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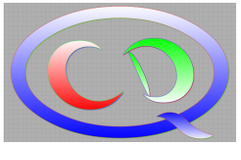
JÜLICH FORSCHUNGSZENTRUM

Nucleons on a Lattice: Symmetry Breaking & Restoration

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

supported by DFG, SFB/TR-110



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CONTENTS

Nuclear lattice EFT: what and why ?

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*

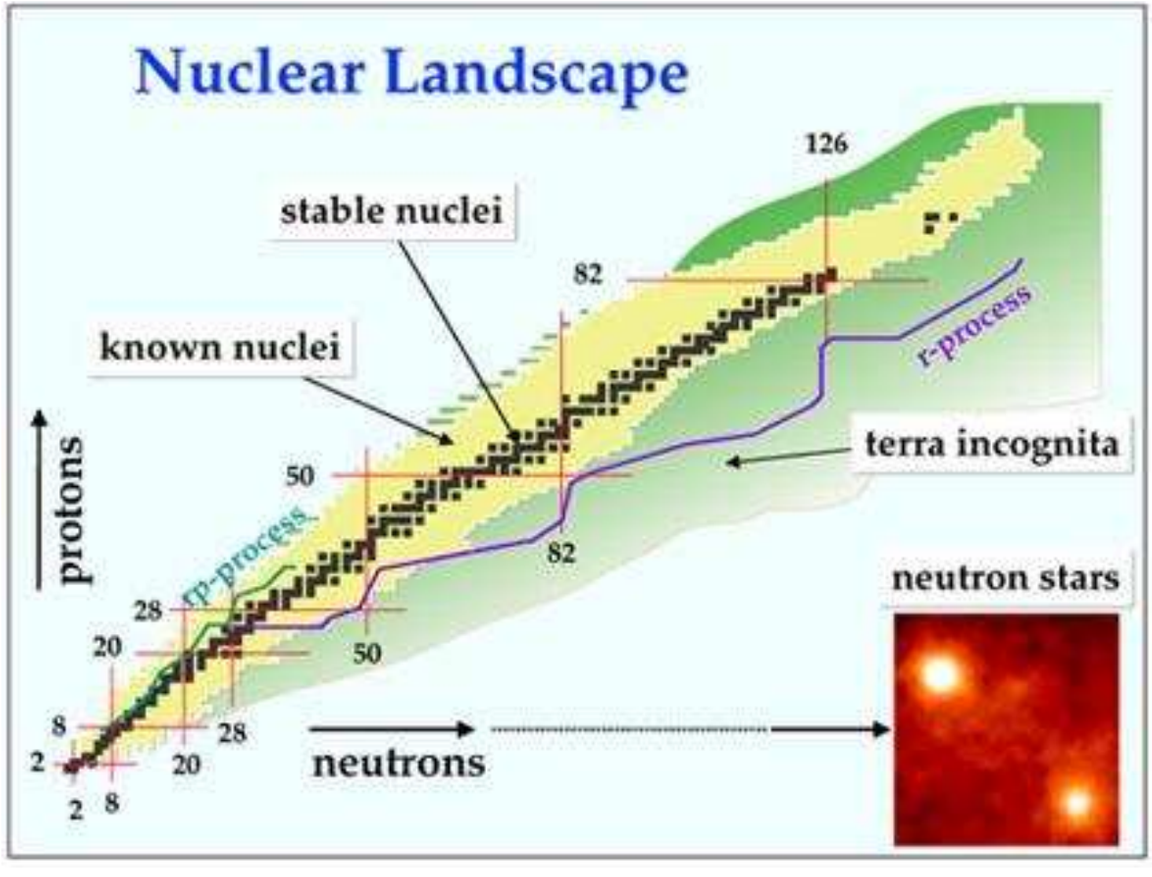
– density functional theory, . . .: *A* $\geq$ *100*

- Chiral EFT:

– provides **accurate 2N, 3N and 4N forces**

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

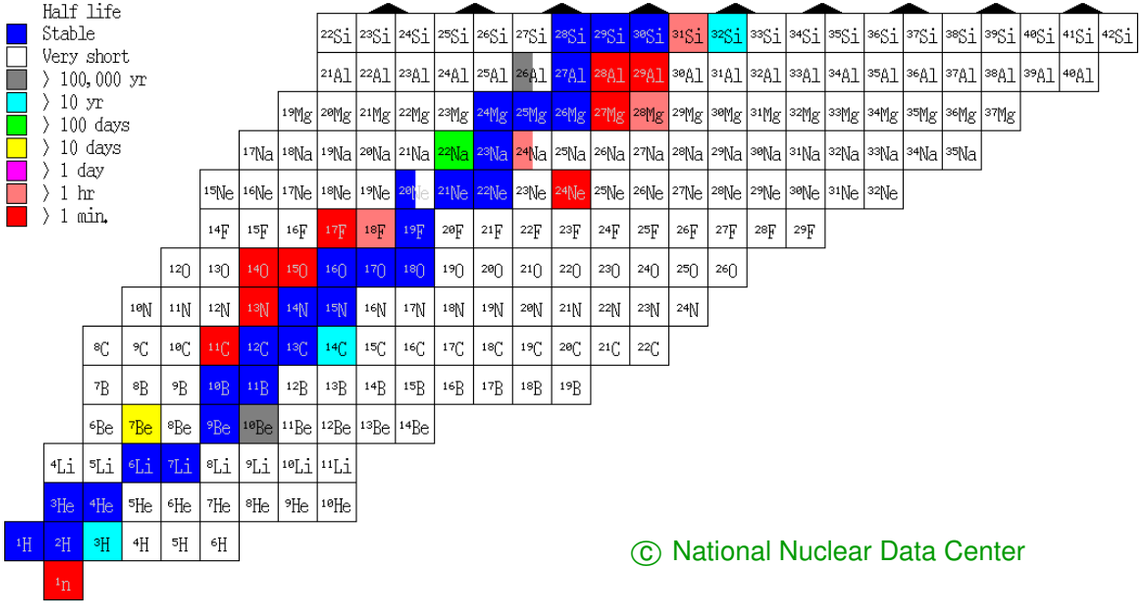
– combine with simulations to get to larger A



⇒ Nuclear Lattice Effective Field Theory

AB INITIO NUCLEAR STRUCTURE and SCATTERING

- Nuclear structure:
  - ⋆ 3-nucleon forces
  - ⋆ limits of stability
  - ⋆ alpha-clustering
  - ⋮



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- Nuclear scattering: processes relevant for nuclear astrophysics
  - ⋆ alpha-particle scattering: $^4\mathrm{He} + {}^4\mathrm{He} \to {}^4\mathrm{He} + {}^4\mathrm{He}$
  - ⋆ triple-alpha reaction: $^4\mathrm{He} + {}^4\mathrm{He} + {}^4\mathrm{He} \to {}^{12}\mathrm{C} + \gamma$
  - ⋆ alpha-capture on carbon: $^4\mathrm{He} + {}^{12}\mathrm{C} \to {}^{16}\mathrm{O} + \gamma$
  - ⋮

MANY–BODY APPROACHES

- nuclear physics = notoriously difficult problem: strongly interacting fermions

- define *ab initio*: combine the precise and well-founded forces from *chiral EFT* with a many-body approach

- two different approaches followed in the literature:

  ⋆ combine chiral NN(N) forces with standard many-body techniques

  Dean, Duguet, Hagen, Navratil, Nogga, Papenbrock, Schwenk, Soma . . .

  → successful, but problems with cluster states (SM, NCSM,...)

  ⋆ combine chiral forces and lattice simulations methods

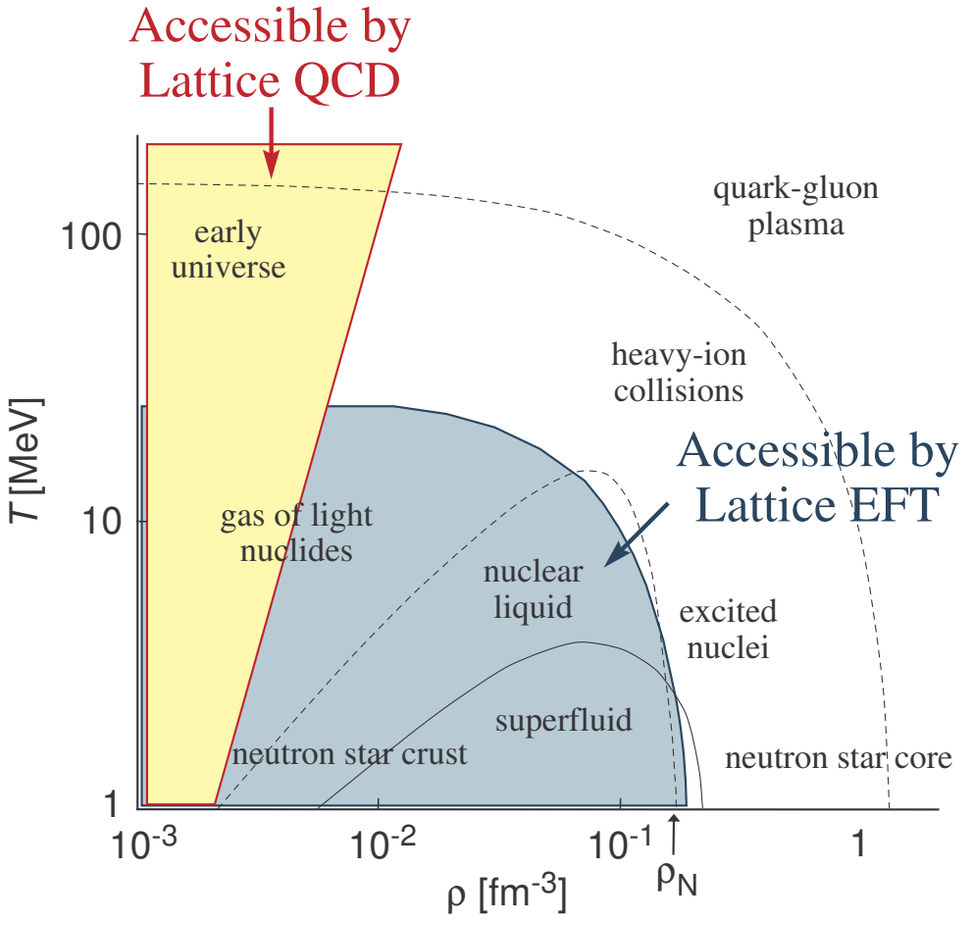
  → this new method is called *nuclear lattice simulations* (NLEFT)

  Borasoy, Elhatisari, Epelbaum, Krebs, Lee, Lähde, UGM, Rupak, . . .

  → rest of the talk

COMPARISON to LATTICE QCD

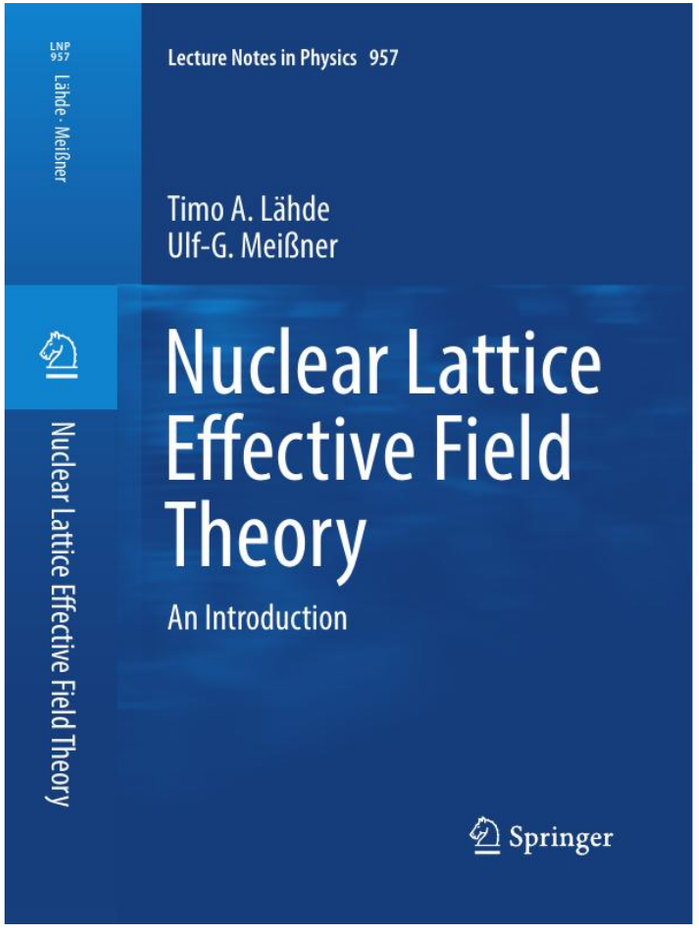
LQCD (quarks & gluons)	NLEFT (nucleons & pions)
relativistic fermions	non-relativistic fermions
renormalizable th'y	EFT
continuum limit	no continuum limit
(un)physical masses	physical masses
Coulomb - difficult	Coulomb - easy
high T/small ρ	small T/nuclear densities
sign problem severe	sign problem moderate



- similar methods:
  hybrid MC, parallel computing, . . .
  ↪ not treated here

- what I want to discuss within the time limitations:
  ↪ how to put the chiral EFT on a lattice
  ↪ scattering on a lattice (**not** the Lüscher approach)
  ↪ the pinhole algorithm / center-of-mass in AFQMC

