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JÜLICH Forschungszentrum

Nuclear Lattice EFT: Status & Perspectives

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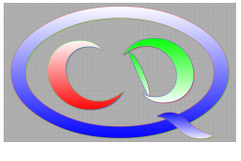


CONTENTS

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* $\geq$ *10(0)*

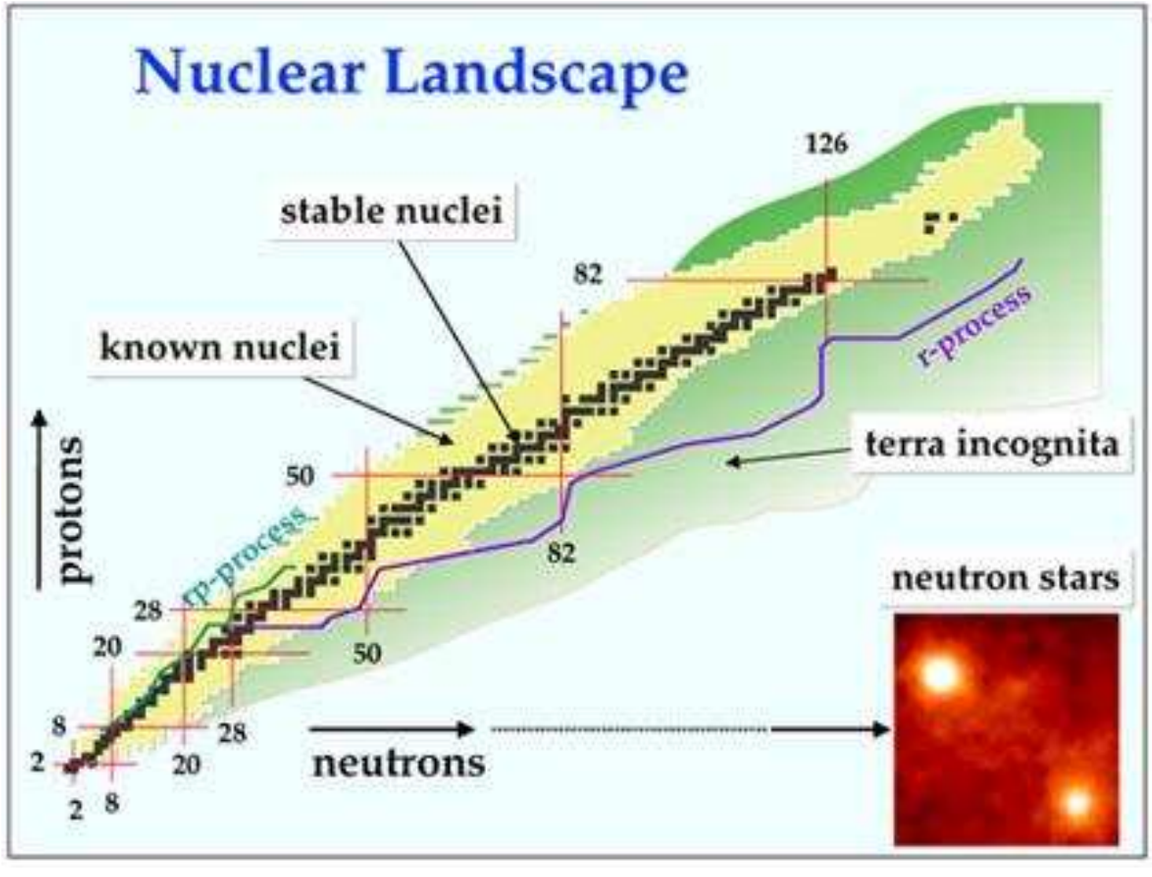
- Chiral EFT:

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

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

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

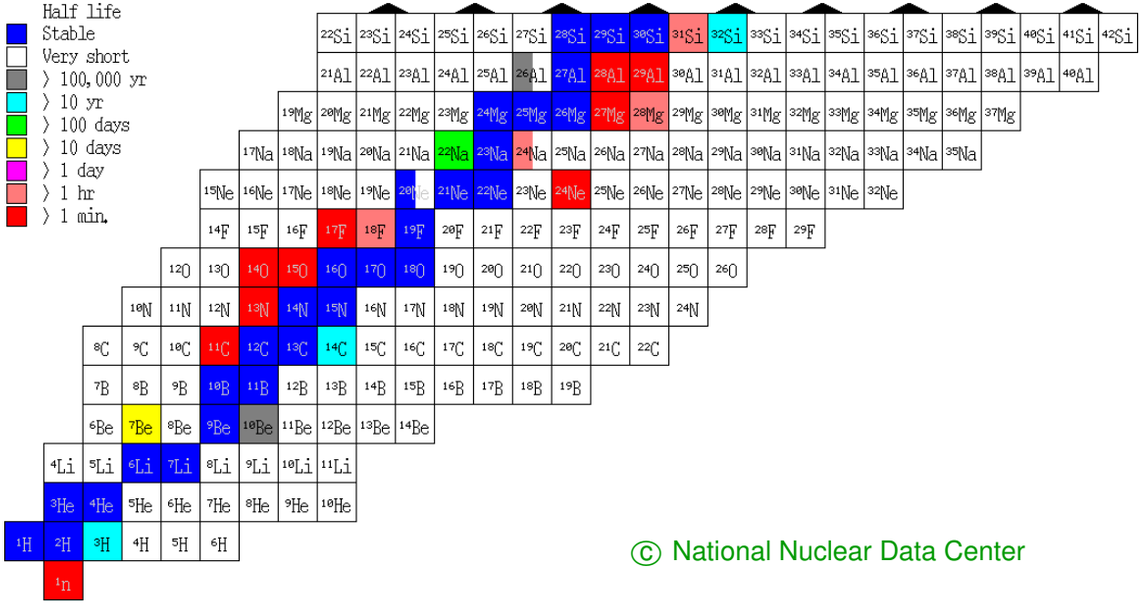
– combine with simulations to get to larger A



⇒ 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

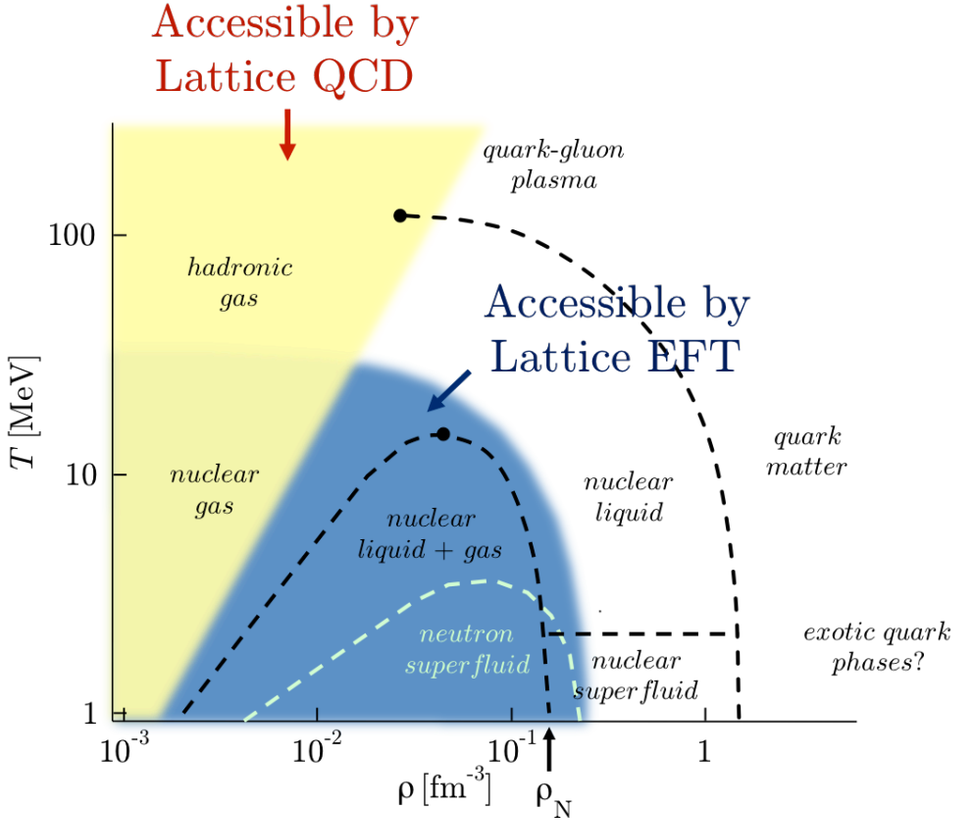
  → this new method is called *Nuclear Lattice Effective Field Theory* (NLEFT)

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

  → rest of the talk

COMPARISON to LATTICE QCD

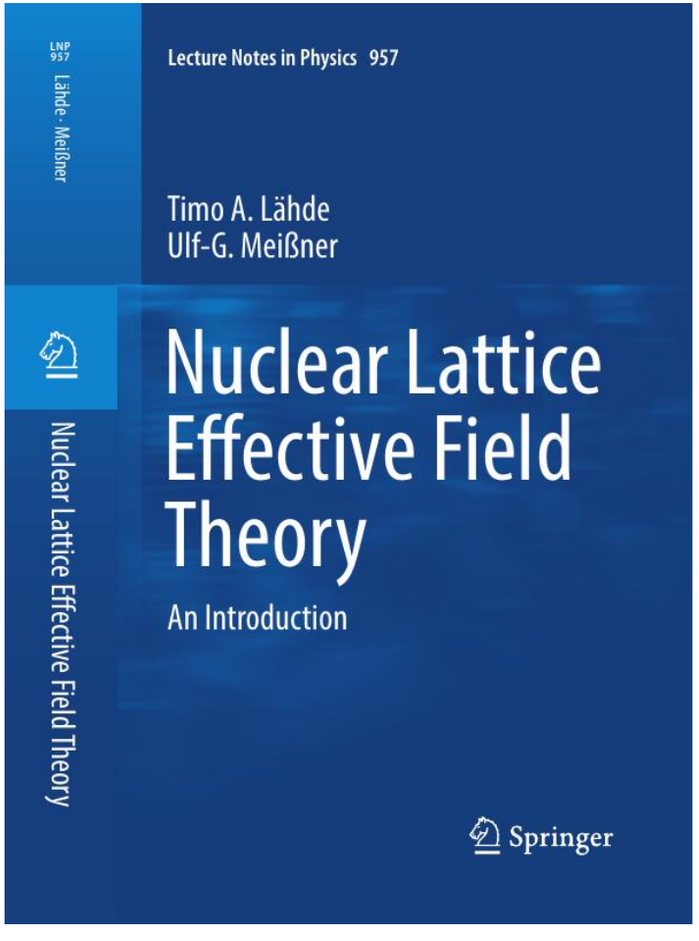
LQCD (quarks & gluons)	NLEFT (nucleons & pions)
relativistic fermions	non-relativistic fermions
renormalizable th'y	EFT
continuum limit	no continuum limit
(un)physical masses	physical masses
Coulomb - difficult	Coulomb - easy
high T/small ρ	small T/nuclear densities
sign problem severe	sign problem moderate



