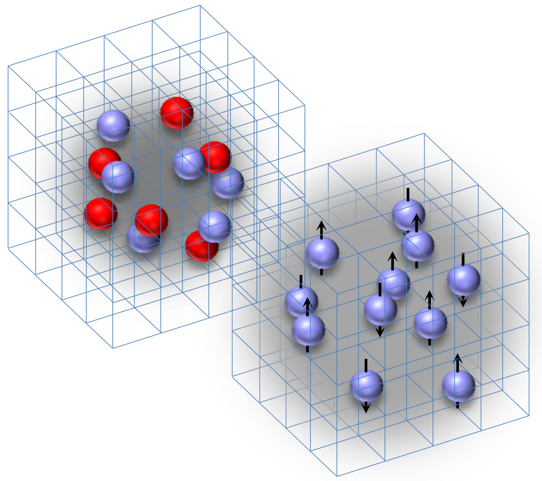
Chiral effective field theory on the lattice: Ab initio calculations of nuclei



Nuclear Lattice EFT Collaboration

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Few Body Physics Working Group
Chiral Dynamics 2012
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Outline

Introduction and motivation

What is lattice effective field theory?

Lattice interactions and scattering

Euclidean time projection and auxiliary fields

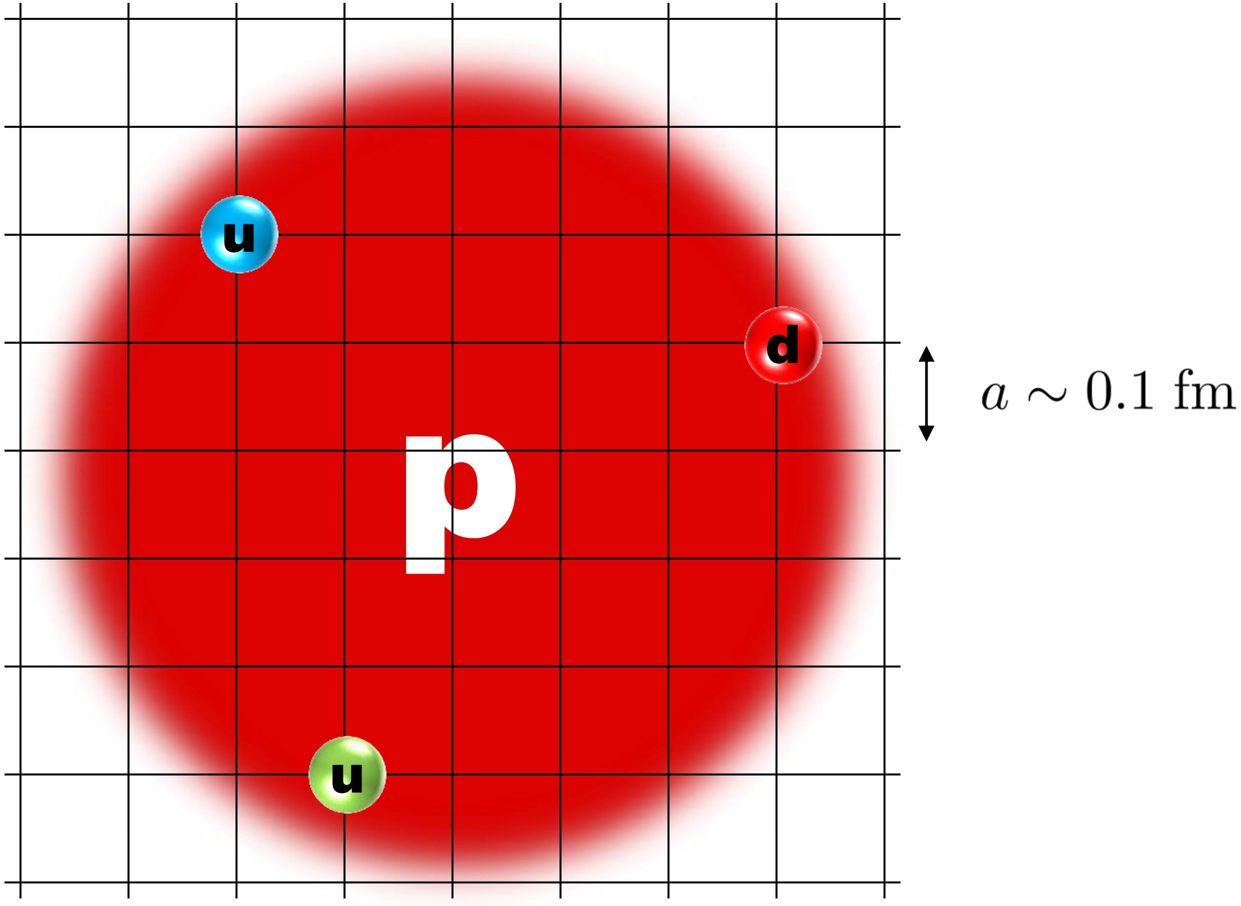
Applications to nuclei

Structure and rotations of the Hoyle state

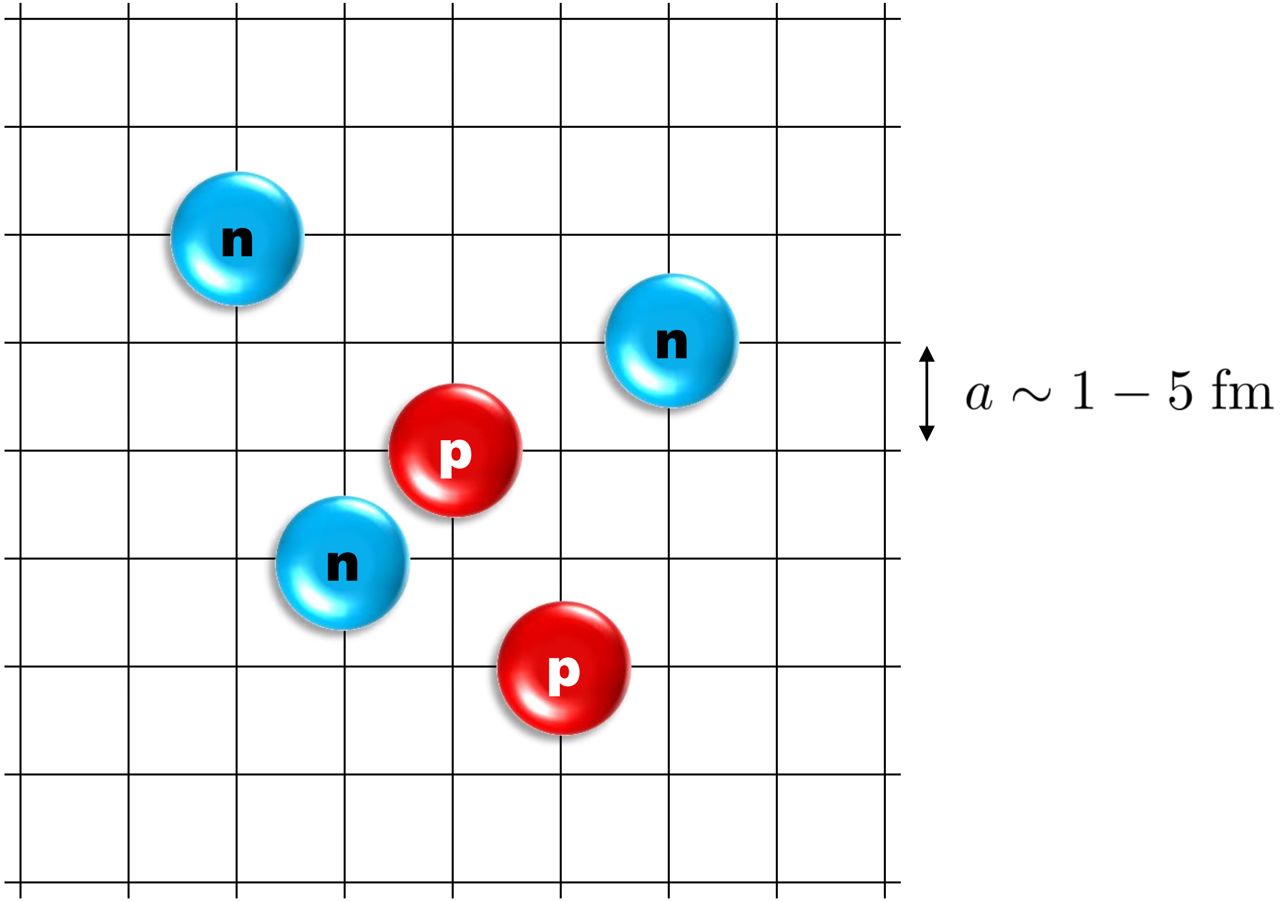
Towards scattering and reactions on the lattice

