Light Nuclei Properties with *ab initio* No-Core Shell Model

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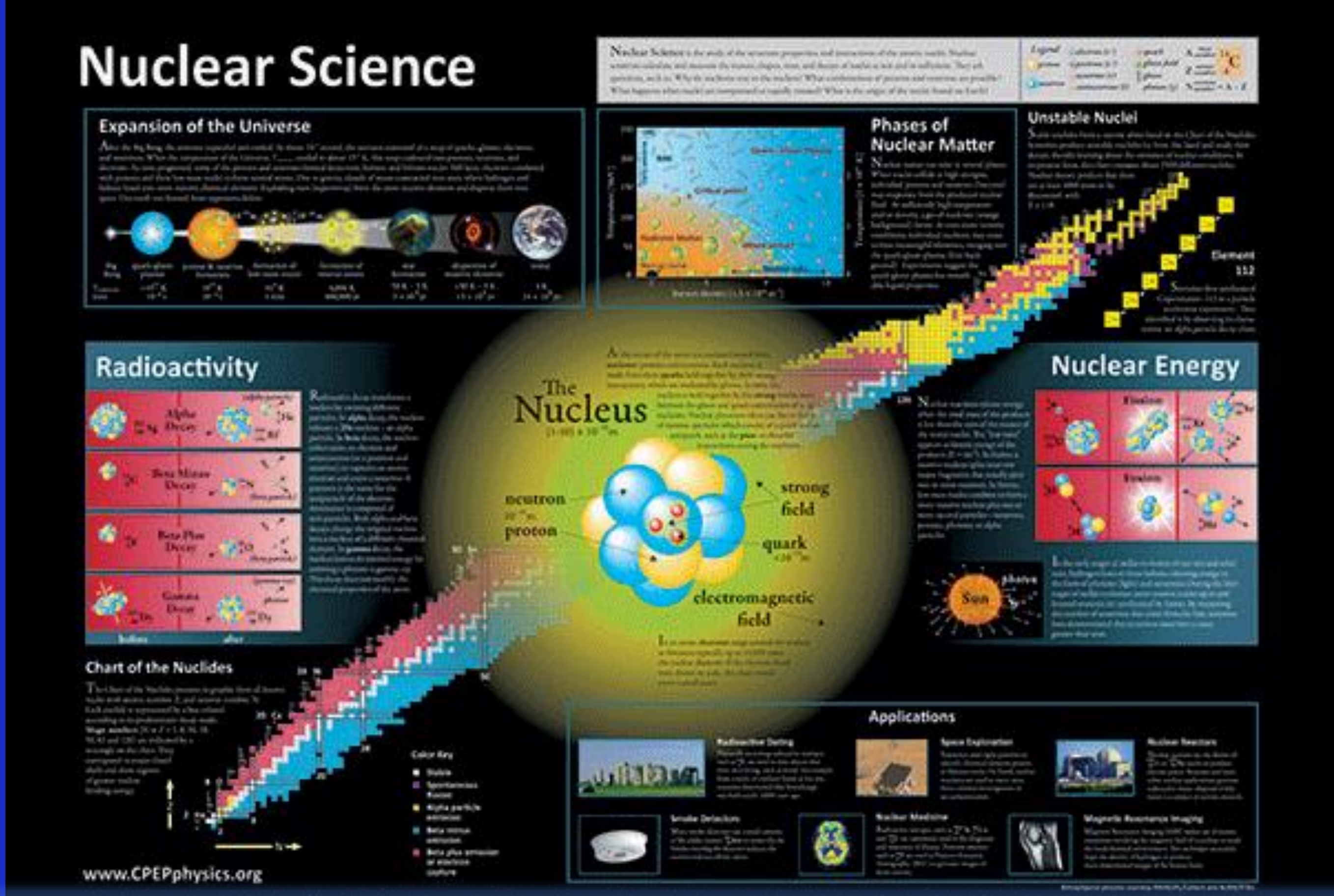
深圳
2024. 11. 15-18



Outline

- No-Core Shell Model
- Sum rules with NCSM
- Monopole transition form factor

Ab initio No-Core Shell Model

What is *ab initio* in nuclear physics?

Few-Body Syst (2023) 64:77
https://doi.org/10.1007/s00601-023-01857-2

R. Machleidt

What is *ab initio*?

Nuclear structure theory at its basic level is not about fitting data to get "good" results. Fundamental nuclear structure theory is about answering the question:

Do the same nuclear forces that explain free-space scattering experiments also explain the properties of finite nuclei and nuclear matter when applied in nuclear many-body theory?

Check for updates

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What is *ab initio* in nuclear

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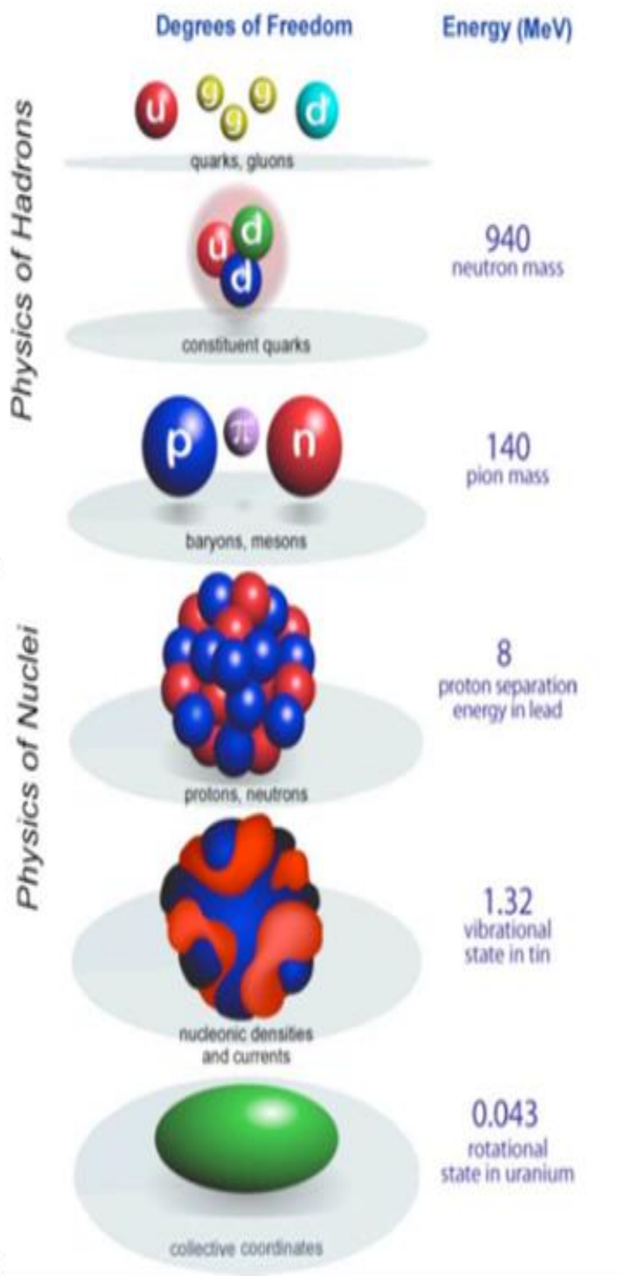
Ab initio has been used as a label in nuclear theory for over two decades. Its meaning has evolved and broadened over the years. We present our interpretation, briefly review its historical use, and discuss its present-day relation to theoretical uncertainty quantification.



