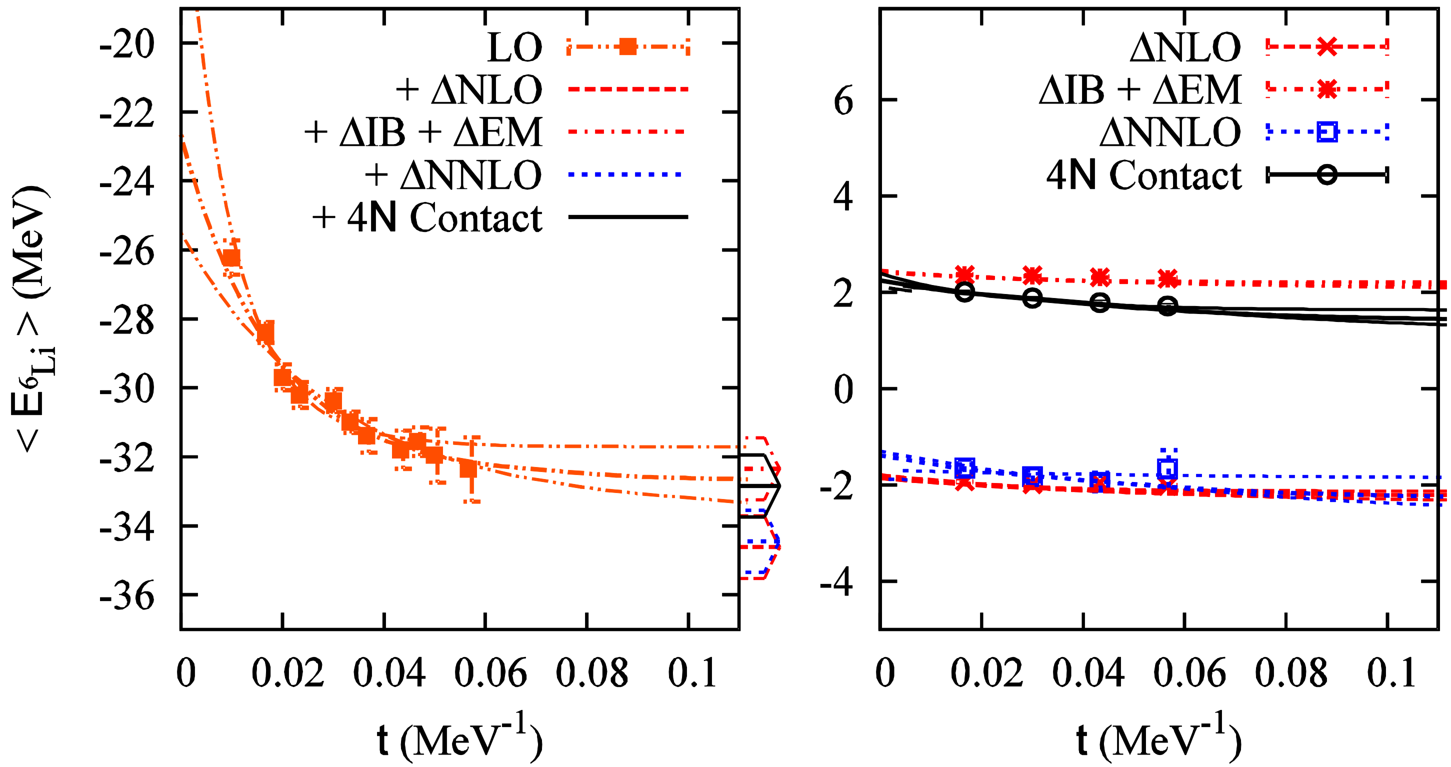
$L = 9.9\,\mathrm{fm}$

LO	–30.5(4) MeV
NLO	–30.6(4) MeV
NLO + IB + EM	–29.2(4) MeV
NNLO + IB + EM	–30.1(5) MeV
NNLO + IB + EM + $4N_{\text{contact}}$	–28.3(5) MeV
Physical (infinite volume)	–28.3 MeV

