Ruprecht Machleidt:
Legacies in the *ab initio* No-Core Shell Model results

(4 PRLs, 1 Nature Commun, 1 PLB)

Presented at NTSE2024 – Busan
by
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"Rup" participated in
NTSE2013 – Ames
& Delivered Keynote Address
NTSE2014 – Khabarovsk
NTSE2018 – Daejeon

Origin of the NCSM: CD-Bonn + AV8' (OLS transformed)

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Properties of ^{12}C in the *Ab Initio* Nuclear Shell Model

P. Navrátil,[1,2] J.P. Vary,[3] and B.R. Barrett[1]

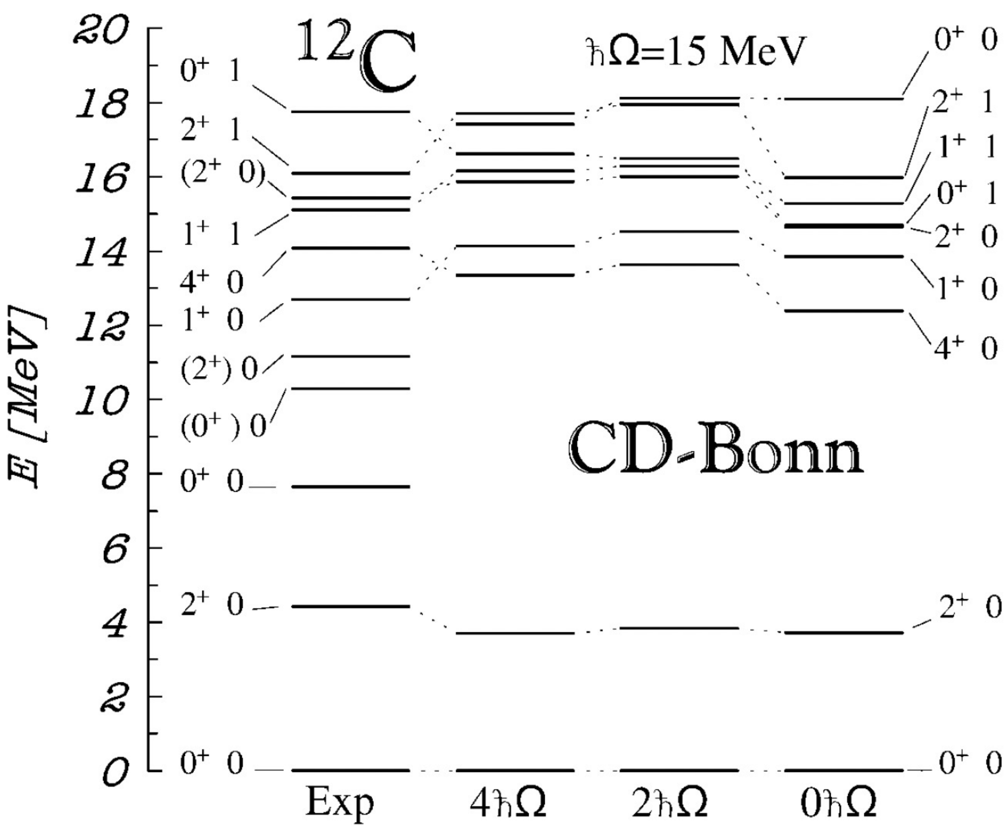


FIG. 1. Experimental and theoretical positive-parity excitation spectra of ^{12}C. Results obtained in $4\hbar\Omega$, $2\hbar\Omega$, and $0\hbar\Omega$ model spaces are compared. The effective interaction was derived from the CD Bonn *NN* potential in a HO basis with $\hbar\Omega = 15$ MeV. The experimental values are from Ref. [21].