Non-relativistic *ab initio* approaches

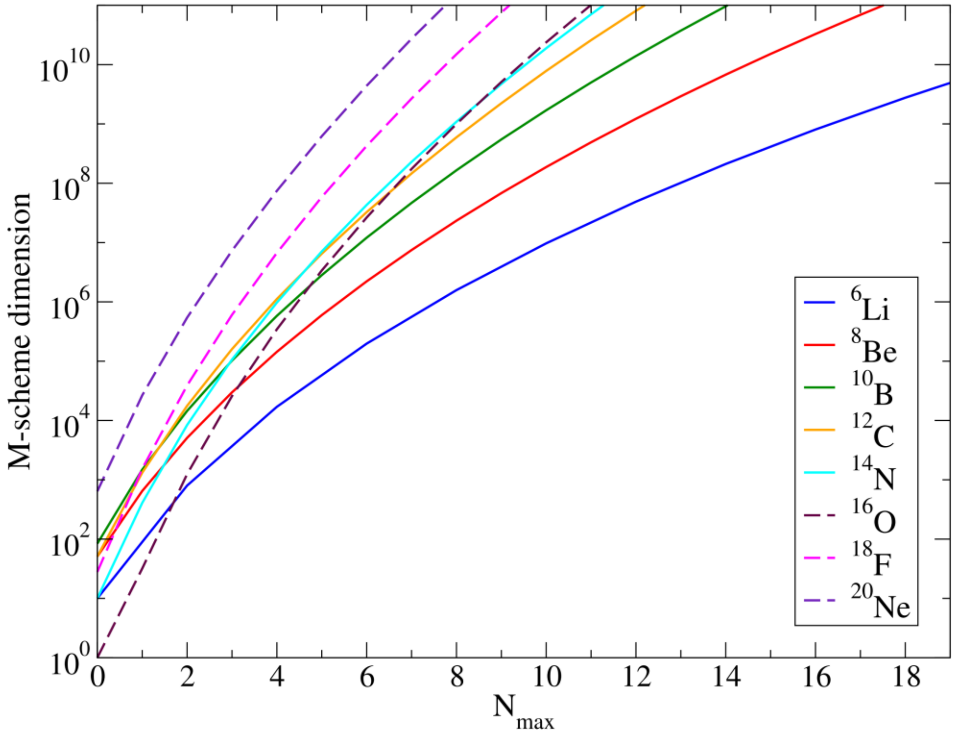
- Few-body methods
  - Faddeev Equation for A=3 system
    - typically in momentum space
  - Faddeev-Yakuboski Equations for A=4 system
    - can nowadays be pushed to A=5 and 6 (Lazauskas)
  - Hyperspherical Harmonics A=6
- Many-body methods
  - Variational Monte-Carlo (A<=12)
  - Green’s Function Monte-Carlo (A<=12)
  - Configuration Interaction (CI) methods (NCSM (A<=20), Coupled Cluster (A<=100))
  - Nuclear Lattice Simulations (A<=40)
- Supercomputer Era
- Quantum computing Era?

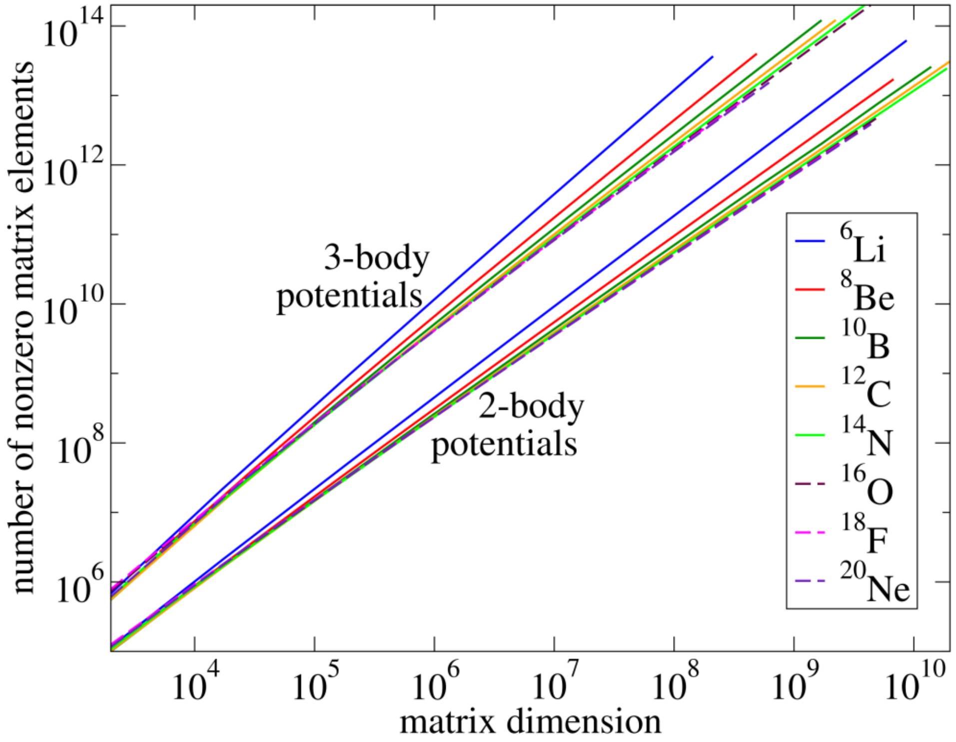
No-Core Shell model

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

- 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 ($10^{10}\times10^{10}$) sparce symmetric matrix
  - Obtain lowest eigenvalues&-vectors corresponding to low-lying spectrum and eigenstates

Main Challenges





- Increase of basis space dimension with A and N_{max}
  - Need calculations up to at least N_{max}=8, preferably N_{max}=10 for meaningful extrapolation and numerical error estimates
- More relevant measure for computational needs
  - Number of nonzero matrix elements

Main Challenge

NERSC
National Energy Research Scientific Computing Center

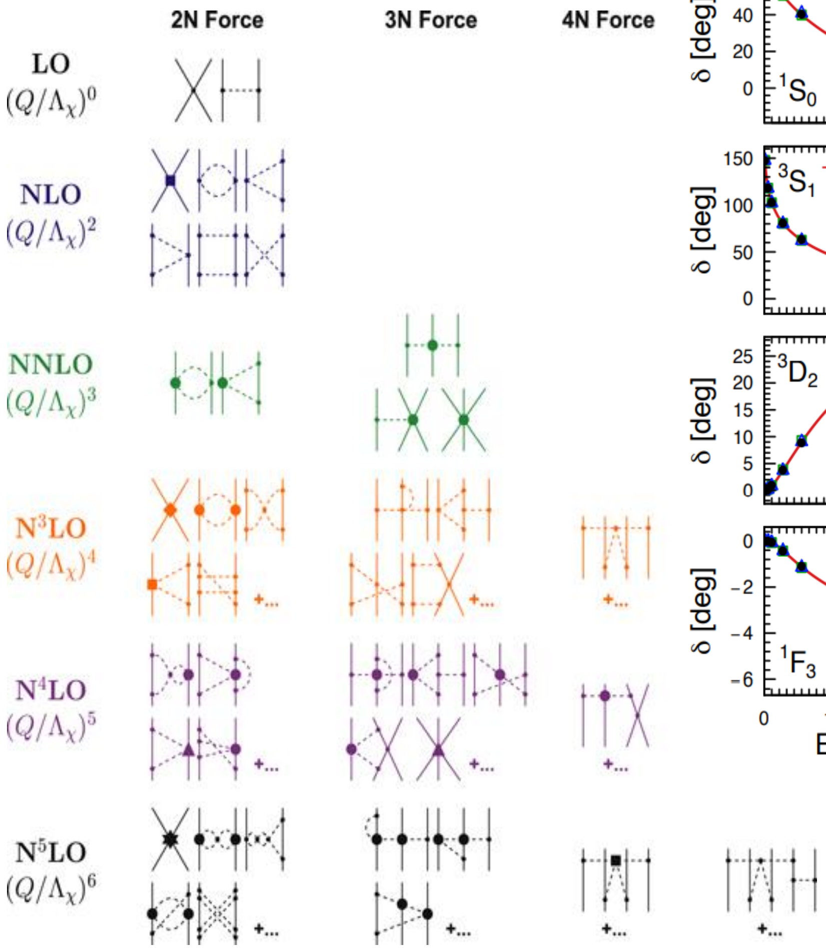
- 2x AMD EPYC 7763 (Milan) CPUs
- 64 cores per CPU
- AVX2 instruction set
- 512 GB of DDR4 memory total
- 204.8 GB/s memory bandwidth per CPU
- 1x HPE Slingshot 11 NIC
- PCIe 4.0 NIC-CPU connection
- 39.2 GFlops per core
- 2.51 TFlops per socket
- 4 NUMA domains per socket (NPS=4)

