Static, Transition & Scattering Observables from the No-Core Shell Model

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LENPIC Annual Meeting

Helmholtz-Institut
fuer Strahlen and Kernphysik
(HISKP)

Bonn, Germany

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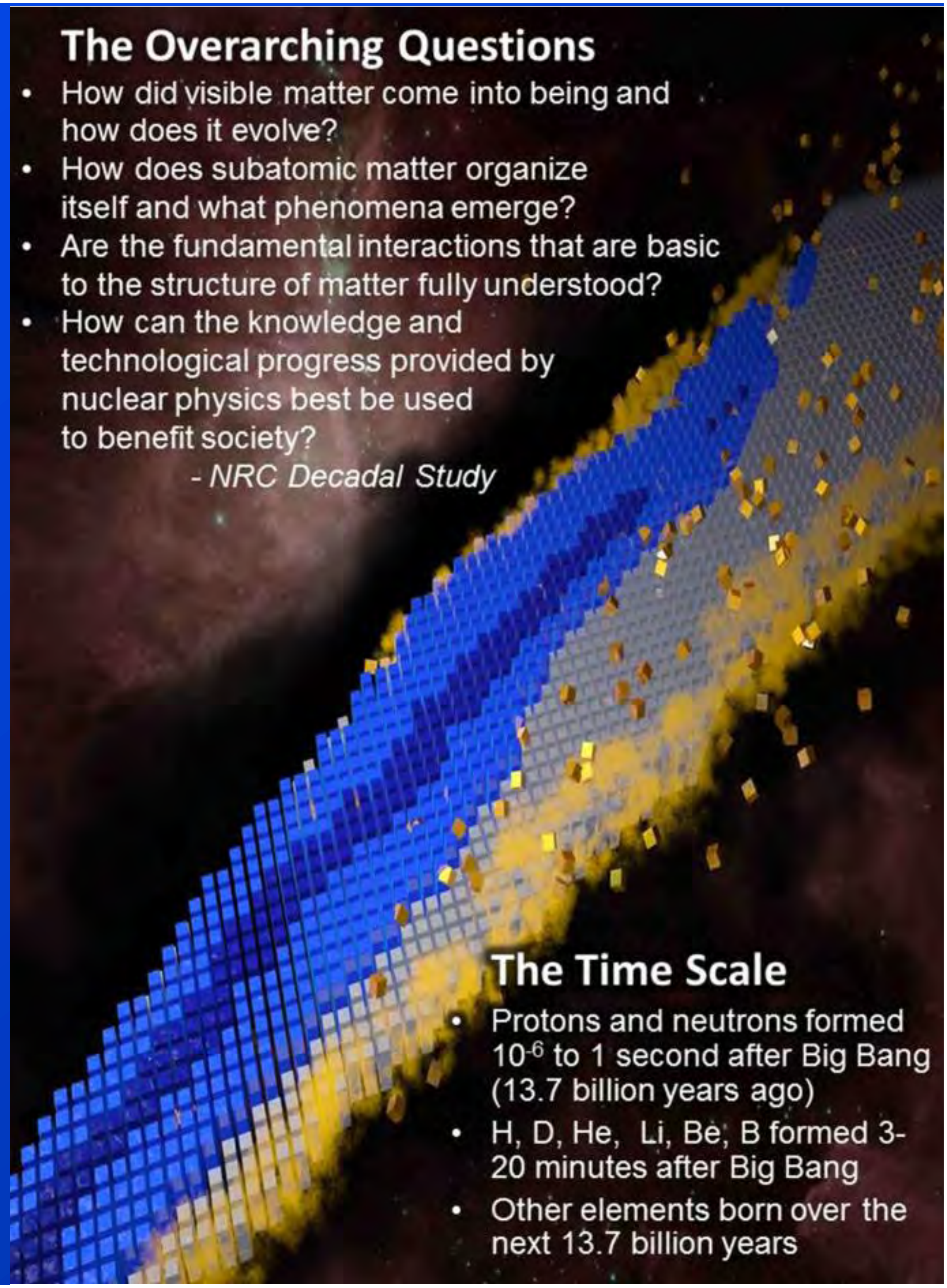
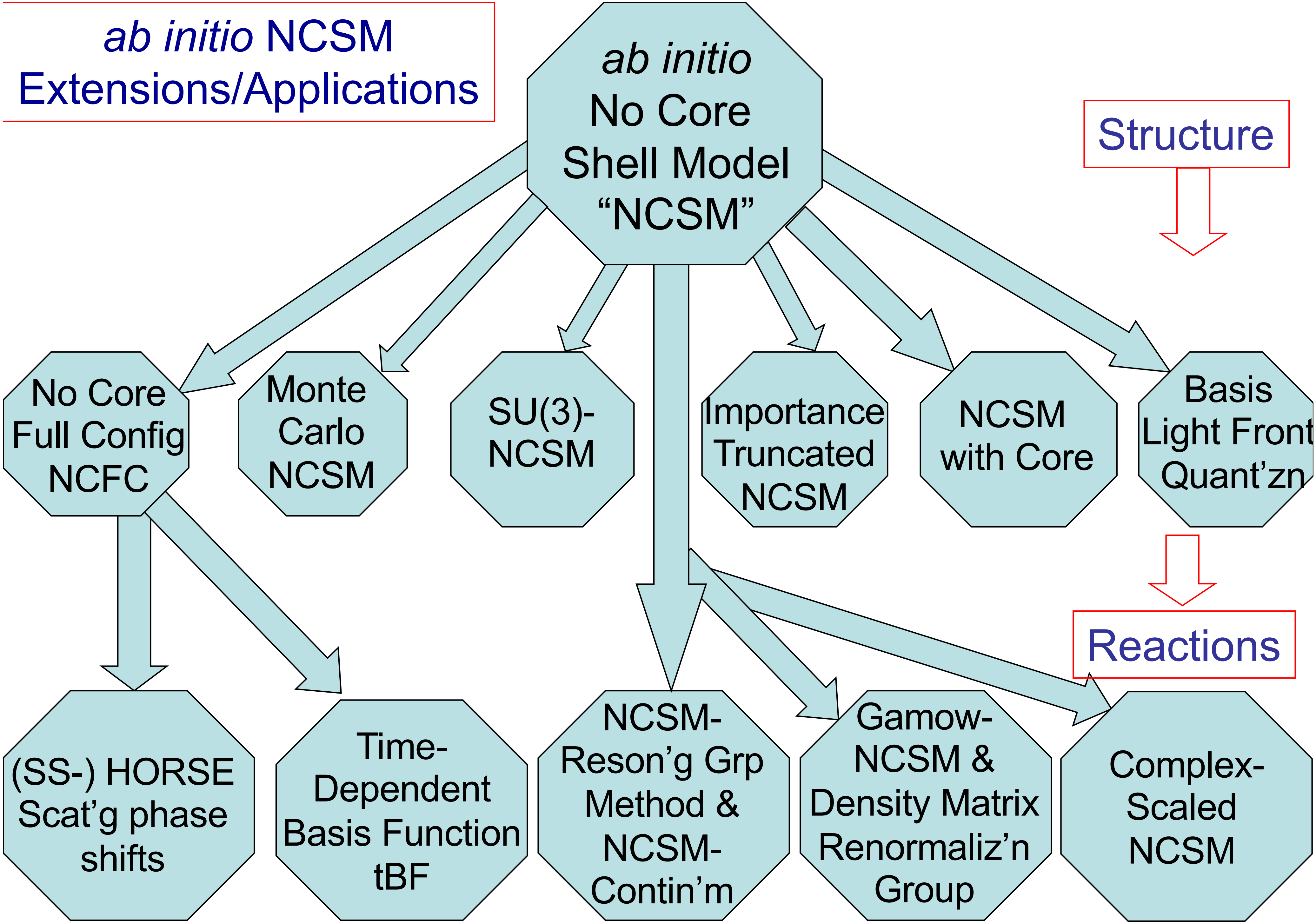


ab initio NCSM Extensions/Applications



Daejeon16 NN interaction

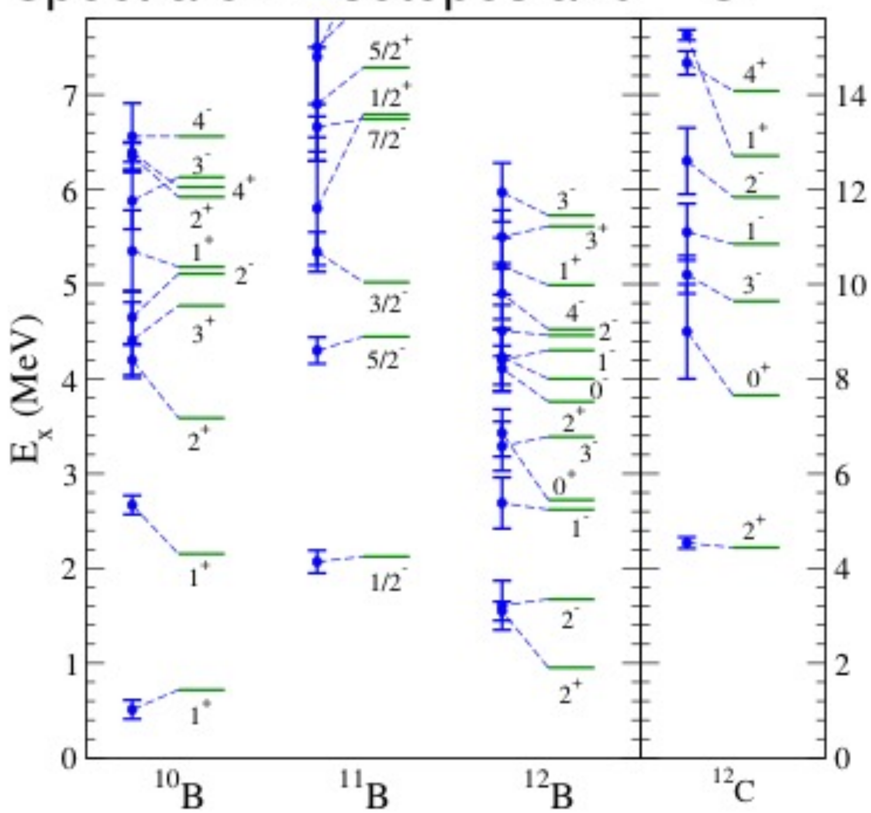
Based on SRG evolution of Entem-Machleidt "500" chiral N3LO to $\lambda = 1.5\ \mathrm{fm}^{-1}$ followed by Phase-Equivalent Transformations (PETs) to fit selected properties of light nuclei.