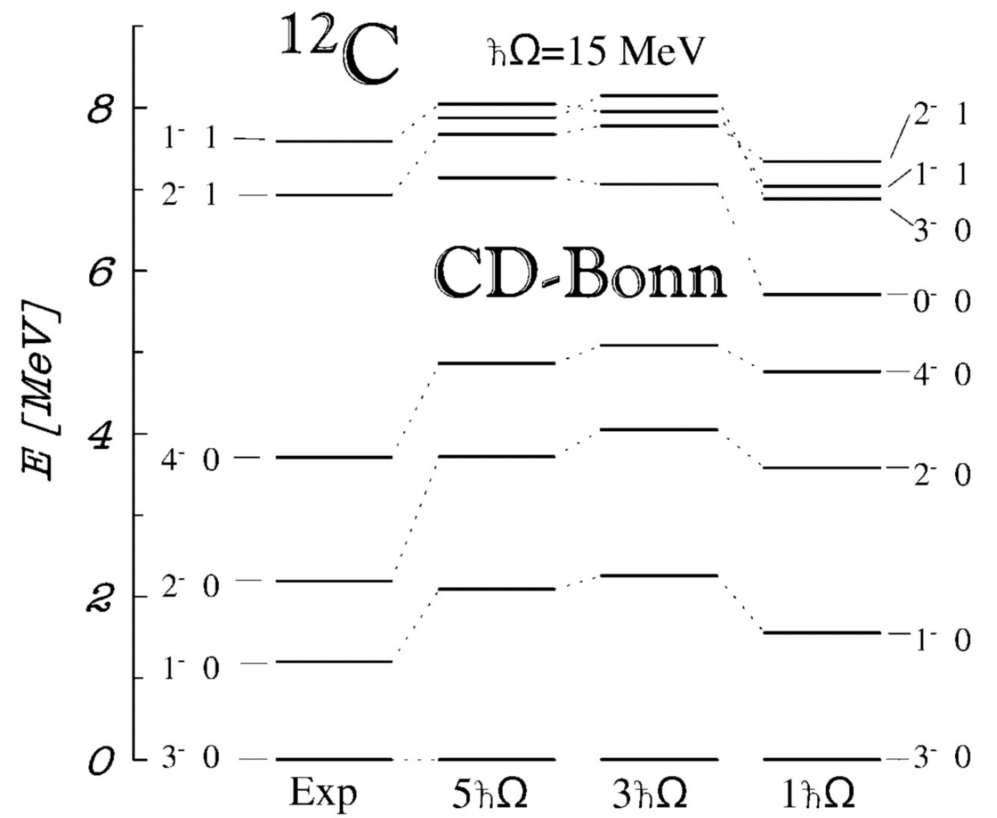


FIG. 2. Experimental and theoretical negative-parity spectra of ^{12}C. Results obtained in $5\hbar\Omega$, $3\hbar\Omega$, and $1\hbar\Omega$ model spaces are compared. Other factors are the same as in Fig. 1.

CD-Bonn: R. Machleidt, F. Sammarruca, and Y. Song, Phys. Rev. C 53, 1483 (1996).

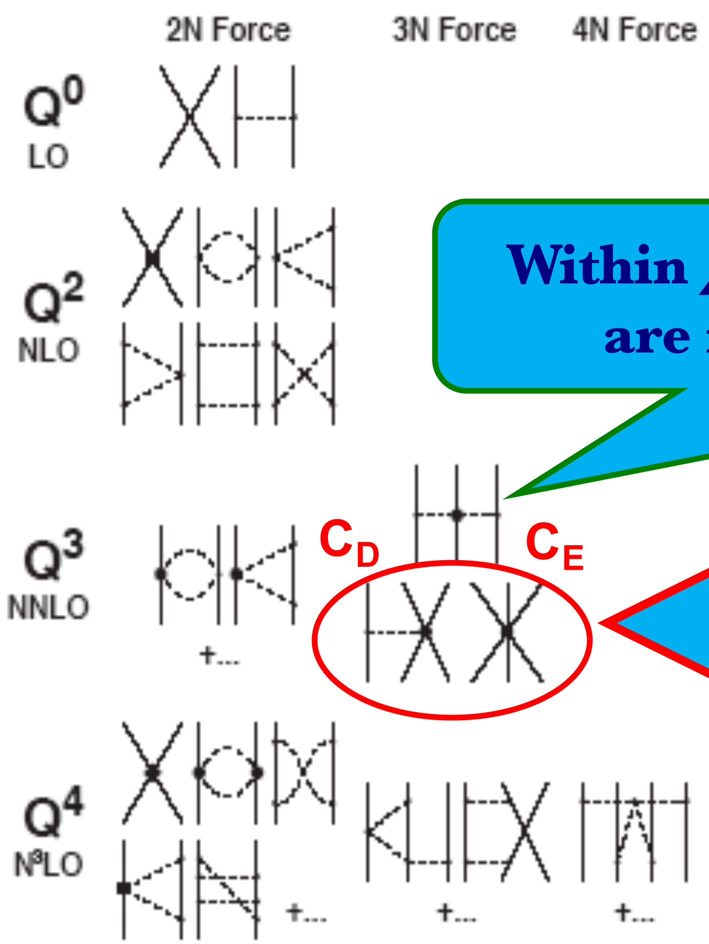
Effective Nucleon Interaction

Chiral Perturbation Theory (χPT)

