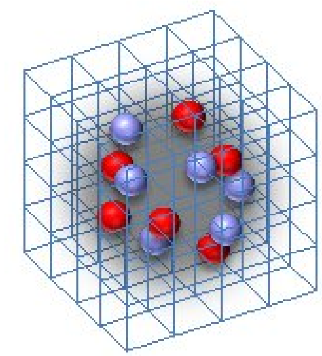
Nuclear Physics from Lattice Simulations

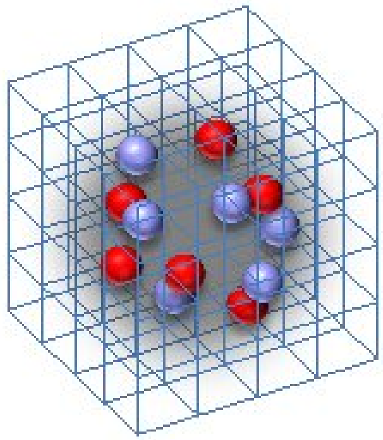
Ulf-G. Meißner, Univ. Bonn & FZ Jülich



NLEFT

Supported by DFG, SFB/TR-16 and by EU, I3HP EPOS and by BMBF 06BN9006 and by HGF VIQCD VH-VI-417

- **Nuclear Lattice Effective Field Theory collaboration**



Evgeny Epelbaum (Bochum)

Hermann Krebs (Bochum)

Timo Lähde (Jülich)

Dean Lee (NC State)

Ulf-G. Meißner (Bonn/Jülich)

CONTENTS

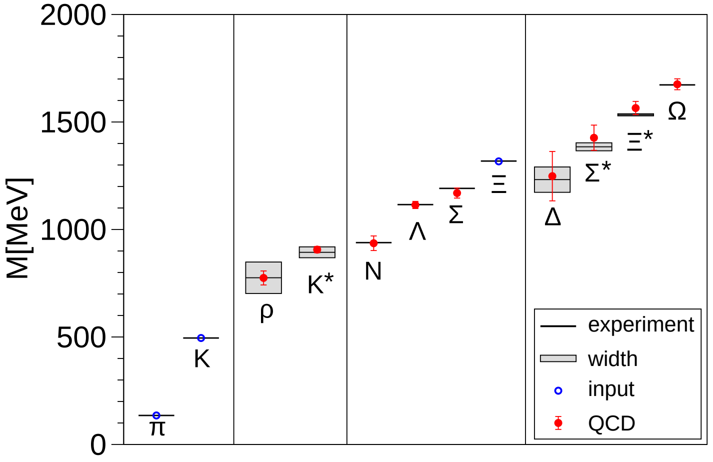
Introduction

FACETS of STRONG QCD

- quarks and gluons form hadrons

  $\Rightarrow$ **lattice QCD**

  $\Rightarrow$ exploring the strong color force

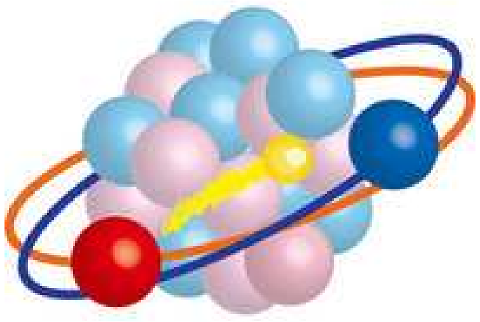


BMW collaboration (2008)

- nucleons and mesons form nuclei

  $\Rightarrow$ **nuclear physics**

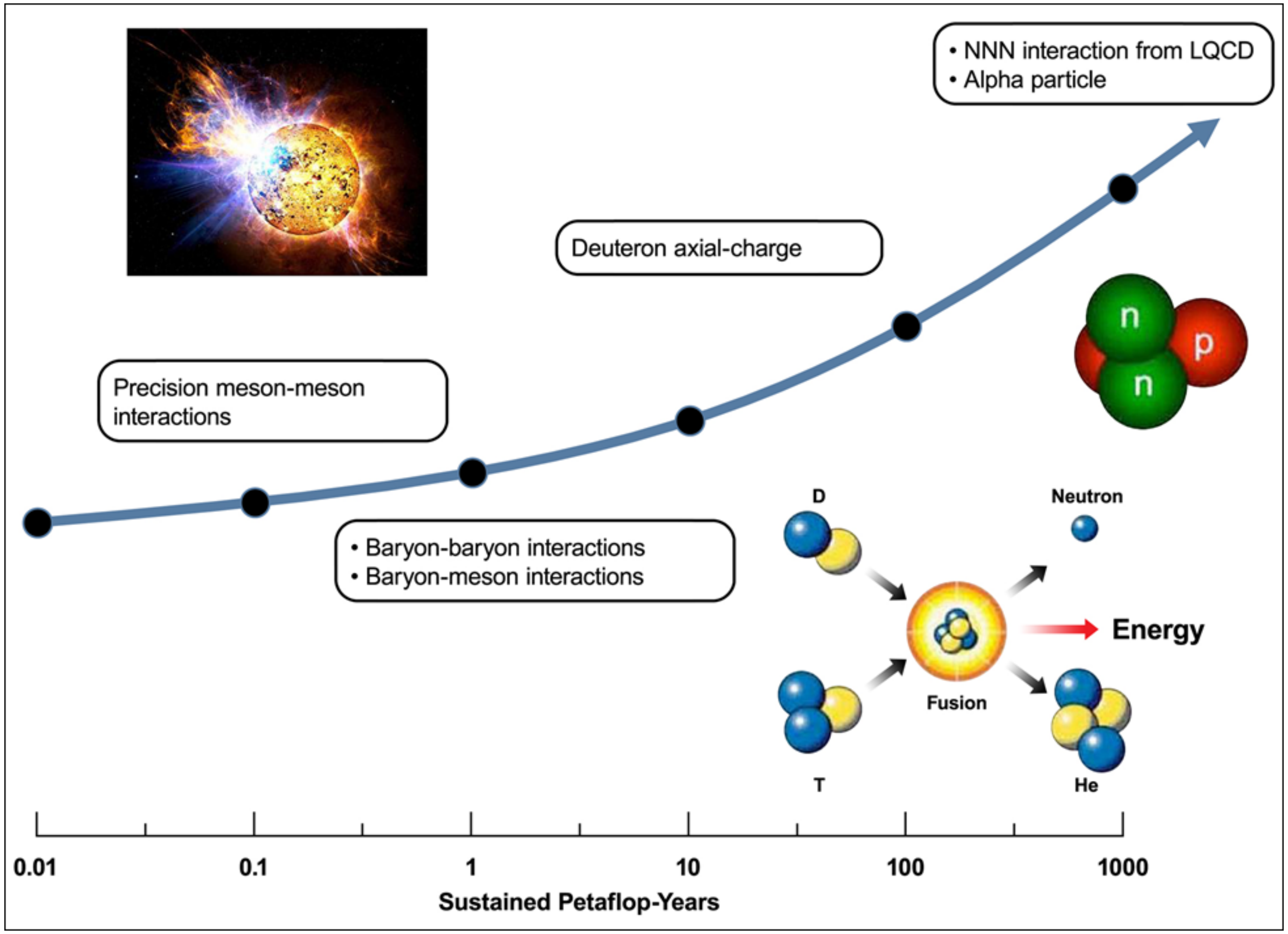
  $\Rightarrow$ exploring the residual color force



NUCLEAR PHYSICS from LATTICE QCD

- LQCD requires hundreds of sustained petaflop-yrs — not quite there yet

USDOE, Computing at the Extreme Scale, 2009



THE NUCLEAR LANDSCAPE: AIMS & METHODS

- Theoretical methods:

– Lattice QCD: *A = 0,1,2, . . .*

– NCSM, Faddeev-Yakubowsky, GFMC, ... : *A = 3 - 16*

– coupled cluster, . . .: *A = 16 -100*

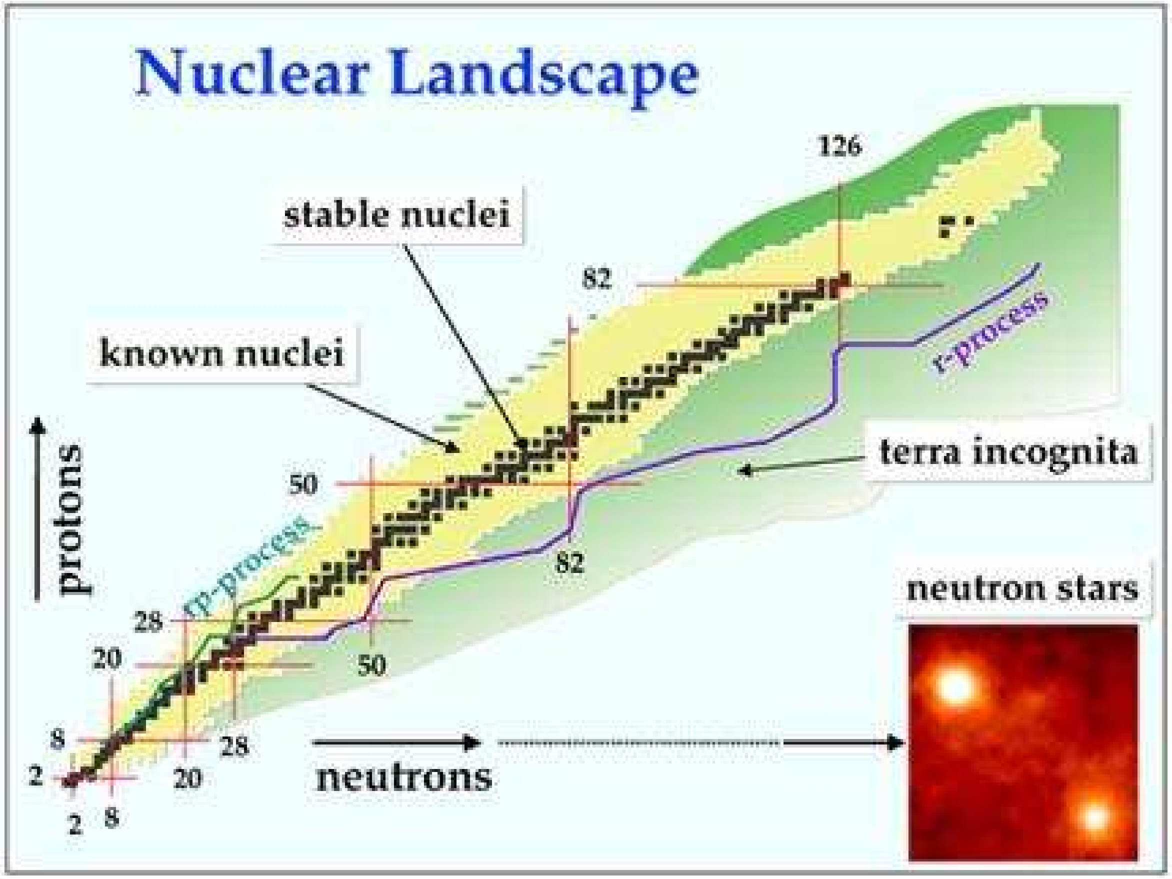
– density functional theory, . . .: $A \geq 100$

