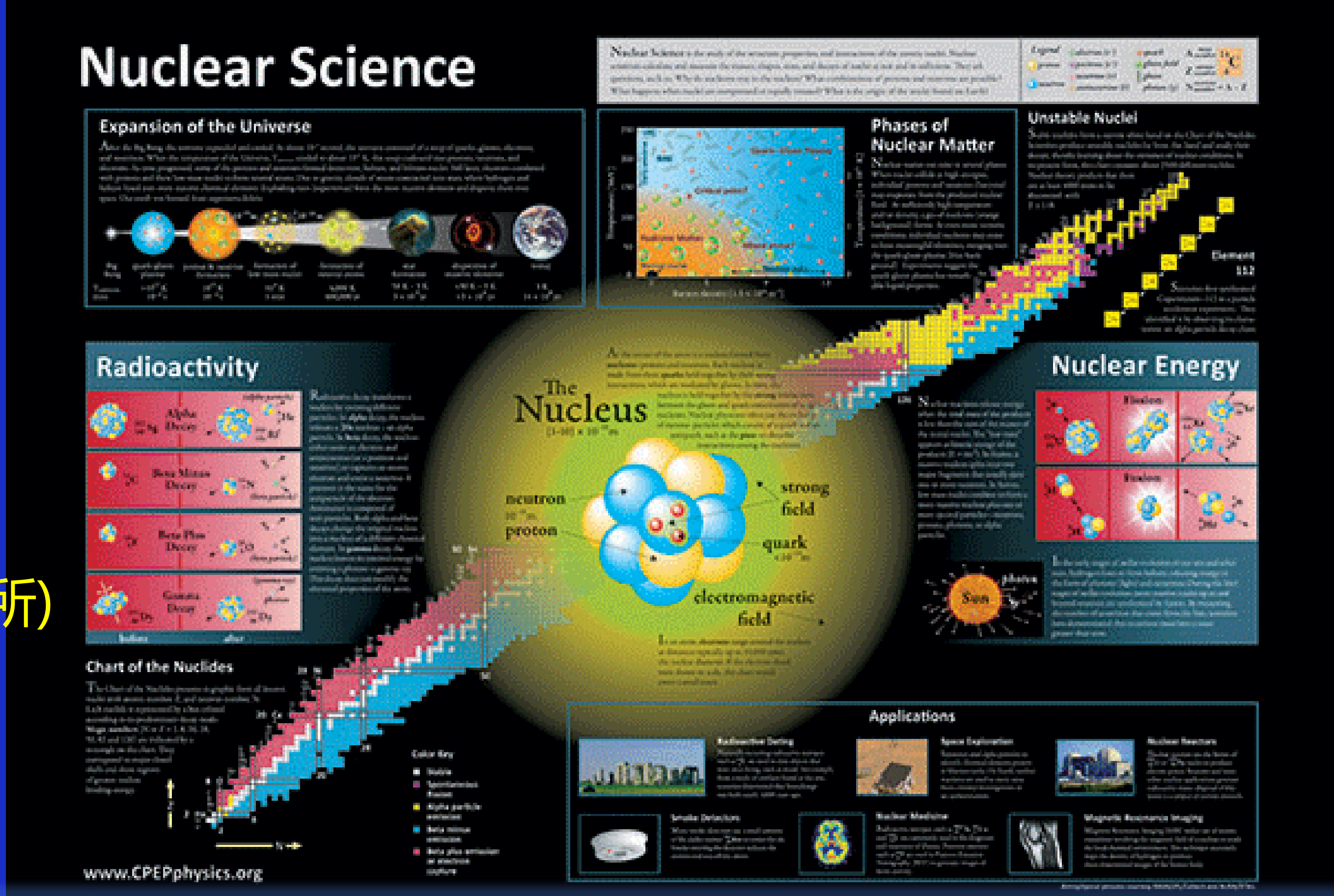
Nuclear structure with *ab initio* No-Core Shell Model

尹鹏 (Peng Yin)

河南科技大学



Collaborators:

左维, 赵行波, 杜伟杰， 李贺, 王惠仁, 房栋梁 (近物所)
周波 （复旦大学)
陈洁 （南方科技大学)
James P. Vary, Pieter Maris (Iowa State University)
Mark Caprio (University of Notre Dame)
Andrey Shirokov (Moscow State University)
Patrick Fasano (Argonne National Laboratory)
Sonia Bacca (Johannes Gutenberg-Universität Mainz)

第二届核结构与反应少体问题研讨会

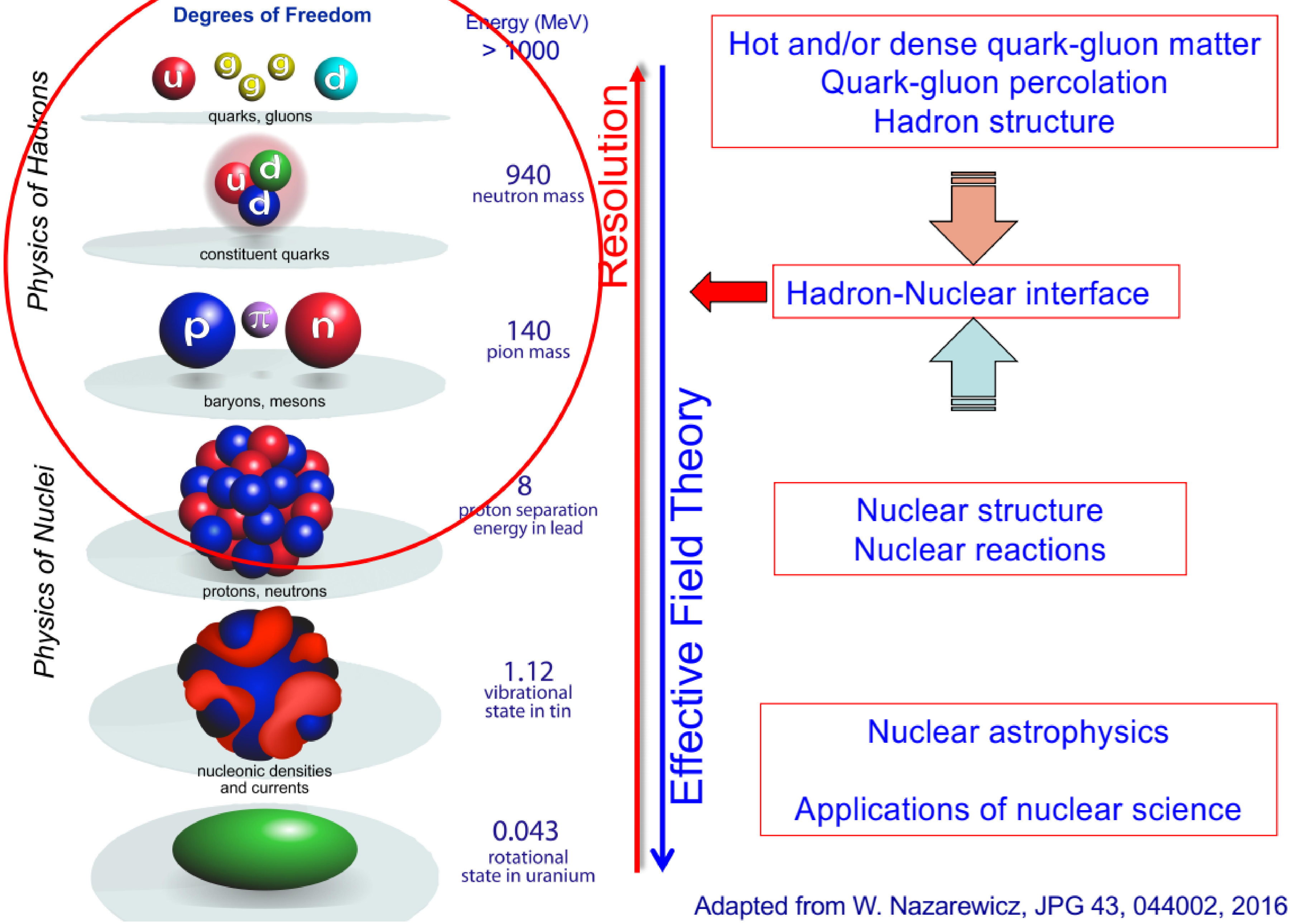
惠州

2025. 1. 13-1. 19

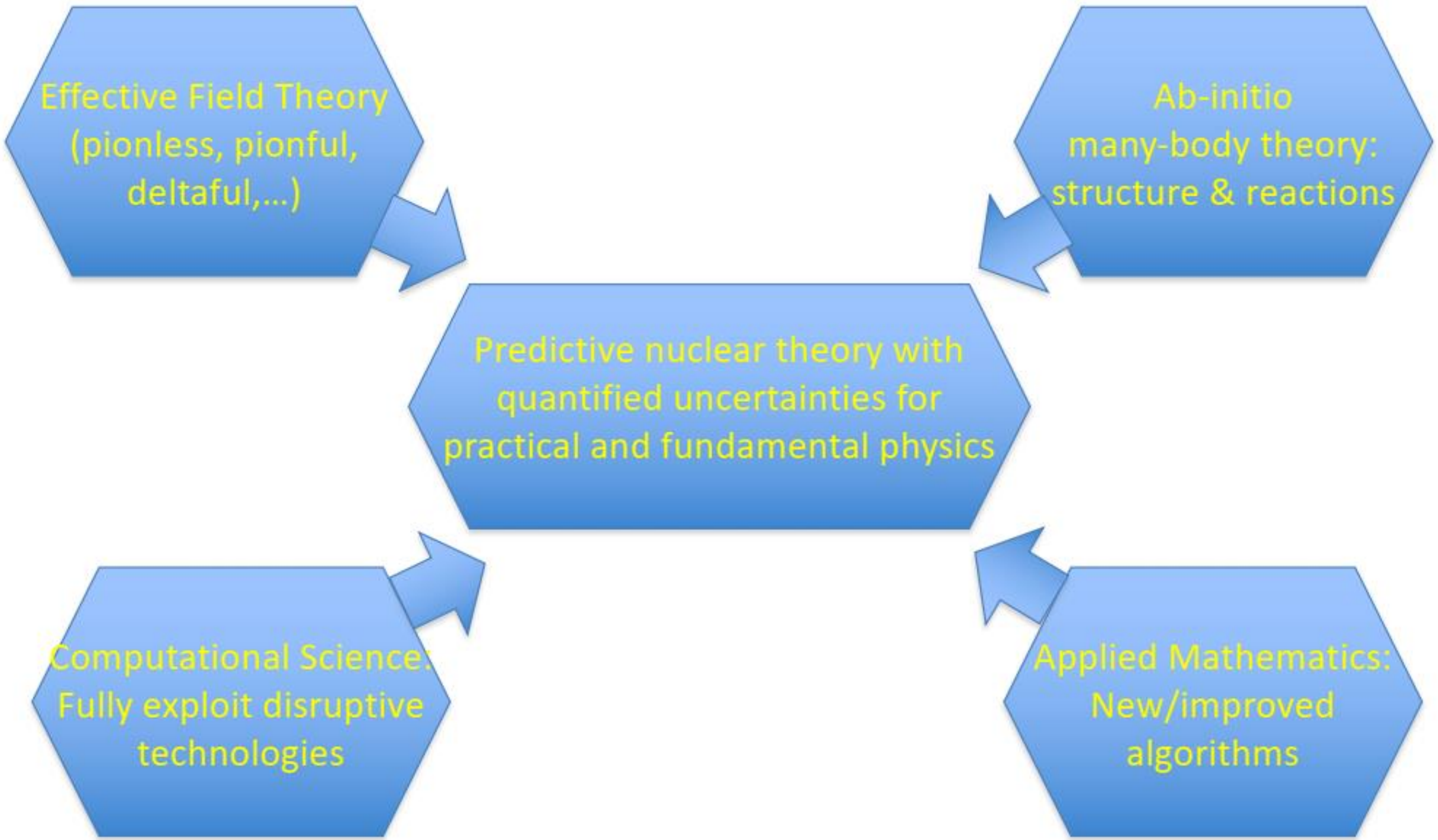
Outline

- No-Core Shell Model
- Long range operators
- Sum rules with NCSM
- Two-body currents of LENPIC interaction
- Monopole transition form factor of ^{4}He
- Time-dependent basis function for nuclear reactions

Heirarchy of first principles problems



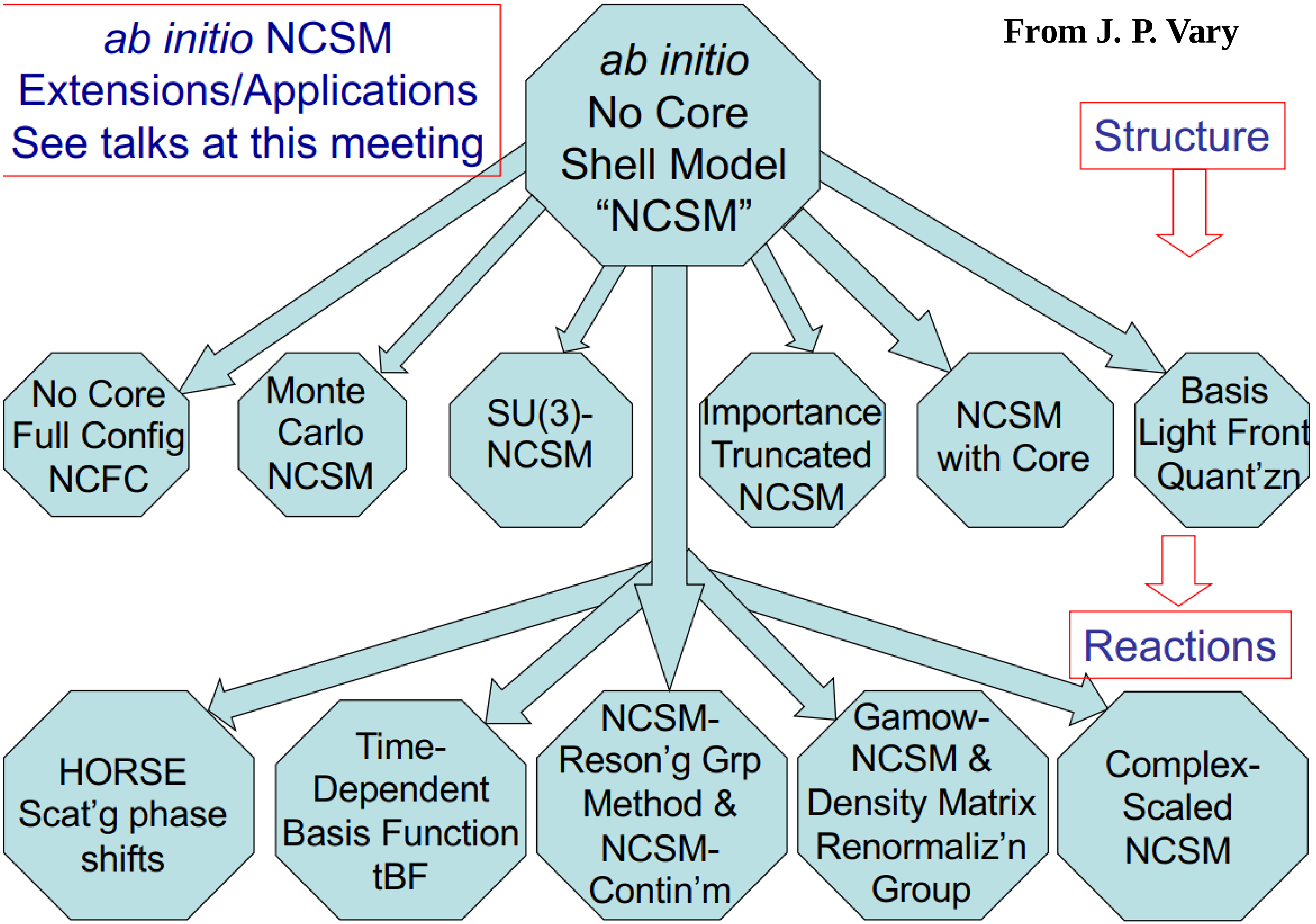
Adapted from W. Nazarewicz, JPG 43, 044002, 2016



SciDAC/NUCLEI: https://nuclei.mps.ohio-state.edu/

Non-relativistic *ab initio* approaches

- Few-body methods
  - Faddeev Equation for A=3 system
    - typically in momentum space
  - Faddeev-Yakuboski Equations for A=4 system
    - can nowadays be pushed to A=5 and 6 (Lazauskas)
  - Hyperspherical Harmonics A=6
- Many-body methods
  - Variational Monte-Carlo (A<=12)
  - Green's Function Monte-Carlo (A<=12)
  - Configuration Interaction (CI) methods (NCSM (A<=20), Coupled Cluster
  - Nuclear Lattice Simulations
  - In-Medium SRG (IM-SRG)
- Supercomputer Era
- Quantum computing Era?


ab initio NCSM
Extensions/Applications
See talks at this meeting
From J. P. Vary
ab initio
No Core
Shell Model
“NCSM”
Structure
Reactions
No Core
Full Config
NCFC
Monte
Carlo
NCSM
SU(3)-
NCSM
Importance
Truncated
NCSM
NCSM
with Core
Basis
Light Front
Quant’zn
HORSE
Scat’g phase
shifts
Time-
Dependent
Basis Function
tBF
NCSM-
Reson’g Grp
Method &
NCSM-
Contin’m
Gamow-
NCSM &
Density Matrix
Renormaliz’n
Group
Complex-
Scaled
NCSM

Ab initio No-Core Shell Model

No-Core Shell model

$$\hat{\mathbf{H}}_{\text{rel}} = \hat{\mathbf{T}}_{\text{rel}} + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} + \ldots$$

- Expand wavefunction in basis states $|\Psi\rangle = \sum a_i |\Phi_i\rangle$
- Express Hamiltonian in basis $\langle\Phi_j|\hat{\mathbf{H}}|\Phi_i\rangle = H_{ij}$
- Diagonalize Hamiltonian matrix H_{ij}
- No-Core: All *A* nucleons are treated equally
- Complete basis: exact results (Caveat: complete basis is infinite dimensional)
- In practice:
  - Truncate basis
  - Study behavior of observables as function of truncation
- Computational challenge:
  - Construct large ($10^{10} \times 10^{10}$) sparce symmetric matrix
  - Obtain lowest eigenvalues&-vectors corresponding to low-lying spectrum and eigenstates

P. Navratil, J. P. Vary and B.R. Barrett, *Phys. Rev. Lett.* **84**, 5728 (2000); *Phys. Rev. C* **62**, 054311 (2000)

Basis Expansion

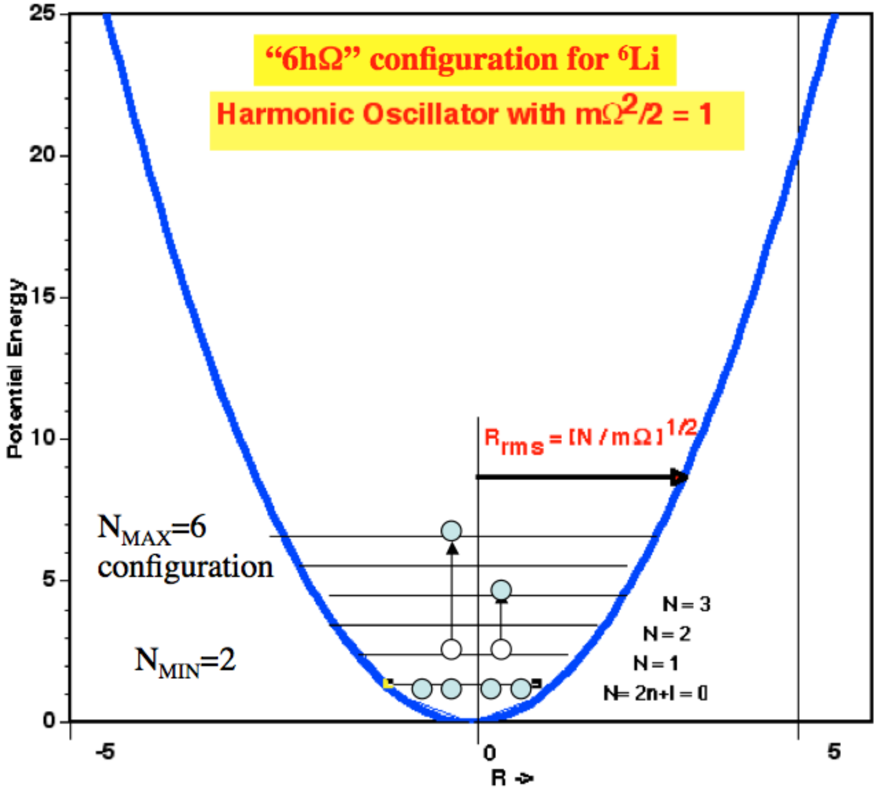
- Expand A-body wave function in basis functions

$$\Psi(r_1, \ldots, r_A) = \sum a_i \Phi_i(r_1, \ldots, r_A)$$

- Use basis of single Slater Determinants of Single-Particle states

$$\Phi_i(r_1, \ldots, r_A) = \frac{1}{\sqrt{(A!)}} \begin{vmatrix} \phi_{i1}(r_1) & \phi_{i2}(r_1) & \ldots & \phi_{iA}(r_1) \\ \phi_{i1}(r_2) & \phi_{i2}(r_2) & \ldots & \phi_{iA}(r_2) \\ \vdots & \vdots & & \vdots \\ \phi_{i1}(r_A) & \phi_{i2}(r_A) & \ldots & \phi_{iA}(r_A) \end{vmatrix}$$

- Single Particle basis states $\phi_{ik}(r_k)$:
  - HO, Coulomb-Sturmian, Natural orbitals
- M-scheme: Many-body basis states: eigenstates of J_z
- N_{max} truncation: $\sum_{k=1}^{A} (2\, n_{ik} + l_{ik}) \leq N_0 + N_{max}$
  - Exact factorization of CoM in HO basis
  - Suitable for excited states



Main Challenges

- 2x AMD EPYC 7763 (Milan) CPUs
- 64 cores per CPU
- AVX2 instruction set
- 512 GB of DDR4 memory total
- 204.8 GB/s memory bandwidth per CPU
- 1x HPE Slingshot 11 NIC
- PCIe 4.0 NIC-CPU connection
- 39.2 GFlops per core
- 2.51 TFlops per socket
- 4 NUMA domains per socket (NPS=4)

National Energy Research Scientific Computing Center

Partition	# of nodes	CPU	GPU
GPU	1536	1x AMD EPYC 7763	4x NVIDIA A100 (40GB)
	256	1x AMD EPYC 7763	4x NVIDIA A100 (80GB)
CPU	3072	2x AMD EPYC 7763	-
Login	40	1x AMD EPYC 7713	1x NVIDIA A100 (40GB)

- Computationally demanding => needs new algorithms & high-performance computers
- Requires convergence assessments and extrapolation tools to retain predictive power
- Current limit 10^{14} (Perlmutter):

  ^{12}C (N_{max}=12), ^{6}He (N_{max}=22)
- Achievable for nuclei up to A~20 with largest computers available

Scientific Computing in the USA

DOE Computer facilities for scientific computing

- National Energy Research Scientific Computing center (NERSC)
  - located at LBNL
  - about 9,000 users
  - many different small and medium-size projects
  - most computing time allocated to DOE Office of Science
    - 12.5% Nuclear Physics (2022)
    - 74 different Nuclear Physics projects (2022)
- Oakridge Leadership Computing Facility (OLCF)
  - relatively small user base
  - limited number of large projects
- Argonne Leadership Computing Facility (ALCF)
  - relatively small user base
  - limited number of large projects

also NSF Computer facilities,
as well as local university computing resources

Supercomputing Era from a personal perspective

- NERSC
  - Seaborg (2002-2008)
    IBM SP, 416 nodes, 6,656 cores, 6,656 GB
  - Franklin (2009-2012)
    Cray XT4, 9,572 nodes, 38,288 cores, 76,576 GB
  - Hopper (2010-2015)
    Cray XE6, 6,384 nodes, 153,216 cores, 216,832 GB
  - Edison (2013-2019)
    Cray XC30, 5,200 nodes, 124,800 cores, 332,800 GB
  - Cori-KNL (2016-2023)
    Cray XC40, 9,688 nodes, 658,784 cores, 893 TB
  - Perlmutter-GPU (2022-), NVIDIA GPUs
    HPE Cray EX, 1,792 GPU nodes, 768 TB
  - Perlmutter (2022-):
    HPE Cray EX, 3,072 CPU nodes, 1,536 TB
  - NERSC-10 planned for 2026

OLCF and ALCF systems

P. Maris, NTSE2024, Busan

- OLCF
  - Jaguar (2008-2012) Cray XT5, 37,538 nodes, 150,152 cores
    - first supercomputer to run scientific application at petaflop rate
    - nuclear theory early science project: ^{14}C$\rightarrow$ ^{14}N β decay
  - ...
  - Frontier (2023-), AMD GPUs, 9,402 nodes, 4.5 PB
- ALCF
  - Intrepid (2009-2013), IBM Blue Gene/P
  - Mira (2013-2019), IBM Blue Gene/Q
    48 racks, 49,152 nodes, 786,432 cores, 768 TB
  - Theta (2017-2023), Cray XC40
    4.2k nodes, 270k cores, 874 TB
  - Aurora (2024-), 63,744 Intel Data Center GPUs, $>$ 7 PB

HPC is entering the Exascale computing era !