Weinberg's χPT allows for controlled power series expansion

Expansion parameter : $\left(\frac{Q}{\Lambda_\chi}\right)^{\upsilon}$, $Q-$momentum transfer,

$\Lambda_\chi \approx 1\ GeV$, χ - symmetry breaking scale



Within χPT 2π-NNN Low Energy Constants (LEC) are related to the NN-interaction LECs $\{c_i\}$

Additional terms from χPT with LECs specific to NNN systems

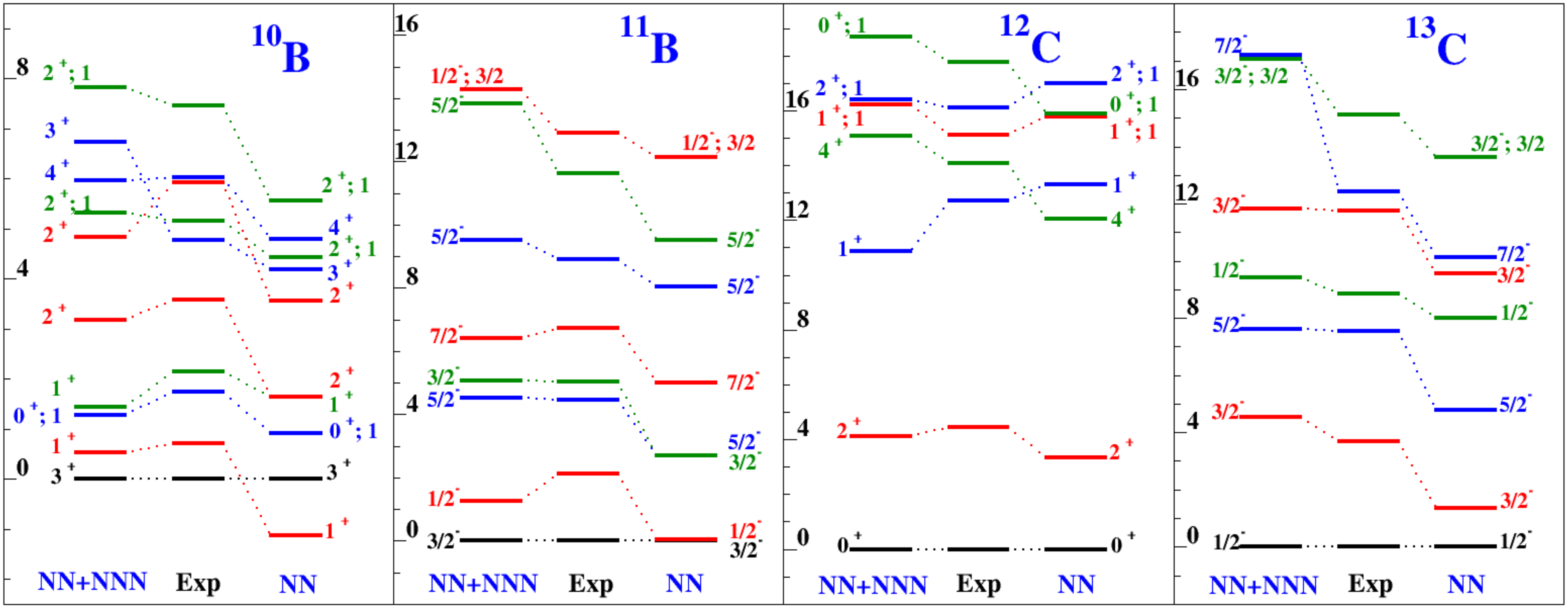
Regularization is essential, which is also implicit within the Harmonic Oscillator (HO) wave function basis (see below)