- Chiral EFT:

– provides accurate NN and 3N forces

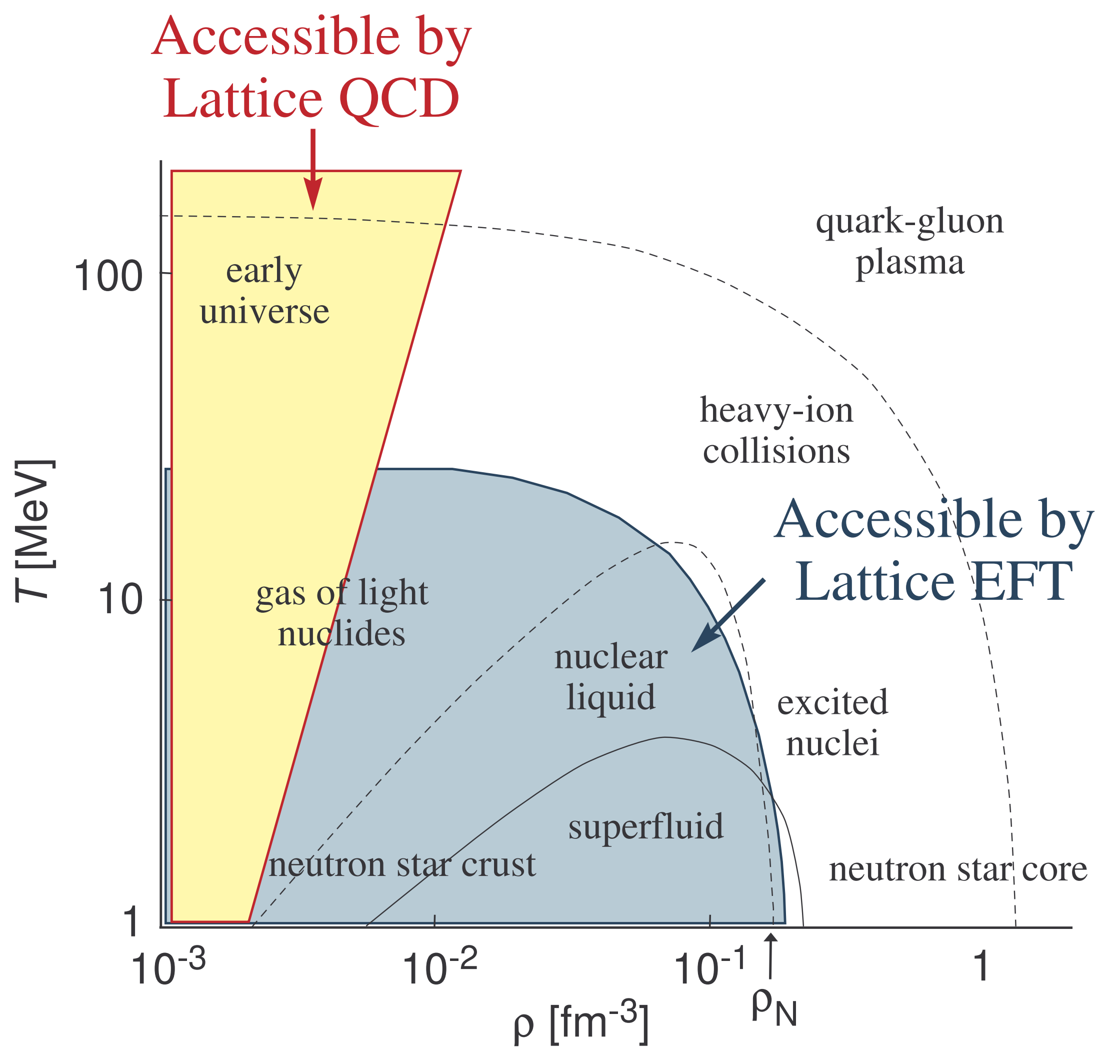
– successfully applied in light nuclei with *A = 2, 3, 4*

– *combine with simulations to go to larger A*



⇒ Nuclear Lattice Simulations

NUCLEAR LATTICE SIMULATIONS: AIMS & SCOPE



Effective Field Theory for Nuclear Physics

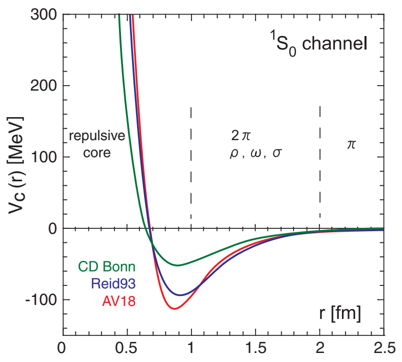
only a brief reminder $\longrightarrow$ details in

E. Epelbaum, H.-W. Hammer, UGM, Rev. Mod. Phys. **81** (2009) 1773
[arXiv:0811.1338 [nucl-th]]

CHIRAL EFT FOR FEW-NUCLEON SYSTEMS

Gasser, Leutwyler, Weinberg, van Kolck, Epelbaum, Bernard, Kaiser, UGM, . . .

- Scales in nuclear physics:



Natural: $\lambda_\pi = 1/M_\pi \simeq 1.5$ fm (Yukawa 1935)

Unnatural: $|a_{np}(^1S_0)| = 23.8\,\mathrm{fm}\,,\ a_{np}(^3S_1) = 5.4\,\mathrm{fm} \gg 1/M_\pi$

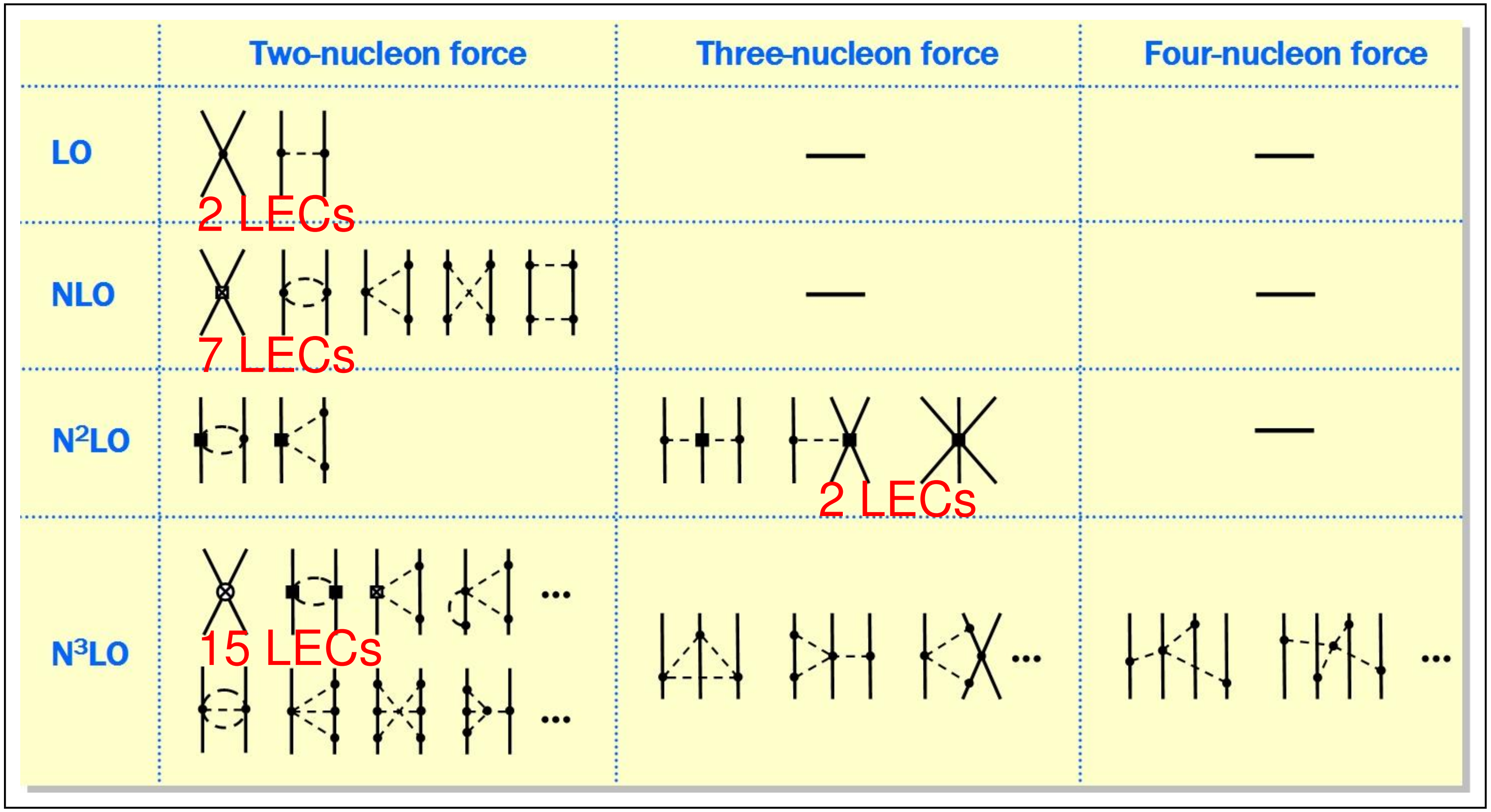
- this can be analyzed in a suitable EFT based on

$$\mathcal{L}_{\rm QCD} \to \mathcal{L}_{\rm EFF} = \mathcal{L}_{\pi\pi} + \mathcal{L}_{\pi N} + \mathcal{L}_{NN} + \ldots$$

