

The nucleus as a quantum laboratory

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(NUMERIQS)

by ERC, EXOTIC



by NRW-FAIR



- Ulf-G. Meißner, The nucleus as a quantum laboratory, ICPS 24, Tiflis, Georgia, August 7, 2024 -

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Introductory remarks

Why nuclear physics?



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Ab initio nuclear structure & reactions



• Nuclear reactions: Scattering processes relevant for nuclear astrophysics

- * alpha-particle scattering: ${}^{4}\text{He} + {}^{4}\text{He} \rightarrow {}^{4}\text{He} + {}^{4}\text{He}$
- \star triple-alpha reaction: ⁴He + ⁴He + ⁴He \rightarrow ¹²C + γ
- \star alpha-capture on carbon: ${}^{4}\text{He} + {}^{12}\text{C} \rightarrow {}^{16}\text{O} + \gamma$

The nucleus as a quantum laboratory

- The nucleus is a challenging and fascinating many-body system
 - \hookrightarrow non-perturbative strong interactions balanced by the Coulomb force
 - \hookrightarrow many interesting phenonema: drip lines, clustering, reactions, ...
 - \hookrightarrow a plethora of few-body/many-body methods already exists
- Macroscopic nuclear matter = neutron stars
 - \hookrightarrow gained prominence again in the multi-messenger aera \hookrightarrow must be able to describe these with the same methods
- I will advocate here a new quantum many-body appraoch
 - \hookrightarrow synthezies chiral EFT w/ stochastic methods
 - \hookrightarrow allows to tackle nuclear structure *and* reactions
 - \hookrightarrow allows to access the multiverse



A brief introduction to nuclear physics

Nuclear physics – a primer

• Nuclei are self-bound system of fermions (protons & neutrons): (Heisenberg (1934)

$$N(ext{ucleon}) = egin{pmatrix} p(ext{roton}) \ n(ext{eutron}) \end{pmatrix}$$

- Bound by the **strong** force (now understood as residual color force of QCD)
- Repulsion also from the **Coulomb** force $(Z_p = +e, Z_n = 0)$
- Nuclear binding energies

 \ll nuclear masses

 $m_p=939.57~{
m MeV}$

 $m_n=928.27~{
m MeV}$

[in nucl. phys. $\hbar = c = 1$]

 DOFs are protons, neutrons and mesons, NOT quarks and gluons! [resolution!]



Nuclear physics – a primer

• Non-relativistic system \rightarrow nuclear Hamiltonian takes the form:

$$H_{
m nuclear} = \sum_{i=1}^A rac{p_i^2}{2m_i} + V \,, \quad V = V_{
m NN} + V_{
m NNN} + \dots$$

- Dominant two-nucleon potential $V_{\rm NN}$, but small three-nucleon force $V_{\rm NNN}$ is required (see pheno forces right)
- The nuclear Hamiltonian can be systematically analyzed using the symmetries of the strong interactions Weinberg, Phys. Lett. B 251 (1990) 288 Weinberg, Nucl. Phys. B 363 (1991) 3



Carlson et al., Rev. Mod. Phys. 87 (2015) 1067

Nuclear interactions – a primer

• Boson-exchange picture of the nucleon-nucleon interaction (V_{NN}) :



- \bullet very successful in describing ~ 10.000 pp and np scattering data
- hadron extension provides parameters
- ullet time-honored parameterization of $V_{
 m NN}$
- But: no error estimate ! [th'y must have errors!]
- But: no consistent three-nucleon force exists!

Bonn, Paris, Nijmegen, Stony Brook, Idaho, ...



Nuclear interactions – a primer

• Modern picture of the nucleon-nucleon interaction (V_{NN}) [and similarly V_{NNN}] based on chiral Lagrangians (symmetry of QCD !):



- ullet equally successful in describing the ~ 10.000 pp and np scattering data
- ullet short- and medium-range interactions parameterized by contact terms o fit LECs C_i
- \bullet two- and three-nucleon forces are related! \checkmark
- \bullet power counting allows for error estimates \checkmark
- worked out to high orders = high precision! \rightarrow next slide



Nuclear interactions – a primer

• State-of-the-art chiral EFT results (N4LO+)

Reinert, Krebs, Epelbaum, Eur. Phys. J. A 54 (2018) 86; Phys. Rev. Lett. 126 (2021) 092501



\hookrightarrow often more precise than the data!

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Nuclear many-body methods – a primer

• Solve the Schrödinger equation for A nucleons in a given nucleus:

$$\left(-\sum_{i=1}^{A}rac{
abla_{i}^{2}}{2m_{N}}+V
ight)|\Psi
angle=E|\Psi
angle\,,\qquad V=V_{
m NN}+V_{
m NNN}+\dots$$

- a variety of classical many-body approaches:
 - the shell-model (independent particles) Goeppert Mayer, Jensen (1949)
 - the deformed shell-model (rotational bands) Nilsson (1957)
 - collective excitations (deformations, vibrations) Bohr, Mottelson (1958)
 - coupled-cluster approach (correlations) Koester, Kümmel (1958)
 - density-functional approach (correlations) Kohn, Sham (1963)
 - and various others....

