



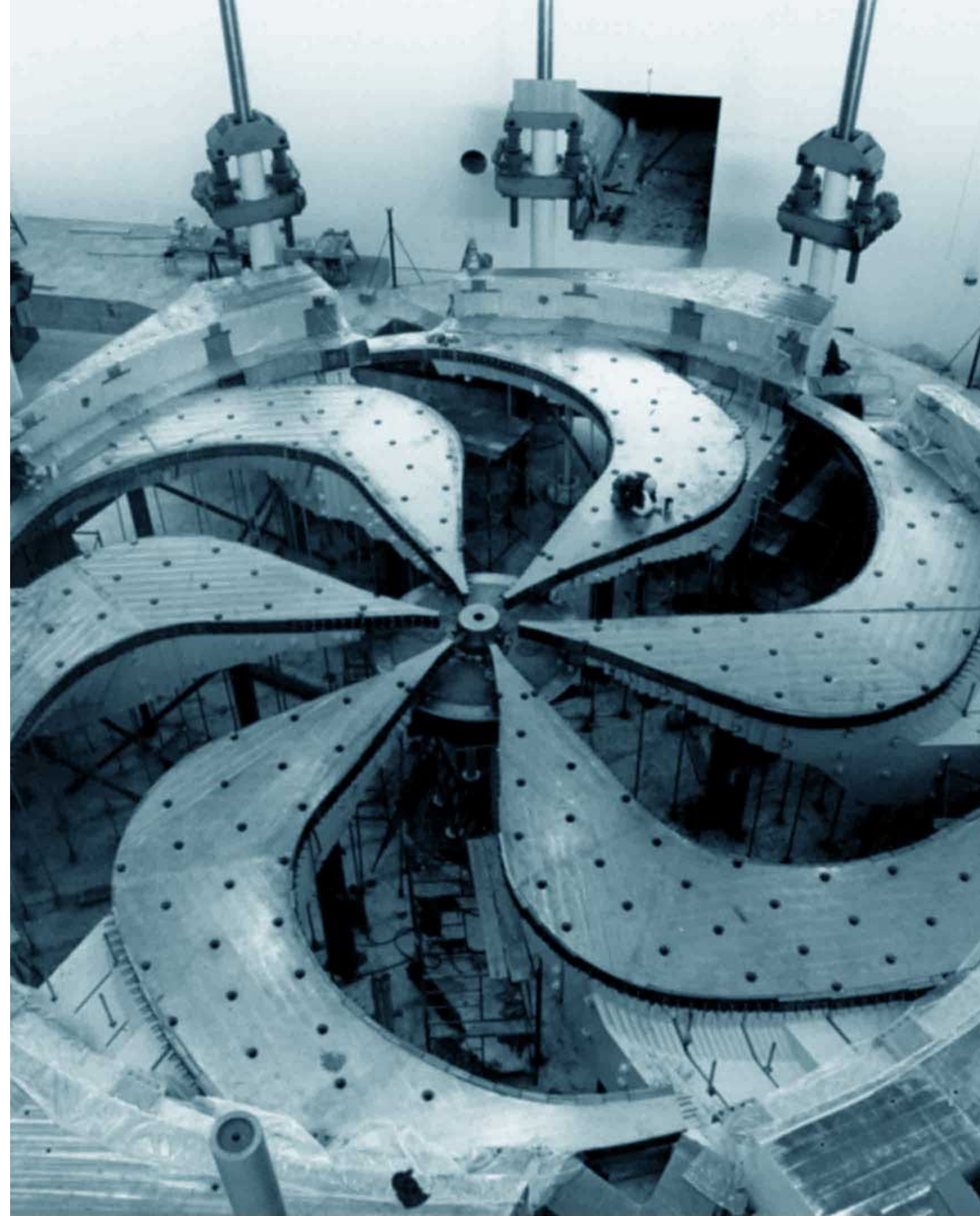
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Light Nuclei from *Ab Initio* Theory

17th International Conference on Meson-Nucleon
Physics and the Structure of the Nucleon (MENU 2026)
Stony Brook University, October 19–23, 2026