- pion and pion-nucleon sectors are perturbative in Q/Λ_χ $\to$ chiral perturbation th'y
- $\mathcal{L}_{NN}$ collects short-distance contact terms, to be fitted
- NN interaction requires non-perturbative resummation

$\to$ chirally expand $\mathrm{V}_{\rm NN(N)}$, use in regularized LS/FY equation

CHIRAL POTENTIAL and NUCLEAR FORCES



$\mathcal{O}((Q/\Lambda_\chi)^0)$

$\mathcal{O}((Q/\Lambda_\chi)^2)$

$\mathcal{O}((Q/\Lambda_\chi)^3)$

$\mathcal{O}((Q/\Lambda_\chi)^4)$

- explains naturally the observed hierarchy of nuclear forces
- MANY successfull tests in few-nucleon systems (continuum calc's)

$\longrightarrow$ talk E. Epelbaum

Nuclear lattice simulations
– Formalism –

NUCLEAR LATTICE SIMULATIONS

Frank, Brockmann (1992), Koonin, Müller, Seki, van Kolck (2000) , Lee, Schäfer (2004), . . .
Borasoy, Krebs, Lee, UGM, Nucl. Phys. **A768** (2006) 179; Borasoy, Epelbaum, Krebs, Lee, UGM, Eur. Phys. J. **A31** (2007) 105

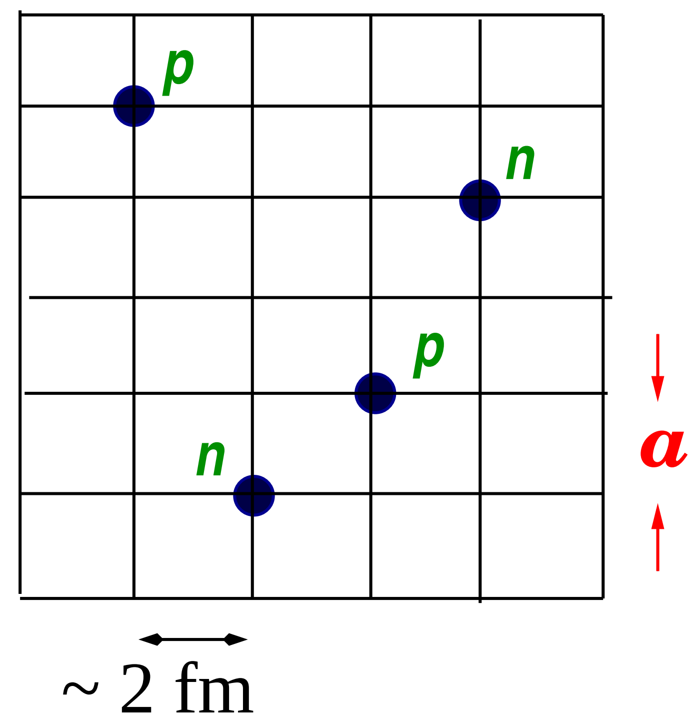
- *new method* to tackle the nuclear many-body problem

- discretize space-time $V = L_s \times L_s \times L_s \times L_t$:
  nucleons are point-like fields on the sites

- discretized chiral potential w/ pion exchanges
  and contact interactions

- typical lattice parameters

$$\Lambda = \frac{\pi}{a} \simeq 300 \text{ MeV [UV cutoff]}$$

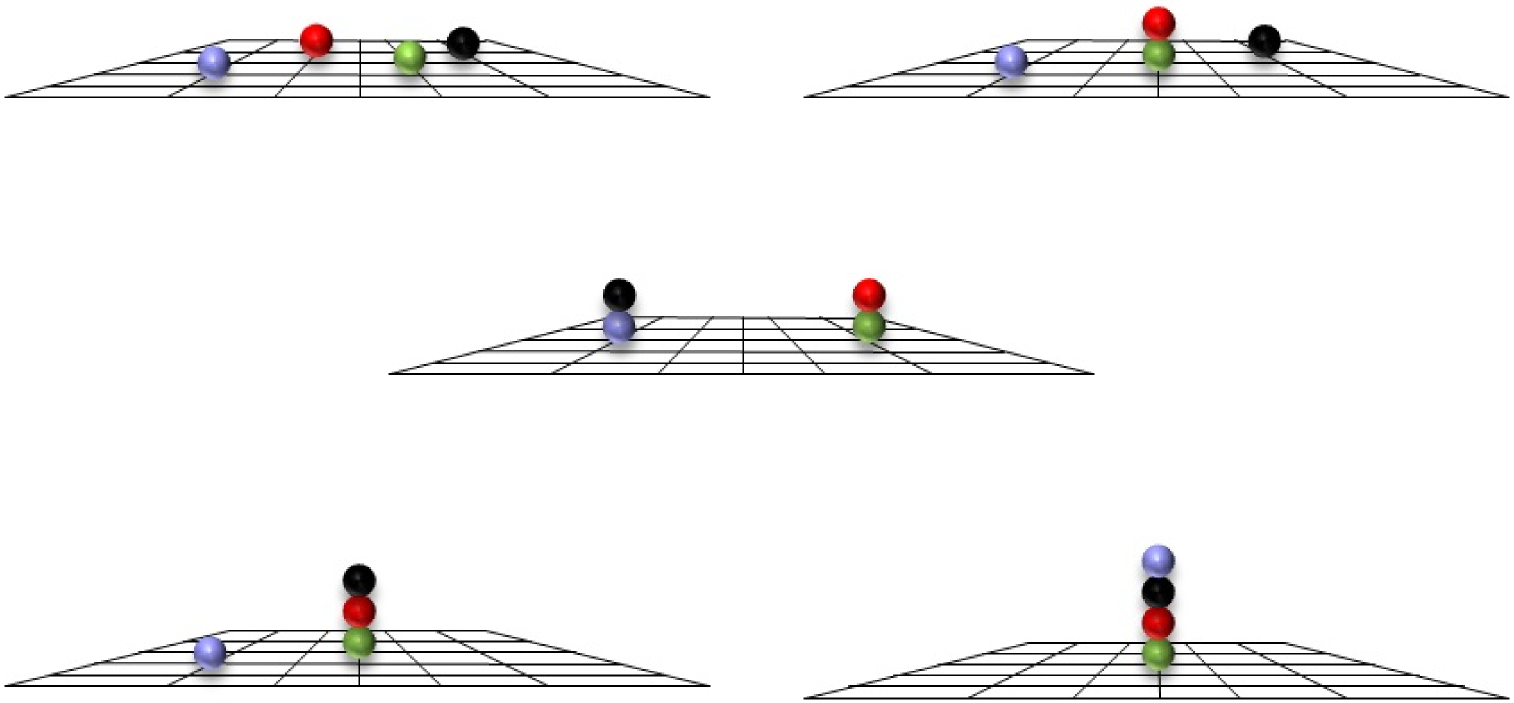


- strong suppression of sign oscillations due to approximate Wigner SU(4) symmetry

J. W. Chen, D. Lee and T. Schäfer, Phys. Rev. Lett. **93** (2004) 242302

- hybrid Monte Carlo & transfer matrix (similar to LQCD)

CONFIGURATIONS



⇒ all *possible* configurations are sampled

⇒ *clustering* emerges *naturally*

TRANSFER MATRIX METHOD

- Correlation–function for A nucleons: $Z_A(t) = \langle \Psi_A | \exp(-tH) | \Psi_A \rangle$

  with Ψ_A a Slater determinant for A free nucleons

  Euclidean time

- Ground state energy from the time derivative of the correlator

$$E_A(t) = -\frac{d}{dt} \ln Z_A(t)$$

$\longrightarrow$ ground state filtered out at large times: $E_A^0 = \lim_{t\to\infty} E_A(t)$

- Expectation value of any normal–ordered operator $\mathcal{O}$

$$Z_A^{\mathcal{O}} = \langle \Psi_A | \exp(-tH/2)\, \mathcal{O}\, \exp(-tH/2)\, | \Psi_A \rangle$$