\hookrightarrow all have limitations, we want to do better (exact solutions w/ modern forces)



1975

998

Chiral EFT on a lattice



ີ≌ຼີ≌ Lähde∙Meißne Lecture Notes in Physics 957 Timo A. Lähde Ulf-G. Meißner **Nuclear** Lattice 2 **Effective Field Nuclear Lattice Effective Field Theory** Theory An Introduction Deringer

T. Lähde & UGM

Nuclear Lattice Effective Field Theory - An Introduction Springer Lecture Notes in Physics **957** (2019) 1 - 396

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More on EFTs

• Much more details on EFTs in light quark physics:



Effective Field Theories

AUTHORS:

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https://www.cambridge.org/de/academic/subjects/physics/theoretical-physics-and-mathematical-physics/effective-field-theories

Nuclear lattice effective field theory (NLEFT)

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

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

• typical lattice parameters

$$p_{
m max} = rac{\pi}{a} \simeq 315 - 630\,{
m MeV}\,[{
m UV}~{
m cutoff}]$$



• 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

ullet physics independent of the lattice spacing for $a=1\dots 2$ fm

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

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]
- Transient energy

$$E_A(au) = -rac{d}{d au}\,\ln Z_A(au)$$

- \rightarrow ground state: $E_A^0 = \lim_{\tau \to \infty} E_A(\tau)$
- Similarly:
 - insert operators / other observables
 - excited states / transitions



Euclidean time





 \Rightarrow all *possible* configurations are sampled \Rightarrow preparation of *all possible* initial/final states \Rightarrow *clustering* operance *paturally*

 \Rightarrow *clustering* emerges *naturally*

Auxiliary field method

• Represent interactions by auxiliary fields (Gaussian quadrature):



Computational equipment

• Present = JUWELS (modular system) + FRONTIER + ...



The Hoyle state and the generation of carbon in stars

Element generation

- Elements are generated in the Big Bang & in stars through the **fusion** of protons & nuclei
 [pp chain or CNO-cycle]
- All is simple until ⁴He
- Only elements up to Be are produced in the Big Bang [BBNucleosynthesis]
- Life-essential elements like ¹²C and ¹⁶O are generated in hot, old stars (triple-alpha reaction !)
- Note also that nuclei make up the visible matter in the Universe



[[]from Wikipedia]

A short history of the Hoyle state

• Heavy element generation in massive stars: triple- α process

Bethe 1938, Öpik 1952, Salpeter 1952, Hoyle 1954, ...

⁴He + ⁴He \Rightarrow ⁸Be ⁸Be + ⁴He \Rightarrow ¹²C+ γ ¹²C + ⁴He \Rightarrow ¹⁶O+ γ [further step to get oxygen]

 \hookrightarrow this generates **order of magnitude** too few carbon and oxygen

- Hoyle's great idea:
 - \Rightarrow need a resonance close to the ⁸Be + ⁴He threshold at $E_R = 0.35$ MeV
 - \Rightarrow ⁸Be + ⁴He \Rightarrow ¹²C* \rightarrow ¹²C+ γ
 - \Rightarrow this corresponds to a 0⁺ excited state 7.7 MeV above the g.s.
- a corresponding state was experimentally confirmed at Caltech at $E E(g.s.) = 7.653 \pm 0.008$ MeV Dunbar et al. 1953, Cook et al. 1957
- this state was an enigma for *ab initio* calculations until 2011 (just hold your breath)

The triple-alpha process



• this reaction involves two fine-tunings [are they related?]

- 1) the ⁸Be nucleus is instable, long lifetime \rightarrow 3 alphas must meet
- 2) the Hoyle state sits just above the continuum threshold
 - \hookrightarrow about 4 out of 10000 decays produce stable carbon

• the reaction rate:

$$au_{3lpha} \sim \exp\left\{-\left(E_{
m Hoyle} - E_{
m (8Be+4He)}
ight)/kT
ight\}$$

An enigma for nuclear theory

- Ab initio calculation in the no-core shell model: $\approx 10^7$ CPU hrs on JAGUAR
- P. Navratil et al., Phys. Rev. Lett. 99 (2007) 042501; R. Roth et al., Phys. Rev. Lett. 107 (2011) 072501



\Rightarrow excellent description, but no trace of the Hoyle state

• Take home message:

If you have a new method, you must solve a problem others could not!



- \hookrightarrow all LECs determined before
- Independent particle and cluster initial states
 - \hookrightarrow results do not depend on this!
 - \hookrightarrow clustering emerges (see later)



A breakthrough - spectrum of carbon-12

Epelbaum, Krebs, Lee, UGM, Phys. Rev. Lett. **106** (2011) 192501 Epelbaum, Krebs, Lähde, Lee, UGM, Phys. Rev. Lett. **109** (2012) 252501

• After 8 • 10⁶ hrs JUGENE/JUQUEEN (and "some" human work)



Spectrum of ¹²C reloaded

Shen, Lähde, Lee, UGM, Nature Commun. 14 (2023) 2777

• New algorithms, new methods, finer & larger lattices \hookrightarrow improved description of ¹²C



ightarrow solidifies earlier NLEFT statements about the structure of the 0^+_2 and 2^+_2 states

Electromagnetic properties

Shen, Lähde, Lee, UGM, Nature Commun. 14 (2023) 2777

• Form factors and transition ffs [parameter-free]:



Sick, McCarthy, Nucl. Phys. A **150** (1970) 631 Strehl, Z. Phys. **234** (1970) 416 Crannell et al., Nucl. Phys. A **758** (2005) 399

Chernykh et al., Phys. Rev. Lett. 105 (2010) 022501

Emergence of geometry

• Use the pinhole algorithm to measure the distribution of α -clusters/matter:



 \hookrightarrow clear signal of alpha (⁴He) particle clustering in these states!