Pre-History: Many-Fermion Dynamics

From P. Maris

- General fortran77 code for (No-Core) Configuration Interaction calculations of many-fermion and many-boson systems, dating back to the early nineties

  Vary, The Many-Fermion Dynamics Shell-Model Code, ISU, 1992 (unpublished)

  Vary and Zheng, ISU report, 1994 (unpublished)
- Contributors in period 1996 - 2006
  - Petr Navratil (now at TRIUMF, Canada)
  - Jim Coyle (still at ISU)
  - Andreas Nogga (now at JUELICH, Germany)
- Lanczos algorithm for obtaining lowest eigenvalues and vectors
- Large scale calculations: distributed-memory systems using MPI
- Mixed precision: matrix elements and vectors in single precision, but overlaps for orthonormalization in double precision
- Observables (besides energies)
  - static: r^2, μ, $\mathcal{Q}$, occupation probabilities, . . .
  - transitions: M1, E2, and GT (assuming isospin symmetry)

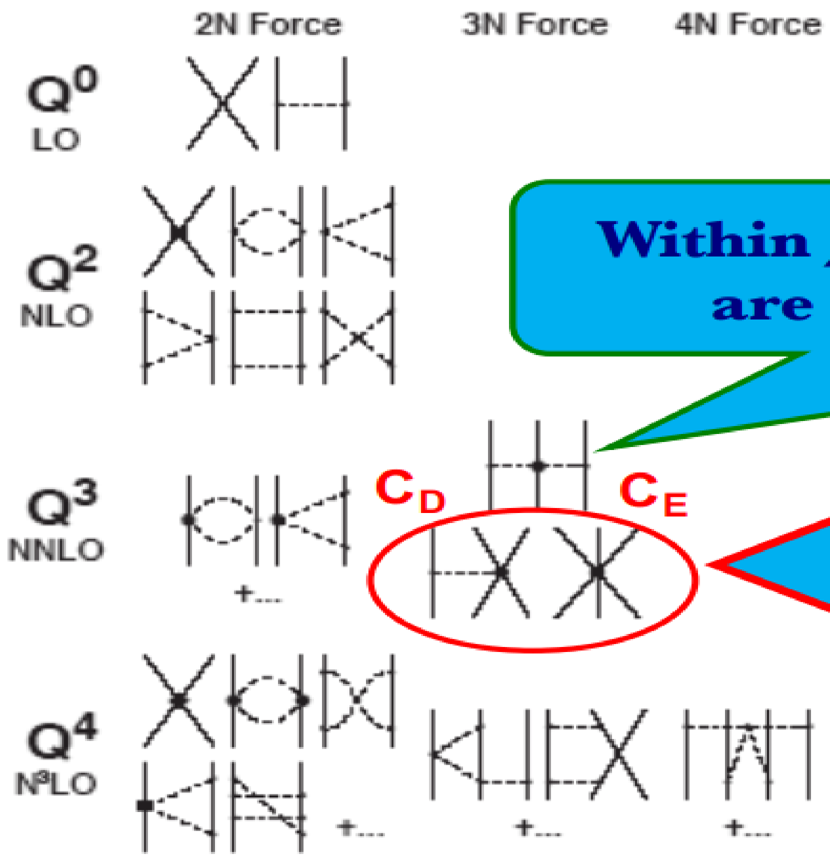
Effective Nucleon Interaction

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 $\{c_i\}$

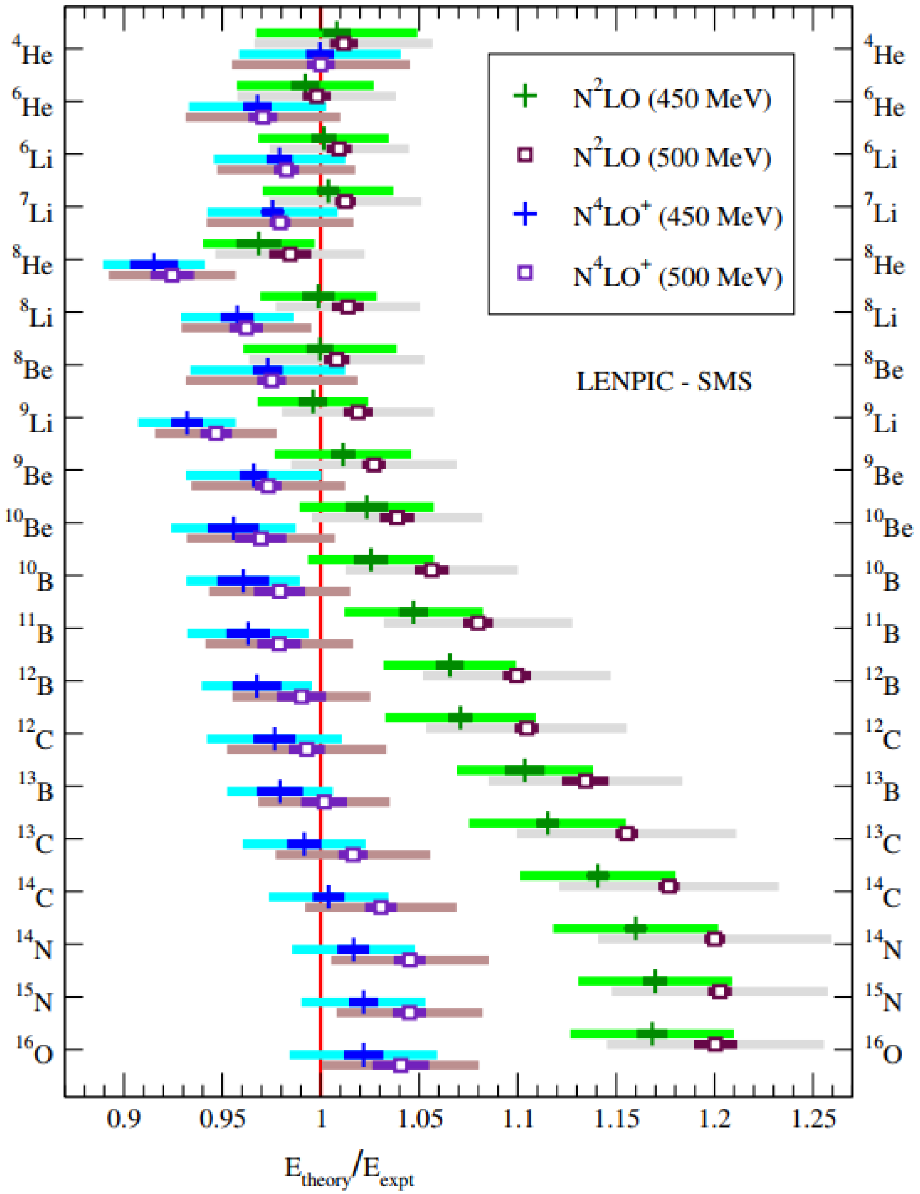
Additional terms from χPT with LECs specific to NNN systems

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

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)

Adapted from P. Navratil slide

Binding Energies with LENPIC-SMS chiral EFT



P. Maris, H. Le, A. Nogga, R. Roth, J.P. Vary
Front. Phys. 11, 1098262 (2023)

- NN potential up to N^{4}LO$^+$
- 3NFs at N^{2}LO
- SRG evolved to $\alpha = 0.08$ fm^4
- LECs fitted to
  - NN scattering data
  - ^{3}H binding energy
  - Nd scattering
- Parameter-free predictions
- Error bars
  - numerical uncertainty
  - chiral EFT uncertainty from Bayesian analysis

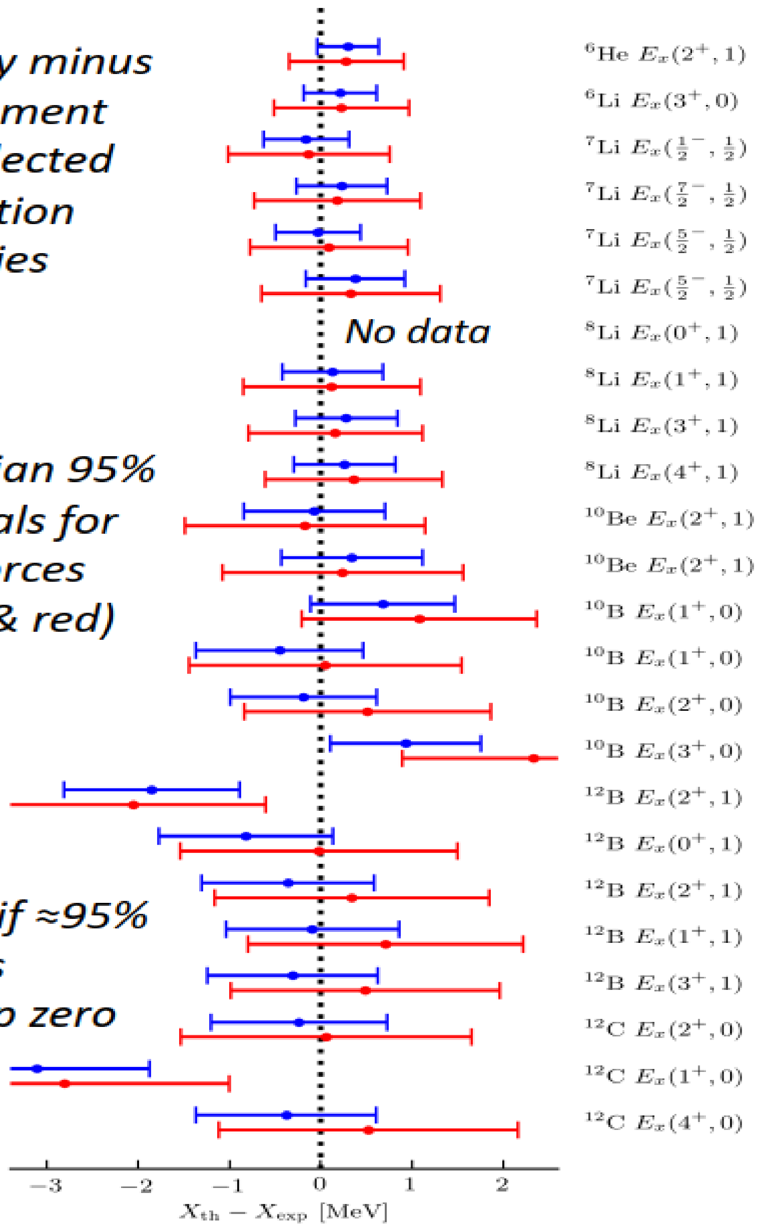
Adapted from P. Maris, LENPIC Annual Meeting, Bonn, March 11-13, 2024

Excitation energies from effective field theory with quantified uncertainties

Theory minus experiment for selected excitation energies

Bayesian 95% intervals for two forces (blue & red)

Check if ≈95% of bars overlap zero



Objectives

- Predict properties of ground and excited states of light nuclei with robust theoretical error estimates.
- Test consistent LENPIC chiral effective field theory (EFT) interactions with 2- and 3-nucleon forces.
- Extend and test a Bayesian statistical model that learns from the order-by-order EFT convergence pattern to account for correlated excitations.

Impact

- First test of novel chiral nucleon-nucleon potentials with consistent three-nucleon forces.
- Demonstrates understanding of theoretical uncertainties due to chiral EFT expansion.
- Accounting for correlations produces agreement with experimental excitation energies (see figure).
- Exceptions in ^{12}C and ^{12}B indicate different theoretical correlations in the nuclear structure.

Accomplishments

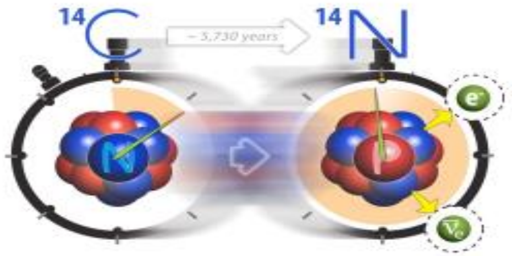
P. Maris et al, Phys. Rev. C **103**, 054001 (2021); Editors' Suggestion; arXiv: 2012.12396 [nucl-th]

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]

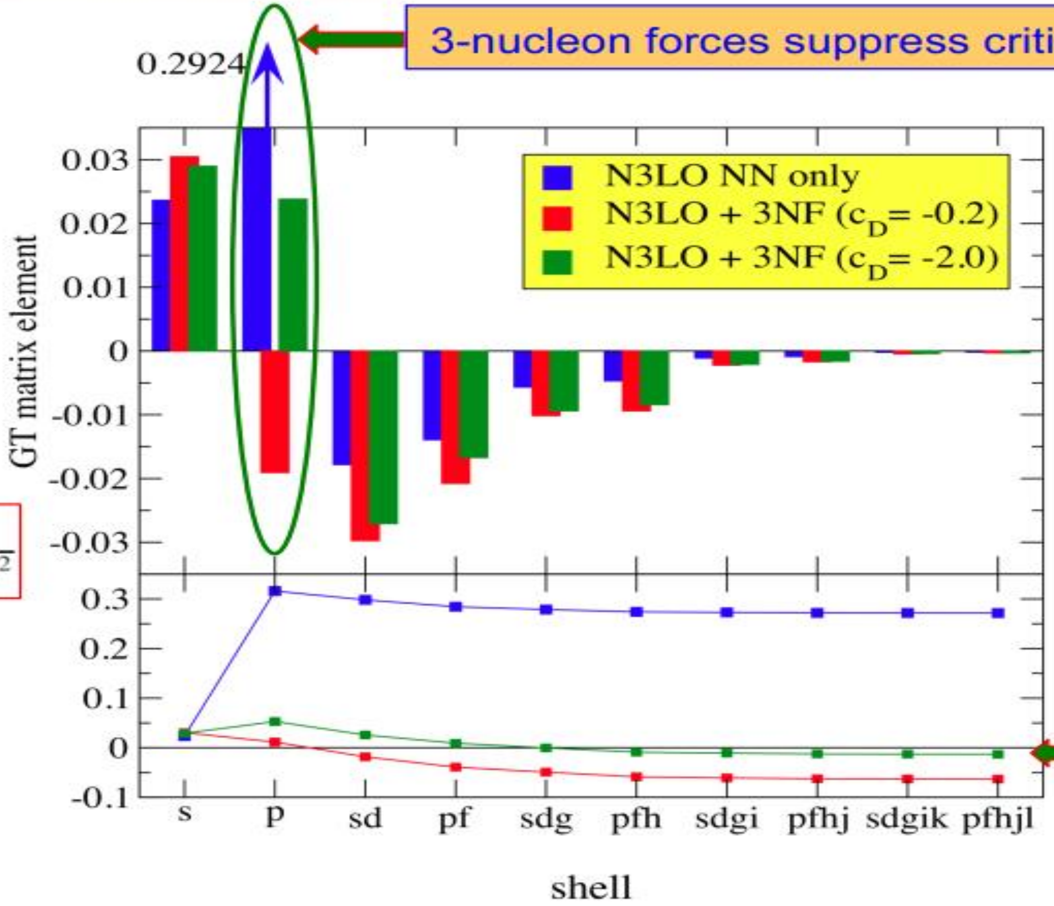
- Solves the puzzle of the long but useful lifetime of ^{14}C
- Establishes a major role for strong 3-nucleon forces in nuclei
- Strengthens foundation for guiding experiments



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

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

3-nucleon forces suppress critical component



net decay rate
Is very small

- 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)

Daejeon16 NN interaction

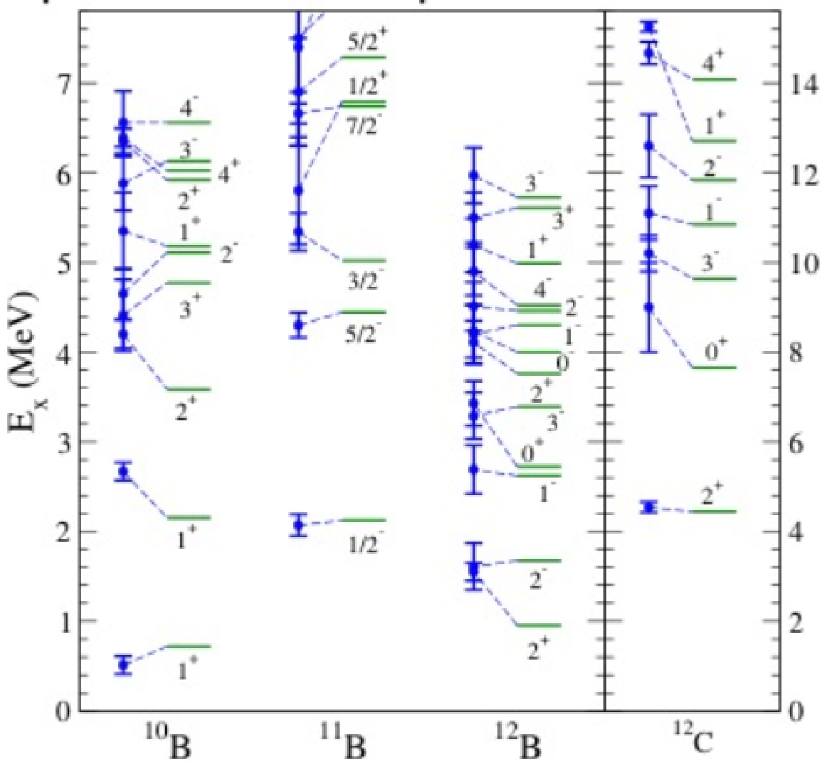
Based on SRG evolution of Entem-Machleidt "500" chiral N3LO to $\lambda = 1.5\ \mathrm{fm}^{-1}$ followed by Phase-Equivalent Transformations (PETs) to fit selected properties of light nuclei.

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

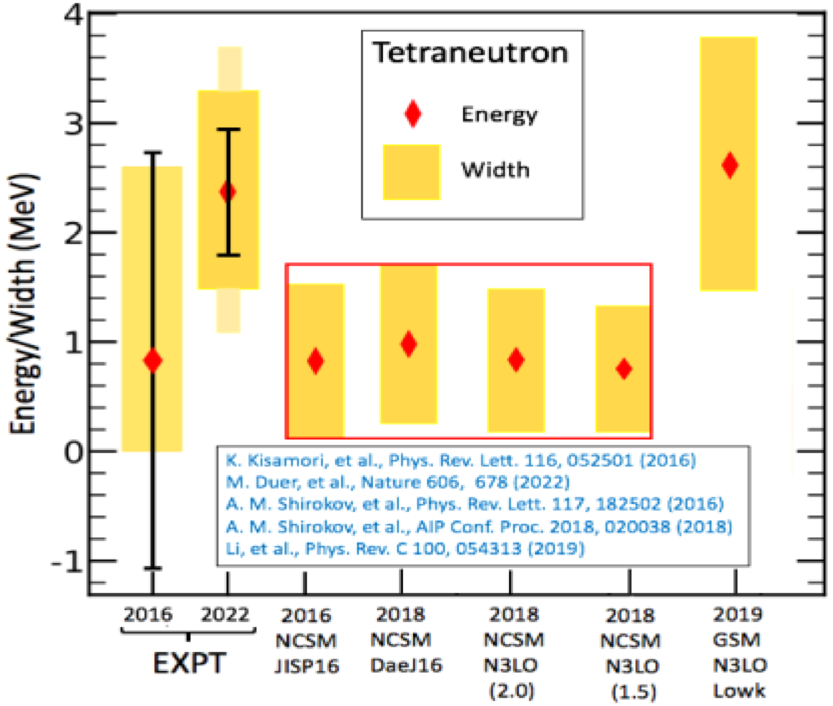
U.S. DEPARTMENT OF ENERGY | Office of Science