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?
  - Otsuka et al, Nature Comm 13:2234 (2022)

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

U.S. DEPARTMENT OF ENERGY | Office of Science

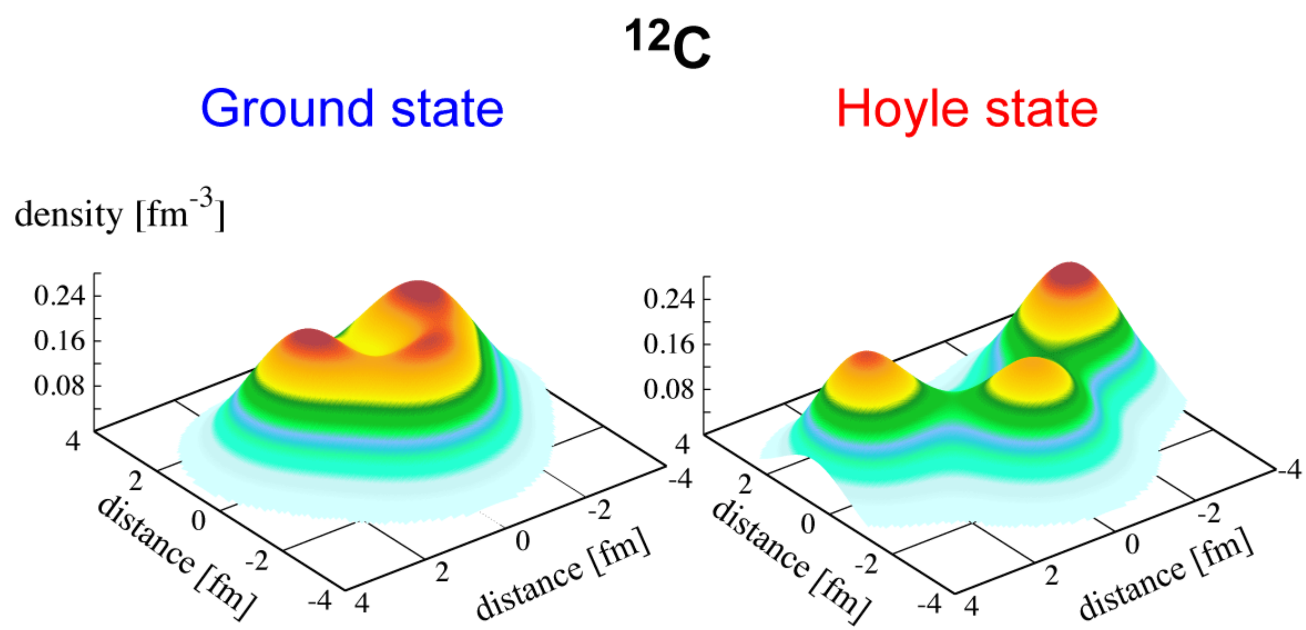
NUCLEI Nuclear Computational Low-Energy Initiative

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.

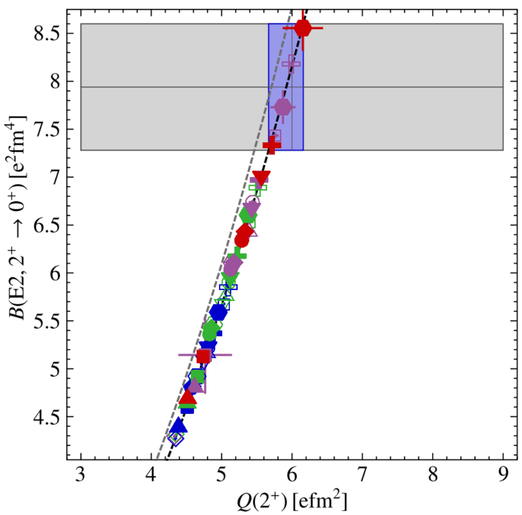
Accomplishments

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)

Electric quadrupole (E2) observables in nuclei

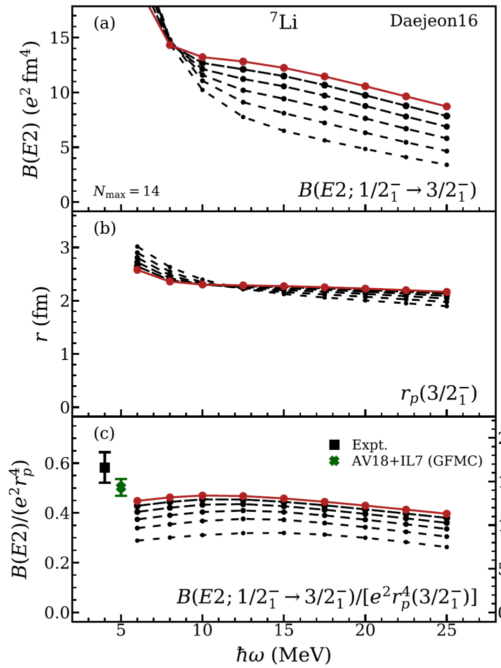
- Electric quadrupole (E2) observables, such as the electric quadrupole moment Q_p, and E2 transition strength B(E2), reveal nuclear collective structure and dynamics.
- To probe the nuclear quadrupole dynamics more completely, both proton and neutron quadrupole observables are needed.
- E2 observables are sensitive to the large-distance tails of the nuclear wave function, they are slowly convergent in ab initio NCSM approaches. Useful predictions for static and dynamic E2 observables have been derived by focusing on selected ratios.

Ratios of E2 observables calculated by NCSM



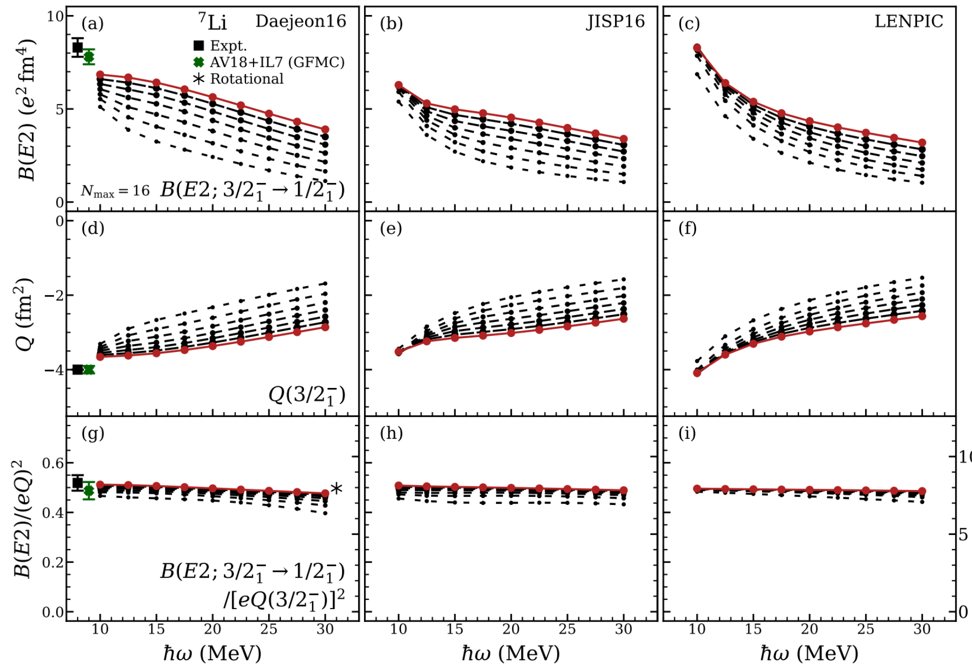
Robust correlation between the two *E2* observables: quadrupole moments and transition strengths

2_1^+ to 0_1^+ in ^{12}C
Chiral *NN* (open symbols)
NN + *3N* (solid symbols)
From N_{max} = 2 to 8, $\hbar\Omega$ = 16 MeV
Grey shaded: experimental result
Blue shaded: NCSM prediction



The convergence patterns of the *E2* transition strengths and radius are strongly correlated

$1/2_1^-$ to $3/2_1^-$ in ^{7}Li
Daejeon16 interaction
From Nmax = 4 to14
Square: experimental result
Cross: GFMC prediction