Emergence of duality

• ¹²C spectrum shows a cluster/shell-model duality



• dashed triangles: strong 1p-1h admixture in the wave function

Nuclear binding: A quantum phase transition

Phase transitions



External conditions (like temperature, pressure) change the state of matter
 e.g. ice ^T→water

• and many other examples (pick your favorite)

What is a quantum phase transition?

A quantum phase transition (QPT) is a phase transition between different quantum phases (phases of matter at zero temperature). Contrary to classical phase transitions, quantum phase transitions can only be accessed by varying a physical parameter – such as magnetic field or pressure – at absolute zero temperature.



Vectorized version by AG Caesar, original by DG85 from Wikipedia

- at T = 0 any system is in its lowest energy state
- \hookrightarrow any QPT is driven by quantum fluctuations (Heisenberg's uncertainty principle)
- much thought after in cond. mat./ UC atom systems (spin chains, spin ice, ...)

Vojta, Rept. Prog. Phys. 66 (2003) 2069

• but nuclear physics provides a real-life example!

Prelude: Local and non-local interactions

- General potential: $V(\vec{r}, \vec{r'})$ • Two types of interactions: local: $\vec{r} = \vec{r'}$ non-local: $\vec{r} \neq \vec{r'}$
- Nuclear physics: both types appear: Pion exchange is non-local, often used as local
 → covariant form

$$V(\vec{q},\vec{q}') = -\frac{g_{\pi N}^2}{4m_N^2} \frac{\omega_N'\omega_N}{(\vec{q}'-\vec{q})^2 + M_\pi^2} \left(\frac{\vec{\sigma}_1'\cdot\vec{q}}{\omega_N'} - \frac{\vec{\sigma}_1\cdot\vec{q}}{\omega_N}\right) \left(\frac{\vec{\sigma}_2'\cdot\vec{q}}{\omega_N'} - \frac{\vec{\sigma}_2\cdot\vec{q}}{\omega_N}\right) \xrightarrow{\text{FT}} V(r',r)$$

 \hookrightarrow static pion-exchange ($\omega'_N\simeq\omega_N\simeq 2m_N, ec{k}=ec{q'}-ec{q}$)

$$V(\vec{q})^{\rm loc} = -\frac{g_{\pi N}^2}{4m_N^2} \frac{(\vec{\sigma}_1 \cdot \vec{k})(\vec{\sigma}_2 \cdot \vec{k})}{\vec{k}^2 + M_\pi^2} \xrightarrow{\rm FT} V(r)$$

• let us explore this freedom on the lattice (optimal tool!)

Local and non-local interactions on the lattice

Elhatisari, et al., Phys. Rev. Lett. 117 (2016) 132501 [arXiv:1602.04539]

- Use the lattice and a simplified interactions [not high precsion]
- Taylor two very different interactions:

Interaction A at LO (+ Coulomb)

Non-local short-range interactions

- + One-pion exchange interaction
 - (+ Coulomb interaction)

 \rightarrow tuned to NN phase shifts

Interaction B at LO (+ Coulomb)

Non-local short-range interactions + Local short-range interactions + One-pion exchange interaction

(+ Coulomb interaction)

 \rightarrow tuned to NN + $\alpha\text{-}\alpha$ phase shifts
Phase shifts for interactions A and B

Elhatisari, et al., Phys. Rev. Lett. 117 (2016) 132501 [arXiv:1602.04539]

• NN and α - α phase shifts:



- \rightarrow both interactions do well for NN, but differ for α - α scattering
- ightarrow lpha-lpha interaction is sensitive to the degree of locality of the NN interaction
- \hookrightarrow consequences for nuclei?

Ground state energies I

• Ground state energies for alpha-type nuclei plus ³He:



Ground state energies II

• Ground state energies for alpha-type nuclei (in MeV):

	A (LO)	A (LO+C.)	B (LO)	B (LO+C.)	Exp.
⁴ He	-29.4(4)	-28.6(4)	-29.2(1)	-28.5(1)	-28.3
⁸ Be	-58.6(1)	-56.5(1)	-59.7(6)	-57.3(7)	-56.6
^{12}C	-88.2(3)	-84.0(3)	-95.0(5)	-89.9(5)	-92.2
^{16}O	-117.5(6)	-110.5(6)	-135.4(7)	-126.0(7)	-127.6
²⁰ Ne	-148(1)	-137(1)	-178(1)	-164(1)	-160.6

 \hookrightarrow B (LO+Coulomb) quite close to experiment (within 2% or better) \hookrightarrow A (LO+Coulomb) also fine for lighter nuclei, deviations for $A \ge 12$ \hookrightarrow A (LO) describes a Bose condensate of particles:

> $E(^{8}Be)/E(^{4}He) = 1.997(6)$ $E(^{12}C)/E(^{4}He) = 3.00(1)$ $E(^{16}O)/E(^{4}He) = 4.00(2)$ $E(^{20}Ne)/E(^{4}He) = 5.03(3)$

Consequences for nuclei & nuclear matter

• Define a one-parameter family of interactions that interpolates between the interactions A and B:

$$\left(V_{\lambda} = \left(1 - \lambda
ight) V_A + \lambda \, V_B
ight)$$

- To discuss the many-body limit, we turn off the Coulomb interaction and explore the zero-temperature phase diagram
- As a function of λ, there is a quantum phase transition at the point where the alpha-alpha scattering length vanishes

Stoff, Phys. Rev. A 49 (1994) 3824

• The transition is a first-order transition from a Bose-condensed gas of alpha particles to a nuclear liquid

Zero-temperature phase diagram



- By adjusting the parameter λ in *ab initio* calculations, one can move the of any α -cluster state up and down to alpha separation thresholds.
- \rightarrow This can be used as a new window to view the structure

of these exotic nuclear states

• In particular, one can tune the α - α scattering length to infinity!