Tetraneutron discovery confirms prediction

NUCLEI
Nuclear Computational Low-Energy Initiative

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

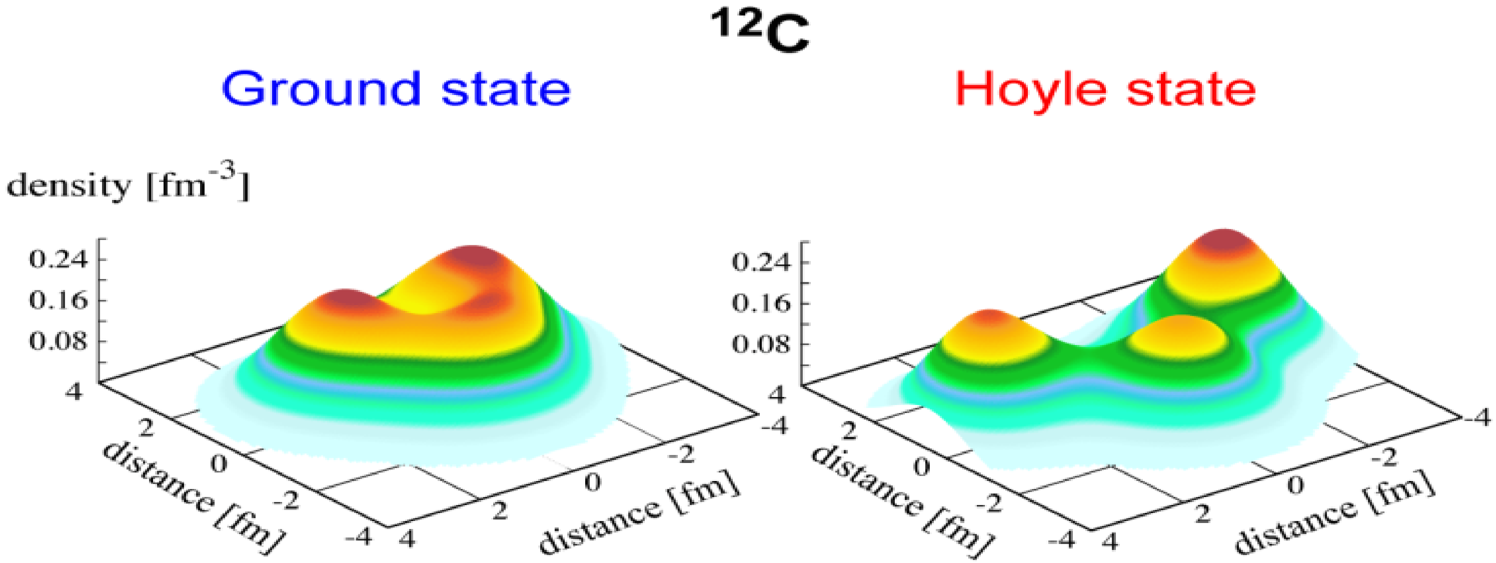
Objectives

- *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

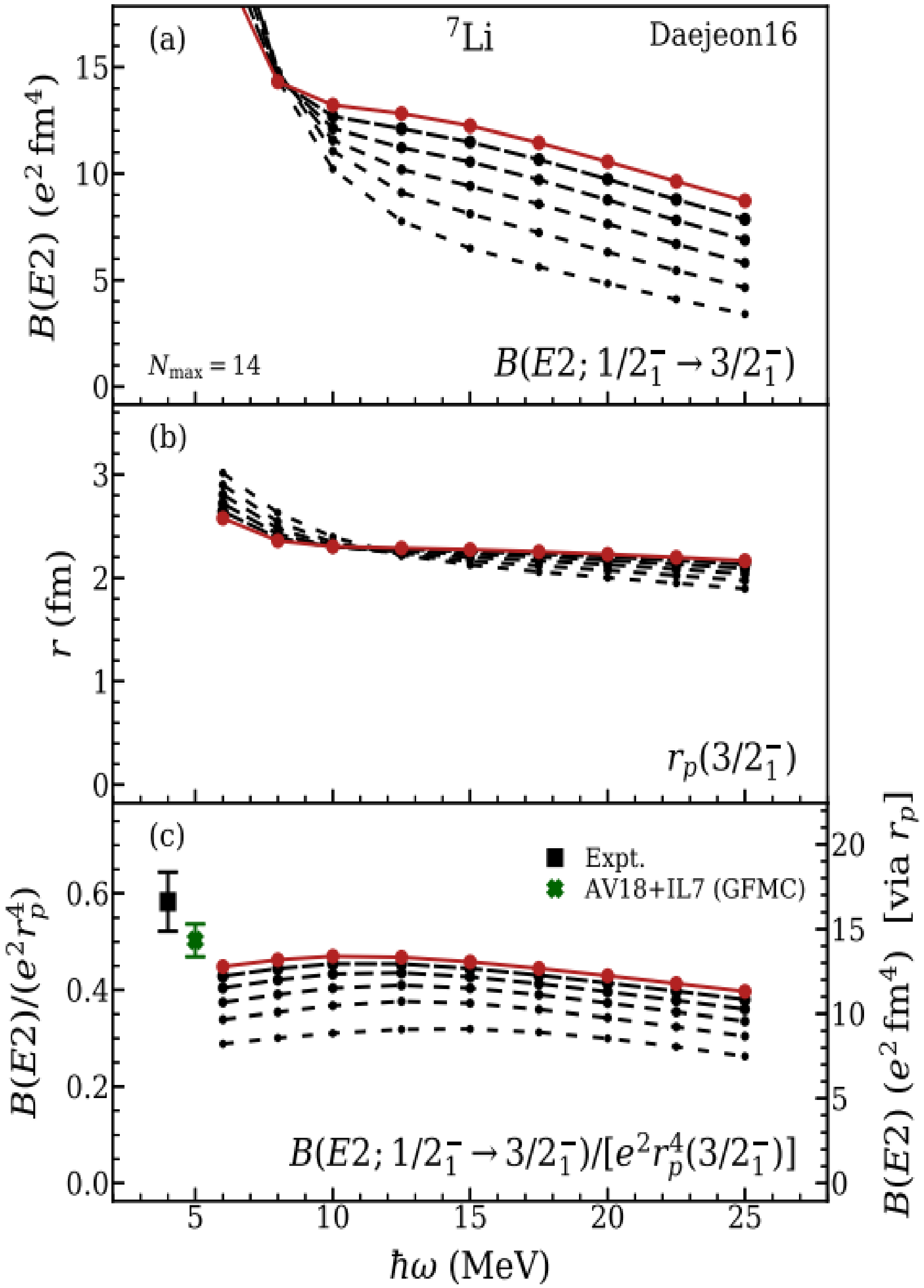
Ab initio Monte-Carlo Shell Model results for density contours of 12C Ground state and first excited 0^+ (Hoyle) state using the Daejeon16 two-nucleon potential. Simulations were performed on Fugaku in Japan, the world's largest supercomputer at the time.

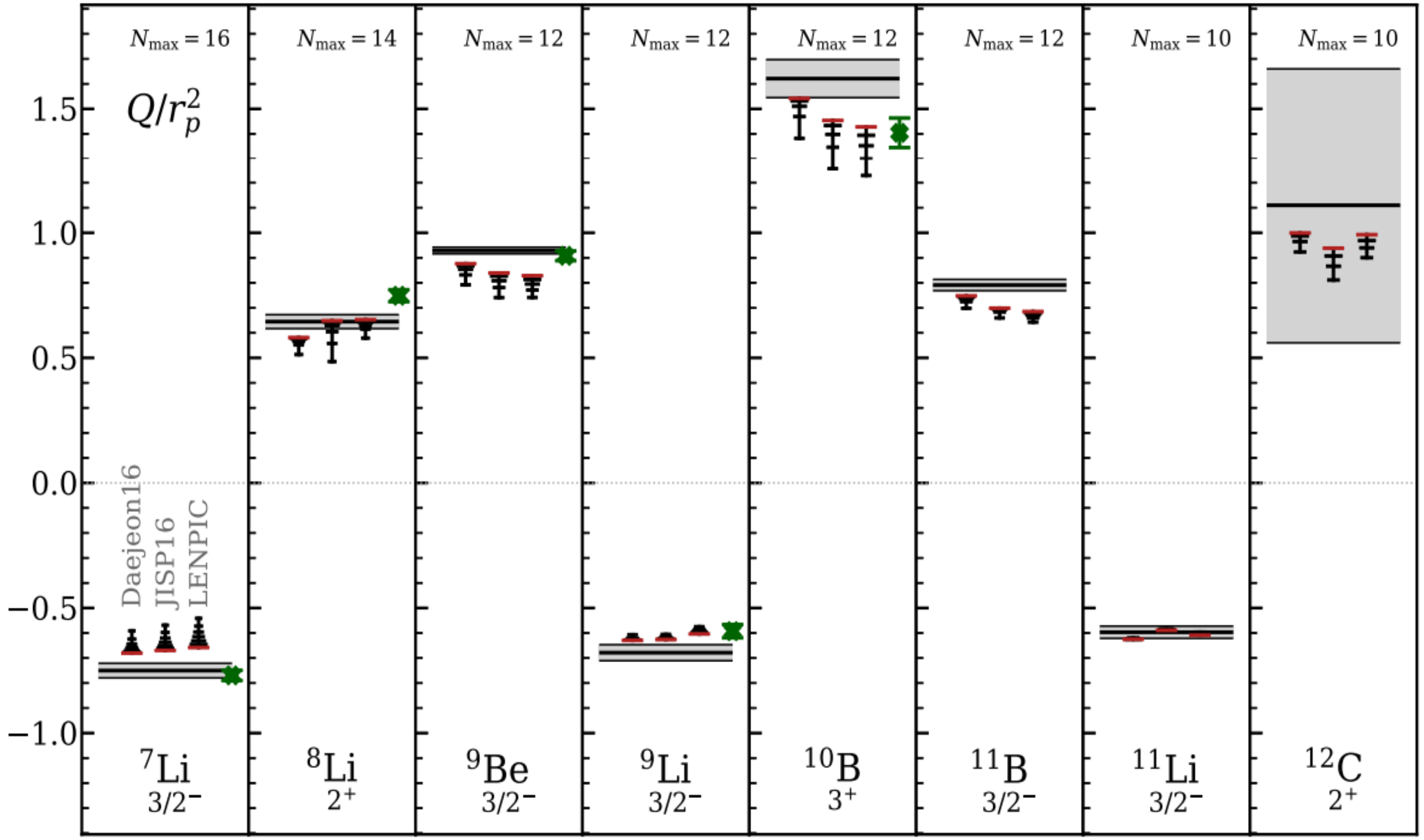


Accomplishments

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)

Long range operators





- Long-range observables converge slowly in HO basis
- Ratio's of long-range observables converge significantly better

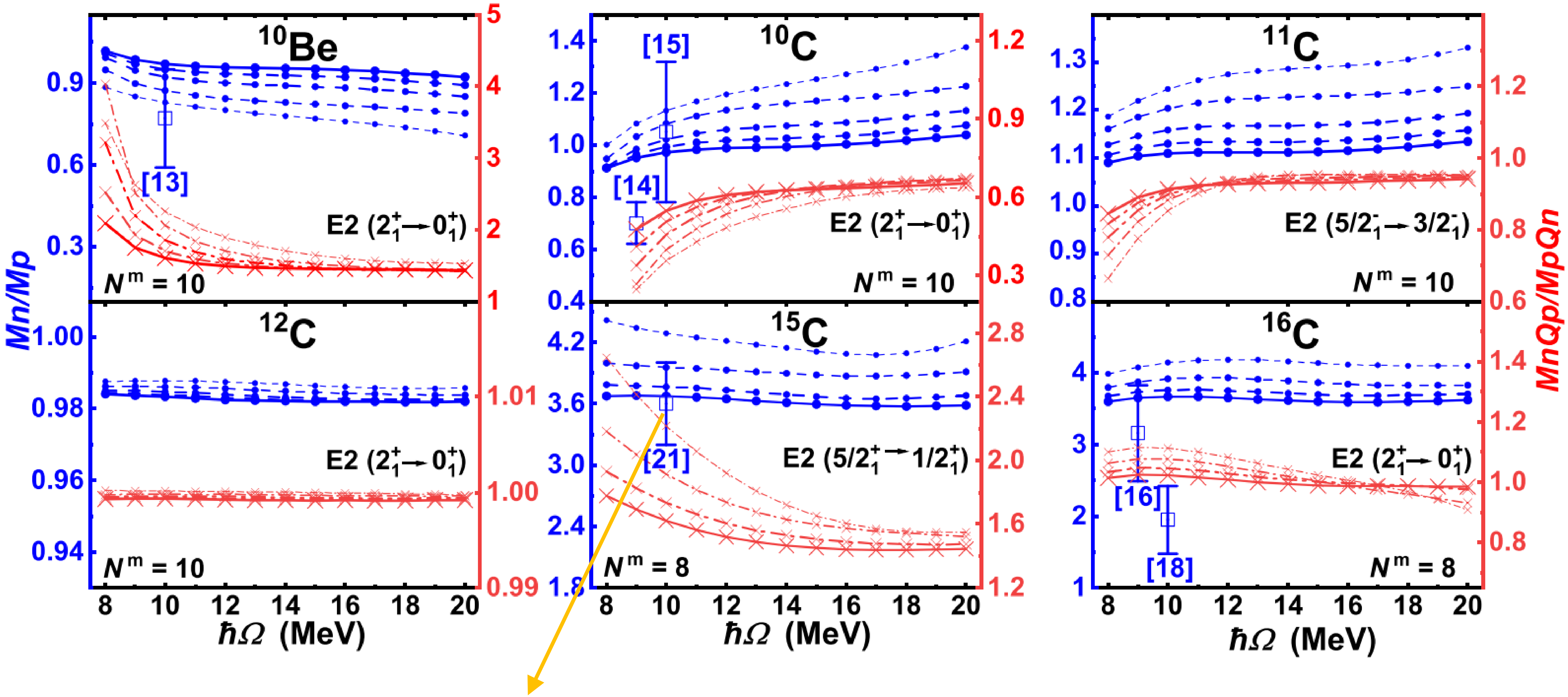
M. Caprio *et al.*, Phys. Rev. C **105**, L061302 (2022)

^{15}C Experiment

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

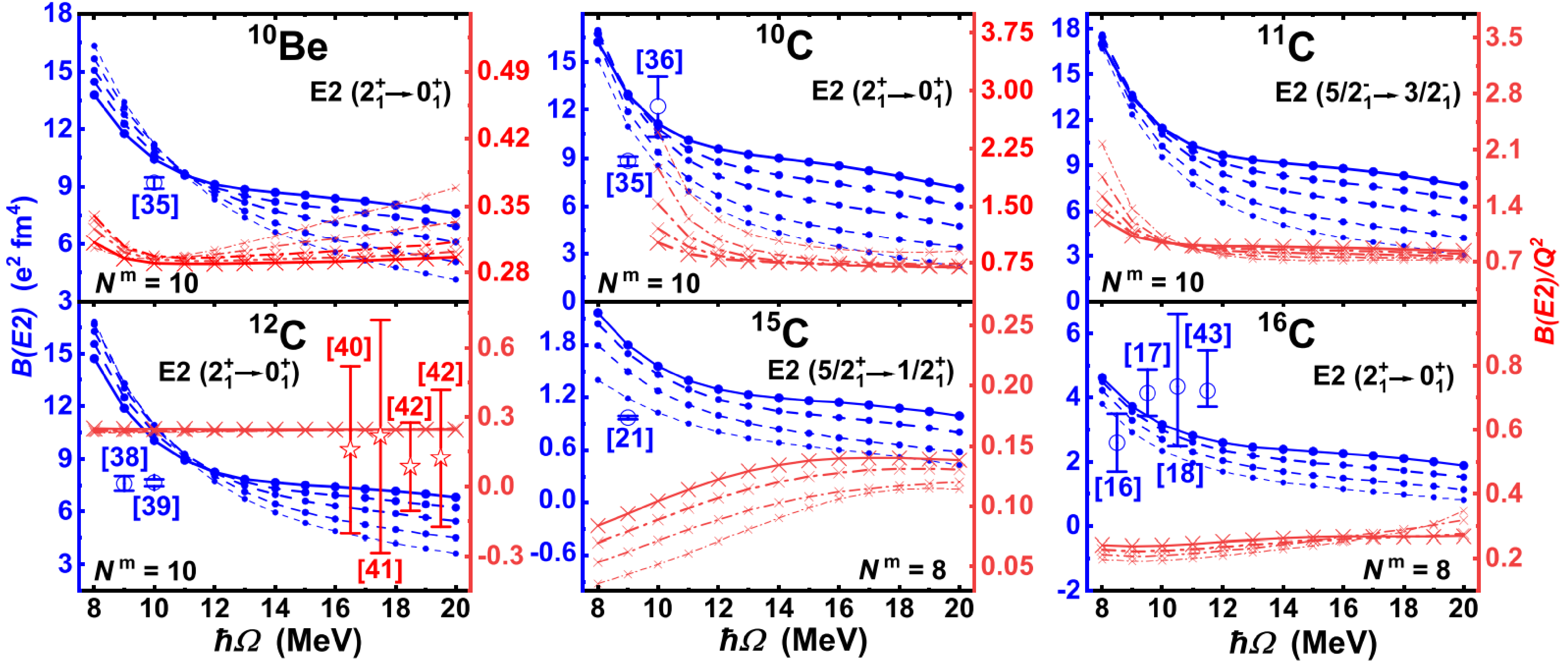
$\hbar\Omega$	17 MeV			18 MeV			Extrapolation	Experiment
N_{max}	4	6	8	4	6	8		
$E_{g.s.}(\frac{1}{2}{}_1^+)$ [MeV]	-100.034	-104.146	-106.091	-100.194	-104.134	-106.019	-107.793(45)	-106.503 [54]
$E_x(\frac{5}{2}{}_1^+)$ [MeV]	0.556	0.941	1.169	0.494	0.908	1.148	1.440(9)	0.740(15) [54]
$B(E2;\frac{5}{2}{}_1^+\rightarrow\frac{1}{2}{}_1^+)$ [e^2fm^4]	0.699	0.938	1.115	0.658	0.899	1.080	2.025(30)	0.97(2) [28]
$\mu_{g.s.}(\frac{1}{2}{}_1^+)$ [μ_N]	-1.723	-1.717	-1.711	-1.720	-1.714	-1.709	-1.633(53)	|1.315(70)| [55]
$\mu(\frac{5}{2}{}_1^+)$ [μ_N]	-1.464	-1.442	-1.428	-1.467	-1.443	-1.429	-1.407(9)	-1.758(30) [55]
M_n/M_p $(\frac{5}{2}{}_1^+\rightarrow\frac{1}{2}{}_1^+)$	3.870	3.649	3.578	3.876	3.652	3.575	3.529(6)	3.6(4)

J. Chen *et al.*, Phys. Rev. C **106**, 064312 (2022)



J. Chen *et al.*, Phys. Rev. C **106**, 064312 (2022)

H. Li, D. Fang, H. J. Ong, A. M. Shirokov, J. P. Vary, P. Yin, X. Zhao, Phys. Rev. C **110** , 064325 (2024)



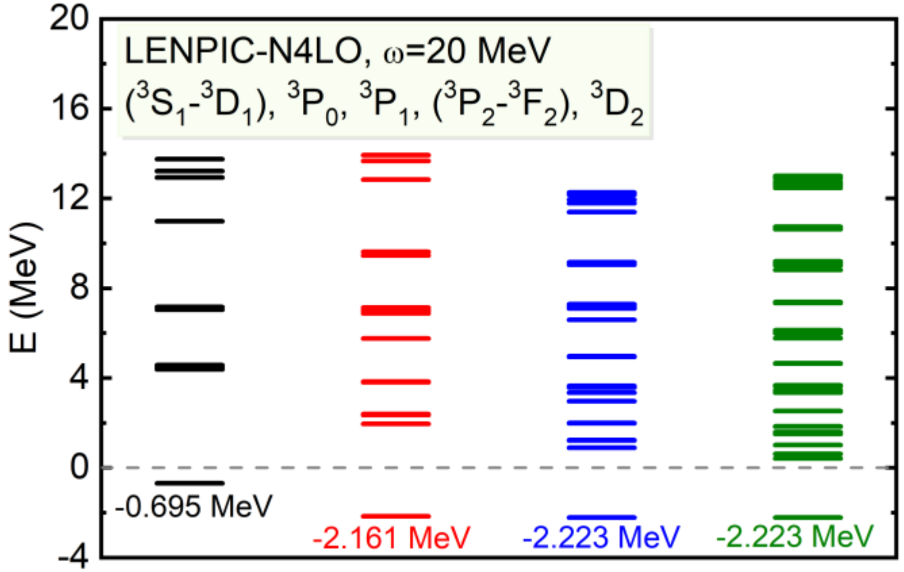
H. Li, D. Fang, H. J. Ong, A. M. Shirokov, J. P. Vary, P. Yin, X. Zhao, Phys. Rev. C **110** , 064325 (2024)

Sum rules with NCSM

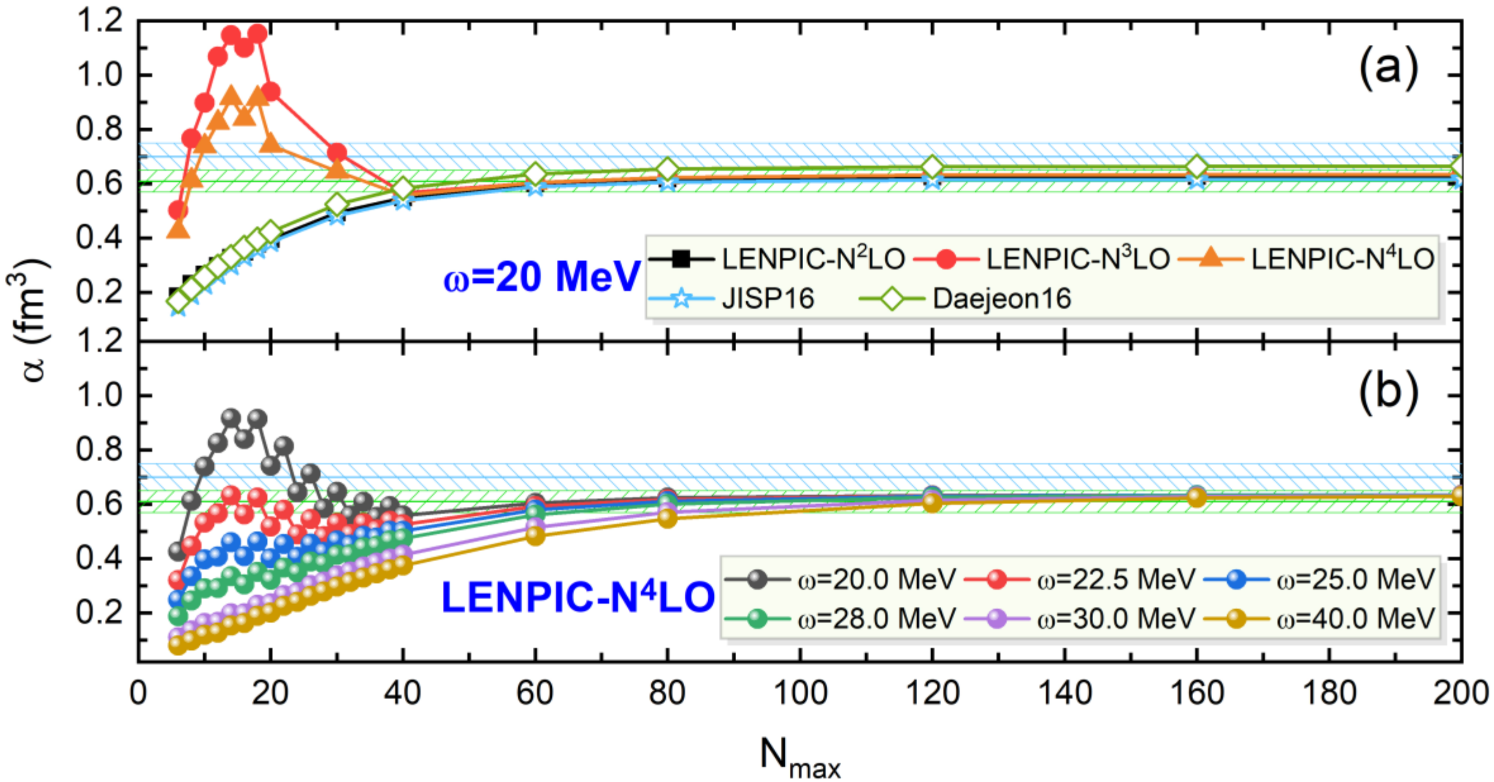
Sum rules with NCSM

$$I_M = \sum_{\mu}^{M} |\langle\mu|\hat{O}|i\rangle|^2 g(\omega_\mu) \qquad \alpha_E = \frac{8\pi}{9}\sum_k \frac{B(E1; J_0 \to J_k)}{E_k - E_0} = \frac{1}{2\pi^2}\int_{\omega_{\rm th}}^{\infty} d\omega \frac{\sigma_\gamma^{\rm ud}(\omega)}{\omega^2}$$

- Sum rule: response of nuclei to external field probe
- Direct techniques: only available for deuteron
- Indirect techniques: Lorentz integral transform, Lanczos sum rule method
- A>2, direct calculation?