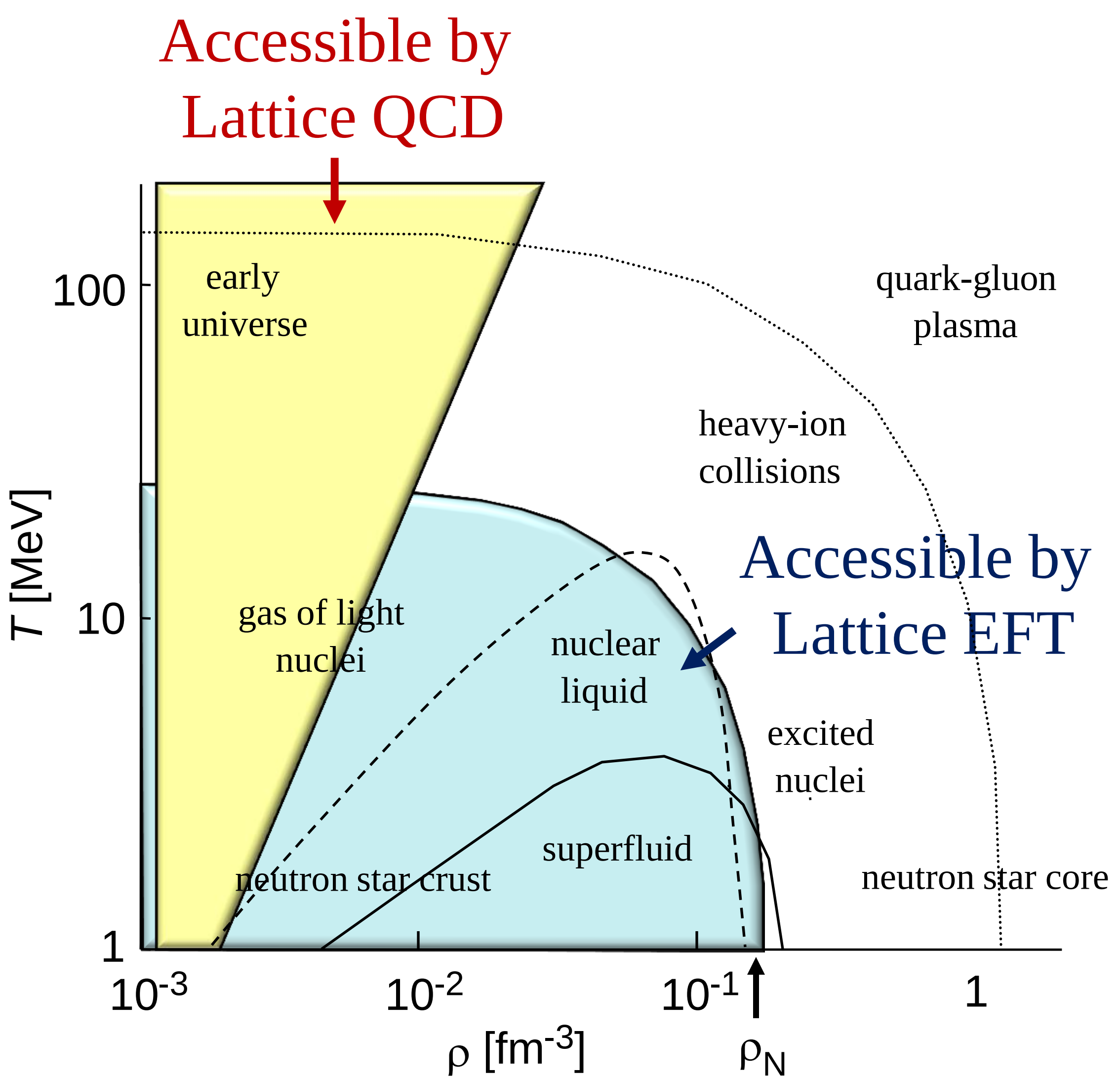
Summary and future directions

Lattice quantum chromodynamics



Lattice effective field theory




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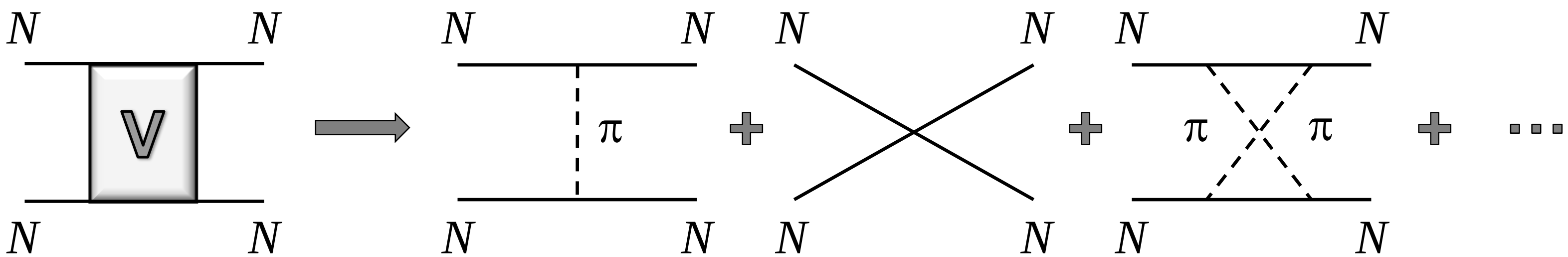
heavy-ion
collisions
Accessible by
Lattice EFT
gas of light
nuclei
nuclear
liquid
excited
nuclei
superfluid
neutron star crust
neutron star core
10-3
10-2
10-1
1
ρ [fm-3]
ρN

Low energy nucleons: Chiral effective field theory

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

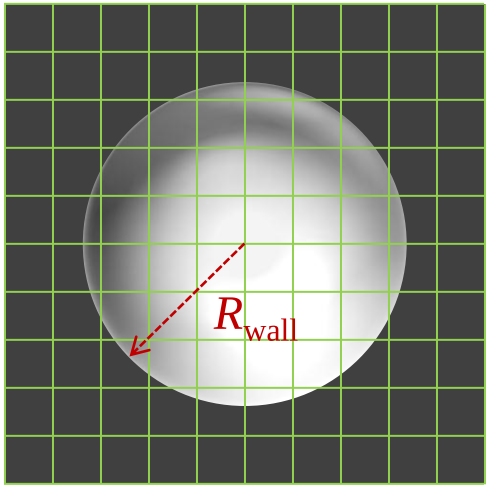
Construct the effective potential order by order



V^{OPEP} Contact interactions $1,\ \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2$ V^{TPEP}

Leading order (LO) Next-to-leading order (NLO)

Physical scattering data → Unknown operator coefficients

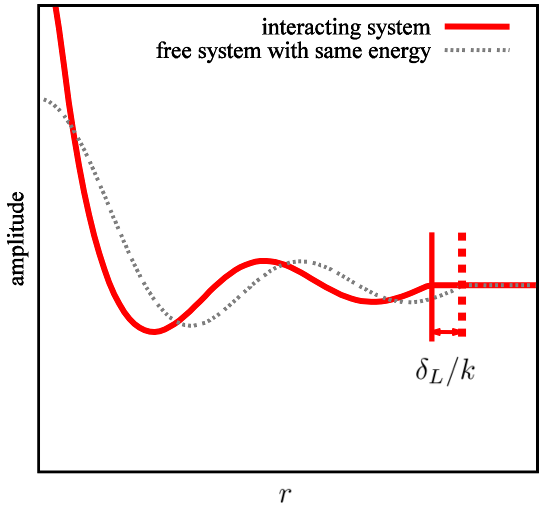


Spherical wall method

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

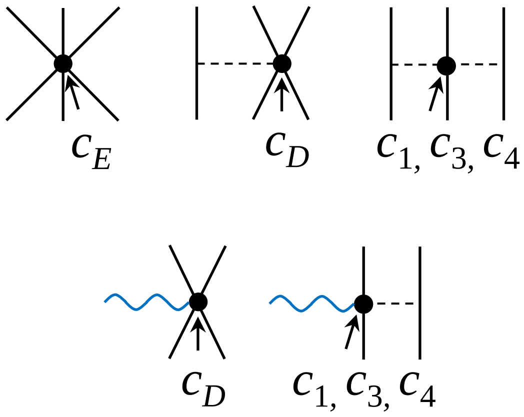
Spherical wall imposed in the center of mass frame

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	$2 \bmod 4$	$\frac{Y_{3,2}-Y_{3,-2}}{\sqrt{2}}$

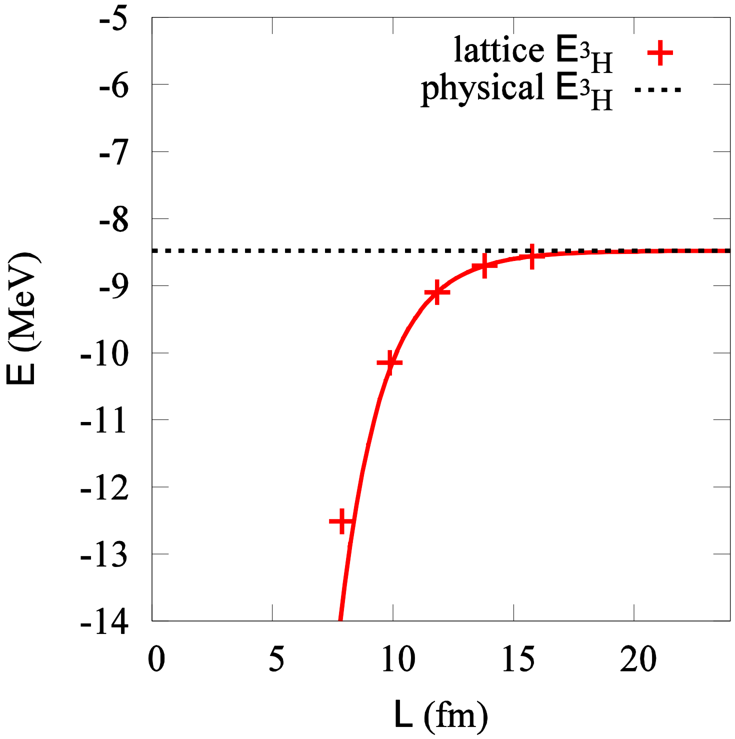


Three nucleon forces

Two unknown coefficients at NNLO from three-nucleon forces. Determine c_D and c_E using ^{3}H binding energy and the weak axial current at low cutoff momentum.