 \rightarrow In the absence of Coulomb interactions, one can thus make contact to **universal Efimov physics**:

for a review, see Braaten, Hammer, Phys. Rept. 428 (2006) 259

Hoyle state of 12 C
$$\lambda \rightarrow$$
Universal Efimov trimerSecond 0+ of 16 O $\lambda \rightarrow$ Universal Efimov tetramer

The anthropic principle: A glimpse into the multiverse

The Anthropic Principle (AP)

• so many parameters in the Standard Model, the landscape of string theory, ...

 \Rightarrow The anthropic principle:

"The observed values of all physical and cosmological quantities are not equally probable but they take on values restricted by the requirement that there exist sites where carbon-based life can evolve and by the requirements that the Universe be old enough for it to have already done so."

Carter 1974, Barrow & Tippler 1988, ...

 \Rightarrow can this be tested? / have physical consequences?

• Ex. 1: "Anthropic bound on the cosmological constant" Weinberg (1987) [1044 cites]

• Ex. 2: "The anthropic string theory landscape"

Susskind (2003) [1136 cites]

A prime example of the AP

• Hoyle (1953):

Prediction of an excited level in carbon-12 to allow for a sufficient production of heavy elements (^{12}C , ^{16}O ,...) in stars

• was later heralded as a prime example for the AP:

"As far as we know, this is the only genuine anthropic principle prediction" Carr & Rees 1989

"In 1953 Hoyle made an anthropic prediction on an excited state – 'level of life' – for carbon production in stars" Linde 2007

"A prototype example of this kind of anthropic reasoning was provided by Fred Hoyle's observation of the triple alpha process..." Carter 2006

The relevant question

Date: Sat, 25 Dec 2010 20:03:42 -0600 From: Steven Weinberg (weinberg@zippy.ph.utexas.edu) To: Ulf-G. Meissner (meissner@hiskp.uni-bonn.de) Subject: Re: Hoyle state in 12C

Dear Professor Meissner,

Thanks for the colorful graph. It makes a nice Christmas card. But I have a detailed question. Suppose you calculate not only the energy of the Hoyle state in C12, but also of the ground states of He4 and Be8. How sensitive is the result that the energy of the Hoyle state is near the sum of the rest energies of He4 and Be8 to the parameters of the theory? I ask because I suspect that for a pretty broad range of parameters, the Hoyle state can be well represented as a nearly bound state of Be8 and He4.

All best,

Steve Weinberg

- How does the Hoyle state move relative to the 4He+8Be threshold, if we change the fundamental parameters of QCD+QED?
- not possible in nature, but on a high-performance computer!

NLO EM+IB NNLO Exper

-70

-100

-110

LO

E (MeV)

46



The non-anthropic scenario

• Weinberg's assumption: The Hoyle state stays close to the 4He+8Be threshold



•The AP strikes back: The Hoyle state moves away from the 4He+8Be threshold



Earlier studies of the AP

• rate of the 3
$$lpha$$
-process: $r_{3lpha}\sim\Gamma_{\gamma}\,\exp\left(-rac{\Delta E_{h+b}}{kT}
ight)$
 $\Delta E_{h+b}=E_{12}^{\star}-3E_{lpha}=379.47(18)\,{
m keV}$

- too few ¹⁶O too few ¹²C 10.00 \bigcirc $M(C,0) / M_0(C,0)$ 1.00 0.10 0.01 -150-100-5050 100 0 $\Delta E_{\rm R}$ (keV)
- how much can ΔE_{h+b} be changed so that there is still enough ¹²C and ¹⁶O?

$$\Rightarrow ig|\Delta E_{h+b}| \lesssim 100 ext{ keV}$$

Oberhummer et al., Science **289** (2000) 88 Csoto et al., Nucl. Phys. A **688** (2001) 560 Schlattl et al., Astrophys. Space Sci. **291** (2004) 27 [Livio et al., Nature **340** (1989) 281]

More recent stellar simulations

- ullet Consider a larger range of masses $M_{\star} = (15-40)\,M_{\odot}$
- Consider low $Z = 10^{-4}$ and high $Z = Z_{\odot} \simeq 0.02$ metallicity



 \Rightarrow carbon constraints somewhat weakened

 \Rightarrow stronger constraints from oxygen production

Huang, Adams, Grohs, Astropart. Phys. 105 (2019) 13

 ΔE_R (keV)