Still to do: infinite volume extrapolation

Lithium-6

$L = 9.9\,\mathrm{fm}$



Epelbaum, Krebs, D.L, Meißner, 0912.4195

Lithium-6

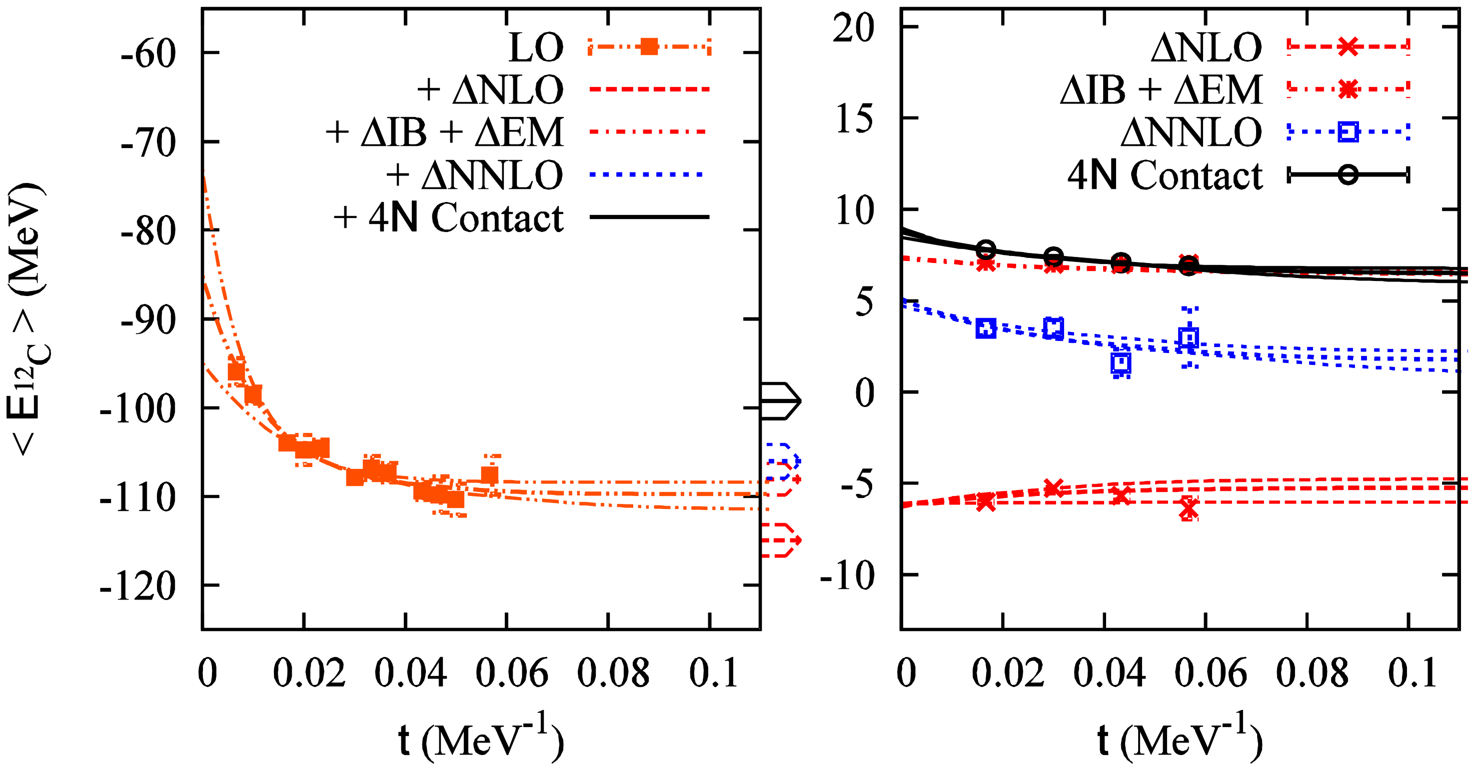
$$L = 9.9\,\mathrm{fm}$$

LO	–32.6(9) MeV
NLO	–34.6(9) MeV
NLO + IB + EM	–32.4(9) MeV
NNLO + IB + EM	–34.5(9) MeV
NNLO + IB + EM + 4N_{contact}	–32.9(9) MeV
Physical (infinite volume)	–32.0 MeV