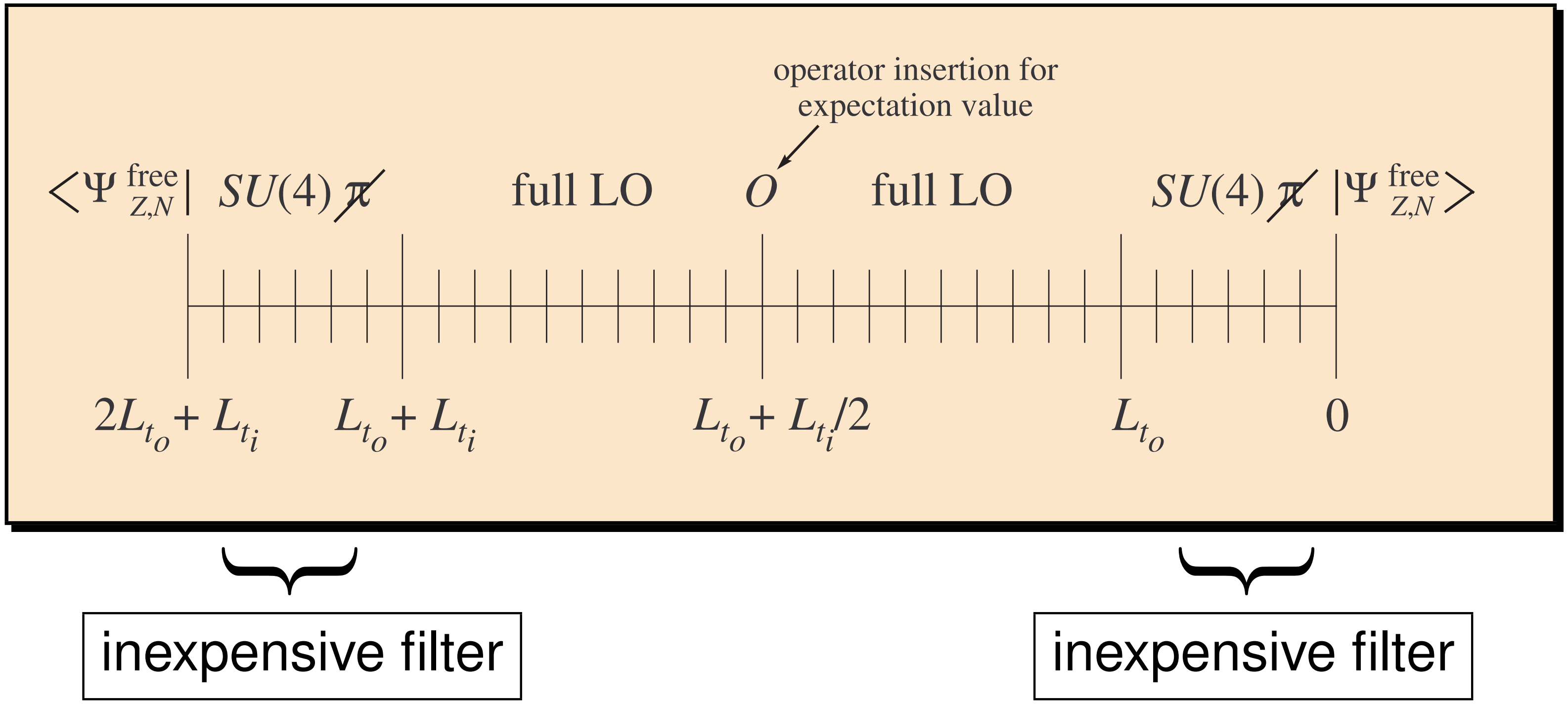
$$\lim_{t\to\infty} \frac{Z_A^{\mathcal{O}}(t)}{Z_A(t)} = \langle \Psi_A | \mathcal{O} \, | \Psi_A \rangle$$

TRANSFER MATRIX CALCULATION

- Expectation value of any normal–ordered operator $\mathcal{O}$

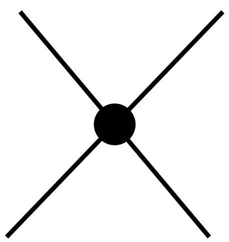
$$\langle \Psi_A | \mathcal{O} \, | \Psi_A \rangle = \lim_{t \to \infty} \frac{\langle \Psi_A | \exp(-tH/2) \, \mathcal{O} \, \exp(-tH/2) \, | \Psi_A \rangle}{\langle \Psi_A | \exp(-tH) | \Psi_A \rangle}$$

- Anatomy of the transfer matrix



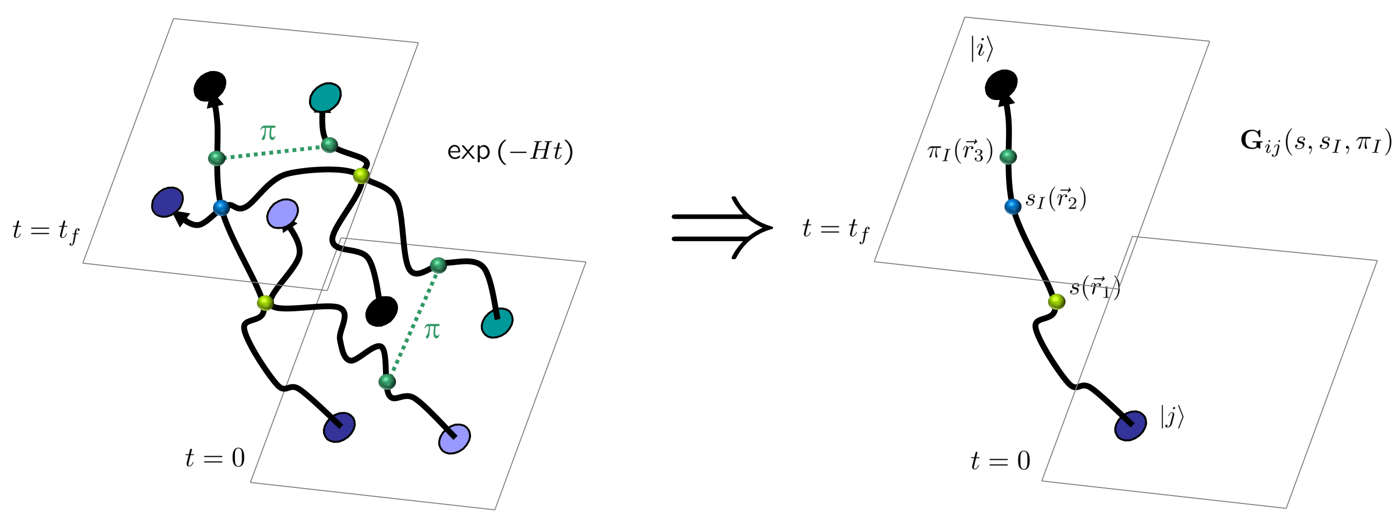
MONTE CARLO with AUXILIARY FILEDS

- Contact interactions represented by auxiliary fields s, s_I



$$\exp(\rho^2/2) \propto \int_{-\infty}^{+\infty} ds \, \exp(-s^2/2 - s\rho) \, , \quad \rho \sim N^\dagger N$$

- Correlation function = path-integral over pions & auxiliary fields

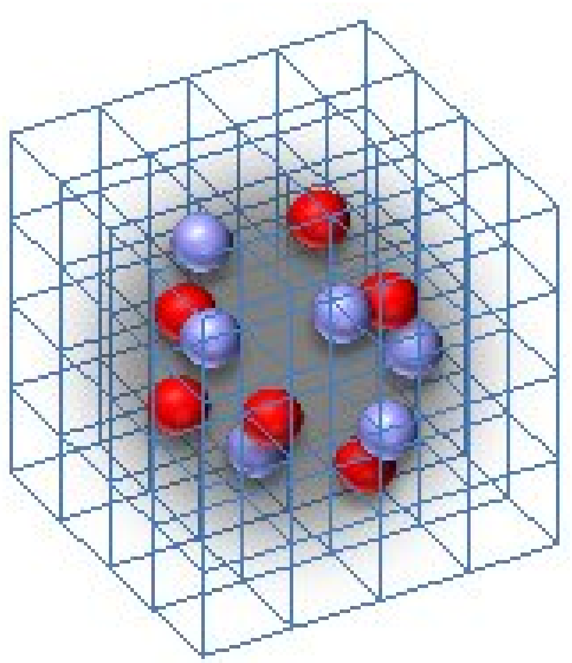


COMPUTATIONAL EQUIPMENT

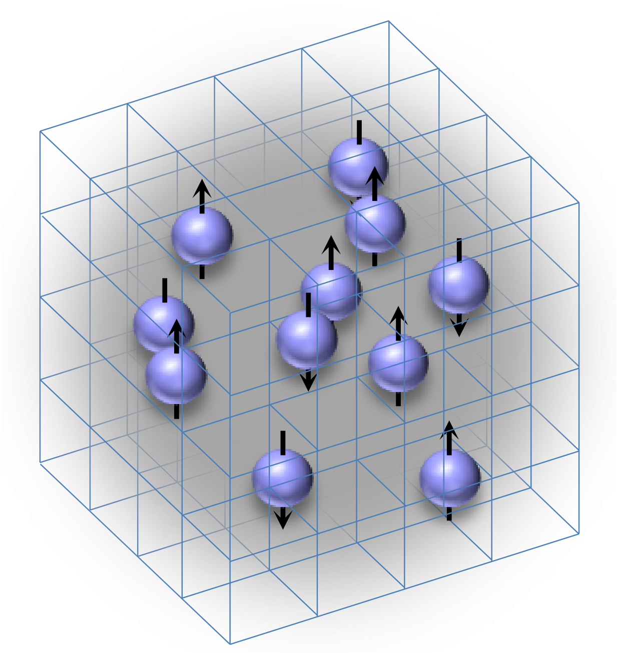
- Present = JUGENE (BlueGene/P)
- Future = JUQUEEN (BlueGene/Q)