Pion mass dependence from MC simulations

• Consider pion mass changes as *small perturbations* for an energy (difference) E_i

$$\begin{split} \frac{\partial E_{i}}{\partial M_{\pi}}\Big|_{M_{\pi}^{\text{ph}}} &= \left.\frac{\partial E_{i}}{\partial M_{\pi}^{\text{OPE}}}\right|_{M_{\pi}^{\text{ph}}} + x_{1} \left.\frac{\partial E_{i}}{\partial m_{N}}\right|_{m_{N}^{\text{ph}}} \\ &+ x_{2} \left.\frac{\partial E_{i}}{\partial g_{\pi N}}\right|_{g_{\pi N}^{\text{ph}}} + x_{3} \left.\frac{\partial E_{i}}{\partial C_{0}}\right|_{C_{0}^{\text{ph}}} + x_{4} \left.\frac{\partial E_{i}}{\partial C_{I}}\right|_{C_{I}^{\text{ph}}} \\ &\text{with} \\ &x_{1} \equiv \left.\frac{\partial m_{N}}{\partial M_{\pi}}\right|_{M_{\pi}^{\text{ph}}}, x_{2} \equiv \left.\frac{\partial g_{\pi N}}{\partial M_{\pi}}\right|_{M_{\pi}^{\text{ph}}} \\ &x_{3} \equiv \left.\frac{\partial C_{0}}{\partial M_{\pi}}\right|_{M_{\pi}^{\text{ph}}}, x_{4} \equiv \left.\frac{\partial C_{I}}{\partial M_{\pi}}\right|_{M_{\pi}^{\text{ph}}} \end{split}$$

- \Rightarrow problem reduces to the calculation of the various derivatives using AFQMC and the determination of the x_i
- x_1 and x_2 can be obtained from LQCD plus CHPT
- $ullet x_3$ and x_4 can be obtained from NN scattering and its M_{π} -dependence $o ar{A}_{s,t}$

Correlations

• vary the quark mass derivatives of $\bar{A}_{s,t} = \partial a_{s,t}^{-1} / \partial M_{\pi}|_{M_{\pi}^{\mathrm{ph}}}$ within $-1, \ldots, +1$:



• clear correlations: the two fine-tunings are not independent

 \Rightarrow has been speculated before but could not be calculated

Weinberg (2001)

The end-of-the-world plot I

 $ullet ~~|\delta(\Delta E_{h+b})| < 100~{
m keV}$

Oberhummer et al., Science (2000)

$$ightarrow \left| \left(0.571(14) ar{A}_s + 0.934(11) ar{A}_t - 0.069(6)
ight) rac{\delta m_q}{m_q}
ight| < 0.0015
ight.$$



An update on fine-tunings in the triple-alpha process 54

Lähde, UGM, Epelbaum, Eur. Phys. J A 56 (2020) 89

• Use lattice data to determine \bar{A}_s and \bar{A}_t :

 $\hookrightarrow ar{A}_s$ is consistent w/ earlier determination $\hookrightarrow ar{A}_t$ changes sign compared to earlier determination

- update x_1 and x_2 using better LQCD data:
 - $x_1 = 0.84(7)$, $x_2 = -0.053(16)$
- $\hookrightarrow x_1$ and x_2 more precise $\hookrightarrow x_2$ now has a definite sign
- \Rightarrow update end-of-the-world plot





New end-of-the-world plots

- Constraints now depend on Z, the nucleus and the sign of δm_q
- lattice values for $\bar{A}_{s,t}$:

The light quark mass is fine-tuned to $\simeq 0.5\,\%$

• chiral EFT values for $\bar{A}_{s,t}$:

The light quark mass is fine-tuned to $\simeq 1...5$ %

• Bound on $\alpha_{\rm EM}$ softened



Lähde, UGM, Epelbaum, Eur. Phys. J A 56 (2020) 89



Bounds from the Big Bang

UGM, Metsch, Meyer, Eur. Phys. J A 59 (2023) 223; Meyer, UGM, JHEP 06 (2024) 074

• Apply the same machinery to element production in the Big Bang

• variations of $\alpha_{\rm EM}$







 \hookrightarrow stronger bounds, in particular from Y_d

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Summary & outlook

Nuclear lattice EFT: a new quantum many-body approach

- \rightarrow based on the successful continuum nuclear chiral EFT
- \rightarrow efficiently combined with stochastic (Monte Carlo) simulations
- \hookrightarrow a number of highly visible results already obtained
- \hookrightarrow much more to come (neutron stars, weak decays, hypernuclei, ...)
- \hookrightarrow amenable to quantum computing

⇒ Nuclear physics is a rich & fascinating field

SPARES

Remarks on Wigner's SU(4) symmetry

- Wigner SU(4) spin-isospin symmetry in the context of pionless nuclear EFT
 - → large scattering lengths Mehen, Stewart, Wise, Phys. Rev. Lett. 83 (1999) 931
- Wigner SU(4) spin-isospin symmetry is particularly beneficial for NLEFT
 - \hookrightarrow suppression of sign oscillations Chen, Lee, Schäfer, Phys. Rev. Lett. **93** (2004) 242302
 - ← provides a very much improved LO action when smearing is included Lu, Li, Elhatisari, Lee, Epelbaum, UGM, Phys. Lett. B **797** (2019) 134863
- Initimately related to α -clustering in nuclei
 - \hookrightarrow cluster states in ¹²C like the famous Hoyle state

Epelbaum, Krebs, Lee, UGM, Phys. Rev. Lett. **106** (2011) 192501

← nuclear physics is close to a quantum phase transition Elhatisari et al., Phys. Rev. Lett. **117** (2016) 132501

Wigner's SU(4) symmetry and the carbon spectrum

 Study of the spectrum of ¹²C Shen, Lähde, Lee, UGM, Eur. Phys.J. A 57 (2021) 276
 → spin-orbit splittings are known to be weak Hayes, Navratil, Vary, Phys. Rev. Lett. 91 (2003) 012502 Johnson, Phys. Rev. C 91 (2015) 034313