Chiral EFT on a lattice



T. Lähde & UGM

Nuclear Lattice Effective Field Theory - An Introduction

Springer Lecture Notes in Physics **957** (2019) 1 - 396

NUCLEAR LATTICE EFFECTIVE FIELD THEORY

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

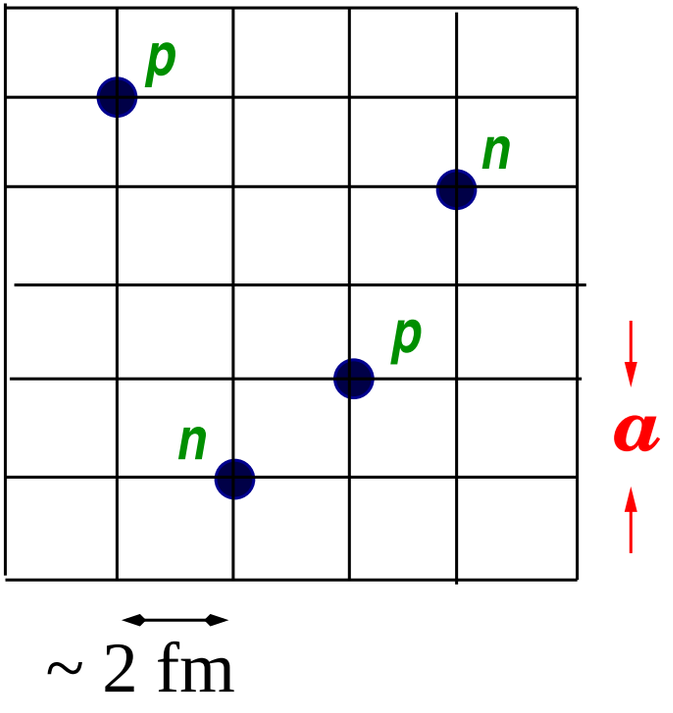
- discretize space-time $V = L_s \times L_s \times L_s \times L_t$:
  nucleons are point-like particles on the sites

- discretized chiral potential w/ pion exchanges
  and contact interactions + Coulomb

  → see Epelbaum, Hammer, UGM, Rev. Mod. Phys. **81** (2009) 1773

- typical lattice parameters

$$p_{\rm max} = \frac{\pi}{a} \simeq 314\,\text{MeV [UV cutoff]}$$



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

E. Wigner, Phys. Rev. **51** (1937) 106; T. Mehen et al., Phys. Rev. Lett. **83** (1999) 931; J. W. Chen et al., Phys. Rev. Lett. **93** (2004) 242302

- physics independent of the lattice spacing for $a = 1 \ldots 2$ fm

Alarcon, Du, Klein, Lähde, Lee, Li, Lu, Luu, UGM, EPJA **53** (2017) 83; Klein, Elhatisari, Lähde, Lee, UGM, EPJA **54** (2018) 121

LATTICE NOTATION

- nucleon annihilation ops: $a_{0,0} \equiv a_{\uparrow,p},\ a_{1,0} \equiv a_{\downarrow,p},\ a_{0,1} \equiv a_{\uparrow,n},\ a_{1,1} \equiv a_{\downarrow,n}$

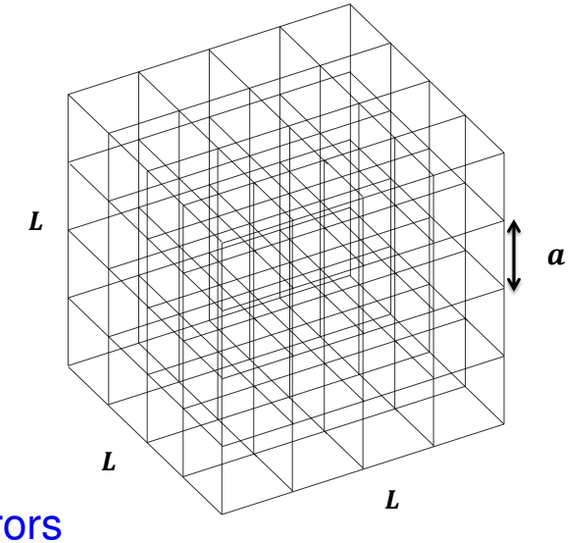
  $\rightarrow$ labeling **spin** and **isospin**

- spatial & temporal lattice spacing: $a,\, a_t \to \alpha_t \equiv a_t/a$

- lattice size: $L \equiv Na,\, L_t \equiv N_t a_t$

- lattice momenta: $\vec{k} = (k_1, k_2, k_3) \equiv \left(\frac{2\pi}{N}\hat{k}_1, \frac{2\pi}{N}\hat{k}_2, \frac{2\pi}{N}\hat{k}_3 \right),$

  $\rightarrow$ in the first Brillouin zone: $|k_i| < \pi$ and $0 \leq |\hat{k}_i| < N/2$



- any derivative operator requires *improvement*, as the simplest representation in terms of two neighboring points is afflicted by the largest discretization errors

$$k_l \equiv \sum_{j=1}^{\nu+1} (-1)^{j+1} \theta_{\nu,j} \sin(jk_l) \ + \mathcal{O}(a^{2\nu+2})$$

$$\frac{k_l^2}{2} \equiv \sum_{j=0}^{\nu+1} (-1)^{j} \omega_{\nu,j} \cos(jk_l) \ + \mathcal{O}(a^{2\nu+2})$$

$\hookrightarrow$ no improvement ($\nu = 0$): $\theta_{0,1} = 1,\ \omega_{0,0} = 1,\ \omega_{0,1} = 1$

LATTICE NOTATION continued

- Order a^2 improvement ($\nu = 1$): $\theta_{1,1} = \frac{4}{3}$, $\theta_{1,2} = \frac{1}{6}$, $\omega_{1,0} = \frac{5}{4}$, $\omega_{1,1} = \frac{4}{3}$, $\omega_{1,2} = \frac{1}{12}$

- Order a^4 improvement ($\nu = 2$): $\theta_{2,1} = \frac{3}{2}$, $\theta_{2,2} = \frac{3}{10}$, $\theta_{2,3} = \frac{1}{30}$
$\omega_{2,0} = \frac{49}{36}$, $\omega_{2,1} = \frac{3}{2}$, $\omega_{2,2} = \frac{3}{20}$, $\omega_{2,3} = \frac{1}{90}$

↪ definition of the first order spatial derivative:

$$\nabla_{l,(\nu)} f(\vec{n}) \equiv \frac{1}{2} \sum_{j=1}^{\nu+1} (-1)^{j+1} \theta_{\nu,j} \Big[f(\vec{n} + j\hat{e}_l) - f(\vec{n} - j\hat{e}_l) \Big]$$

↪ second order spatial derivative:

$$\tilde{\nabla}^2_{l,(\nu)} f(\vec{n}) \equiv - \sum_{j=0}^{\nu+1} (-1)^{j} \omega_{\nu,j} \Big[f(\vec{n} + j\hat{e}_l) + f(\vec{n} - j\hat{e}_l) \Big]$$

has two zeros in per Brillouin zone → beneficial feature for tuning NLO coefficients

↪ improved lattice dispersion relation: $\omega^{(\nu)}(\vec{p}) \equiv \frac{1}{\tilde{m}_N} \sum_{j=0}^{\nu+1} \sum_{l=1}^{3} (-1)^j \omega_{\nu,j} \cos(j p_l)$

$$\boxed{\tilde{m}_N \equiv m_N a}$$

TRANSFER MATRIX METHOD

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

  with Ψ_A a Slater determinant for A free nucleons

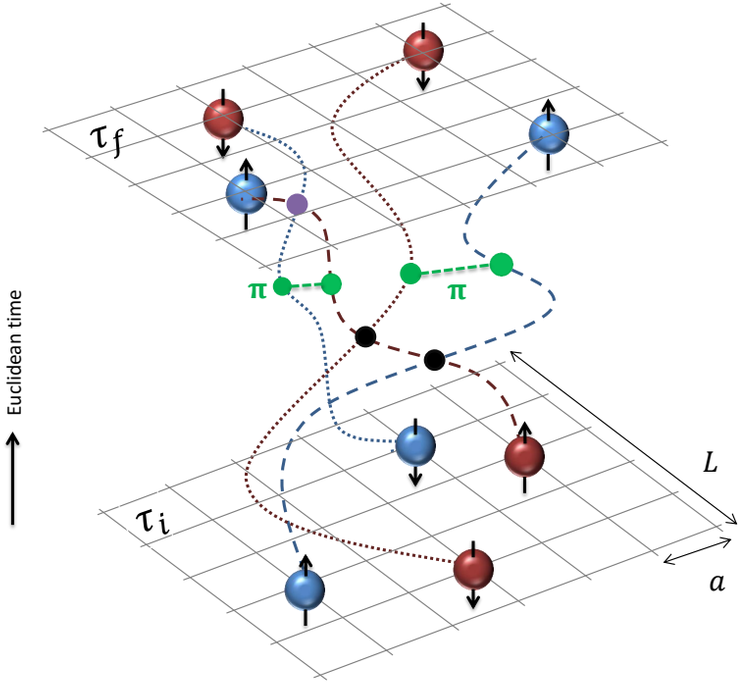
  [or a more sophisticated (correlated) initial/final state]

Euclidean time

- Transient energy

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

$\rightarrow$ ground state: $E_A^0 = \lim_{\tau \to \infty} E_A(\tau)$

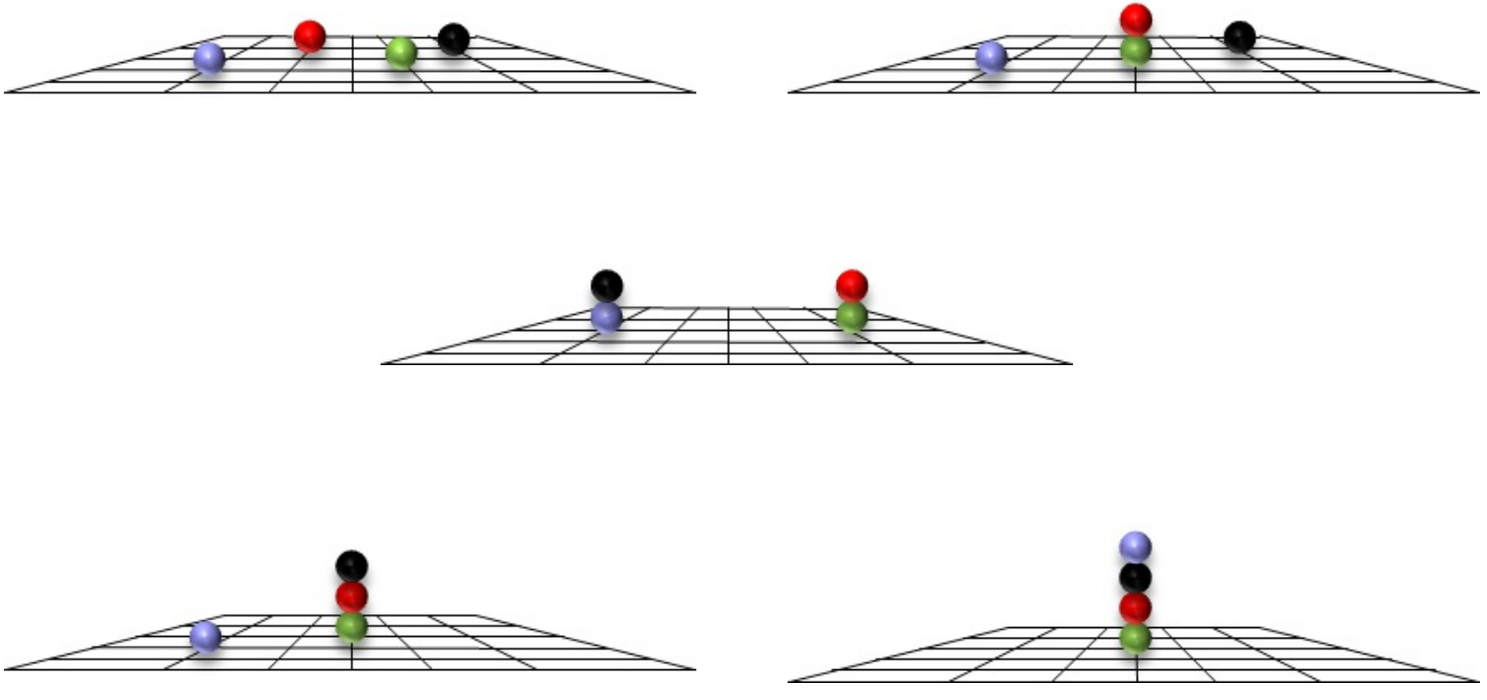


- Exp. value of any normal–ordered operator $\mathcal{O}$

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

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

CONFIGURATIONS



$\Rightarrow$ all *possible* configurations are sampled

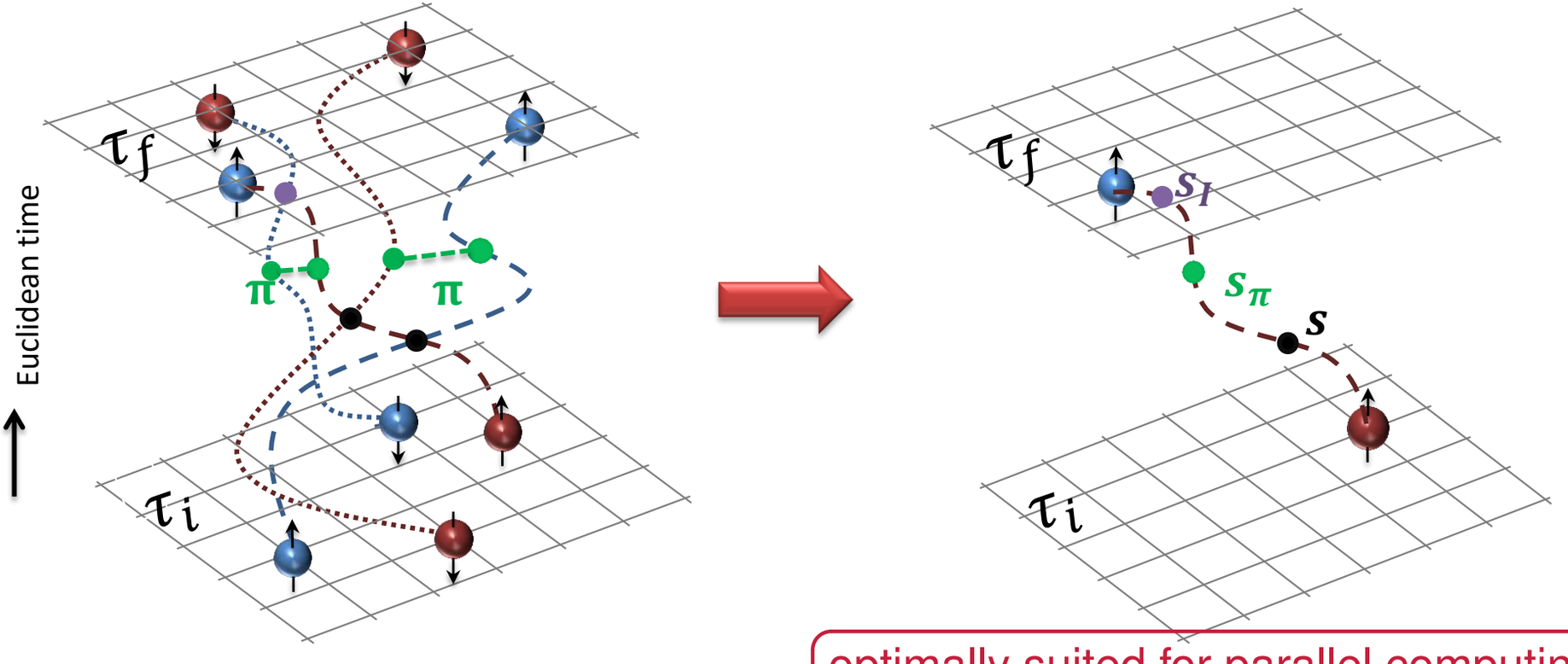
$\Rightarrow$ preparation of *all possible* initial/final states

$\Rightarrow$ *clustering* emerges *naturally*

AUXILIARY FIELD METHOD

- Represent interactions by auxiliary fields:

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



optimally suited for parallel computing!

