Nuclear lattice simulations

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Outline

What is lattice effective field theory?

Chiral effective field theory for nucleons

Computational strategies on the lattice

Auxiliary fields, signs, and complex actions

Phase shifts and unknown operator coefficients

Dilute neutron matter at NLO

Studies of light nuclei at NNLO

Summary and future directions

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

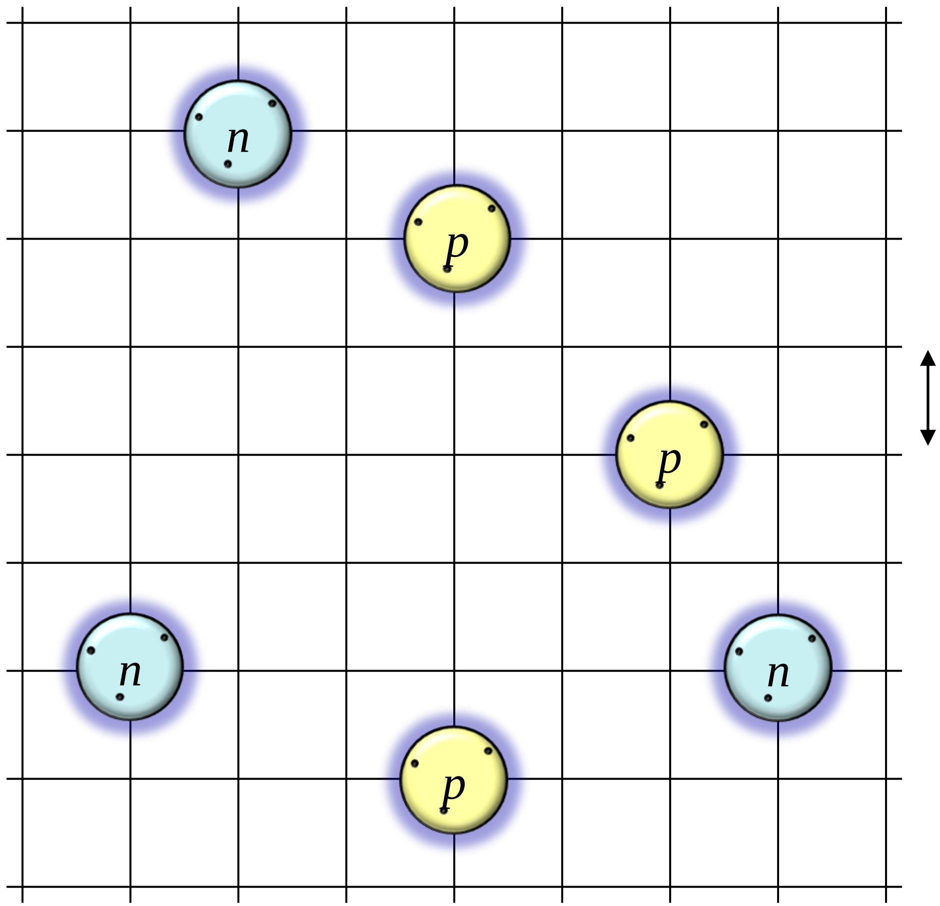
Juillet, New J. Phys. 9 (2007)163

Wingate, cond-mat/0502372

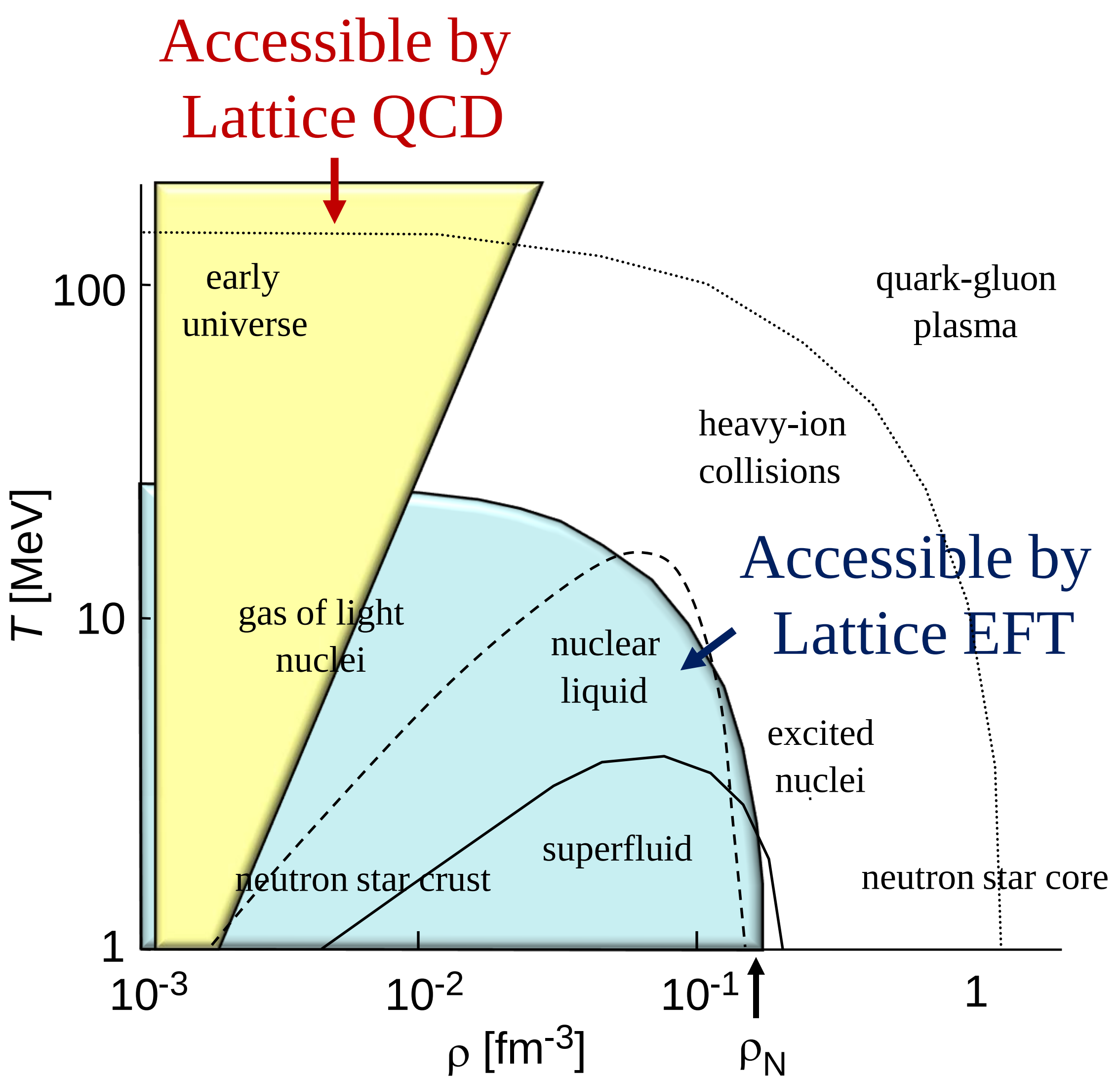
D.L., Schaefer, PRC 73 (2006) 015202; …

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

Lattice EFT for nucleons



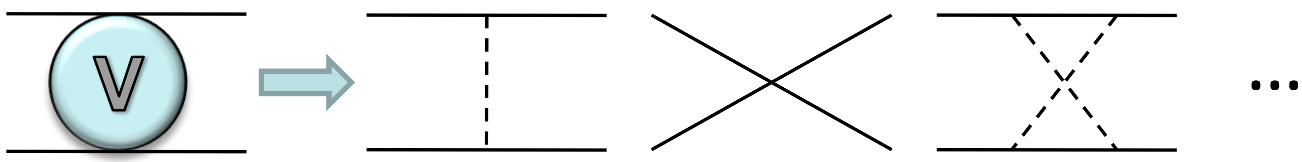
$a \sim 1 - 5$ fm


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
100
10
1
T [MeV]
10-3
10-2
10-1
1
ρ [fm-3]
ρN