 \hookrightarrow start with cluster and shell-model configurations \rightarrow next slide

• Locally and non-locally smeared SU(4) invariant interaction:

$$V = C_{2} \sum_{n',n,n''} \rho_{NL}(n') f_{s_{L}}(n'-n) f_{s_{L}}(n-n'') \rho_{NL}(n'') :, \quad f_{s_{L}}(n) = \begin{cases} 1, & |n| = 0, \\ s_{L}, & |n| = 1, \\ 0, & \text{otherwise} \end{cases}$$
$$\rho_{NL}(n) = a_{NL}^{\dagger}(n) a_{NL}(n)$$
$$a_{NL}^{(\dagger)}(n) = a^{(\dagger)}(n) + s_{NL} \sum_{|n'|=1} a^{(\dagger)}(n+n'), \quad s_{NL} = 0.2$$

 \hookrightarrow only two adjustable parameters (C_2, s_L) fitted to $E_{^4\mathrm{He}}$ & $E_{^{12}\mathrm{C}}$

 \hookrightarrow investigate the spectrum for a = 1.64 fm and a = 1.97 fm

1 1

Configurations

• Cluster and shell model configurations



- Ulf-G. Meißner, The nucleus as a quantum laboratory, ICPS 24, Tiflis, Georgia, August 7, 2024 -

Transient energies

• Transient energies from cluster and shell-model configurations



Spectrum of ¹²C

Shen, Lähde, Lee, UGM, Eur. Phys.J. A 57 (2021) 276 [arXiv:2106.04834]

 \bullet Amazingly precise description \rightarrow great starting point



 \rightarrow solidifies earlier NLEFT statements about the structure of the 0^+_2 and 2^+_2 states

A closer look at the spectrum of ^{12}C

Shen, Lähde, Lee, UGM, Nature Commun. 14 (2023) 2777

• Include also 3NFs:
$$V = \frac{C_2}{2!} \sum_{n} \tilde{\rho}(n)^2 + \frac{C_3}{3!} \sum_{n} \tilde{\rho}(n)^3$$

- Fit the four parameters:
 - C_2, C_3 ground state energies of ⁴He and ¹²C
 - $s_{\rm L}$ radius of ¹²C around 2.4 fm
 - *s*_{NL} best overall description of the transition rates
- Calculation of em transitions
 requires coupled-channel approach
 e.g. 0⁺ and 2⁺ states



The hidden spin-isospin exchange symmetry

Nucleon-nucleon interaction in large- N_C

Kaplan, Savage, Phys. Lett. 365B (1996) 244; Kaplan, Manohar, Phys. Rev. C 56 (1997) 96

• Performing the large- N_C analysis:

$$V_{\text{large}-N_c}^{2\text{N}} = V_C + W_S \,\vec{\sigma}_1 \cdot \vec{\sigma}_2 \vec{\tau}_1 \cdot \vec{\tau}_2 + W_T \,S_{12} \vec{\tau}_1 \cdot \vec{\tau}_2 + \dots$$

- Leading terms are $\sim N_C$
- First corrections are $1/N_C^2$ suppressed, fairly strong even for $N_C = 3$
- Velocity-dependent corrections can be incorporated
- Based on spin-isospin exchange symmetry of the nucleon w.f. $d_\uparrow \leftrightarrow u_\downarrow$ or on the nucleon level $n_\uparrow \leftrightarrow p_\downarrow$
- Constraints on 3NFs: Phillips, Schat, PRC 88 (2013) 034002; Epelbaum et al., EPJA 51 (2015) 26

Hidden spin-isospin symmetry: Basic ideas

Lee, Bogner, Brown, Elhatisari, Epelbaum, Hergert, Hjorth-Jensen, Krebs, Li, Lu, UGM, Phys. Rev. Lett. 127 (2021) 062501 [2010.09420 [nucl-th]]

• $V_{large-N_c}^{2N}$ is not renomalization group invariant:

$$rac{dV_{\mu}(p,p')}{d\mu}
eq 0$$

 \simeq implicit setting of a preferred renormalization/resolution scale

• How does this happen?

- high energies: corrections to the nucleon w.f. are $\sim v^2$
 - ightarrow these high-energy modes must be $\mathcal{O}(1/N_C^2)$ in our low-energy EFT
 - ightarrow momentum resolution scale $\Lambda \sim m_N/N_C \sim {\cal O}(1)$
 - ightarrow consistent with the cutoff in a Δ less th'y $\sim \sqrt{2m_N(m_\Delta-m_N)}$
- low energies: the resolution scale must be large enough,

so that orbital angular momentum and spin are fully resolved

ightarrow as nucleon size is independent of N_C , so should be $\Lambda_{-}\sqrt{}$

• as will be shown, the optimal scale (where corrections are $\sim 1/N_C^2$) is:

 $\Lambda_{\mathrm{large}-N_c}\simeq 500\,\mathrm{MeV}$

Nucleon-nucleon phase shifts – lattice

Lee, Bogner, Brown, Elhatisari, Epelbaum, Hergert, Hjorth-Jensen, Krebs, Li, Lu, UGM, Phys. Rev. Lett. **127** (2021) 062501 [2010.09420 [nucl-th]]