- similar methods:
  hybrid MC, parallel computing, . . .
  ↪ only treated briefly (shuttle algorithm)

- what I want to discuss within the time limitations:
  ↪ how to put the chiral EFT on a lattice
  ↪ the pinhole algorithm / center-of-mass in AFQMC
  ↪ the pinhole trace algorithm
  ↪ going to larger A, increasing the precision
  ↪ ab initio nuclear thermodynamics

Chiral EFT on a lattice



T. Lähde & UGM

Nuclear Lattice Effective Field Theory - An Introduction

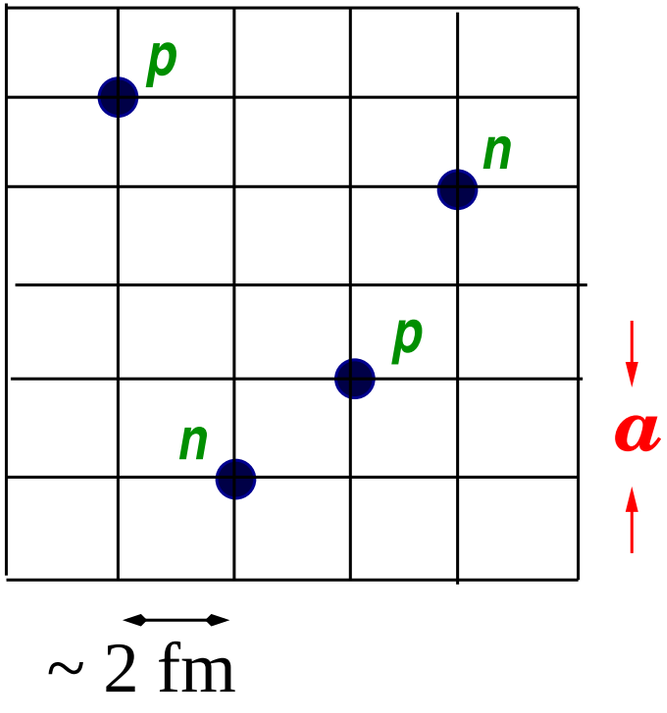
Springer Lecture Notes in Physics **957** (2019) 1 - 396

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: $a_{0,0} \equiv a_{\uparrow,p},\ a_{1,0} \equiv a_{\downarrow,p},\ a_{0,1} \equiv a_{\uparrow,n},\ a_{1,1} \equiv a_{\downarrow,n}$

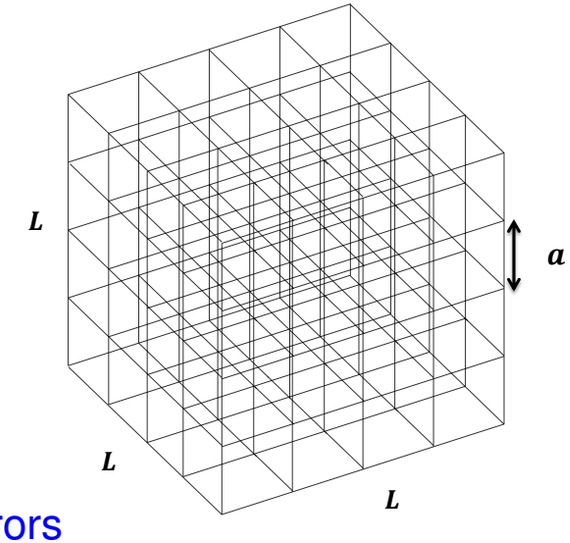
  $\rightarrow$ labeling **spin** and **isospin**

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

$\hookrightarrow$ definition of the first order spatial derivative:

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

$\hookrightarrow$ 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 $\longrightarrow$ beneficial feature for tuning NLO coefficients

$\hookrightarrow$ 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

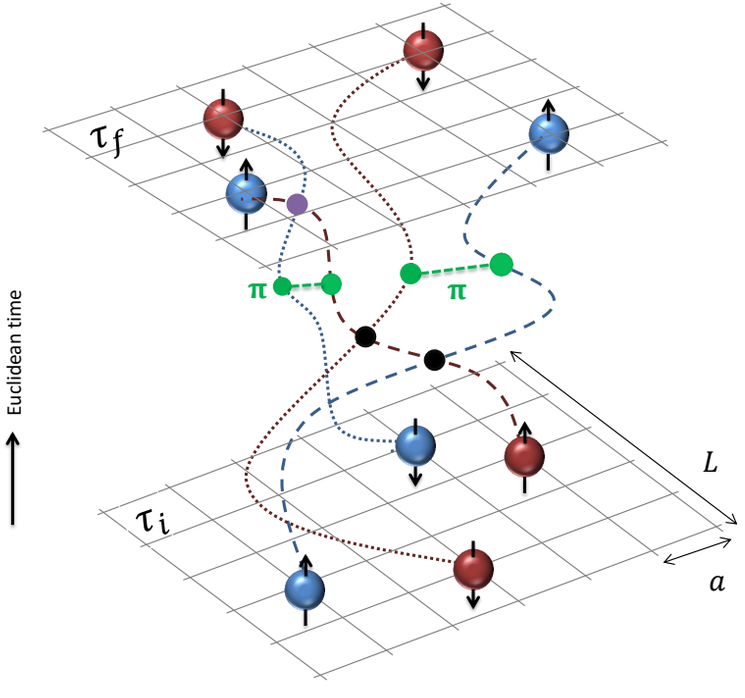
  [or a more sophisticated (correlated) initial/final state]