Adapted from P. Navratil slide

R. Machleidt and D.R. Entem, Phys. Rep. 503, 1 (2011);
E. Epelbaum, H. Krebs, U.-G Meissner, Eur. Phys. J. A51, 53 (2015); Phys. Rev. Lett. 115, 122301 (2015)

ab initio NCSM with χ_{EFT} Interactions

NNN interactions produce correct ^{10}B ground state spin and overall spectral improvements



$c_D = -1$

Chiral EFT NN (N3LO): D. R. Entem and **R. Machleidt**, Phys. Rev. C 68, 041001(R) (2003).
Chiral EFT NNN (N2LO): U. van Kolck, Phys. Rev. C 49, 2932 (1994);
E. Epelbaum, A. Nogga, W. Glöckle, H. Kamada, Ulf-G. Meißner, and H. Witała, Phys. Rev. C 66, 064001 (2002).
R. Machleidt and D.R. Entem, Phys. Rep. 503, 1 (2011)

P. Navratil, V.G. Gueorguiev, J. P. Vary, W. E. Ormand and A. Nogga, Phys Rev Lett 99, 042501(2007); ArXiV: nucl-th 0701038.

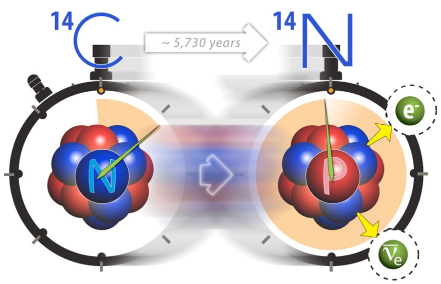
PRL **106,** 202502 (2011) PHYSICAL REVIEW LETTERS week ending 20 MAY 2011

Origin of the Anomalous Long Lifetime of ^{14}C

P. Maris,[1] J. P. Vary,[1] P. Navrátil,[2,3] W. E. Ormand,[3,4] H. Nam,[5] and D. J. Dean[5]

Employed the same Chiral NN + NNN as above

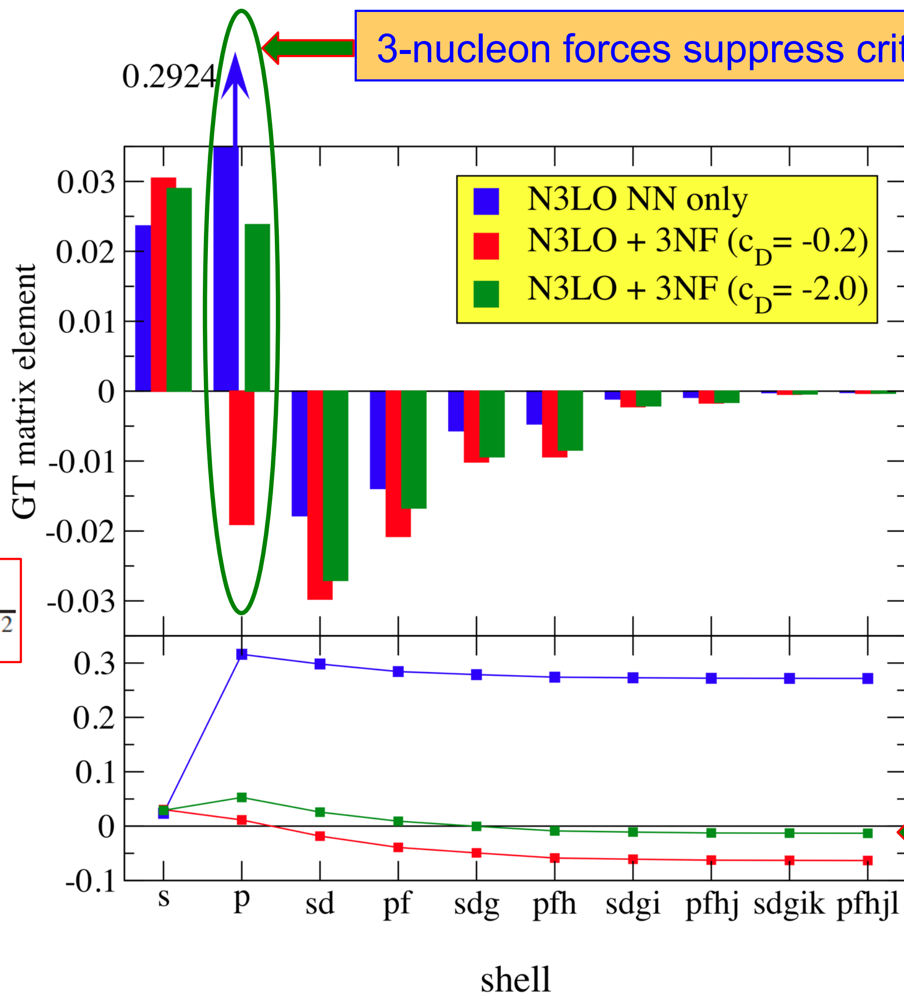
- Solves the puzzle of the long but useful lifetime of ^{14}C
- Establishes a major role for strong 3-nucleon forces in nuclei
- Strengthens foundation for guiding experiments