• Use N3LO action (w/ TPE absorbed in contact interactions) at a=1.32 fm

 $\hookrightarrow \Lambda = \pi/a = 470 \, {\rm MeV}$

- \bullet compare S=0, T=1 w/ S=1, T=0
- S-waves: switch off the tensor force in 3S_1
- D-waves: average the spin-triplet channel
- NLEFT low-energy constants

ch., order	LEC (l.u.)	ch., order	LEC (l.u.)
$^1\mathrm{S}_0, Q^0$	1.45(5)	$^3\mathrm{S}_1, Q^0$	1.56(3)
$^1\mathrm{S}_0, Q^2$	-0.47(3)	$^3\mathrm{S}_1,Q^2$	-0.53(1)
$^1\mathrm{S}_0, Q^4$	0.13(1)	$^3\mathrm{S}_1,Q^4$	0.12(1)
$^1\mathrm{D}_2,Q^4$	-0.088(1)	$^{3}\mathrm{D_{all}},Q^{4}$	-0.070(2)

 \Rightarrow works pretty well



Nucleon-nucleon phase shifts – continuum

• Consider various (chiral) continuum potentials \rightarrow also works $\sqrt{}$



····· IDAHO N3LO

--- IDAHO N4LO ($\Lambda = 500$ MeV)

• - • - CD-Bonn Bochum N4⁺LO ($\Lambda = 400 - 550$ MeV)

• • • Nijmegen PWA

Entem, Machleidt, PRC **68** (2003) 041001 Entem, Machleidt, Nosyk PRC **96** (2017) 024004 Machleidt, PRC **63** (2001) 024001 eV) Reinert, Krebs, Epelbaum, EPJA **54** (2018) 86 Wiringa, Stoks, Schiavilla, PRC **51** (1995) 38

Two-nucleon matrix elements

 Consider the ME between any two-nucleon states A and B. Both have total spin S and total isospin T. Then (for isospin-inv. H):

$$M(S,T) = rac{1}{2S+1} \sum_{S_z=-S}^{S} \langle A; S, S_z; T, T_z | H | B; S, S_z; T, T_z
angle$$

- Spin-isospin exchange symmetry: $\left(M(S,T)=M(T,S)\right)$
- Ex: ³⁰P has 1 proton + 1 neutron in the $1s_{1/2}$ orbitals (minimal shell model)
- ightarrow if spin-isospin exchange symmetry were exact, the S=0, T=1 & S=1, T=0 states should be degenerate
- Data: The 1⁺ g.s. is 0.677 MeV below the 0⁺ excited state ($E_{g.s.} \simeq 220$ MeV)
- ightarrow fairly good agreement, consistent w/ $1/N_C^2$ corrections
- \rightarrow explanation: interactions of the np pair with the ²⁸Si core are suppressing spatial correlations of the 1⁺ w.f. caused by the tensor interaction

Two-nucleon matrix elements in the s-d shell

- Test the spin-isospin echange symmetry for general two-body MEs 1s-0d shell
- Use the spin-tensor analysis developed by Kirson, Brown et al.
 Kirson, PLB 47 (1973) 110; Brown et al., JPhysG 11 (1985) 1191; Ann. Phys. 182 (1988) 191
- Seven two-body MEs for (S,T) = (1,0) and (S,T) = (0,1)

ME	L_1	L_2	L_3	L_4	L_{12}	L_{34}
1	2	2	2	2	0	0
2	2	2	2	2	2	2
3	2	2	2	2	4	4
4	2	2	2	0	2	2
5	2	2	0	0	0	0
6	2	0	2	0	2	2
7	0	0	0	0	0	0

 L_1, L_2 : orbital angular momenta of the outgoing orbitals of A L_{12} : total angular momentum of state A L_3, L_4 : orbital angular momenta of the outgoing orbitals of B L_{34} : total angular momentum of state AME 7 corresponds to the $1s_{1/2}$ orbitals discussed before set $L_Z = (L_{12})_z = (L_{34})_z$, average over L_z

 \rightarrow Work out M(S,T) for various forces at $\Lambda = 2.0, 2.5, 3.0, 3.5$ fm⁻¹

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Two-nucleon matrix elements in the s-d shell

• Results for the AV18 and N3LO chiral potentials


Two-nucleon matrix elements: Conclusions

- As anticipated:
 - The optimal resolution scale is obviously $\Lambda \sim 500\,\text{MeV}$
 - For $\Lambda < \Lambda_{\mathrm{large}-N_c}$, the (S,T)=(1,0) channel is more attractive
 - For $\Lambda > \Lambda_{\mathrm{large}-N_c}$, the (S,T)=(0,1) channel is more attractive
 - These results do not depend on the type of interaction, while AV18 is local, chiral N3LO has some non-locality (and similar for more modern interactions like chiral N4⁺LO)
 - \hookrightarrow consistent with the results for NN scattering

 \Rightarrow Validates Weinberg's power counting! \checkmark

Three-nucleon forces

• Leading central three-nucleon force at the optimal resolution scale:

$$\begin{split} V^{3\mathrm{N}}_{\mathrm{large}-N_c} &= V^{3\mathrm{N}}_C + [(\vec{\sigma}_1 \times \vec{\sigma}_2) \cdot \vec{\sigma}_3] [(\vec{\tau}_1 \times \vec{\tau}_2) \cdot \vec{\tau}_3] W^{3\mathrm{N}}_{123} \\ &+ \vec{\sigma}_1 \cdot \vec{\sigma}_2 \vec{\tau}_1 \cdot \vec{\tau}_2 W^{3\mathrm{N}}_{12} + \vec{\sigma}_2 \cdot \vec{\sigma}_3 \vec{\tau}_2 \cdot \vec{\tau}_3 W^{3\mathrm{N}}_{23} \\ &+ \vec{\sigma}_3 \cdot \vec{\sigma}_1 \vec{\tau}_3 \cdot \vec{\tau}_1 W^{3\mathrm{N}}_{31} + \dots, \end{split}$$