Still to do: infinite volume extrapolation

Carbon-12

$L = 13.8\,\text{fm}$



Epelbaum, Krebs, D.L, Meißner, 0912.4195

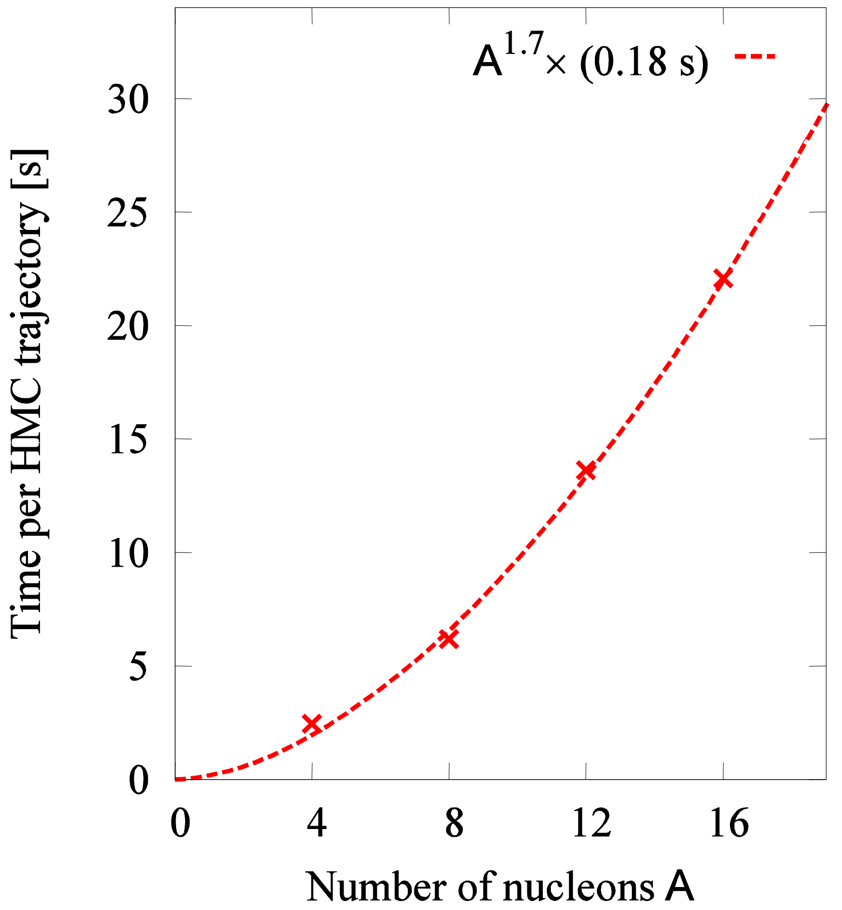
Carbon-12

$L = 13.8\,\mathrm{fm}$

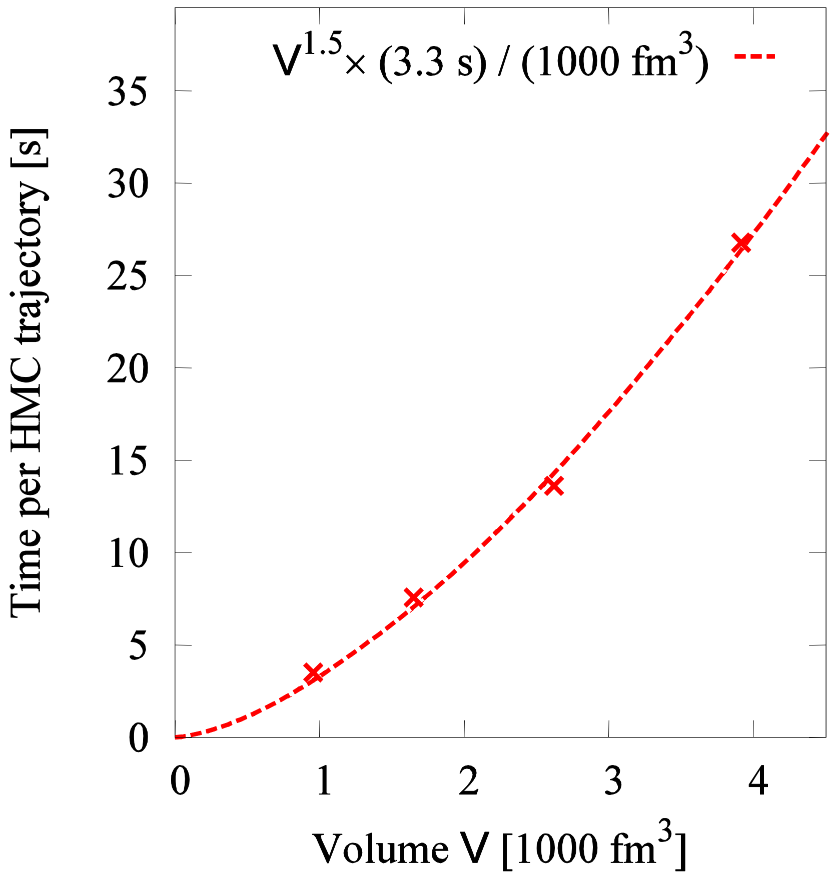
LO	–109(2) MeV
NLO	–115(2) MeV