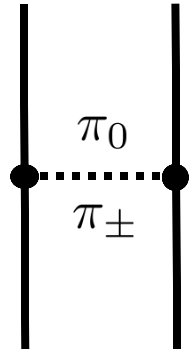
Park, et al., PRC 67 (2003) 055206,
Gårdestig, Phillips, PRL 96 (2006) 232301,
Gazit, Quaglioni, Navratil, PRL 103 (2009) 102502



Neutrons and protons: Isospin breaking and Coulomb

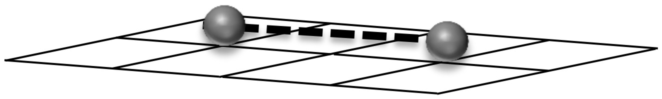
Isospin-breaking and power counting *[Friar , van Kolck, PRC 60 (1999) 034006; Walzl, Meißner, Epelbaum NPA 693 (2001) 663; Friar, van Kolck, Payne, Coon, PRC 68 (2003) 024003; Epelbaum, Meißner, PRC72 (2005) 044001…]*

Pion mass difference

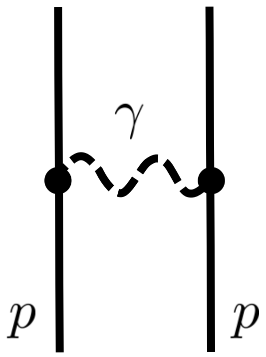


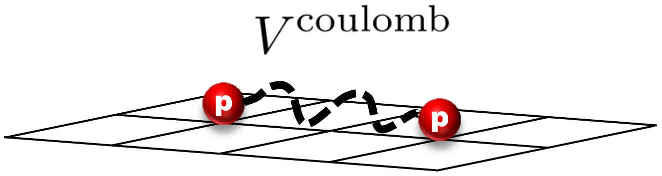
$m_{\pi_0} \neq m_{\pi_\pm}$

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

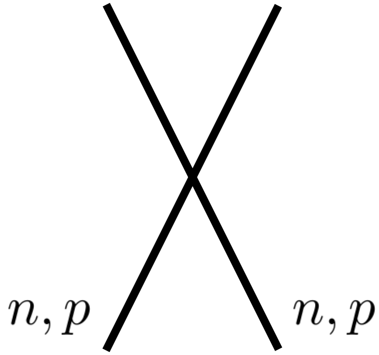


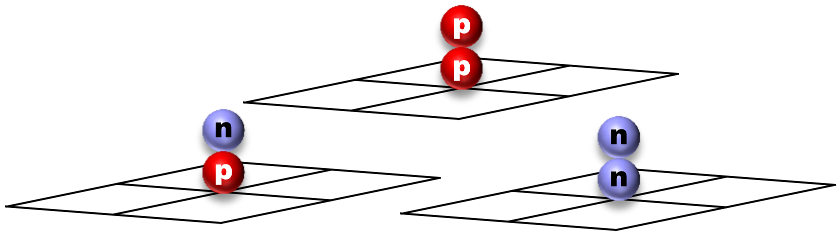
Coulomb potential



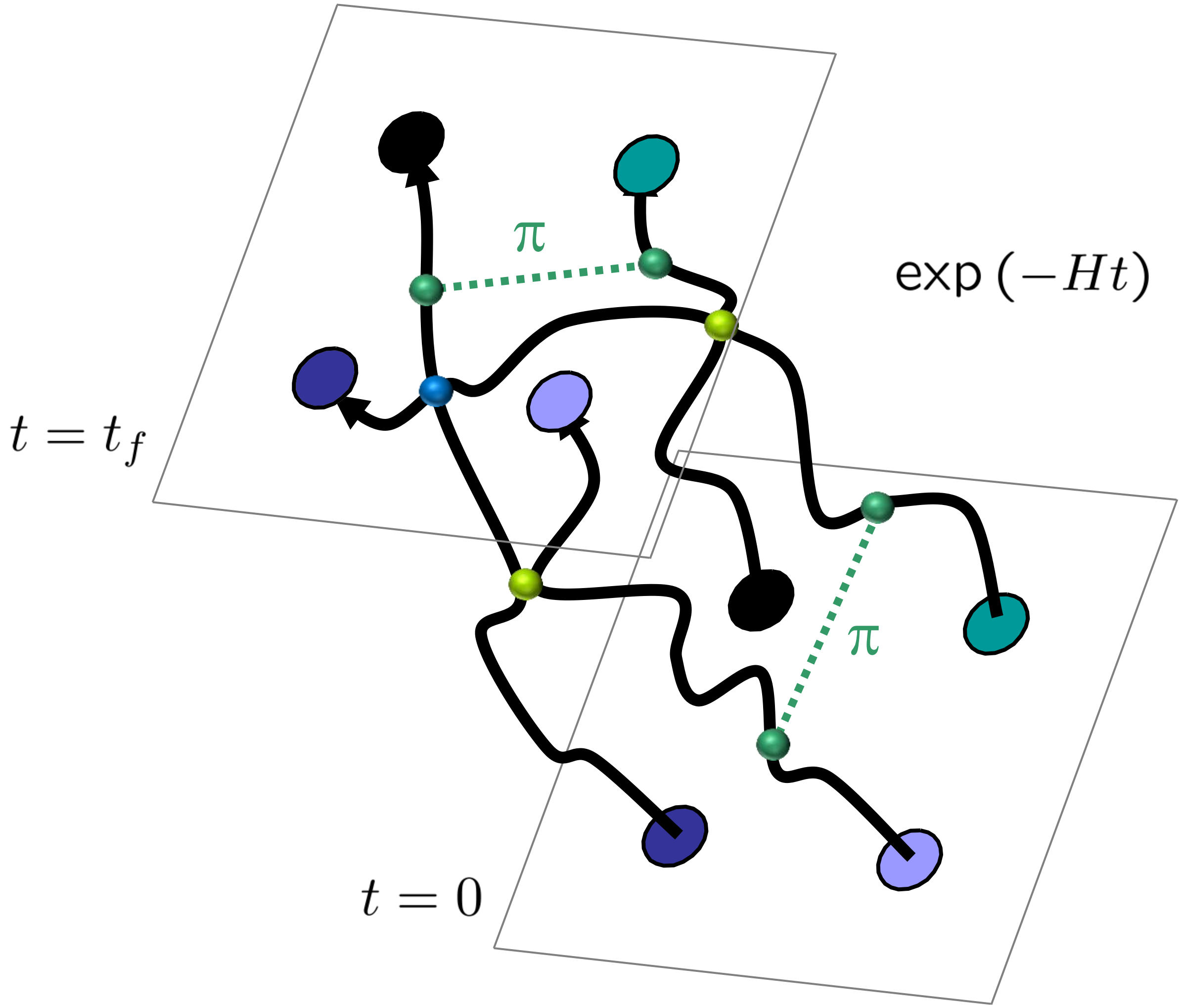


Charge symmetry breaking
Charge independence breaking





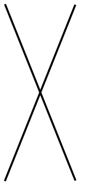
Euclidean time projection



Auxiliary field method

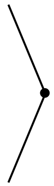
We can write exponentials of the interaction using a Gaussian integral identity