Euclidean time

- Transient energy

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

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

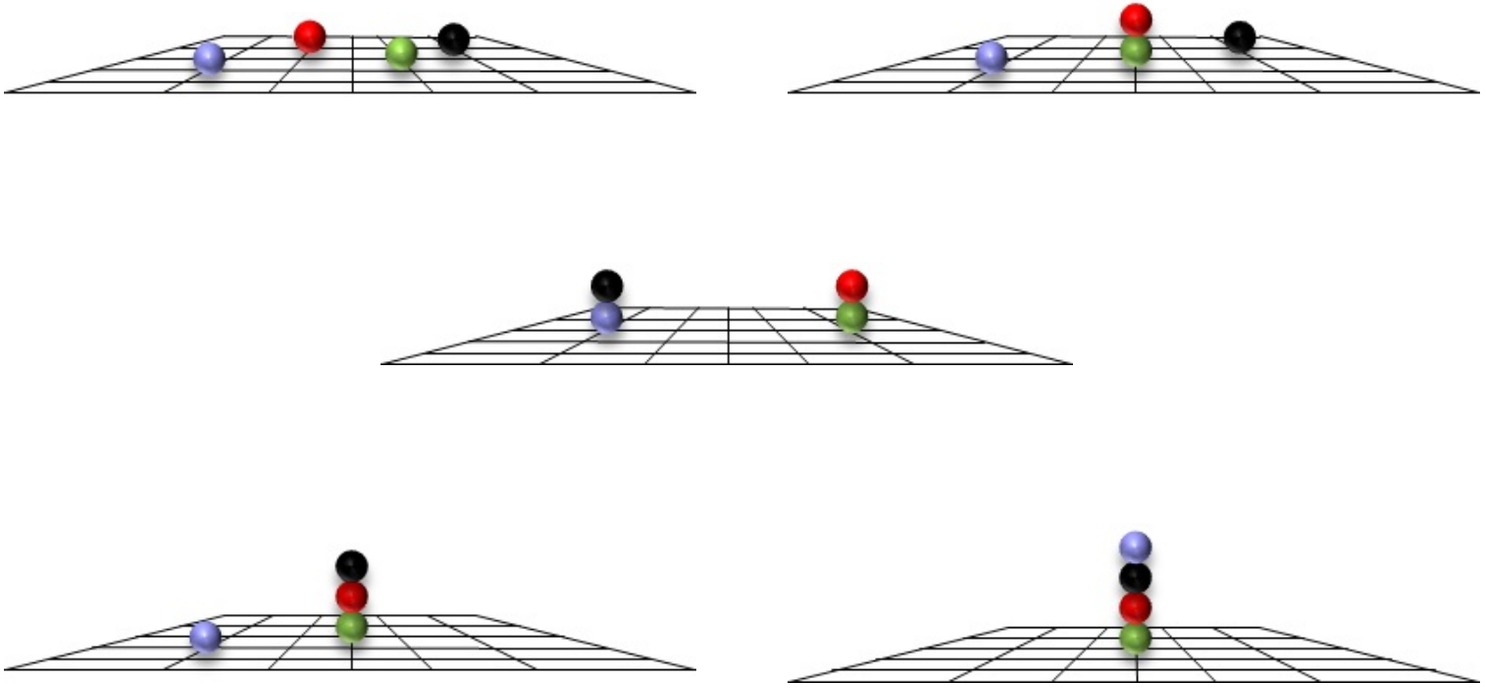


- Exp. value of any normal–ordered operator $\mathcal{O}$

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

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

CONFIGURATIONS



$\Rightarrow$ all *possible* configurations are sampled

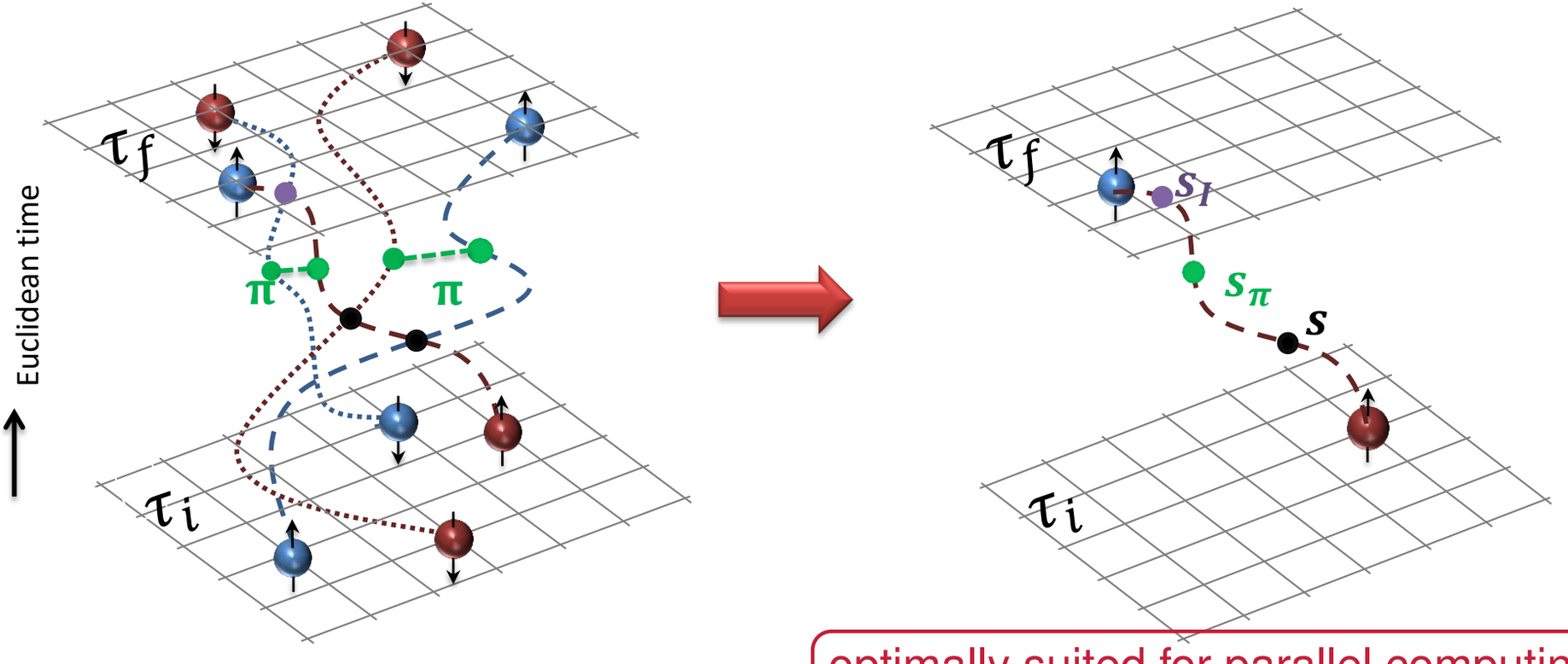
$\Rightarrow$ preparation of *all possible* initial/final states

$\Rightarrow$ *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

Algorithmic developments

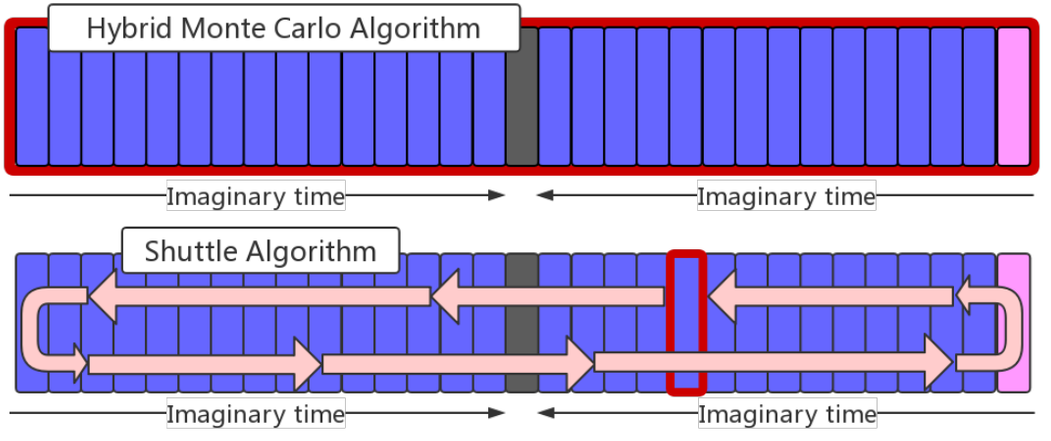
shuttle algorithm: Lu et al., Phys. Lett. B**797** (2019) 134863

pinhole algorithm: Elhatisari et al., Phys. Rev. Lett. **19** (2017) 222505

pinhole trace algorithm: Lu et al., arXiv:1912.05105, subm. for publication

THE SHUTTLE ALGORITHM

- Auxiliary fields $s(n_t, \vec{n})$ are updated on one time slice only
- Proceed to the next time slice, update, ... , turn around at the end of the time series



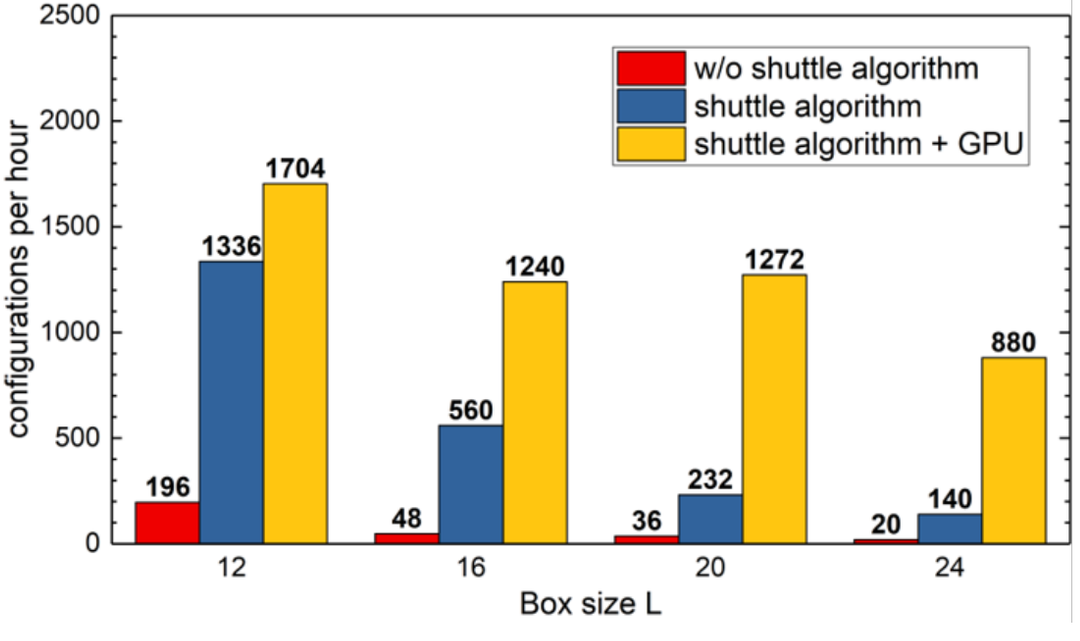
$\rightarrow$ very efficient for small temporal lattice spacings, $a_t = 0.001$ MeV^{-1}

$\rightarrow$ high acceptance rate, typically $\sim 50\%$

$\rightarrow$ more efficient than HMC

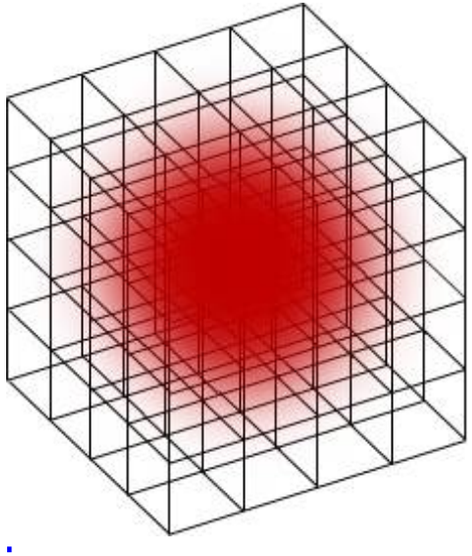
$\rightarrow$ about 10 times more configurations per hour generated