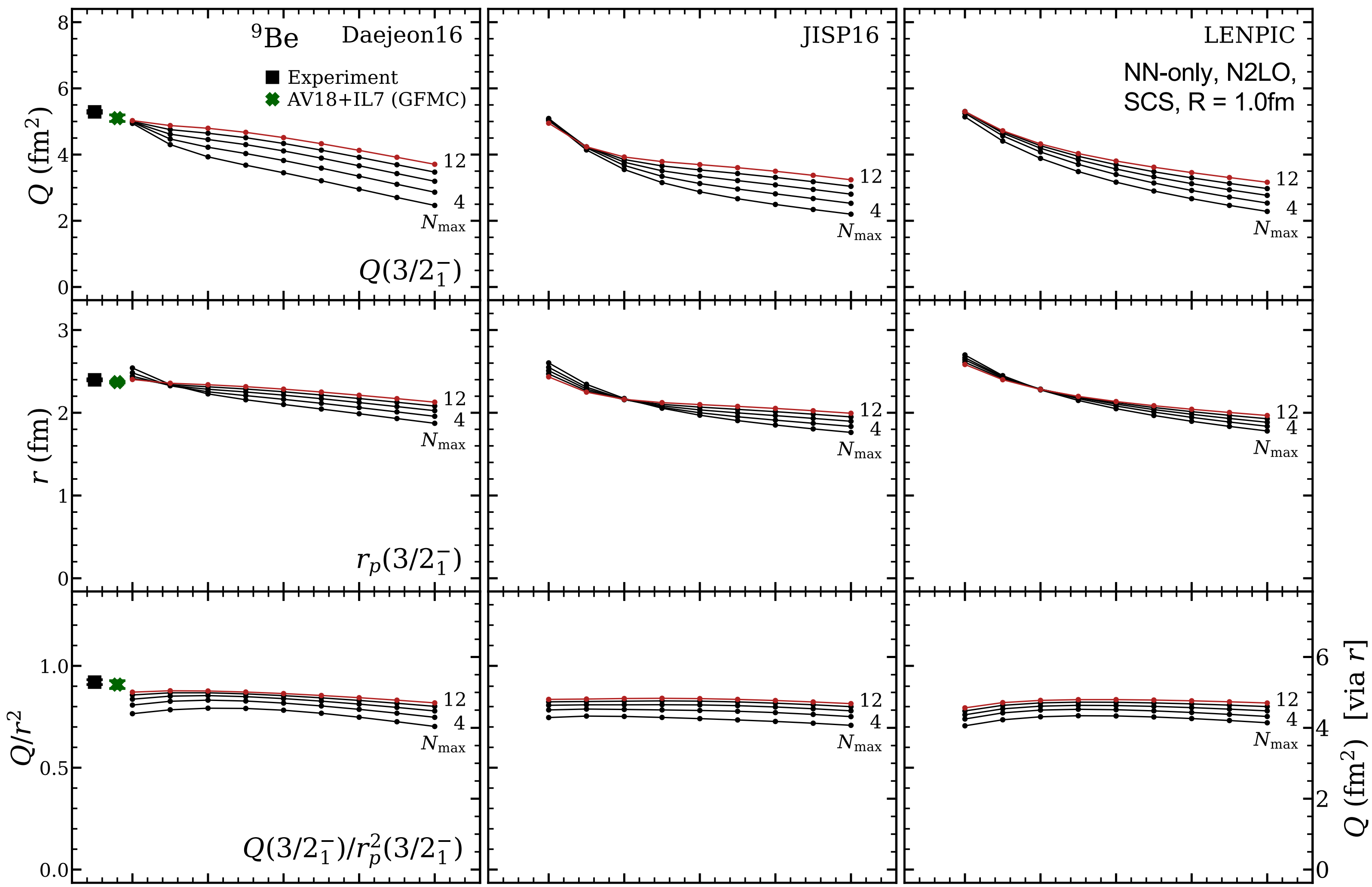


A near-complete elimination of the *hω* dependence at the higher N_{max} is shown with the dimensionless ratio $B(E2)/Q^2$

$3/2_1^-$ to $1/2_1^-$ in ^{7}Li with Daejeon16, JISP16 and LENPIC
From Nmax = 4 to16
Square: experimental result
Cross: GFMC prediction
Asterisk: rotational ratio

A. Calci et al., Phys. Rev. C (2016)
M. Caprio et al., Phys. Rev. C (2021)
M. Caprio et al., Phys. Rev. C (2022)

^{9}Be: $E2$ moment correlation with radius



M. A. Caprio, University of Notre Dame

GFMC: S. Pastore, S. C. Pieper, R. Schiavilla, and R. B. Wiringa, Phys. Rev. C **87**, 035503 (2013).

M. A. Caprio, P. J. Fasano, and P. Maris, Phys. Rev. C 105, L061302 (2022), and new paper in preparation

$$\frac{B(E2)}{Q_p^2} = \frac{\langle J_f || \sum_{i\in p} r_i^2 Y_2(\hat{r}_i) || J_i \rangle^2}{\langle J_i || \sum_{i\in p} r_i^2 Y_2(\hat{r}_i) || J_i \rangle^2},$$

Ratios of observables converge better
He Li, et al., arXiv: 2401.05776

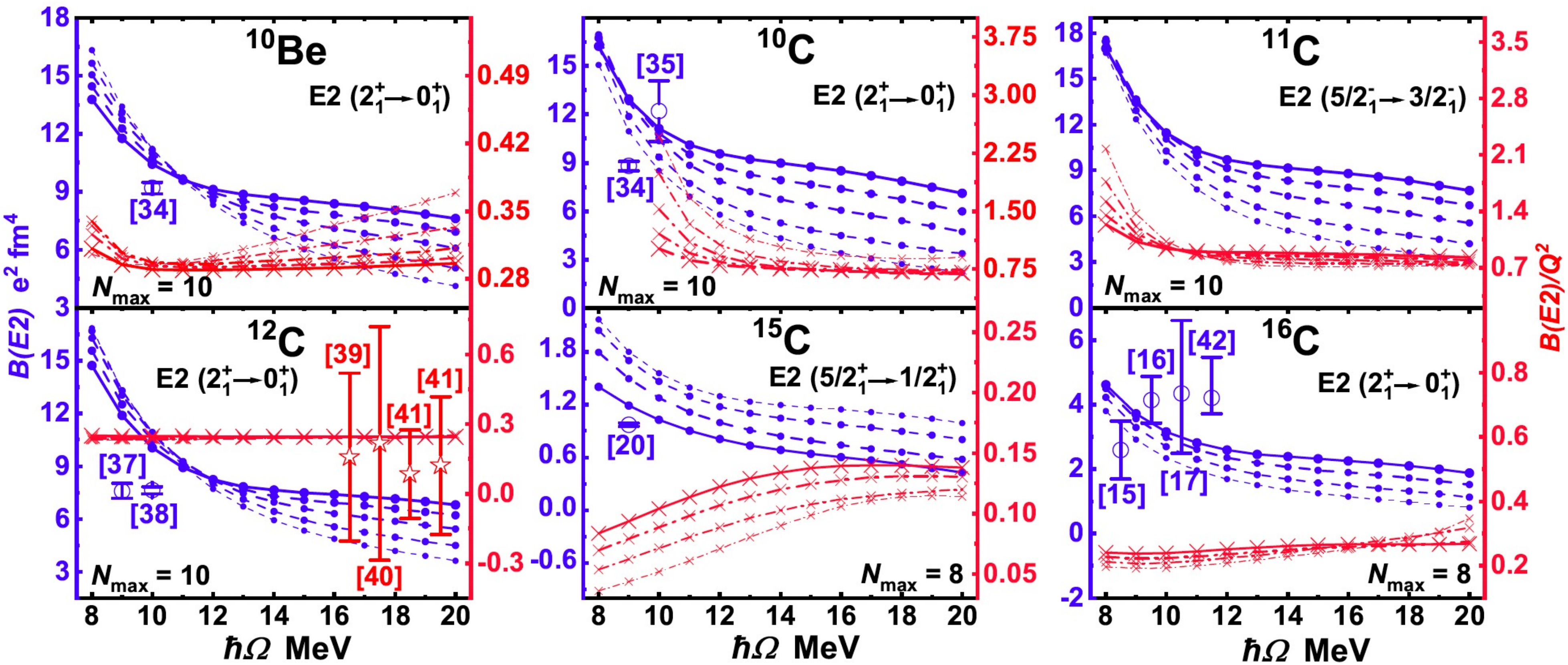


FIG. 1. (Color online) $B(E2)$ (blue and scales to the left) and the ratios $B(E2)/Q_p^2$ (red and scales to the right) in ^{10}Be, ^{10}C, ^{11}C, ^{12}C, ^{15}C, ^{16}C for the indicated transitions are shown as functions of $\hbar\Omega$. NCSM results with Daejeon16 NN interaction are shown by the dashed curves with thickness increasing with $N_{\max}$ for $N_{\max} = 2, 4, 6$ for ^{15,16}C, and $N_{\max} = 2, 4, 6, 8$ for the other nuclei. The maximal $N_{\max}$ value is indicated at the bottom of each panel and is represented by the solid curves. For comparison, the available experimental $B(E2)$ and $B(E2)/Q_p^2$ data with their uncertainties are shown by open circles and stars respectively, with the citation indicated in square brackets.

$$\frac{M_n}{M_p} = \frac{\langle J_f || \sum_{i \in n} r_i^2 Y_2(\hat{r}_i) || J_i \rangle}{\langle J_f || \sum_{i \in p} r_i^2 Y_2(\hat{r}_i) || J_i \rangle},$$

Ratios of observables and
ratios of ratios converge better
He Li, et al., arXiv: 2401.05776