Nuclear lattice simulations – Results –

nuclei

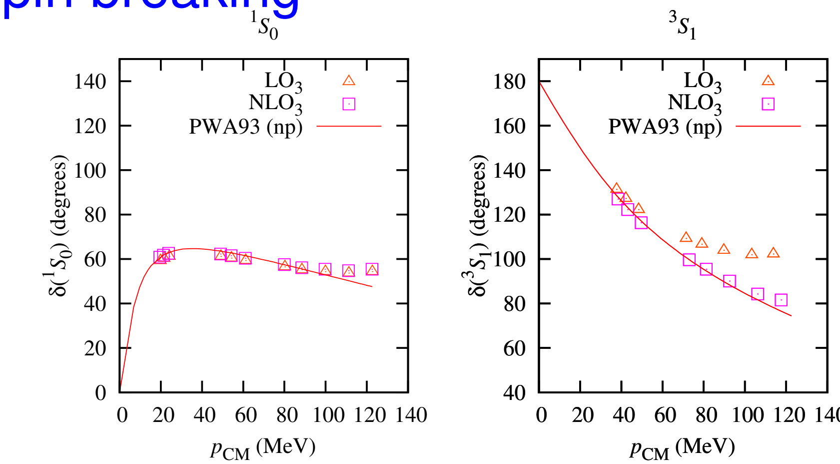


neutron matter



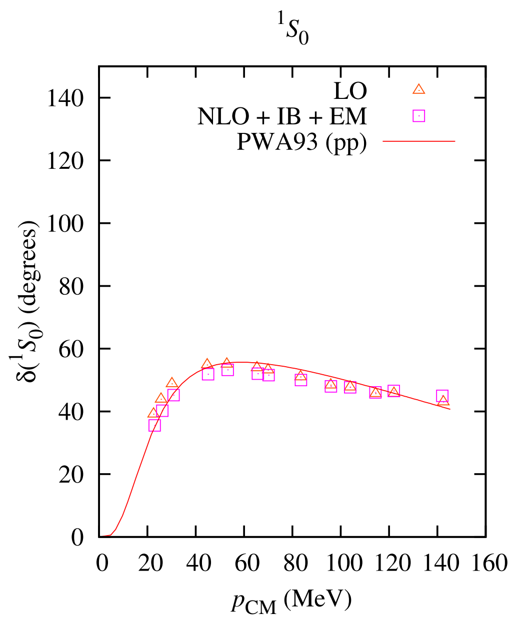
FIXING PARAMETERS & FIRST PREDICTIONS

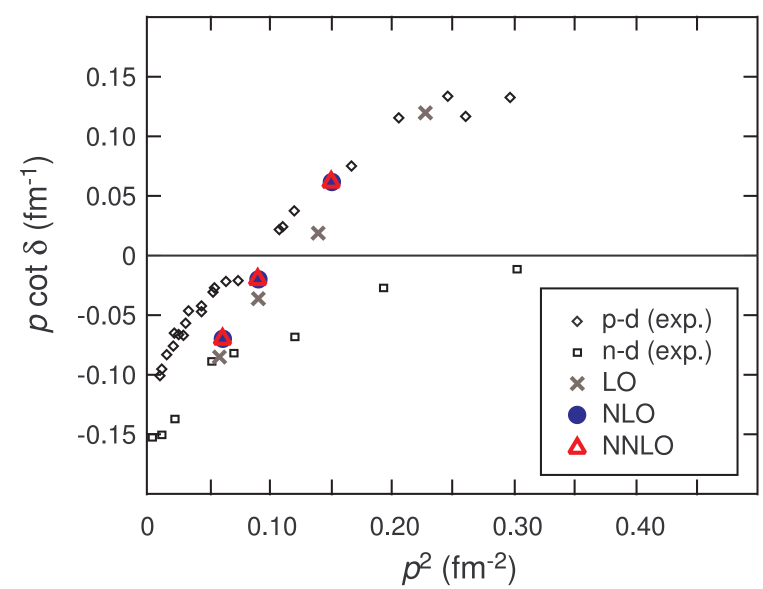
- work at NNLO including strong and em isospin breaking
- 9 NN LECs from np scattering and Q_d
- 2 LECs for isospin-breaking (np, pp, nn)
- 2 LECs D, E related to the leading 3NF



$\Rightarrow$ make predictions

- pp vs np scattering
- nd spin-3/2
  quartet channel
- . . .





Ground states

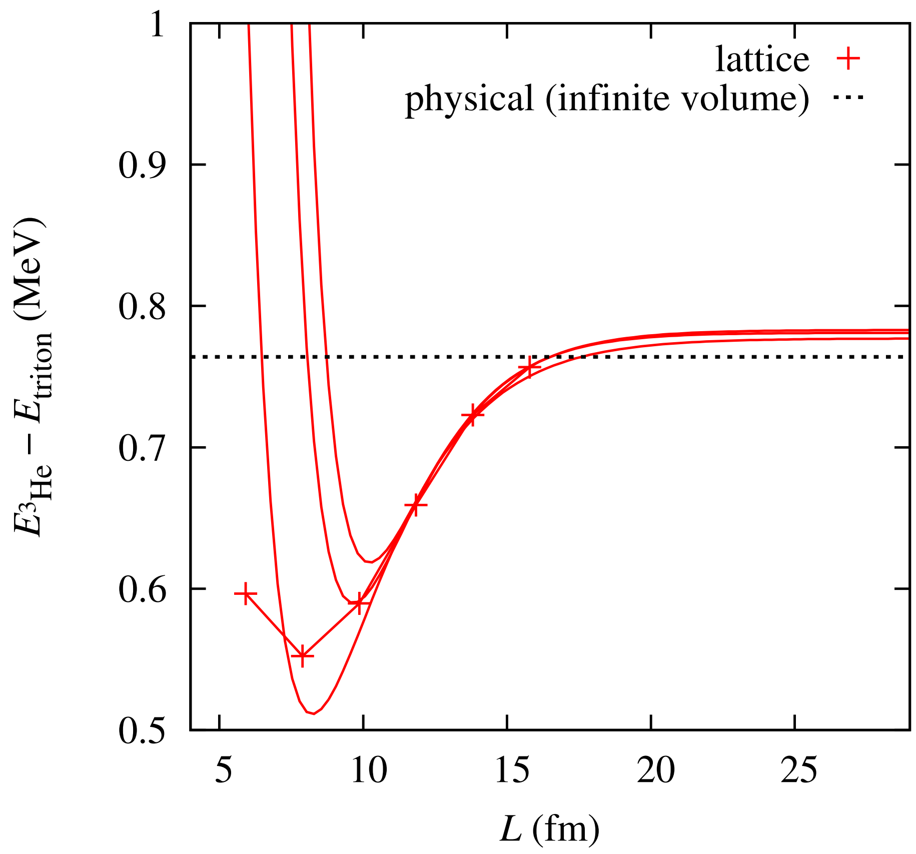
PREDICTIONS: TRITON & HELIUM-3

Epelbaum, Krebs, Lee, UGM, Phys. Rev. Lett. **104** (2010) 142501; Eur. Phys. J. **A 45** (2010) 335

• binding energies of 3N systems: $E(L) = \mathrm{B.E.} - \frac{a}{L}\exp(-bL)$

see also Hammer, Kreuzer (2011)

$\Rightarrow$ predict the energy difference $E(^3He) - E(^3H)$

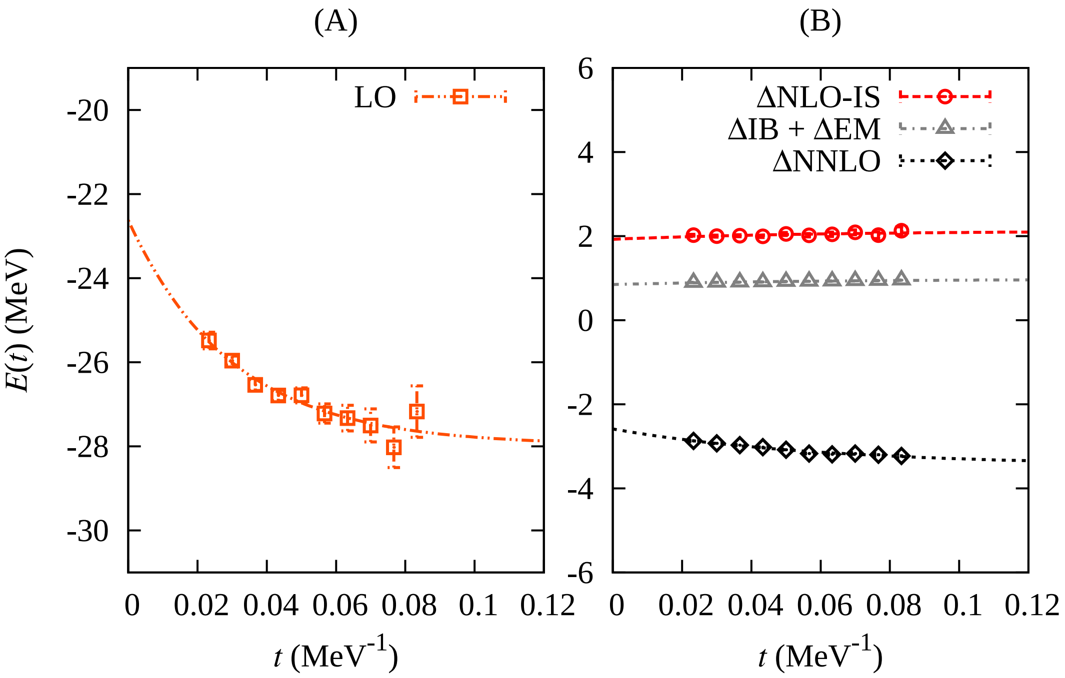


0.78(5) MeV

0.76 MeV [exp.]

Ground state of ^{4}He

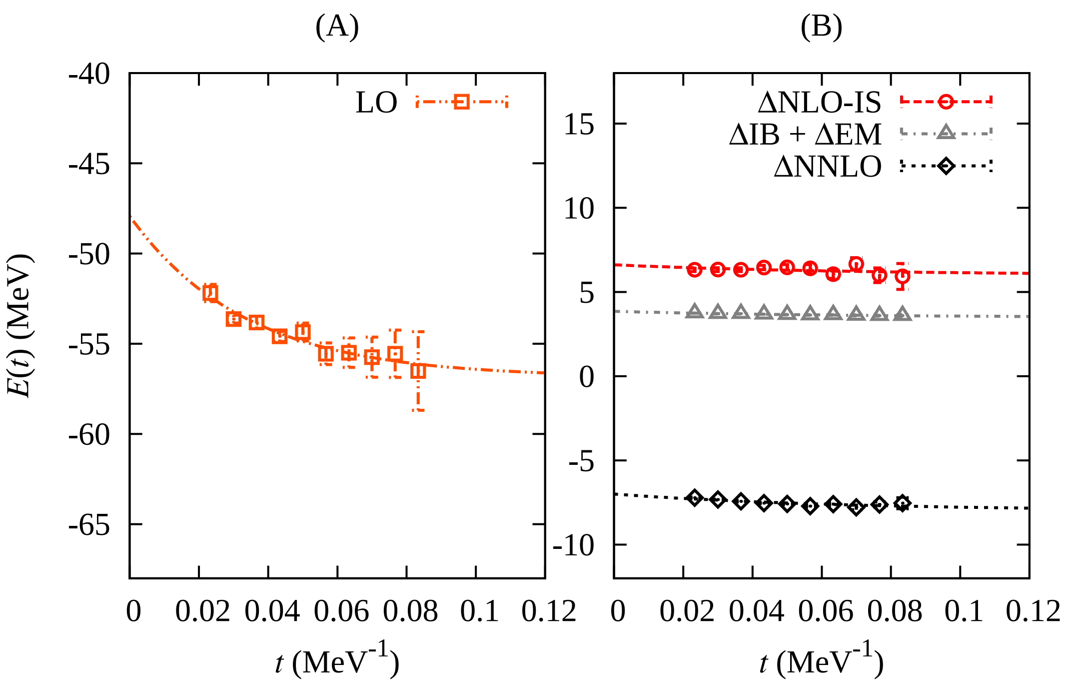
$L = 11.8$ fm



LO ($\mathcal{O}(Q^0)$)	$-28.0(3)$ MeV
NLO ($\mathcal{O}(Q^2)$)	$-24.9(5)$ MeV
NNLO ($\mathcal{O}(Q^3)$)	$-28.3(6)$ MeV
Exp.	-28.3 MeV