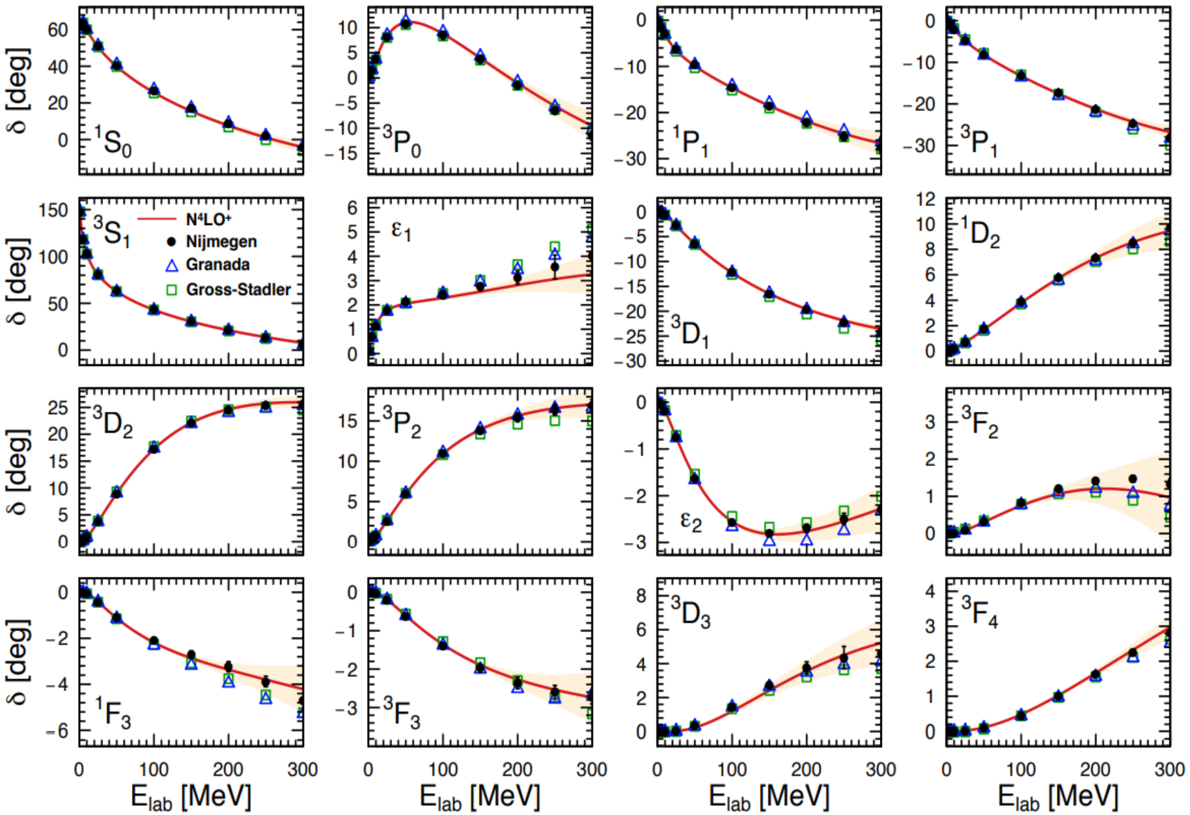
Partition	# of nodes	CPU	GPU
GPU	1536	1x AMD EPYC 7763	4x NVIDIA A100 (40GB)
	256	1x AMD EPYC 7763	4x NVIDIA A100 (80GB)
CPU	3072	2x AMD EPYC 7763	-
Login	40	1x AMD EPYC 7713	1x NVIDIA A100 (40GB)

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

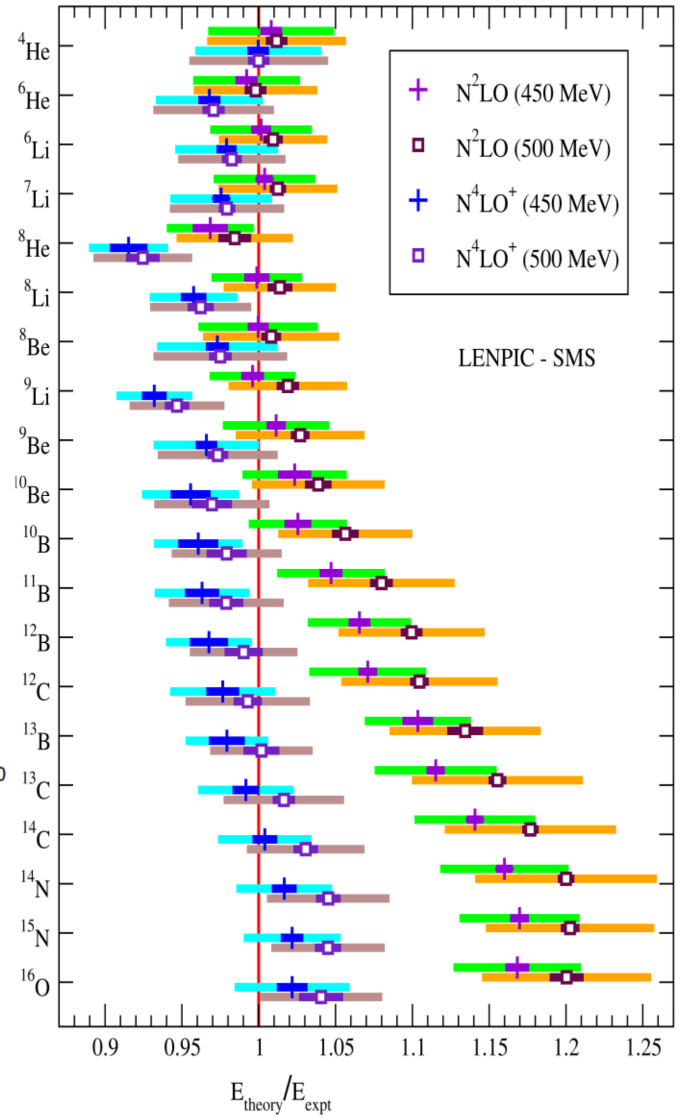
  ^{12}C (N_{max}=12), ^{6}He (N_{max}=22)
- Achievable for nuclei up to A~20 with largest computers available

LENPIC chiral EFT *NN* potential up to N^4LO+





P. Reinert, H. Krebs, E. Epelbaum
Eur. Phys. J. A 54, 86 (2018)



LENPIC Collaboration,
Phys. Rev. C 106, 064002 (2022)

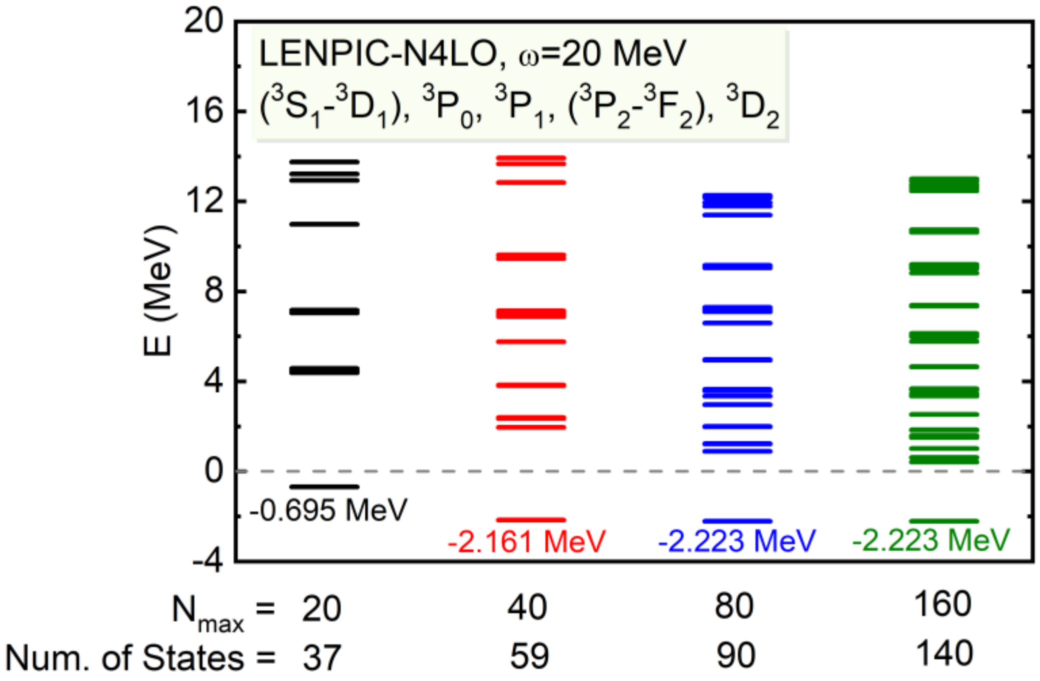
RUB universitätbonn TECHNISCHE UNIVERSITÄT DARMSTADT JAGIELLONIAN UNIVERSITY IN KRAKOW JÜLICH FORSCHUNGSZENTRUM Kyutech THE OHIO STATE UNIVERSITY IPN ORSAY TRIUMF