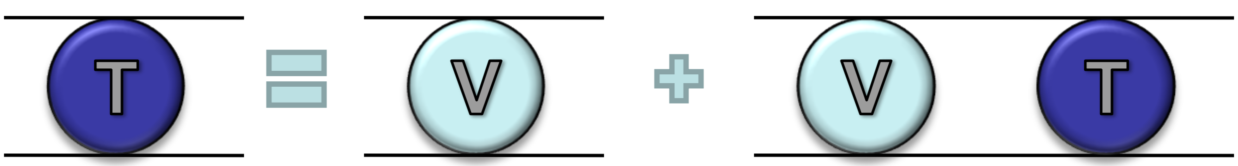
Chiral EFT for low-energy nucleons

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

Construct the effective potential order by order



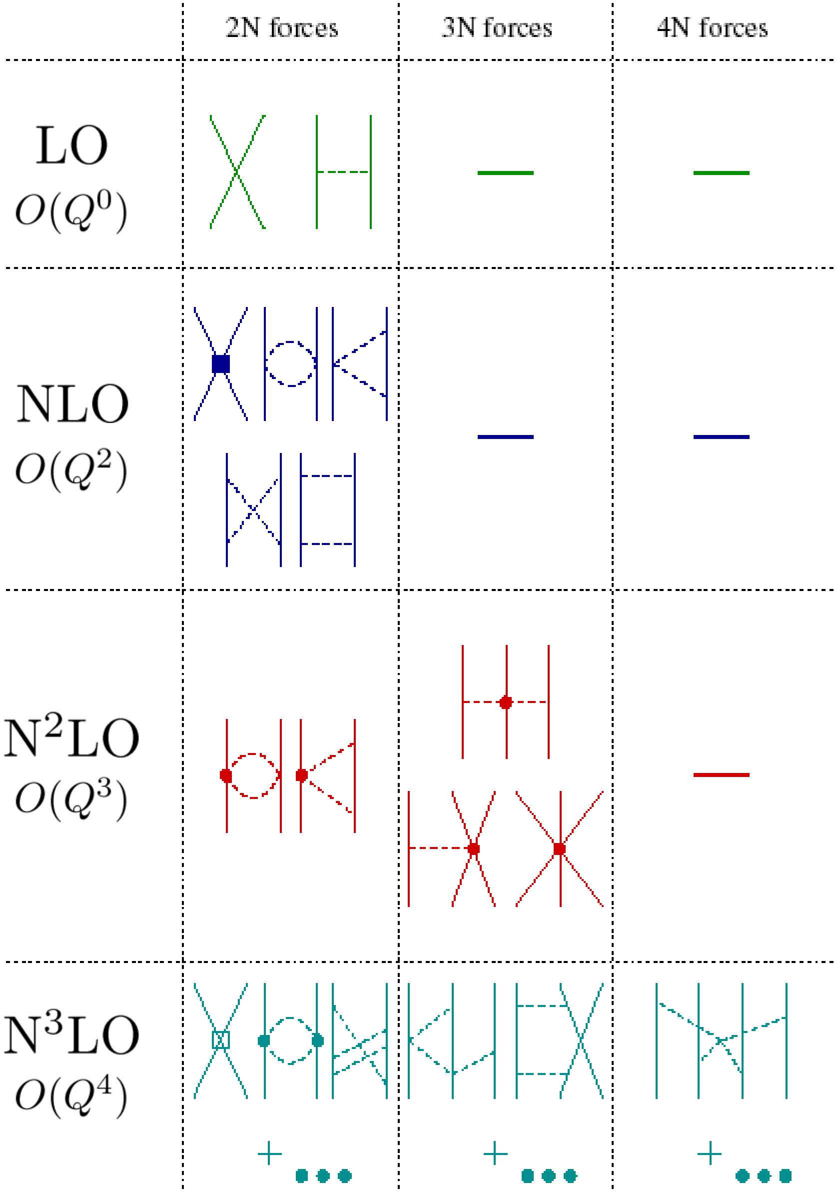
Solve Lippmann-Schwinger equation non-perturbatively



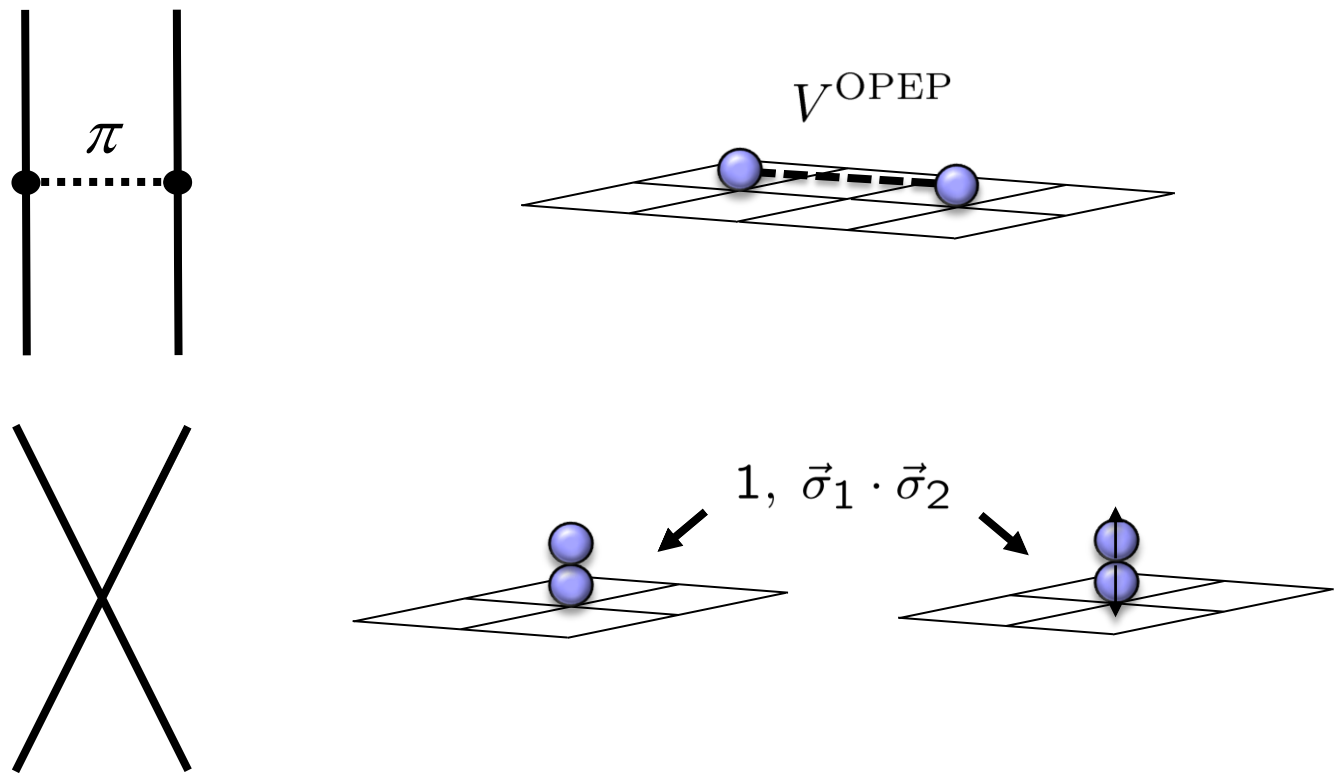
Nuclear
Scattering Data

Effective
Field Theory

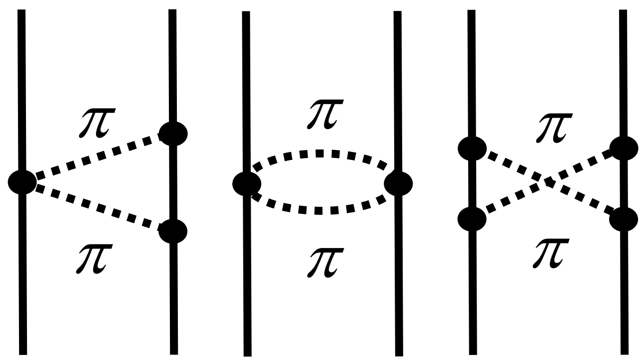
Ordonez et al. ’94; Friar & Coon ’94;
Kaiser et al. ’97; Epelbaum et al. ’98,‘03;
Kaiser ’99-’01; Higa et al. ’03; …



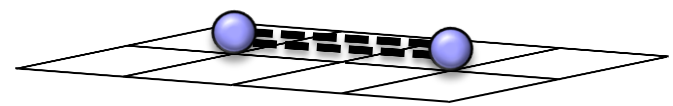
Leading order on lattice

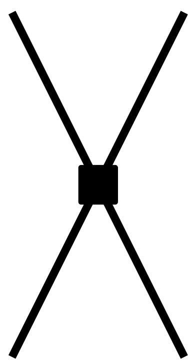


Next-to-leading order on lattice

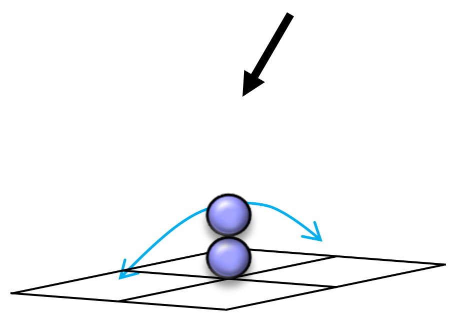


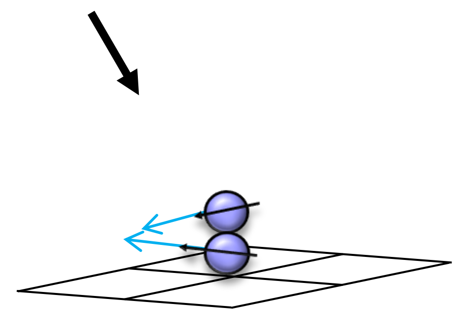
V^{TPEP}



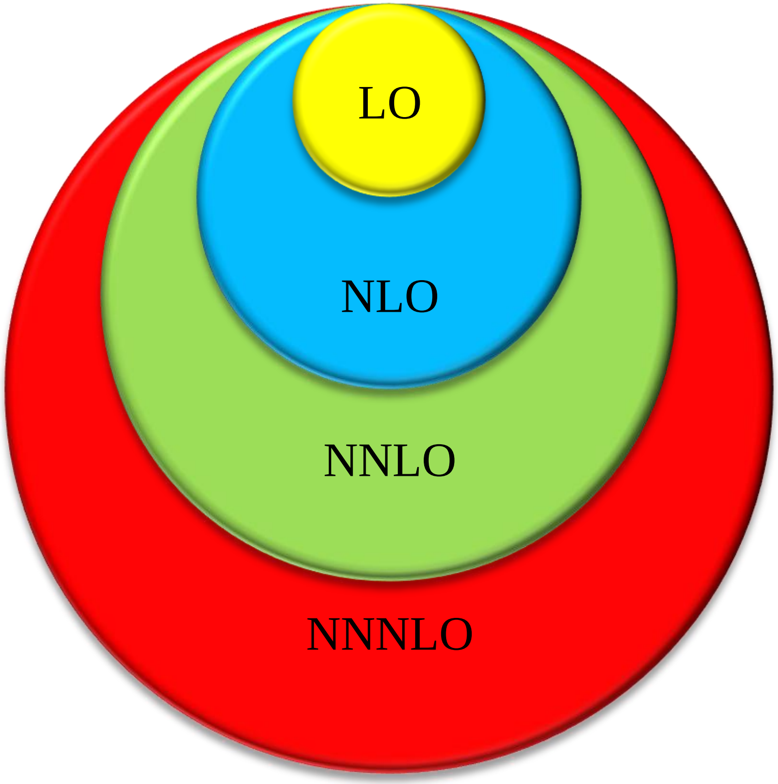


$\vec{\nabla}_1 \cdot \vec{\nabla}_2 \qquad (\vec{\sigma}_1 \cdot \vec{\nabla}_1)\,(\vec{\sigma}_2 \cdot \vec{\nabla}_2) \qquad \cdots$