Ground state of ^{8}Be

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

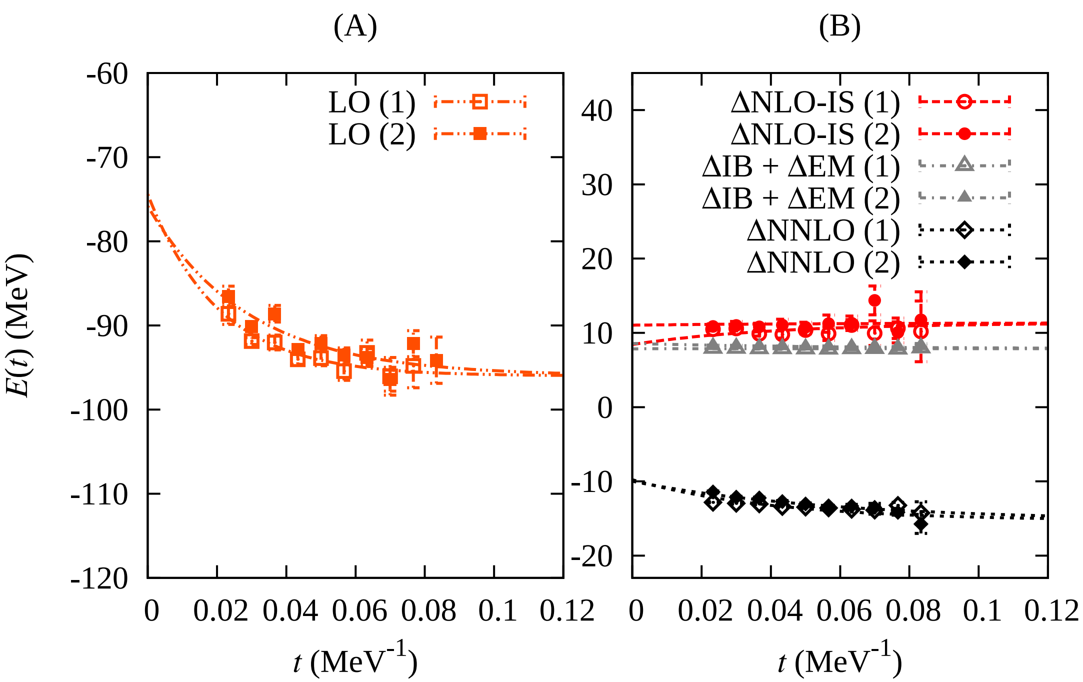


to be published

LO ($\mathcal{O}(Q^0)$)	$-57(2)$ MeV
NLO ($\mathcal{O}(Q^2)$)	$-47(2)$ MeV
NNLO ($\mathcal{O}(Q^3)$)	$-55(2)$ MeV
Exp.	-56.5 MeV

Ground state of ^{12}C

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

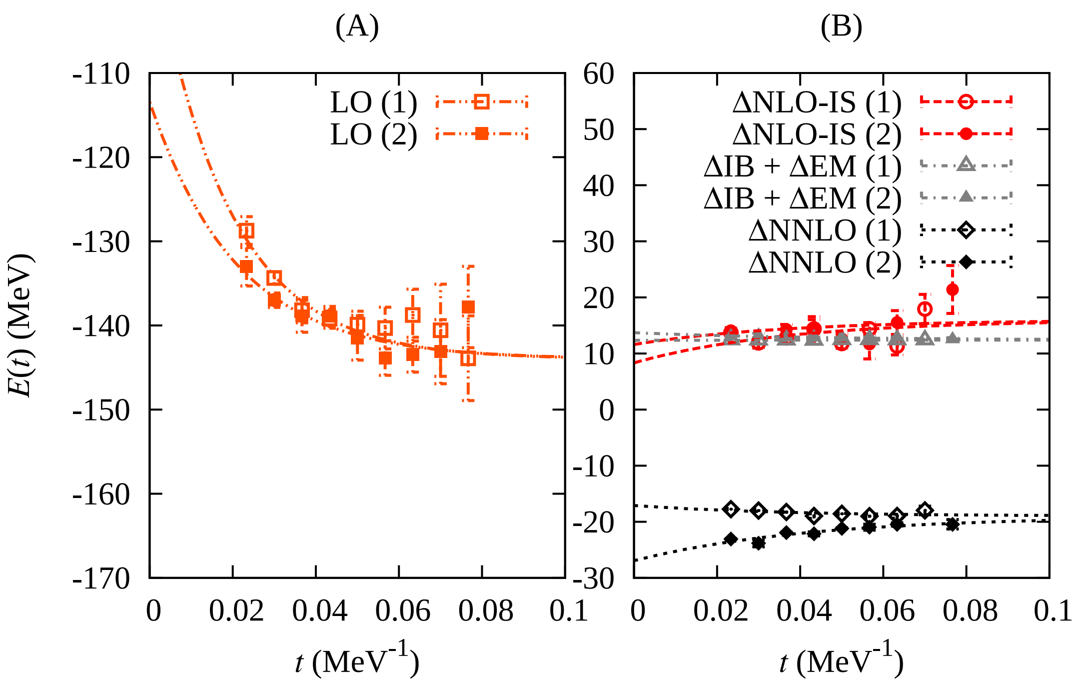


to be published

LO ($\mathcal{O}(Q^0)$)	$-96(2)$ MeV
NLO ($\mathcal{O}(Q^2)$)	$-77(3)$ MeV
NNLO ($\mathcal{O}(Q^3)$)	$-92(3)$ MeV
Exp.	-92.2 MeV

Ground state of ^{16}O

$L = 11.8$ fm

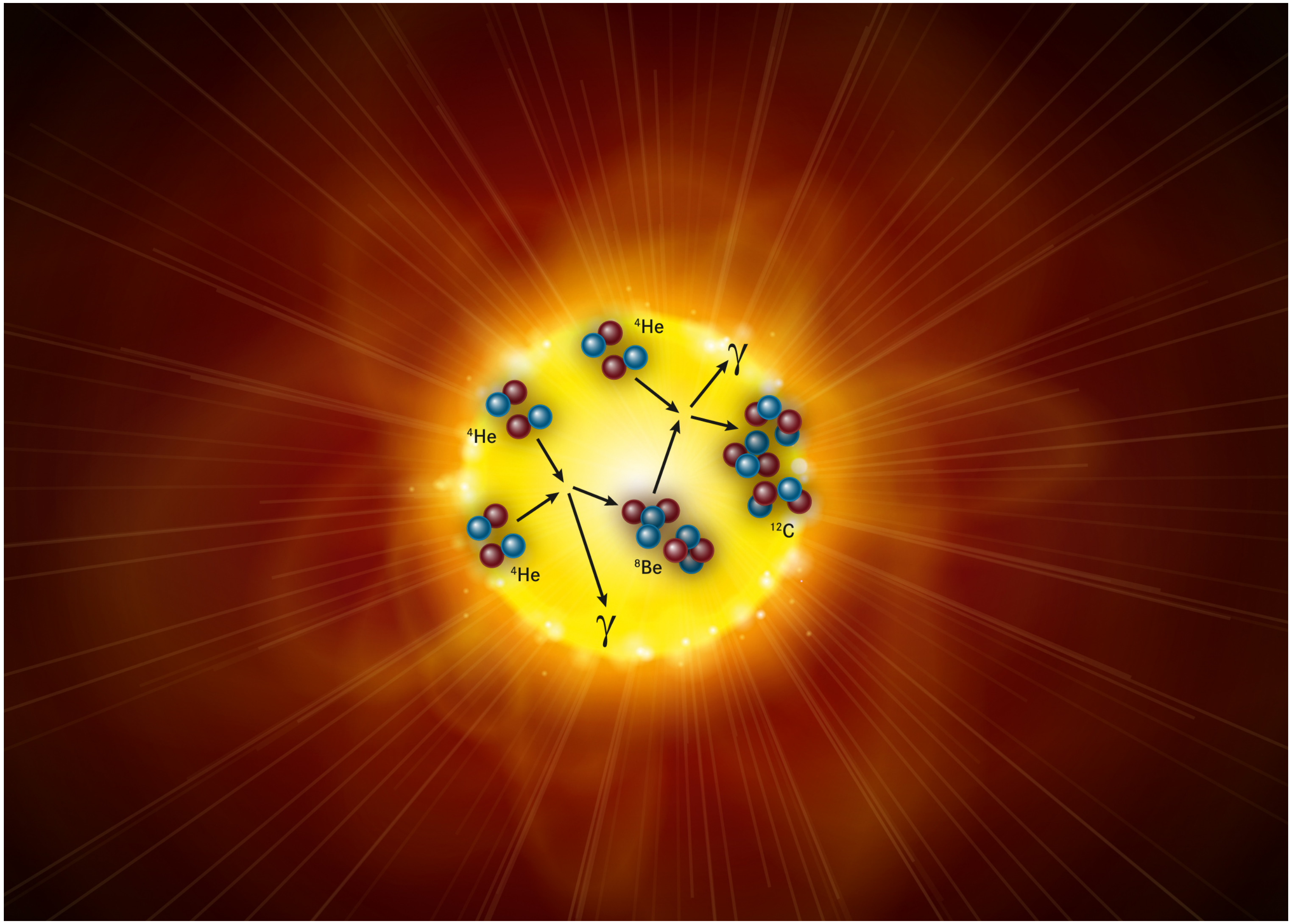


to be published

LO ($\mathcal{O}(Q^0)$)	$-144(4)$ MeV
NLO ($\mathcal{O}(Q^2)$)	$-116(6)$ MeV
NNLO ($\mathcal{O}(Q^3)$)	$-135(6)$ MeV
Exp.	-127.6 MeV