Petr Navratil

TRIUMF



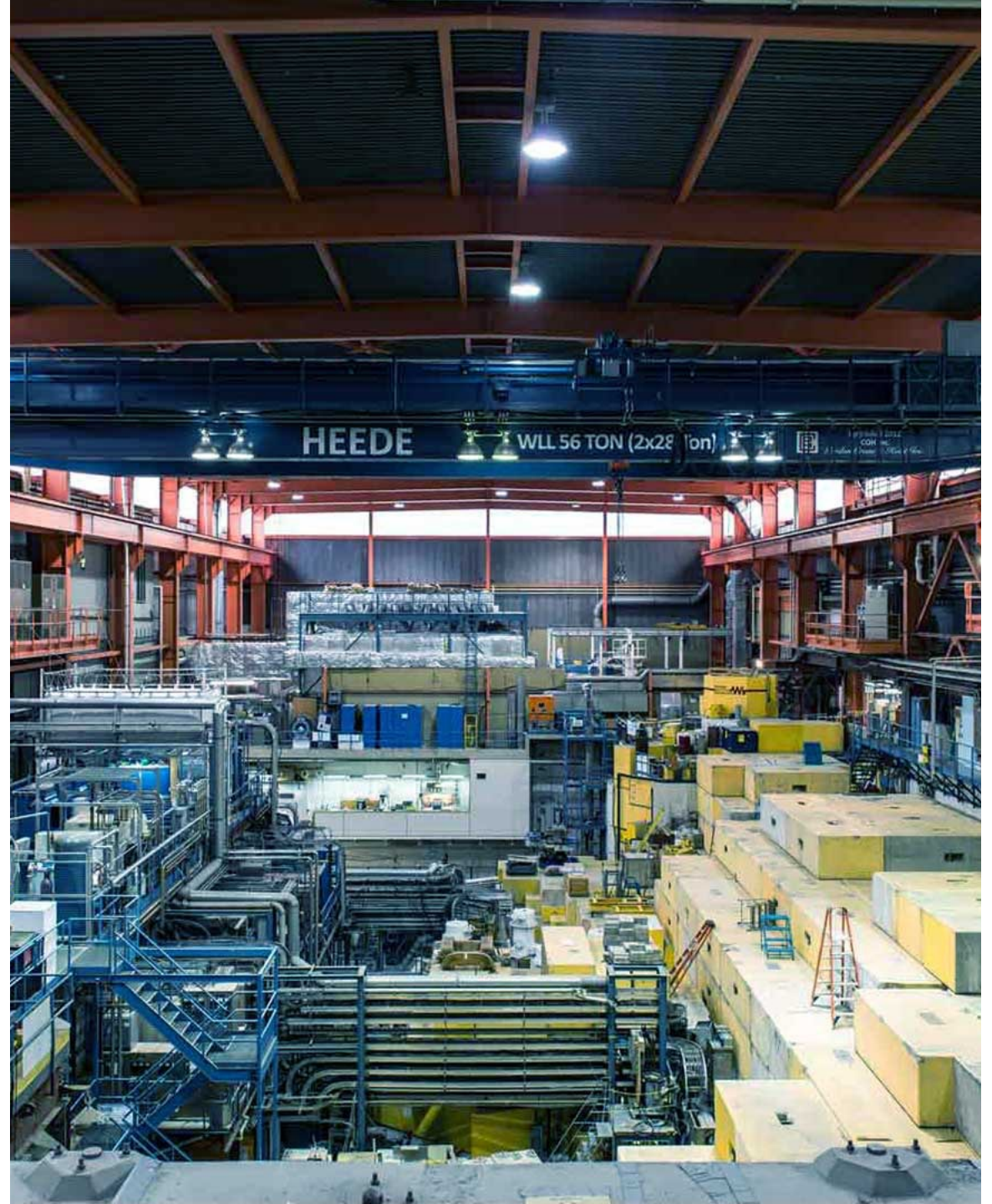
Outline

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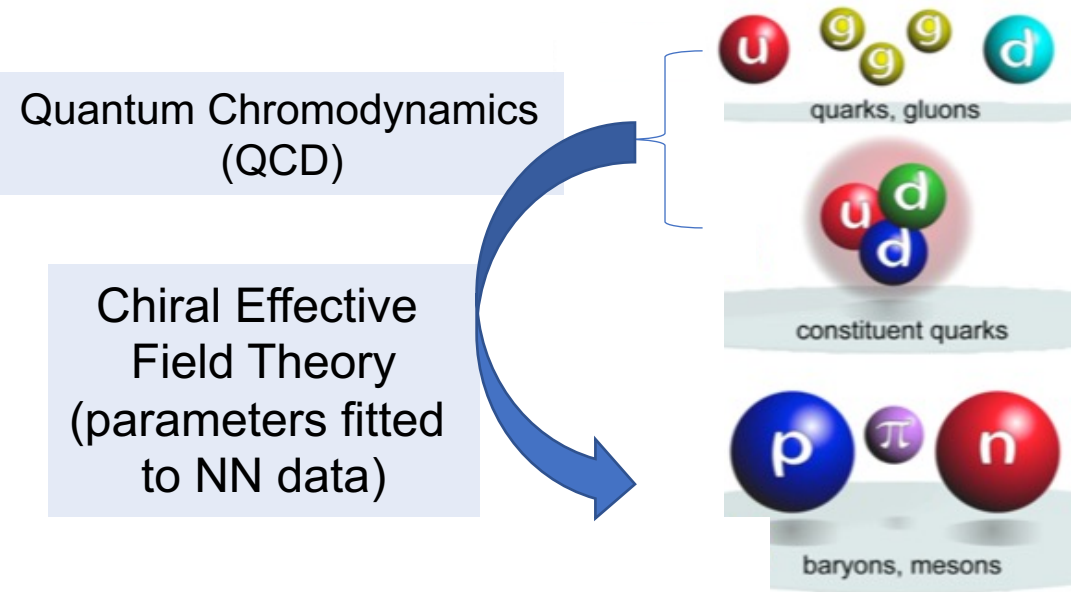
- *Ab initio* nuclear theory – no-core shell model (NCSM) & NCSM with continuum (NCSMC)
- Precision chiral EFT NN + 3N forces
- Applications of NCSM to electroweak processes
 - Superaligned Fermi transitions – electroweak radiative correction δ_{NS}
 - Muonic atoms – two-photon exchange nuclear correction
- Applications of NCSMC with chiral EFT forces to nuclear scattering and reactions
 - Nucleon - α scattering
 - DT fusion – ${}^3\text{H}(\text{d},\text{n}){}^4\text{He}$
 - Structure of ${}^6\text{Li}$ and ${}^2\text{H}(\alpha,\gamma){}^6\text{Li}$ radiative capture
 - Internal pair creation and the X17 anomaly - ${}^7\text{Li}(\text{p},\text{e}^+\text{e}^-){}^8\text{Be}$
- Conclusions

Ab initio nuclear theory - no-core shell model (NCSM)

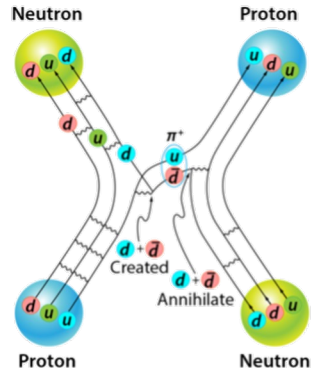
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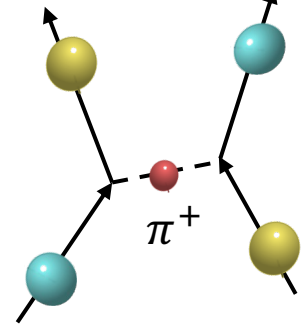
First principles or *ab initio* nuclear theory



Quantum Chromodynamics

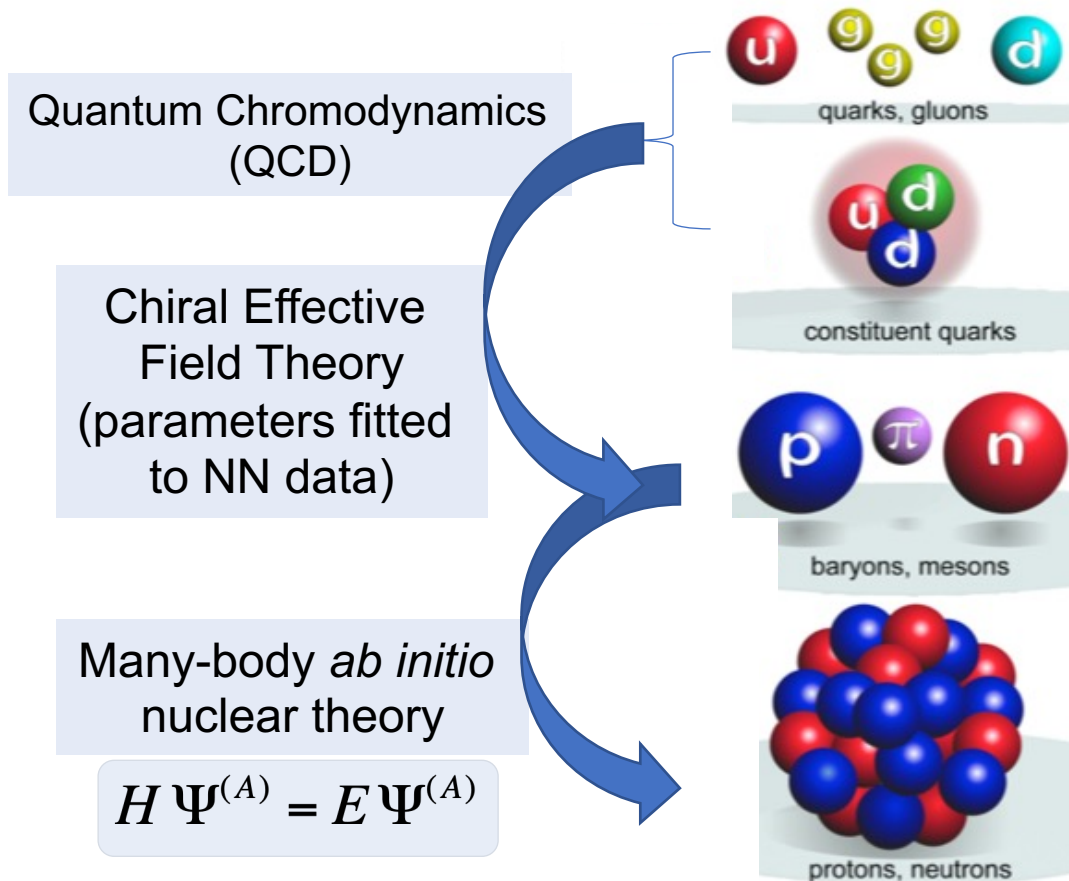


Chiral Effective Field Theory

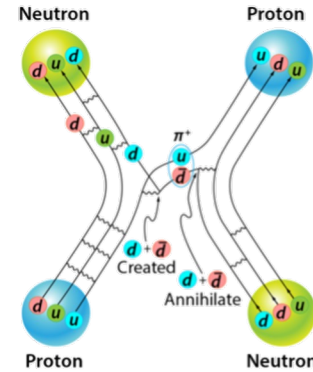


	NN force	NNN force	NNNN force
Q^0 LO			
Q^2 NLO			
Q^3 N ² LO			
Q^4 N ³ LO			
	+ ...	+ ...	+ ...