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



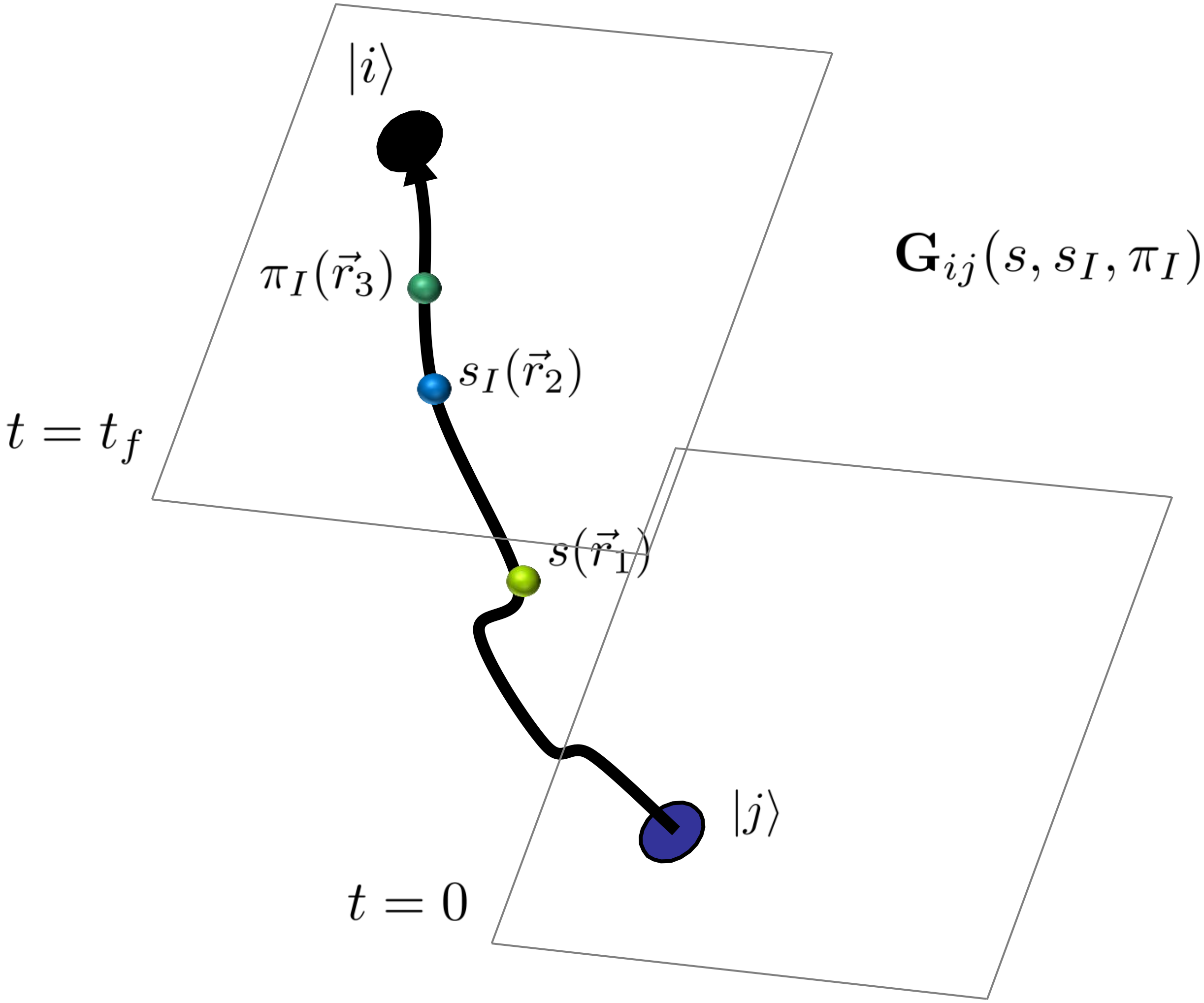
$(N^{\dagger}N)^{2}$

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

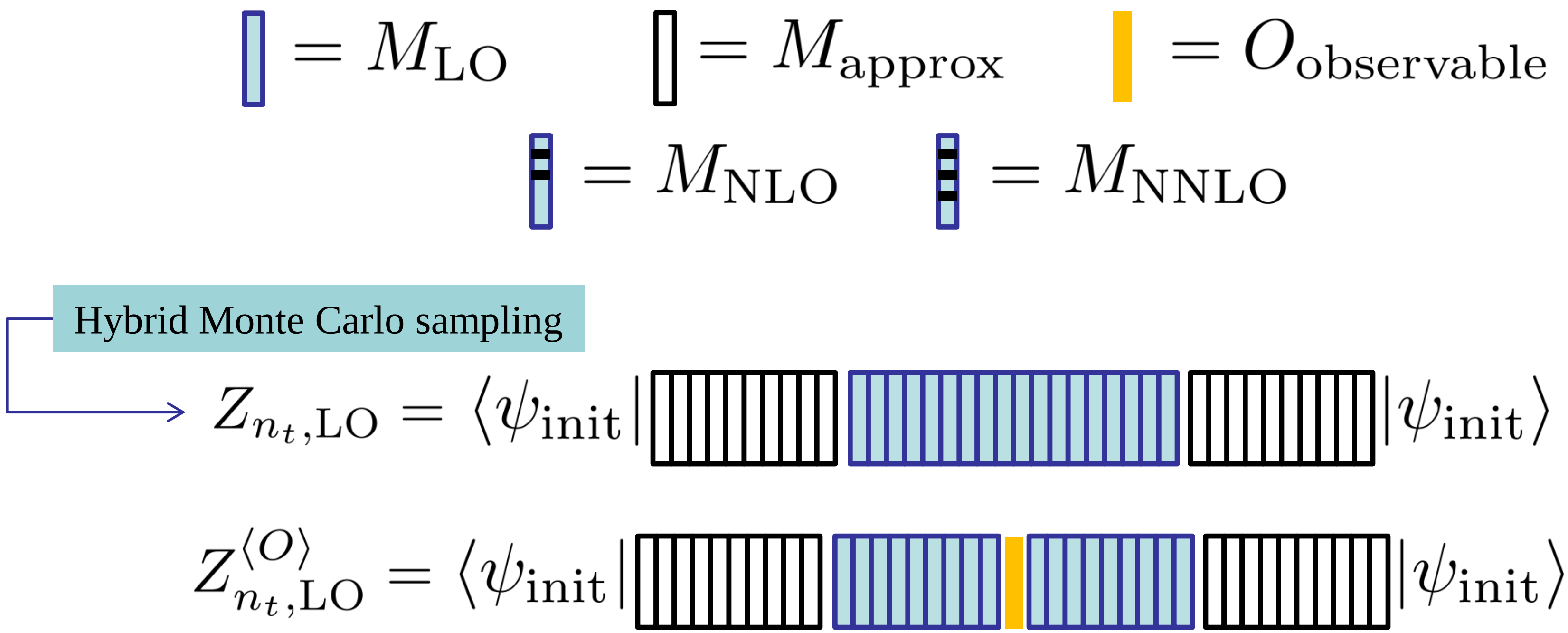


$sN^{\dagger}N$

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

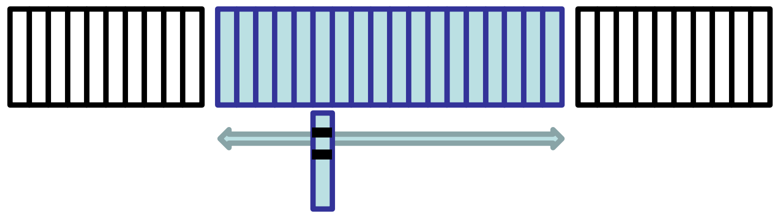

$|i\rangle$
$\pi_I(\vec{r}_3)$
$s_I(\vec{r}_2)$
$t = t_f$
$s(\vec{r}_1)$
$\mathbf{G}_{ij}(s, s_I, \pi_I)$
$|j\rangle$
$t = 0$

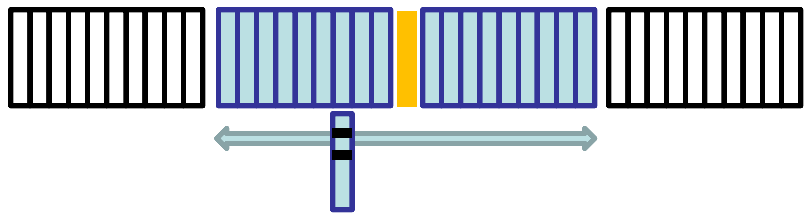
Schematic of lattice Monte Carlo calculation