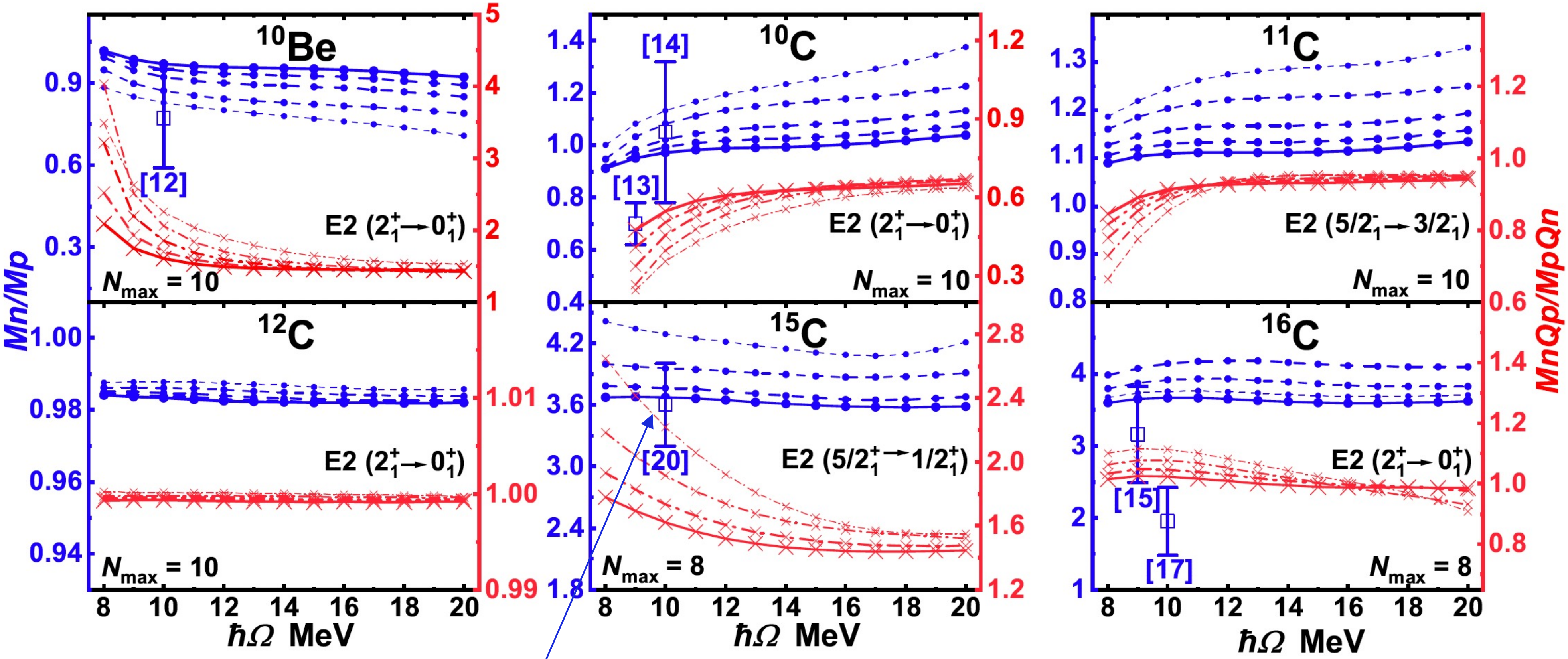
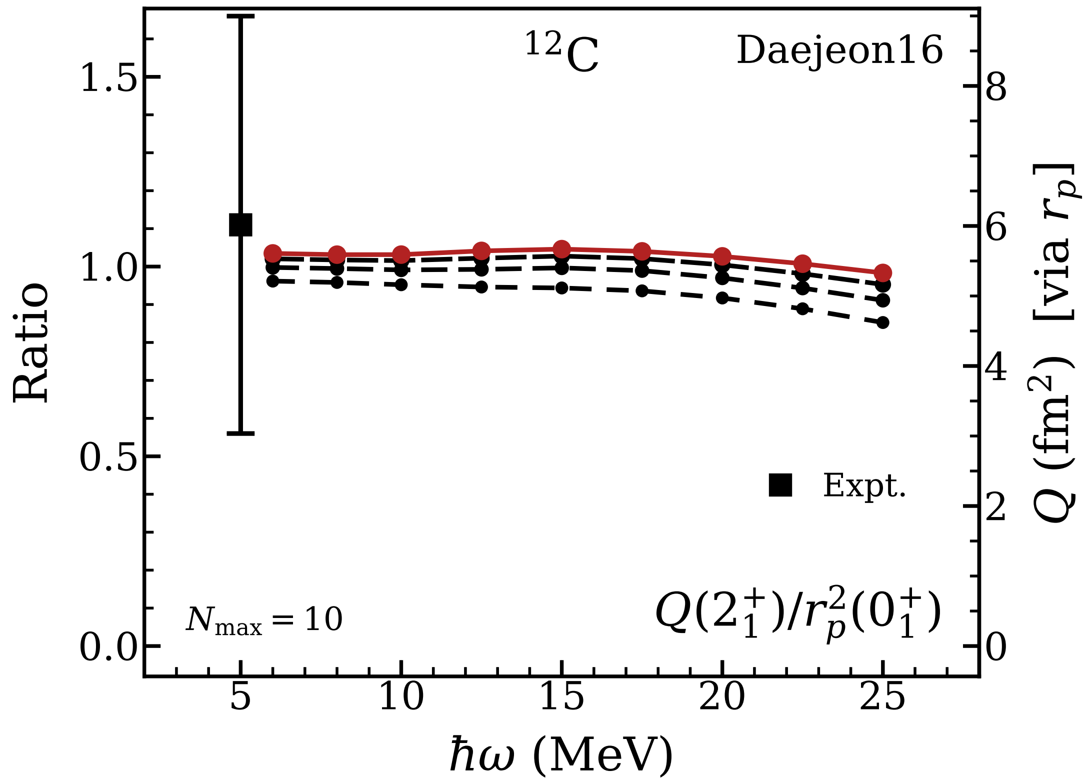
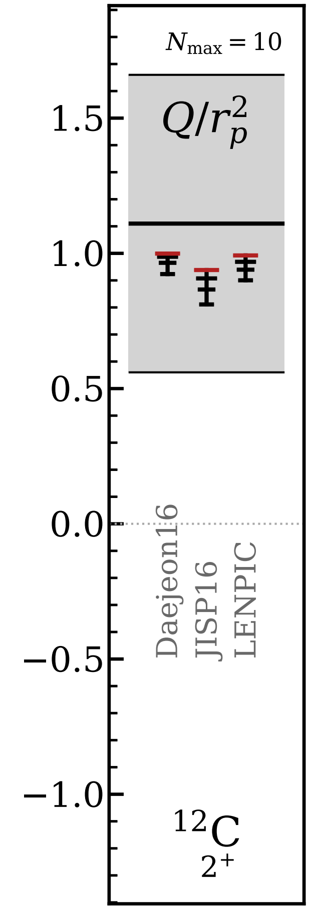


FIG. 2. (Color online) Ratios M_n/M_p (blue and scales to the left) and M_nQ_p/M_pQ_n (red and scales to the right) in the same nuclei and for the same transitions as in Fig. 1. See Fig. 1 for more details. Available experimental M_n/M_p results with their uncertainties are shown by open squares with the citation indicated in square brackets.

Jie Chen et al.,
PRC 106, 064312 (2022)

Excited-state quadrupole moment from radius in ^{12}C





$Q(2_1^+) = +6(3)\,\mathrm{fm}^2$ Vermeer 1983 (Stone 2016)

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Ab Initio Nucleon-Nucleus scattering

INSTITUTE OF NUCLEAR & PARTICLE PHYSICS INPP

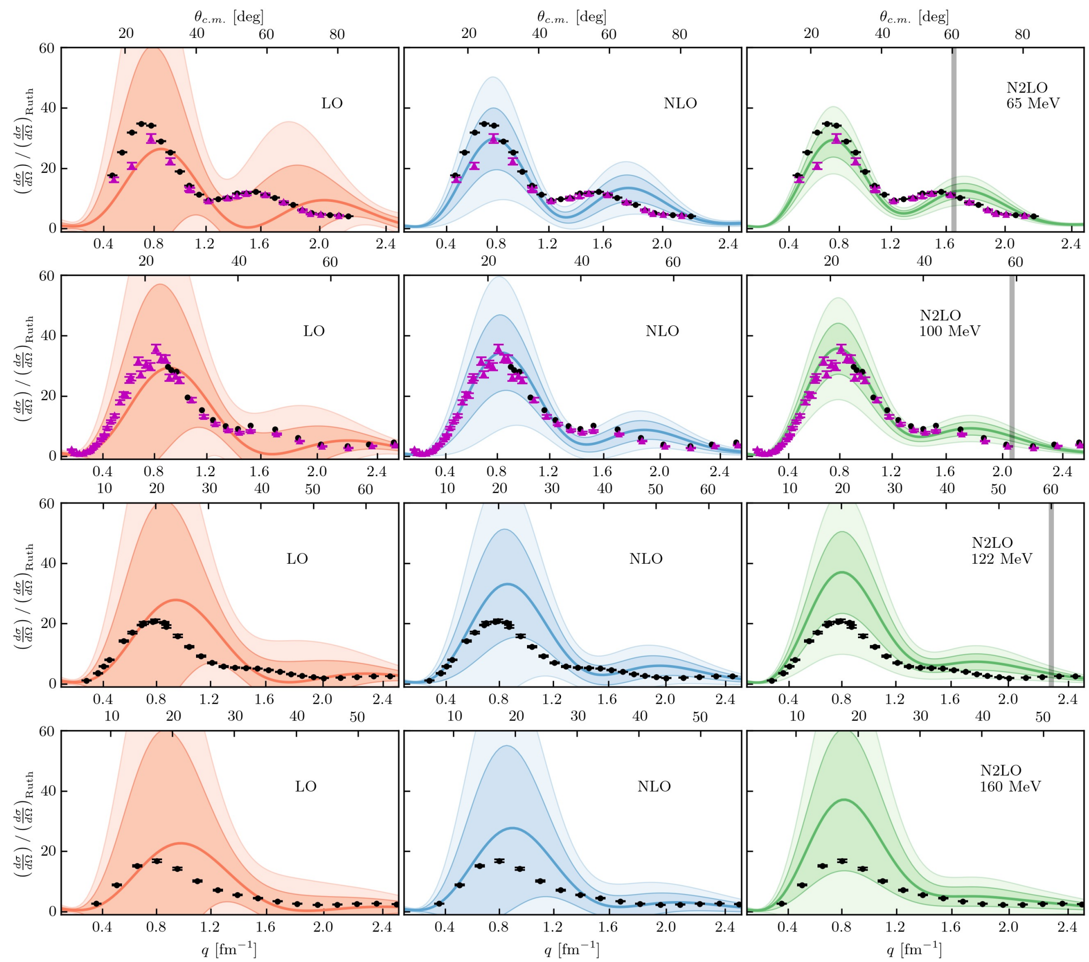
NUCLEI Nuclear Computational Low-Energy Initiative

Objectives

- Predict elastic scattering of nucleons on light nuclei with theoretical uncertainty estimates.
- Use consistent effective field theory (EFT) nucleon-nucleon interactions for both scattering and bound state calculations.
- Apply Bayesian statistical model to infer EFT truncation uncertainties.

Impact

- First nucleon-nucleus scattering calculations using nucleon-nucleon interactions with quantified EFT truncation uncertainties.
- Uncertainties increase with increasing scattering energies.
- Need to incorporate higher orders, as well as consistent three-nucleon interactions.



Differential cross section for elastic proton scattering on Carbon-12 with quantified uncertainties.

Accomplishments

R.B. Baker, B. McClung, Ch. Elster, P. Maris, S.P. Weppner, M. Burrows, G. Popa, Phys. Rev. C106, 064605 (2022);
R.B. Baker, M. Burrows, Ch. Elster, K.D. Launey, P. Maris, G. Popa, S.P. Weppner, Front. Phys. 10, 1071971 (2022)

General idea of the HORSE formalism

"Harmonic Oscillator Representation of Scattering Equations"

$$T + V$$

NCSM with:
$\lambda(N,\hbar\Omega)$ & $\Lambda(N,\hbar\Omega)$

Infinite set of algebraic equations in HO basis of relative motion:

$$\sum_{n'=0}^{N}\left(T^{l}_{nn'}+V^{l}_{nn'}-\delta_{nn'}E\right)a_{n'l}(E)=0. \qquad n\le N-1$$

Matching condition at $n = N$

$$\sum_{n'=0}^{N}\left(T^{l}_{Nn'}+V^{l}_{Nn'}-\delta_{Nn'}E\right)a_{n'l}(E)+T^{l}_{N,N+1}a_{N+1,l}(E)=0. \quad n\le N-1$$

Then for $n\ge N+1$

$$\sum_{n'=0}^{\infty}\left(T^{l}_{nn'}-\delta_{nn'}E\right)a_{n'l}(E)=0,$$ which produces:

$$T^{l}_{n,n-1}a_{n-1,l}(E)+\left(T^{l}_{nn}-E\right)a_{nl}(E)+T^{l}_{n,n+1}a_{n+1,l}(E)=0.$$

"think outside the box"=> T

Arises as a natural extension of NCSM where both potential and kinetic energies are truncated

This is an exactly solvable algebraic problem!