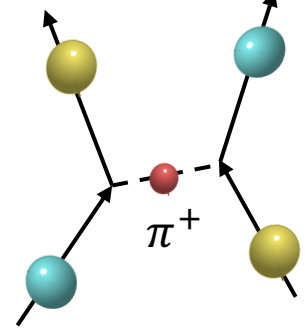
First principles or *ab initio* nuclear theory



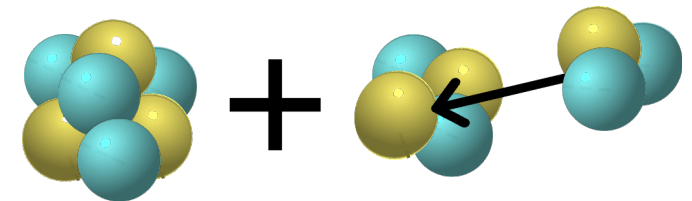
Quantum Chromodynamics



Chiral Effective Field Theory



No Core Shell Model with continuum (NCSMC)





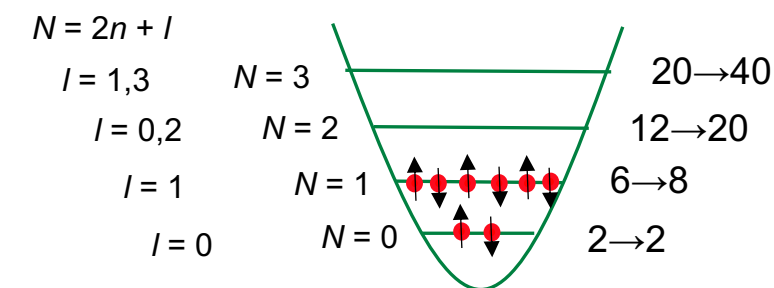
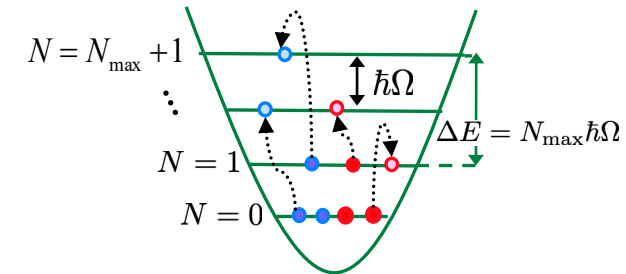
Review

Ab initio no core shell modelBruce R. Barrett^a, Petr Navrátil^b, James P. Vary^{c,*}

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Conceptually simplest *ab initio* method: No-Core Shell Model (NCSM)

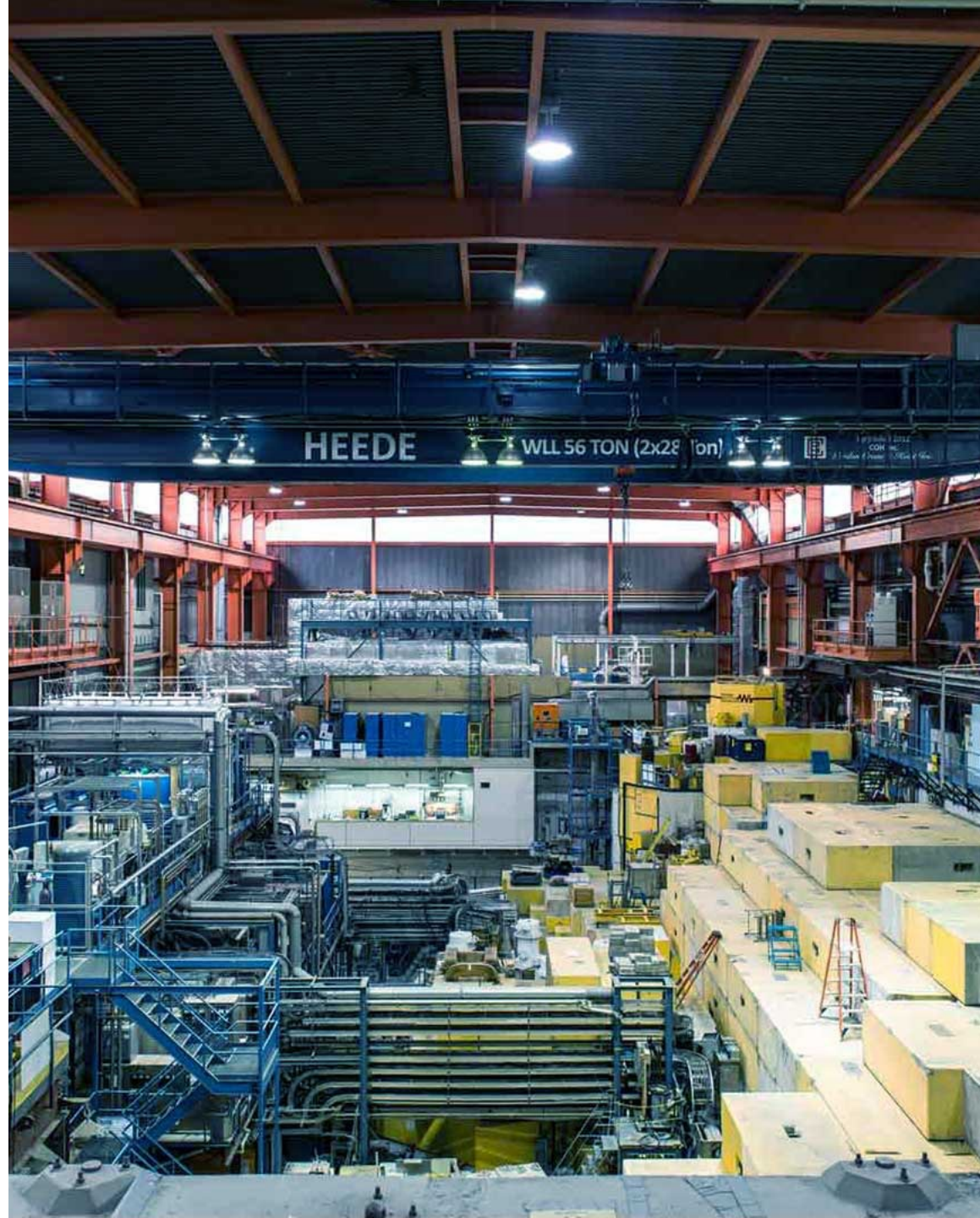
- Basis expansion method (CI)
 - Harmonic oscillator (HO) basis truncated in a particular way ($N_{\max}$)
 - Why HO basis?
 - Lowest filled HO shells match magic numbers of light nuclei (2, 8, 20 – ^4He , ^{16}O , ^{40}Ca)
 - Equivalent description in relative(Jacobi)-coordinate and Slater determinant basis – **nuclei self-bound**, $[\mathbf{H}, \mathbf{P}_{\text{CM}}]=0$
 - Exact factorization of CM and intrinsic eigenfunctions at each $N_{\max}$
 - Good for well-bound states, approximation of weakly-bound states and narrow resonances