NLO + IB + EM	–108(2) MeV
NNLO + IB + EM	–106(2) MeV
NNLO + IB + EM + $4N_{\mathrm{contact}}$	–99(2) MeV
Physical (infinite volume)	–92.2 MeV

Still to do: infinite volume extrapolation

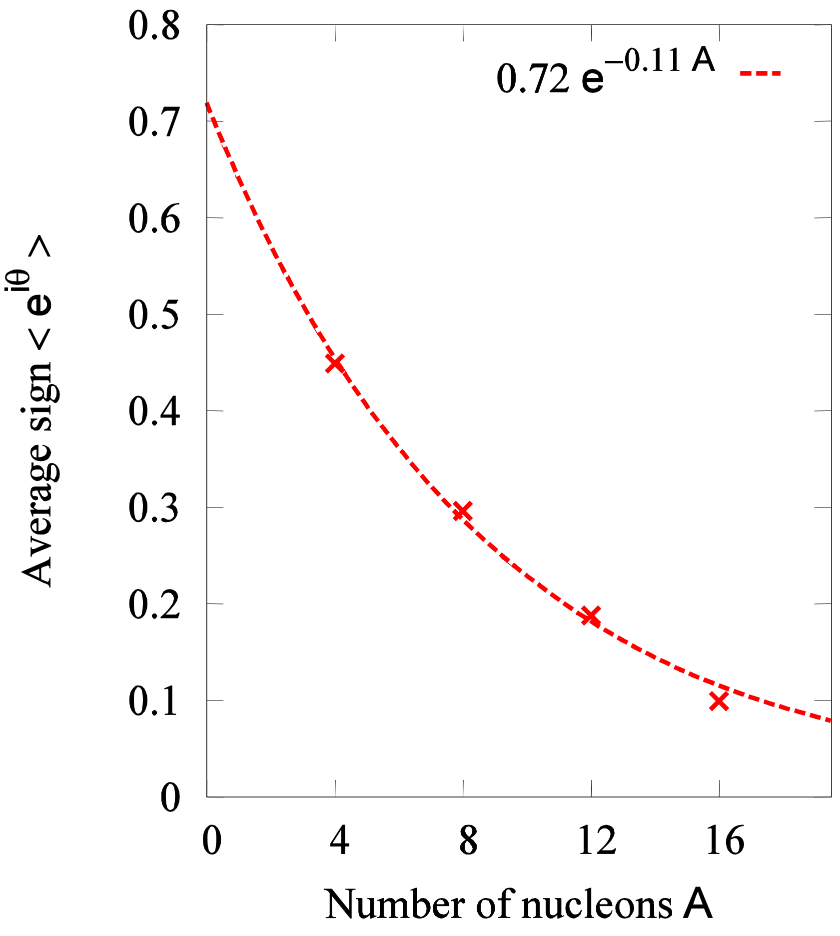
Computational time versus number of nucleons