$\rightarrow$ further acceleration by GPUs



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

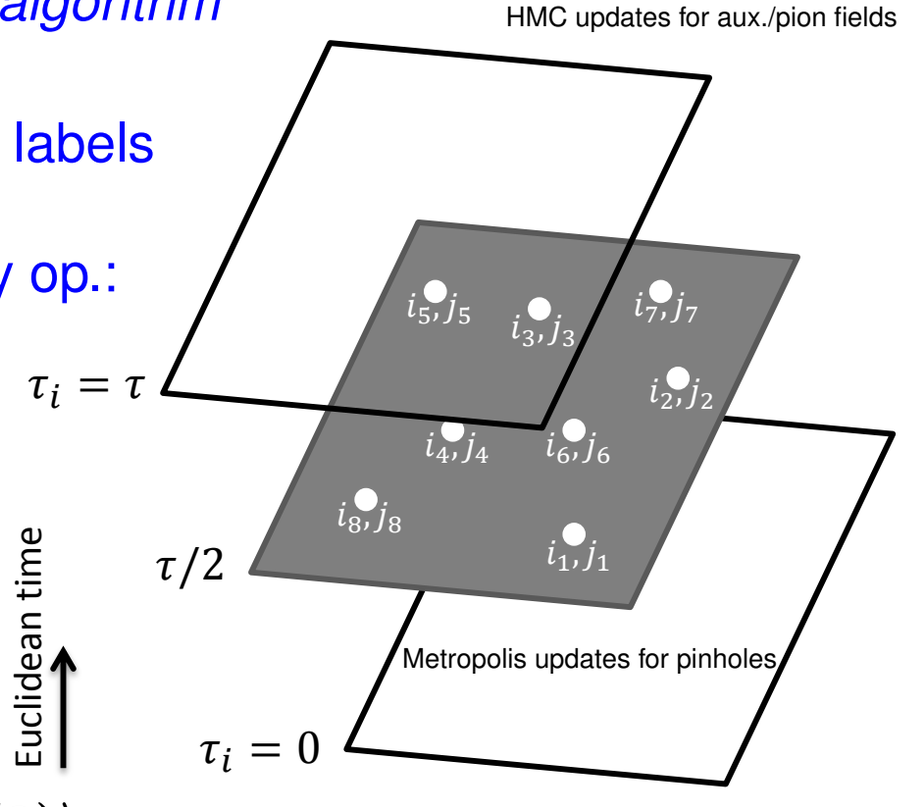
PINHOLE ALGORITHM

- 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

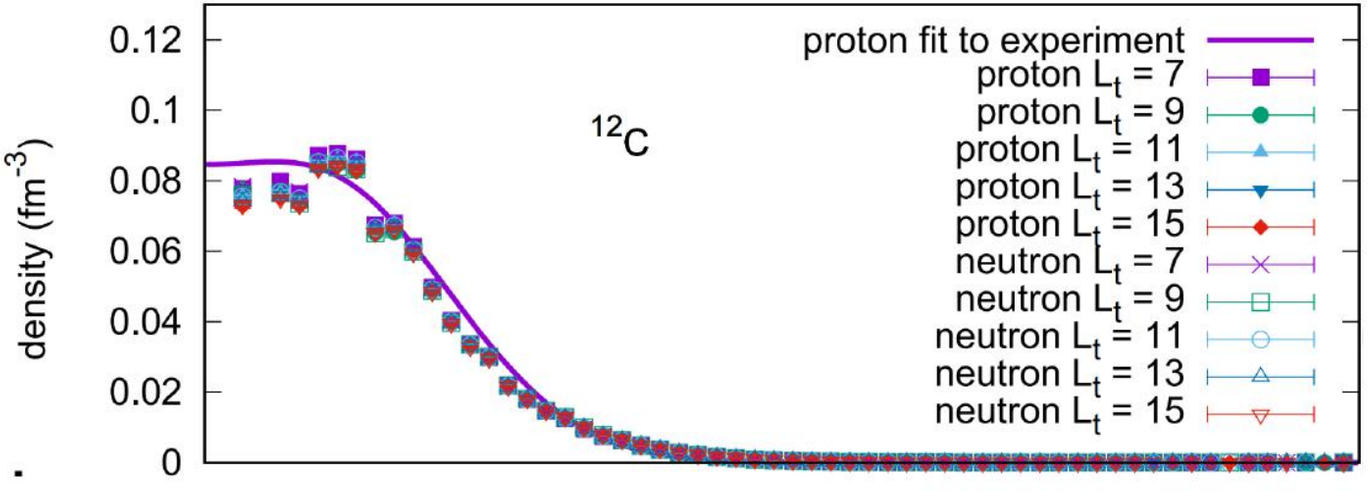
- Resolution scale $\sim a/A$ as cm position $\mathbf{r}_{\mathbf{cm}}$ is an integer $\mathbf{n}_{\mathbf{cm}}$ times a/A

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

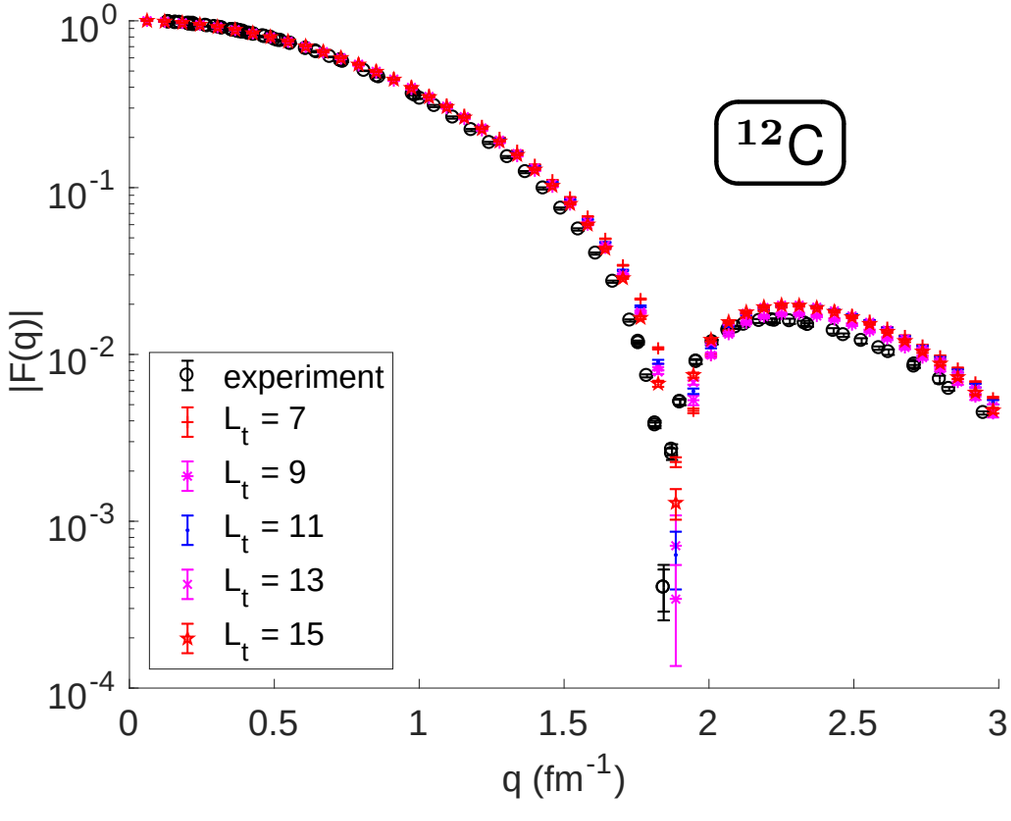


$\Rightarrow$ independent of projection time $\rightarrow$ ground state

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

FORM FACTORS

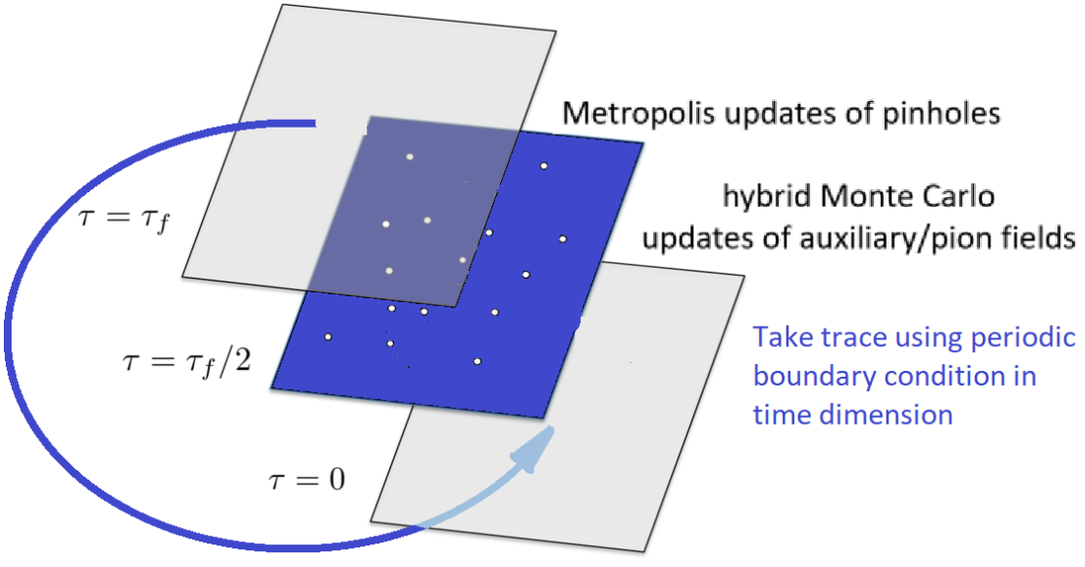
- Fit charge distributions by a Wood-Saxon shape
  ↪ get the form factor from the Fourier-transform (FT)
  ↪ uncertainties from a direct FT of the lattice data



$\Rightarrow$ detailed structure studies become possible

PINHOLE TRACE ALGORITHM (PTA)

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



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

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

- allows to study: liquid-gas phase transition → this talk

  thermodynamics of finite nuclei

  thermal dissociation of hot nuclei

  cluster yields of dissociating nuclei

Essentials of Nuclear Binding

B. N. Lu, N. Li, S. Elhatisari, D. Lee, E. Epelbaum, UGM,
Phys. Lett. **B 797** (2019) 134863

TOWARDS HEAVY NUCLEI in NLEFT

- Two step procedure:

  1) Further improve the LO action

  ↪ minimize the sign oscillations

  ↪ minimize the higher-body forces

  ↪ gain an understanding of the essentials of nuclear binding

  2) Work out the corrections to N3LO

  ↪ first on the level of the NN interaction

  ↪ second for the spectra of nuclei

  ↪ third for nuclear reactions (nuclear astrophysics)

ESSENTIAL ELEMENTS for NUCLEAR BINDING I

Lu, Li, Elhatisari, Epelbaum, Lee, UGM. Phys. Lett. B **797** (2019) 134863 [arXiv:1812.10928]

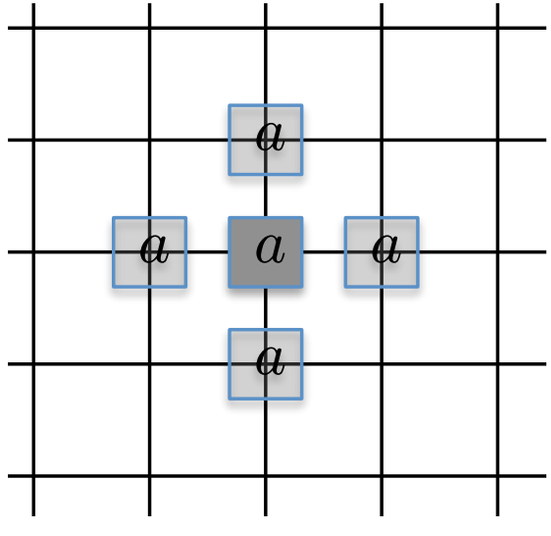
- **Step 1**: construct a highly improved LO action, **free** of any sign problem

- Highly SU(4) symmetric LO action without pions, local and non-local smearing:

$$H_{\rm SU(4)} = H_{\rm free} + \frac{1}{2!} C_2 \sum_n \tilde{\rho}(n)^2 + \frac{1}{3!} C_3 \sum_n \tilde{\rho}(n)^3$$

$$\tilde{\rho}(n) = \sum_i \tilde{a}_i^\dagger(n) \tilde{a}_i(n) + s_L \sum_{|n'-n|=1} \sum_i \tilde{a}_i^\dagger(n') \tilde{a}_i(n')$$

$$\tilde{a}_i(n) = a_i(n) + s_{NL} \sum_{|n'-n|=1} a_i(n')$$



- Only **four** parameters!