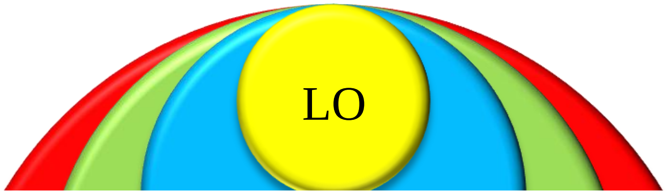


Computational strategy



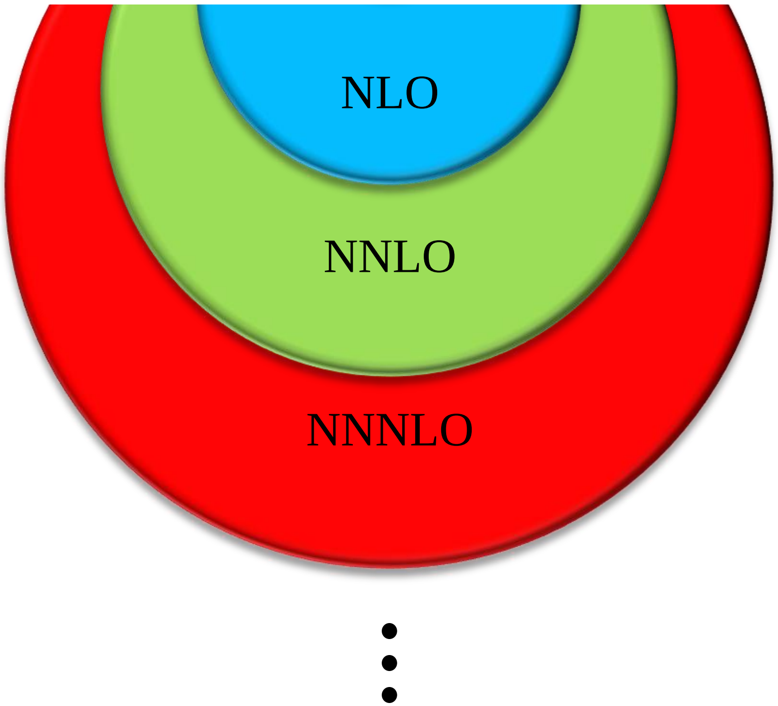
⋮

Non-perturbative – Monte Carlo



“Improved LO”

Perturbative corrections



Lattice formulations

Grassmann path integral $\exp\left[-S(c, c^{*})\right]$	$=$	Transfer matrix operator M	$\xrightarrow{a_t \to 0}$	Hamiltonian operator H
$\parallel$		$\parallel$		$\parallel$
Grassmann path integral with auxiliary/pion field $\exp\left[-S_A(c, c^{*}, \pi, s)\right]$	$=$	Transfer matrix operator with auxiliary/pion field $M_A(s, \pi, n_t)$	$\xrightarrow{a_t \to 0}$	Hamiltonian operator with auxiliary/pion field $M_A(s, \pi, t)$

Euclidean-time transfer matrix

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

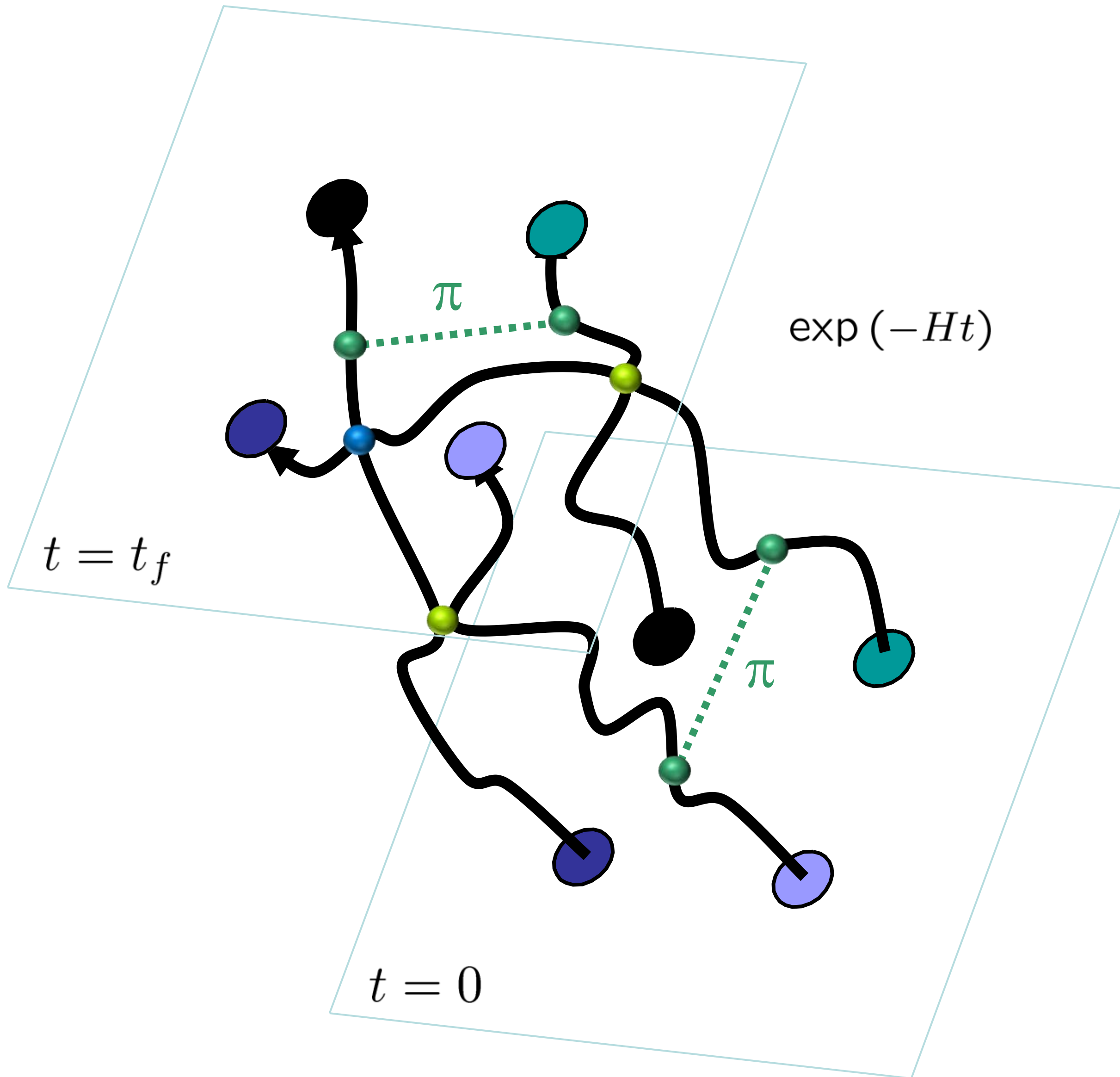
… with auxiliary fields

C contact interaction:

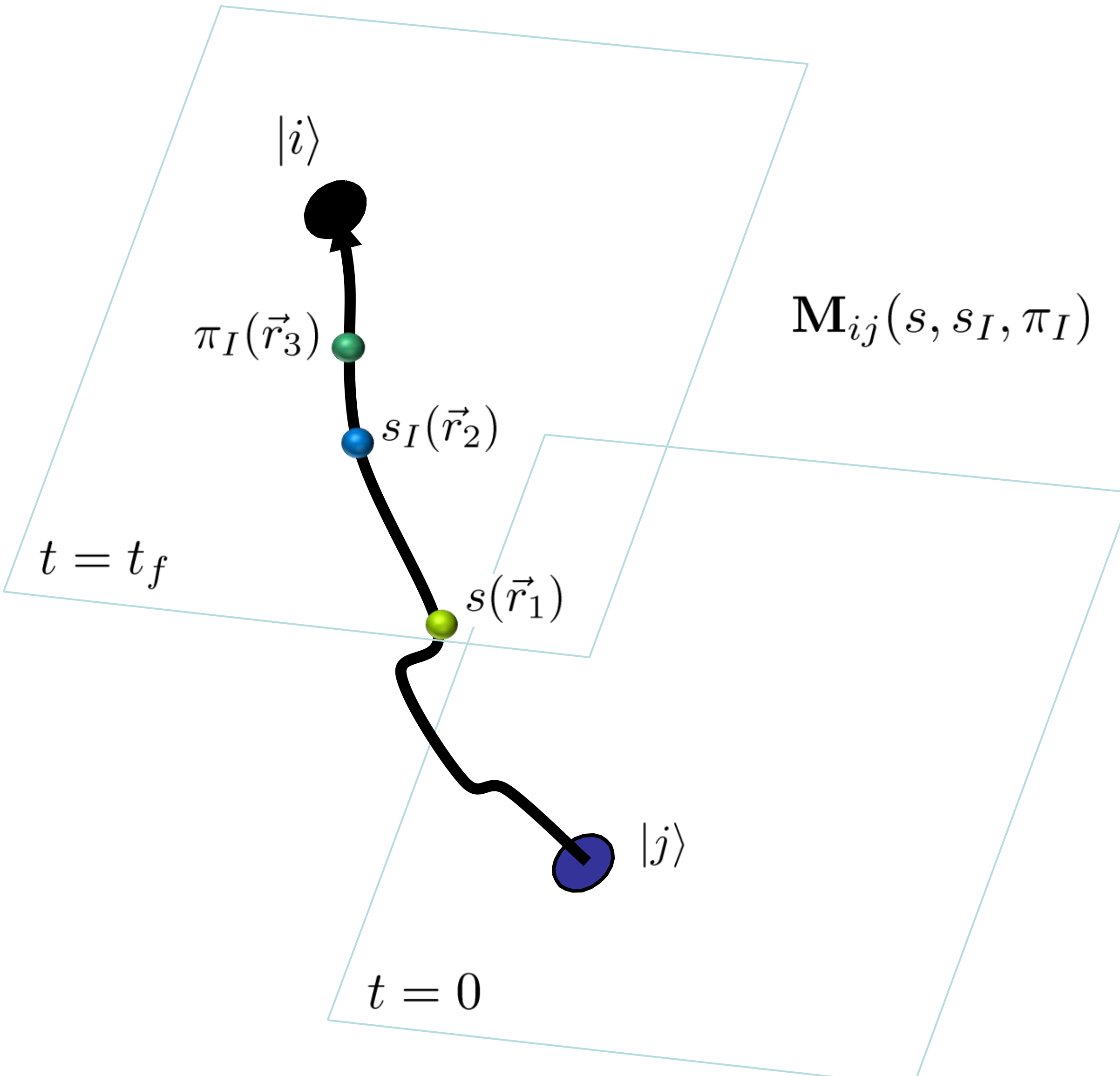
$$\exp\left[-\frac{1}{2}CN^\dagger NN^\dagger N\Delta t\right] \quad (C<0)$$
$$= \frac{1}{\sqrt{2\pi}}\int ds \exp\left[-\frac{1}{2}s^2 + sN^\dagger N\sqrt{-C\Delta t}\right]$$

C_I contact interaction:

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



π
$\exp(-Ht)$
$t = t_f$
π
$t = 0$


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

Auxiliary-field determinantal Monte Carlo

$$\langle\psi_{\text{init}}|\, M^{(L_t-1)}(s,s_I,\pi_I)\cdot\cdots\cdot M^{(0)}(s,s_I,\pi_I)\,|\psi_{\text{init}}\rangle = \det\mathbf{M}(s,s_I,\pi_I)$$

$$\mathbf{M}_{ij}(s,s_I,\pi_I) = \langle\vec{p}_i|\, M^{(L_t-1)}(s,s_I,\pi_I)\cdots M^{(0)}(s,s_I,\pi_I)\,|\vec{p}_j\rangle$$

For *A* nucleons, the matrix is *A* by *A*.

For the leading-order calculation, if there is no pion coupling and the quantum state is an isospin singlet then

$$\tau_2\mathbf{M}\tau_2 = \mathbf{M}^*$$

This shows the determinant is real. Actually can show the determinant is positive semi-definite.

With nonzero pion coupling the determinant is real for a spin-singlet isospin-singlet quantum state

$$\sigma_2 \tau_2 \mathbf{M} \sigma_2 \tau_2 = \mathbf{M}^*$$

but the determinant can be both positive and negative

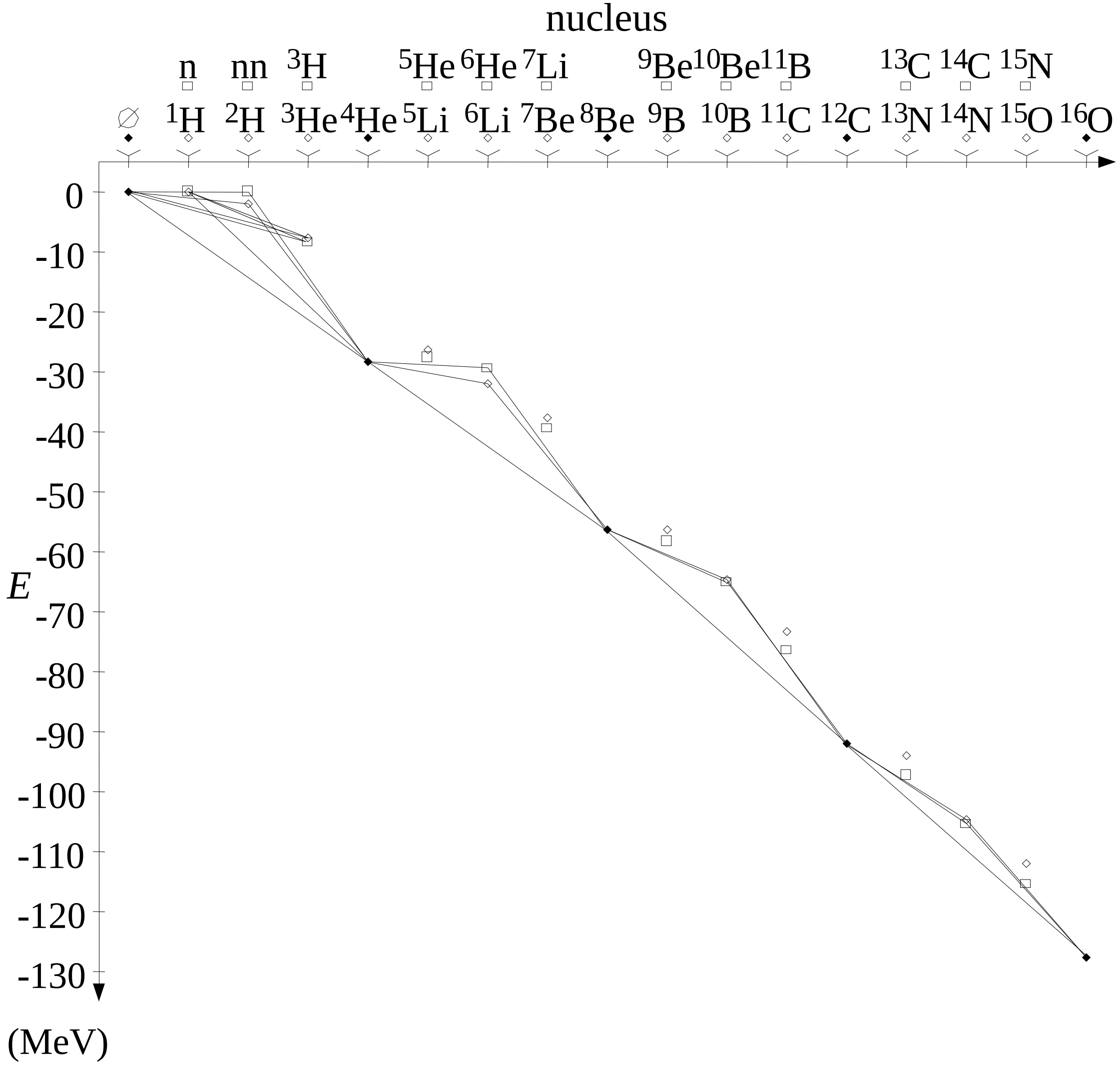
Some comments about Wigner's approximate SU(4) symmetry…

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

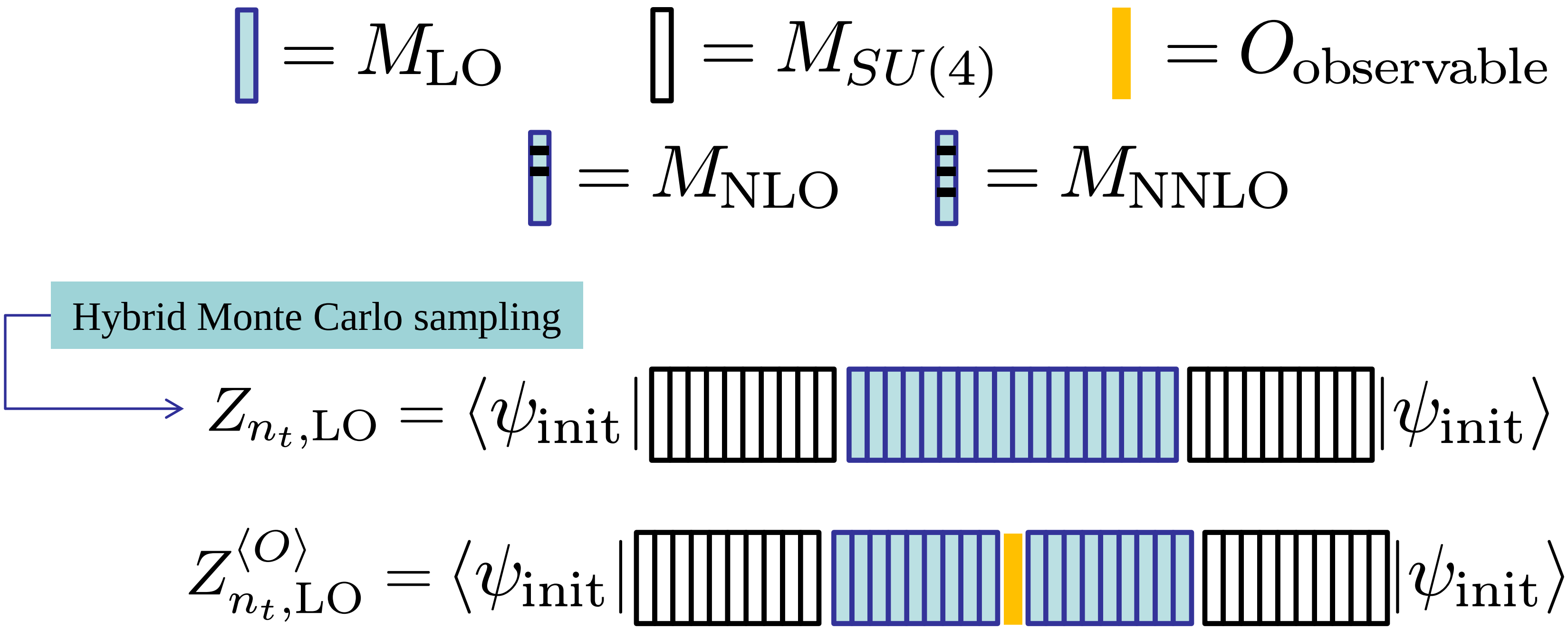
Corollary: It can be simulated without sign oscillations