Sum rules with NCSM

Sum rules with NCSM

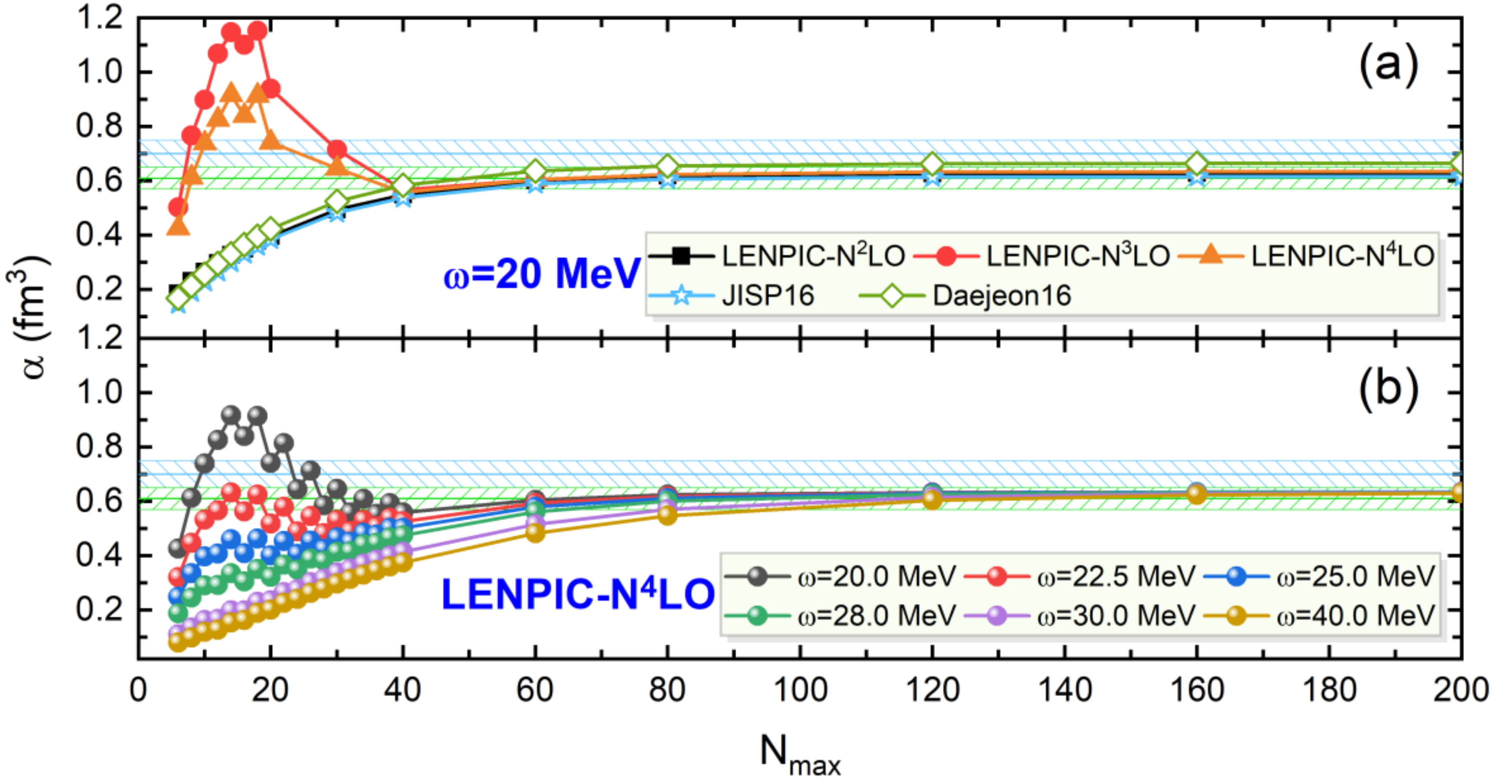
$$I_M = \sum_{\mu}^{M} |\langle \mu | \hat{O} | i \rangle|^2 g(\omega_\mu) \qquad \alpha_E = \frac{8\pi}{9} \sum_k \frac{B(E1; J_0 \to J_k)}{E_k - E_0} = \frac{1}{2\pi^2} \int_{\omega_{\rm th}}^{\infty} d\omega \frac{\sigma_\gamma^{\rm ud}(\omega)}{\omega^2}$$

- 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?



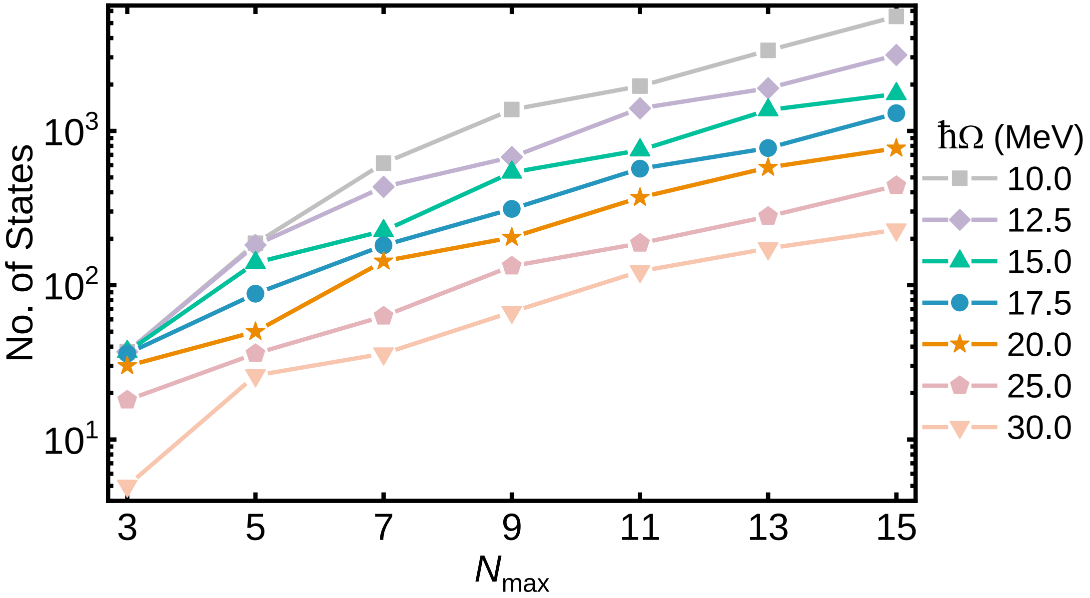
P. Yin *et al, J.Phys.G* 49, 125102 (2022)