$$T_{1/2} = \frac{1}{f(Z, E_0)} \frac{2\pi^3\hbar^7 \ln 2}{m_e^5 c^4 G_V^2} \frac{1}{g_A^2 |M_{GT}|^2}$$

$$M_{GT} = \sum_k \langle \Psi_f || \sigma(k)\tau_+(k) || \Psi_i \rangle$$

3-nucleon forces suppress critical component



- Dimension of matrix solved for 8 lowest states ~ 1x10^9
- Each run takes ~ 6 hours on 215,000 cores on Cray XT5 Jaguar at ORNL
- "Scaling of *ab initio* nuclear physics calculations on multicore computer architectures," P. Maris, M. Sosonkina, J. P. Vary, E. G. Ng and C. Yang, 2010 Intern. Conf. on Computer Science, Procedia Computer Science 1, 97 (2010)

net decay rate
Is very small

Daejeon16 NN interaction

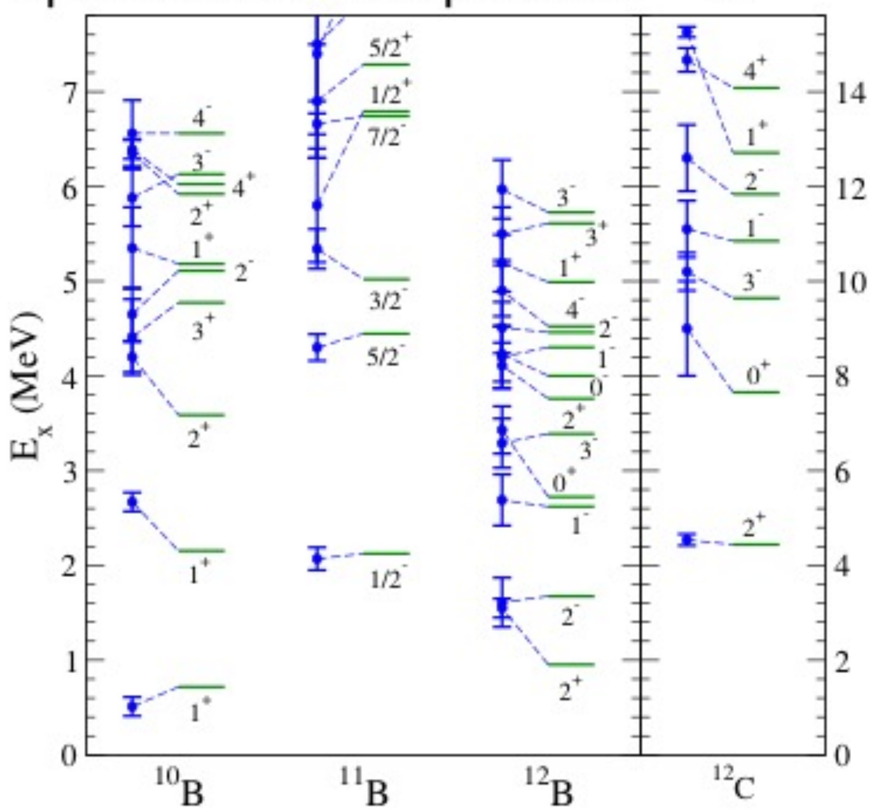
Based on SRG evolution of Entem-Machleidt "500" chiral N3LO to $\lambda = 1.5\ \mathrm{fm}^{-1}$ followed by Phase-Equivalent Transformations (PETs) to fit selected properties of light nuclei.