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

SU(4) convexity bounds

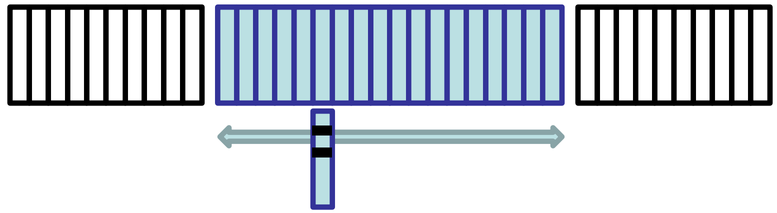


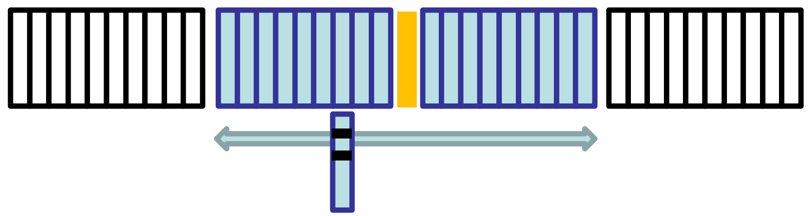
Schematic of projection calculations



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

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

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

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

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

LO_1: Pure contact interactions

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

LO_2: Gaussian smearing

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

LO_3: Gaussian smearing only in even partial waves

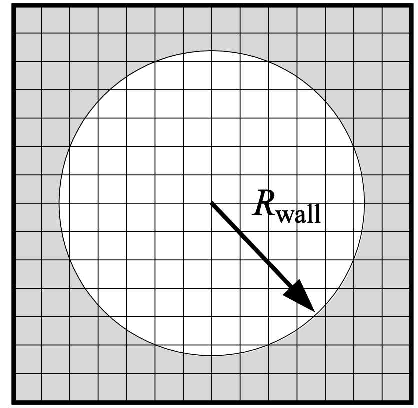
$$\begin{aligned}\mathcal{A}(V_{\text{LO}_3}) = {} & C_{1S0} f(\vec{q}^{\,2}) \left(\tfrac{1}{4} - \tfrac{1}{4}\vec{\sigma}_1 \cdot \vec{\sigma}_2\right) \left(\tfrac{3}{4} + \tfrac{1}{4}\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2\right) \\ & + C_{3S1} f(\vec{q}^{\,2}) \left(\tfrac{3}{4} + \tfrac{1}{4}\vec{\sigma}_1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

Physical scattering data → Unknown operator coefficients

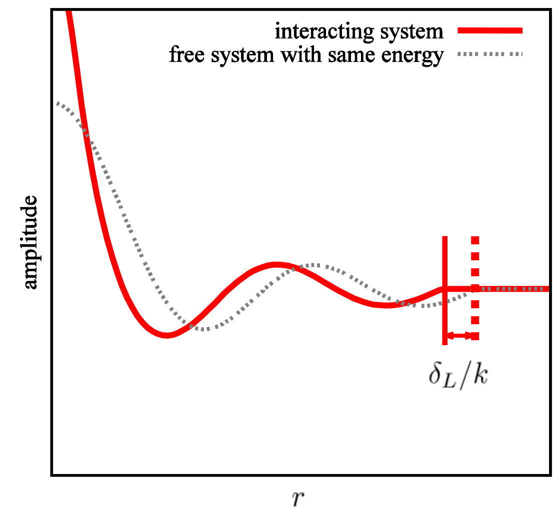
Spherical wall method

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

Spherical wall imposed in the center of mass frame

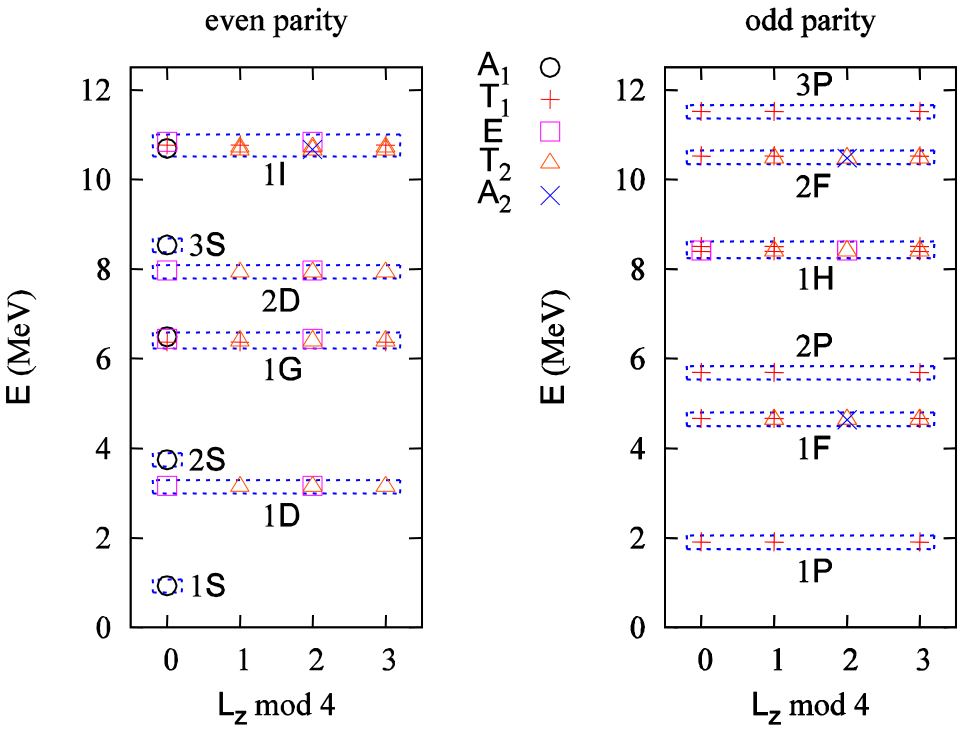


Representation	J_z	Example
A_1	$0 \bmod 4$	$Y_{0,0}$
T_1	$0, 1, 3 \bmod 4$	$\{Y_{1,0}, Y_{1,1}, Y_{1,-1}\}$
E	$0, 2 \bmod 4$	$\left\{Y_{2,0}, \frac{Y_{2,-2}+Y_{2,2}}{\sqrt{2}}\right\}$
T_2	$1, 2, 3 \bmod 4$	$\left\{Y_{2,1}, \frac{Y_{2,-2}-Y_{2,2}}{\sqrt{2}}, Y_{2,-1}\right\}$
A_2	$2 \bmod 4$	$\frac{Y_{3,2}-Y_{3,-2}}{\sqrt{2}}$