COMPUTATIONAL EQUIPMENT

- Past = JUQUEEN (BlueGene/Q)
- Present = JUWELS (modular system) + SUMMIT + ...

12 Pflops

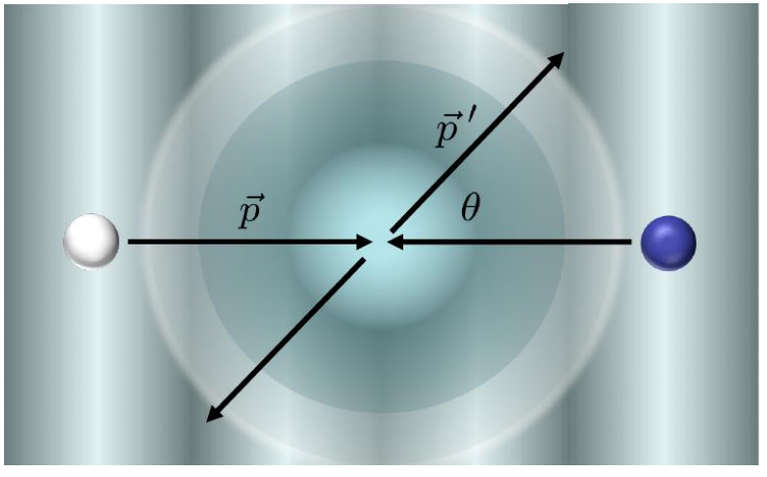
Rotational symmetry on the lattice: Breaking and restoration

spherical wall method: Borasoy, Epelbaum, Krebs, Lee, UGM, EPJA **34** (2007) 185

auxiliary potential method: Lu, Lähde, Lee, UGM, Phys. Lett. B**760** (2016) 309

REMINDER: SCATTERING THEORY

- Two-body scattering theory in the center-of-mass (CMS) frame

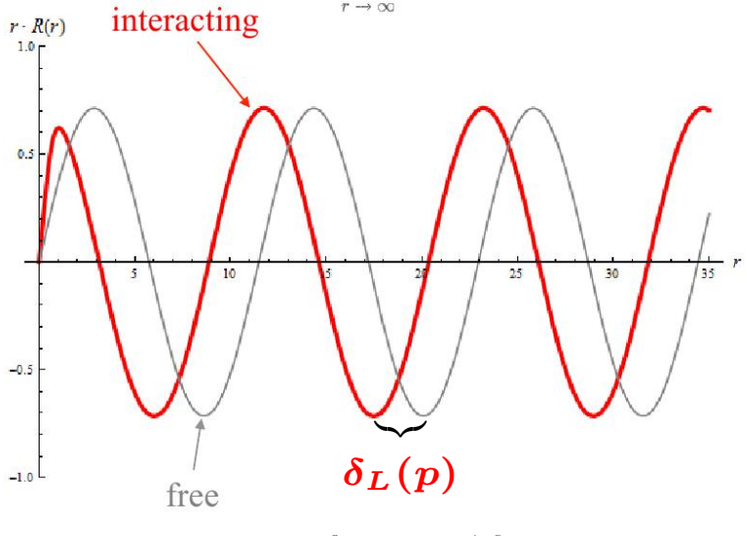


$$\psi(\vec{r}\,) \underset{r\to\infty}{\longrightarrow} \exp(i\vec{p}\cdot\vec{r}) + f(\vec{p}\,',\vec{p})\,\frac{\exp(ipr)}{r}$$

- Phase-shift and partial-wave decomposition:

$$f(\vec{p}\,',\vec{p}) = \sum_{L=0}^{\infty} f_L(p) P_L(\cos\theta)$$

$$f_L(p) = \frac{-i}{2p}\Big[\underbrace{e^{2i\delta_L(p)}}_{S_L(p)} - 1\Big] = \frac{1}{p[\cot\delta_L(p) - i]}$$



- partial wave mixing can also be dealt with in more complex cases → phase shifts & mixing angles

SCATTERING in a FINITE VOLUME

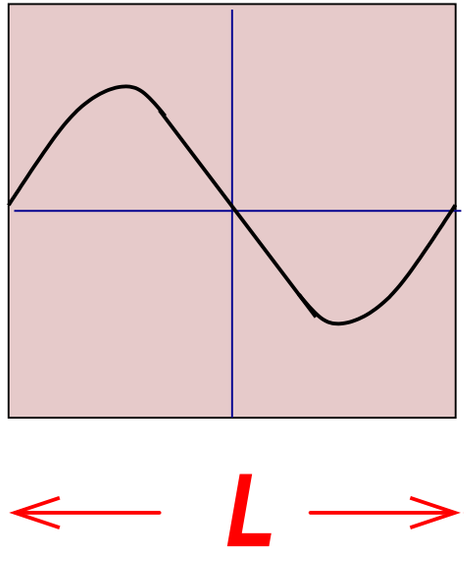
Lüscher, Comm. Math. Phys. **104** (1986) 177; **105** (1986) 153; Nucl. Phys, B **354** (1991) 531

- cubic lattice: rotation group SO(3) broken to SO(3,Z)
- 5 irreducible representations (A_1, T_1, E, T_2, A_2) include definite J modulo 4
- Lüscher's formula for phase shifts ($LM_{\rm light} \gg 1$)

$$\exp(2i\delta_0) = \frac{Z_{00}(1;q^2) + i\pi^{3/2}q}{Z_{00}(1;q^2) - i\pi^{3/2}q}$$

$$q = 2\pi n/L\,, \quad n \in \mathbb{Z}^3$$

$$Z_{00}(s;q^2) = \frac{1}{\sqrt{4\pi}} \sum_{n\in\mathbb{Z}^3} \frac{1}{(n^2-q^2)^s}$$



- standard method in lattice QCD, see e.g. NPLQCD on hadron-hadron scattering

Beane, Orginos, Savage, Int. J. Mod. Phys. E **17** (2008) 1517

- however: not well suited for nuclear physics, need a different formalism

SO(3,Z) REPRESENTATIONS

- Irreducible SO(3,Z) representations

	J_z (mod 4)	$Y_{L,M}(\theta,\phi)$
A_1	0	$Y_{0,0}$
T_1	0, 1, 3	$\{Y_{1,0}, Y_{1,1}, Y_{1,-1}\}$
E	0, 2	$\left\{Y_{2,0}, (Y_{2,-2}+Y_{2,2})/\sqrt{2}\right\}$
T_2	1, 2, 3	$\left\{Y_{2,1}, (Y_{2,-2}-Y_{2,2})/\sqrt{2}, Y_{2,-1}\right\}$
A_2	2	$\left\{(Y_{3,2}-Y_{3,-2})/\sqrt{2}\right\}$

- SO(3,Z) decompositions

SO(3)	SO(3,Z)
$J=0$	A_1
$J=1$	T_1
$J=2$	$E \oplus T_2$
$J=3$	$T_1 \oplus T_2 \oplus A_2$

SO(3)	SO(3,Z)
$J=4$	$A_1 \oplus T_1 \oplus E \oplus T_2$
$J=5$	$T_1 \oplus T_1 \oplus E \oplus T_2$
$J=6$	$A_1 \oplus T_1 \oplus E \oplus T_2 \oplus T_2 \oplus A_2$
$J=7$	$T_1 \oplus T_1 \oplus E \oplus T_2 \oplus T_2 \oplus A_2$

SPHERICAL WALL METHOD

Borasoy, Epelbaum, Krebs, Lee, M., Eur. Phys. J. **A 34** (2007) 185

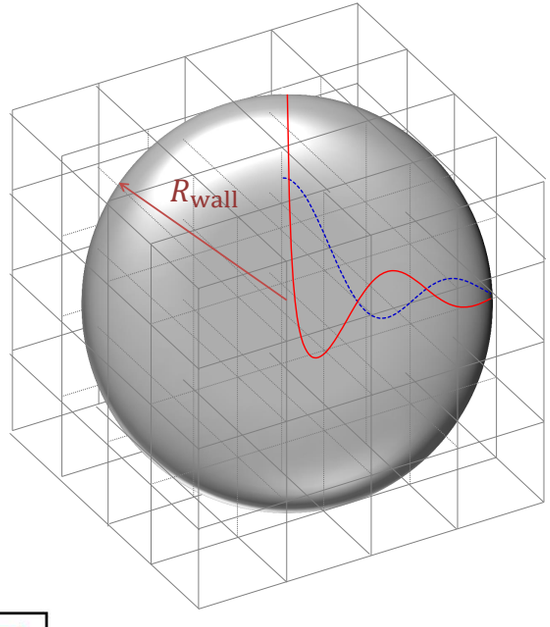
see also: Carlson et al., Nucl. Phys. **A 424** (1984) 47

- Spherical wall method:

  place a wall at sufficiently large R

  $\rightarrow$ standing wave allows to extract phase shifts δ_L

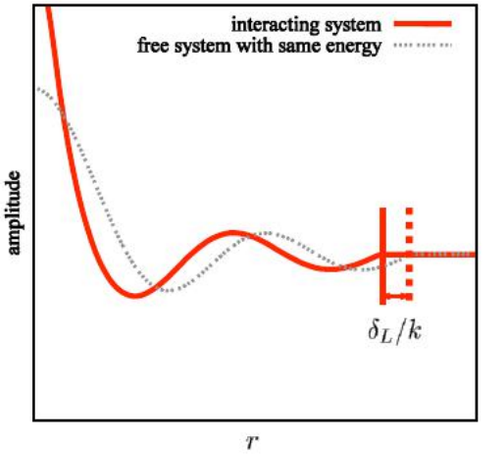
  and mixings ϵ_L



$$\Psi(\vec{r}\,) = [\cos\delta_L j_L(kr) - \sin\delta_L y_L(kr)]Y_{L,m}(\theta,\phi)$$

$$\Psi(R) = 0 \Rightarrow \boxed{\tan\delta_L = \frac{j_L(kR)}{y_L(kR)}}$$

(similar for triplet case)



MEASURING PHASE SHIFTS on the LATTICE II

- Toy model: attractive Gaussian potential w/ central & tensor forces

  reproduces continuum phase shifts accurately

  extra copies of the 2-particle interaction due to periodic b.c. removed

  much better than standard boxes

$$V(r) = C\left\{1 + \frac{r^2}{R_0^2}\, S_{12}(\hat{r})\right\} \exp\left(-\frac{1}{2}\frac{r^2}{R_0^2}\right)$$

$$S_{12}(\hat{r}) = 3(\hat{r}\cdot\vec{\sigma}_1)(\hat{r}\cdot\vec{\sigma}_2) - \vec{\sigma}_1\cdot\vec{\sigma}_2$$