A.M. Shirokov, I.J. Shin, Y. Kim, M. Sosonkina, P. Maris and J.P. Vary,
"N3LO NN interaction adjusted to light nuclei in ab exitu approach,"
Phys. Letts. B 761, 87 (2016); arXiv: 1605.00413

Application to excited states of p-shell nuclei

(Maris, Shin, Vary, in preparation)

Spectra of B isotopes and ^{12}C

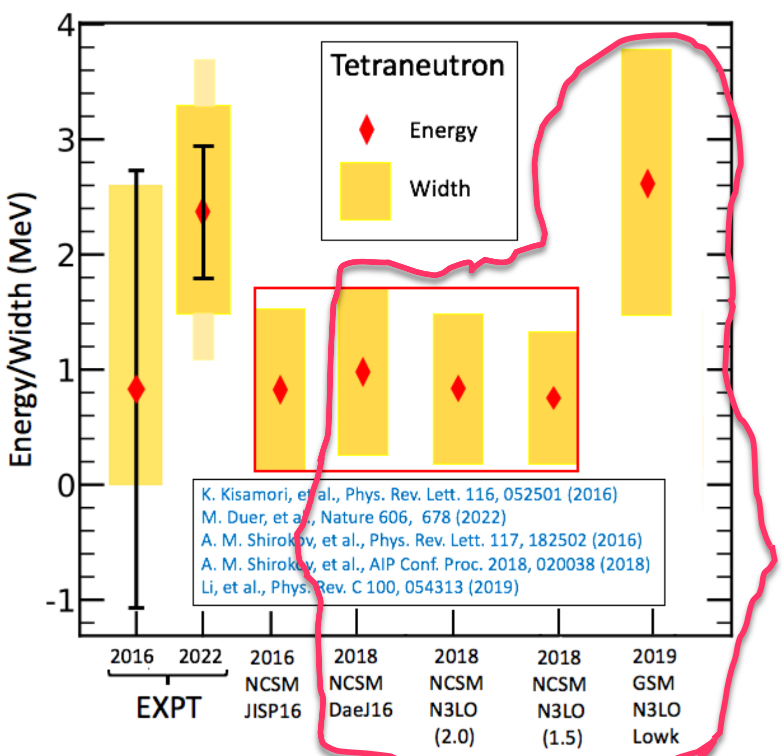


- difference of extrapolated E_b
- extrapolation uncertainties: max of E_b uncertainties
- good agreement with positive and negative parity spectra
- need large bases for 'intruder' and 'non-normal parity' states
- spectrum ^{10}B
  - correct gs 3^+ and excited 1^+
  - third 1^+ 'intruder' state
- excited 0^+ state in ^{12}C
  - Hoyle state?
  - see MCNCSM results below

Tetraneutron discovery confirms prediction

Objectives

- *Ab initio* nuclear theory aims for parameter-free predictions of nuclear properties with controlled uncertainties using supercomputer simulations
- Specific goal is to predict if the tetraneutron (4-neutron system) has a bound state, a low-lying resonance or neither



Experiment and theory for the tetraneutron's resonance energy and width. *Ab initio* No-Core Shell Model (NCSM) and Gamow Shell Model (GSM) predictions use different neutron-neutron interactions and different basis function techniques.

Impact

- Discovery in 2022 announced in Nature [1] confirms *ab initio* theory predictions from 2016 [2] of a short-lived tetraneutron resonance at low energy and the absence of a tetraneutron bound state
- Demonstrates the predictive power of *ab initio* nuclear theory since theory and experiment are within their combined uncertainties
- Sets stage for further experimental and theoretical research on new states of matter formed only of neutrons
- Shows need to anticipate a long wait time for experimental confirmation of such an exotic phenomena, ~ 6 years in this case
- Emphasizes the value of DOE supercomputer allocations (NERSC) and support for multi-disciplinary teamwork (SciDAC/NUCLEI)

Accomplishments

[1] M. Duer, et al., Nature 606, 678 (2022)