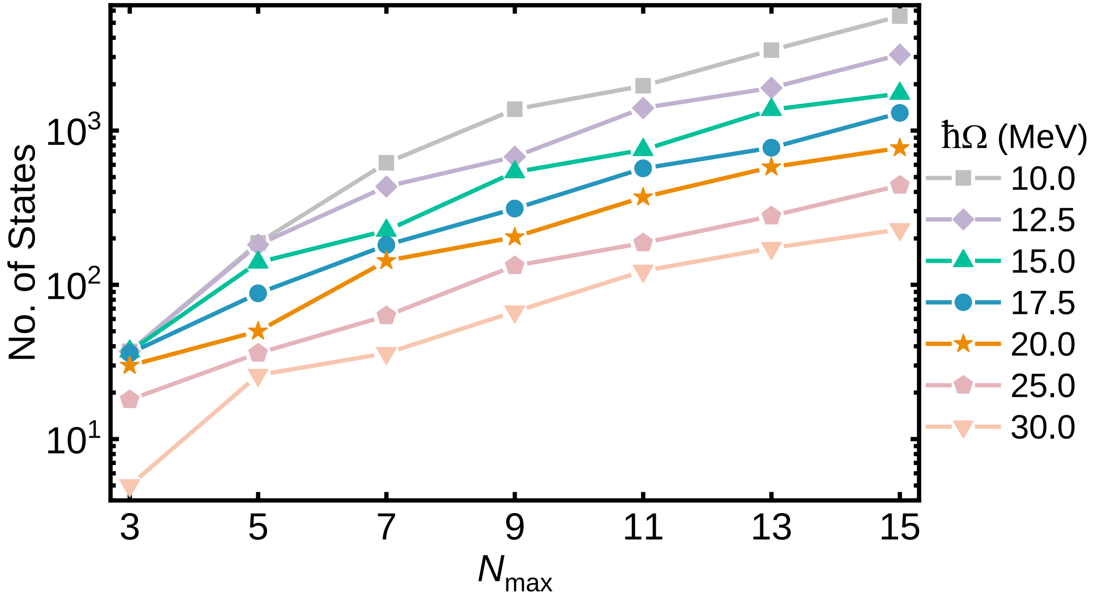
N_{max} =	20	40	80	160
Num. of States =	37	59	90	140



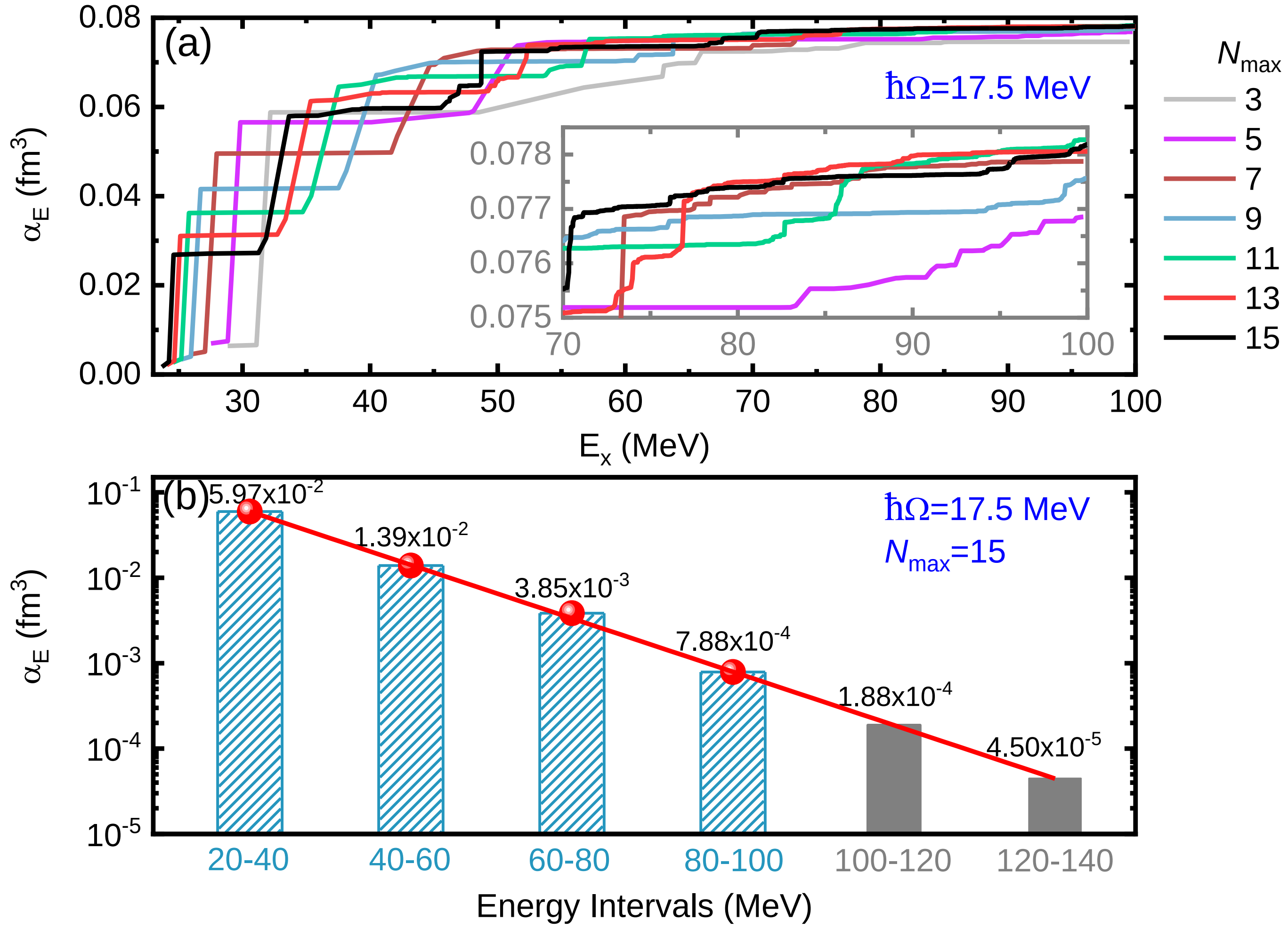
P. Yin *et al, J.Phys.G* 49, 125102 (2022)
P. Yin *et al,* [arXiv:2208.00267 [nucl-th]]

Sum rules with NCSM

- ^{4}He: polarizability $\alpha_E = \frac{8\pi}{9}\sum_k \frac{B(E1; J_0 \rightarrow J_k)}{E_k - E_0}$
- *E1* selection rule: 1^- states
- Retain only 1^- states
  - M-scheme with M=1 (1^-,2^-,…)
  - Lagrangian multiplier $H_{J^2} = \lambda\left(\boldsymbol{J}^2 - 2\right)$

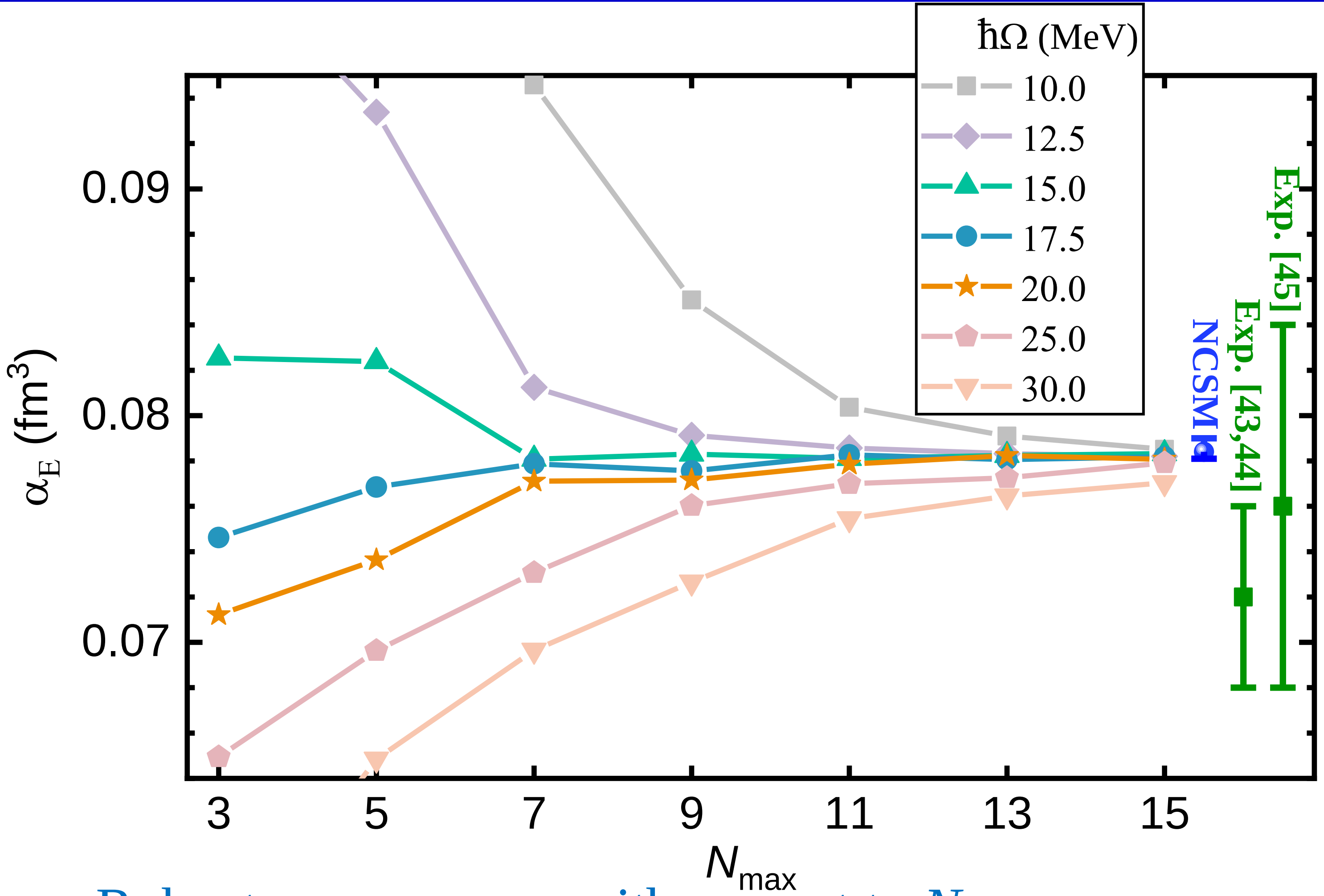


- Up through 100 MeV
- N_{max}=15, hΩ=10 MeV
- 5522 1- states
- 30 GPU nodes, 16800 Lanczos iterations, 21 hours



P. Yin, A. M. Shirokov, P. Maris, P. J. Fasano, M. A. Caprio, H. Li, W. Zuo, J. P. Vary, Phys. Lett. B **855**, 138857 (2024)

Sum rules with NCSM



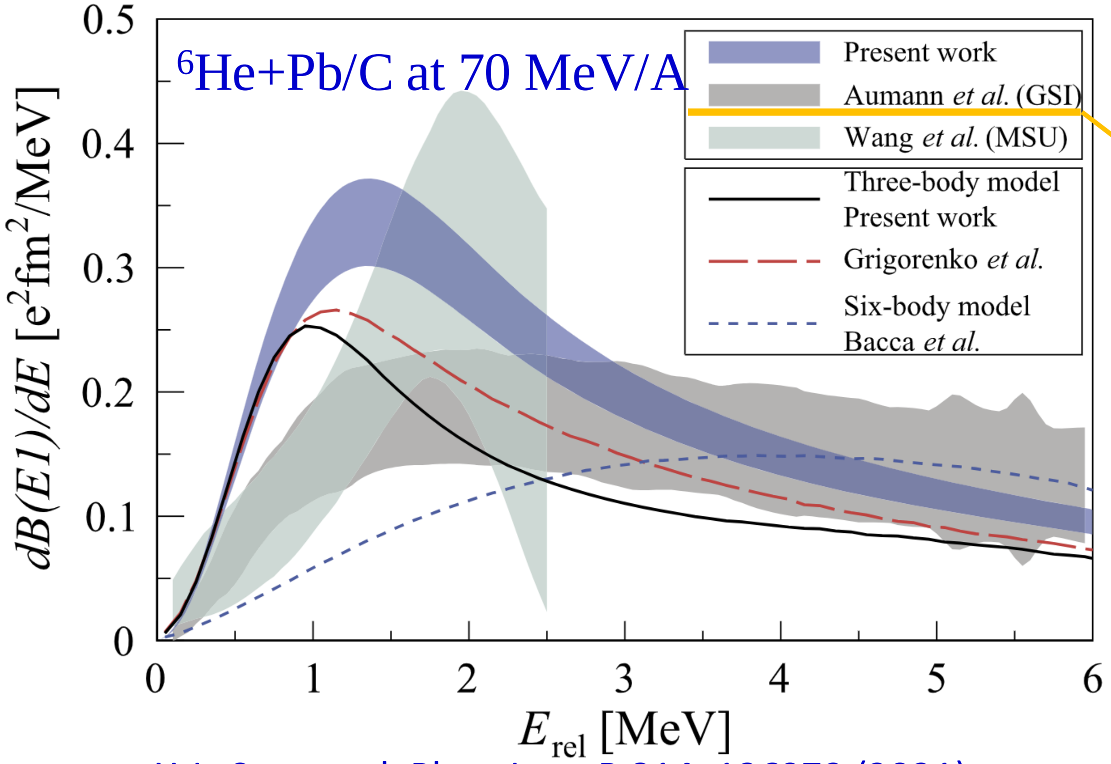
Theo./Exp.	Interaction	α_E (fm^3)
NCSM [This work]	*NN* (Daejeon16)	$0.0782^{+0.0006}_{-0.0003}$
HH [11]	*NN* (AV18) + 3*N* (UIX)	0.0655(4)
HH [12]	*NN* (MT-I/III)	0.076
HH [13]	[*NN* (N^3LO) + 3*N* (N^2LO)]$_{OLS}$	0.0694
NCSM [22]	[*NN* (N^3LO) + 3*N* (N^2LO)]$_{OLS}$	0.0683(14)
NCSM [23]	[*NN* (N^3LO) + 3*N* (N^2LO)]$_{1.8}$ [*NN* (N^3LO) + 3*N* (N^2LO)]$_{3.0}$	0.07093(5) 0.06861(5)
NCSM [24]	*NN* (N^3LO)	0.084(3)
SA-NCSM [24]	*NN* (N^3LO)	0.077(3)
NCSM SA-NCSM [24]	*NN* ($NNLO_{opt}$)	0.0680
CC [16]	*NN* + 3*N* ($NNLO_{sat}$)	0.0735(1)
Exp. [43, 44]	-	0.072(4)
Exp. [45]	-	0.076(8)

- Robust convergence with respect to N_{max}
- Uncertainty due to N_{max} truncation and energy truncation
- Direct calculation is feasible and robust
- Independent of diagonalization techniques

P. Yin, A. M. Shirokov, P. Maris, P. J. Fasano, M. A. Caprio, H. Li, W. Zuo, J. P. Vary, Phys. Lett. B **855**, 138857 (2024).

Sum rule with NCSM

$$\alpha_E = \frac{8\pi\alpha}{9}\int_{E_T}\frac{dE}{E}\frac{1}{e^2}\frac{dB(E1)}{dE}$$



Y. L. Sun, et al. Phys. Lett. B 814, 136072 (2021)

Fig. 3. The B(E1) distribution obtained by the present work compared with previous results from GSI [5] and MSU [23]. The experimental B(E1) distributions are also compared with the three-body calculations (black solid line from this work, red dashed line from Ref. [90]) and *ab initio* six-body calculation (blue dotted line) [91].

PHYSICAL REVIEW C **86**, 064316 (2012)

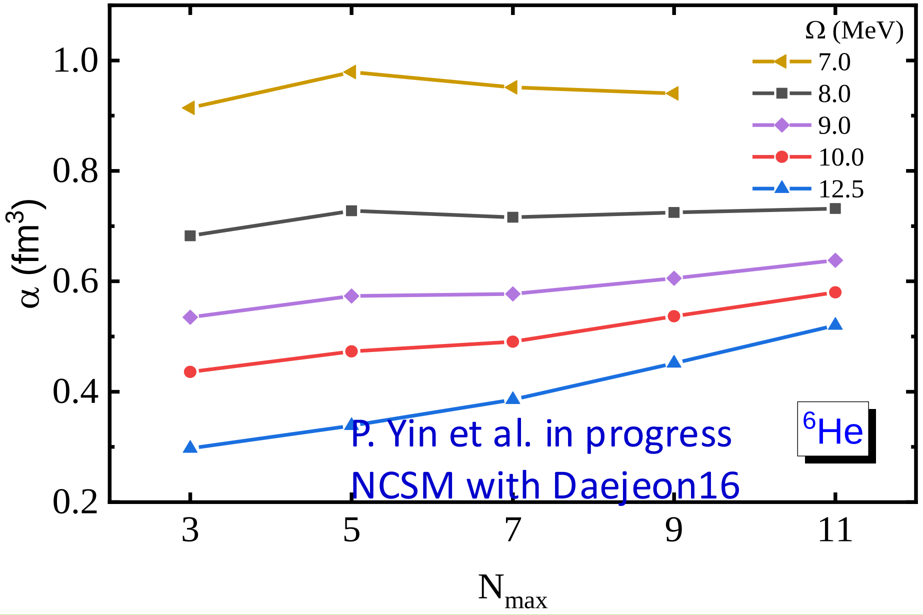
Nuclear electric polarizability of ^{6}He

R. Goerke,[1,2,*] S. Bacca,[2,†] and N. Barnea[3,‡]

[1]*Department of Physics, University of Toronto, 60 St. George St., Toronto, Ontario M5S 1A7, Canada*
[2]*TRIUMF, 4004 Wesbrook Mall, Vancouver, British Columbia V6T 2A3, Canada*
[3]*Racah Institute of Physics, Hebrew University, 91904, Jerusalem, Israel*

(Received 11 September 2012; revised manuscript received 19 November 2012; published 19 December 2012)

We present an estimate of the nuclear electric polarizability α_E of the ^{6}He halo nucleus based on six-body microscopic calculations. Wave functions are obtained from semirealistic two-body interactions using the hyperspherical harmonics expansion method. The polarizability is calculated as a sum rule of the dipole response function using the Lanczos algorithm and also by integrating the photoabsorption cross section calculated via the Lorentz integral transform method. We obtain $\alpha_E = 1.00(14)$ fm^3, which is much smaller than the published value $\alpha_E^{exp} = 1.99(40)$ fm^3 [Pachucki and Moro, Phys. Rev. A **75**, 032521 (2007)] extracted from experimental data. This points toward a potential disagreement between microscopic theories and experimental observations.



- Slow convergence
- ~0.7 fm^3
- Support HH results
- Larger nuclei, total-J

PHYSICAL REVIEW C 74, 061001(R) (2006)

Photonuclear sum rules and the tetrahedral configuration of ^{4}He

Doron Gazit,[1] Nir Barnea,[1] Sonia Bacca,[2] Winfried Leidemann,[3,4,*] and Giuseppina Orlandini[3,4,*]
[1]*The Racah Institute of Physics, The Hebrew University, 91904 Jerusalem, Israel*
[2]*Gesellschaft für Schwerionenforschung, Planckstr. 1, D-64291 Darmstadt, Germany*
[3]*Department of Physics, George Washington University, Washington DC 20052, USA*
[4]*Istituto Nazionale di Fisica Nucleare, Gruppo Collegato di Trento, Italy*
(Received 15 September 2006; published 14 December 2006)

$$m_n(\bar{\omega}) \equiv \int_{\omega_{\rm th}}^{\bar{\omega}} d\omega\, \omega^n\, \sigma_\gamma^{\rm E1UR}(\omega), \qquad (1)$$

$$\Sigma^{\rm TRK} \equiv m_0(\infty) = \frac{\mathcal{G}}{2} \langle 0|\,[\mathbf{D},[H,\mathbf{D}]]\,|0\rangle \qquad (4)$$

$$\Sigma^{\rm BSR} \equiv m_{-1}(\infty) = \mathcal{G}\,\langle 0|\mathbf{D}\cdot\mathbf{D}|0\rangle \qquad (5)$$

$$\Sigma^{\rm PSR} \equiv m_{-2}(\infty) = \mathcal{G}\sum_n (E_n - E_0)^{-1}|\langle n|\mathbf{D}|0\rangle|^2 . \qquad (6)$$

$$\Sigma^{\rm BSR} = \mathcal{G}\left[Z^2\langle r_p^2\rangle - \frac{Z(Z-1)}{2}\langle r_{pp}^2\rangle\right] \qquad (14)$$

$$\langle r_{pp}^2\rangle \equiv \frac{1}{Z(Z-1)}\langle 0|\sum_{i,j=1}^{Z}(\mathbf{r}_i - \mathbf{r}_j)^2|0\rangle. \qquad (15)$$

r_{pp} with NCSM: Daejeon 16

^{4}He: 2.487 fm

^{6}He: 2.645 fm

r_p with NCSM: Daejeon 16

^{4}He: 1.90 fm

^{6}He: 1.514 fm

M. Huang, T. Frederico, P. Maris, P. Yin, R. Basili, P. Fasano, J. P. Vary, in preparation

Table 1

Numerical values of $\langle r_{pp}^2\rangle^{1/2}$, $\langle r'^2\rangle^{1/2}$ and ρ as extracted from experimental values of σ_{-1} and $\mathcal{R}$

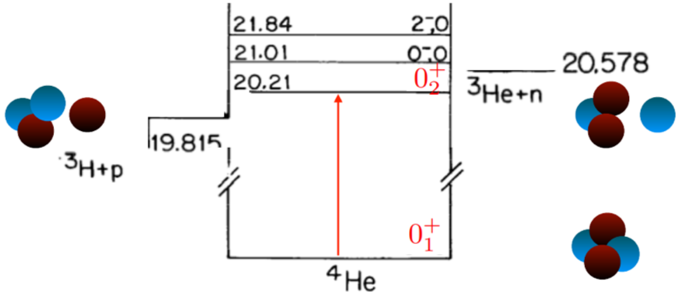
Nucleus	σ_{-1} (exp) (mb)	$\mathcal{R}$ (exp) $^{e)}$ (fm)	$\langle r_{pp}^2\rangle^{1/2}$ (fm)	$\langle r'^2\rangle^{1/2}$ (fm)	ρ
^{4}He	2.3 $^{a)}$	1.63±0.04	2.38	1.19	0.16
	2.1 $^{b)}$		2.43	1.22	0.14
^{7}Li	4.64 $^{c)}$	2.41	3.73	2.15	0.05
^{9}Be	5.19 $^{c)}$	2.51	3.77	2.31	0.03
^{12}C	8.81 $^{c)}$	2.45	3.50	2.26	0.03
^{16}O	14.5 $^{c)}$	2.72	3.86	2.56	0.02
^{40}Ca	45.5 $^{c)}$	3.48	4.89	3.37	0.01
^{90}Zr	70.6 $^{d)}$	4.28	6.01	4.20	~0
^{208}Pb	229.2 $^{d)}$	5.50	7.74	5.43	~0

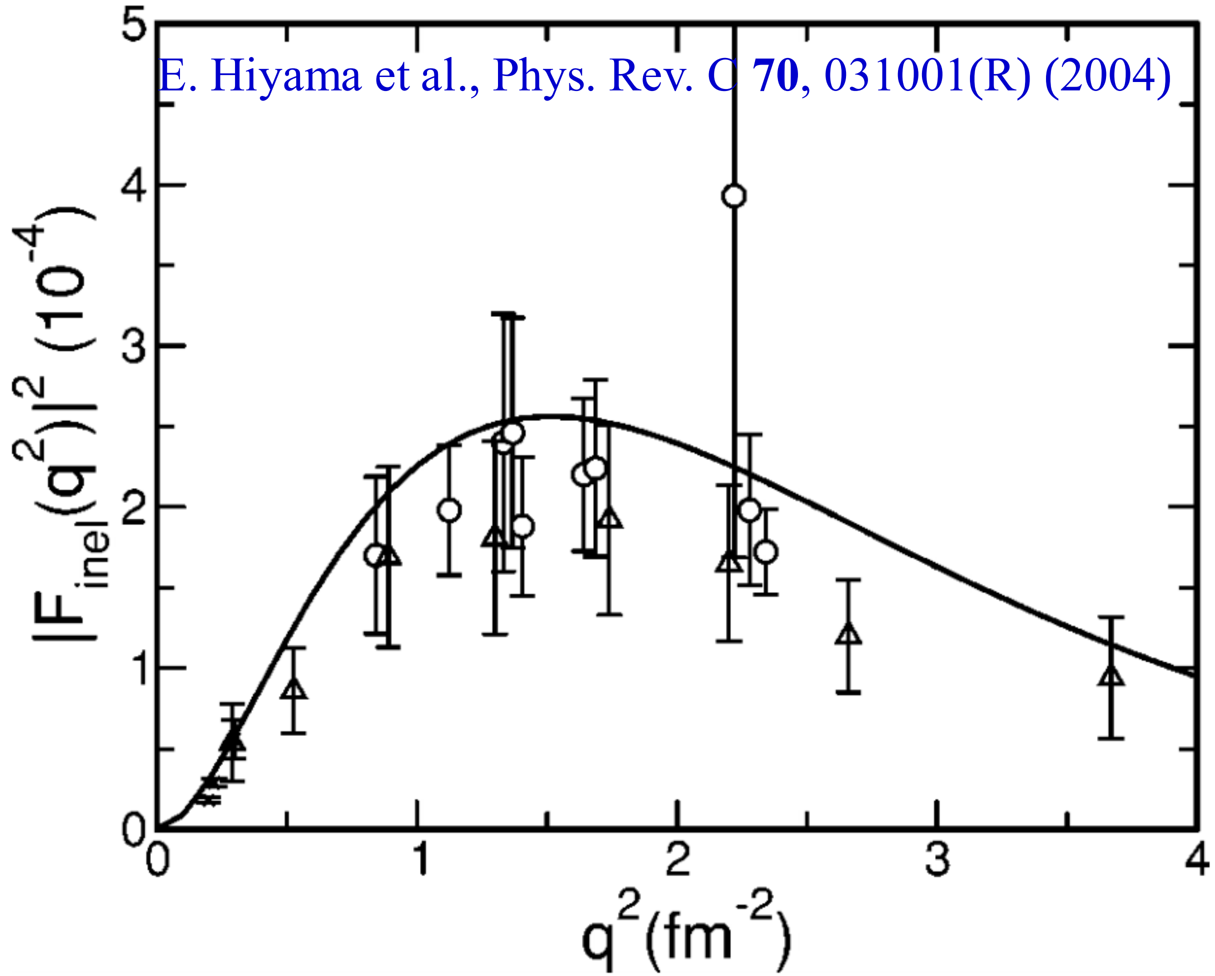
Constrain photoabsorption/strength function with nuclear structure calculations!