Single-State HORSE (SS-HORSE)

$$\sum_{n'=0}^{N} H^{l}_{nn'} \langle n' | \lambda \rangle = E_{\lambda} \langle n | \lambda \rangle, \qquad n \le N$$

$$(H-E)^{-1}_{nn'} \equiv -G_{nn'} = \sum_{\lambda'=0}^{N} \frac{\langle n | \lambda' \rangle \langle \lambda' | n' \rangle}{E_{\lambda'} - E}$$

← Standard HORSE

$$\tan\delta(E) = -\frac{S_{Nl}(E) - G_{NN} T^{l}_{N,N+1} S_{N+1,l}(E)}{C_{Nl}(E) - G_{NN} T^{l}_{N,N+1} C_{N+1,l}(E)}.$$ Also, S-matrix = $S(G_{NN})$

Suppose $E = E_{\lambda'}$ ← Single-State HORSE

$$\tan\delta(E_{\lambda}) = \frac{S_{N+1,l}(E_{\lambda})}{C_{N+1,l}(E_{\lambda})} = (-1)^{l} q^{2l+1} \Gamma(-l+\tfrac{1}{2}) \frac{L^{l+1/2}_{(N-l)/2}(q^{2})}{\Phi(-N/2 - l/2 - 1/2, -l+1/2; q^{2})}$$

where $L^{l+1/2}_{(N-l)/2}$ are associated Laguerre polynomials, Φ are confluent hyper-geometric functions and $q = \sqrt{\frac{2E_{\lambda}}{\hbar\Omega}}$.

E_{λ} are (obtained from) eigenvalues of the NCSM (for given $\hbar\Omega$ and N_{max}). Once a scattering channel is defined (sets the continuum energy scale) the phase shift is calculated. Analog of Lüscher's method for a plane-wave basis.

A.M. Shirokov, A.I. Mazur, I.A. Mazur and J.P. Vary, PRC 94, 064320 (2016); arXiv:1608.05885

Example of nα scattering

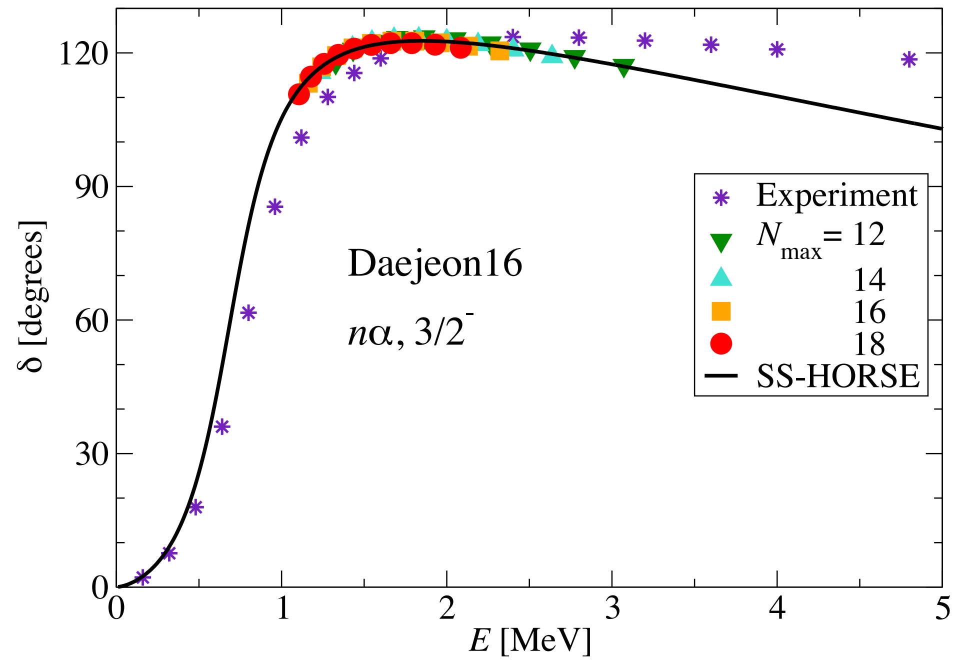
1. No Core Shell Model calculations with Daejeon 16 interaction: $E^{5He}(N_{max},\hbar\Omega)$, $E^{4He}(N_{max},\hbar\Omega)$

2. $E_{rel.n\alpha} = E = E^{5He} - E^{4He}$
   $\tan\delta = f(E)$: obtaining phases at points E with *f* as known function

3. Selection criteria for N_{max} and $\hbar\Omega$: phases form smooth curve

4. Parameterization: $\delta = \delta_r$ + smooth func.

5. Extracting E_r, Γ from δ_r



Adapted from: A. M. Shirokov, A. I. Mazur, I. A. Mazur, E. A. Mazur, I. J. Shin, Y. Kim, L. D. Blokhintsev, and J. P. Vary, Phys. Rev. C 98, 044624 (2018)

PRELIMINARY

SS-HORSE Results for 3n resonances search

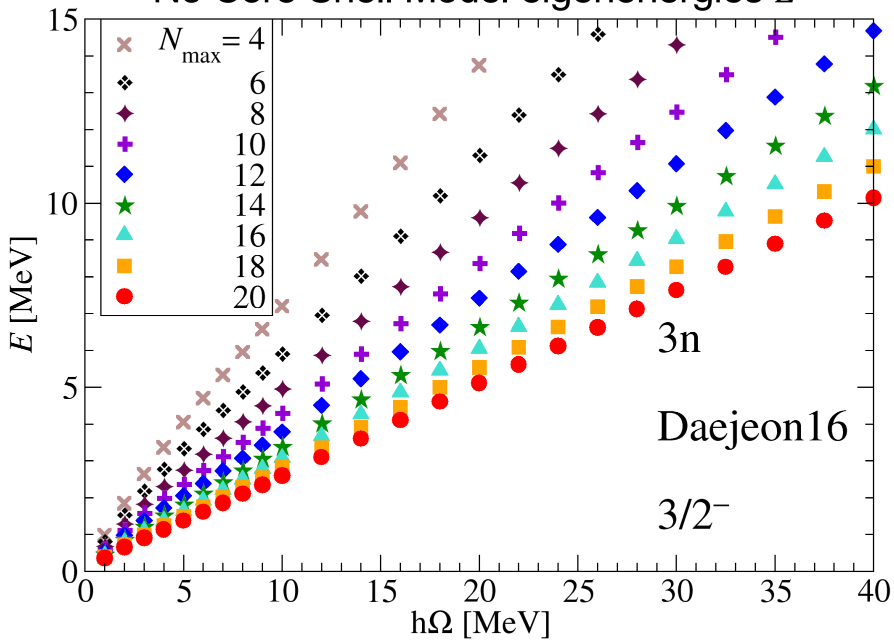
Daejeon16 is modern version of *NN* force that

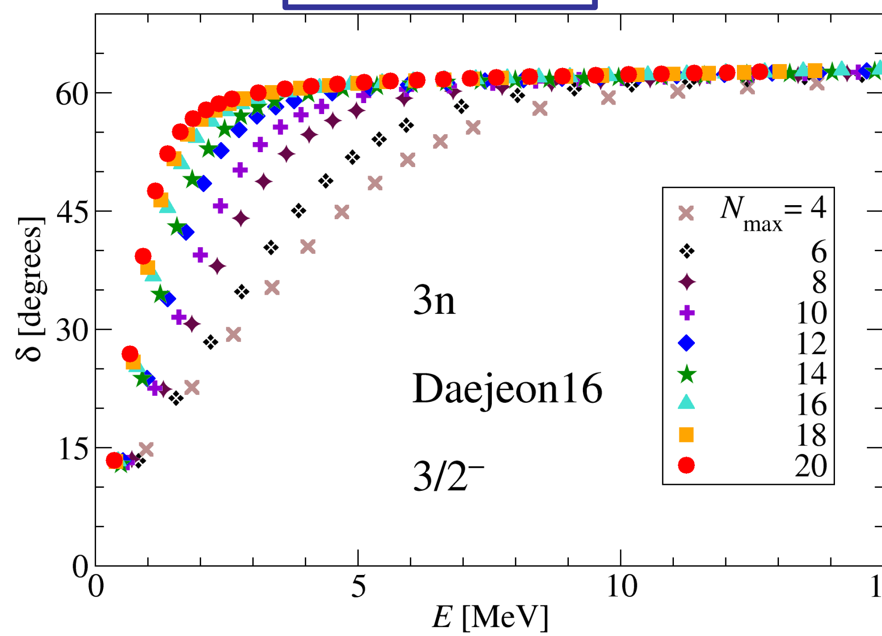
- Started from chiral Idaho N^{3}LO (SRG evolved) interaction
- Effectively included 3*N* forces (due to phase-shift equivalent fit to stable nuclei with up to 16 nucleons)