$$E = (2n + l + \frac{3}{2})\hbar\Omega$$

Precision chiral EFT NN + 3N forces

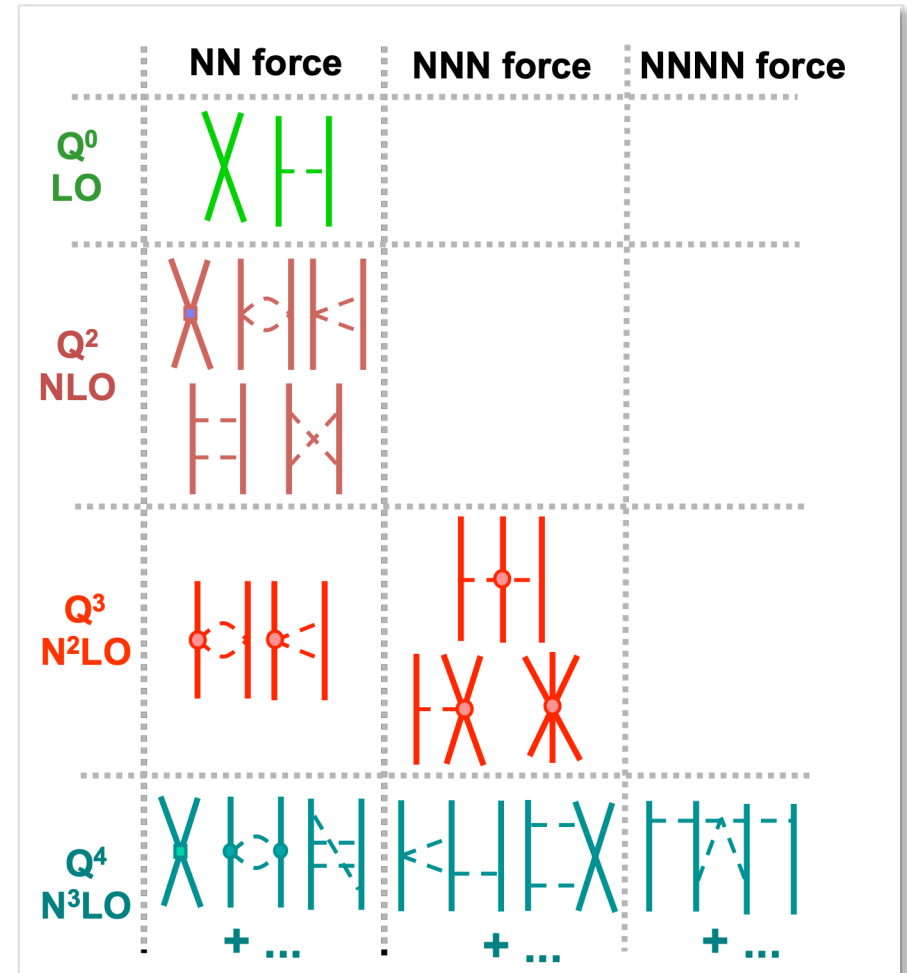
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Nuclear forces from chiral Effective Field Theory

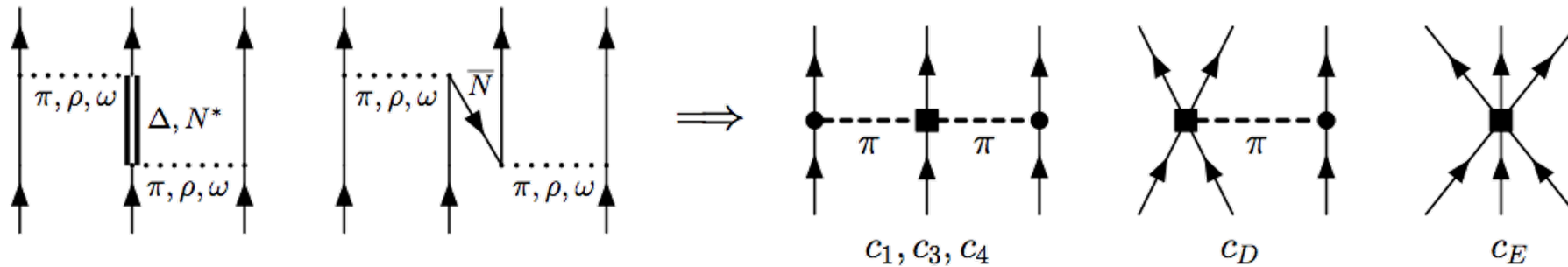
■ Modern approach

- Based on the symmetries of QCD
 - Chiral symmetry of QCD ($m_u \approx m_d \approx 0$), spontaneously broken with pion as the Goldstone boson
 - Degrees of freedom: nucleons + pions
- Systematic low-momentum expansion to a given order (Q/Λ_χ)
- Hierarchy
- Consistency
- Low energy constants (LEC)
 - Fitted to data
 - Can be calculated by lattice QCD



$\Lambda_\chi \sim 1 \text{ GeV}$:
Chiral symmetry breaking scale

Why three-nucleon forces?



Eliminating degrees of freedom leads to three-body forces.

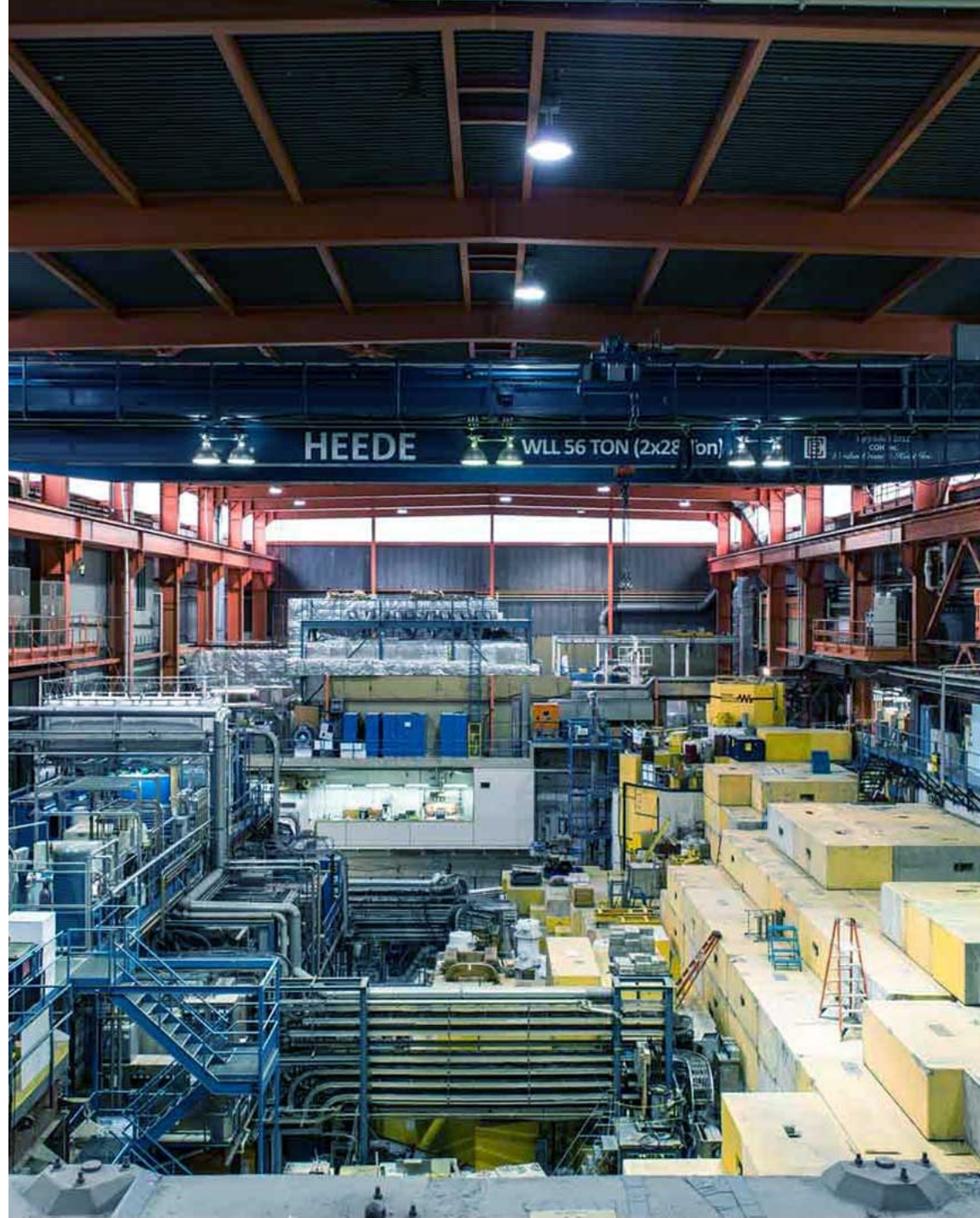
Two-pion exchange with **virtual Δ excitation** – Fujita & Miyazawa (1957)