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

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

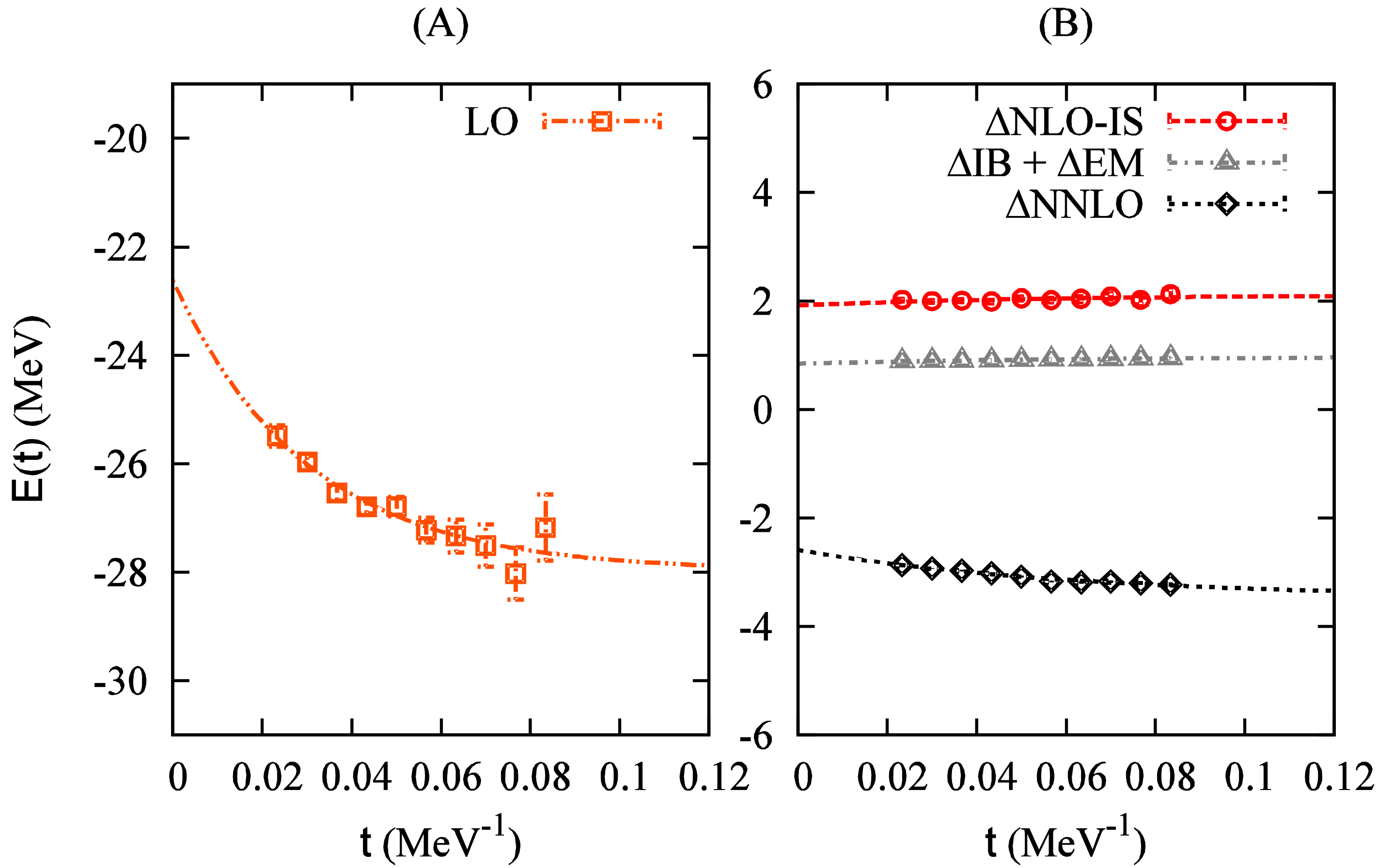
$Z_{n_t,\mathrm{NLO}} = \langle\psi_{\mathrm{init}}|$  $|\psi_{\mathrm{init}}\rangle$

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

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

Ground state of Helium-4

$L = 11.8\,\mathrm{fm}$



Epelbaum, Krebs, D.L, Meißner, PRL 104 (2010) 142501;
EPJA 45 (2010) 335; PRL 106 (2011) 192501

Ground state of Helium-4

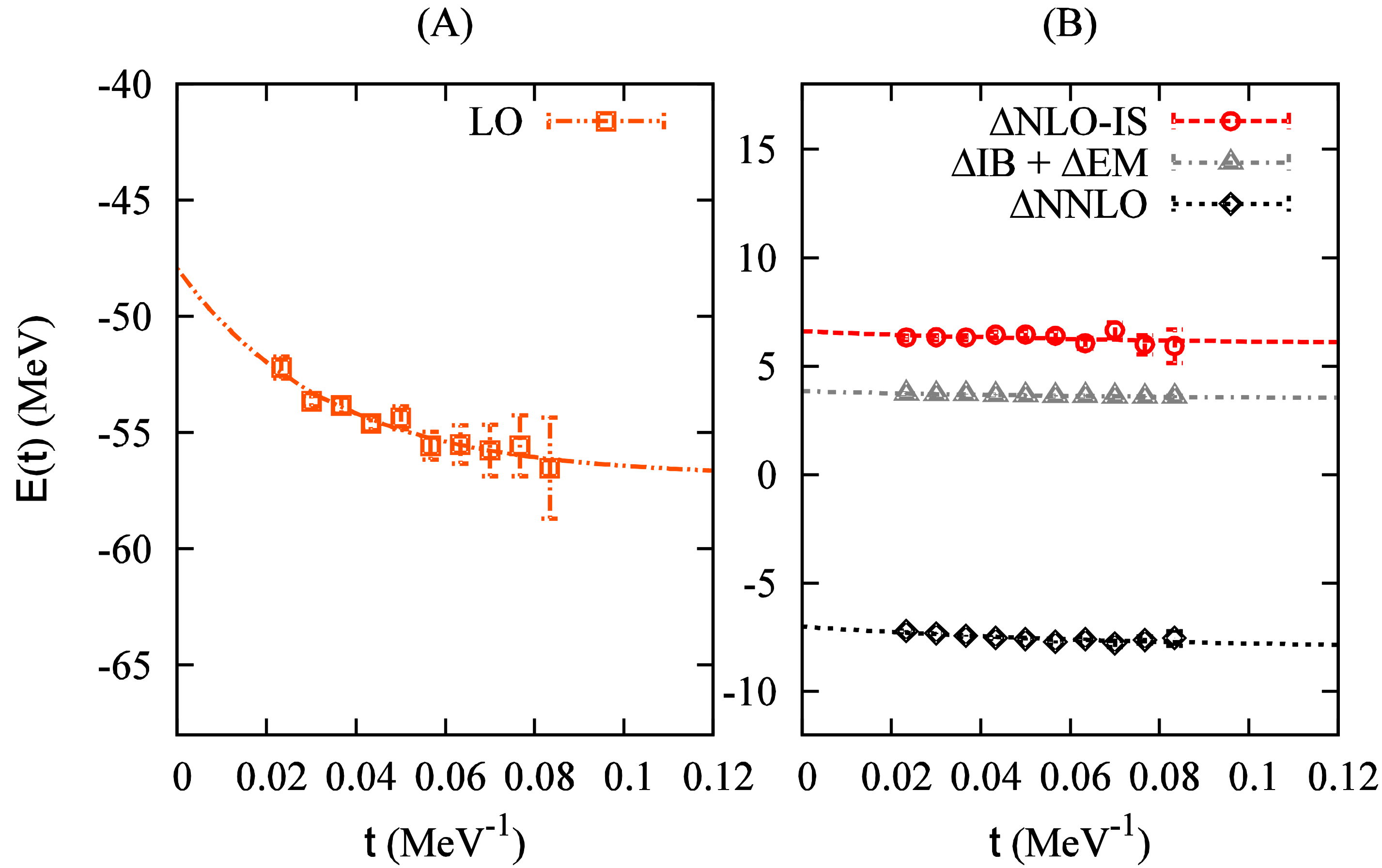
$$L = 11.8\,\mathrm{fm}$$

LO ($O(Q^0)$)	–28.0(3) MeV
NLO ($O(Q^2)$)	–24.9(5) MeV
NNLO ($O(Q^3)$)	–28.3(6) MeV
Experiment	–28.3 MeV

c_1, c_3, c_4 three-nucleon	–0.2(1) MeV
c_D three-nucleon	–1.0(2) MeV
c_E three-nucleon	–2.1(3) MeV