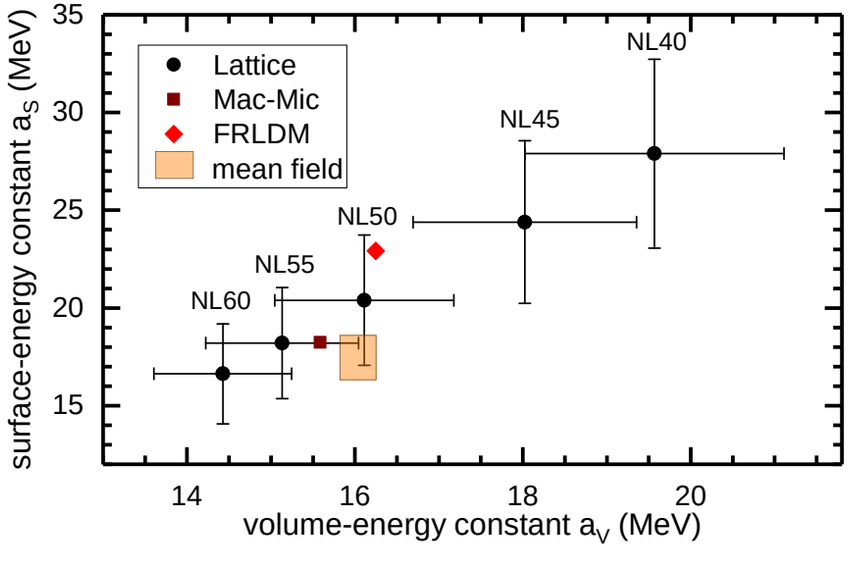
  C_2 and C_3 = strength of the leading two- and three-body interactions

  s_L and s_{NL} = strength of the local and the non-local interaction

ESSENTIAL ELEMENTS for NUCLEAR BINDING II

- Fixing the parameters:
  - ⋆ interaction strength C_2 and range s_L from the average S-wave scattering lengths and effective ranges (requires SU(4) breaking later)
  - ⋆ interaction strength C_3 from the ^{3}H binding energy
  - ⋆ interaction range s_{NL} can not be determined in light nuclei
  - ↪ calculate the volume- and surface energy of mid-mass nuclei $16 \leq A \leq 40$
  - compare w/ existing calculations:

↪ $\boxed{s_{NL} = 0.5}$



Mac-Mic: Wang et al., Phys. Lett. B **734** (2014) 215

FRLDM: Möller et al., Atom Data Nucl. Data Tabl. **59** (1995) 184

mean field: Bender et al., Rev. Mod. Phys. **75** (2003) 121

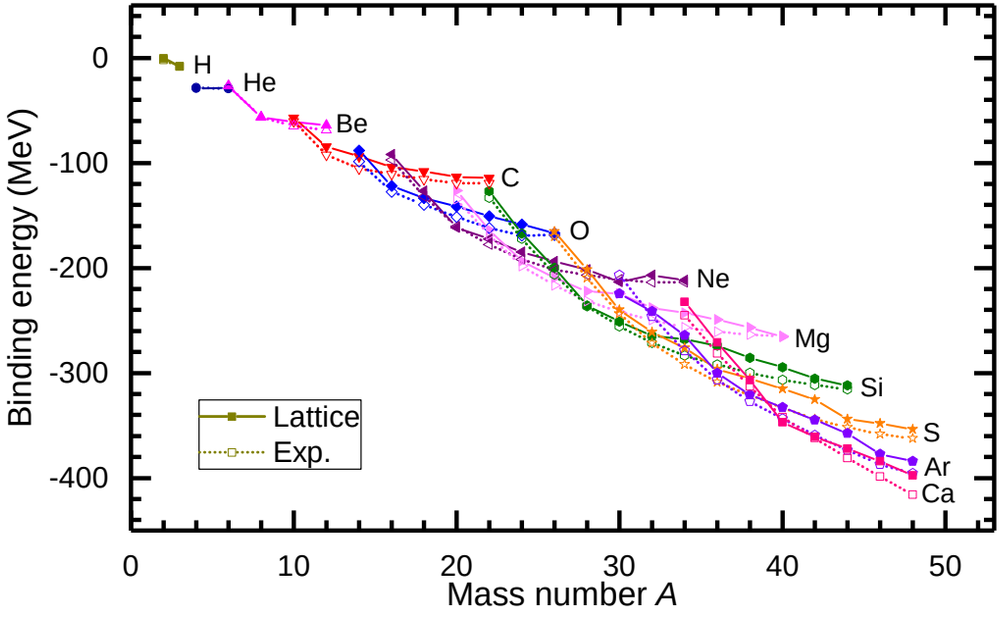
ENERGIES for SELECTED NUCLEI

- Calculated binding energies for 3N & alpha-type nuclei:

	B [MeV]	Coul. [MeV]	B/Exp.
^{3}H	8.48(2)*	0.0	1.00
^{3}He	7.75(2)	0.73(1)	1.00
^{4}He	28.89(1)	0.80(1)	1.02
^{16}O	121.9(3)	13.9(1)	0.96
^{20}Ne	161.6(1)	20.2(1)	1.01
^{24}Mg	193.5(17)	28.0(2)	0.98
^{28}Si	235.8(17)	37.1(4)	1.00
^{40}Ca	346.8(8)	71.7(6)	1.01

[* = input]

- Binding energies for 86 even-even nuclei



- selected nuclei: amazingly precise, largest deviation about 4% in ^{16}O
- even-even isotopic chains come out amazingly precise, general trends reproduced

↪ on the proton-rich side better than on the neutron-rich one → spin-dep. effects

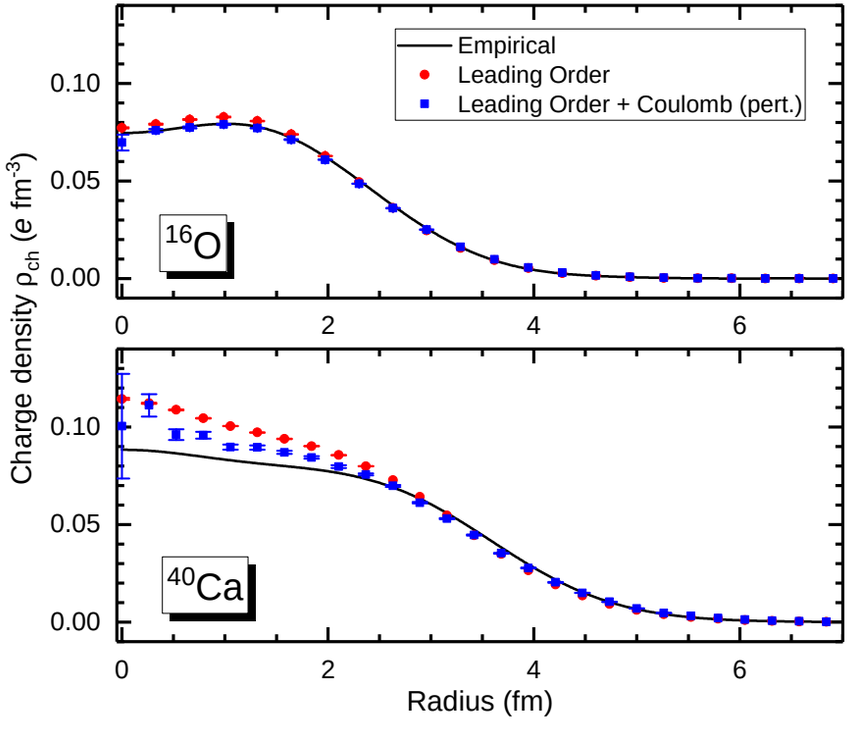
- but remember: this is only leading order!

RADII for SELECTED NUCLEI

- Calculated charge radii for 3N & alpha-type nuclei:

	$R_{\rm ch}$	Exp.	$R_{\rm ch}$/Exp.
^{3}H	1.90(1)	1.76	1.08
^{3}He	1.99(1)	1.97	1.01
^{4}He	1.72(3)	1.68	1.02
^{16}O	2.74(1)	2.70	1.01
^{20}Ne	2.95(1)	3.01	0.98
^{24}Mg	3.13(2)	3.06	1.02
^{28}Si	3.26(1)	3.12	1.04
^{40}Ca	3.42(3)	3.48	0.98