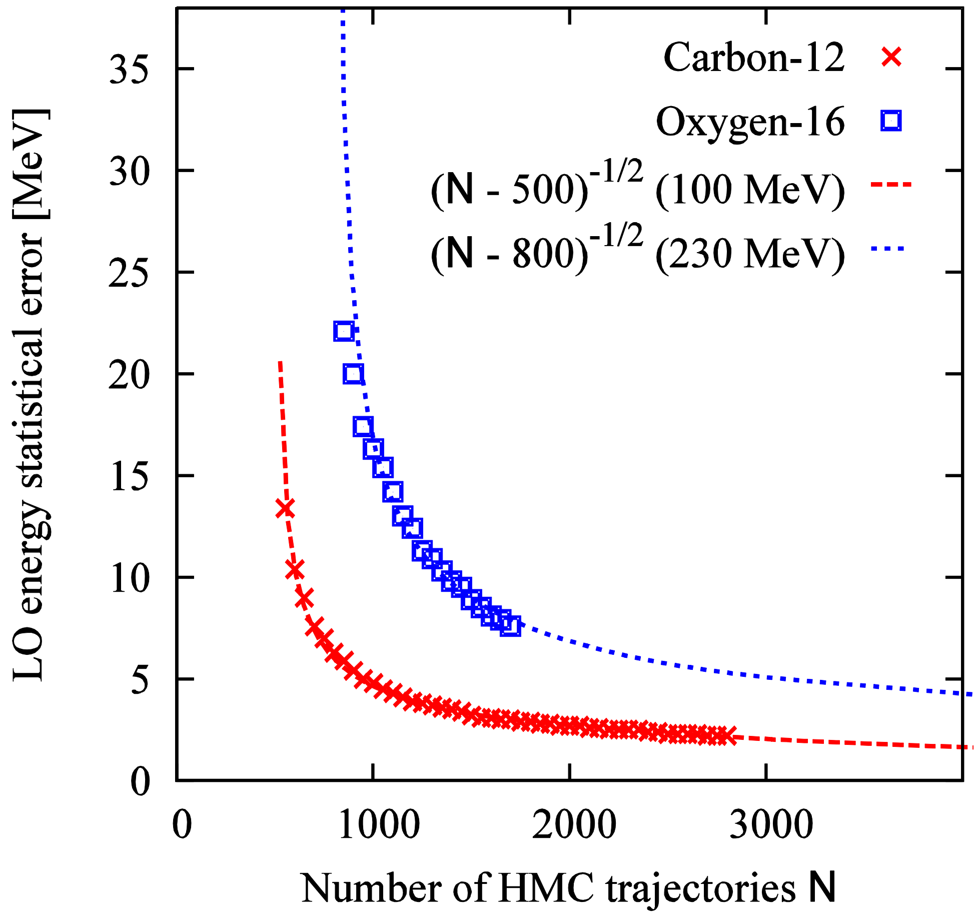
Computational time versus volume



Average sign versus number of nucleons



Statistic error versus number of HMC trajectories



Summary and future directions

Lattice effective field theory is promising tool that combines framework of effective field theory and computational lattice methods

Applications to zero and nonzero temperature simulations of nuclei, neutron matter, nuclear matter, etc.

To do: Infinite volume extrapolations, different boundary conditions, larger nuclei, smaller lattice spacing, higher orders

To do: Storing lattice configurations to calculate correlation functions, scattering, electroweak transitions, etc.