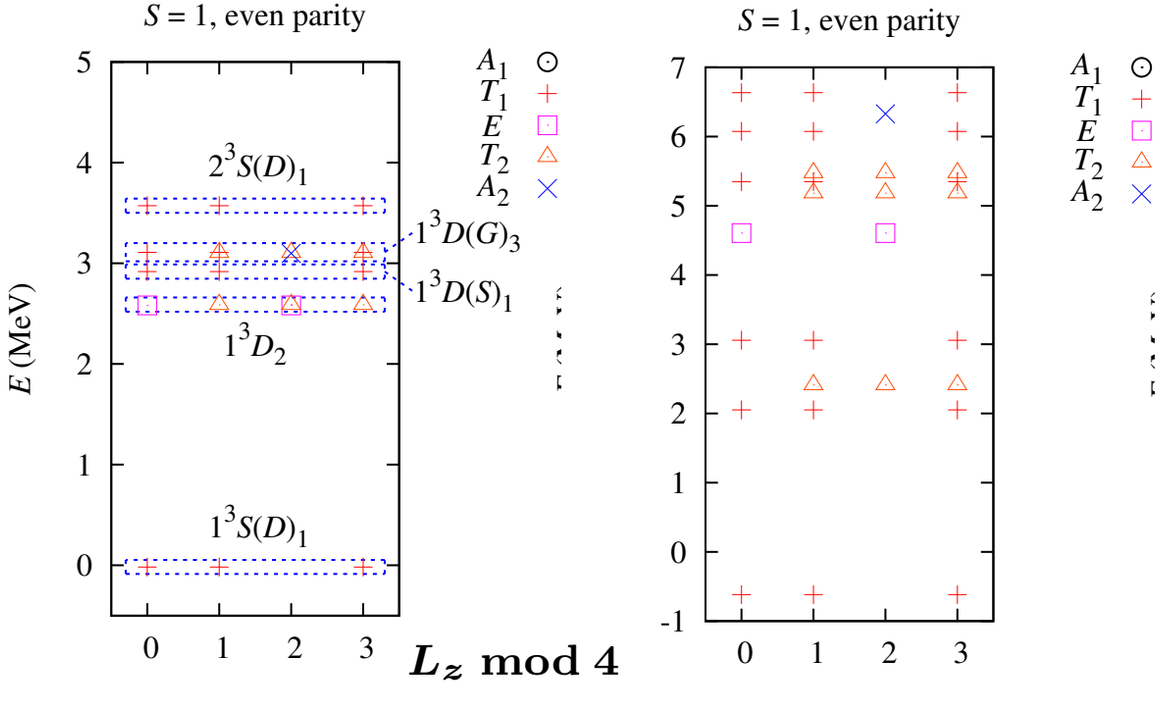
$$C = -2\,\text{MeV}, \quad R_0 = 0.02\,\text{MeV}^{-1}$$

$$m = 938.92\,\text{MeV}$$

$\Downarrow$

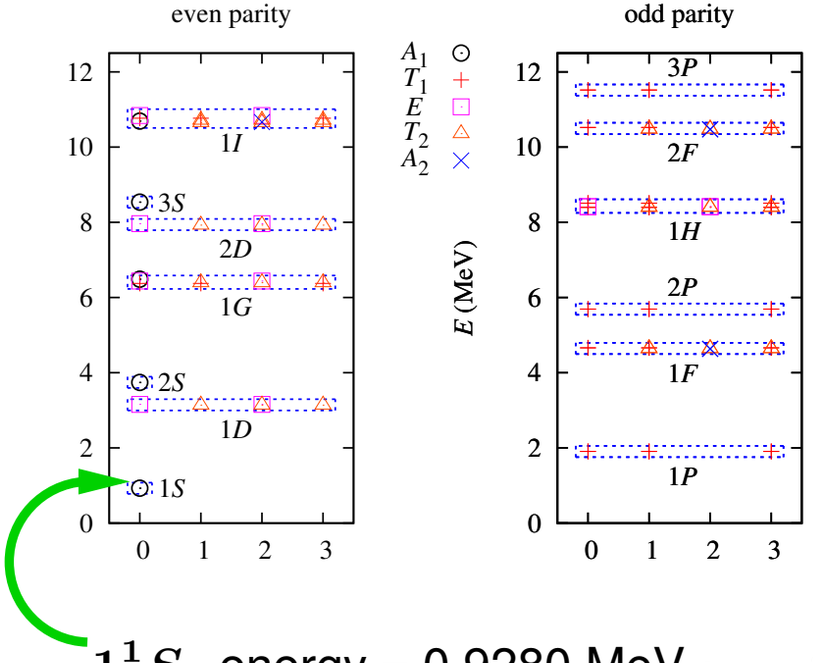
a shallow bound-state in the ${}^3S_1$-${}^3D_1$ channel with a binding energy of -0.155 MeV

$R = 10 + \epsilon$ vs $V = 12^3$



MEASURING PHASE SHIFTS on the LATTICE II

- Free particle spectrum for $R = 10 + \epsilon$



1^1S_0 energy = 0.9280 MeV $[E = k^2/m]$

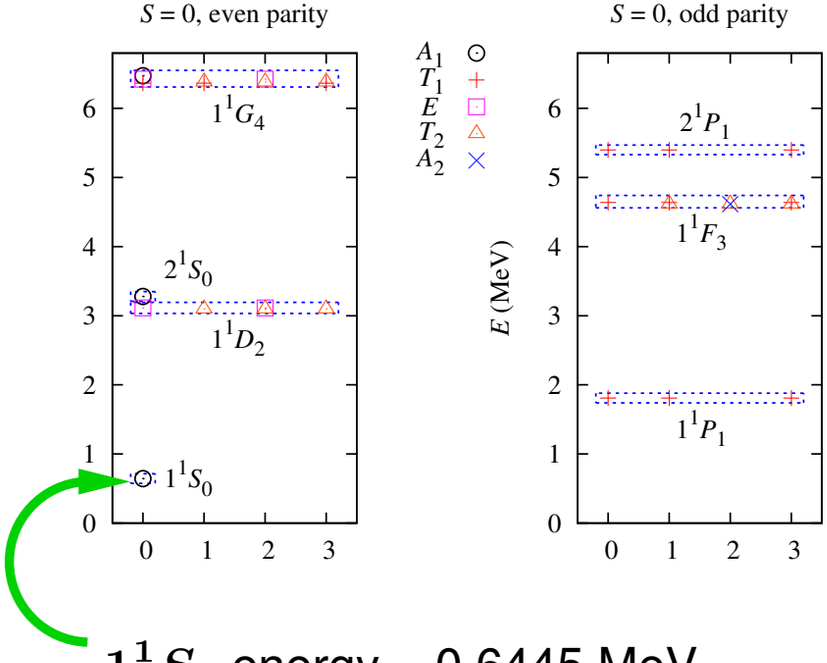
$\Downarrow$

$k_{\rm free} = 29.52$ Mev, $j_0(k_{\rm free} R) = 0$

$\Downarrow$

$$R = \frac{\pi}{k_{\rm free}} = 0.1064\,{\rm MeV}^{-1}$$

- Interacting spectrum for $S = 0$



L_z mod 4

1^1S_0 energy = 0.6445 MeV

$\Downarrow$

$k = 24.60$ MeV

$\Downarrow$

$$\delta(^1S_0) = \tan^{-1}\left[\frac{j_0(kR)}{y_0(kR)}\right] = 30^\circ$$

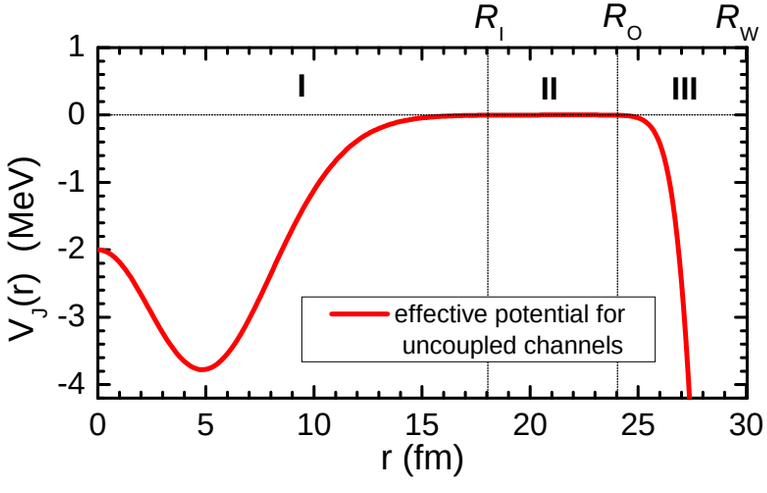
AUXILIARY POTENTIAL METHOD

Lu, Lähde, Lee, UGM, Phys. Lett. **B 760** (2016) 309

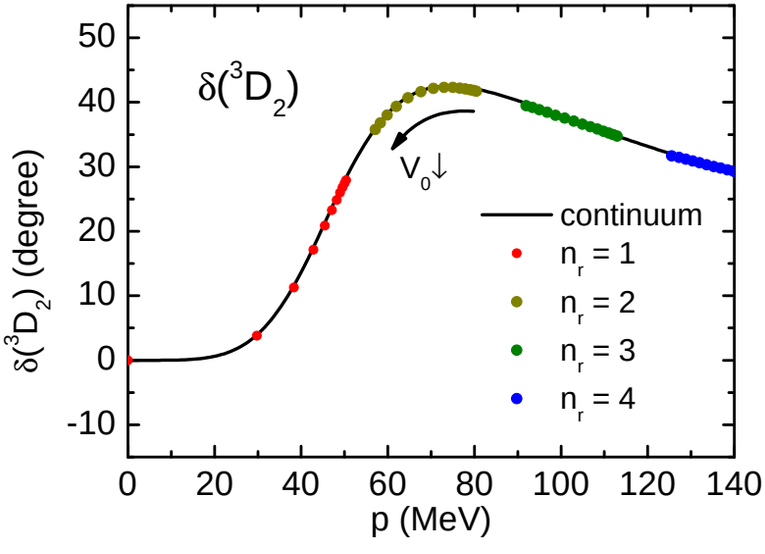
- Spherical wall: small energies require large volumes, accuracy limited
- Improved method: auxiliary potential $\rightarrow$ shift energy levels

$$V_{\rm aux} = V_0 \exp\left[-(r - R_W)^2/a^2\right] \ , \quad R_0 \leq r \leq R_W$$

- Single channel potential ($V_0 = -25$ MeV)



- typical phase shift



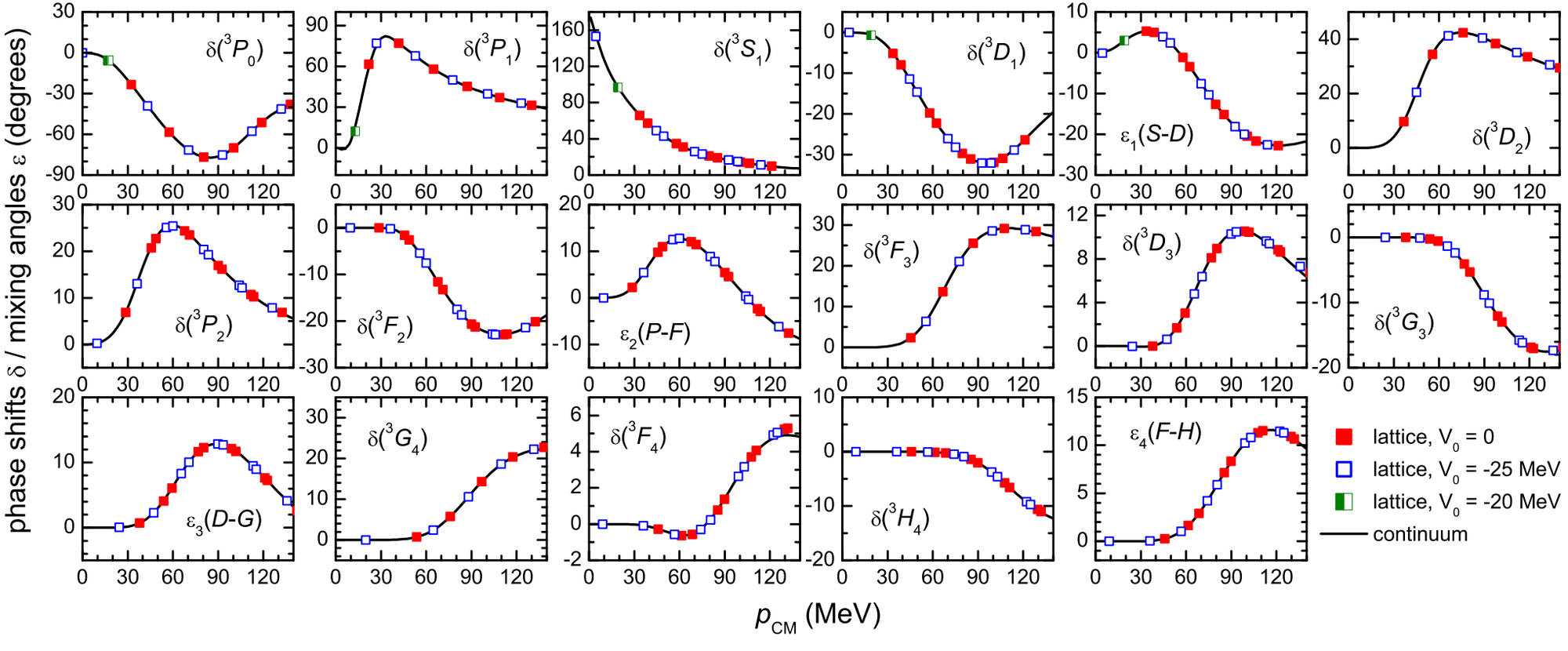
- Extension to coupled channels requires time-reversal symmetry breaking

$\hookrightarrow$ details see in the above reference

AUXILIARY POTENTIAL METHOD: RESULTS

Lu, Lähde, Lee, UGM, Phys. Lett. **B 760** (2016) 309

- same toy model with $R_I = 9.02a, R_0 = 12.02a, R_W = 15.02a$ and $U_0 = 20.0$ MeV
- continuum results from solving the LS equation



ROTATIONAL SYMMETRY BREAKING OPERATORS

- SO(3) $\to$ SO(3,Z): new operators at NLO $O(Q^2)$:

$$\sum_{l=1}^{3} q_l^2 \, (\sigma_A)_l \, (\sigma_B)_l \, , \quad (\tau_A \cdot \tau_B) \sum_{l=1}^{3} q_l^2 \, (\sigma_A)_l \, (\sigma_B)_l$$

$\to$ terms with total spin $S = 0, 2, 4$. $S = 0$ terms already included in NLO contact operators. Others introduce unphysical mixing such as ${}^3D_3$ into ${}^3S_1 - {}^3D_1$

$\to$ introduce two lattice operators

$$\tilde{V}_{R1} = \tfrac{1}{2} \, \tilde{C}_{R1} : \sum_{S=1}^{3} \sum_{\vec{n}} \left[\nabla_{S,(\nu)} \rho_S^{a^\dagger,a}(\vec{n}) \right] \nabla_{S,(\nu)} \rho_S^{a^\dagger,a}(\vec{n}) :$$

$$\tilde{V}_{R2} = \tfrac{1}{2} \, \tilde{C}_{R2} : \sum_{S=1}^{3} \sum_{I=1}^{3} \sum_{\vec{n}} \left[\nabla_{S,(\nu)} \rho_{S,I}^{a^\dagger,a}(\vec{n}) \right] \nabla_{S,(\nu)} \rho_{S,I}^{a^\dagger,a}(\vec{n}) :$$