- Leading three-nucleon force terms
 - Long-range two-pion exchange
 - Medium-range one-pion exchange + two-nucleon contact
 - Short range three-nucleon contact

Nucleons are not
fundamental particles,
have internal structure

NN $N^3\text{LO}$ + $3N_{\text{Inl}}$ Hamiltonian

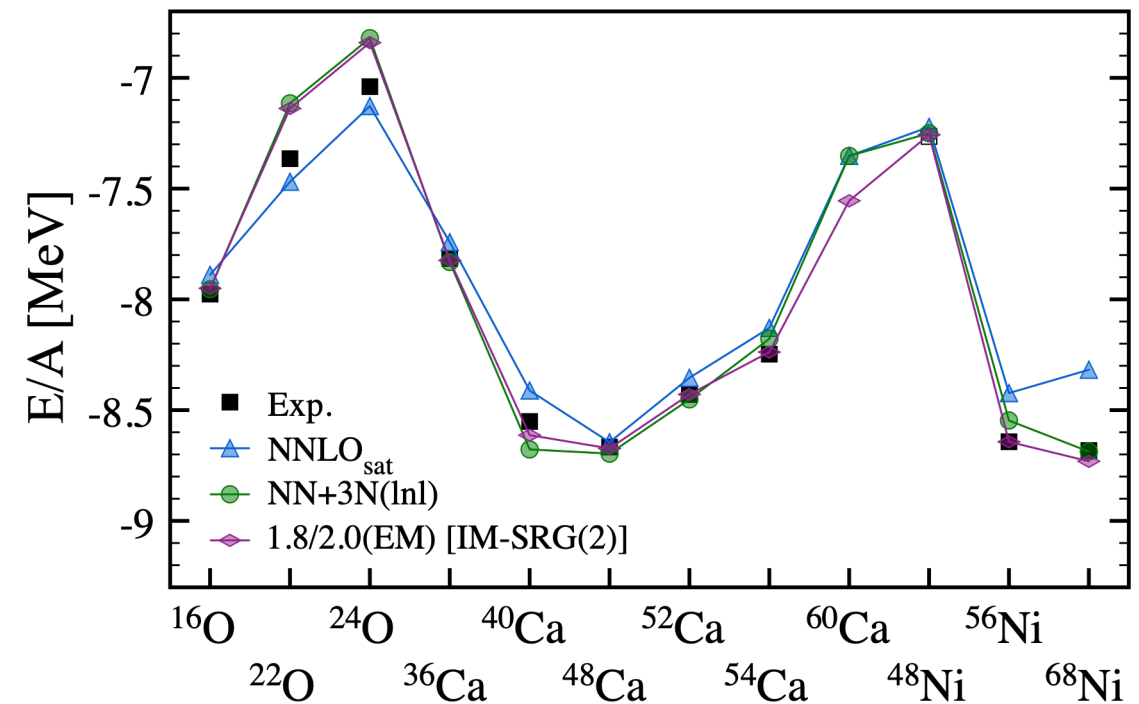
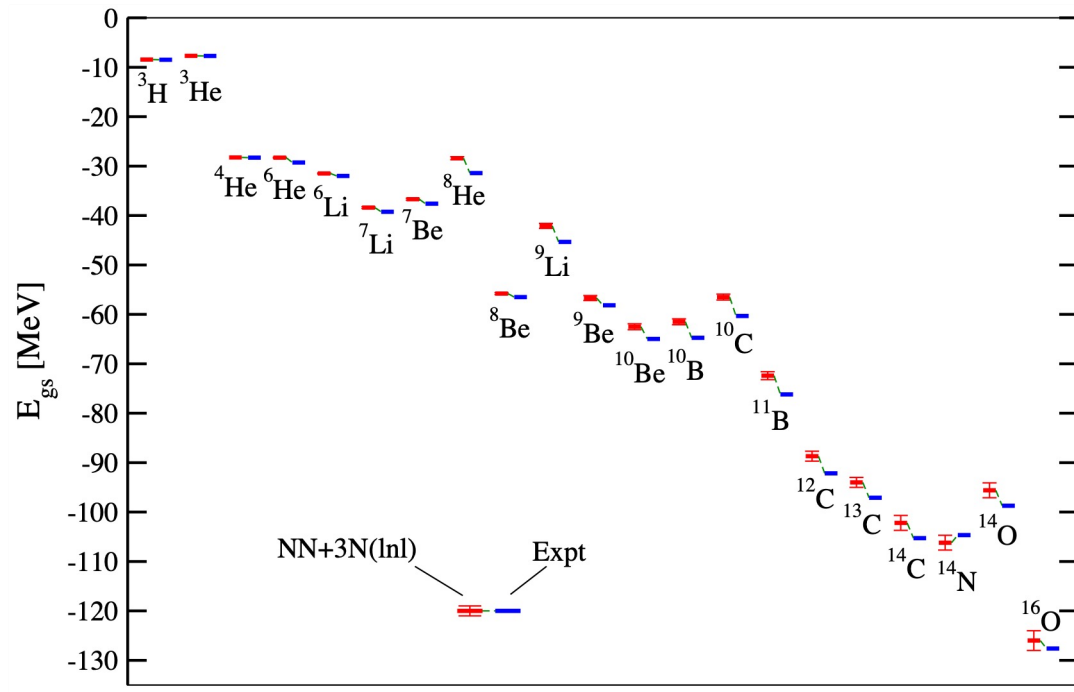
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Binding energies of atomic nuclei from nuclear forces from chiral Effective Field Theory

- Quite reasonable description of binding energies across the nuclear charts becomes feasible
 - **The Hamiltonian fully determined in $A=2$ and $A=3,4$ systems**
 - Nucleon–nucleon scattering, deuteron properties, ^3H and ^4He binding energy, ^3H half life
 - Light nuclei – NCSM
 - Medium mass nuclei – Self-Consistent Green’s Function method