SPECTRUM OF ^{12}C & the HOYLE STATE

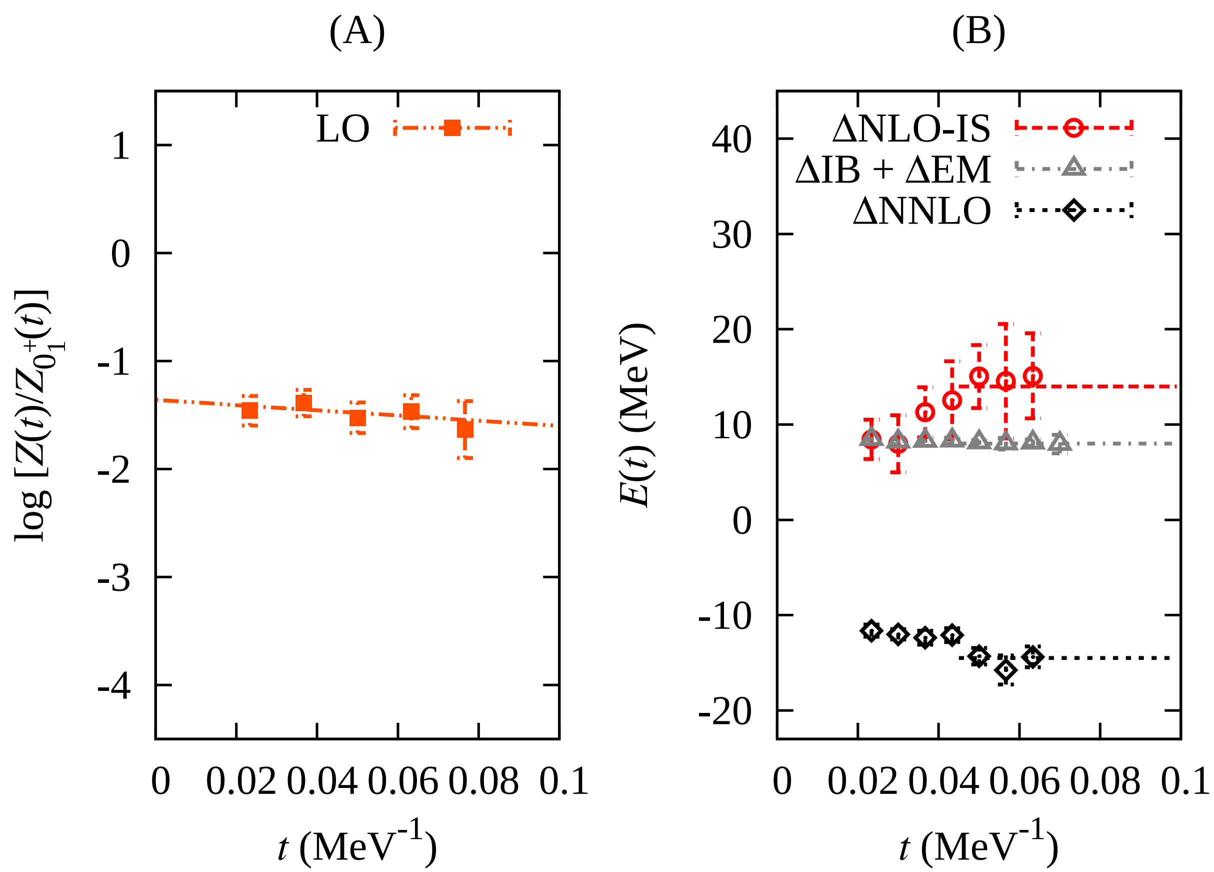
Epelbaum, Krebs, Lee, UGM, Phys. Rev. Lett. **106** (2011) 192501
Viewpoint: Hjorth-Jensen, Physics **4** (2011) 38



EXCITED STATES of ^{12}C

- Multi-channel projection MC: start with many different initial standing waves
- Extract four orthogonal energy levels with even parity and zero total momentum
- Two states have $J_z = 0$, two has $J_z = 2$ $\rightarrow$ clean signals!
- 2_1^+ state:

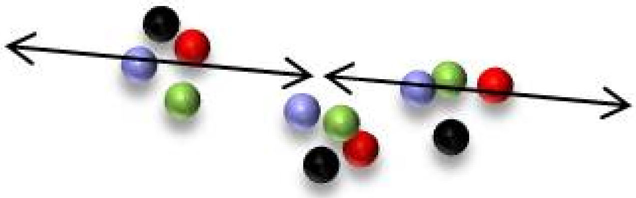
$$E(2_1^+) = -86(3)\ \text{MeV}$$
$$[-87.7\ \text{MeV}]$$

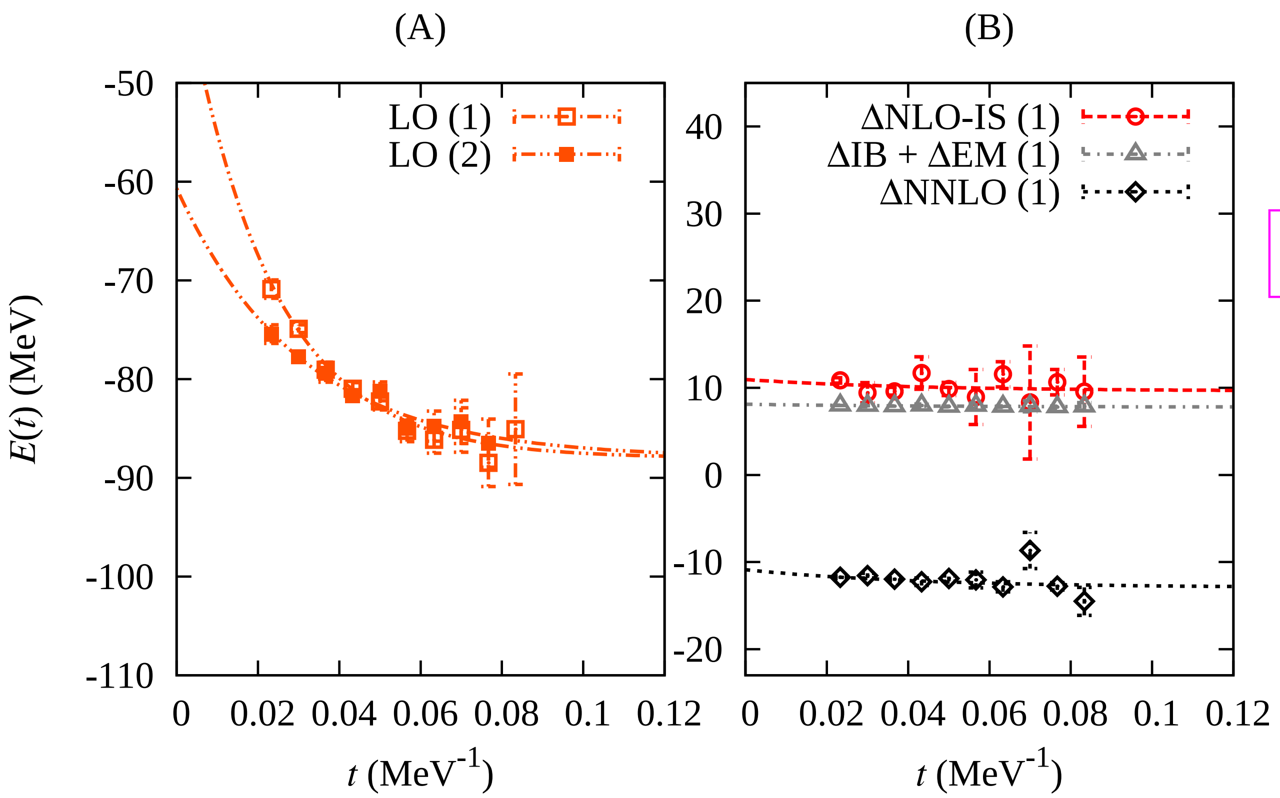


to be published

THE HOYLE STATE (0_2^+)

- energy: $E(0_2^+) = -84(3)$ MeV
- close to $E(^4\mathrm{He}) + E(^8\mathrm{Be}) = -83.8(2.0)$ MeV
- structure: “bent” alpha-chain like (not “BEC”)