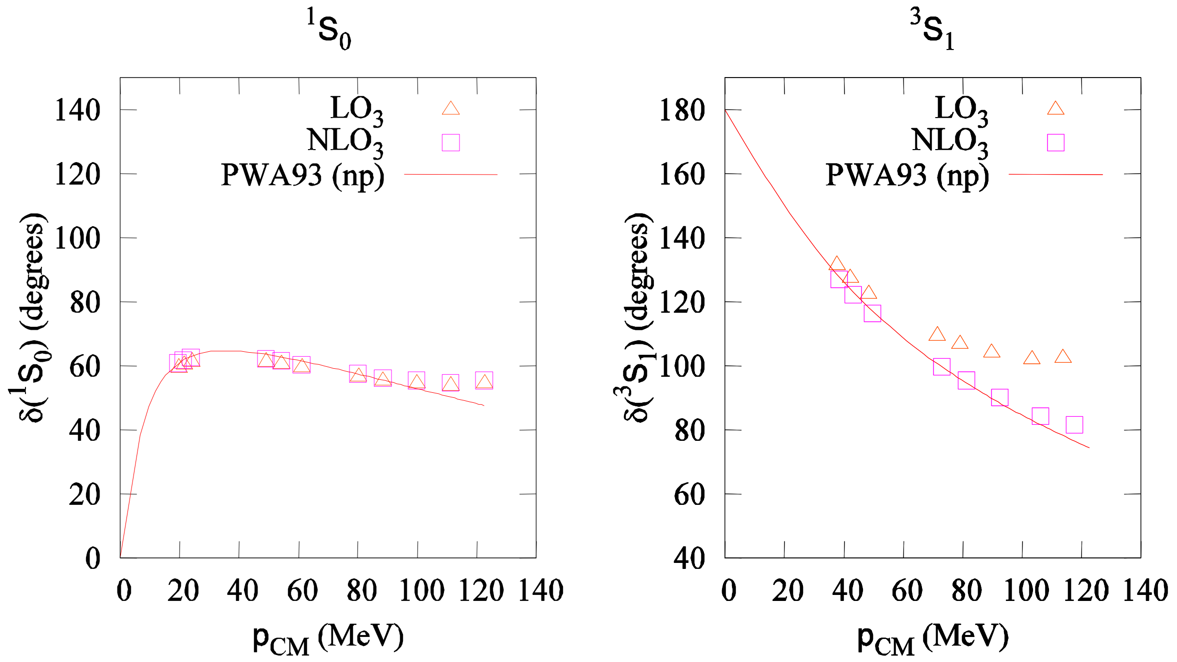
Energy levels with hard spherical wall

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

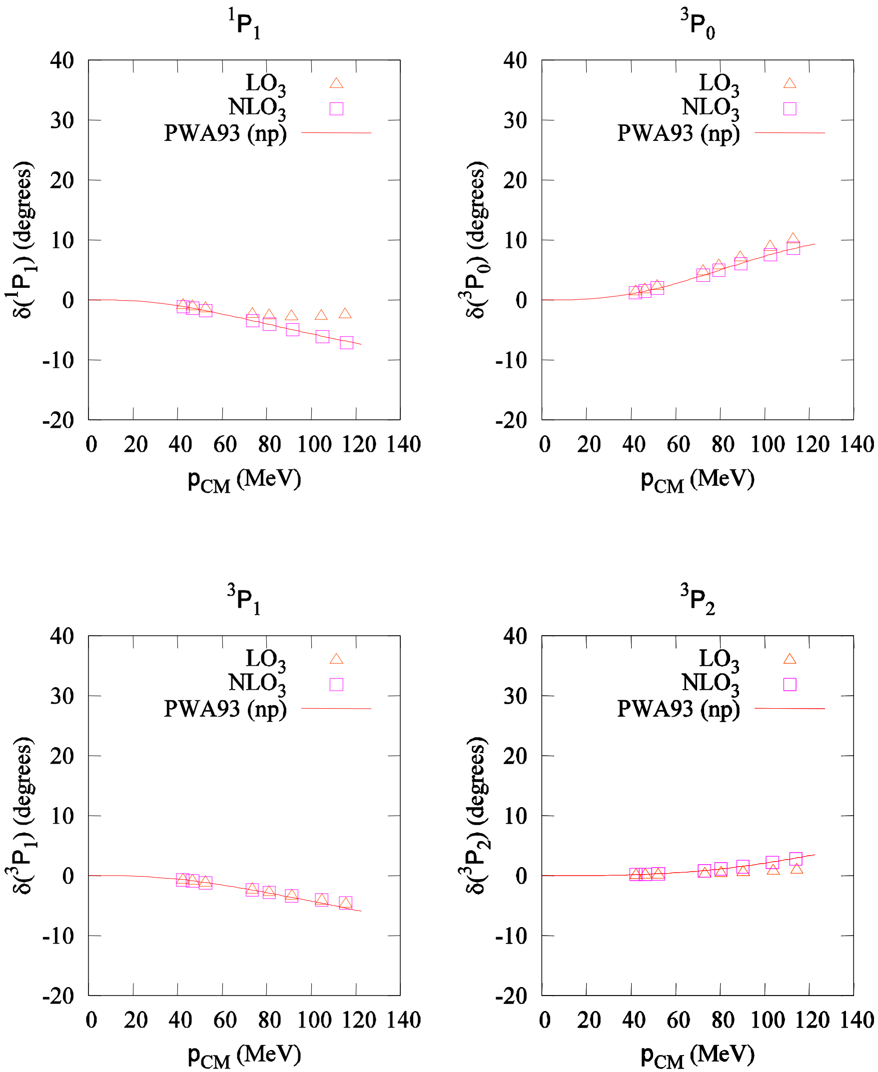


Energy shift from free-particle values gives the phase shift

LO_3: S waves $\quad a = 1.97$ fm



LO_3: P waves $a = 1.97$ fm



Dilute neutrons and the unitarity limit

Neutron-neutron scattering amplitude: $f_0(k) = \frac{1}{k\cot\delta_0(k) - ik}$

$$k\cot\delta_0(k) \approx -a_0^{-1} + \frac{1}{2}r_0 k^2$$

Unitarity limit: $r_0 \to 0, a_0 \to \infty$ $f_0(k) \to \frac{i}{k}$

Free Fermi gas ground state

$$\frac{E_0^{\text{free}}}{A} = \frac{3}{5}E_F$$

$$E_F = \frac{k_F^2}{2m}$$

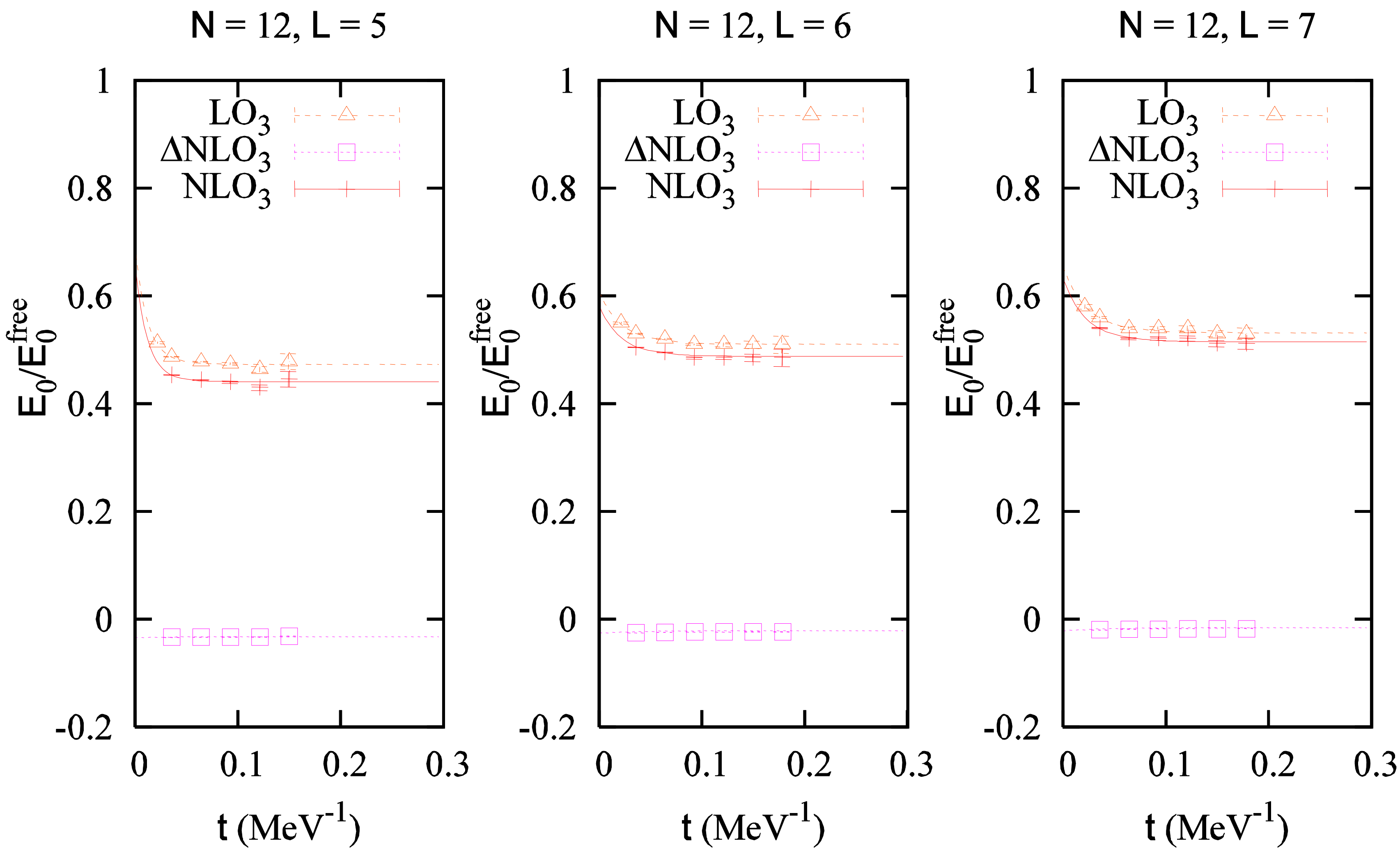
Unitarity limit ground state

$$\frac{E_0}{A} = \xi \cdot \frac{E_0^{\text{free}}}{A} = \xi \cdot \frac{3}{5}E_F$$