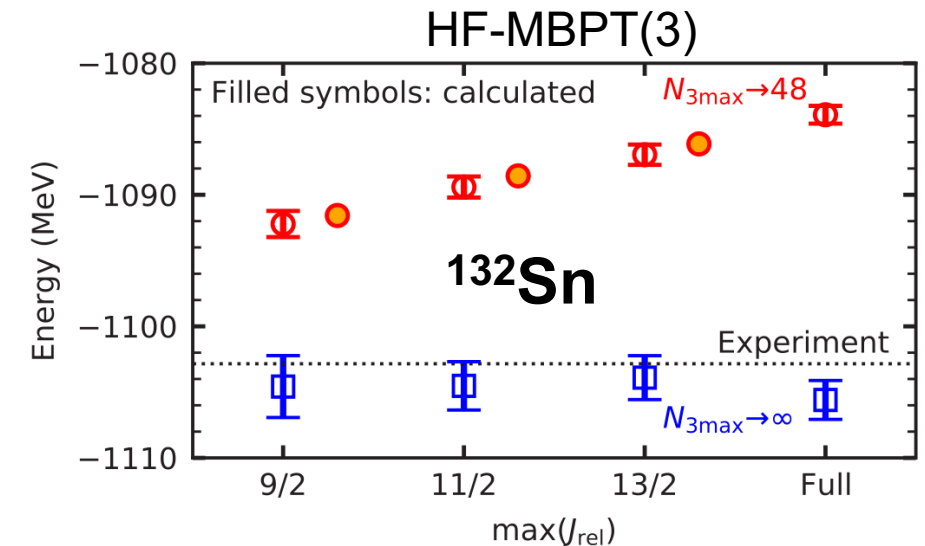
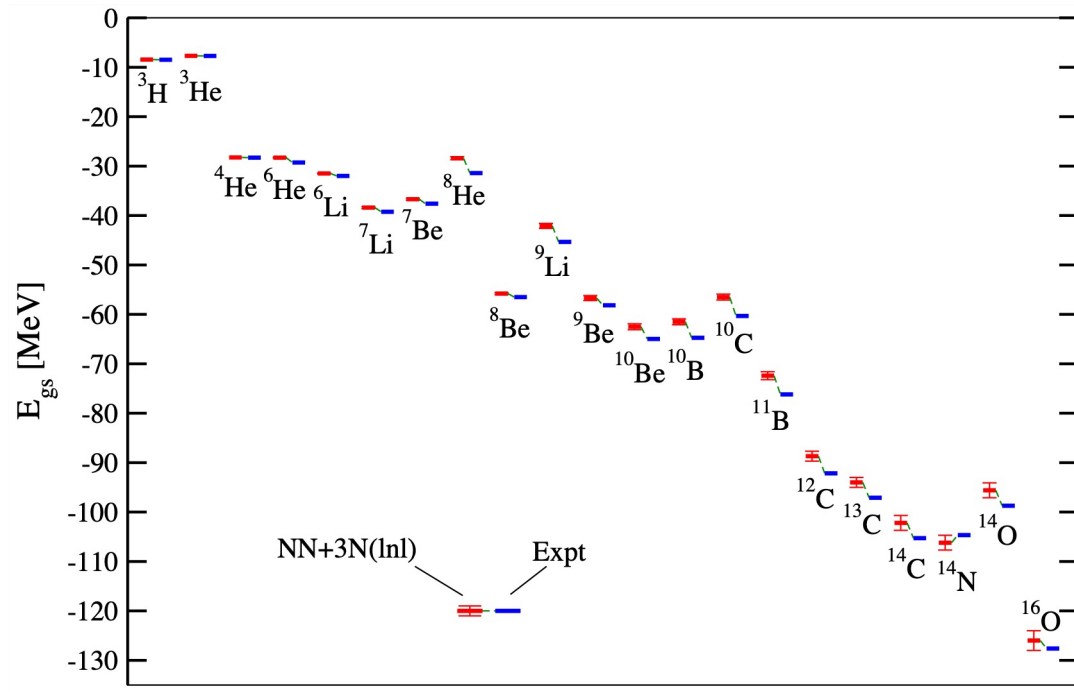
NN N³LO (Entem-Machleidt 2003)
3N N²LO w local/non-local regulator



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 - Heavy nuclei – HF-MBPT(3)

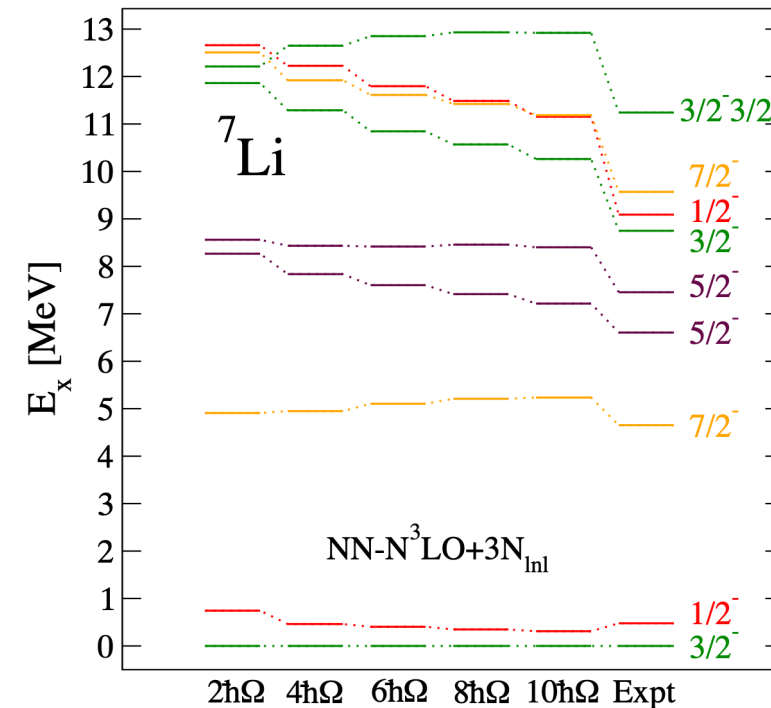
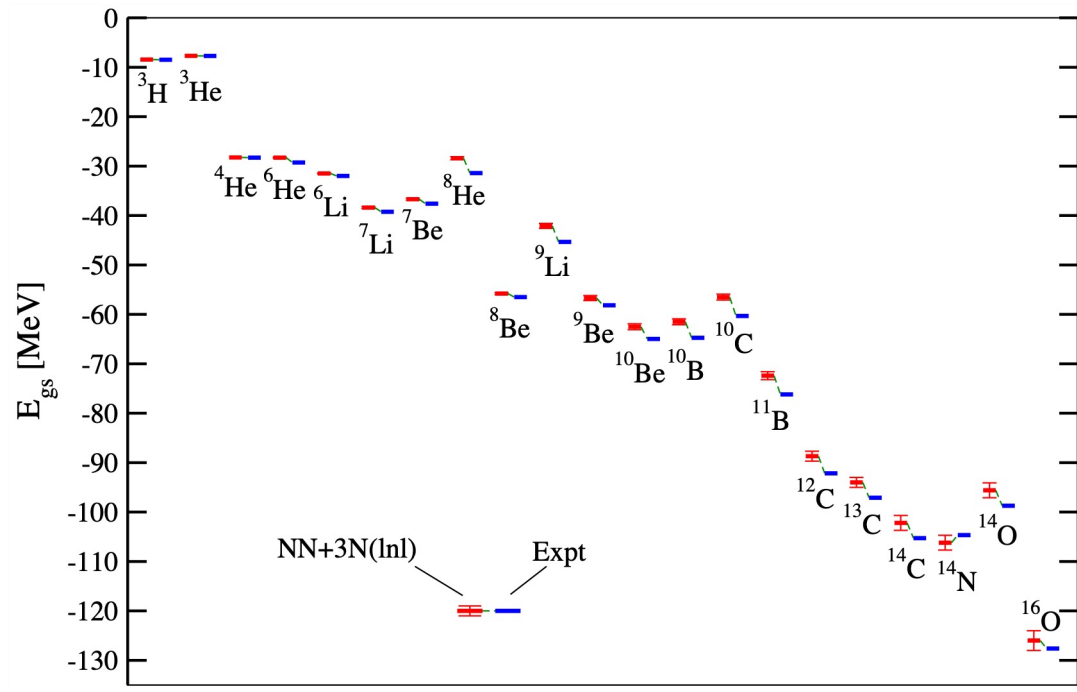
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Binding and excitation energies of atomic nuclei from nuclear forces from chiral Effective Field Theory

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 - Light nuclei – NCSM
 - Denoted as $\text{NN } N^3\text{LO} + 3N_{\text{Inl}}$