- Charge distributions for ^{16}O and ^{40}Ca



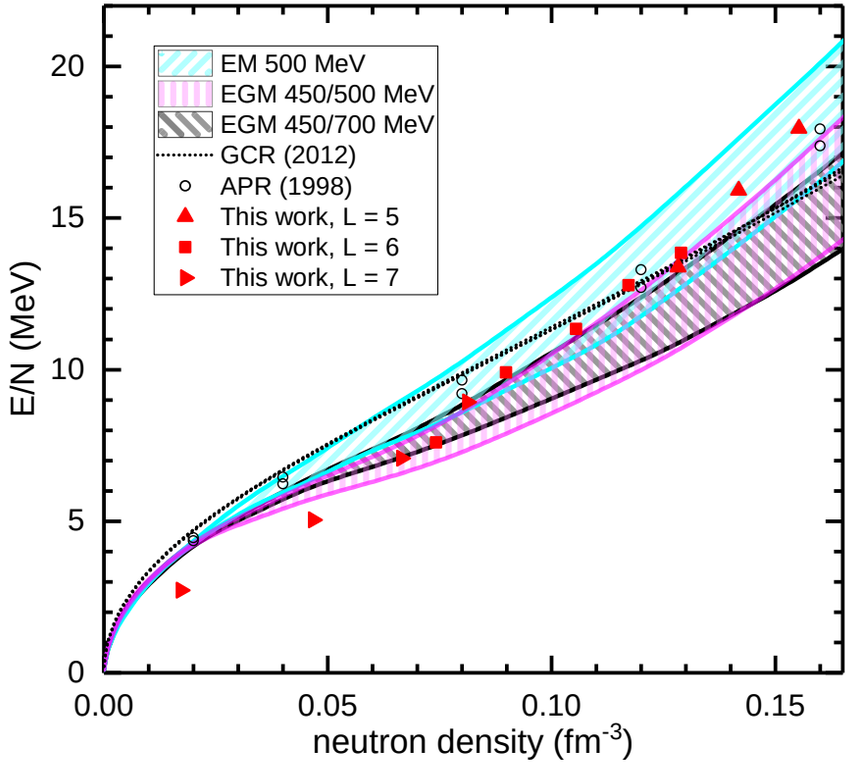
- Radii quite well described

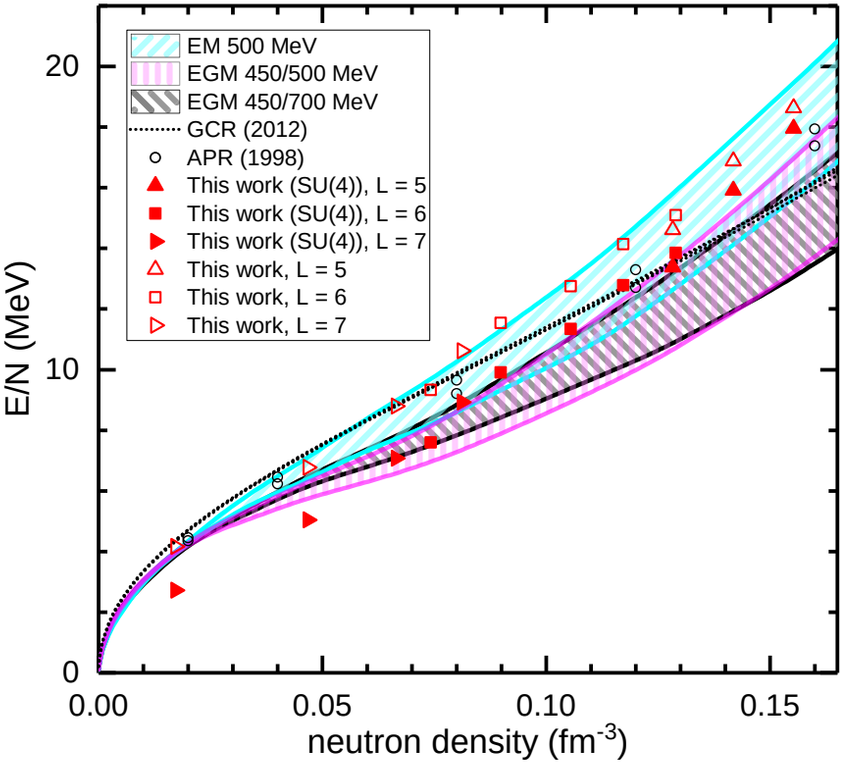
↪ overcomes earlier problems (see PRL 109 (2012) 252501, 112 (2014) 102501)

- Also a fair description of the charge distributions at LO!

NEUTRON MATTER

- 14 to 66 neutrons in $L = 5, 6, 7 \to \rho = 0.02 - 0.15\,\text{fm}^{-3}$





- exact SU(4)

↪ deviations at low densities

- SU(4) breaking term $\to a_{nn}$ ✓

↪ good overall description

APR = Akmal, Pandharipande, Ravenhall, Phys. Rev. C **58** (1998) 1804; GCR = Gandolfi, Carlson, Reddy, Phys. Rev. C **85** (2012) 032801;
all others in: Tews et al., Phys. Rev. Lett. **110** (2013) 032504.

GOING to HIGHER ORDERS

- **Step 2**: Work out NN phase shifts to N3LO

  $\hookrightarrow$ calculate nuclear properties based on NN forces only $\surd$

  $\hookrightarrow$ add three-nucleon forces (in the works)

- Starting Hamiltonian:

$$H_{\mathrm{2N}} = H_{\mathrm{free}} + H_{\mathrm{SU(4)}}(C_3 = 0) + H_{\mathrm{OPE}}$$

  $\hookrightarrow$ consistent with the power counting (3NFs appear at N2LO)

  $\hookrightarrow$ OPE induces some sign problem (but manageable)

- NN forces to N3LO worked out for 4 latt. spacings $a = 0, 99, 1.32, 1.64, 1.98$ fm with local and non-local smearing and restoration of Galilean invariance breaking

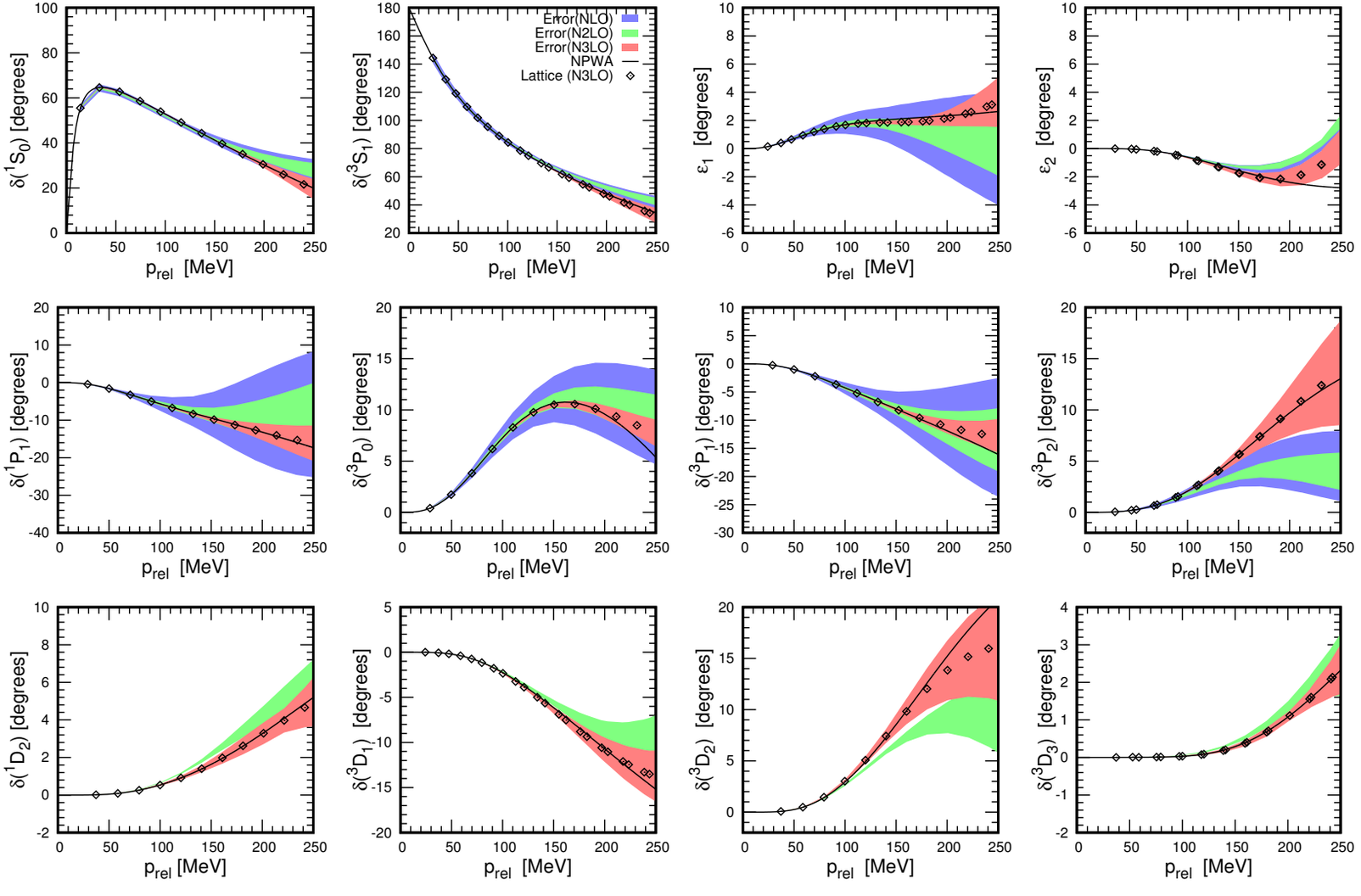
  $\hookrightarrow$ used as input for nuclear structure calculations

Li et al., Phys. Rev. C **98** (2018) 044002; Phys. Rev. C **99** (2019) 064001

NN INTERACTION at N3LO

- np phase shifts including uncertainties for $a = 1.64$ fm (cf. Nijmegen PWA)