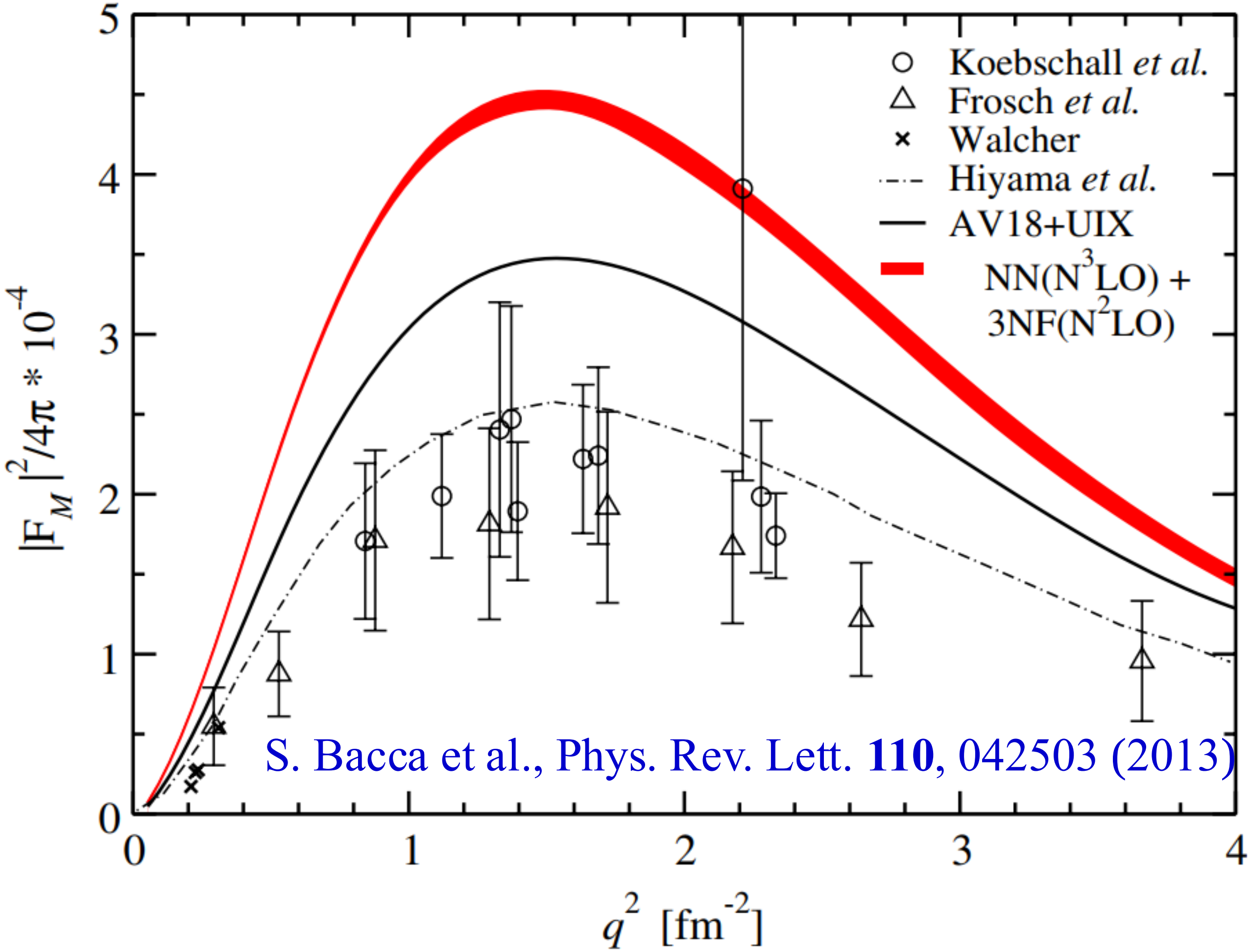
Monopole form factor with NCSM

Monopole transition form factor of ^{4}He

- Ground state: benchmark few-body methods
- Hiyama: Gaussian expansion, simplified force
- Bacca: HH+LIT, realistic *NN*+3*N* from chiral EFT







New experiment

Mainz

Status quo in 2023

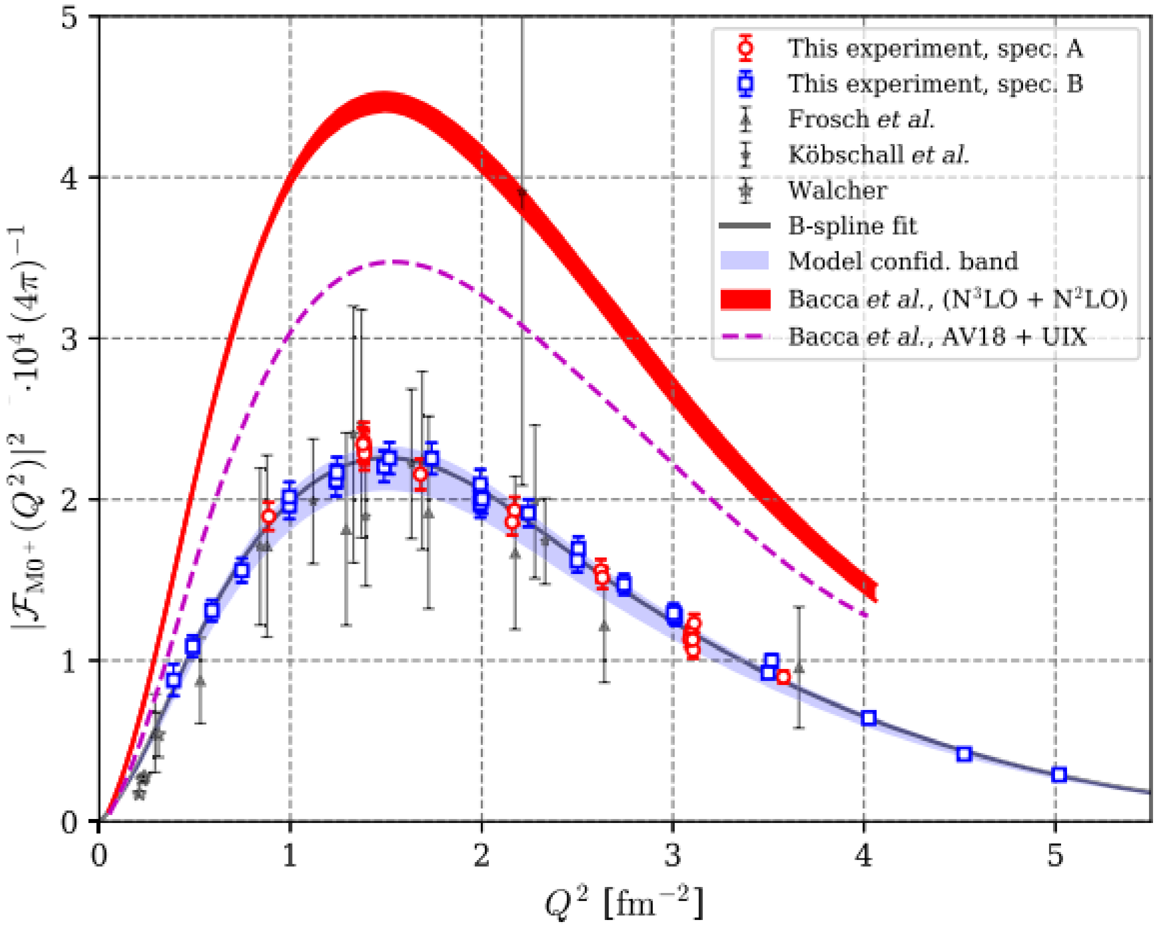
Problem with chiral EFT becomes stronger

PHYSICAL REVIEW LETTERS **130**, 152502 (2023)

Editors' Suggestion | Featured in Physics

Measurement of the α-Particle Monopole Transition Form Factor Challenges Theory: A Low-Energy Puzzle for Nuclear Forces?

S. Kegel,[1] P. Achenbach,[1] S. Bacca,[1,2] N. Barnea,[3] J. Beričič,[4] D. Bosnar,[5] L. Correa,[6,1] M. O. Distler,[1] A. Esser,[1] H. Fonvieille,[6] I. Friščić,[5] M. Heilig,[1] P. Herrmann,[1] M. Hoek,[1] P. Klag,[1] T. Kolar,[7,4] W. Leidemann,[8,9] H. Merkel,[1] M. Mihovilovič,[1,4] J. Müller,[1] U. Müller,[1] G. Orlandini,[8,9] J. Pochodzalla,[1] B. S. Schlimme,[1] M. Schoth,[1] F. Schulz,[1] C. Sfienti,[1,*] S. Širca,[7,4] R. Spreckels,[1] Y. Stöttinger,[1] M. Thiel,[1] A. Tyukin,[1] T. Walcher,[1] and A. Weber[1]

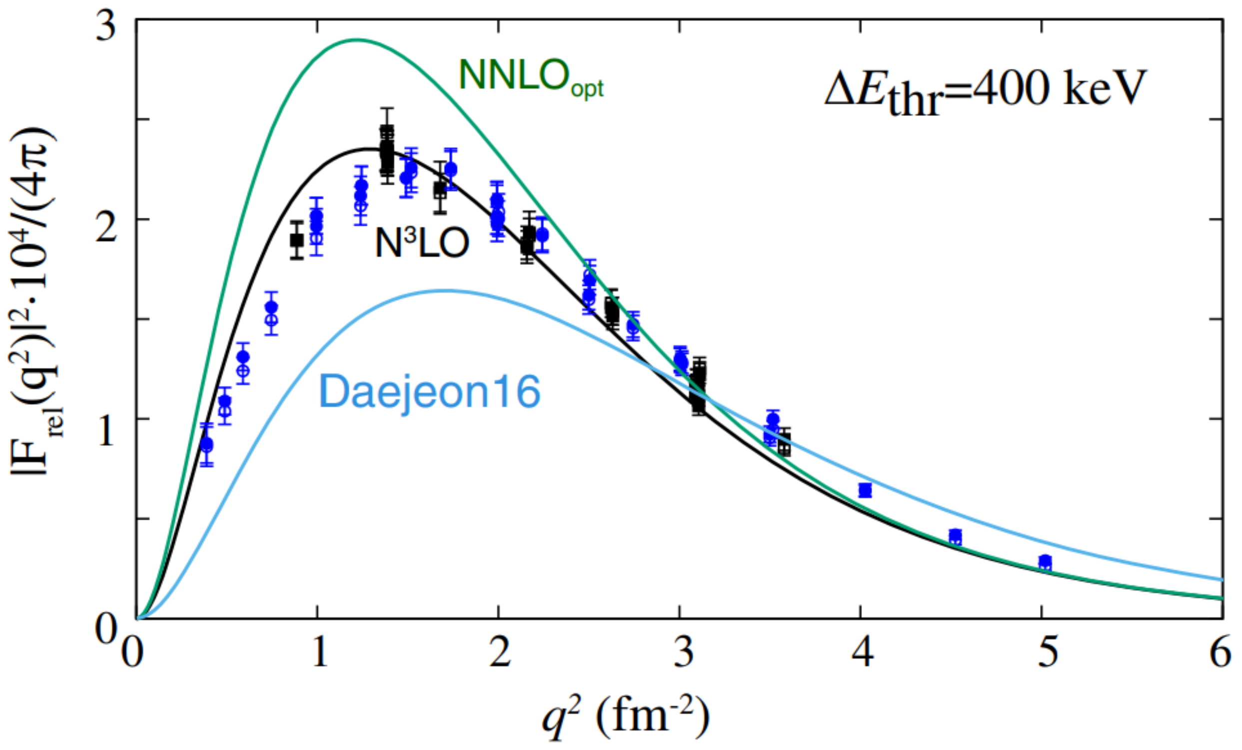


PHYSICAL REVIEW LETTERS **131**, 242502 (2023)

Featured in Physics

Description of the Proton-Decaying 0_2^+ Resonance of the α Particle

N. Michel,[1,2,3] W. Nazarewicz,[4] and M. Płoszajczak[3]



$$|F(q^2)|^2 = \left|\frac{4\pi}{Z}\int \rho_{tr}(r) j_0(qr) r^2 dr\right|^2 f_p^2(q^2)$$

$$\rho_{tr}(r) = \langle 0_1^+|\hat{\rho}(\vec{r})|0_2^+\rangle$$

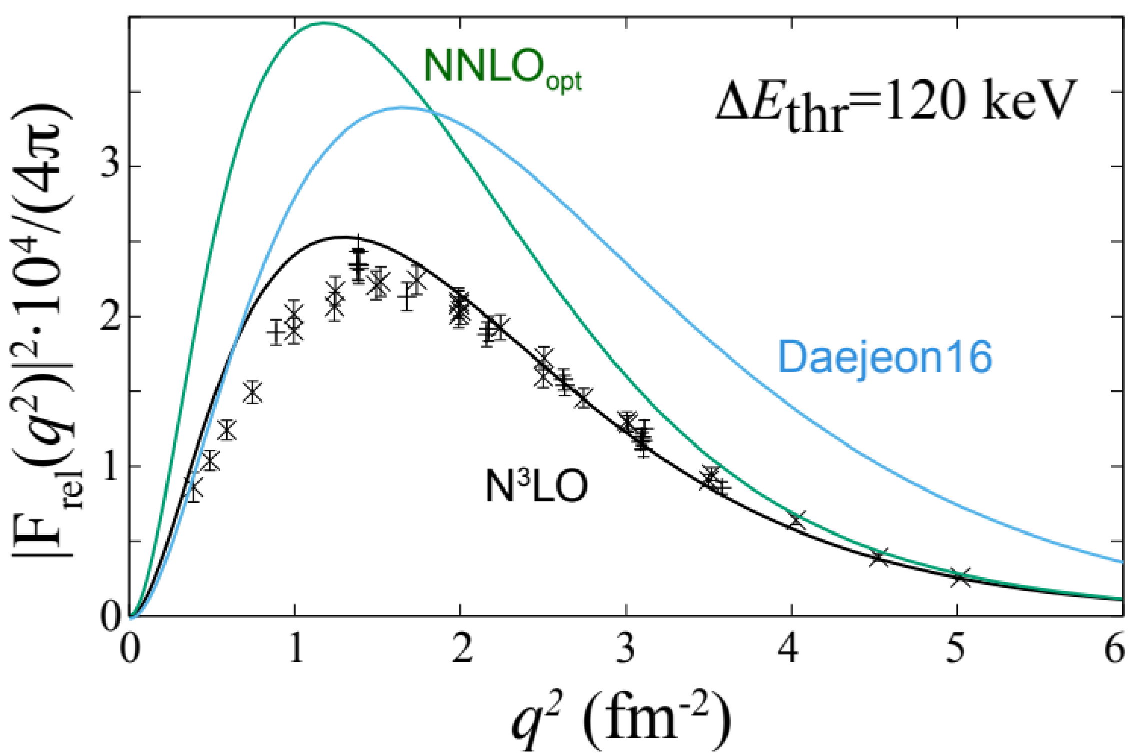
- NCGSM-CC with V_{lowk}
- E_r=400 keV

PHYSICAL REVIEW LETTERS **133**, 239901(E) (2024)

Erratum: Description of the Proton-Decaying 0_2^+ Resonance of the α Particle [Phys. Rev. Lett. 131, 242502 (2023)]

N. Michel, W. Nazarewicz, and M. Płoszajczak

(Received 15 July 2024; revised 9 October 2024; published 4 December 2024)

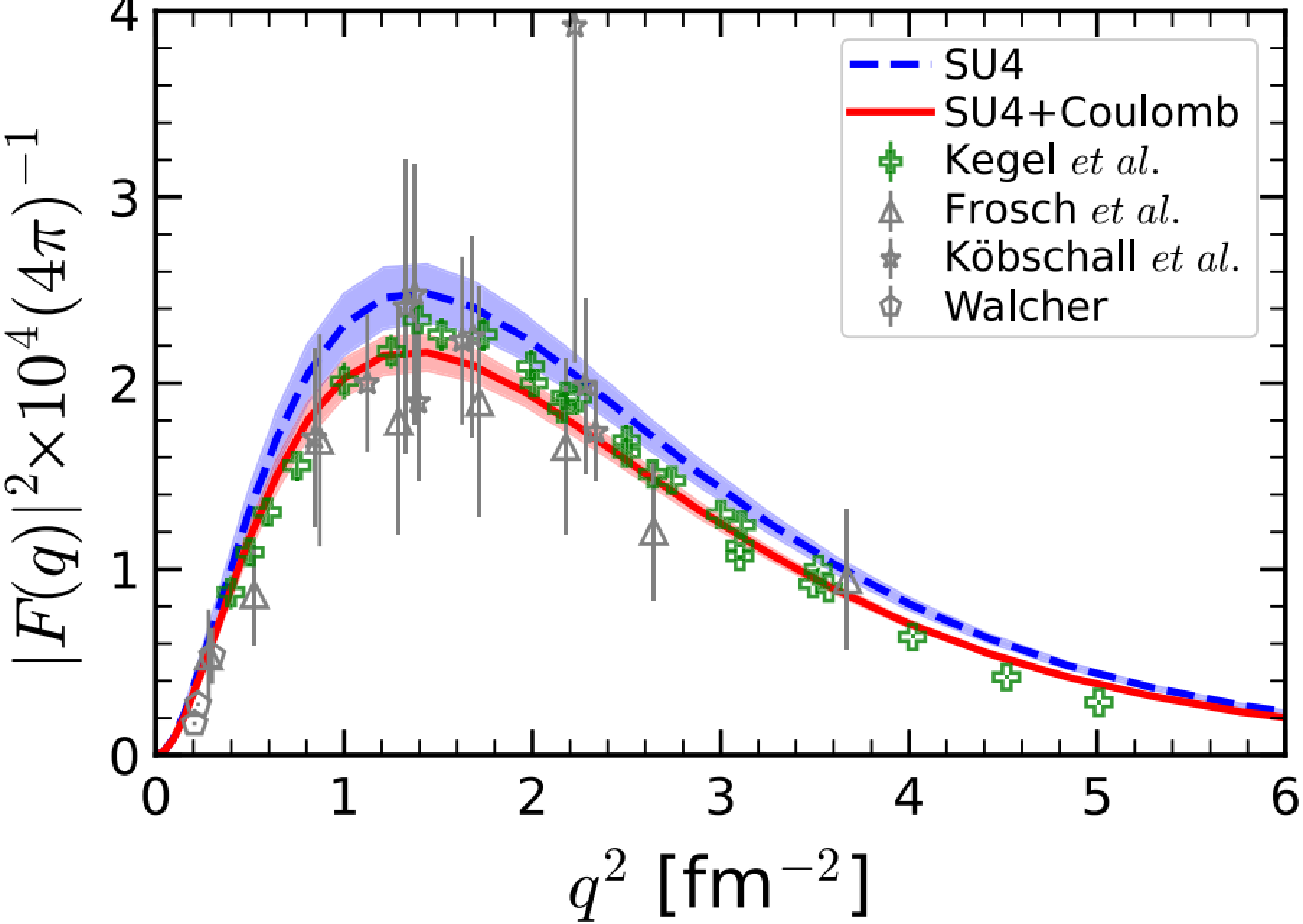


- E_r=120 keV

PHYSICAL REVIEW LETTERS **132,** 062501 (2024)