ξ is a dimensionless number

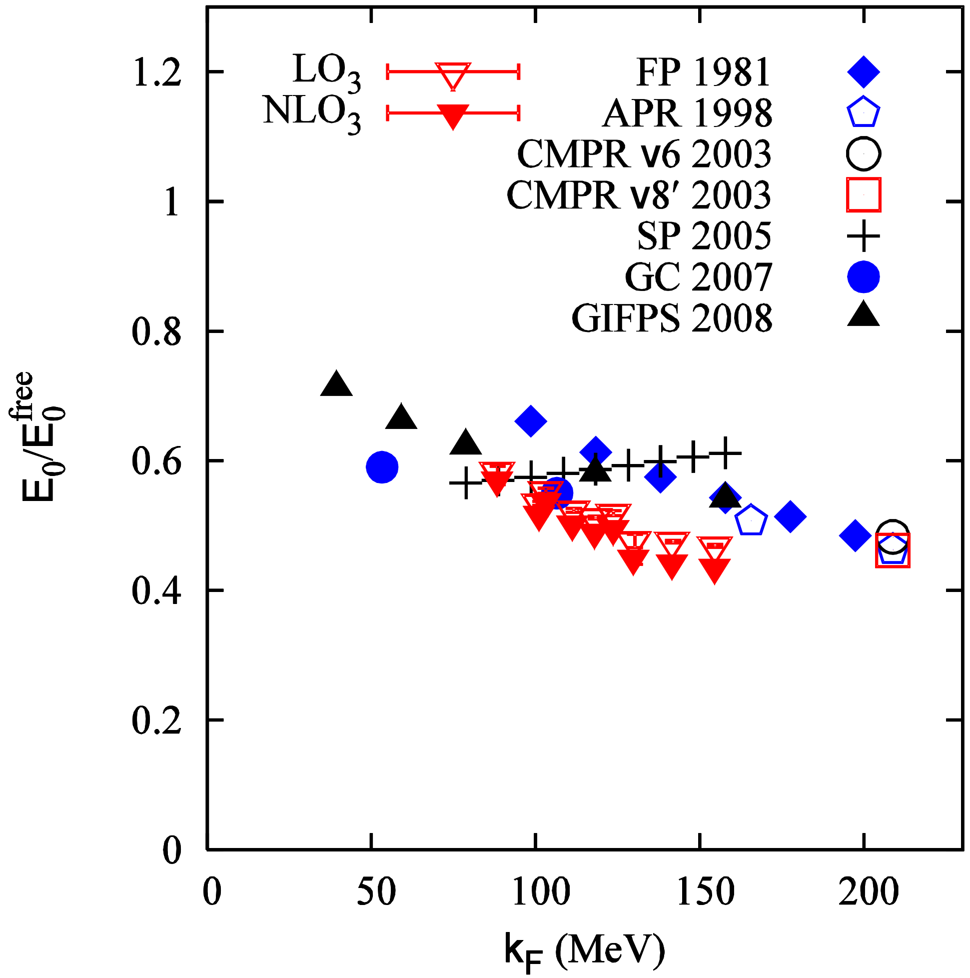
Neutron matter close to unitarity limit for $k_F \sim 80\ \mathrm{MeV}$

Dilute neutron matter at NLO



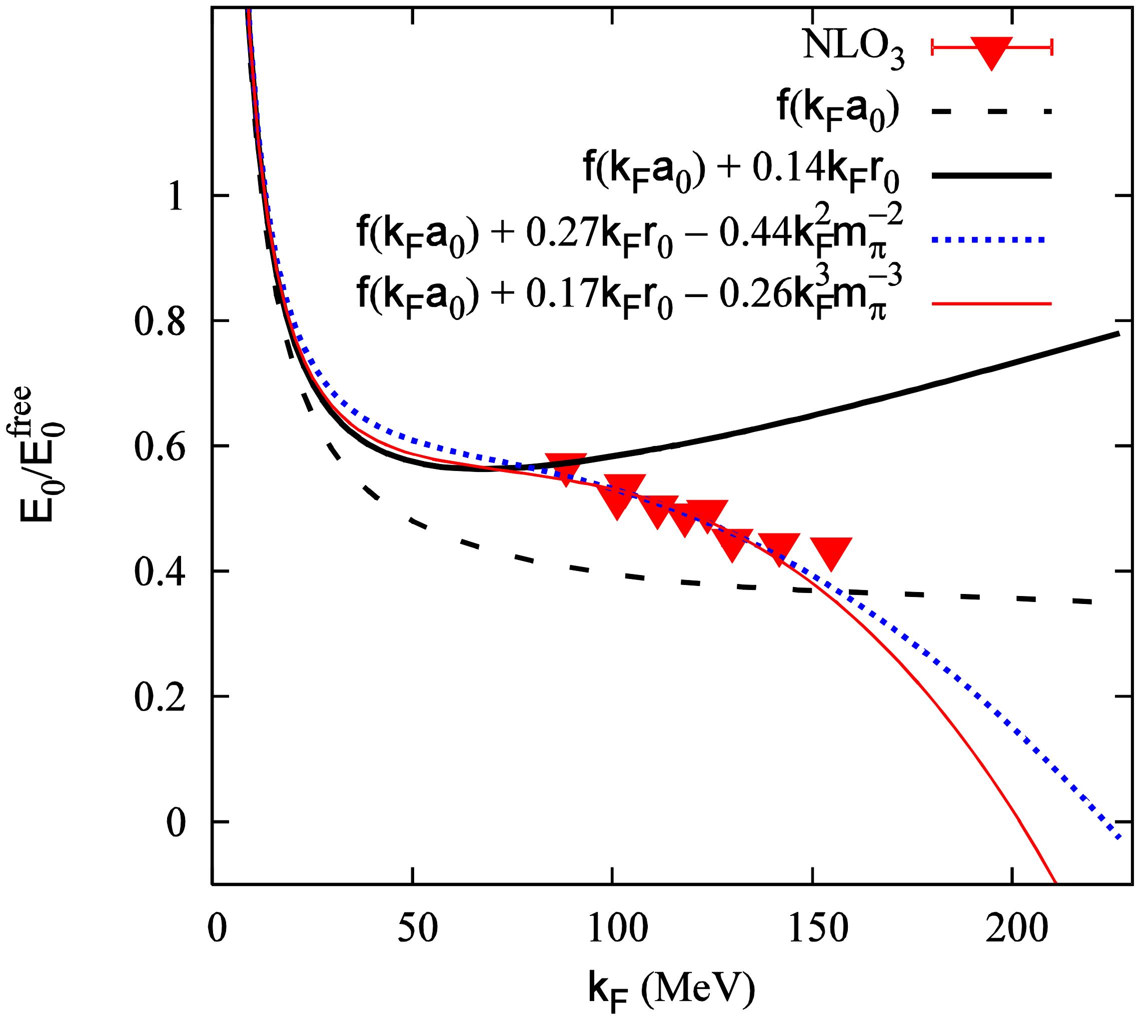
$N = 8, 12, 16$ neutrons at $L^3 = 4^3, 5^3, 6^3, 7^3$

$a = 1.97$ fm



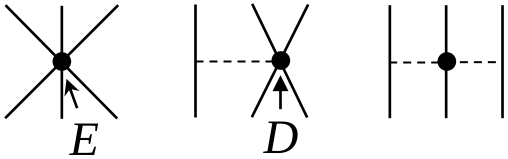
Epelbaum, Krebs, D.L, Meißner, 0812.3653 [nucl-th], EPJA 40 (2009) 199

$$\frac{E_0}{E_0^{\text{free}}} = \underbrace{\xi - \frac{\xi_1}{k_F a_0}}_{f(k_F a_0)} + c k_F r_0 + \ldots \qquad \xi = 0.31(1), \quad \xi_1 \approx 0.8$$

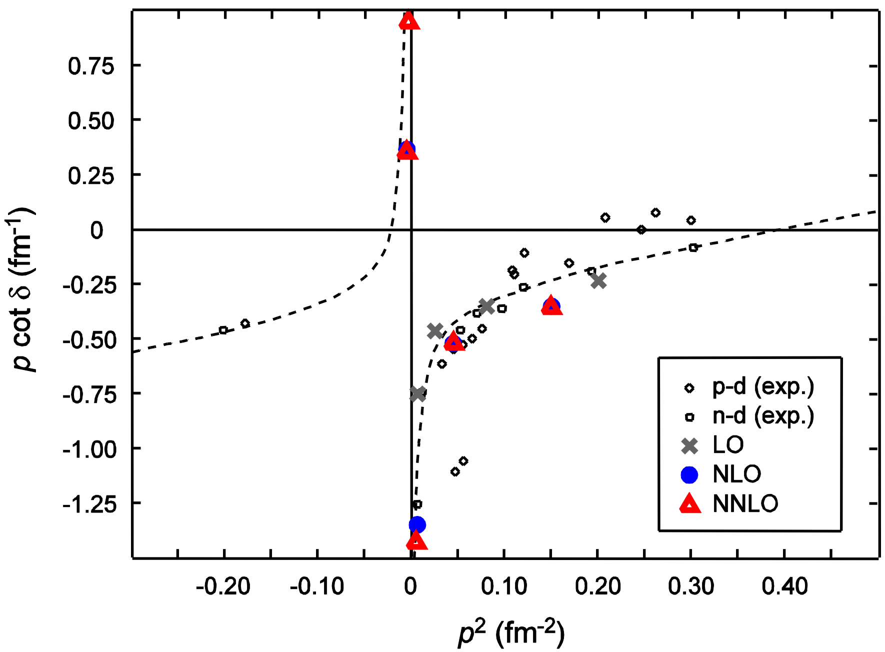


Three-body forces at NNLO

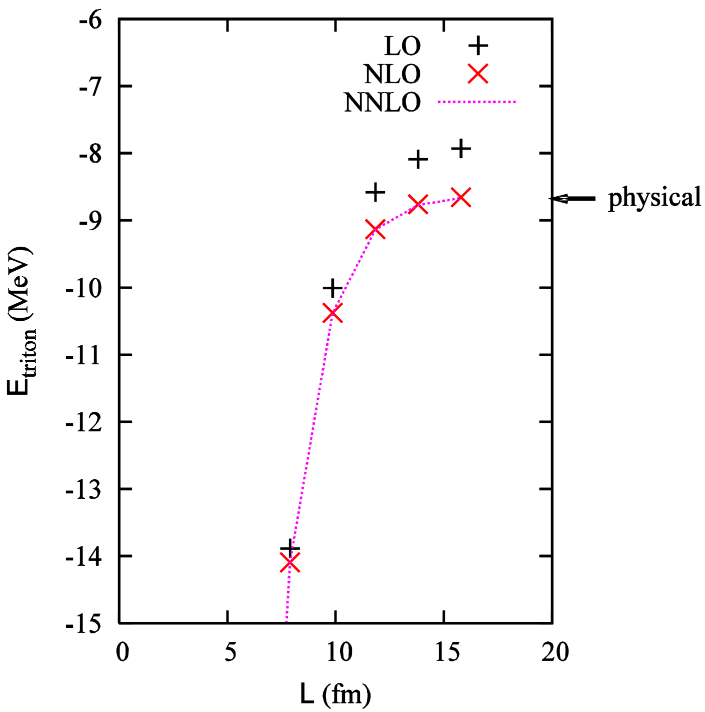
Fit c_D and c_E to spin-1/2 nucleon-deuteron scattering and ^{3}H binding energy