P. Yin *et al,* [arXiv:2208.00267 [nucl-th]]

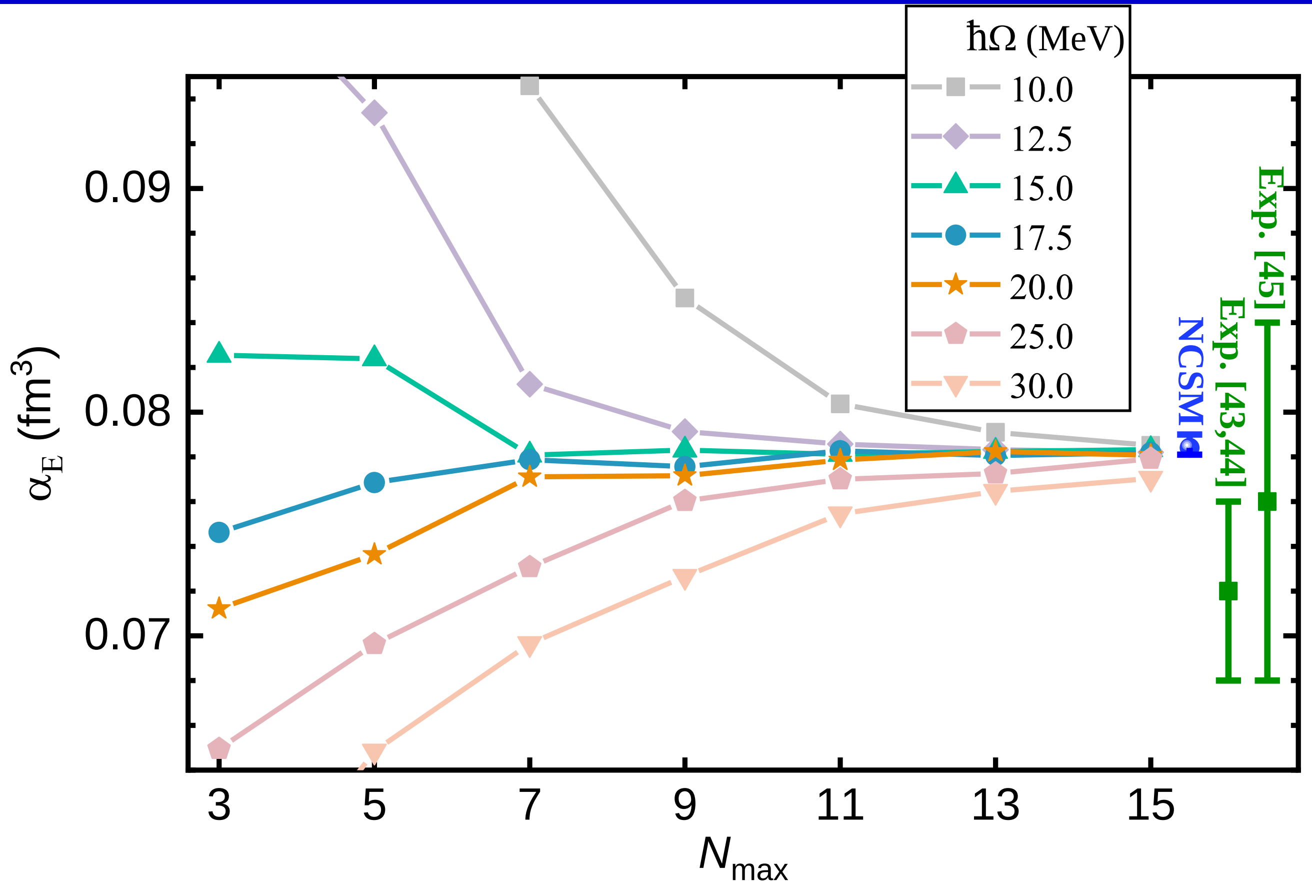


Sum rules with NCSM

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



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



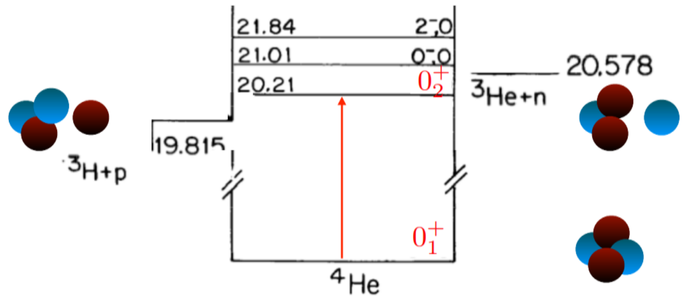
- Robust convergence with respect to N_{max}
- Uncertainty due to N_{max} truncation and energy truncation

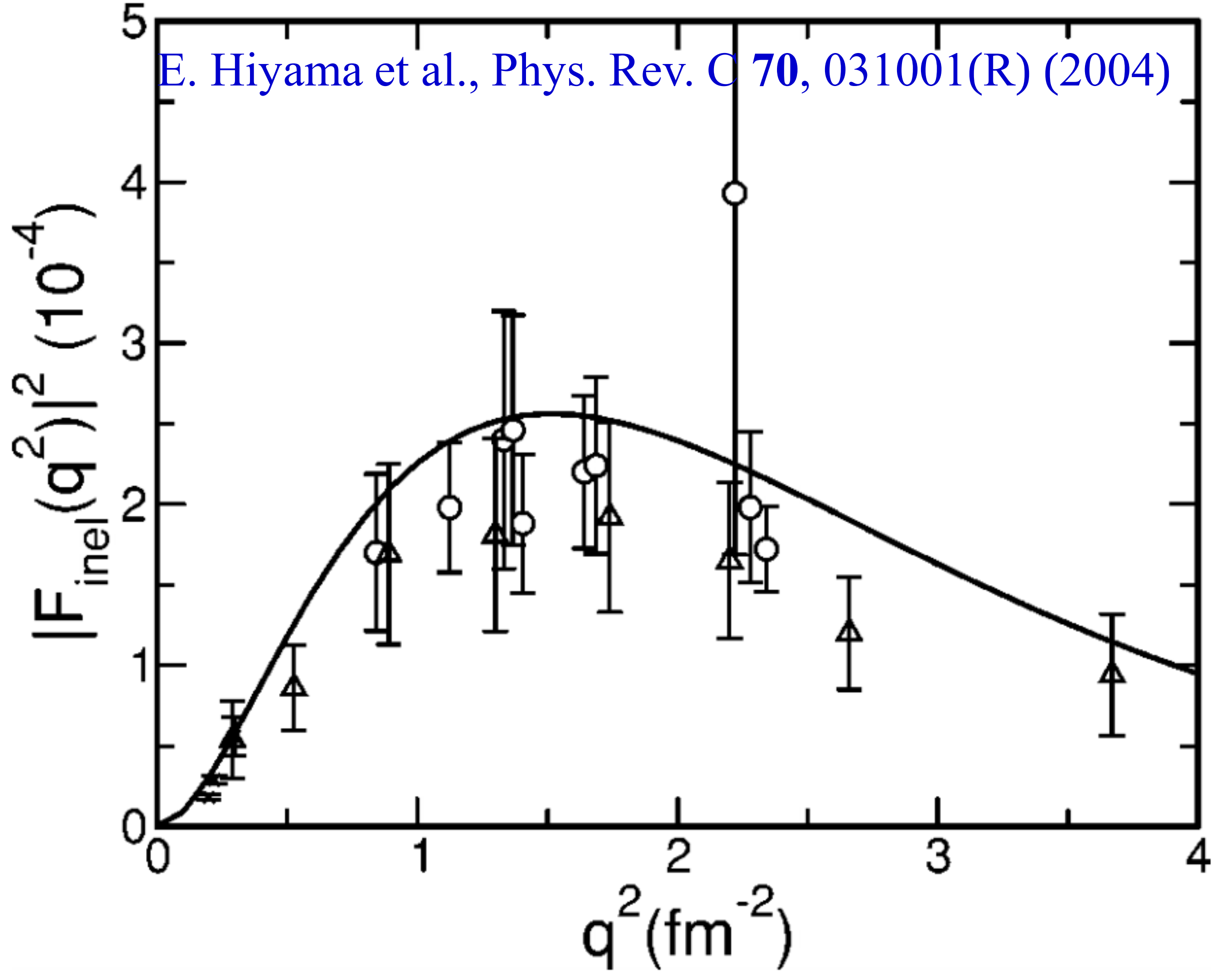
P. Yin, A. M. Shirokov, P. Maris, P. J. Fasano, M. A. Caprio, H. Li, W. Zuo, J. P. Vary, Phys. Lett. B **855**, 138857 (2024)