Ab Initio Calculation of the Alpha-Particle Monopole Transition Form Factor

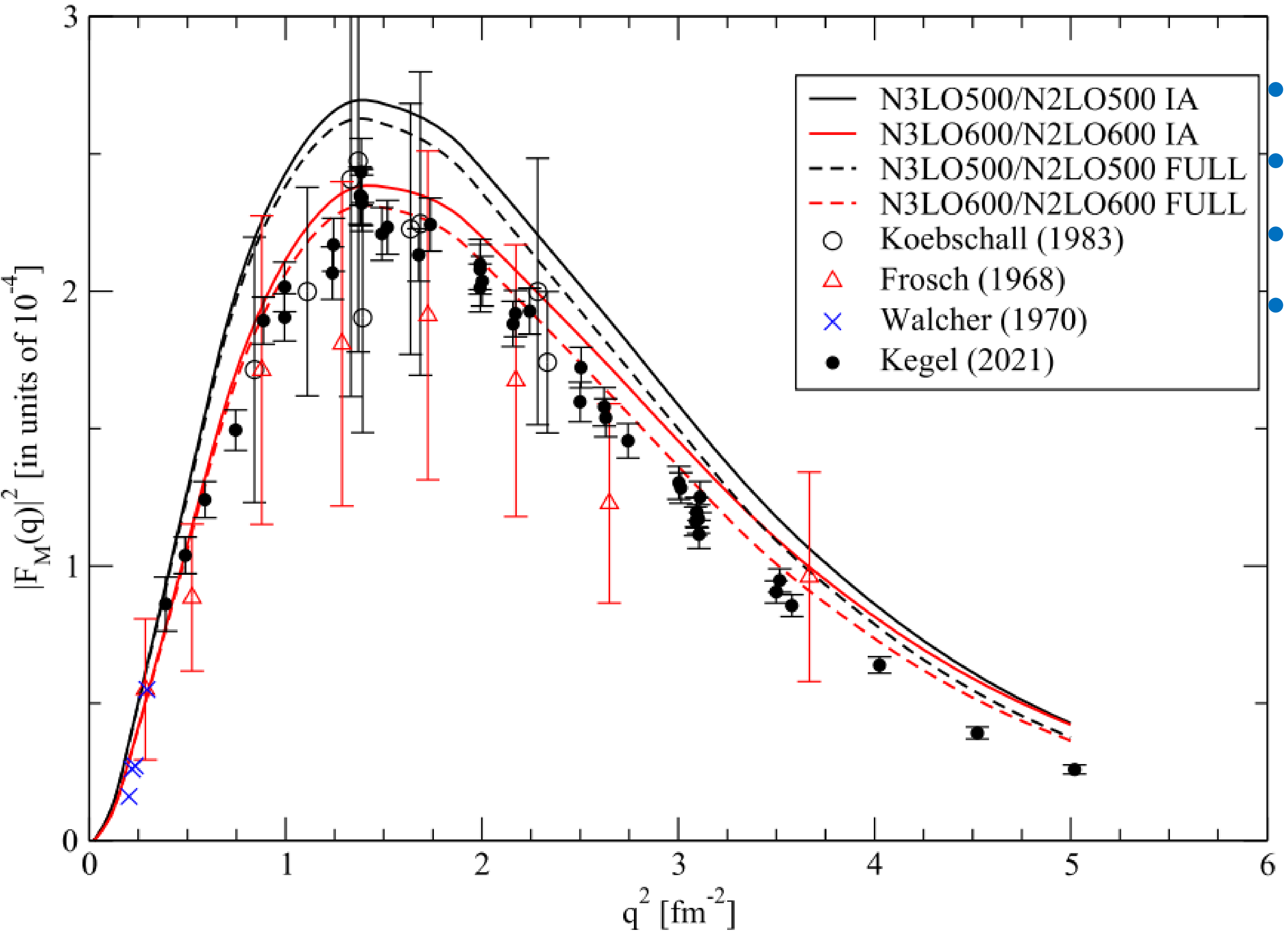
Ulf-G. Meißner,[1,2,3] Shihang Shen,[4,*] Serdar Elhatisari,[5,1] and Dean Lee[6]



Few-Body Syst (2024) 65:74
https://doi.org/10.1007/s00601-024-01940-2

M. Viviani · A. Kievsky · L. E. Marcucci · L. Girlanda

Study of the Alpha-particle Monopole Transition form Factor



- Viviani: HH ^3He+n, ^3H+p, chiral $NN+3N$
- Two-body current
- First successful calculation with chiral EFT?
- Large T=1 components

K	P(T=1)	P(T=2)
28	0.35593	0.00297
30	0.45106	0.00297
32	0.56375	0.00297

In the news

From Sonia Bacca

From Sonia Bacca

Two important comments

E. Epelbaum, Physics **16** (2023) 58

Threshold energy:

"The form factor may depend on the energy difference between the position of the resonance and the two-body breakup threshold, so any uncertainties in calculating the excitation energy would translate into relatively large uncertainties in the form factor predictions."

⇒ investigate role of threshold energy

Kamimura, Prog. Theor. Exp. Phys. (Letter) Vol. 2023, 071D01 (2023)

Bound vs Continuum:

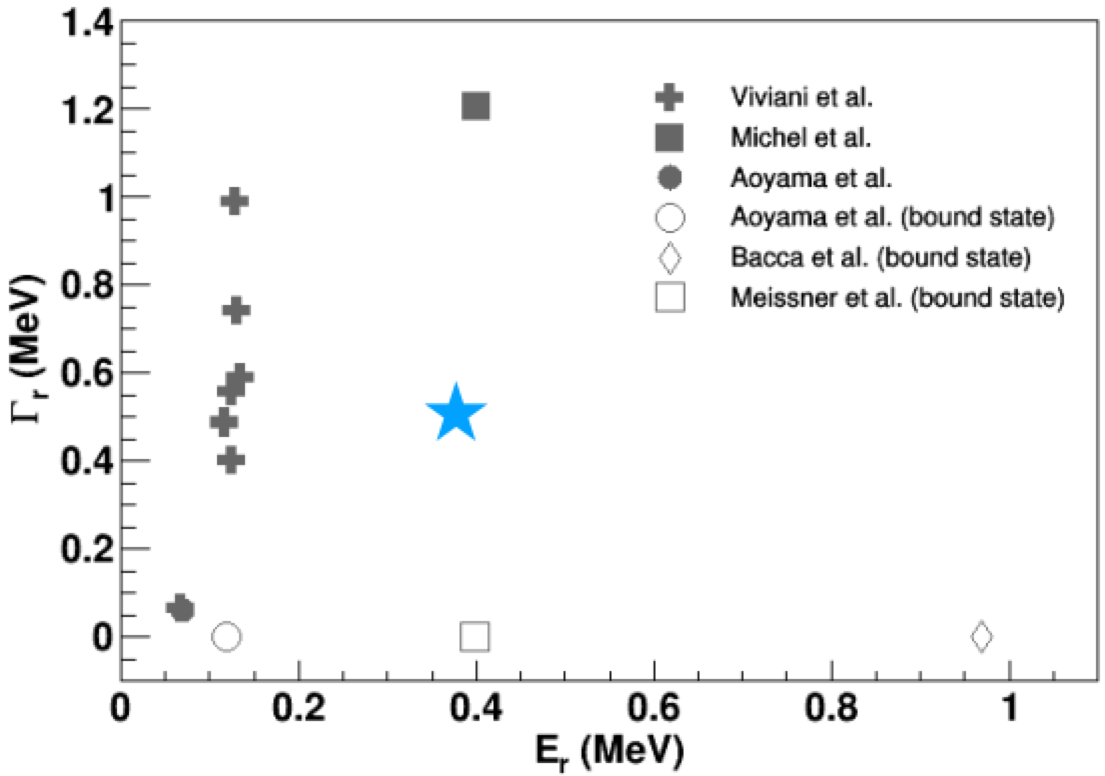
Claim that "*the large difference between the calculated form factors does not stem from numerical methods but from the Hamiltonian. However, the comparison between the methods was performed only for the calculation based on the bound-state approximation.*"

⇒ investigate role of continuum

From Sonia Bacca

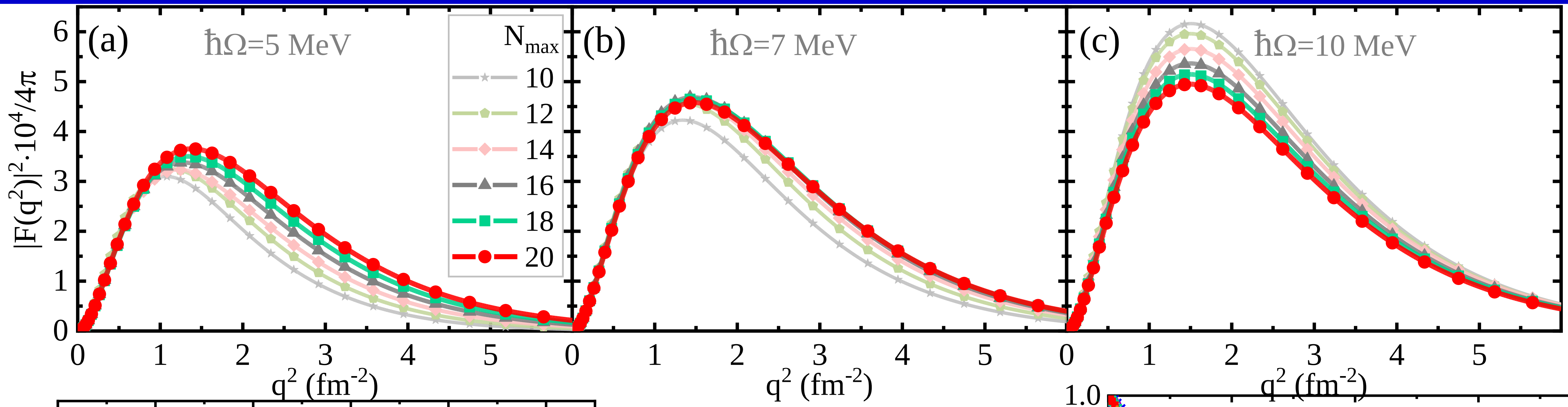
None of the theories gets E_r and Γ_r correct

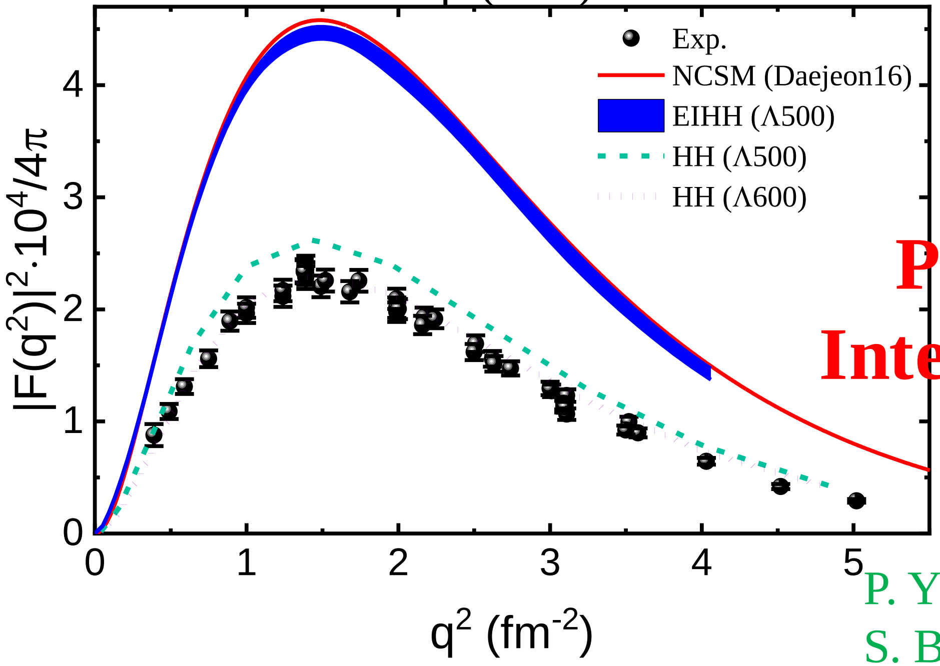
Evaluation by Tilley et al, NPA 541 (1992) 1-104 ★ $E_r = 0.39$ MeV $\Gamma_r = 0.50$ MeV



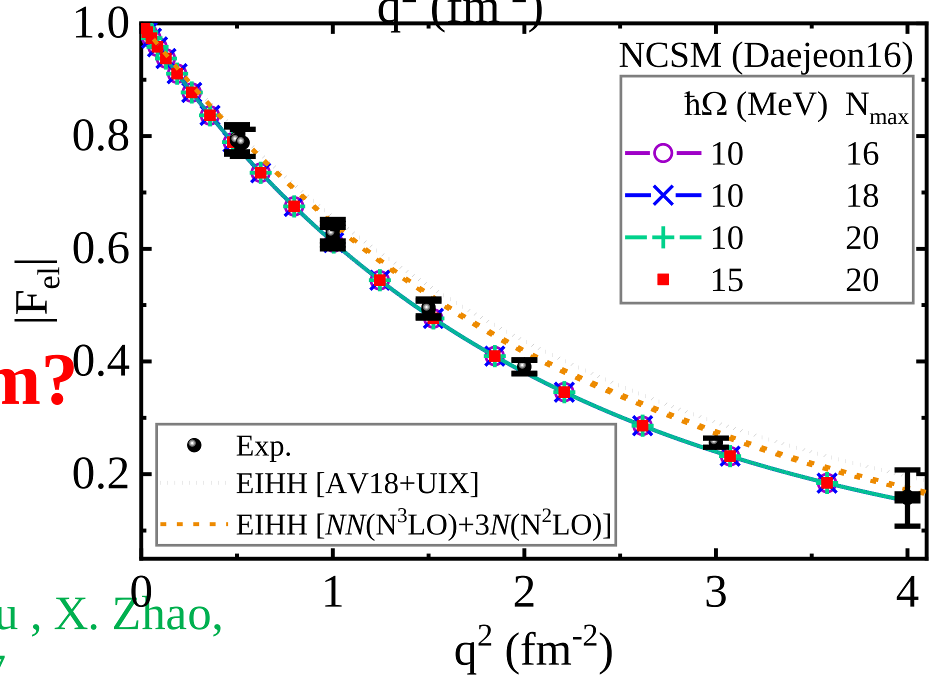
Pionless EFT with RGM: Kirscher and Griesshammer, EPJA **54**, 137 (2018) $E_r = 0.38 \pm 0.25$MeV

Monopole transition form factor of ^{4}He





Puzzle NOT resolved!
Interaction or continuum?



P. Yin, A. M. Shirokov, H. Li, B. Zhou , X. Zhao,
S. Bacca, J. P. Vary, arXiv2412.18037

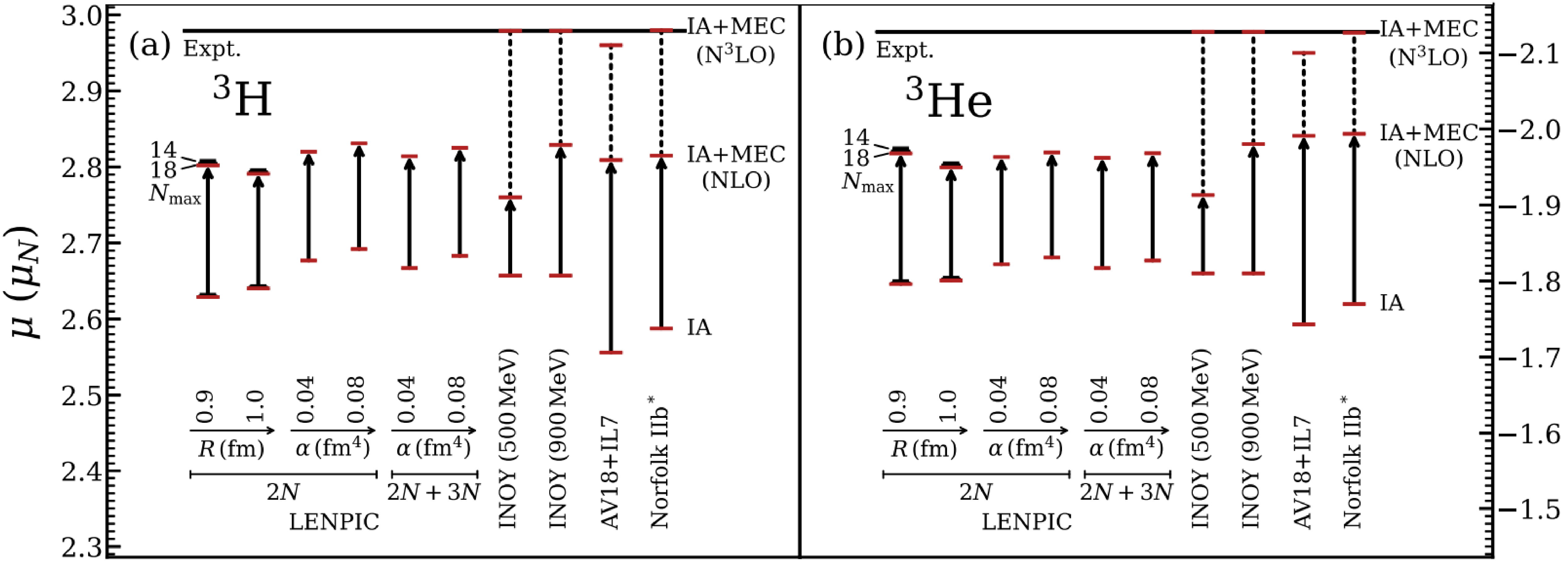
Two-body currents
LENPIC interaction

$$\boldsymbol{\mu} = \frac{1}{2}\int_{\mathbb{R}^3} d^3x\, \boldsymbol{x} \times \bar{\boldsymbol{j}}(\boldsymbol{x})$$

PHYSICAL REVIEW C **108**, 024001 (2023)

Magnetic moments of $A = 3$ nuclei obtained from chiral effective field theory operators

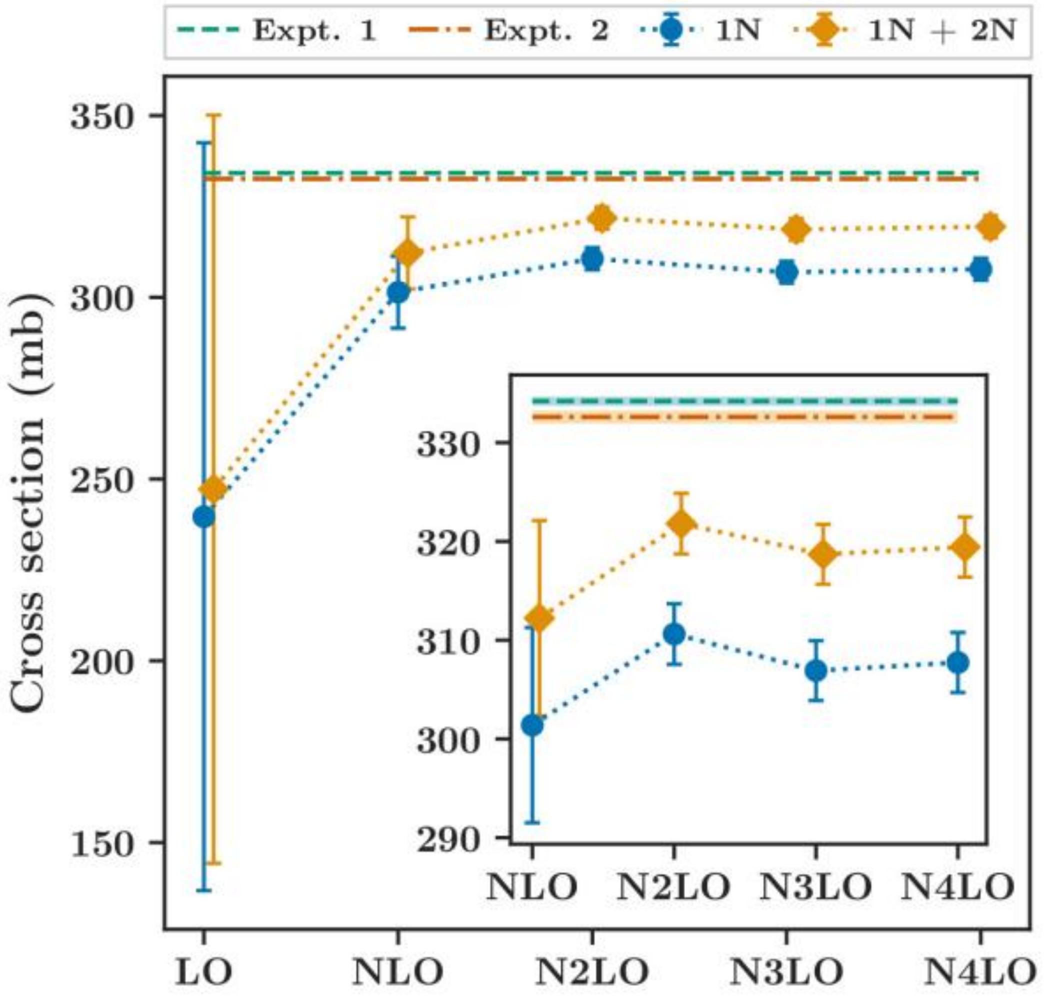
Soham Pal,[1,*] Shiplu Sarker,[1] Patrick J. Fasano,[2,†] Pieter Maris,[1] James P. Vary,[1]
Mark A. Caprio,[2] and Robert A. M. Basili[3]
[1]*Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011-3160, USA*
[2]*Department of Physics and Astronomy, University of Notre Dame, Notre Dame, Indiana 46556-5670, USA*
[3]*Department of Electrical and Computer Engineering, Iowa State University, Ames, Iowa 50011-3160, USA*



PHYSICAL REVIEW C **106**, 054608 (2022)

Calculations of the $np \rightarrow d\gamma$ reaction in chiral effective field theory

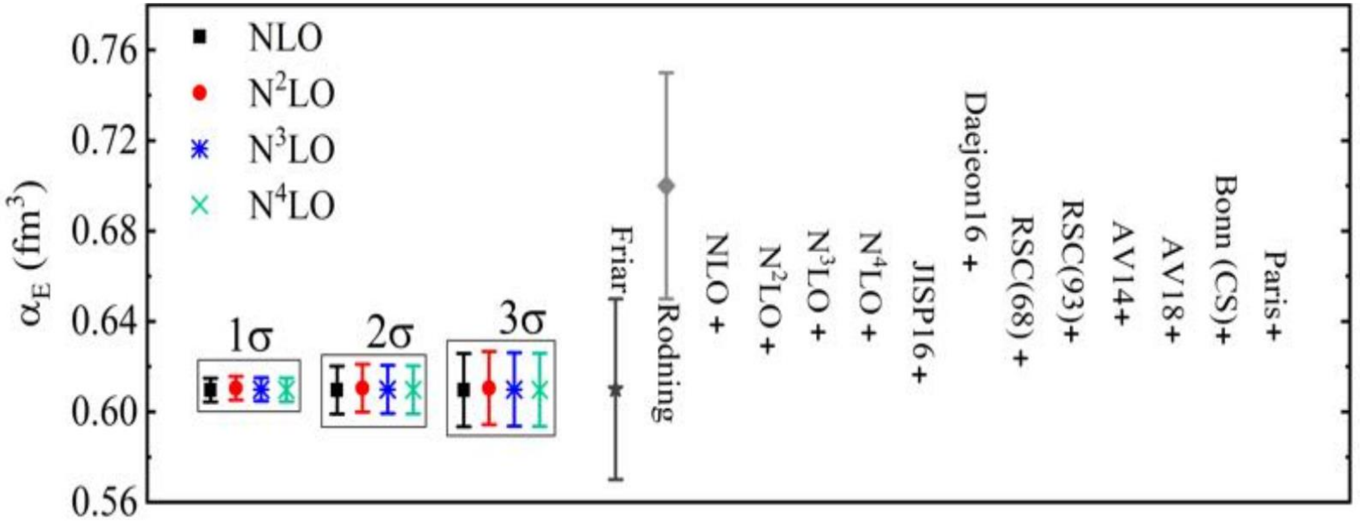
Weijie Du,[1,*] Soham Pal,[1] Mamoon Sharaf,[1] Peng Yin,[1,2] Shiplu Sarker,[1] Andrey M. Shirokov,[3] and James P. Vary[1]
[1]*Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50010, USA*
[2]*Institute of Modern Physics, Chinese Academy of Sciences, Lanzhou 730000, China*
[3]*Skobeltsyn Institute of Nuclear Physics, Lomonosov Moscow State University, Moscow 119991, Russia*



$$\bar{\sigma}_{-2} \equiv \frac{1}{2\pi^2}\int_{E_B}^{\infty} \frac{\sigma(E_\gamma)}{E_\gamma^2}\, dE_\gamma = \bar{\alpha} + \bar{\beta}$$

$$\bar{\alpha} = \alpha_E + \frac{Z\alpha \langle \boldsymbol{r}^2 \rangle}{3Am_N} + \alpha_N + \cdots$$