[2] A.M. Shirokov, G. Papadimitriou, A.I. Mazur, I.A. Mazur, R. Roth and J.P. Vary, "Prediction for a four-neutron resonance," Phys. Rev. Lett. 117, 182502 (2016)

Alpha clusters in Carbon-12 from ab initio theory & statistical learning

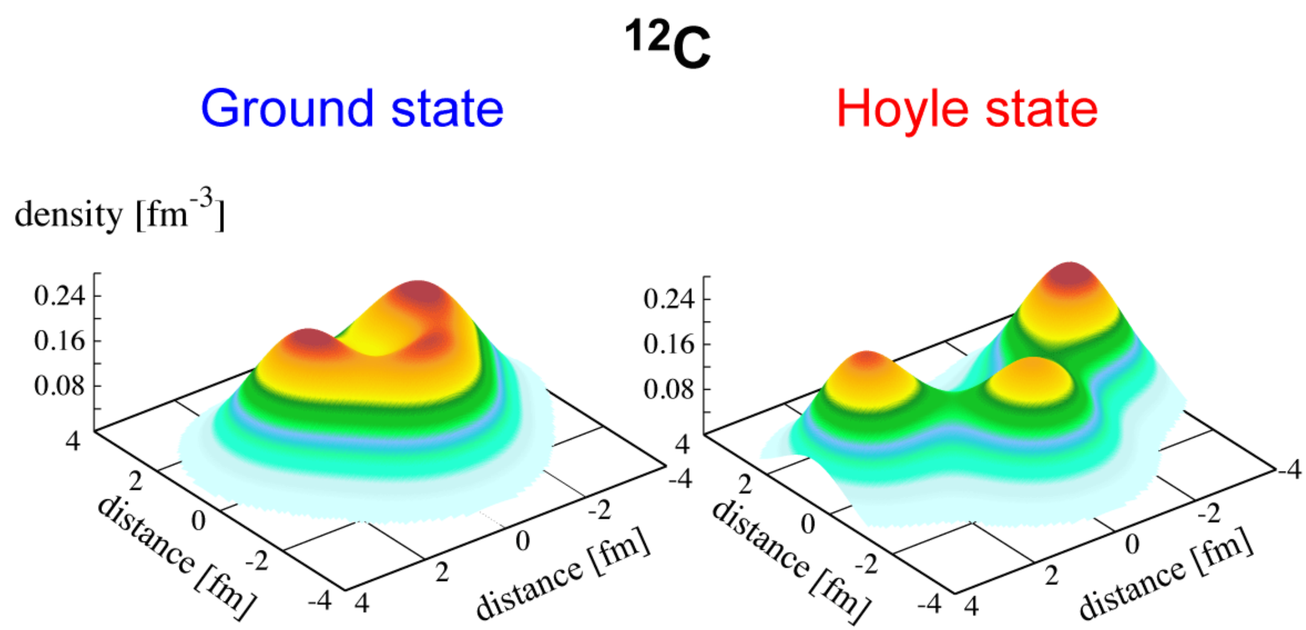
Objectives

- *Ab initio* nuclear theory aims for parameter-free predictions of critical nuclear properties with controlled uncertainties using supercomputer simulations
- Specfic goal is to determine extent of alpha clustering in the Ground state and the Hoyle state of Carbon-12 (^{12}C)

Impact

- Ground state found to have 6% alpha clustering while Hoyle state discovered to be 3-alphas 61% of the time
- With this high percentage of 3-alphas, the Hoyle state is confirmed as a natural gateway state for the cosmic formation of ^{12}C, the key element for organic life
- Statistical learning confirms 3-alpha feature of Hoyle state

Ab initio Monte-Carlo Shell Model results for density contours of 12C Ground state and first excited 0^+ (Hoyle) state using the Daejeon16 two-nucleon potential. Simulations were performed on Fugaku in Japan, the world's largest supercomputer at the time.



Accomplishments

T. Otsuka, T. Abe, T. Yoshida, Y. Tsunoda, N. Shimizu, N. Itagaki, Y. Utsuno, J. Vary, P. Maris and H. Ueno, "Alpha-Clustering in Atomic Nuclei from First Principles with Statistical Learning and the Hoyle State Character," Nature Communications 13:2234 (2022)

Thank you, Rup,

for your pioneering contributions to Physics