$\to$ adjust the isoscalar combination of these terms to eliminate the unphysical mixing of the ${}^3D_3$ partial wave. The isovector combination is set to zero (unphysical mixing tiny)

- also rotational symmetry breaking terms in the OPE, can be dealt with by a perturbative improvement of the πN coupling

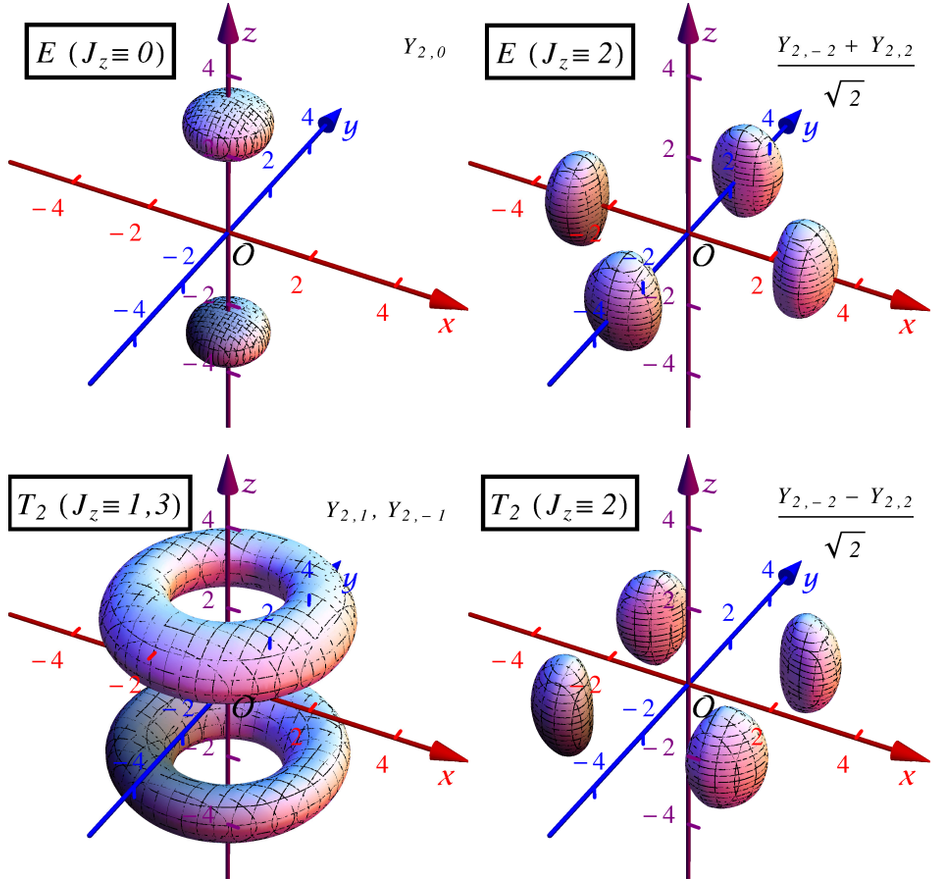
FURTHER ROTATIONAL SYMMETRY BREAKING

- The $2J+1$ magnetic quantum number degeneracy is broken:

$$\mathcal{H}_{J=0} = A_1$$
$$\mathcal{H}_{J=1} = T_1$$
$$\mathcal{H}_{J=2} = E \oplus T_2$$
$$\mathcal{H}_{J=0} = A_2 \oplus T_1 \oplus T_2$$

- The $J=2$ eigenfunctions are:

$$\mathcal{H}_{J=2} = E \left[\sqrt{\tfrac{1}{2}}Y_{2,2} + \sqrt{\tfrac{1}{2}}Y_{2,-2}, Y_{2,0}\right] \oplus T_2 \left[\sqrt{\tfrac{1}{2}}Y_{2,2} - \sqrt{\tfrac{1}{2}}Y_{2,-2}, Y_{2,\pm 1}\right]$$



⇒ Detailed studies in cluster models

FURTHER ROTATIONAL SYMMETRY BREAKING cont'd

- Improved kinetic energy/dispersion relation

  $\rightarrow$ standard use in NLEFT (discussed before)

- Further methods developed in cluster models:

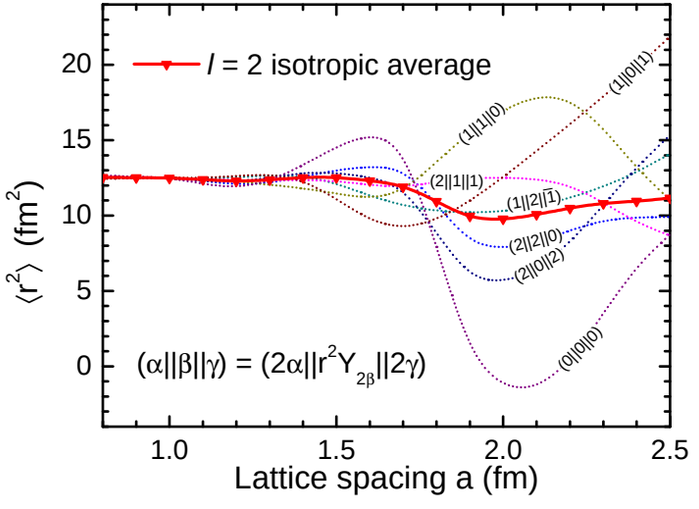
  – weighted average for the energy

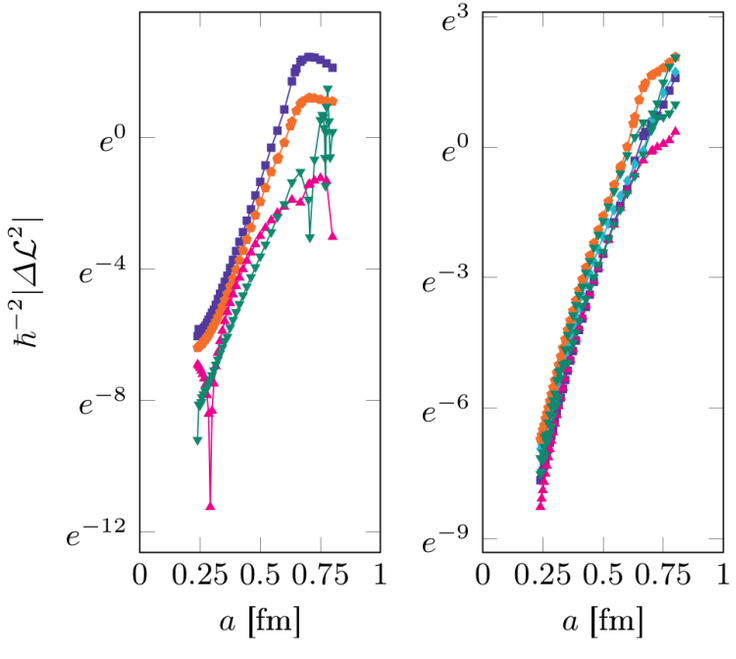
  – orientation average for tensor ops

  Ex: quadrupole moment $\langle r^2 Y_{2\mu} \rangle$ of ^{12}C

  – finite volume angular momentum corrections

  Ex: squared ang. mom. in ^{8}Be $(4_2^+, 6_2^+)$





Lu, Lähde, Lee, UGM, Phys. Rev. **D90** (2014) 034507

Lu, Lähde, Lee, UGM, Phys. Rev. **D92** (2015) 014506

Stellin, Elhatisari, UGM, EPJA **54** (2018) 232

Galilean invarince on the lattice: Breaking and restoration

NN system: Li, Elhatisari, Epelbaum, Lu, Lee, UGM, [arXiv:1902.01295]

pinhole algorithm: Elhatisari, Epelbaum, Krebs, Lähde, Lee, Li, Lu, UGM, Rupak, Phys. Rev. Lett. **119** (2017) 222505

GALILEAN INVARIANCE BREAKING: NN SYSTEM

- Consider np scattering first with total momentum $\vec{P} = \mathbf{0}$, match to Nijmegen PWA
- then boost to a moving frame with $\vec{P} = (2\pi/L)\vec{k}$

$\Rightarrow$ if the results are different, then there is Galilean invariance breaking $\rightarrow$slide

- introduce operators to compensate for GIB (up-to-next-to-next-to-nearest neighbors)

$$
\begin{aligned}
V_{\rm GIR} &= V^0_{\rm GIR} + V^1_{\rm GIR} + V^2_{\rm GIR} \\
V^0_{\rm GIR} &= C^0_{\rm GIR} \sum_{\mathbf{n},i,j,i',j'} a^\dagger_{i,j}(\mathbf{n}) a^\dagger_{i',j'}(\mathbf{n}) a_{i',j'}(\mathbf{n}) a_{i,j}(\mathbf{n} \\
V^1_{\rm GIR} &= C^1_{\rm GIR} \sum_{\mathbf{n},i,j,i',j'} \sum_{|\mathbf{n}'|=1} a^\dagger_{i,j}(\mathbf{n}+\mathbf{n}') a^\dagger_{i',j'}(\mathbf{n}+\mathbf{n}') a_{i',j'}(\mathbf{n}) a_{i,j}(\mathbf{n}) \\
V^2_{\rm GIR} &= C^2_{\rm GIR} \sum_{\mathbf{n},i,j,i',j'} \sum_{|\mathbf{n}'|=\sqrt{2}} a^\dagger_{i,j}(\mathbf{n}+\mathbf{n}') a^\dagger_{i',j'}(\mathbf{n}+\mathbf{n}') a_{i',j'}(\mathbf{n}) a_{i,j}(\mathbf{n})
\end{aligned}
$$

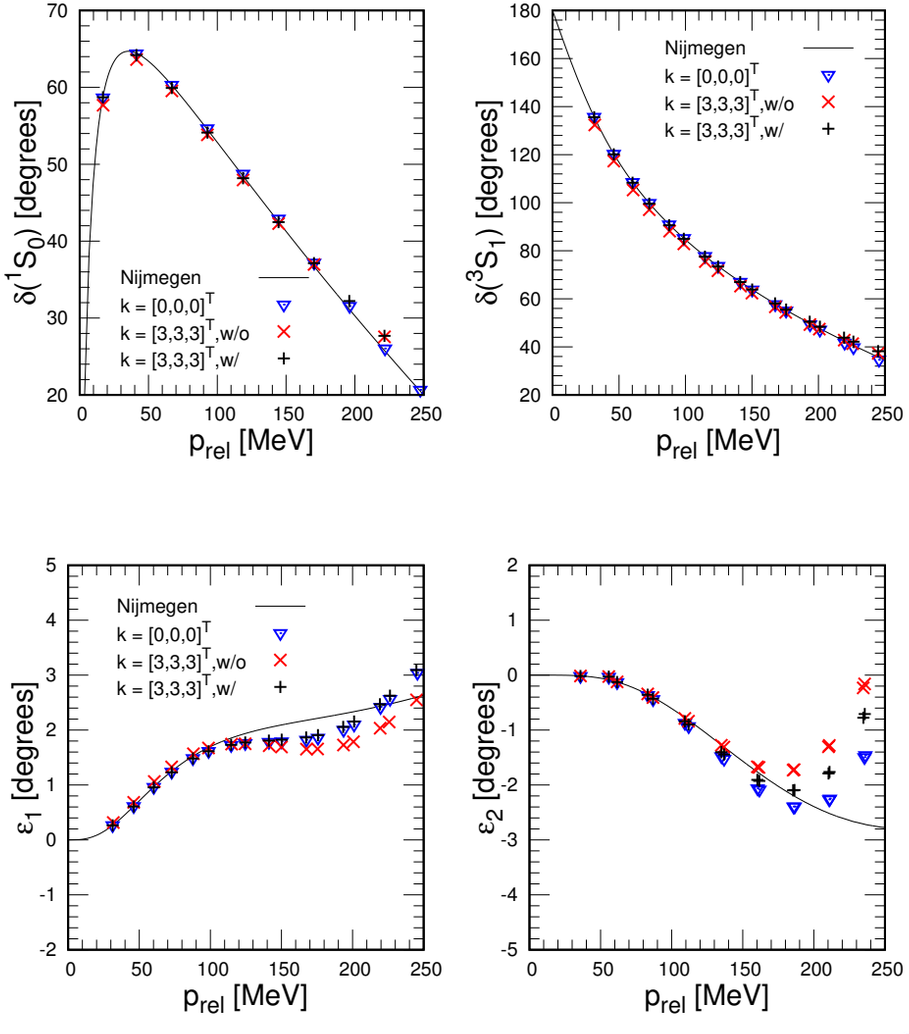
- restore GI by fixing the coefficients (in each partial wave such that)

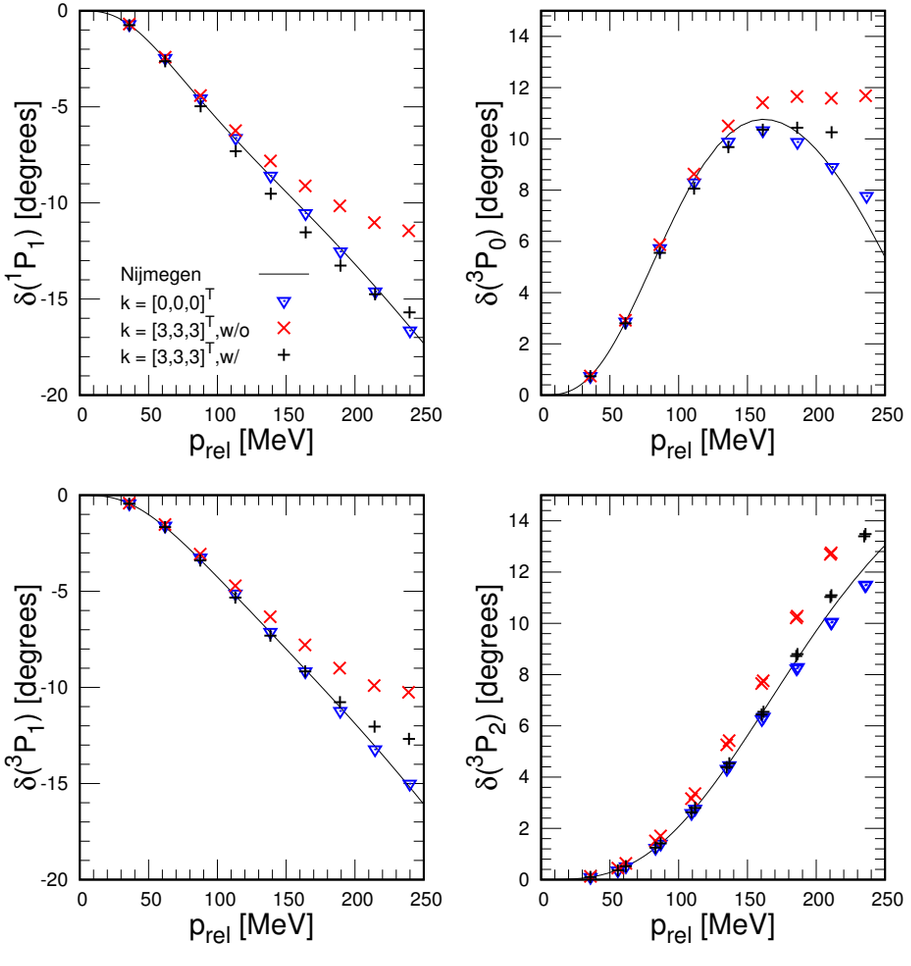
$$
\boxed{C^0_{\rm GIR} + 6C^1_{\rm GIR} + 12C^2_{\rm GIR} = 0}
$$

BREAKING and RESTORATION of GALILEAN INV.