Ground state of Beryllium-8

$$L = 11.8\,\mathrm{fm}$$



Epelbaum, Krebs, D.L, Meißner, PRL 106 (2011) 192501

Ground state of Beryllium-8

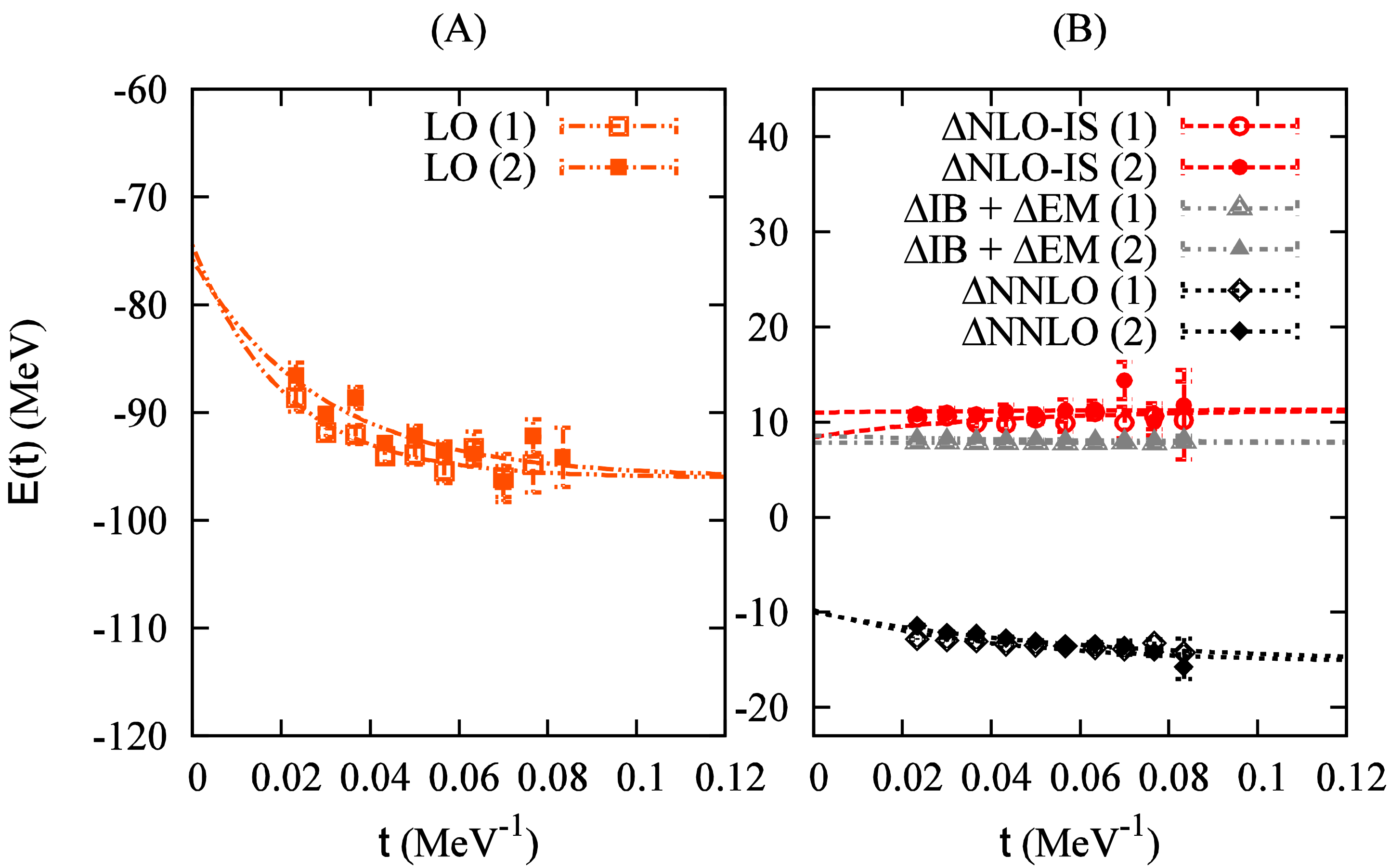
$$L = 11.8\,\text{fm}$$

LO ($O(Q^0)$)	–57(2) MeV
NLO ($O(Q^2)$)	–47(2) MeV
NNLO ($O(Q^3)$)	–55(2) MeV
Experiment	–56.5 MeV

c_1, c_3, c_4 three-nucleon	–0.7(2) MeV
c_D three-nucleon	–3.4(5) MeV
c_E three-nucleon	–4(1) MeV

Ground state of Carbon-12

$L = 11.8\,\mathrm{fm}$



Epelbaum, Krebs, D.L, Meißner, PRL 104 (2010) 142501; EPJA 45 (2010) 335; PRL 106 (2011) 192501

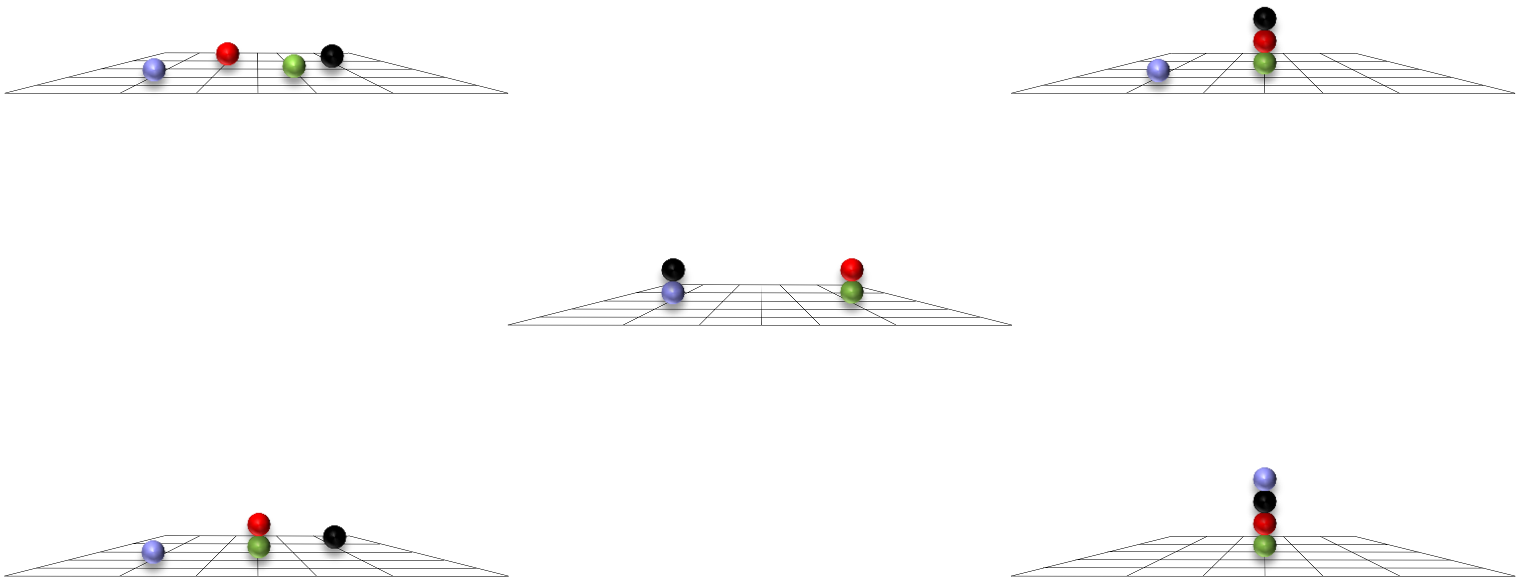
Ground state of Carbon-12

$$L = 11.8\,\text{fm}$$

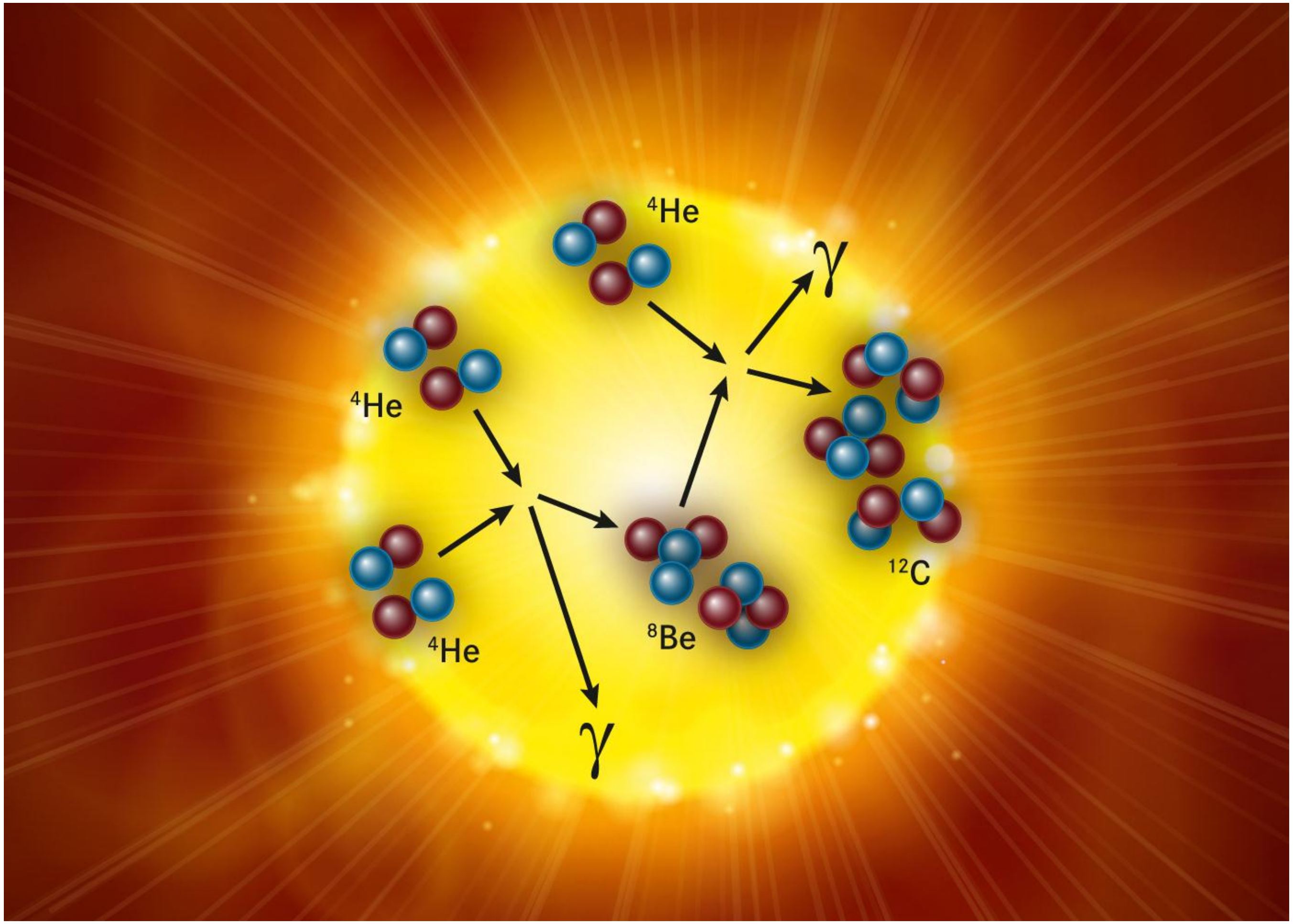
LO ($O(Q^0)$)	–96(2) MeV
NLO ($O(Q^2)$)	–77(3) MeV
NNLO ($O(Q^3)$)	–92(3) MeV
Experiment	–92.2 MeV

c_1, c_3, c_4 three-nucleon	–2.5(5) MeV
c_D three-nucleon	–6(1) MeV
c_E three-nucleon	–6(2) MeV