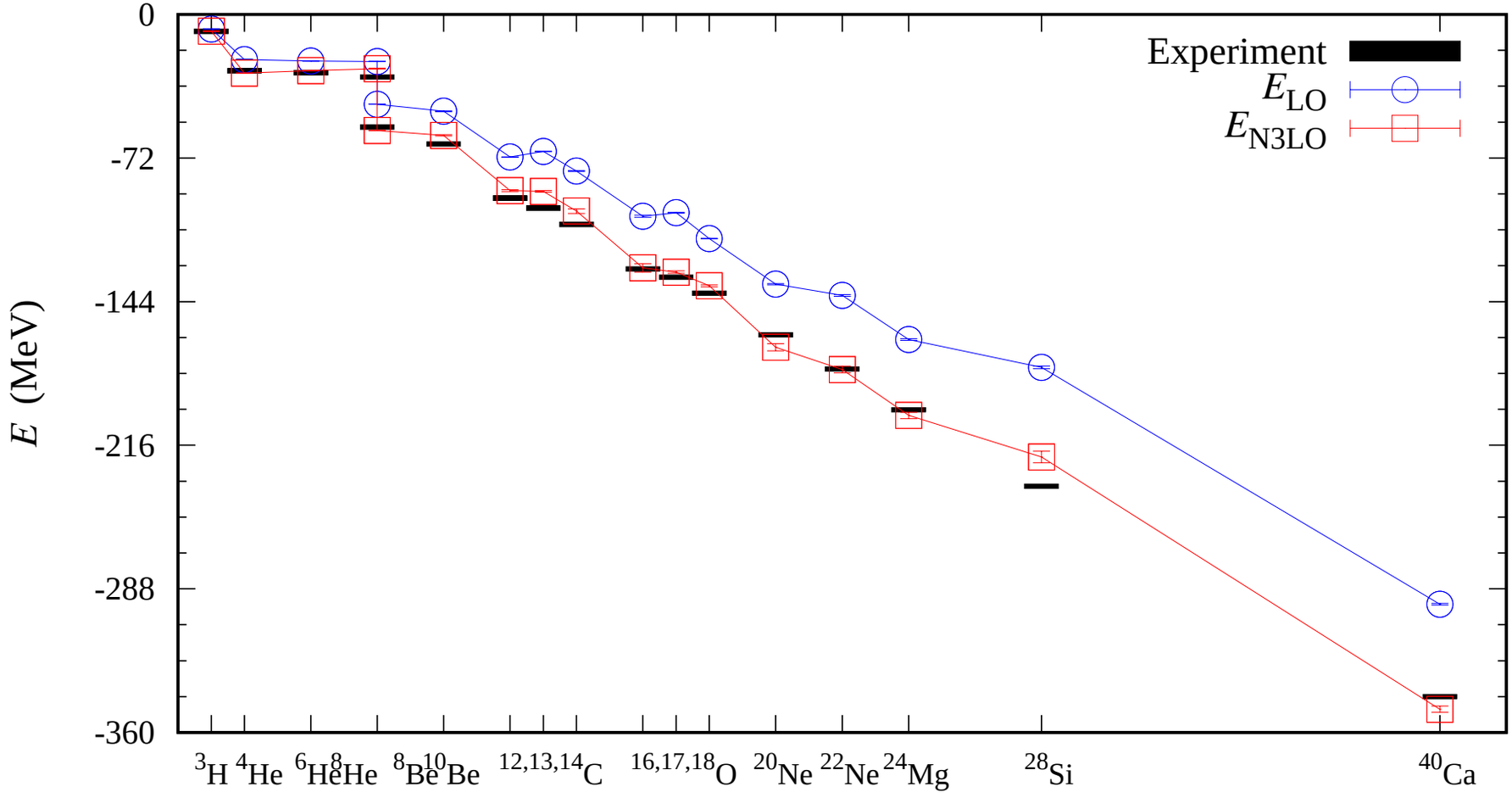
NLO
N2LO
N3LO



uncertainty estimates á la Epelbaum, Krebs, UGM, Eur. Phys. J. A **51** (2015) 53

NUCLEI at N3LO

- Binding energies of nuclei for $a = 1.64$ fm



$\rightarrow$ excellent starting point for precision studies

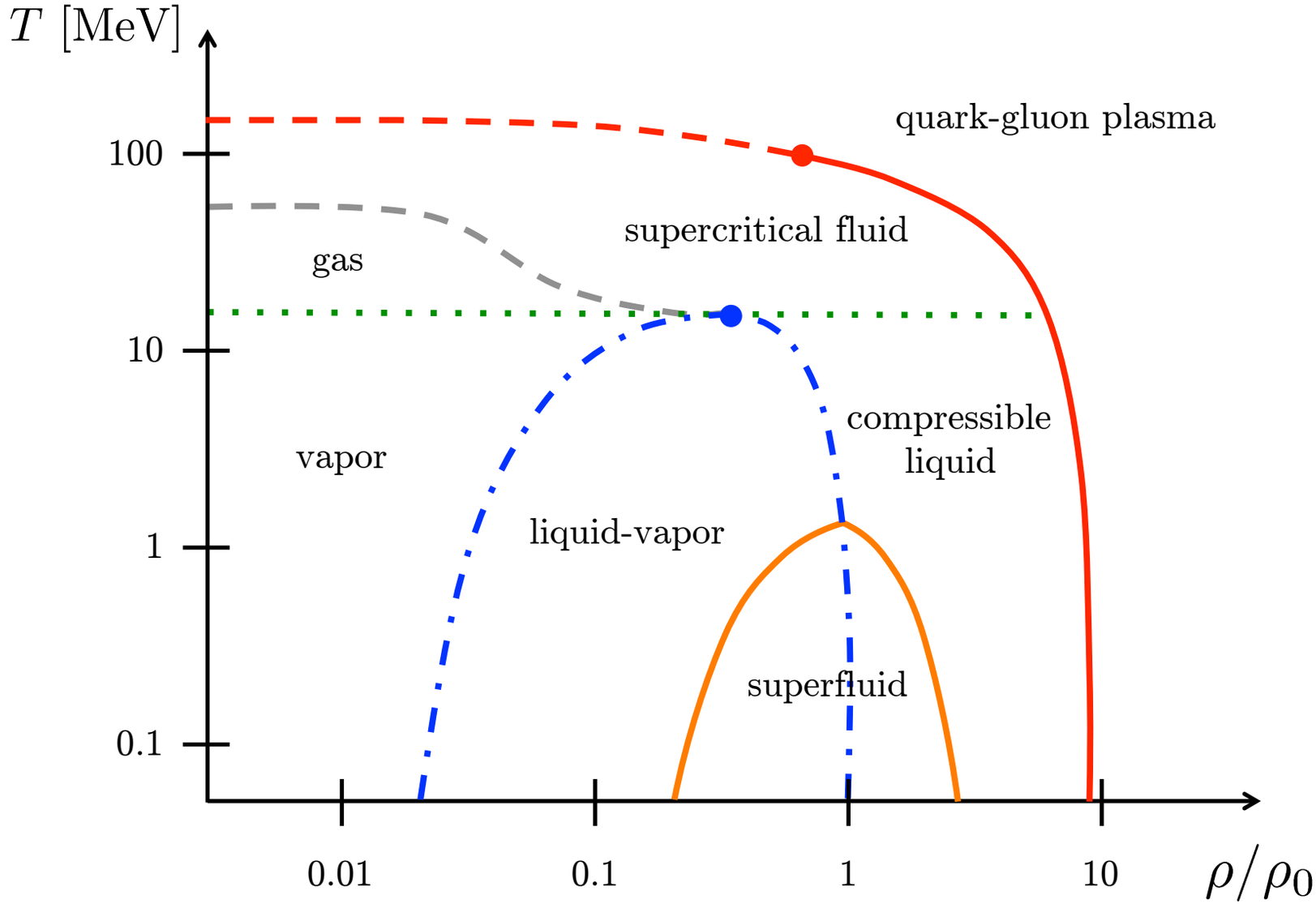
Ab Initio Nuclear Thermodynamics

B. N. Lu, N. Li, S. Elhatisari, D. Lee, J. Drut, T. Lähde, E. Epelbaum, UGM, [arXiv:1912.05105], submitted for publication

PHASE DIAGRAM

- Phase diagram of strongly interacting matter

Fig. courtesy B.-N. Lu



NEW PARADIGM for NUCLEAR THERMODYNAMICS

- The PTA allows for simulations with fixed neutron & proton numbers at non-zero T

$\hookrightarrow$ thousands to millions times faster than existing codes using the grand-canonical ensemble ($t_{\rm CPU} \sim V N^2$ vs. $t_{\rm CPU} \sim V^3 N^2$)

- Only a mild sign problem $\to$ pinholes are dynamically driven to form pairs

- Typical simulation parameters:

  up to $N = 144$ nucleons in volumes $L^3 = 4^3, 5^3, 6^3$

  $\hookrightarrow$ densities from 0.008 fm^{-3} ... 0.20 fm^{-3}

  $a = 1.32$ fm $\to \Lambda = \pi/a = 470$ MeV , $a_t \simeq 0.1$ fm

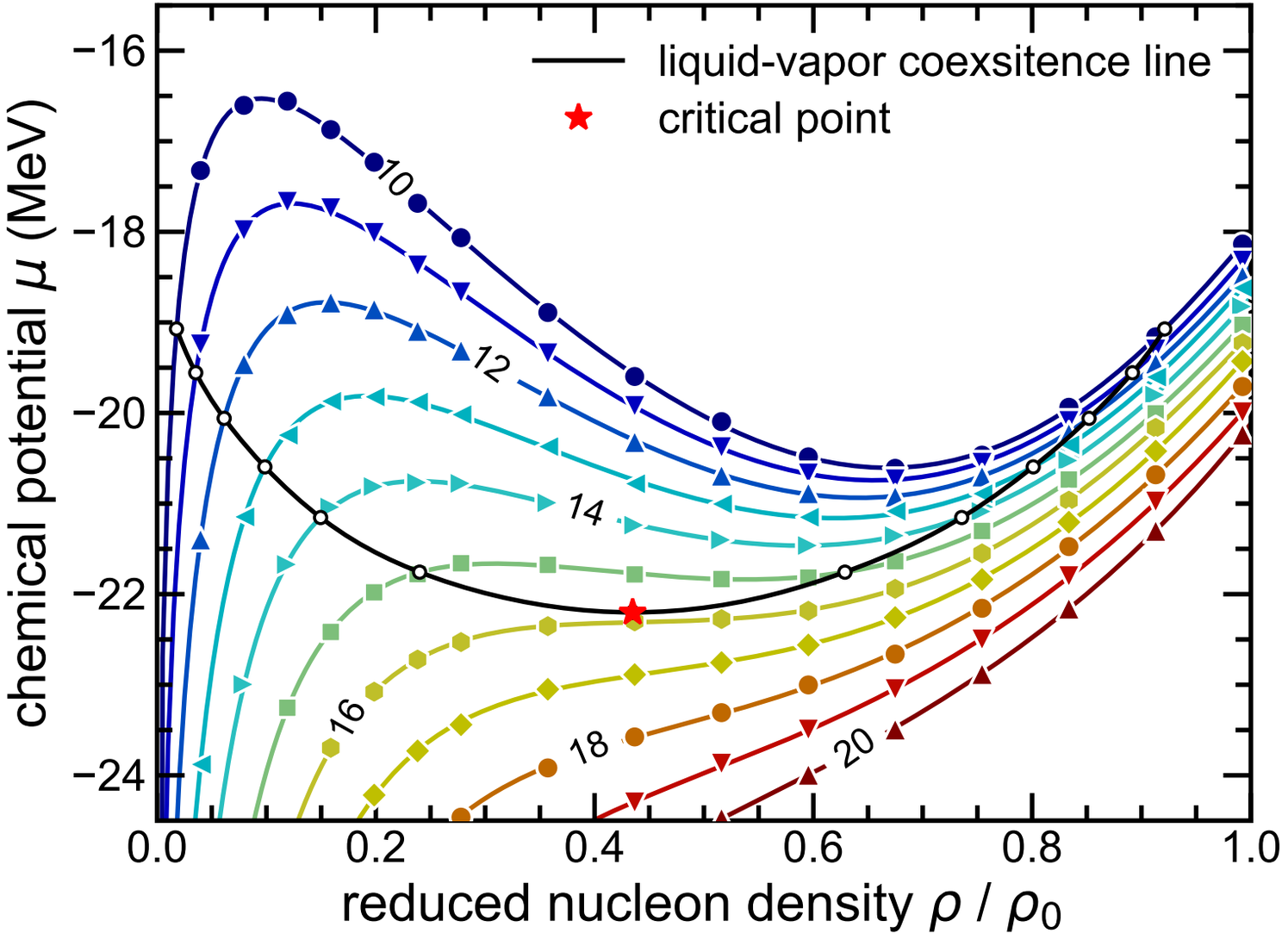
  consider $T = 10 \ldots 20$ MeV

- use twisted bc's, average over twist angles $\to$ acceleration to the td limit

- very favorable scaling for generating config's: $\boxed{\Delta t \sim N^2 L^3}$