- Consider highly smeared N3LO interactions,

  compare rest-frame $\boldsymbol{k} = [\mathbf{0}, \mathbf{0}, \mathbf{0}]$ with moving frame $\boldsymbol{k} = [\mathbf{3}, \mathbf{3}, \mathbf{3}]$

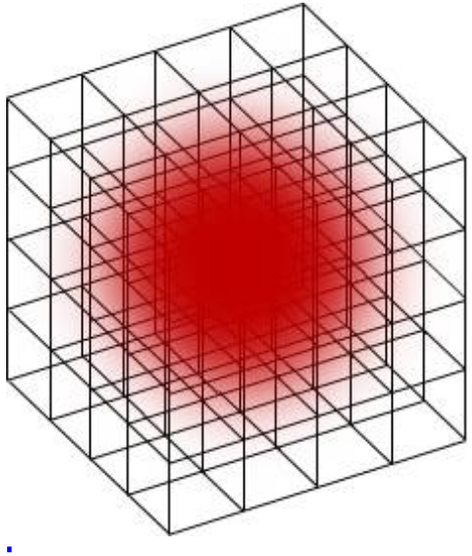




$\Rightarrow$ effects i.g. small but must be taken care of

CENTER-of-MASS PROBLEM

- AFQMC calculations involve states that are superpositions of many different center-of-mass (com) positions



$$Z_A(\tau) = \langle \Psi_A(\tau) | \Psi_A(\tau) \rangle$$

$$|\Psi_A(\tau)\rangle = \exp(-H\tau/2) |\Psi_A\rangle$$

- but: translational invariance requires summation over all transitions

$$Z_A(\tau) = \sum_{i_{\rm com}, j_{\rm com}} \langle \Psi_A(\tau, i_{\rm com}) | \Psi_A(\tau, j_{\rm com}) \rangle \,, \quad {\rm com} = {\rm mod}((i_{\rm com} - j_{\rm com}), L)$$

$i_{\rm com}$ $(j_{\rm com})$ = position of the center-of-mass in the final (initial) state

$\rightarrow$ density distributions of nucleons can not be computed directly, only moments

$\rightarrow$ need to overcome this deficieny

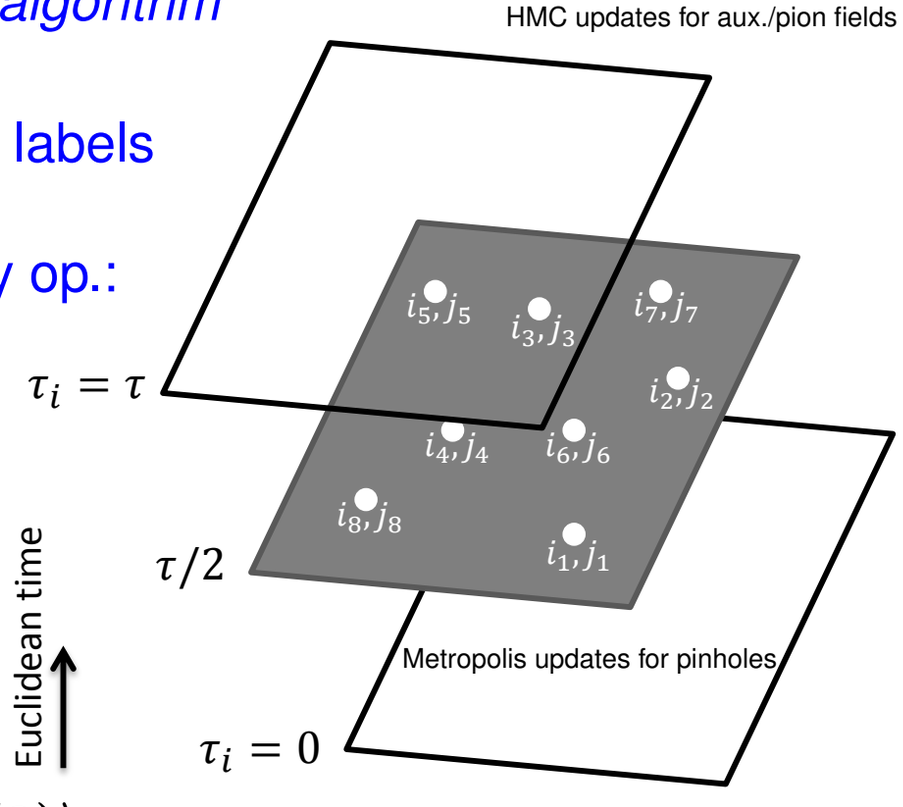
PINHOLE ALGORITHM

- Solution to the CM-problem:

  track the individual nucleons using the *pinhole algorithm*

- Insert a screen with pinholes with spin & isospin labels that allows nucleons with corresponding spin & isospin to pass = insertion of the A-body density op.:

$$\rho_{i_1,j_1,\cdots i_A,j_A}(\mathbf{n}_1,\cdots \mathbf{n}_A) =: \rho_{i_1,j_1}(\mathbf{n}_1)\cdots\rho_{i_A,j_A}(\mathbf{n}_A):$$



- MC sampling of the amplitude:

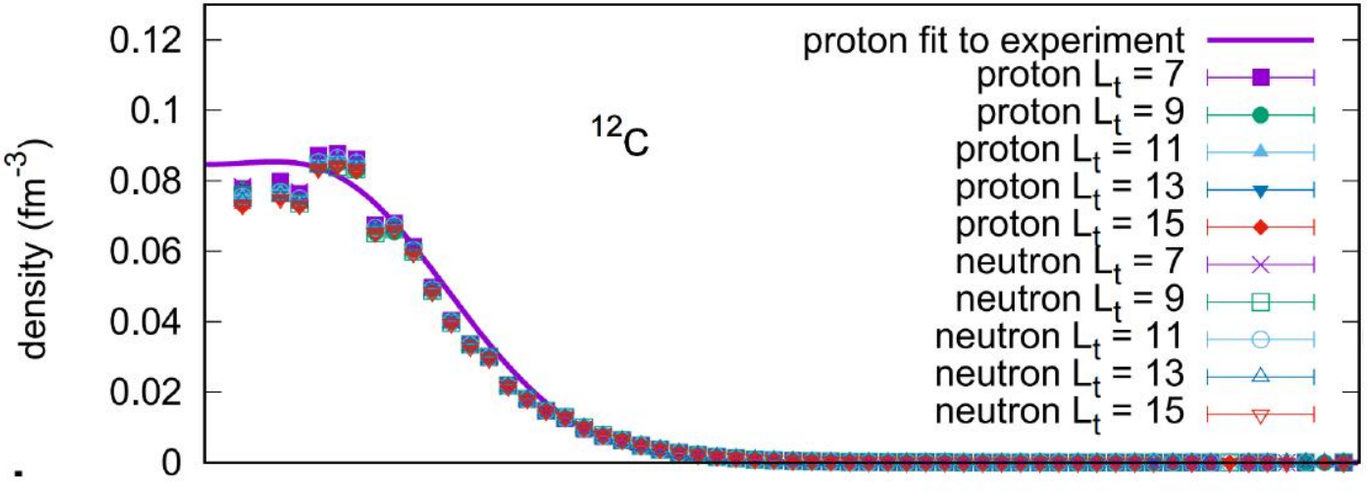
$$A_{i_1,j_1,\cdots i_A,j_A}(\mathbf{n}_1,\ldots,\mathbf{n}_A,L_t) = \langle\Psi_A(\tau/2)|\rho_{i_1,j_1,\cdots i_A,j_A}(\mathbf{n}_1,\ldots,\mathbf{n}_A)|\Psi_A(\tau/2)\rangle$$

- Allows to measure proton and neutron distributions

- Resolution scale $\sim a/A$ as cm position $\mathbf{r}_{\mathbf{cm}}$ is an integer $\mathbf{n}_{\mathbf{cm}}$ times a/A

PROTON and NEUTRON DENSITIES in CARBON

- first NLEFT calculation of the charge density in ^{12}C [proton size accounted for]
- asymptotic properties of the distributions from the volume dependence of N-body bound states König, Lee, Phys. Lett. B779 (2018) 9
- open symbols: neutron / closed symbols: proton

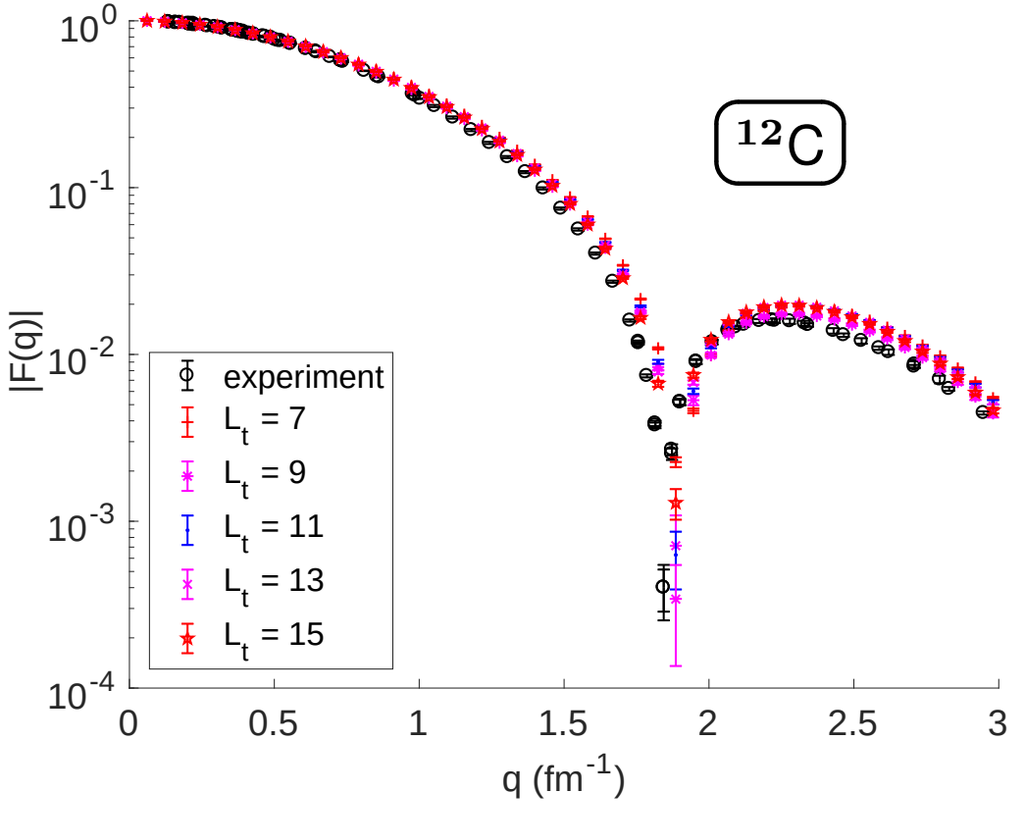


$\Rightarrow$ independent of projection time $\rightarrow$ ground state

$\Rightarrow$ small error bars $\rightarrow$ sign problem under control

FORM FACTORS

- Fit charge distributions by a Wood-Saxon shape
  ↪ get the form factor from the Fourier-transform (FT)
  ↪ uncertainties from a direct FT of the lattice data