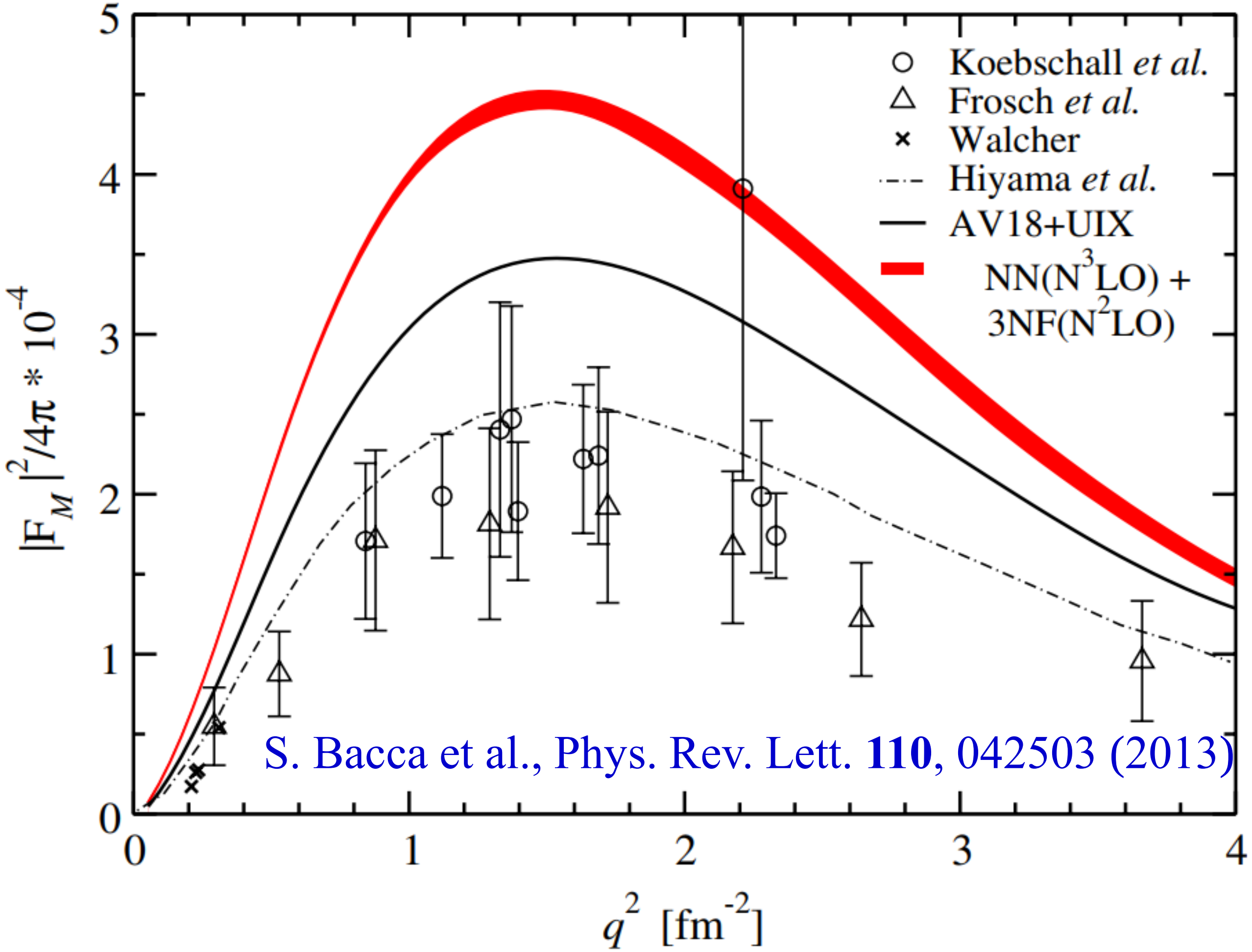
Monopole form factor with NCSM

Monopole transition form factor of ^{4}He

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







New experiment

Mainz

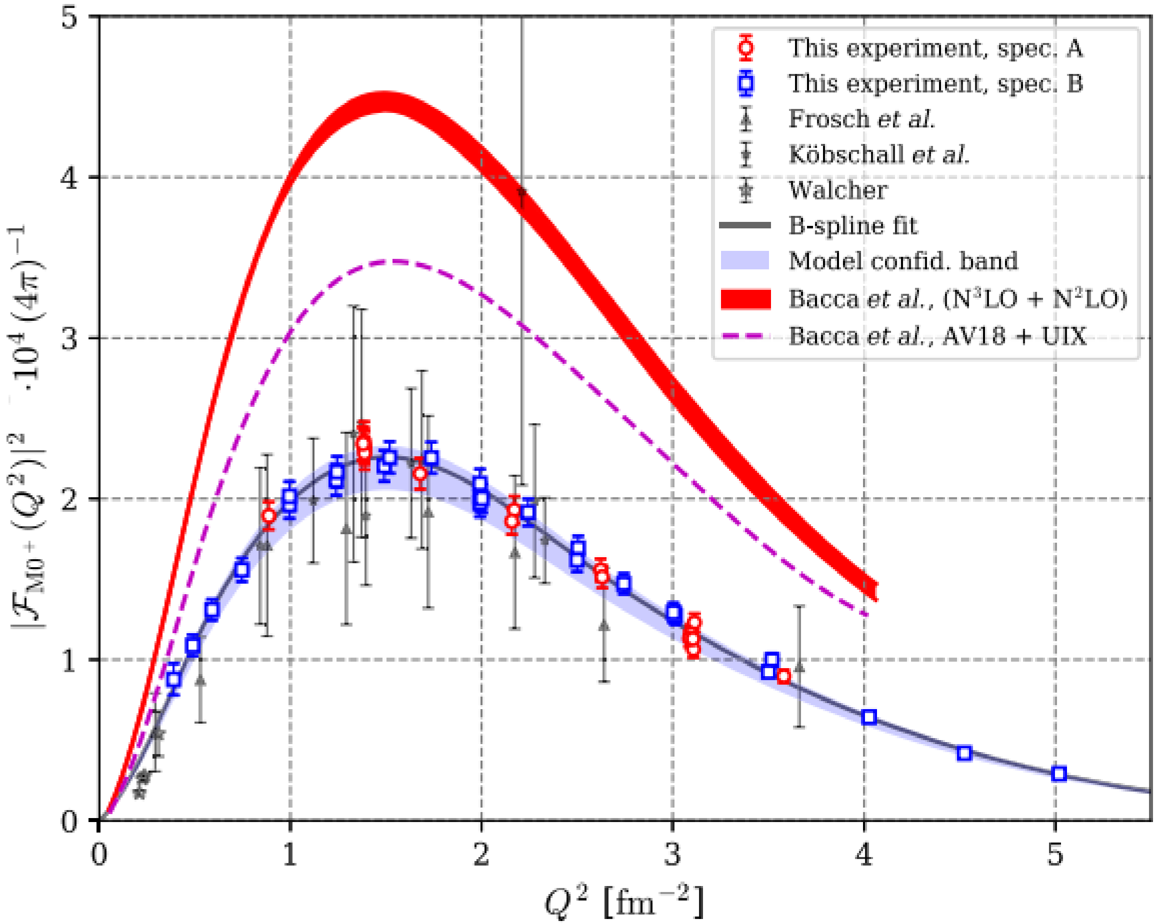
Status quo in 2023

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]



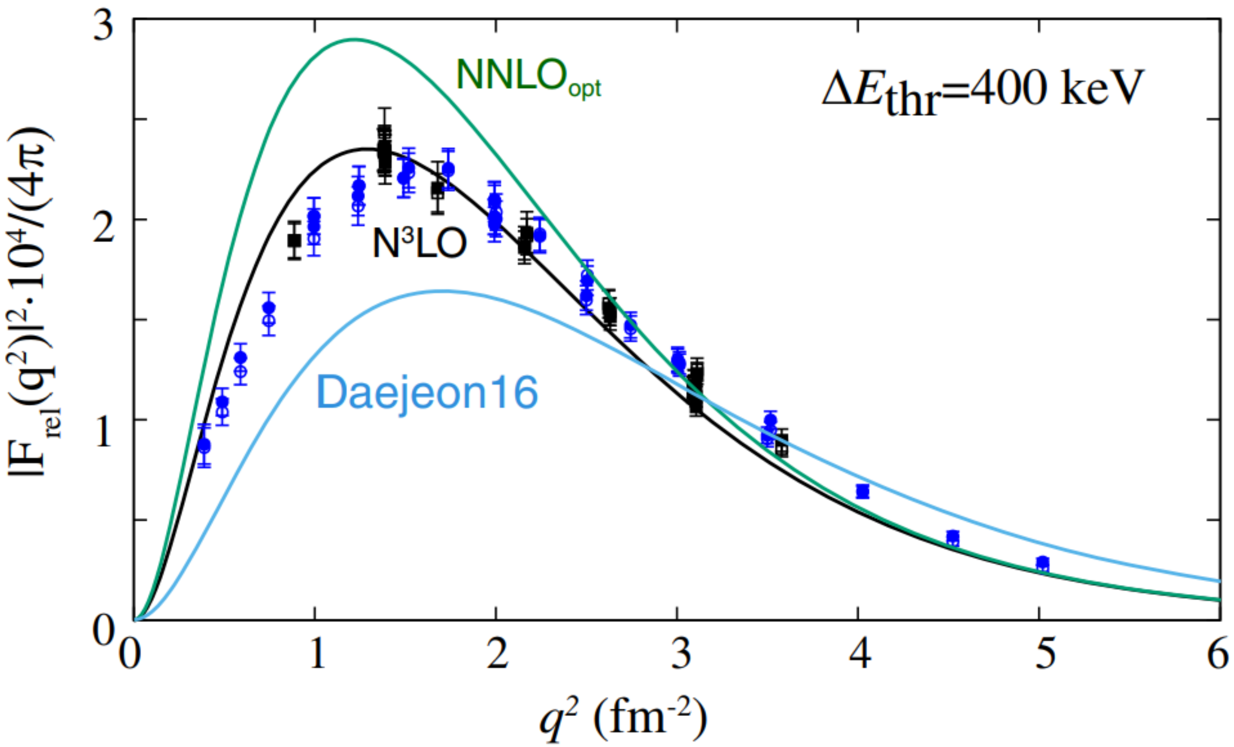
Problem with chiral EFT becomes stronger