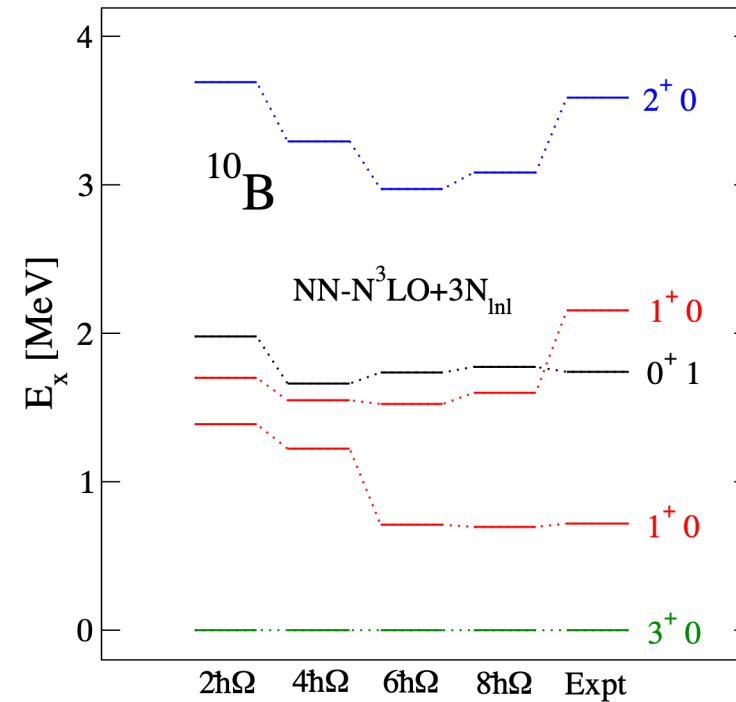
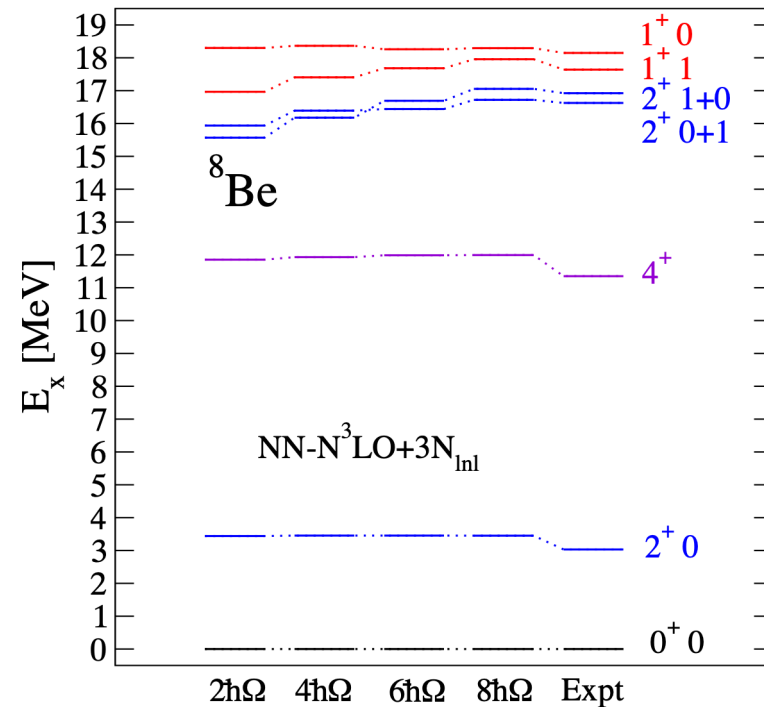
NN $N^3\text{LO}$ (Entem-Machleidt 2003)
 3N $N^2\text{LO}$ w local/non-local regulator



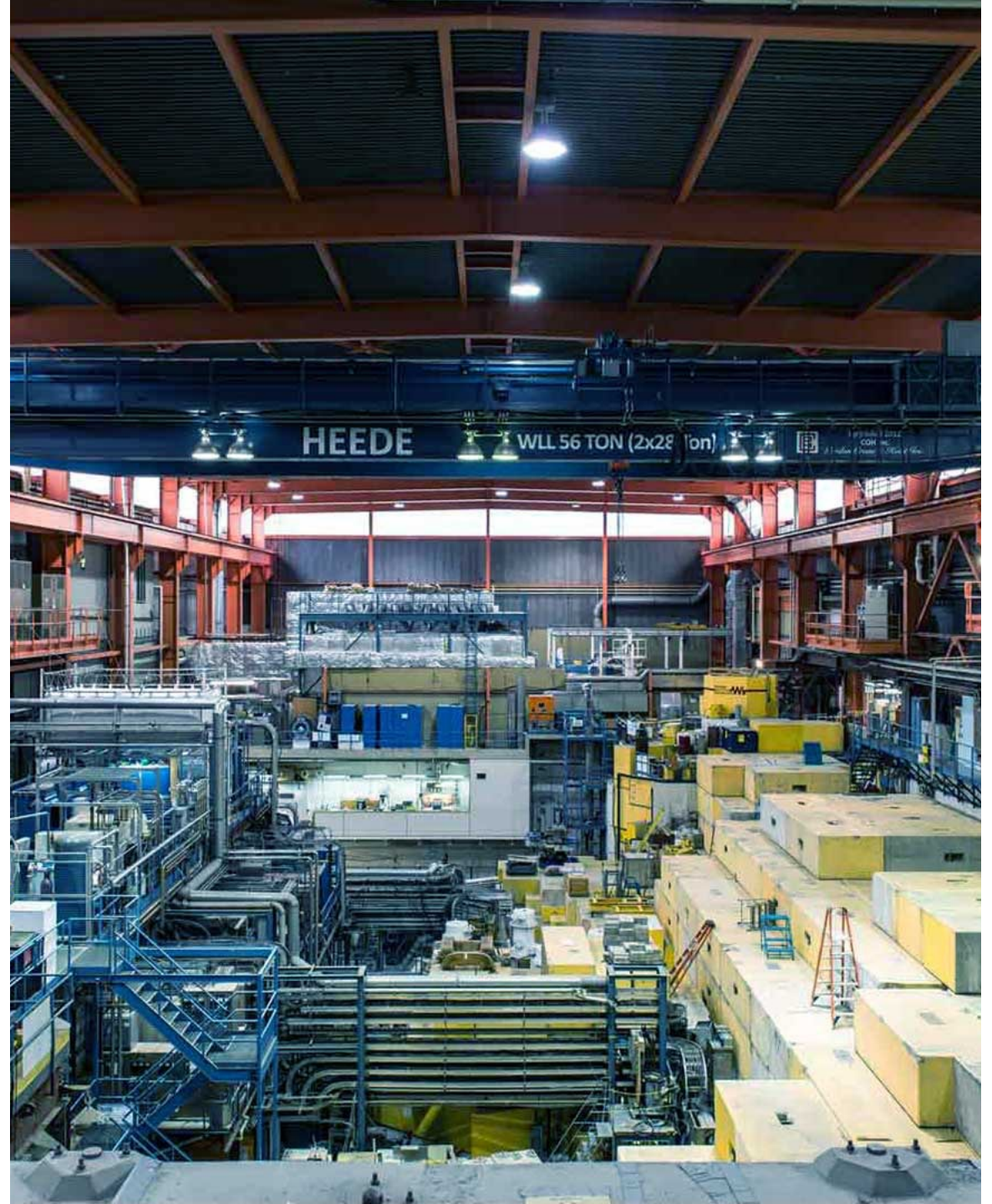
Excitation energies of atomic nuclei from nuclear forces from chiral Effective Field Theory

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$\text{NN } N^3\text{LO}$ (Entem-Machleidt 2003)
 $3N$ $N^2\text{LO}$ w local/non-local regulator