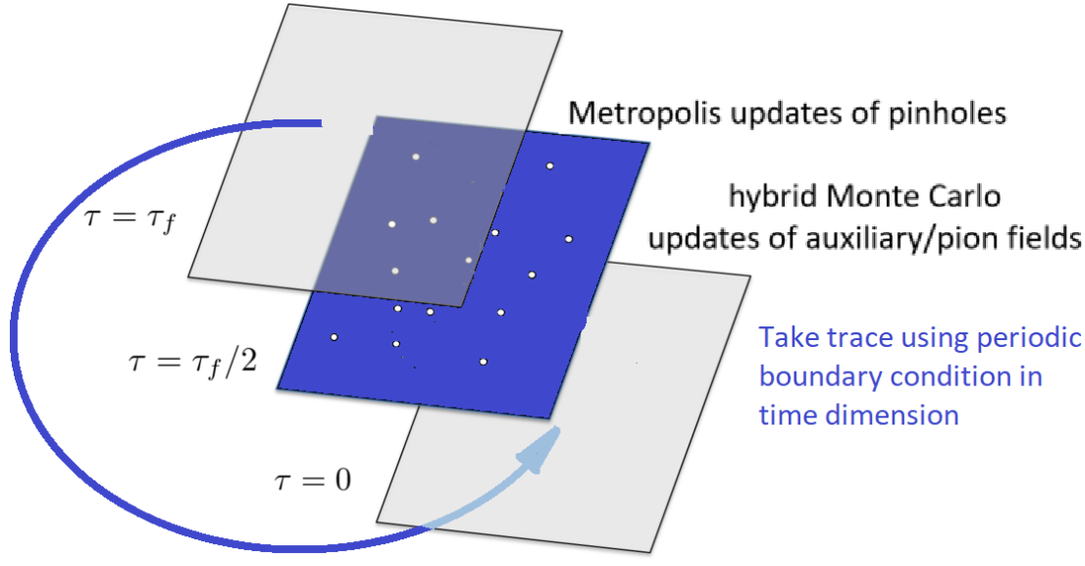
⇒ detailed structure studies become possible

Nuclear Thermodynamics

B. N. Lu, D. Lee, UGM, et al., *in preparation*

TRACE PINHOLE ALGORITHM

- The pinhole states span the whole A-body Hilbert space
- The canonical partition function can be expressed using pinholes:



$$Z_A = \mathrm{Tr}_A\left[\exp(-\beta H)\right], \ \beta = 1/T$$

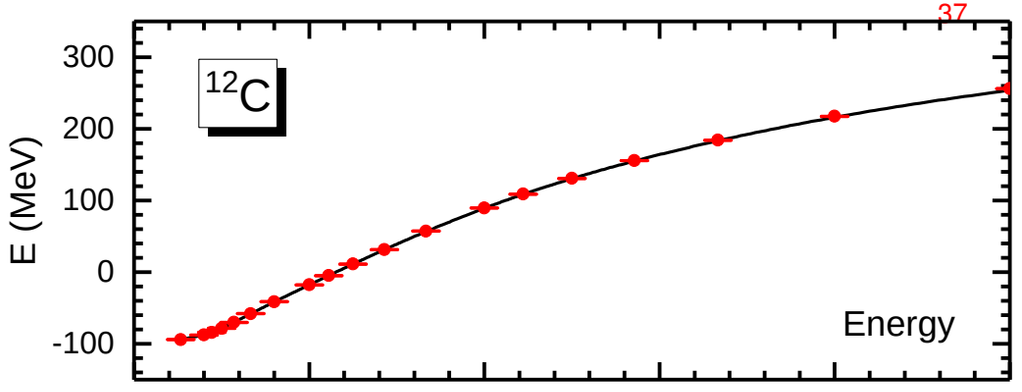
$$= \sum_{n_1,\cdots,n_A} \int \mathcal{D}s\mathcal{D}\pi \langle n_1,\cdots,n_A|\exp[-\beta H(s,\pi)]|n_1,\cdots,n_A\rangle$$

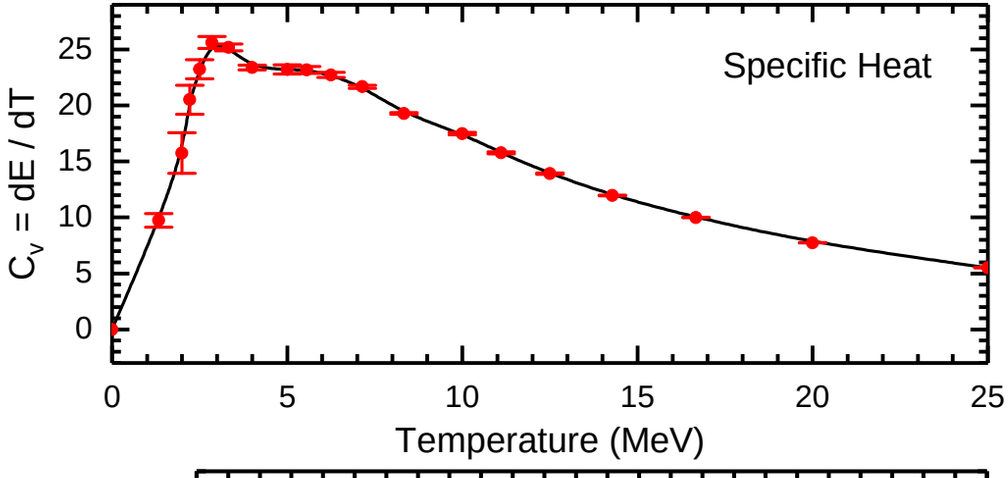
- allows to study: liquid-gas phase transition at $T \simeq 10$ MeV
  thermodynamics of finite nuclei
  thermal dissociation of hot nuclei
  cluster yields of dissociating nuclei

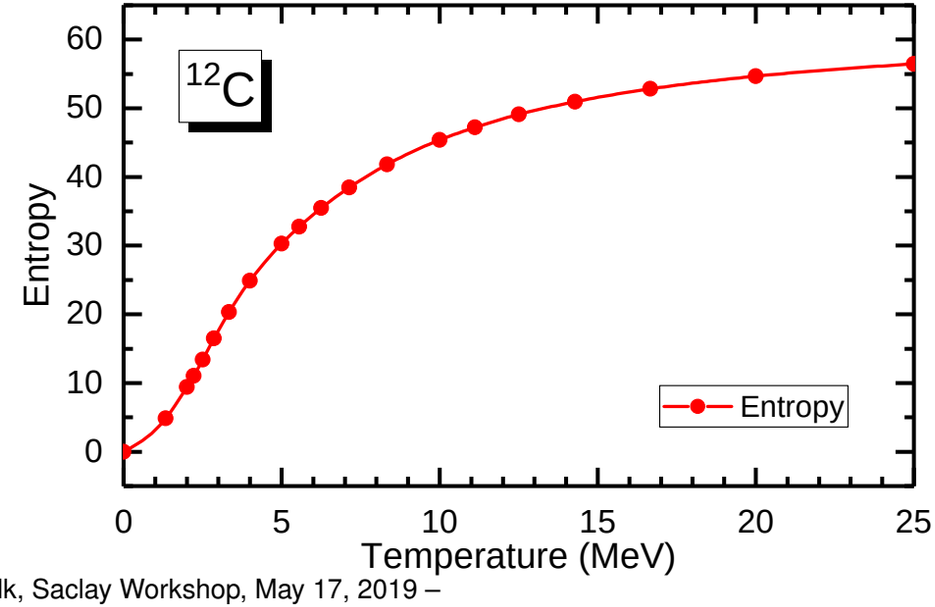
HOT CARBON in a BOX

- 6 protons and 6 neutrons in a box with $L = 12$ fm w/periodic b.c.
- specific heat peaks at $T = 3.3$ MeV
- rise of the entropy w/ temperature, saturates at $T \simeq 25$ MeV
- similar behavior of the level density
- liquid to alpha-particle gas transition smeared due to finite size effects

$\rightarrow$ look at this in more detail

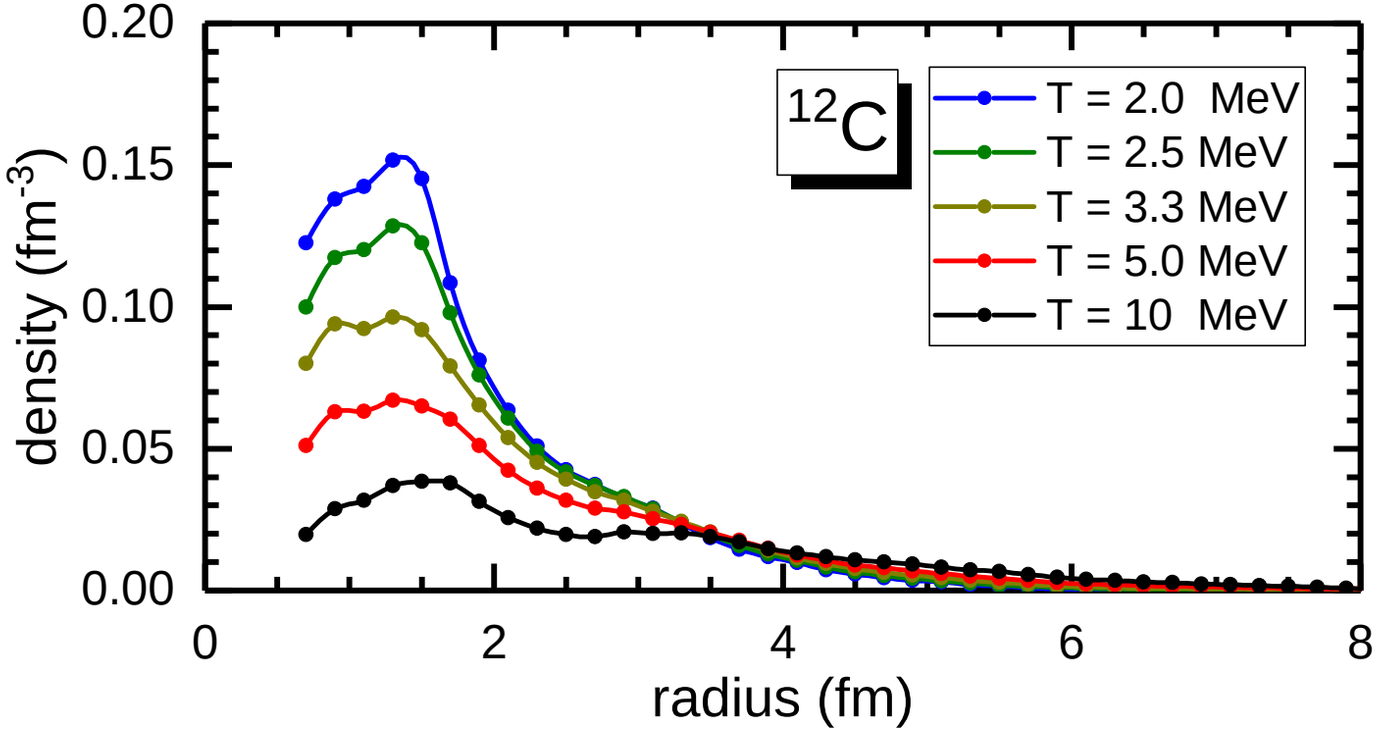






HOT CARBON in a BOX: DENSITY PROFILE

- intrinsic density profile collapses w/ increasing temperature
- α-clusters evaporate form the liquid drop
- radius increases gradually, evidencing a smeared phase transition



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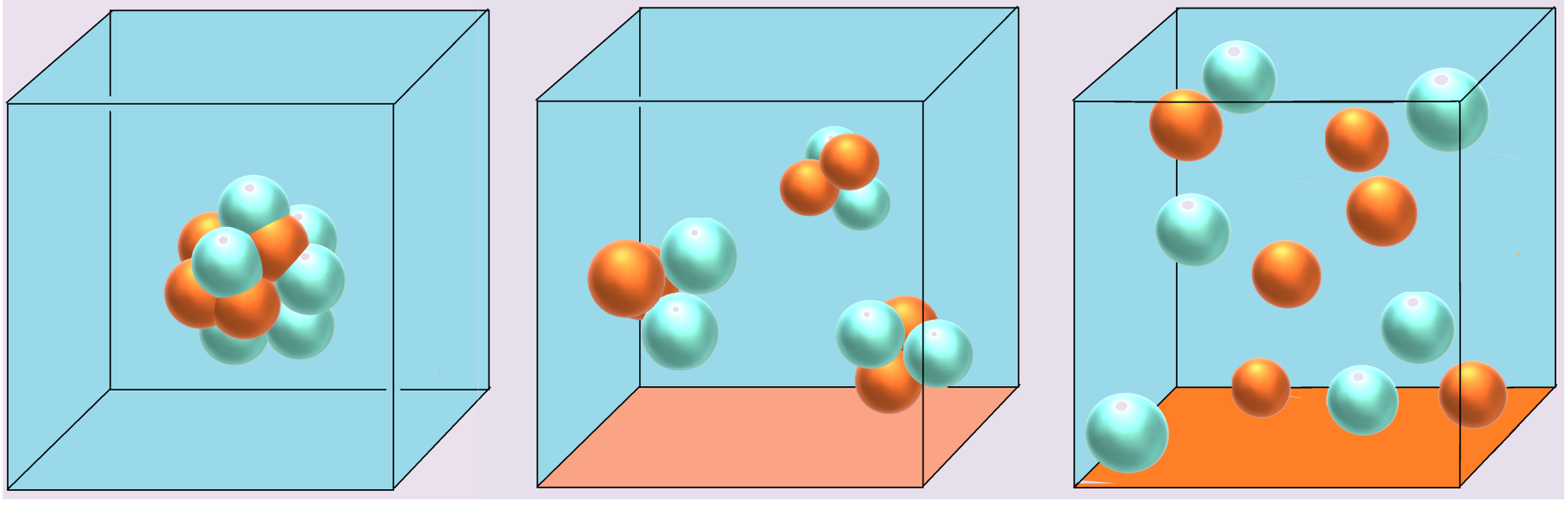
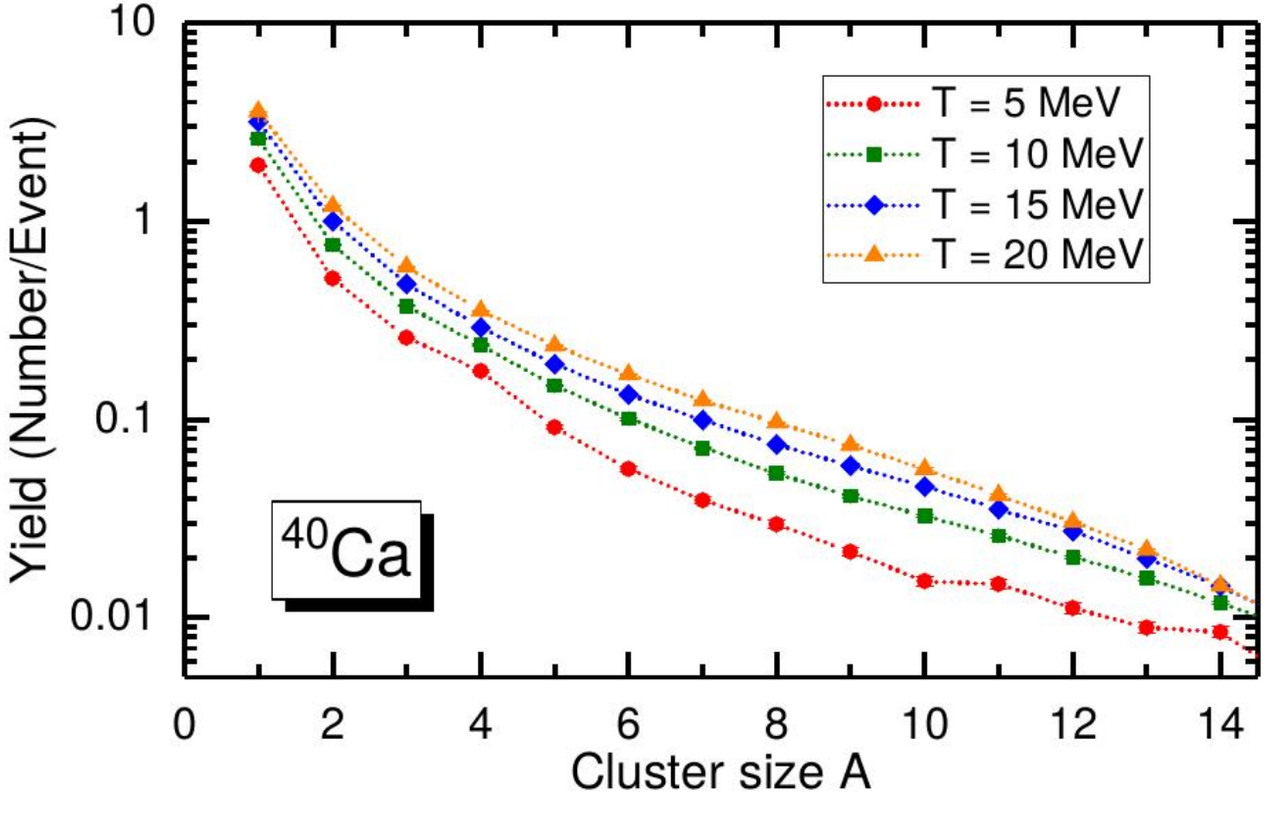