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]



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

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

- NCGSM-CC with V_{lowk}
- E_r=400 keV, fit to Exp

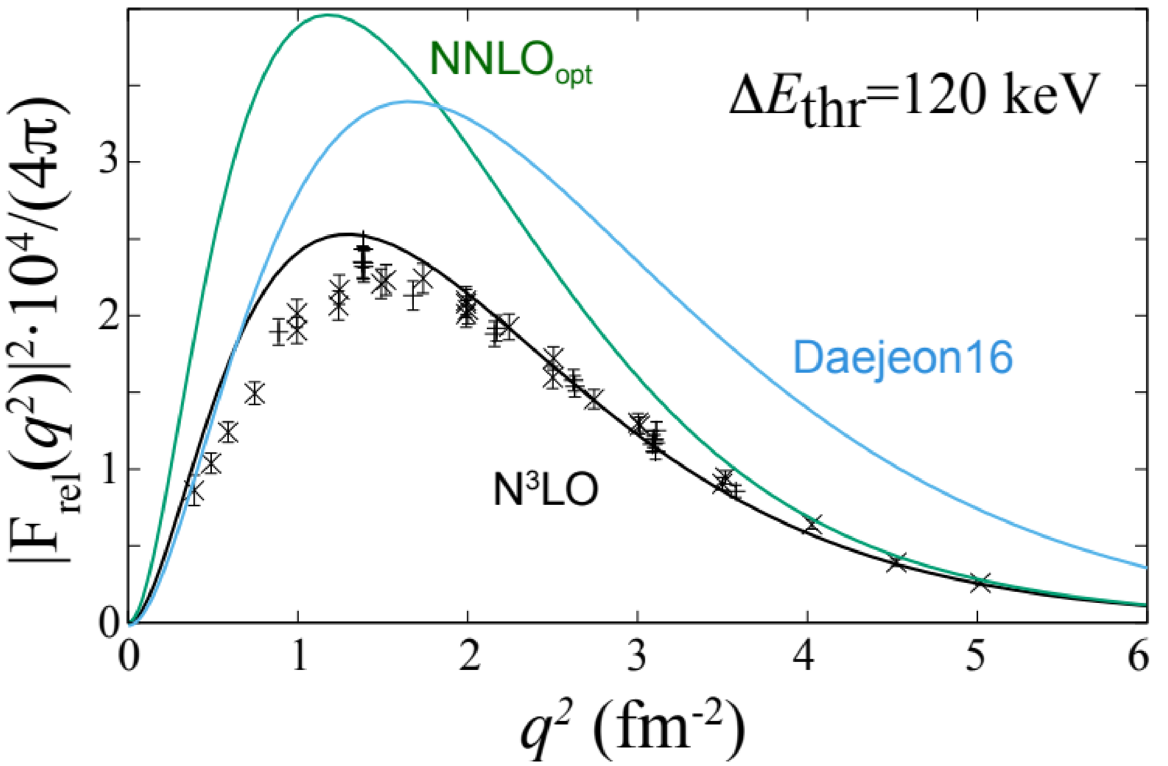
Accepted Paper

Erratum: Description of the proton-decaying 0_2^+ resonance of the α particle [Phys. Rev. Lett. **131**, 242502 (2023)]

Phys. Rev. Lett.

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

Accepted 28 October 2024

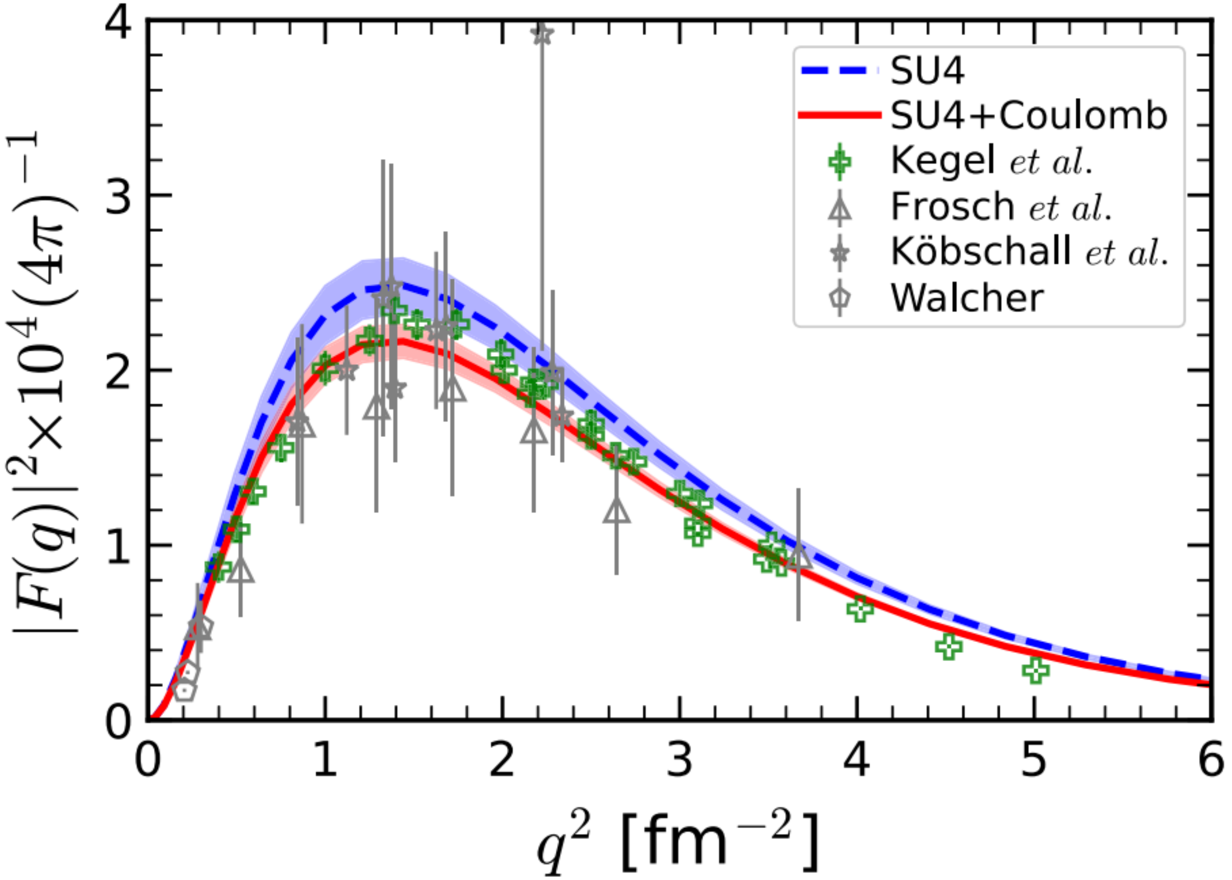


- E_r=120 keV, fit to Exp

PHYSICAL REVIEW LETTERS 132, 062501 (2024)