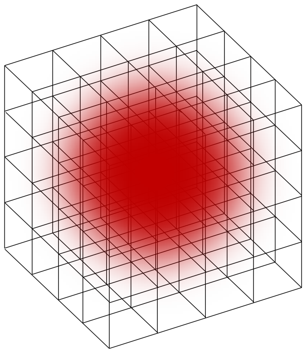
Particle clustering included automatically



Carbon-12 spectrum and the Hoyle state



Simulations using general initial/final state wavefunctions



$$\psi_j(\vec{n}) \quad j = 1, \cdots A$$

Construct states with well-defined momentum using all possible translations.

$$L^{-3/2} \sum_{\vec{m}} \psi_j(\vec{n} + \vec{m})\, e^{i\vec{P}\cdot\vec{m}} \quad j = 1, \cdots A$$

Shell model wavefunctions

$$\psi_j(\vec{n}) = \exp(-c\vec{n}^2)$$
$$\psi'_j(\vec{n}) = n_x \exp(-c\vec{n}^2)$$
$$\psi''_j(\vec{n}) = n_y \exp(-c\vec{n}^2)$$
$$\psi'''_j(\vec{n}) = n_z \exp(-c\vec{n}^2)$$
$$\vdots$$

Alpha cluster wavefunctions

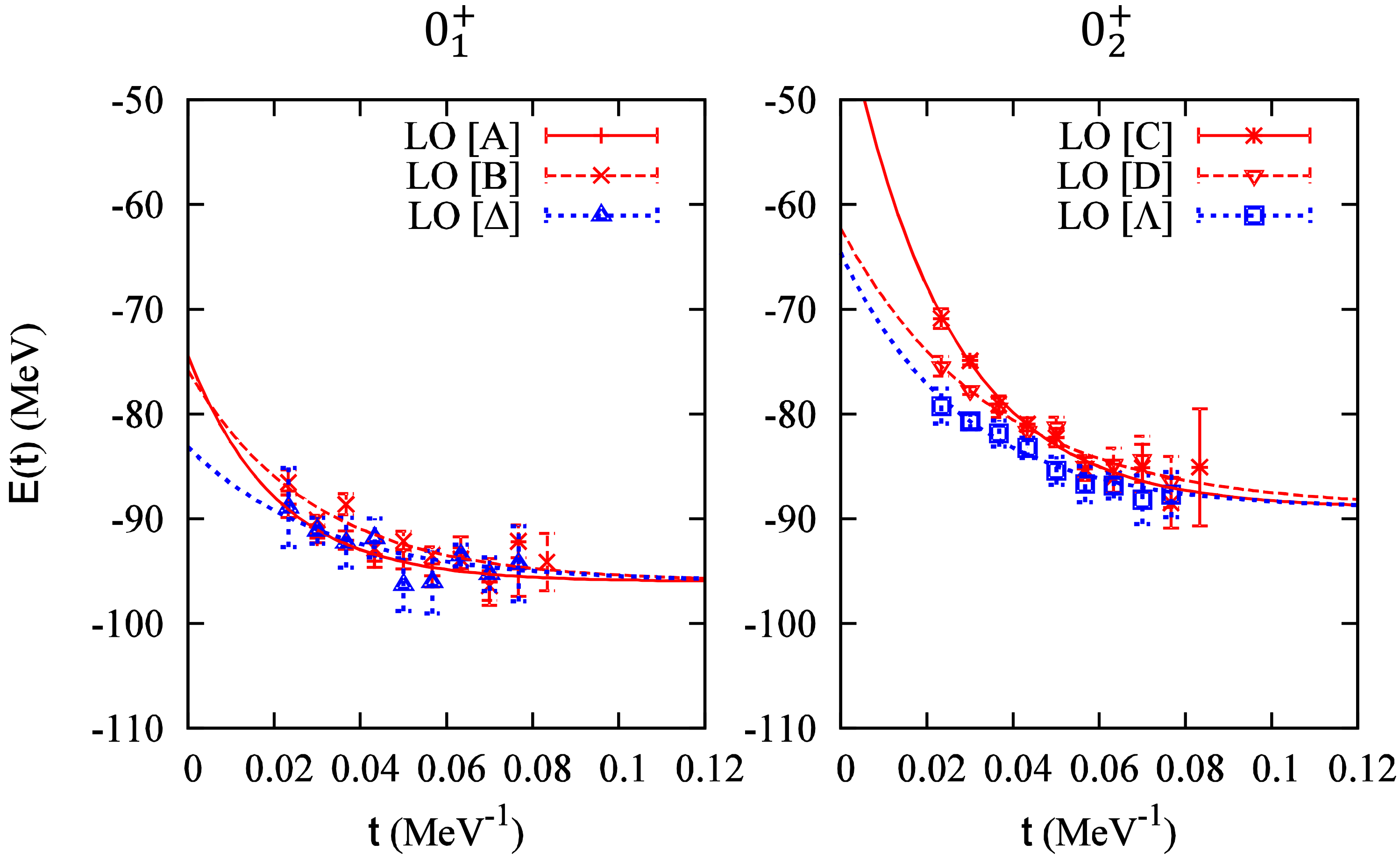
$$\psi_j(\vec{n}) = \exp[-c(\vec{n} - \vec{m})^2]$$
$$\psi'_j(\vec{n}) = \exp[-c(\vec{n} - \vec{m}')^2]$$
$$\psi''_j(\vec{n}) = \exp[-c(\vec{n} - \vec{m}'')^2]$$
$$\vdots$$

Shell model wavefunctions do not have enough local four nucleon correlations,

$$< (N^\dagger N)^4 >$$

Needs to develop the four nucleon correlations via Euclidean time projection.

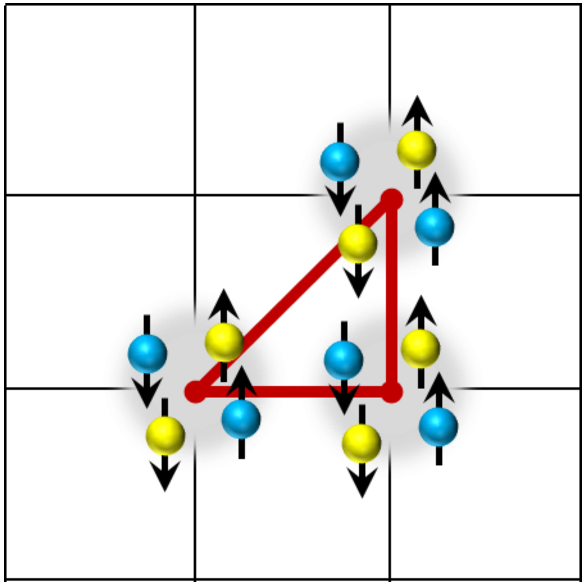
But can reproduce same results starting directly from alpha cluster wavefunctions [Δ and Λ in plots on next slide].