• Subleading central 3N interactions are of size $1/N_C$, of type

 $ec{\sigma}_1\cdotec{\sigma}_2[(ec{ au}_1 imesec{ au}_2)\cdotec{ au}_3]\,, \qquad [(ec{\sigma}_1 imesec{\sigma}_2)\cdotec{\sigma}_3]ec{ au}_1\cdotec{ au}_2$

- ⇒ helps in constraining the many short-range three-nucleon interactions that appear at higher orders in chiral EFT
- The spin-isospin exchange symmetry of the leading interactions also severely limits the isospin-dependent contributions of the 3N interactions to the nuclear EoS
- ⇒ relevant for calculations of the nuclear symmetry energy and its density dependence in dense nuclear matter

Ab Initio Nuclear Thermodynamics

 B. N. Lu, N. Li, S. Elhatisari, D. Lee, J. Drut, T. Lähde, E. Epelbaum, UGM, Phys. Rev. Lett. **125** (2020) 192502 [arXiv:1912.05105]

Phase diagram of strongly interacting matter



- Ulf-G. Meißner, The nucleus as a quantum laboratory, ICPS 24, Tiflis, Georgia, August 7, 2024 -

Pinhole trace algorithm (PTA)

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



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

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

 allows to study: liquid-gas phase transition → this talk thermodynamics of finite nuclei
 thermal dissociation of hot nuclei
 cluster yields of dissociating nuclei

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 ($t_{
 m CPU} \sim V N^2$ vs. $t_{
 m CPU} \sim V^3 N^2$)
- \bullet Only a mild sign problem \rightarrow 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 $\rightarrow \Lambda = \pi/a = 470$ MeV , $a_t \simeq 0.1$ fm consider $T = 10 \dots 20$ MeV

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

• very favorable scaling for generating config's:

$$\Delta t \sim N^2 L^3$$

Chemical potential

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



[–] Ulf-G. Meißner, The nucleus as a quantum laboratory, ICPS 24, Tiflis, Georgia, August 7, 2024 –

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/fm³, $\rho_c = 0.089(18)$ fm⁻³



⁻ Ulf-G. Meißner, The nucleus as a quantum laboratory, ICPS 24, Tiflis, Georgia, August 7, 2024 -

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0.06(2)

 $\rho_{\rm c}$

 $0.31(7) \text{MeV/fm}^3$ Experiment: T_c

P_c fm

15.0(3) MeV,

Vapor-liquid phase transition

- Vapor-liquid phase transition in a finite volume $V \& T < T_c$
- the most probable configuration for different nucleon number ${oldsymbol{A}}$

• the free energy

• chemical potential $\mu = \partial F / \partial A$



CENTER-of-MASS PROBLEM

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

 $egin{aligned} Z_A(au) &= \langle \Psi_A(au) | \Psi_A(au)
angle \ &| \Psi_A(au)
angle &= \exp(-H au/2) | \Psi_A
angle \end{aligned}$



• but: translational invariance requires summation over all transitions

 $Z_A(au) = \sum_{i_{
m com}, j_{
m com}} \langle \Psi_A(au, i_{
m com}) | \Psi_A(au, j_{
m com})
angle, \ \ {
m com} = {
m mod}((i_{
m com} - j_{
m com}), L)$

 $i_{\rm com}~(j_{\rm com})=$ 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.:

$$egin{aligned} &
ho_{i_1,j_1,\cdots i_A,j_A}(\mathrm{n}_1,\cdots \mathrm{n}_A)\ &=:
ho_{i_1,j_1}(\mathrm{n}_1)\cdots
ho_{i_A,j_A}(\mathrm{n}_A): \end{aligned}$$

MC sampling of the amplitude:

$$\begin{array}{l} \text{MC sampling of the amplitude:} & & & \\ A_{i_1,j_1,\cdots i_A,j_A}(\mathbf{n}_1,\ldots,\mathbf{n}_A,L_t) & & \\ = \langle \Psi_A(\tau/2) | \rho_{i_1,j_1,\cdots i_A,j_A}(\mathbf{n}_1,\ldots,\mathbf{n}_A) | \Psi_A(\tau/2) \rangle \end{array}$$

- Allows to measure proton and neutron distributions
- Resolution scale $\sim a/A$ as cm position $\mathbf{r_{cm}}$ is an integer $\mathbf{n_{cm}}$ times a/A

 $\tau_i = \tau$



Similarity renormalization group studies

Timoteo, Szpigel, Ruiz Arriola, Phys. Rev. C 86 (2012) 034002

• Investigation of Wigner SU(4) symmetry using the SRG, use AV18:



• At the scale $\lambda_{\text{Wigner}} \simeq 3 \text{ fm}^{-1}$ one has $V_{^{1}S_{0},\text{Wigner}}(p',p) \approx V_{^{3}S_{1},\text{Wigner}}(p',p)$