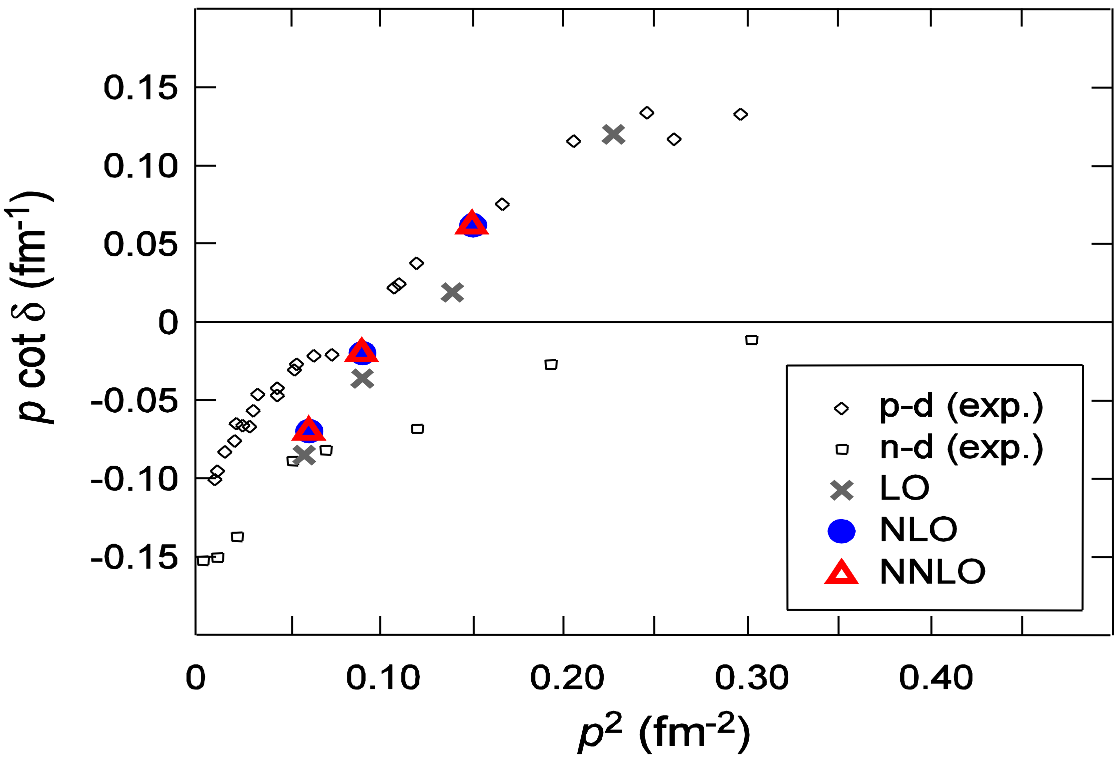
Spin-1/2 nucleon-deuteron



^{3}H binding energy



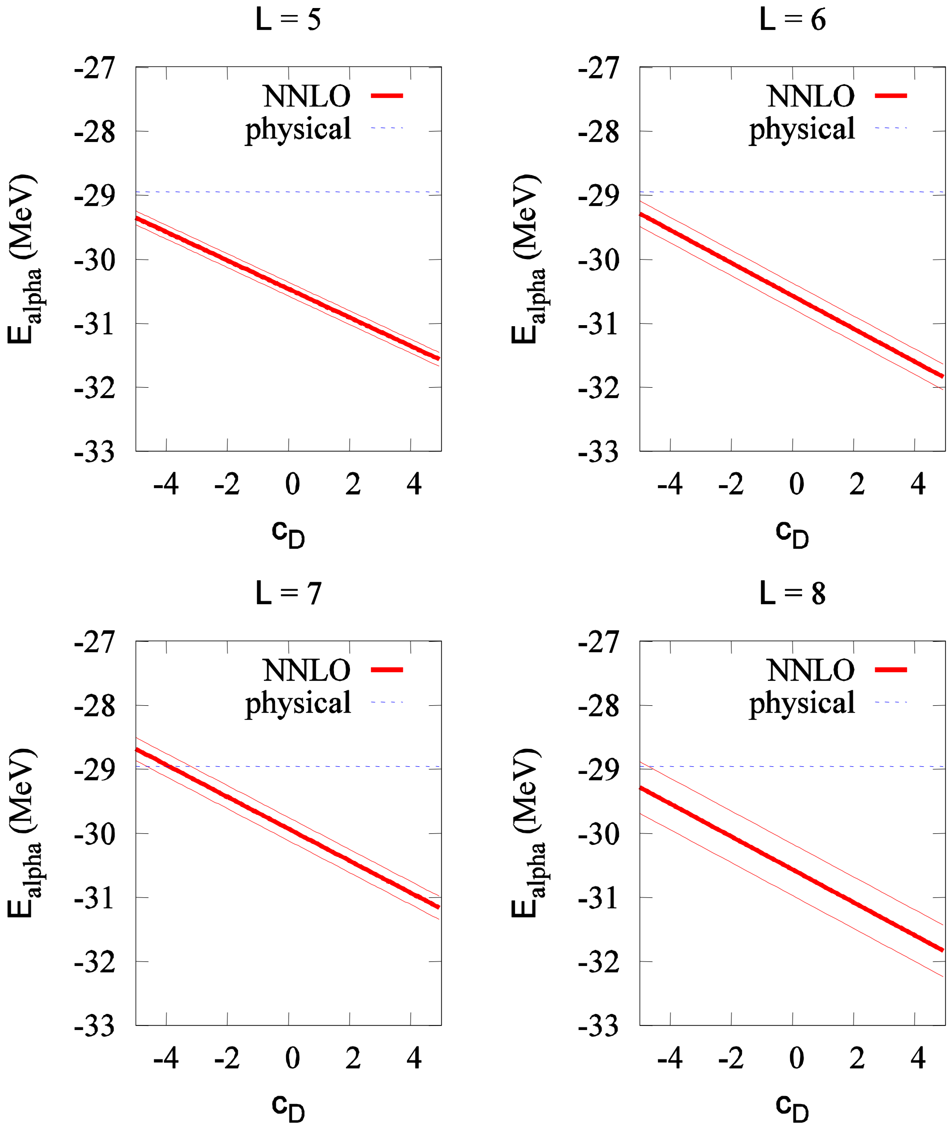
Spin-3/2 nucleon-deuteron scattering



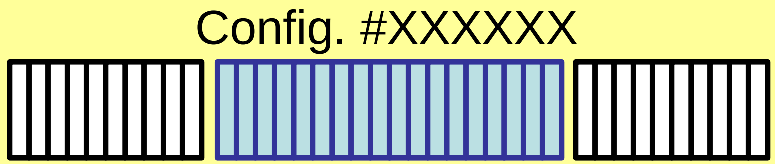
Epelbaum, Krebs, D.L, Meißner, 0812.3653 [nucl-th], EPJA 41 (2009) 125

Alpha-particle energy

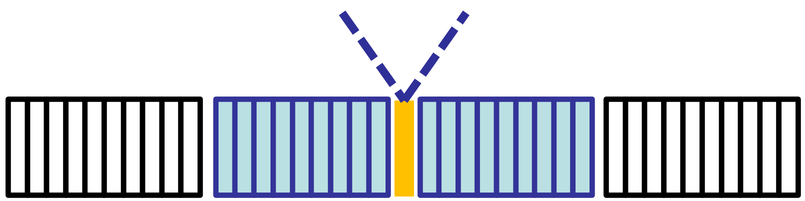
(no Coulomb, isospin symmetric)



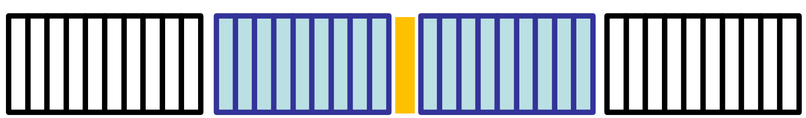
What can you do with lattice EFT configurations?

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

Correlation functions, soft scattering processes, etc.

$\langle \psi_{\mathrm{init}} |$  $| \psi_{\mathrm{init}} \rangle$

Transition matrix elements of light nuclei

$\langle \psi'_{\mathrm{init}} |$  $| \psi_{\mathrm{init}} \rangle$

Summary

Relatively new and promising tool that combines framework of effective field theory and computational lattice methods

Applications to zero and nonzero temperature simulations of light nuclei, neutron matter, cold atoms, etc.

Future directions

Include Coulomb interactions and isospin breaking

Keep going – higher orders, improved actions, smaller lattice spacing, larger volume, more nucleons

Storing lattice EFT configurations – calculate correlation functions, scattering, transitions, etc.