Epelbaum, Krebs, Lähde, D.L, Meißner, arXiv:1208.xxxx

Structure of ground state and first 2+

Strong overlap with compact triangle configuration

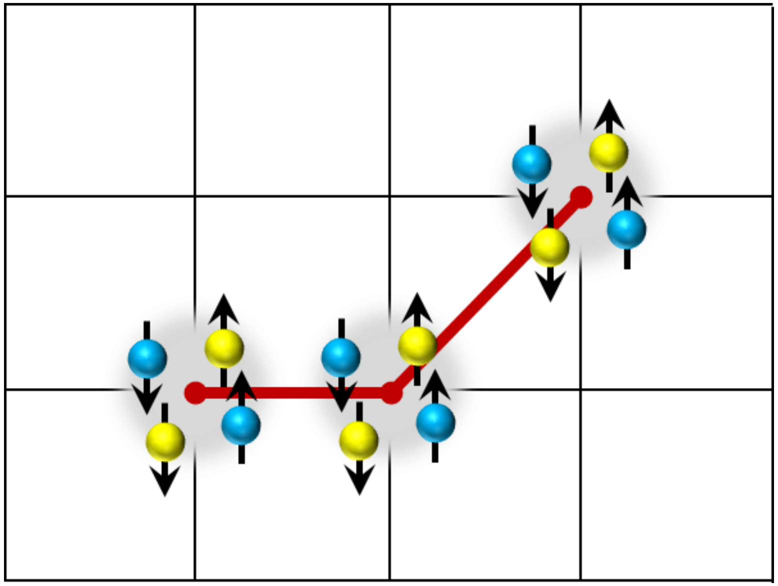


$a = 1.97$ fm

12 rotational orientations

Structure of Hoyle state and second 2+

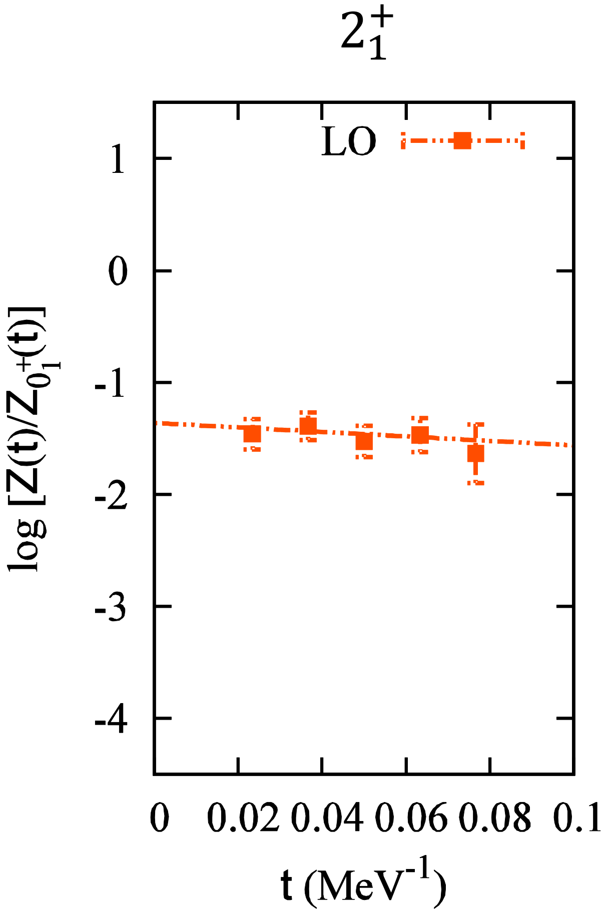
Strong overlap with bent arm configuration

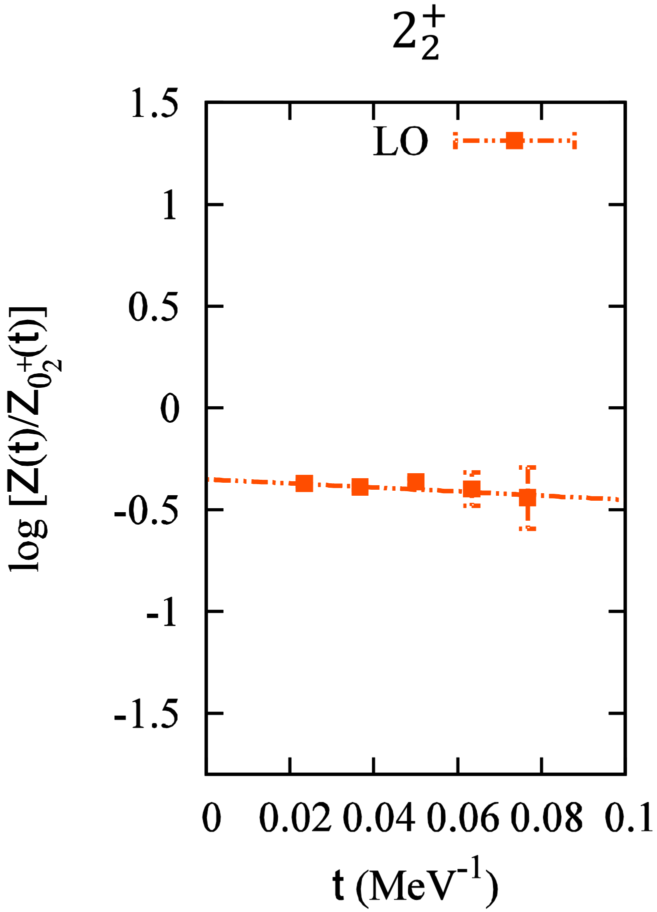


24 rotational orientations

$a = 1.97 \text{ fm}$

Rotational excitations – 2_1^+, 2_2^+





Excited state spectrum of carbon-12 (even parity)

	2_1^+	0_2^+	2_2^+
LO ($O(Q^0)$)	–94(2) MeV	–89(2) MeV	–88(2) MeV
NLO ($O(Q^2)$)	–74(3) MeV	–72(3) MeV	–70(3) MeV
NNLO ($O(Q^3)$)	–89(3) MeV	–85(3) MeV	–83(3) MeV
Experiment	–87.72 MeV	–84.51 MeV	–82.6(1) MeV –82.32(6) MeV –81.1(3) MeV –82.13(11) MeV*

*See W. Zimmerman's talk for new experimental results from TUNL/HIγS

Epelbaum, Krebs, Lähde, D.L, Meißner, arXiv:1208.xxxx

RMS charge radius

bound states at leading order

	LO	Experiment
$r_{0_1^+}$ [fm]	2.2(2)	2.47(2)
$r_{2_1^+}$ [fm]	2.2(2)	–
$r_{0_2^+}$ [fm]	2.4(2)	–
$r_{2_2^+}$ [fm]	2.4(2)	–

Quadrupole moment

	LO	Experiment
$Q_{2_1^+}$ [e fm^2]	6(2)	6(3)
$Q_{2_2^+}$ [e fm^2]	–7(2)	–

Electromagnetic transition strengths

	LO	Experiment
$B(E2, 2_1^+ \to 0_1^+)$ $[e^2 \text{ fm}^4]$	5(2)	7.6(4)
$B(E2, 2_1^+ \to 0_2^+)$ $[e^2 \text{ fm}^4]$	1.5(7)	2.6(4)
$B(E2, 2_2^+ \to 0_1^+)$ $[e^2 \text{ fm}^4]$	2(1)	0.73(13)*
$B(E2, 2_2^+ \to 0_2^+)$ $[e^2 \text{ fm}^4]$	6(2)	–
$m(E0, 0_2^+ \to 0_1^+)$ $[e \text{ fm}^2]$	3(1)	5.5(1)

*See W. Zimmerman's talk for new experimental results from TUNL/HIγS

See also other recent calculations using fermionic molecular dynamics

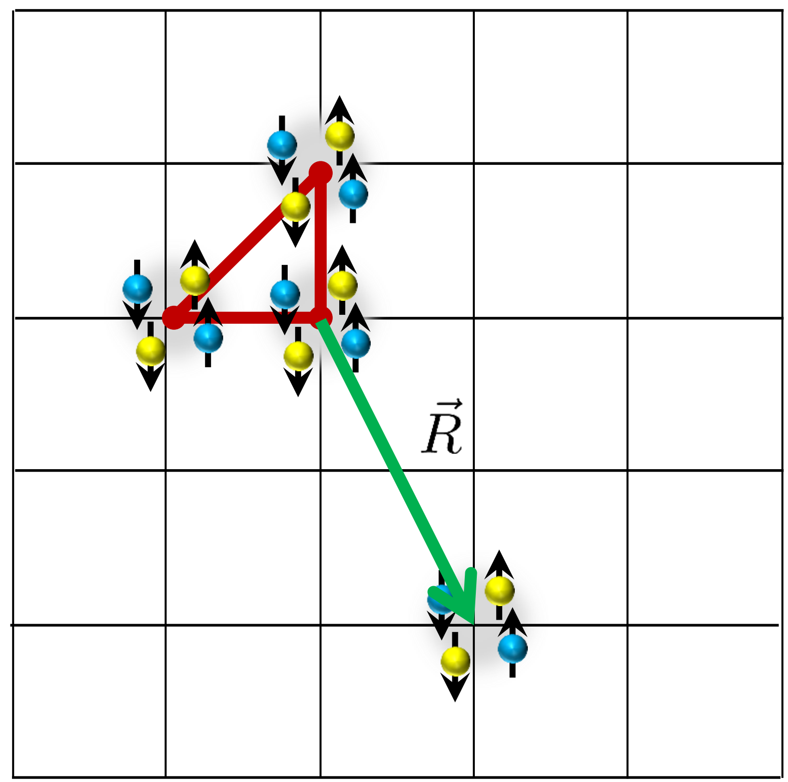
Chernykh, et al., PRL 98 (2007) 032501

and no-core shell model

Forssen, Roth, Navratil, arXiv:1110.0634v2

Towards nucleus scattering and reactions

Work in progress with Gautam Rupak and Michelle Pine



initial state

$|\vec{R}>$

Use Monte Carlo simulations to propagate in Euclidean time and then construct norm matrix and adiabatic Hamiltonian matrix

$$|\vec{R}>_t = e^{-Ht}|\vec{R}>$$

$$_t < \vec{R}'|\vec{R}>_t$$

$$_t < \vec{R}'|H|\vec{R}>_t$$

Similar in spirit to no-core shell model with resonating group method. But some differences.

Complete antisymmetrization is automatic in the auxiliary field formulation when computing single nucleon amplitude determinants.

Distortion of the nucleus wavefunctions is automatic due to Euclidean time projection. Formalism is being tested on the lattice for $n + p \to d + \gamma$ and elastic dimer-fermion scattering.

Summary and future directions

A golden age for nuclear theory from first principles. Big science discoveries being made and many more around the corner.

Lattice effective field theory is a relatively new and promising tool that combines the framework of effective field theory and computational lattice methods. May play a significant role in the future of *ab initio* nuclear theory.

Topics to be addressed in the near future…

Different lattice spacings, quark mass dependence of Hoyle state, electromagnetic transitions, spectrum of oxygen-16, alpha clustering in nuclei, ground state of nitrogen-14, ground state of neon-20, transition from S-wave to P-wave pairing in superfluid neutron matter, weak matrix elements, adiabatic Hamiltonians for scattering and reactions, etc.