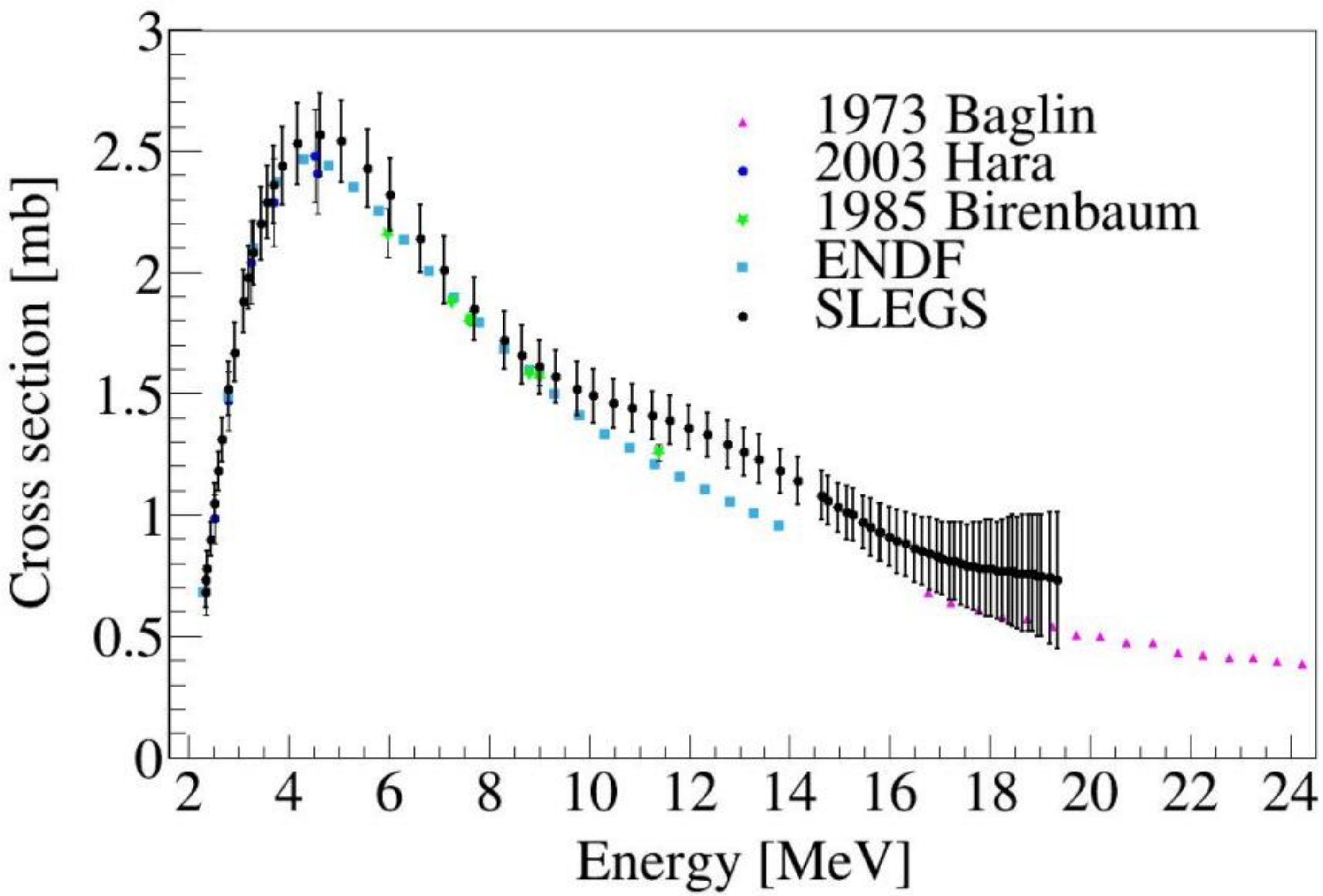
$$\bar{\beta} = \frac{2\alpha}{3}\sum_{n\neq 0}\sum_{M_n,\lambda} \frac{|\langle \Psi_n, M_n|\mu_{1,\lambda}|\Psi_0, M_0\rangle|^2}{E_n - E_0} - \frac{Z\alpha\langle \boldsymbol{r}^2\rangle}{6m_N} - \frac{\alpha\langle \boldsymbol{D}^2\rangle}{2Am_N} + \beta_N + \beta_\pi +$$



- Updated photoabsorption data
- Two-body current: 5%

Shiplu Sarker, P. Yin et al., in preparation

$$\sigma_{-2} = \bar{\alpha} + \bar{\beta} = \frac{1}{2\pi}\int_{S_n}^{\infty} \sigma(E) E^{-2} \mathrm{d}E$$



对测量得到的D(γ,n)p截面计算σ_{-2}：

- S_n-15.66MeV：
  0.6843 fm³
  ±0.0065 fm³(stat)
  ±0.0125 fm³(meth)
  ±0.0432 fm³(syst)
- S_n-19.33 MeV：
  0.6943 fm³
  ±0.0068 fm³(stat)
  ±0.0137 fm³(meth)
  ±0.0449 fm³(syst)

如果结合[2H(γ, p) absolute cross section and angular distribution at 17–25 MeV]的数据，σ_{-2}结果为:

0.7013±0.0479 fm³

可以看出该数据的贡献仅为0.0069 fm³，与统计误差相当，因此可以认为

$$\sigma_{-2} = \frac{1}{2\pi}\int_{S_n}^{19.34\mathrm{MeV}} \sigma(E) E^{-2} \mathrm{d}E + \Delta$$

where, $\Delta <$ statistical uncertainty

Summary

- Introduction to *ab initio* NCSM approach
- Long range operators
- Sum rules with NCCI
- Monopole transition form factor of ^4He
- Two-body currents

Outlook

- Photoabsorption reaction
- Neutrino-nucleus reaction
- n+α, p+^3H, n+^3He… scatterings
- Coulomb dissociation of light nuclei

NCSM with continuum (P. Navratil)

- 3He(α,γ)7Be and 3H(α,γ)7Li
- 7Li(p,e+e−)8Be: X17
- α+α
- p+7Be and p+7Li
- 8Li(n,γ)9Li, 7Be(p,γ) 8B

Time Dependent Basis Function

Scattering at sub-barrier with the tBF approach

1. *Ab initio* structure calculation

$$H_0 = T_{rel} + V$$

$$H_0|\beta_i\rangle = E_i|\beta_i\rangle$$

$$\{|\beta_1\rangle, |\beta_2\rangle, \cdots, |\beta_n\rangle\}$$

2. Time-dependent process

$$i\frac{d}{dt}|\psi(t)\rangle = H(t)|\psi(t)\rangle$$

$$H(t) = H_0 + V(t)$$

$$|\psi(t)\rangle_I = \sum_{j=1}^{n} A_j^I(t)|\beta_j\rangle$$

- Natural extension of *ab initio* nuclear structure approaches, e.g., NCSM
- Non-perturbative
- Full quantal coherence

- Weijie Du, Peng Yin*, Yang Li, Guangyao Chen, Wei Zuo, Xingbo Zhao, and James P. Vary, ***Phys. Rev. C* 97**, 064620 (2018);
- Weijie Du, Peng Yin, Guangyao Chen, Xingbo Zhao, and James P. Vary, *in Proceedings of the International Conference "Nuclear Theory in the Supercomputing Era–2016" (NTSE-2016), Khabarovsk, Russia, September 19–23,* 2016;
- Peng Yin, Weijie Du, Wei Zuo, Xingbo Zhao and James P. Vary, **J. Phys. G** (2022);
- Weijie Du, James P. Vary, Xingbo Zhao, Wei Zuo, **Phys. Rev. A** 104, 012611 (2021).
- Peng Yin, Weijie Du, Wei Zuo, Xingbo Zhao and James P. Vary, arXiv 2208.00267

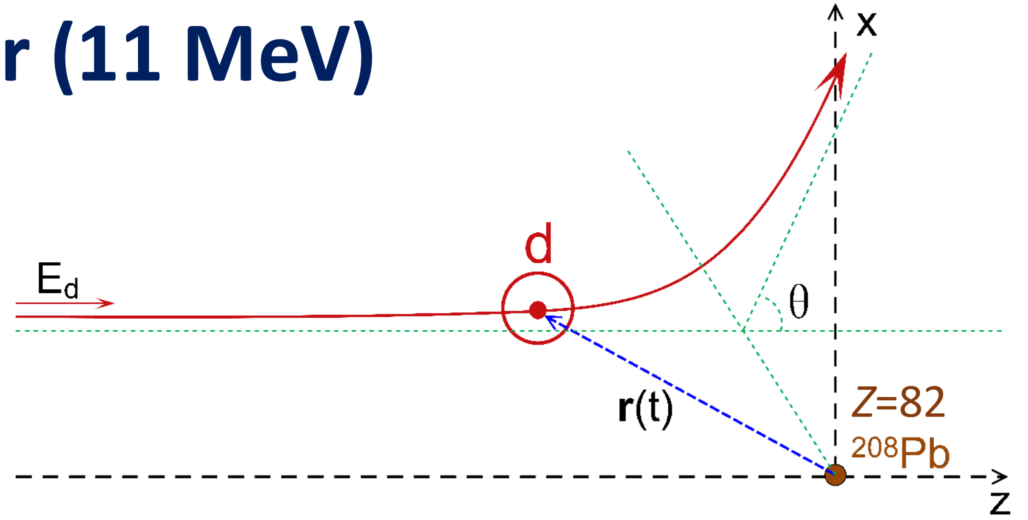
d+^{208}Pb scatterings below Coulomb barrier (11 MeV)

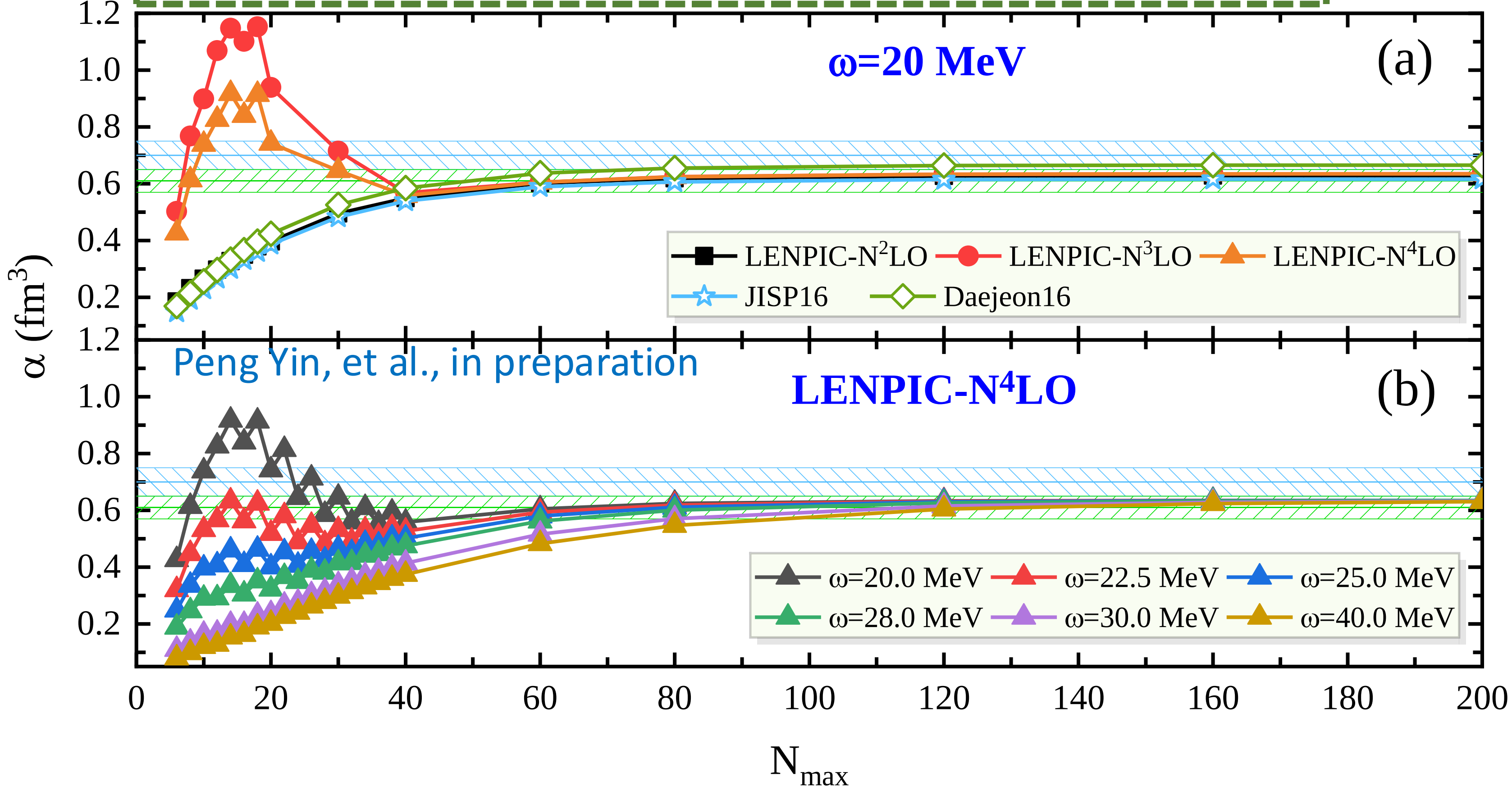
Solving EOM for CM motion of deuteron in external field:

$V = V_{coul} + V_{pol}$

$$V_{pol} = -\frac{1}{2}\alpha Z^2 e^2 \frac{1}{r^4}$$

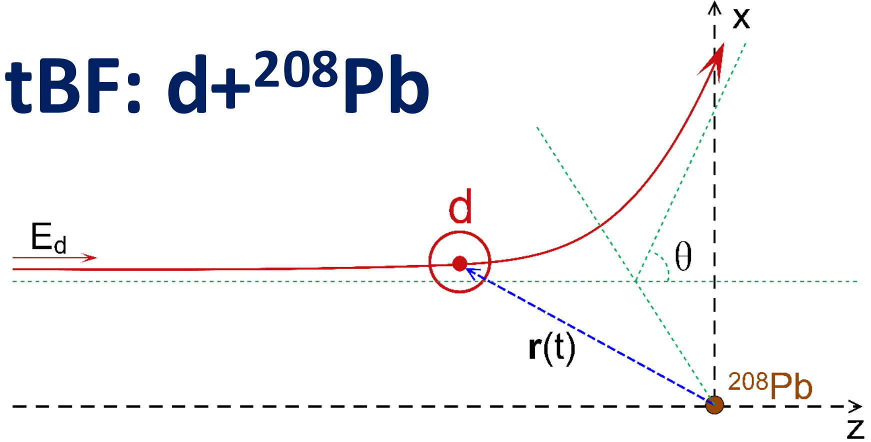
$$\alpha = \frac{8\pi}{9} \sum_{n\neq 0} \frac{B(E1; 0 \to n)}{(E_n - E_0)}$$





- Harmonic oscillator (HO) basis;
- Parameters of HO basis: N_{max} and ω, $(2n + l \leq N_{max})$;
- α is converged with respect to N_{max} and ω;
- LENPIC interactions: regulator R=1.0 fm.

tBF: d+^{208}Pb



Time-independent:

$$H_0 = T_{rel} + V_{np}$$

$$H_0|\beta_i\rangle = E_i|\beta_i\rangle$$

Basis set $\{|\beta_j\rangle\}$

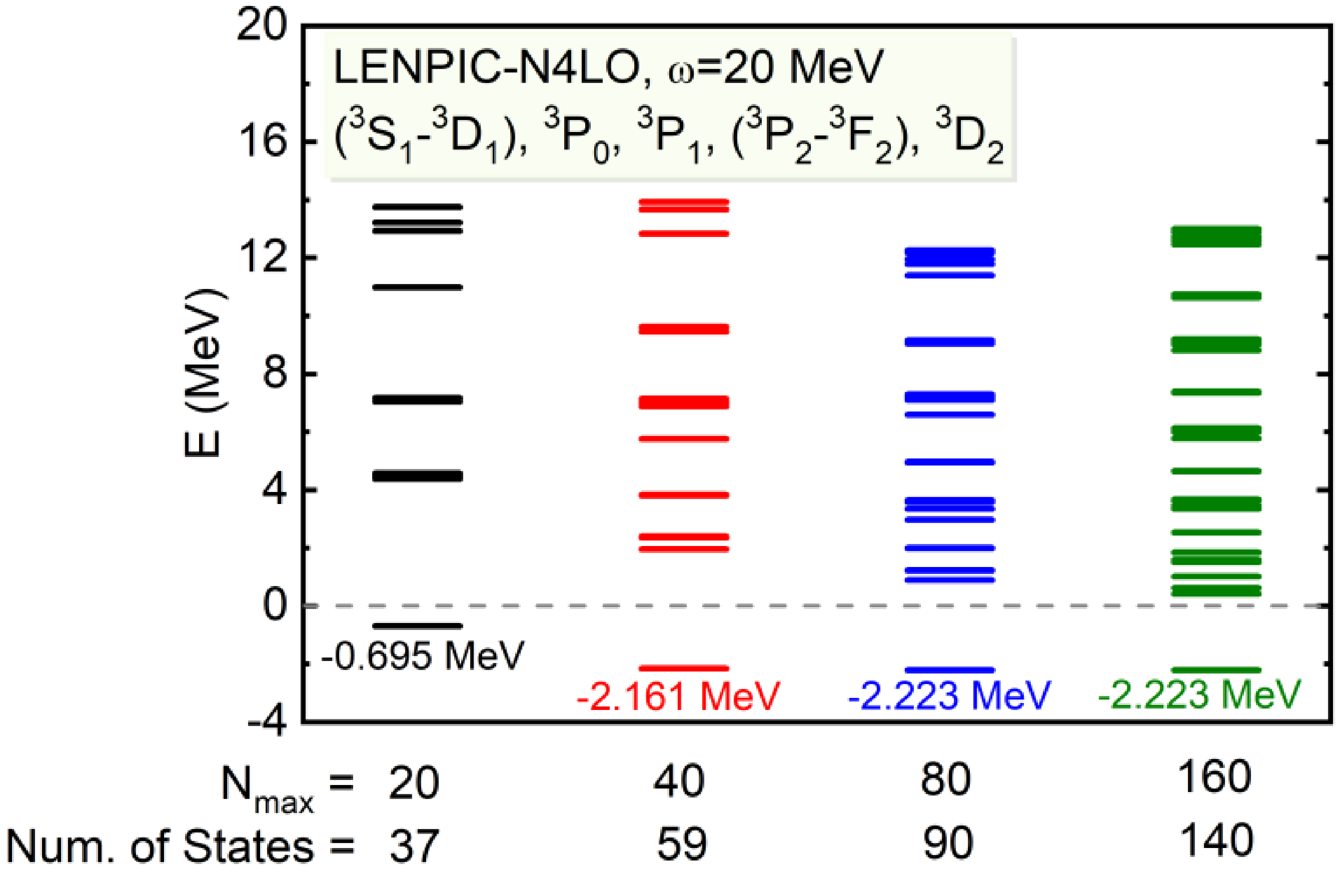
$$H(t) = H_0 + V(t)$$

E1 is dominant

Time-dependent:

$$i\frac{\partial}{\partial t}|\psi(t)\rangle_I = V_I(t)|\psi(t)\rangle_I$$

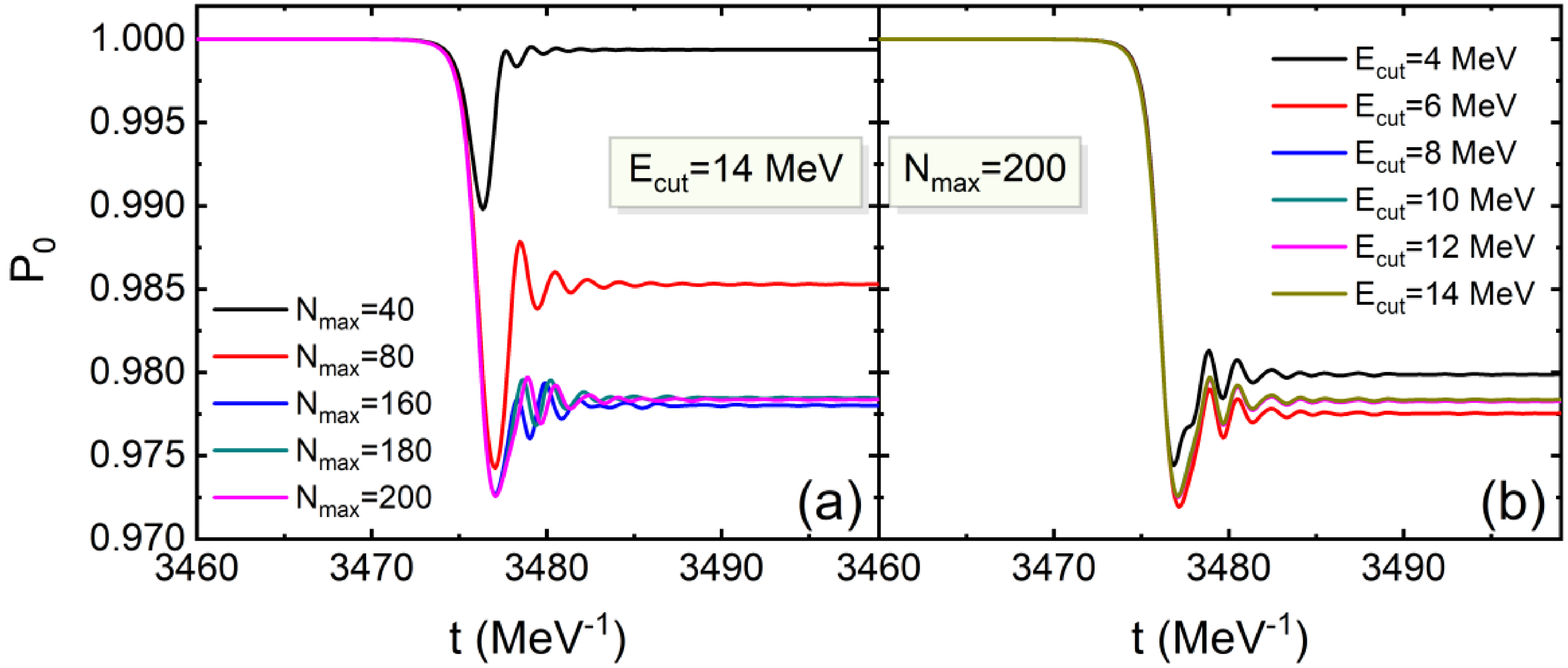
$$|\psi(t)\rangle_I = \sum_{j=1}^{n} A_j^I(t)|\beta_j\rangle$$



- *NN* interaction: LENPIC-N^{4}LO
- 3DHO basis: N_{max}, $\omega = 20$ MeV
- S=1, J_{max}=2

Peng Yin, Weijie Du, Wei Zuo, Xingbo Zhao and James P. Vary, arXiv 2208.00267

$d+^{208}Pb$ scatterings at E_d=7 MeV and θ=150°
Convergence with respect to N_{max} and E_{cut}



- Initial state: deuteron ground state with M=-1;
- P_0 is the probability of the initial state;
- The asymptotic value is well converged with respect to Nmax and Ecut.