Using this interaction looks reasonable because there are no 3body interactions that are fit to Isospin=3/2 states

$$\tan\delta = -\frac{S_{N+1,\mathcal{L}}(E)}{C_{N+1,\mathcal{L}}(E)}$$

No Core Shell Model eigenenergies *E*

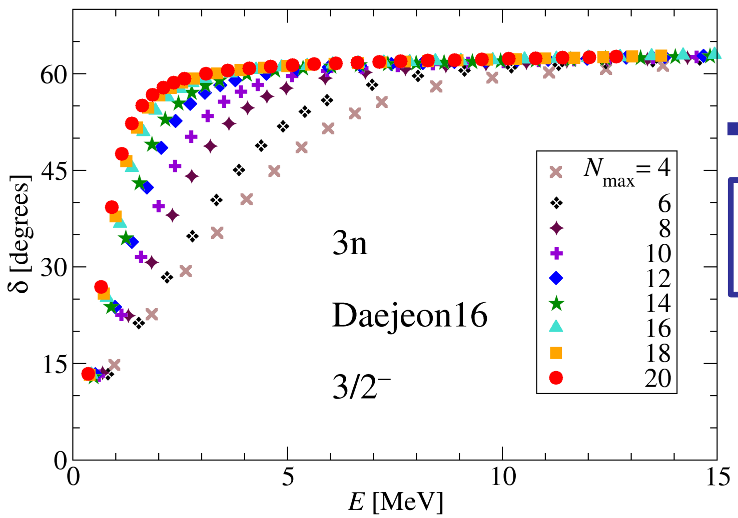




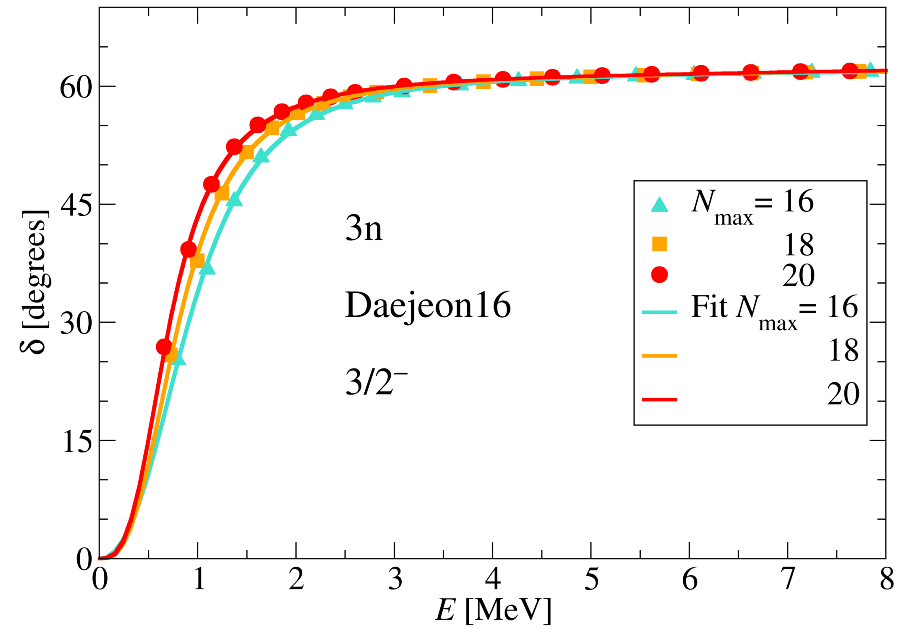
Igor Mazur, IMP Workshop, Huizhou, China, Nov. 21, 2023; I. Mazur et al, in preparation

PRELIMINARY

SS-HORSE Results for 3n resonances search



Selection of points, parameterization



Extraction of S-matrix pole position

N_{max}	$3/2^-$		$1/2^-$	
	E_r [MeV]	Γ [MeV]	E_r [MeV]	Γ [MeV]
16	0.607	1.524	0.606	1.604
18	0.537	1.176	0.531	1.133
20	0.481	0.963	0.481	0.962

Igor Mazur, IMP Workshop, Huizhou, China, Nov. 21, 2023; I. Mazur et al, in preparation

PRELIMINARY

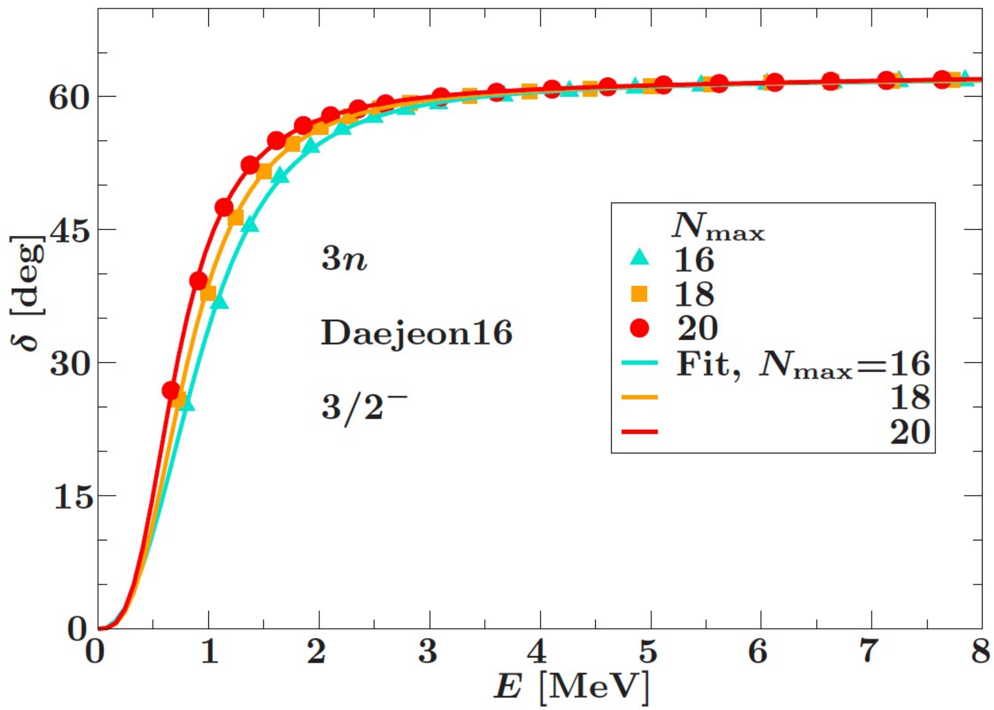


FIG. 2: Fits of $3 \to 3$ phase shifts in the $3/2^-$ trineutron state obtained with NN interaction Daejeon16 and $W = 5$ in the $X(k)$ expansion (18).

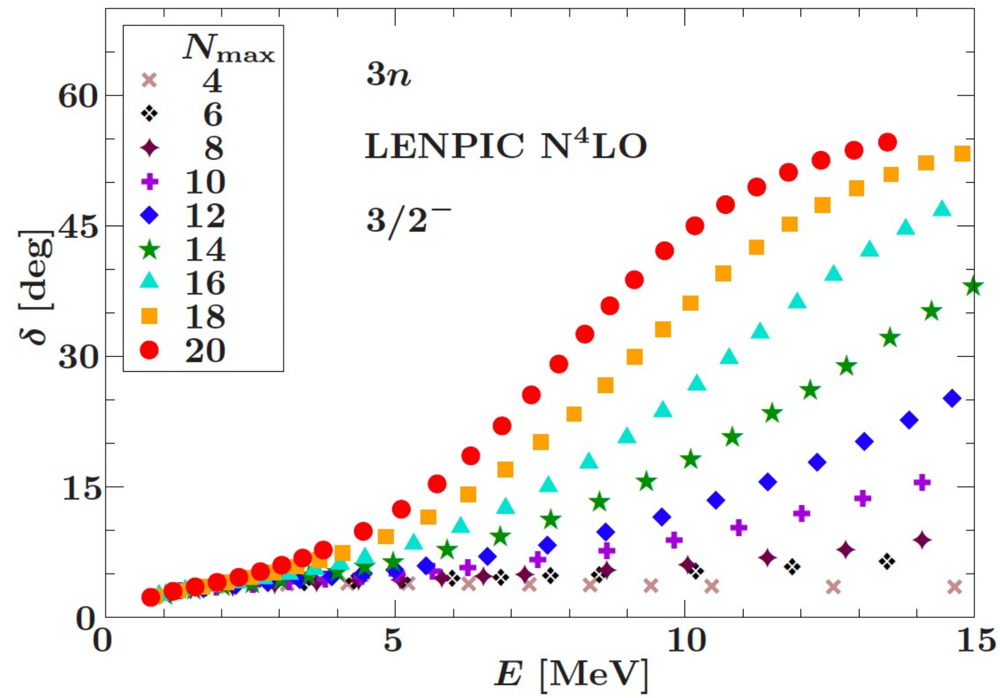


FIG. 3: $3 \to 3$ phase shifts in the $3/2^-$ state at the NCSM eigenenergies obtained with LENPIC N^{4}LO NN interaction [49] using Eq. (3).

I. Mazur et al, in preparation

PRELIMINARY

Our results vs recent results

Our results

Interaction	3/2⁻		1/2⁻	
	E_r [MeV]	Γ [MeV]	E_r [MeV]	Γ [MeV]
Daejeon16	0.51 ± 0.06	1.1 ± 0.3	0.55 ± 0.09	1.0 ± 0.3
JISP16	0.37 ± 0.09	0.74 ± 0.21	0.37 ± 0.09	0.7 ± 0.3
Idaho-N^3LO SRG Λ=2 fm^{-1}	0.34 ± 0.09	0.79 ± 0.24	0.35 ± 0.12	0.8 ± 0.3
Bare N^3LO, N^4LO (no NNN interaction), R = 0.9 fm: no resonance				

Recent results

Approach	Interaction	E_r [MeV]	Γ [MeV]	Reference
Q Monte Carlo, trap	N^2LO (incl. 3N)	0.37(7)		Gandolfi *et al*, PRL 118, 232501 (2017)
NC Gamov SM	N^3LO $V_{low\text{-}k}$	0.91	1.29	Li, Michel, Hu, Zuo, Xu, PRC 100, 054313 (2019)
Transition operators	various “hard” interactions	no resonance		Deltuva, PRC 97, 034001 (2018)
Complex scaling	various “hard” interactions	no resonance		Hiyama, Lazauskas *et al*, PRC 93, 044004 (2016)

Igor Mazur, IMP Workshop, Huizhou, China, Nov. 21, 2023; I. Mazur et al, in preparation

M. Duer, et al., Nature **606**, 678 (2022)

Experimental setup in the Lab frame and in the Center-of-mass frame

Basic idea: the proton knocks out the ^{4}He nucleus from the ^{8}He system so fast as to leave the 4n system behind and, apparently, in a resonant state for a significant fraction of the time (~20%). In the remaining ~80% of the cases, the 4n system is left in some excited “continuum” configuration.