CHEMICAL POTENTIAL

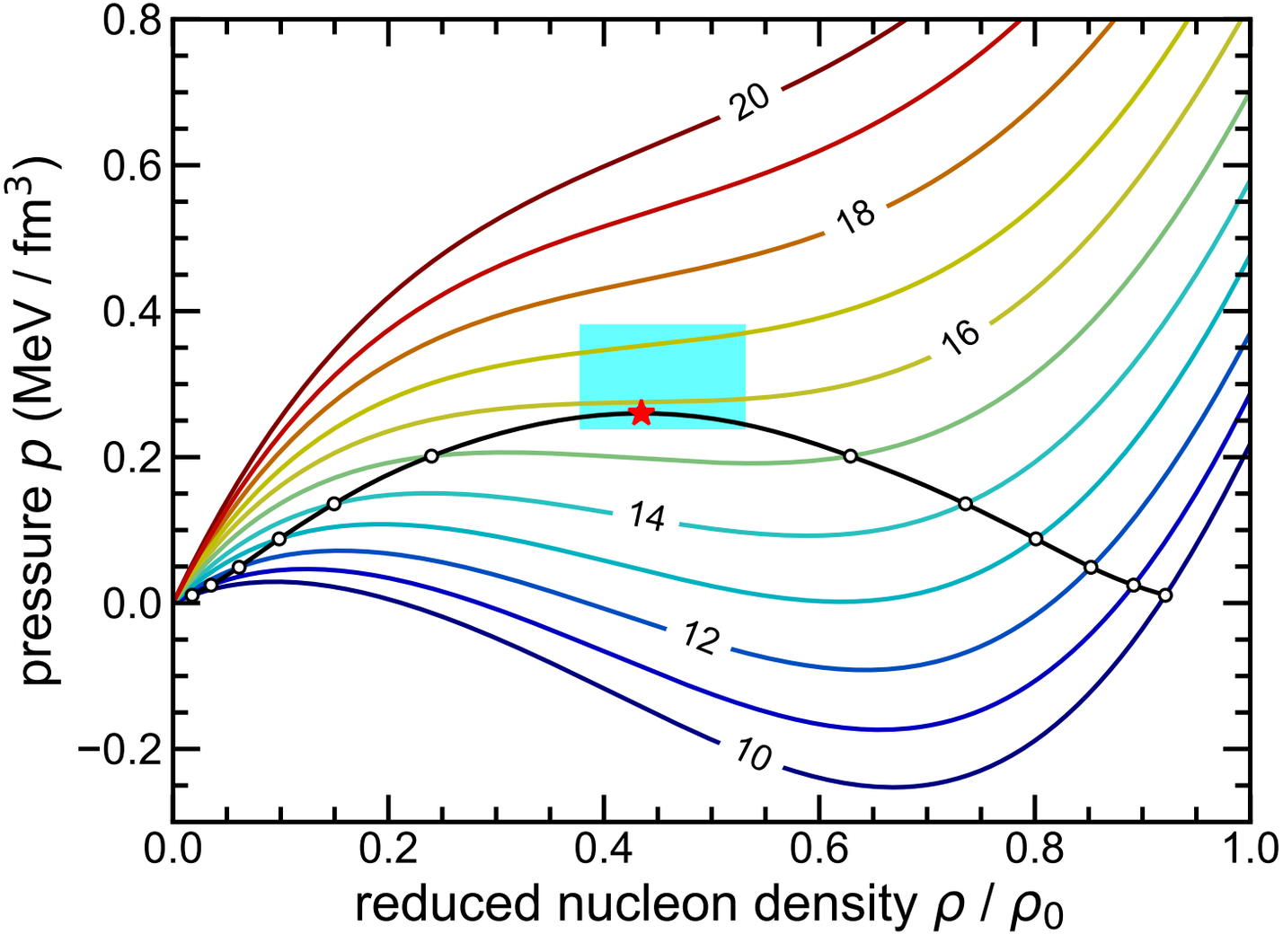
- Calculated from the free energy: $\mu = (F(N+1) - F(N-1))/2$



at very low densities like the ideal gas $\mu \propto \log(\rho)$

EQUATION of STATE

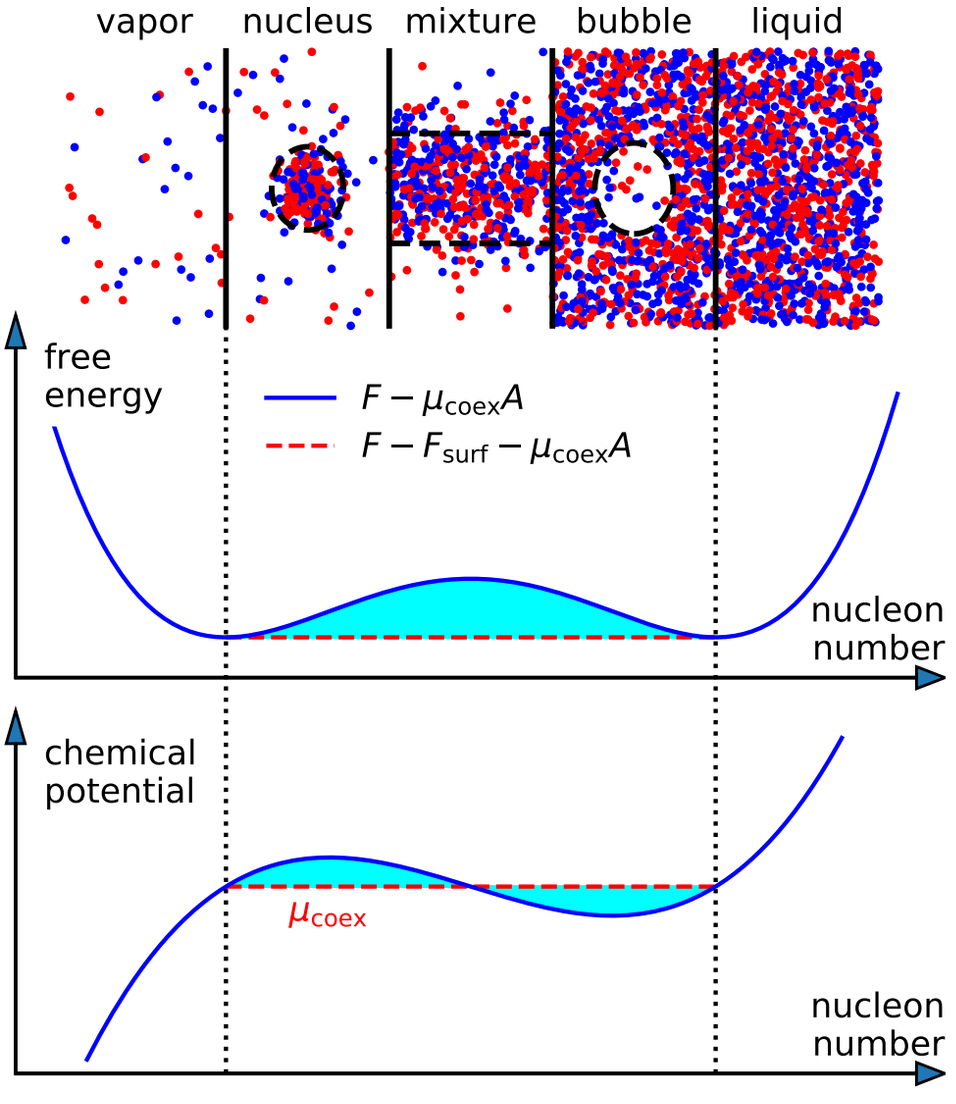
- Calculated by integrating: $dP = \rho\, d\mu$
- Crtitical point: $T_c = 15.8(1.6)$ MeV, $P_c = 0.26(3)$ MeV/fm^3, $\rho_c = 0.089(18)$ fm^{-3}



Experiment: $T_c = 15.0(3)$ MeV, $P_c = 0.31(7)$ MeV/fm^3, $\rho_c = 0.06(2)$ fm^{-3}

VAPOR-LIQUID PHASE TRANSITION

- Vapor-liquid phase transition
  in a finite volume V & $T < T_c$
- the most probable configuration
  for different nucleon number A
- the free energy
- chemical potential $\mu = \partial F / \partial A$



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
- Algorithmic developments
  - → shuttle algorithm speeds up the simulations considerably
  - → pinhole algorithm allows to fix the center-of-mass: charge distributions etc
  - → pinhole trace algorithm: thermodynamics with fixed nucleon number
- Towards heavier nuclei & higher precision
  - → highly improved LO action baed on SU(4) → nuclei & neutron matter
  - → NN interaction at N3LO, first results for nuclei at N3LO
- Ab initio nuclear thermodynamics
  - → partition function via the pinhole trace algorithm
  - → first promising results for the phase diagram of nuclear matter at finite temperature
  - → prediction of the vapor-liquid phase transition within reasonable accuracy