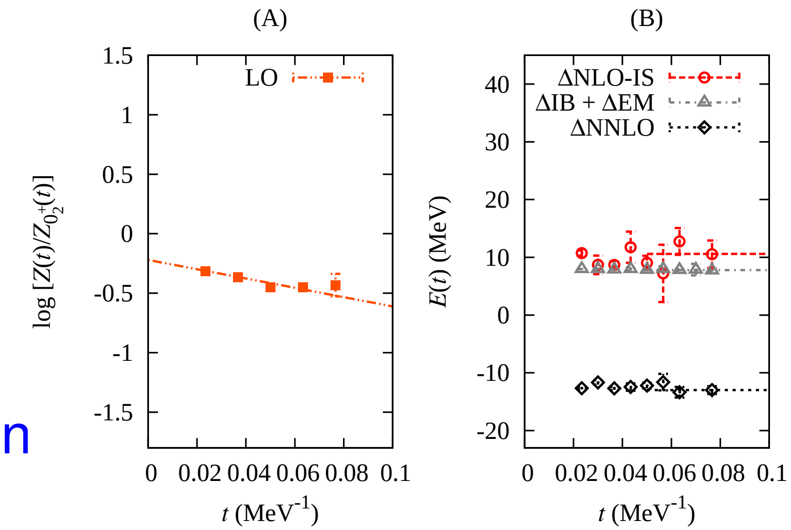




to be published

A HOYLE STATE EXCITATION (2_2^+)

to be published



- a 2^+ state 4 MeV above the Hoyle state
- interpretation:
  a rotational band of the Hoyle state
  generated from excitations of the alpha-chain
- what's in the data ?
  a 2^+ state 3.51 MeV above the Hoyle state seen in ${}^{11}B(d,n){}^{12}C$
  not included in the level scheme! Ajzenberg-Selove, Nucl. Phys. A506 (1990) 1

  a 2^+ state 3.8(4) MeV above the Hoyle state seen in ${}^{12}C(\alpha,\alpha){}^{12}C$
  Bency John et al., Phys. Rev. C 68 (2003) 014305

$\Rightarrow$ ab initio prediction requires experimental confirmation

SPECTRUM OF ^{12}C

- Summarizing the results for carbon-12:

	0_1^+	2_1^+	0_2^+	2_2^+
LO	$-96(2)$ MeV	$-94(2)$ MeV	$-88(2)$ MeV	$-84(2)$ MeV
NLO	$-77(3)$ MeV	$-72(3)$ MeV	$-71(3)$ MeV	$-66(3)$ MeV
NNLO	$-92(3)$ MeV	$-86(3)$ MeV	$-84(3)$ MeV	$-79(3)$ MeV
Exp.	-92.2 MeV	-87.7 MeV	-84.5 MeV	$-80.7(4)$ MeV

- importance of consistent 2N & 3N forces
- good agreement w/ experiment, can be improved
- test of the *Anthropic Principle* possible

to be published

TOPOLGICAL PHASES

Bour, Hammer, König, Lee, UGM, Phys. Rev. D **84** (2011) 091503(R)

- consider a moving finite-size particle in a box

$\Rightarrow$ the wavefunction picks up a *topological phase*
i.e. the particle touches all walls $\longrightarrow$ energy shift

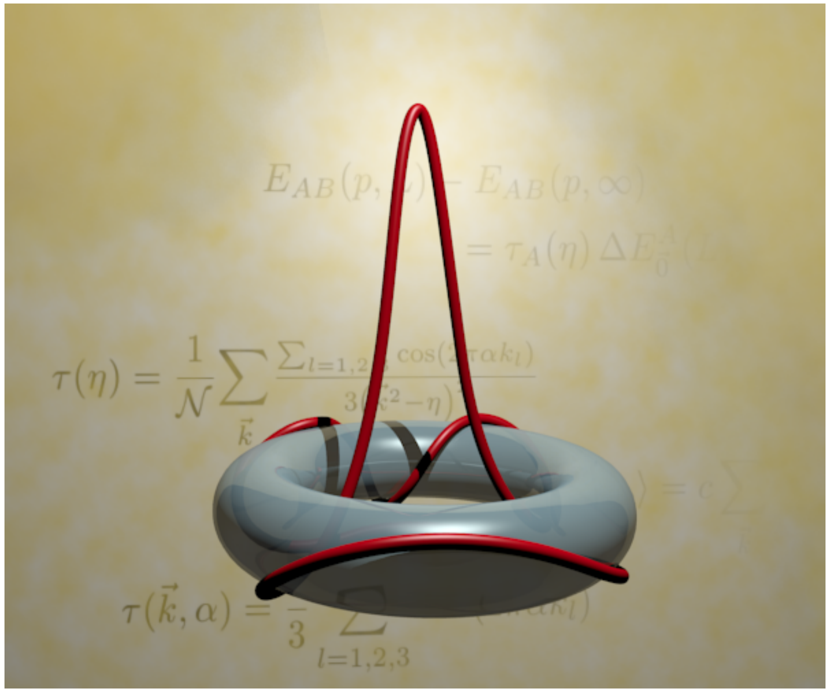


Figure courtesy S. König

- e..g a moving dimer with momentum $\vec{k}$
(b.s. of two particles with masses m_1, m_2)

$$\Rightarrow \boxed{\frac{\Delta E_{\vec{k}}(L)}{\Delta E_{\vec{0}}(L)} = \sum_{i=1,2,3} \cos(2\pi\alpha k_i) \equiv \tau(\vec{k},\alpha)}$$

$$\alpha = \frac{m_1}{m_1 + m_2}$$

$\hookrightarrow$ result is **universal**

$\hookrightarrow$ easily generalized to other waves and more constituents

$\hookrightarrow$ easily generalized to the scattering of composite particles

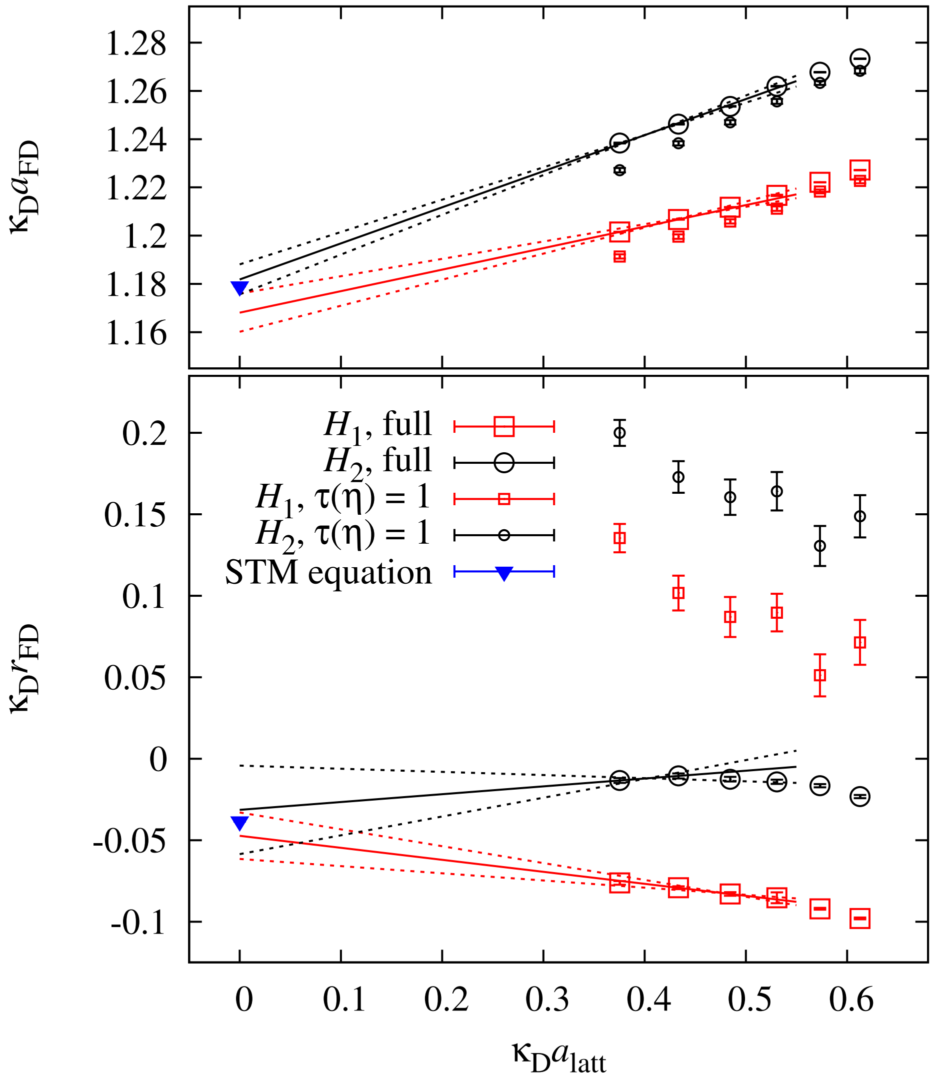
FERMION-DIMER SCATTERING

Bour, Hammer, König, Lee, UGM, Phys. Rev. D **84** (2011) 091503(R)

- consider fermion-dimer scattering on the lattice
- consider two lattice Hamiltonians $\mathcal{H}_{1,2}$ that reproduce the same continuum limit
  Bour et al., Phys.Rev. A **83** (2011) 063619
- compare with exact solution of the STM eq.
  Skorniakov, Ter-Martirosian (1957)

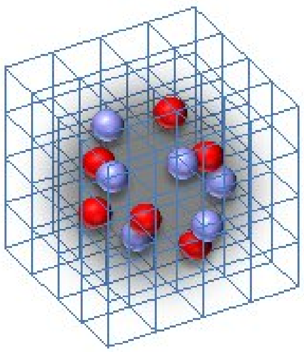
> $\Rightarrow$ topological volume factor τ must be included for obtaining the correct continuum result !

- extension to bound nuclear systems from lattice QCD
  Davoudi, Savage, Phys. Rev. D **84** (2011) 114502



SUMMARY & OUTLOOK

- Nuclear lattice simulations as a new quantum many-body approach
- Formulate continuum EFT on space-time lattice $V = L_s \times L_s \times L_s \times L_t$
- New method to extract phase shifts & mixing angles
- Fix parameters in few-nucleon systems $\longrightarrow$ predictions
- Promising results for $A = 2, 3, 4, 8, 12, 16$ at NNLO
- ^{12}C spectrum at NNLO $\longrightarrow$ Hoyle state & 2^+ excitation
- First ever ab initio MC calculation of ^{16}O
- Reaction theory is in reach $\longrightarrow$ topological phases
- Computational scaling $\longrightarrow$ medium nuclei in reach



$\Rightarrow$ larger A and higher precision