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

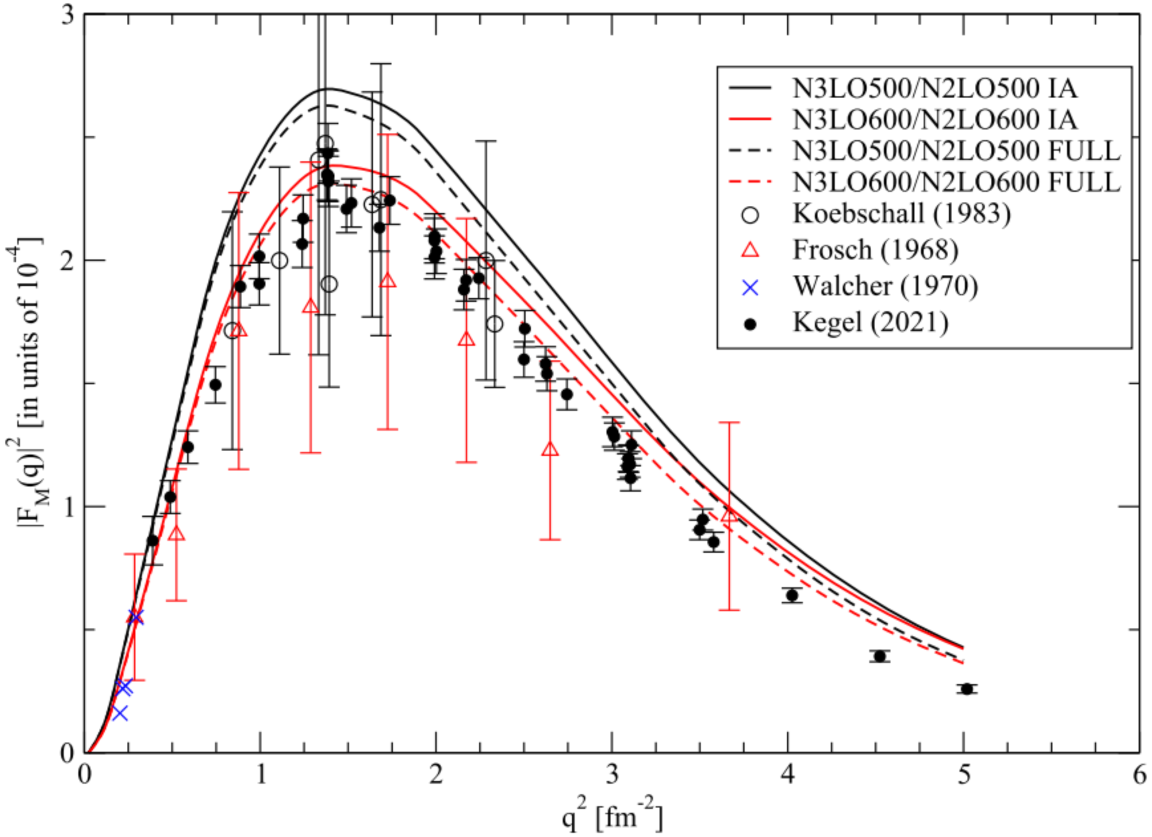
Ulf-G. Meißner,[1,2,3] Shihang Shen,[4,*] Serdar Elhatisari,[5,1] and Dean Lee[6]



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

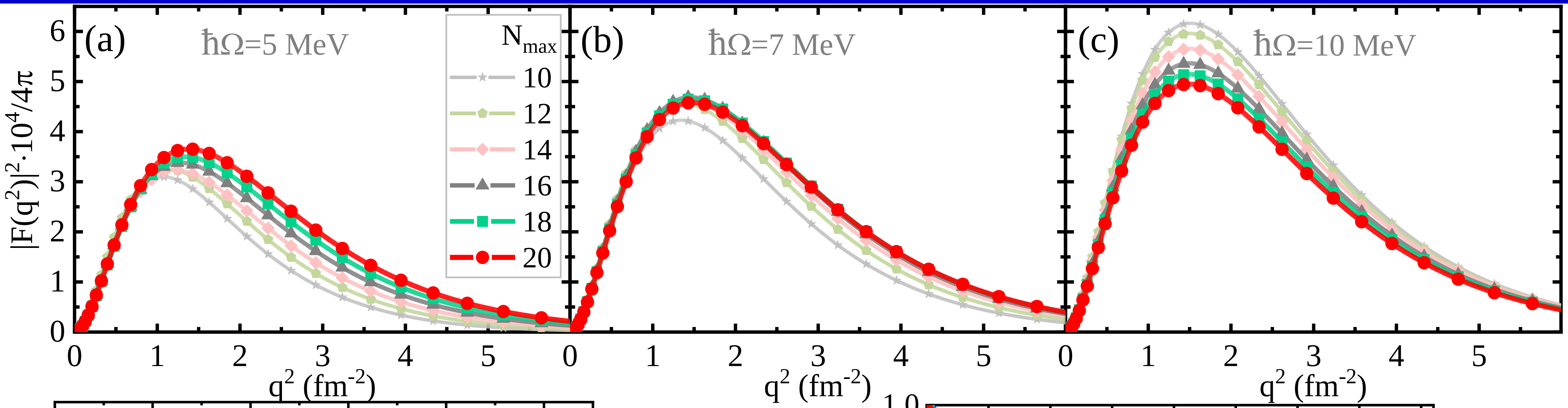


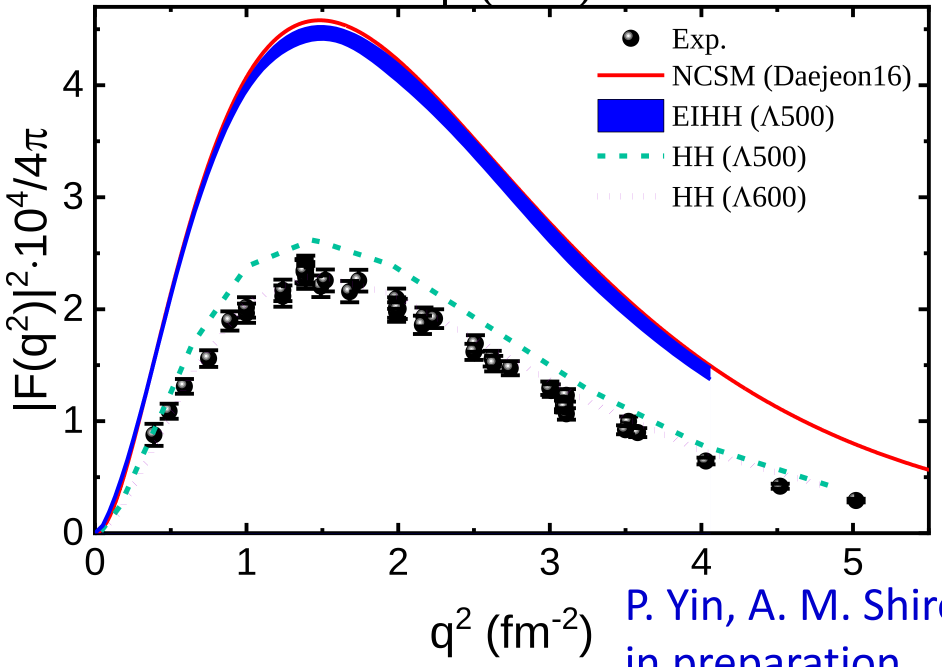
- Viviani: HH ^{3}He+n, ^{3}H+p, chiral NN+3N
- Two-body current
- First successful calculation with chiral EFT?

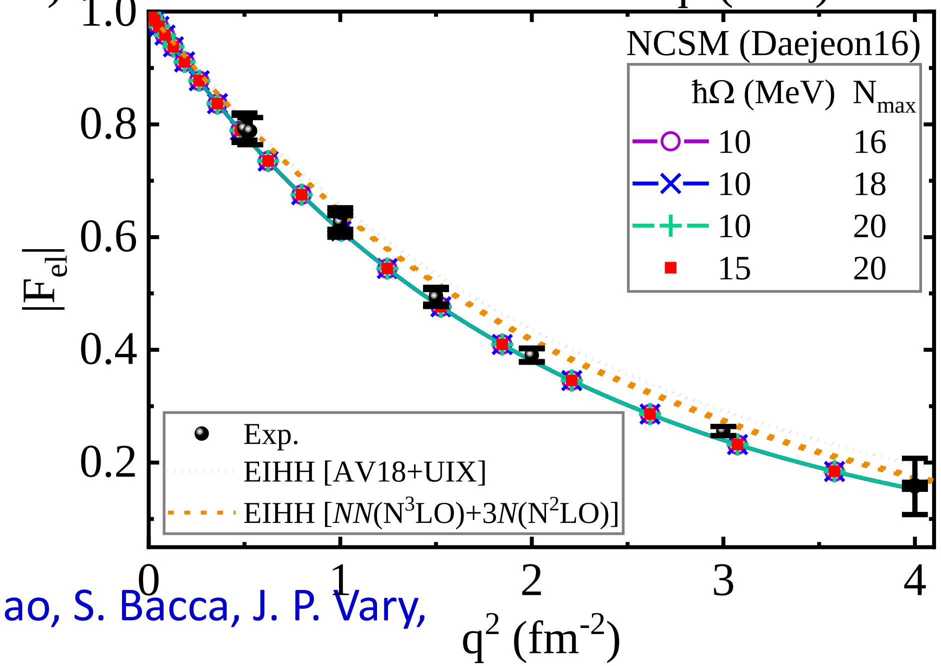
In the news

From Sonia Bacca

Transition monopole form factor of ^{4}He







P. Yin, A. M. Shirokov, H. Li, X. B. Zhao, S. Bacca, J. P. Vary, in preparation

Summary

- Introduction to *ab initio* NCSM approach
-
- Sum rules with NCSM
- Transition monopole form factor of ^{4}He

Outlook

- Photoabsorption reaction
- Coulomb dissociation of light nuclei
- Two-body current