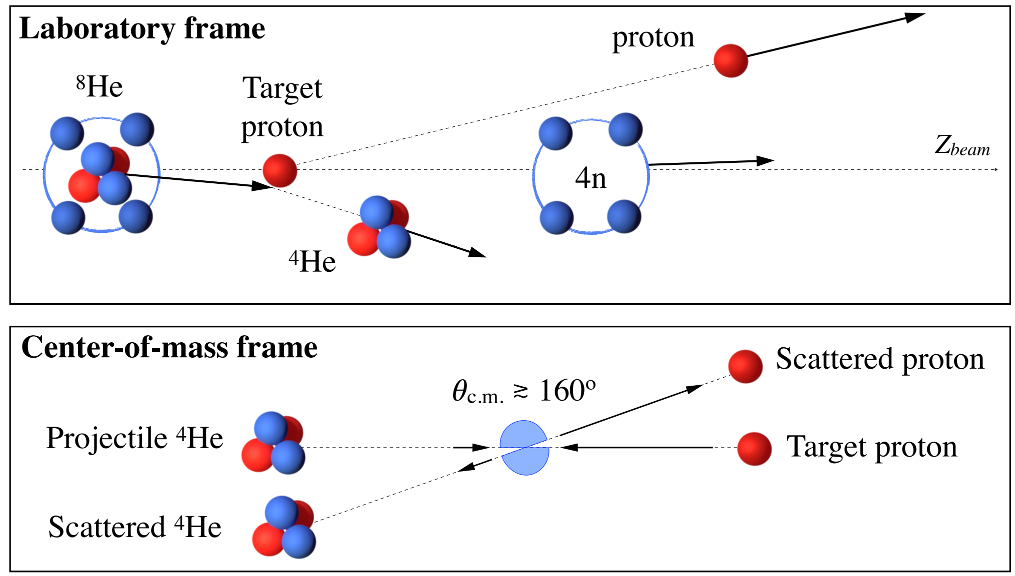
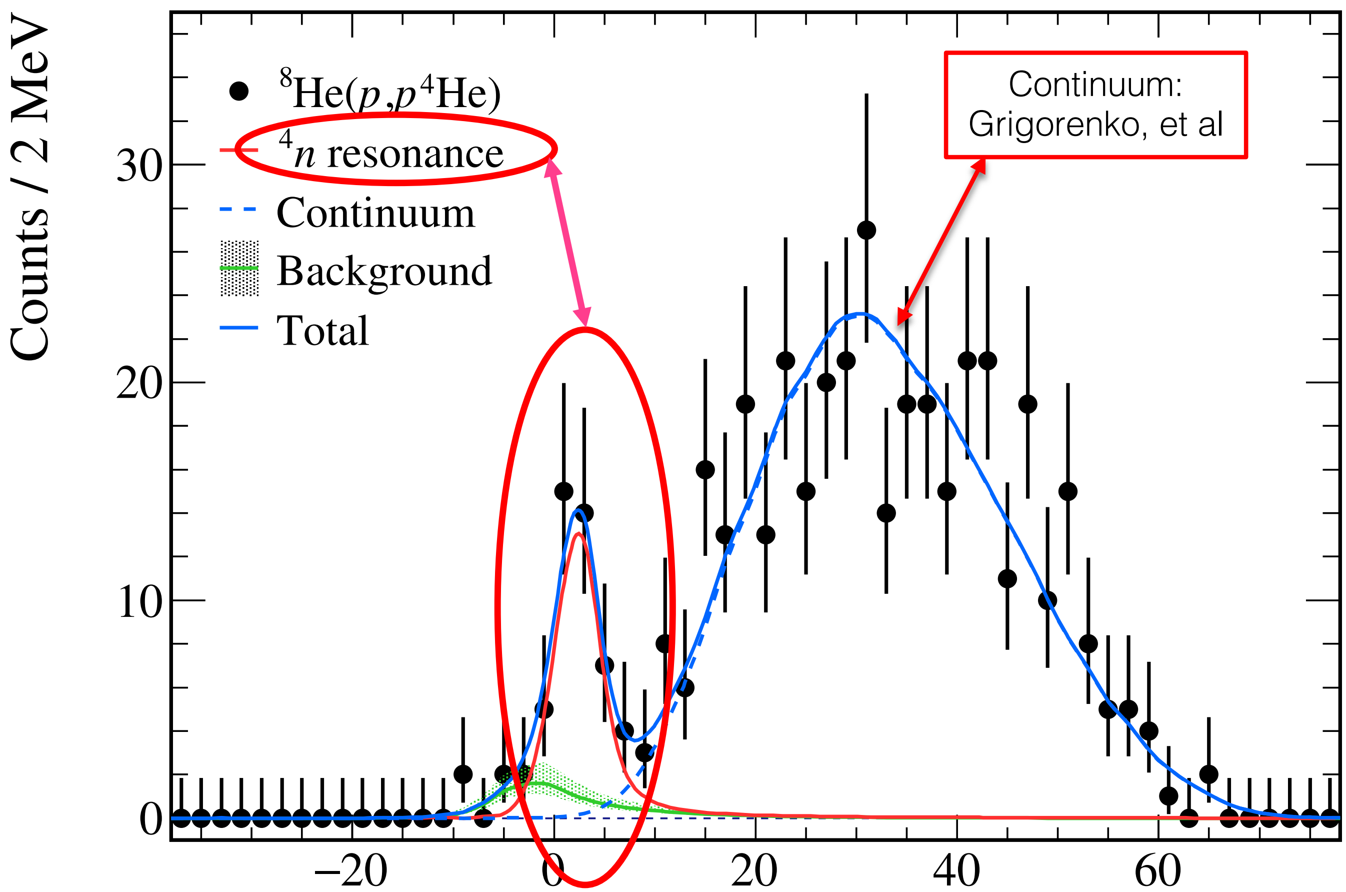
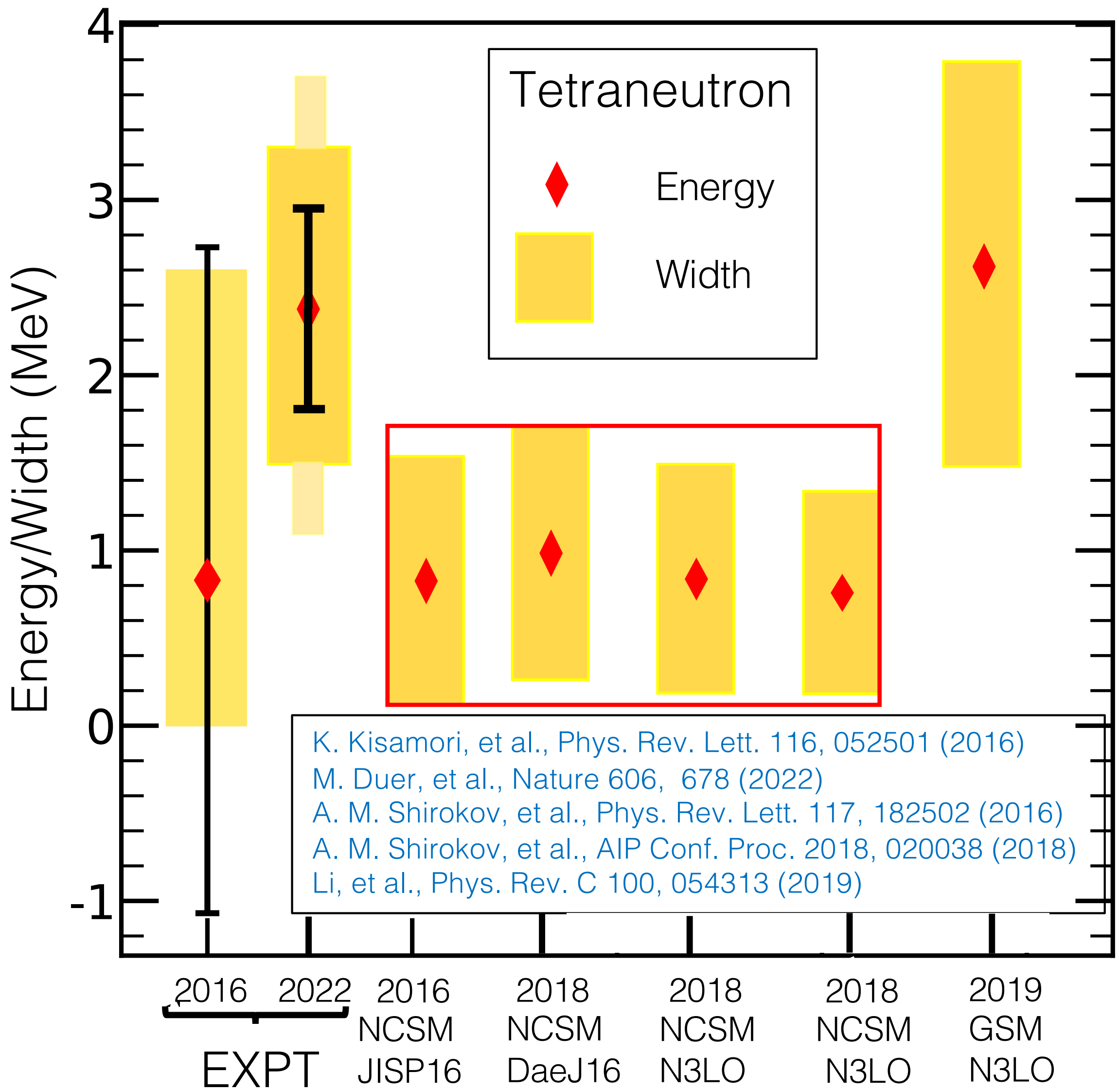


Figure 1: | **Schematic illustration of the quasi-elastic reaction investigated in this work.** Top: Quasi-elastic scattering of the ^{4}He core from a ^{8}He projectile off a proton target in the laboratory frame. The length of the arrows represents the momentum/nucleon (the velocity) of the incoming and outgoing particles. Bottom: The equivalent $p-{}^4$He elastic scattering in their center-of-mass frame, where we consider reactions at backward angles close to 180°. In this frame, the momentum of the proton balances that of the ^{4}He, $\boldsymbol{P}_p = -\boldsymbol{P}_{^4\mathrm{He}}$, *i.e.*, the proton is four times faster than the ^{4}He.