$\rightarrow$ similar results for ^{16}O and ^{40}Ca

HOT CALCIUM in a BOX: CLUSTER YIELDS

- A hot nucleus is hard to detect, can not control temperature, pressure etc
- but we can measure cluster yields in nuclear collisions
- *ab initio* calculation of the cluster yields of ^{40}Ca:



SUMMARY & OUTLOOK

- Nuclear lattice simulations: a new quantum many-body approach
  - → based on the successful continuum nuclear chiral EFT
  - → a number of highly visible results already obtained
- Rotational symmetry breaking and its consequences
  - → scattering can be treated using the spherical wall & aux. potential method
  - → cures: improvement, averaging over multiplets and unphysical operators
- Galilean invariance breaking and its consequences
  - → GIR operators in the two-nucleon system
  - → COM problem in AFQMC calculations: pinhole algorithm to the rescue
- Nuclear thermodynamics
  - → partition function via the trace pinhole algorithm
  - → first promising results for nuclei at finite temperature

SPARES

COULOMB INTERACTION

- Proton-proton repulsion in coordinate space:

$$\mathcal{A}[V_{\rm em}] = \frac{\alpha_{\rm EM}}{r} \left(\frac{1+\tau_3}{2}\right)_A \left(\frac{1+\tau_3}{2}\right)_B , \; \alpha_{\rm EM} \simeq 1/137$$

- Lattice operator:

$$\tilde{V}_{\rm em} = \frac{1}{2} : \sum_{\vec{n},\vec{n}'} \frac{\alpha_{\rm em}}{R(\vec{n}-\vec{n}')} \frac{1}{4} \left[\rho^{a^\dagger,a}(\vec{n}) + \rho^{a^\dagger,a}_{I=3}(\vec{n})\right] \left[\rho^{a^\dagger,a}(\vec{n}') + \rho^{a^\dagger,a}_{I=3}(\vec{n}')\right] :$$

$$R(\vec{n}) = \max(1/2, |\vec{n}|)$$

$\rightarrow$ effect of two protons on the same site **not** observable, $R(\vec{n}) = |\vec{n}|$ absorbed in pp contact term

$\rightarrow$ include pp and nn contact terms to allow for $a_{np} \neq a_{nn} \neq a_{pp}$ & other IB terms

$$\mathcal{A}[V_{nn}] = C_{nn} \left(\frac{1-\tau_3}{2}\right)_A \left(\frac{1-\tau_3}{2}\right)_B , \;\; \mathcal{A}[V_{pp}] = C_{pp} \left(\frac{1+\tau_3}{2}\right)_A \left(\frac{1+\tau_3}{2}\right)_B$$

HYBRID MONTE CARLO

Duane et al., Phys. Lett. B **195** (1986) 216

- apply hybrid MC to fields s, s_I, π_I for the calculation of the path-integral

- introduce conjugate fields p_{π_I}, p_s, p_{S_I}

$$H_{HMC} = \frac{1}{2} \sum_{I,\vec{n}} \left(p^2_{\pi_I}(\vec{n}\,) + p^2_s(\vec{n}\,) + p^2_{s_I}(\vec{n}\,) \right) + V(\pi_I, s, s_I)$$

$$V(\pi_I, s, s_I) = S_{\pi\pi} + S_{ss} - \log\{|\det \mathcal{M}|\}$$

generate new configs for $p_{\pi_I}, p_s, p_{S_I}, \pi_I, S, s_I$ by molecular dynamics trajectories

$\Downarrow$

apply Metropolis accept/reject step for new config according to the probability $\exp(-H_{HMC})$

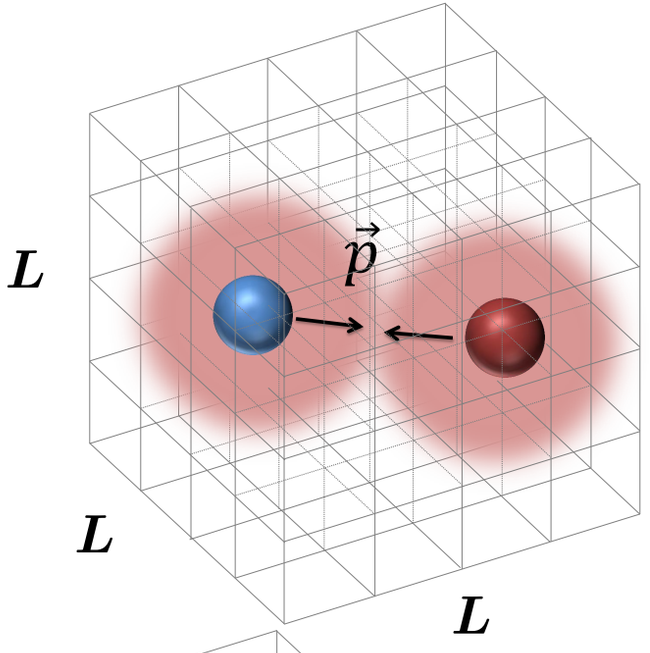
repeat steps many times

EXTRACTING PHASE SHIFTS on the LATTICE

- Lüscher's method:

  Two-body energy levels below the inelastic threshold on a periodic lattice are related to the phase shifts in the continuum

  Lüscher, Comm. Math. Phys. **105** (1986) 153
  Lüscher, Nucl. Phys. B **354** (1991) 531

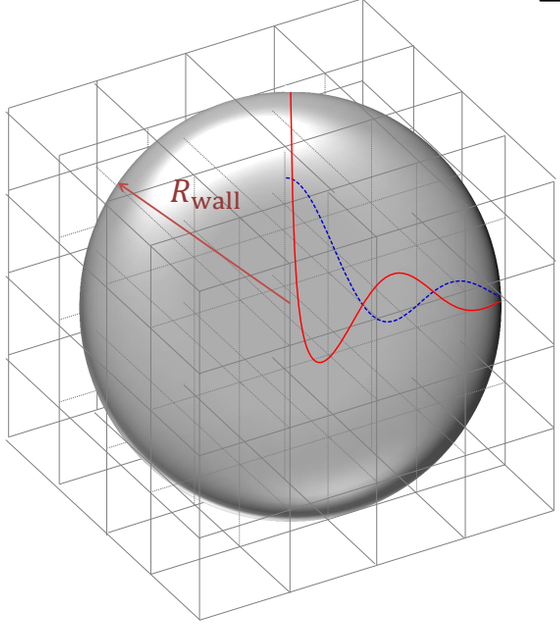


- Spherical wall method:

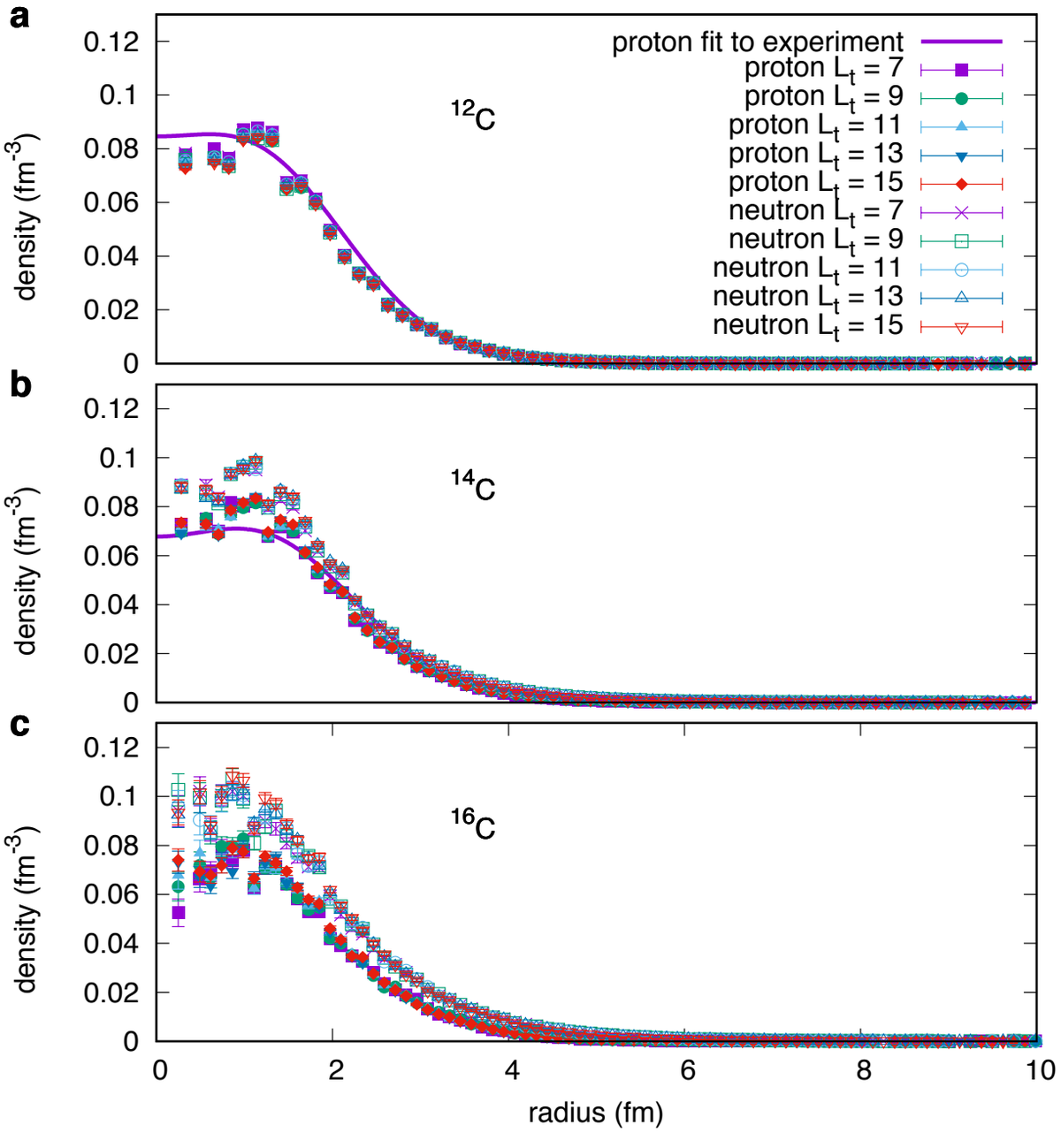
  Impose a hard wall on the lattice and use the fact that the wave function vanishes for $r = R_{\rm wall}$:

$$\psi_\ell(r) \sim [\cos\delta_\ell(p) F_\ell(pr) + \sin\delta_\ell(p) G_\ell(pr)]$$

  Borasoy, Epelbaum, Krebs, Lee, UGM, EPJA **34** (2007) 185
  Carlson, Pandharipande, Wiringa, NPA **424** (1984) 47



PROTON and NEUTRON DENSITIES in CARBON



- open symbols: neutron
- closed symbols: proton
- proton size accounted for
- asymptotic properties of the distributions from the volume dependence of N-body bound states

  König, Lee, Phys. Lett. B779 (2018) 9
- consistent with data
- fit to data from

  Kline et al., Nucl. Phys. A209 (1973) 381