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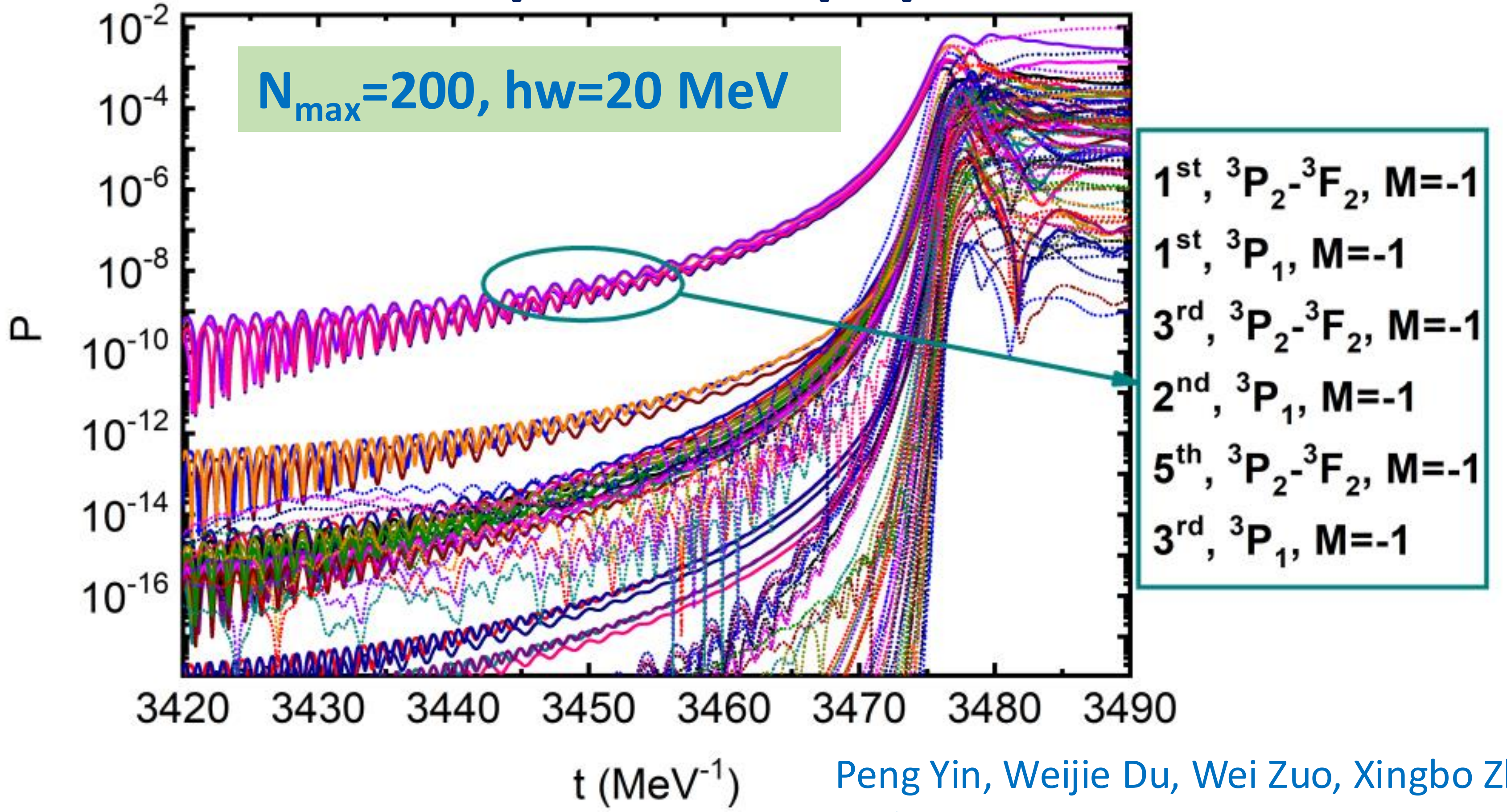
$d+^{208}Pb$ scatterings at E_d=7 MeV and θ=150°
Sequence of population



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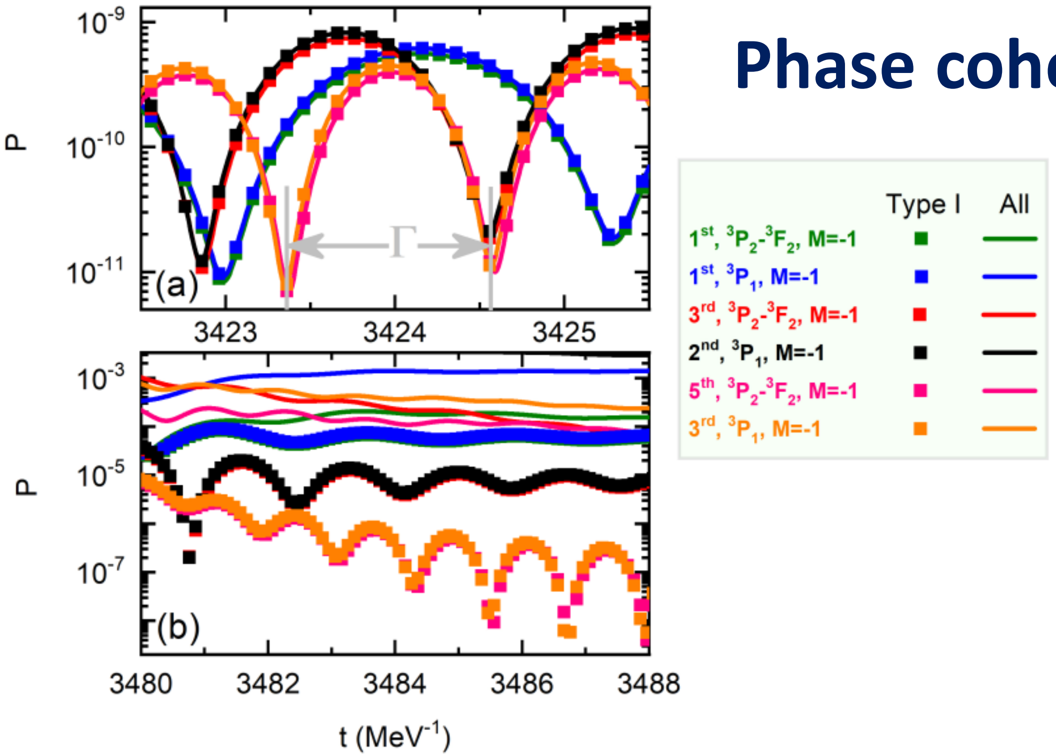
- Initial state: deuteron ground state $^3S_1$-$^3D_1$ with M=-1;
- P is the probability of states other than the initial state;
- Allowed states (solid lines) populate first. Forbidden states (dotted lines) populate afterward;
- 6 allowed states populate dominantly in the early stage of the time evolution.

d+^{208}Pb scatterings at E_d=7 MeV and θ=150°
Phase coherence and decoherence



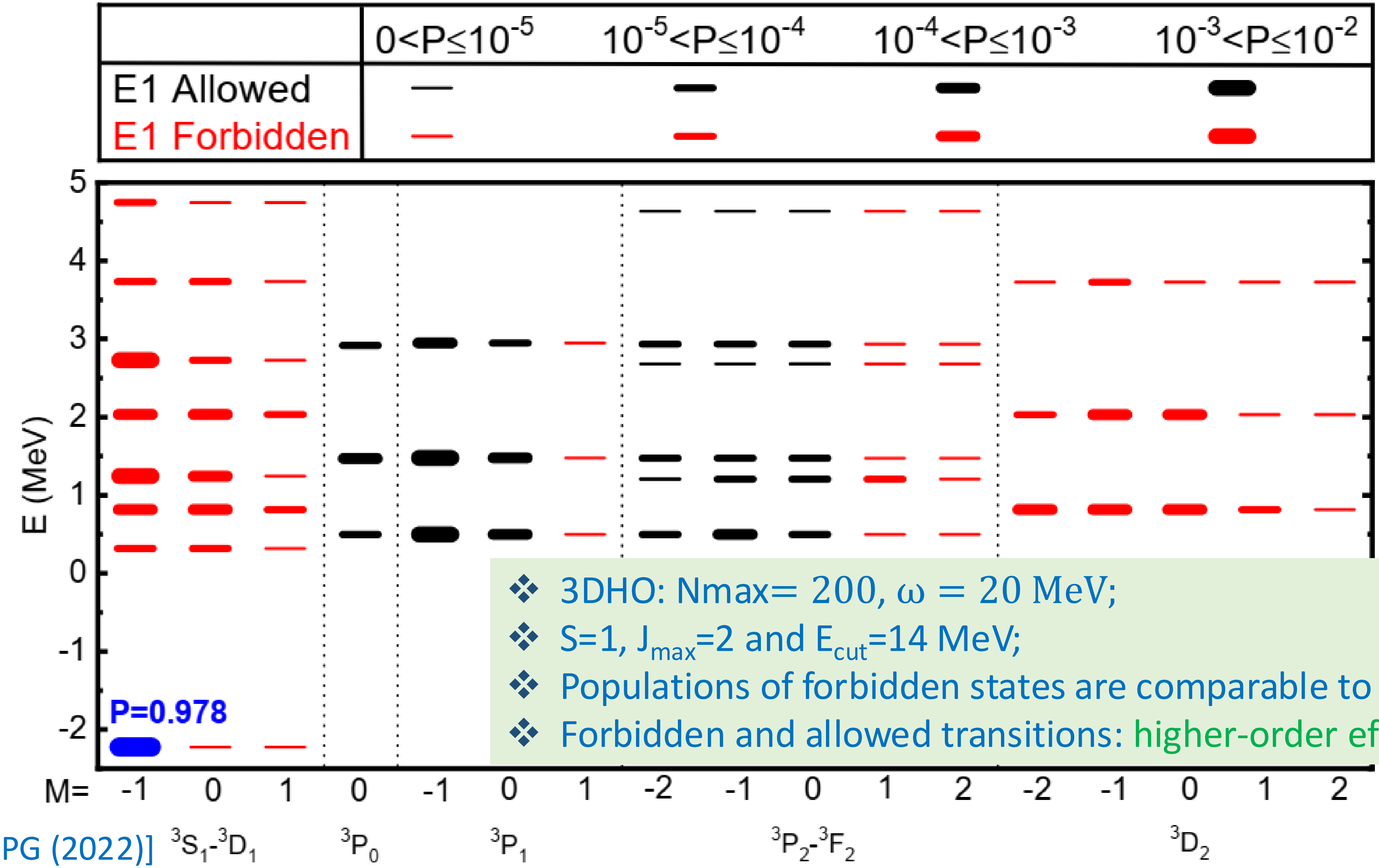
Transitions to forbidden states generate phase decoherence.

~2π ~2π ~?

	E_x (MeV)	Γ(MeV^{-1})				κ			
		Incoming		Outgoing		Incoming		Outgoing	
		Type I	All	Type I	All	Type I	All	Type I	All
1st $^3P_2$-$^3F_2$	2.72	2.31	2.31	2.30	2.10	6.28	6.28	6.26	5.71
1st $^3P_1$	2.72	2.31	2.31	2.30	2.13	6.28	6.28	6.26	5.79
3rd $^3P_2$-$^3F_2$	3.69	1.70	1.70	1.69	2.16	6.27	6.27	6.24	7.97
2nd $^3P_1$	3.70	1.70	1.70	1.69	2.12	6.29	6.29	6.25	7.84
5th $^3P_2$-$^3F_2$	5.15	1.22	1.22	1.17	1.32	6.28	6.28	6.03	6.80
3rd $^3P_1$	5.17	1.22	1.22	1.17	1.31	6.31	6.31	6.05	6.77

$$\kappa = \Gamma E_x$$

Occupation probabilities of np states after d+^{208}Pb scattering
E_d=7 MeV and θ=150° : LENPIC-N^{4}LO



- ❖ 3DHO: Nmax= 200, ω = 20 MeV;
- ❖ S=1, J_{max}=2 and E_{cut}=14 MeV;
- ❖ Populations of forbidden states are comparable to allowed states;
- ❖ Forbidden and allowed transitions: higher-order effects.

[Peng Yin *et al.*, JPG (2022)]

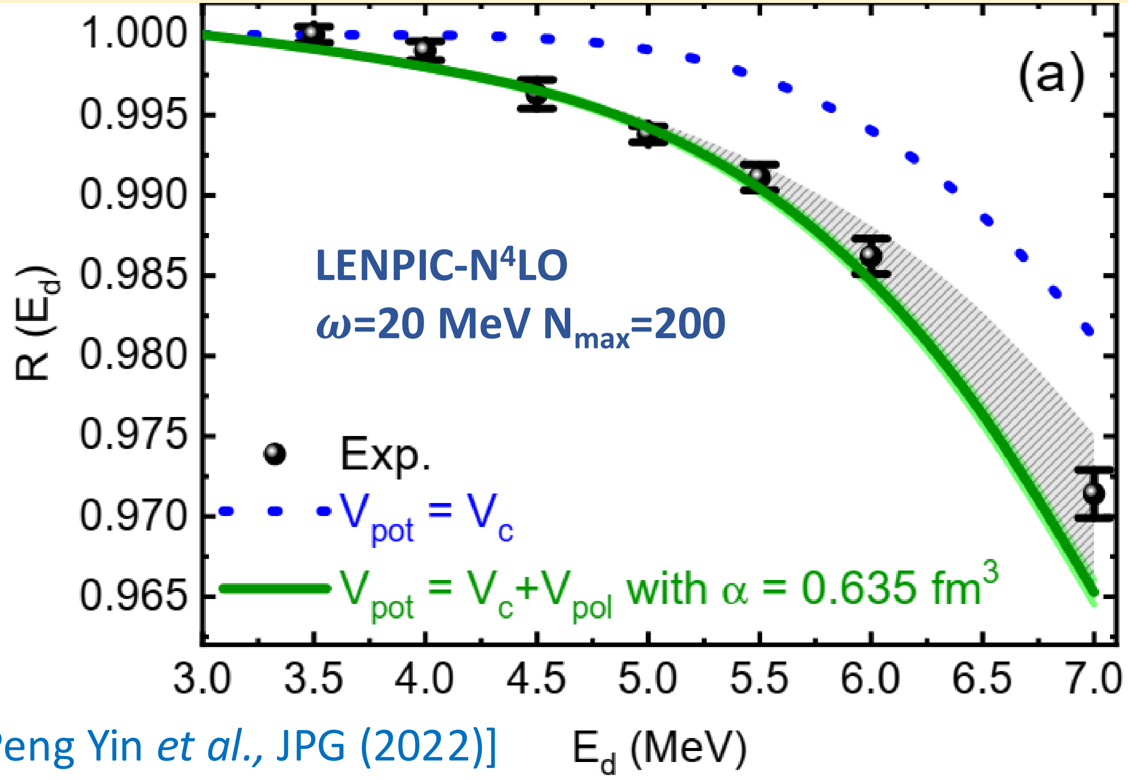
Observables for d+^{208}Pb scattering

$$V_{\rm pol} = -\frac{1}{2}\alpha Z^2 e^2 \frac{1}{r^4}$$

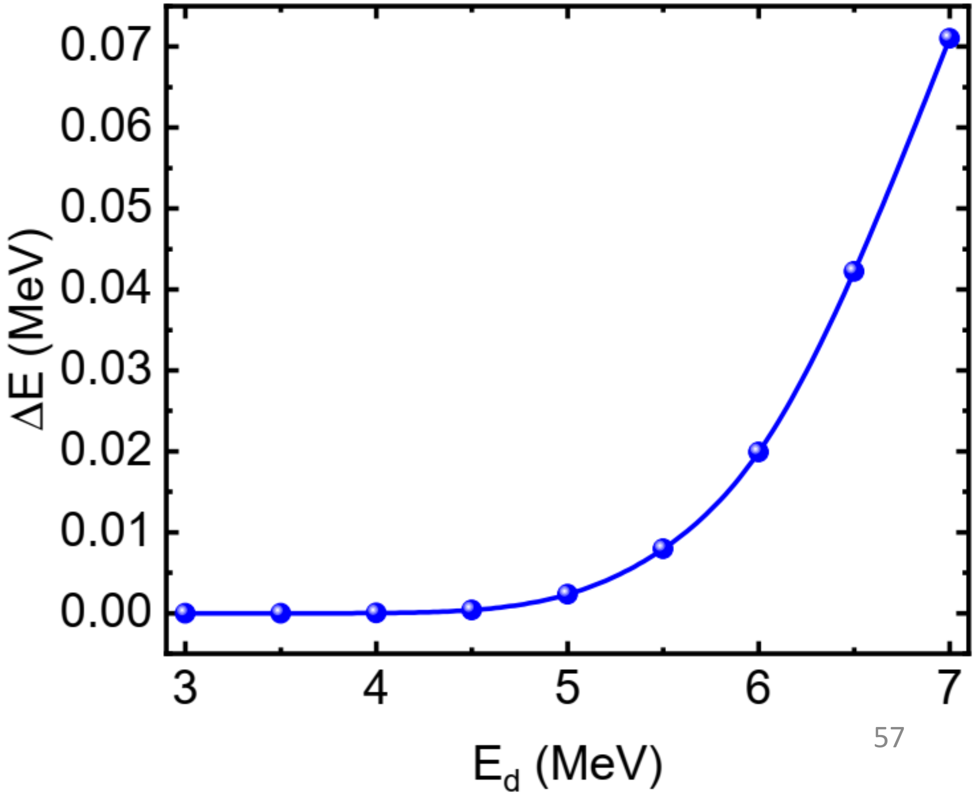
$$R(E_d) = \frac{\sigma(E_d = 3\ \mathrm{MeV}, \theta_1 = 60^\circ)}{\sigma(E_d = 3\ \mathrm{MeV}, \theta_2 = 150^\circ)} \frac{\sigma(E_d, \theta_2 = 150^\circ)}{\sigma(E_d, \theta_1 = 60^\circ)}$$

- ❖ Exp: N. L. Rodning, L. D. Knutson, W. G. Lynch and M. B. Tsang, Phys. Rev. Lett. 49, 909 (1982);
- ❖ No adjustable parameter;
- ❖ No optical potential;
- ❖ Energy loss correction.

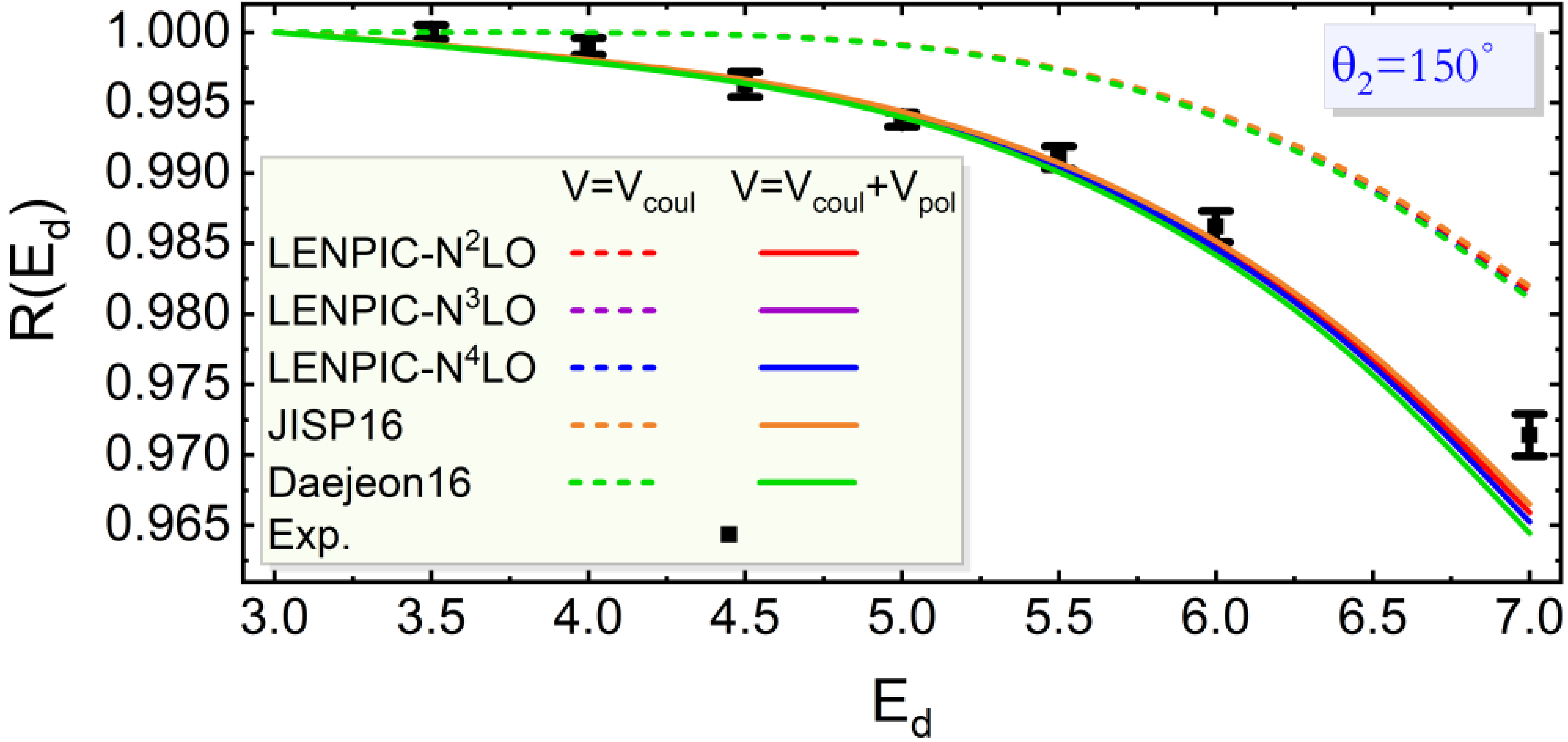
	α (fm^3)
LENPIC-N^{2}LO	0.6292(1)
LENPIC-N^{3}LO	0.6352(1)
LENPIC-N^{4}LO	0.6349(1)
JISP16	0.6164(1)
Daejeon16	0.6658(1)



[Peng Yin *et al.*, JPG (2022)]



$d+^{208}Pb$ scattering E_d=3-7 MeV
Sensitivity to *NN* interactions



Peng Yin, Weijie Du, Wei Zuo, Xingbo Zhao and James P. Vary, arXiv 2208.00267

Conclusions/Perspectives

- Non-perturbative time-dependent basis function approach;
- Application to d+^{208}Pb scattering;
- Extension of the tBF method to heavier projectiles, e.g., rare isotopes,…:
  using wavefunctions from NCSM.
- Extension to higher incident energies: adding strong interaction between scattering nuclei.
- Two-body electromagnetic operators from chiral effective field theory.
- Quantum consideration of center of mass motion of the projectile.
- Quantum computing