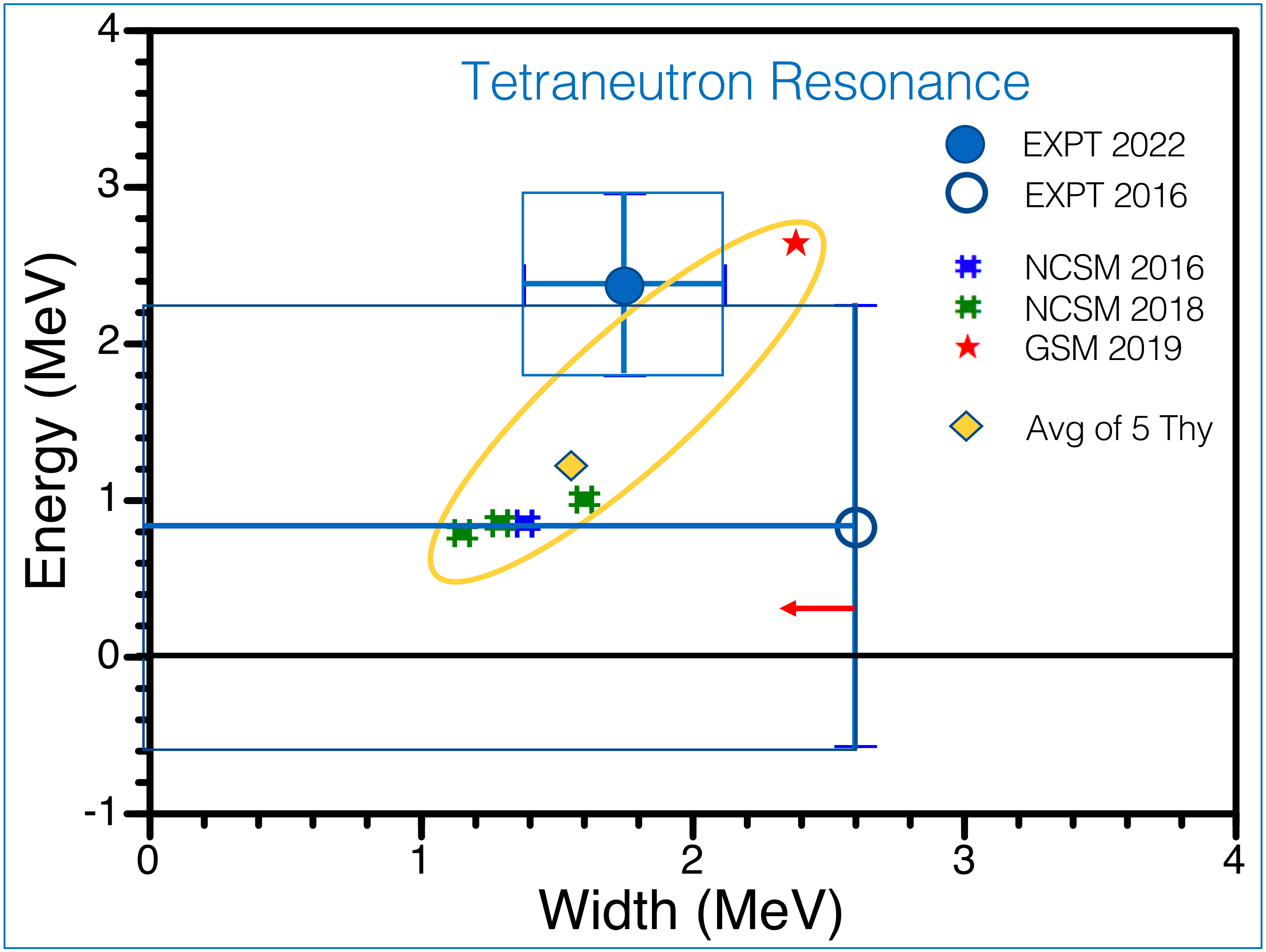
M. Duer, et al., Nature **606**, 678 (2022)

$$E_r = 2.37 \pm 0.38(\text{stat.}) \pm 0.44(\text{sys.})\ \text{MeV},$$
$$\Gamma = 1.75 \pm 0.22(\text{stat.}) \pm 0.30(\text{sys.})\ \text{MeV}.$$





Tetraneutron
Energy
Width
Energy/Width (MeV)
4
3
2
1
0
-1
K. Kisamori, et al., Phys. Rev. Lett. 116, 052501 (2016)
M. Duer, et al., Nature 606, 678 (2022)
A. M. Shirokov, et al., Phys. Rev. Lett. 117, 182502 (2016)
A. M. Shirokov, et al., AIP Conf. Proc. 2018, 020038 (2018)
Li, et al., Phys. Rev. C 100, 054313 (2019)
2016
2022
EXPT
2016 NCSM JISP16
2018 NCSM DaeJ16
2018 NCSM N3LO (2.0)
2018 NCSM N3LO (1.5)
2019 GSM N3LO Lowk


Tetraneutron Resonance
EXPT 2022
EXPT 2016
NCSM 2016
NCSM 2018
GSM 2019
Avg of 5 Thy
Energy (MeV)
Width (MeV)
4
3
2
1
0
-1
0
1
2
3
4

What about 4n resonances for J > 0 channels?

Put the 4n system in a trap which confines the system: states with different J values appear above the J = 0 ground state raising the question of possible additional resonances in the physical system.

"Neutron drops" in a 10 MeV harmonic oscillator trap

2014-2016 INCITE Closeout Report Highlight

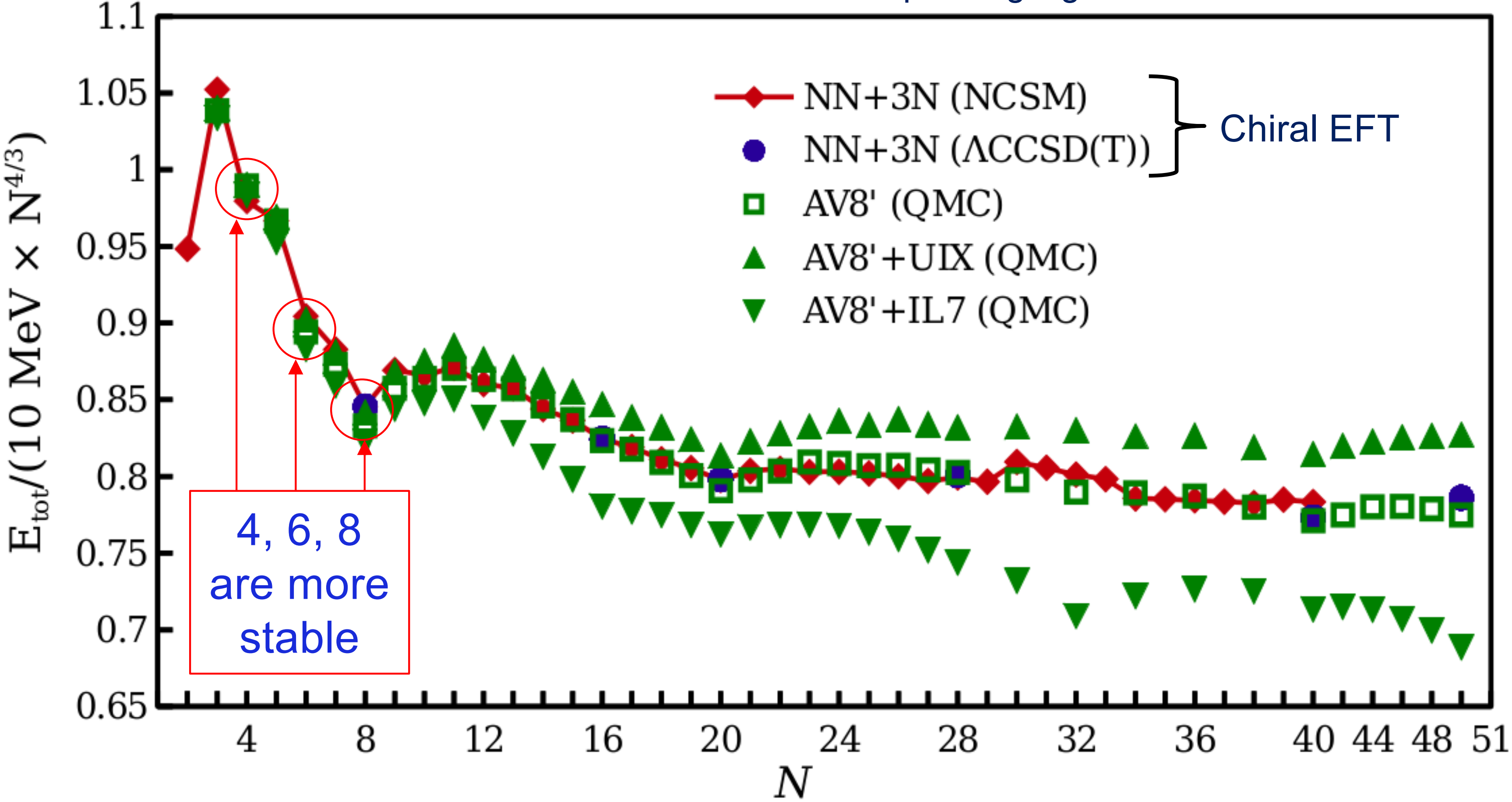


Fig. 6 Scaled ground state energies for neutron drop systems when confined to a harmonic oscillator trap with strength 10 MeV. The results are obtained with NN + 3N interactions from chiral Effective Field Theory (those labeled "NN+3N") and compared with results from meson exchange interactions using other methods (P. Maris et al., Phys. Rev. C 87, 054318 (2013)). These results help quantify the uncertainty due to interaction dependence. NCSM results (labeled "NCSM") are obtained on Titan using the GPUs for decoupling transformations of the 3N interaction from a compressed coupled angular momentum and isospin basis to an m-scheme basis that is employed in MFDn. Results from coupled-cluster calculations using the same interaction are labeled "ΛCCSD(T)".

P. Maris, J.P. Vary, S. Gandolfi, J. Carlson, S.C. Pieper, Phys. Rev. C87, 054318 (2013);
H. Potter, S. Fischer, P. Maris, J.P. Vary, S. Binder, A. Calci, J. Langhammer and R.Roth, Phys. Lett. B739, 445 (2014)

Overall Conclusions for static, transition and scattering observables from ab initio theory

- Large classes of parameter-free predictions emerging
- Ratios of well-chosen observables have small uncertainties and show remarkable agreements with experiment where available
- Ab-initio, non-perturbative and time-dependent scattering theory is developing rapidly – could become a fundamental physics “killer app” for Quantum Computers which will provide a sensitive probe into nuclear dynamics.

Thank you for your attention

I welcome your questions