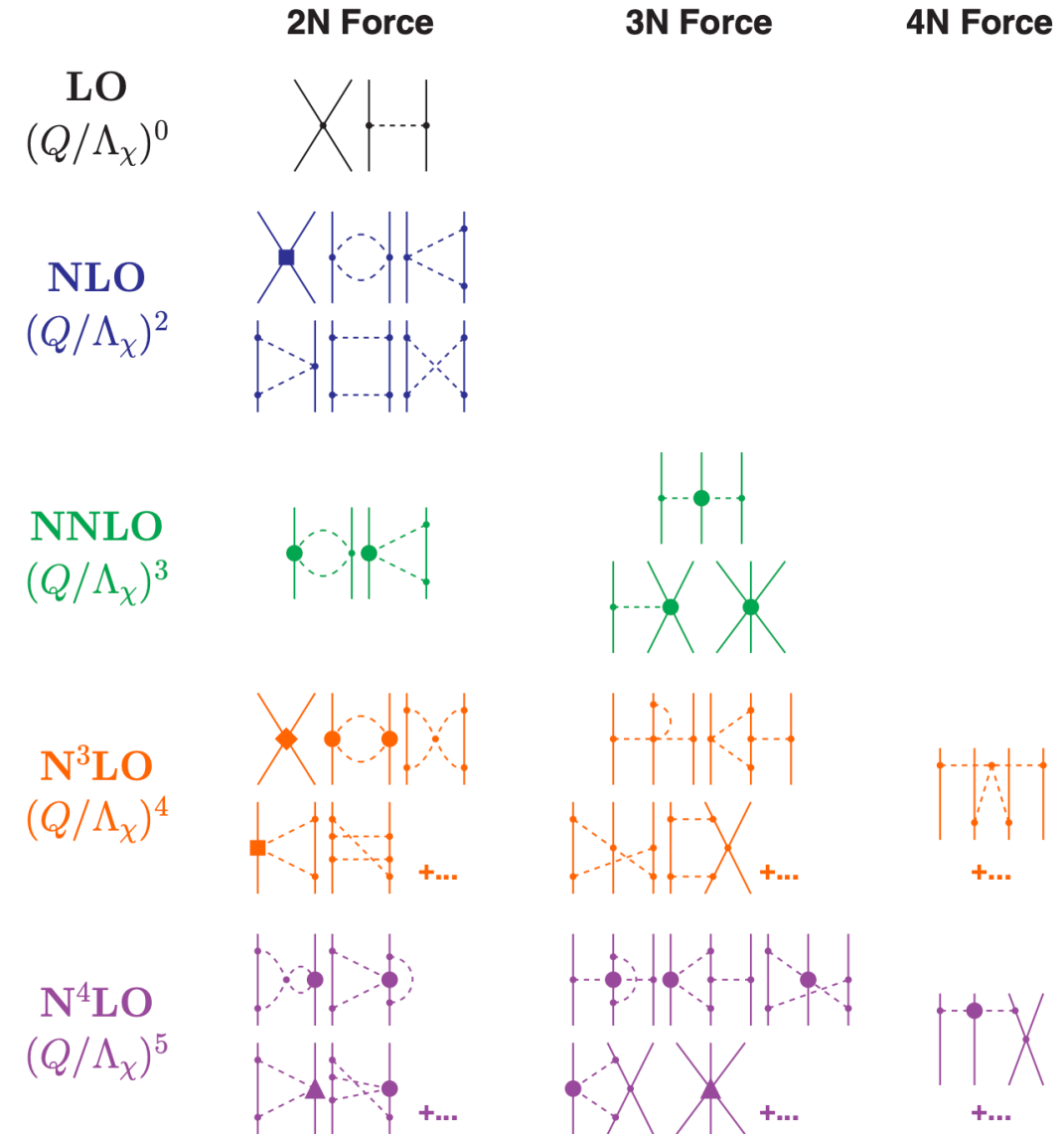


NN N^4LO + $3N_{\text{in}E7}$ Hamiltonian
with a sub-leading $3N$ interaction term



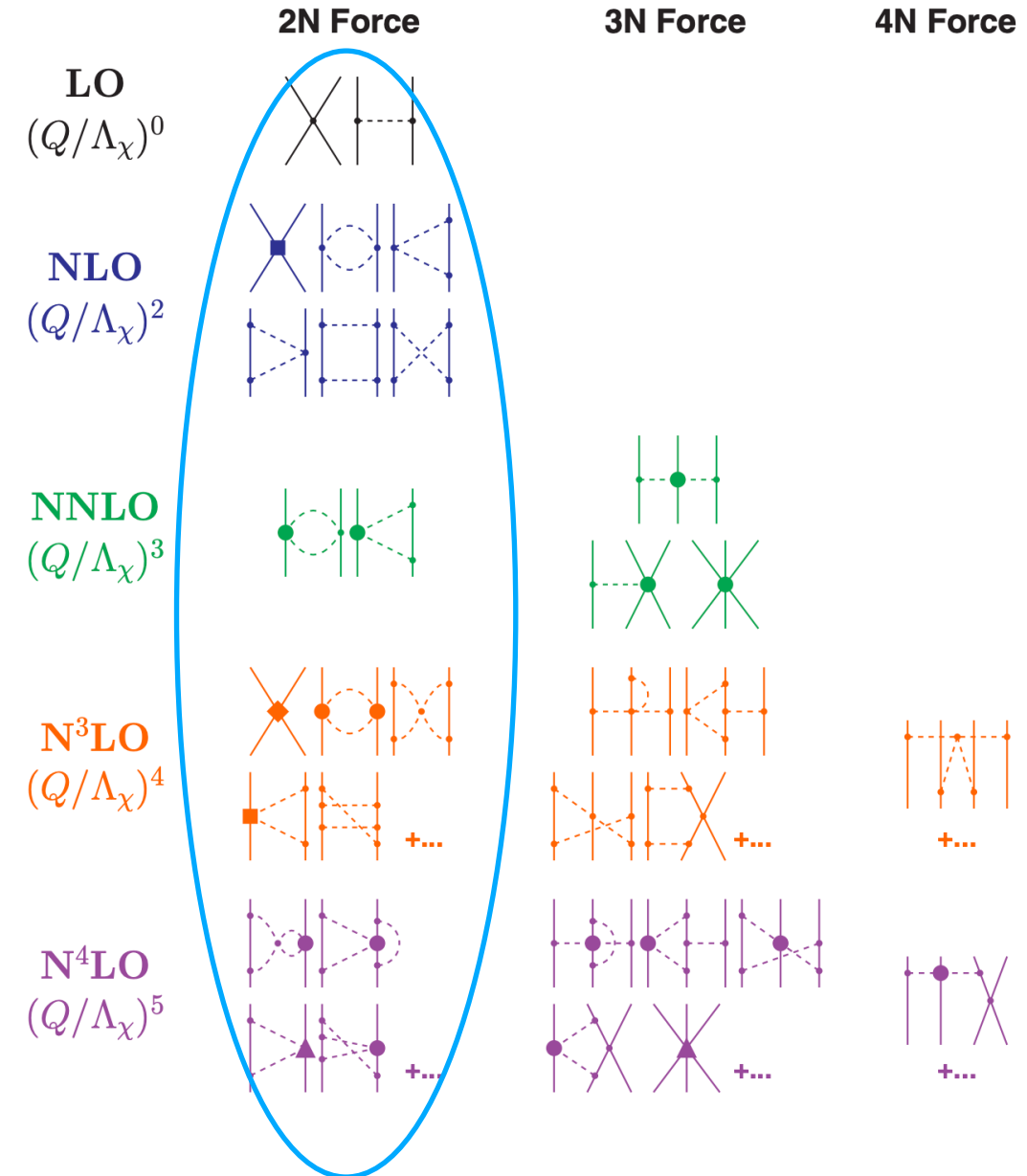
Precision chiral EFT Hamiltonian with a sub-leading 3N interaction term

- NN N⁴LO 500 interaction by Entem-Machleidt-Nosyk (2017)
- 3N N²LO plus a sub-leading spin-orbit enhancing term with a new LEC (E_7) – Girlanda 2011
 - local/non-local regulator
 - **The Hamiltonian fully determined in $A=2$, $A=3,4$, and ${}^6\text{Li}$ systems**
 - Nucleon–nucleon scattering, deuteron properties, ${}^3\text{H}$ and ${}^4\text{He}$ binding energy, ${}^3\text{H}$ half life
 - New LEC (E_7) fitted to improve ${}^6\text{Li}$ excitation levels
- Denoted as NN N⁴LO + 3N_{InlE7}



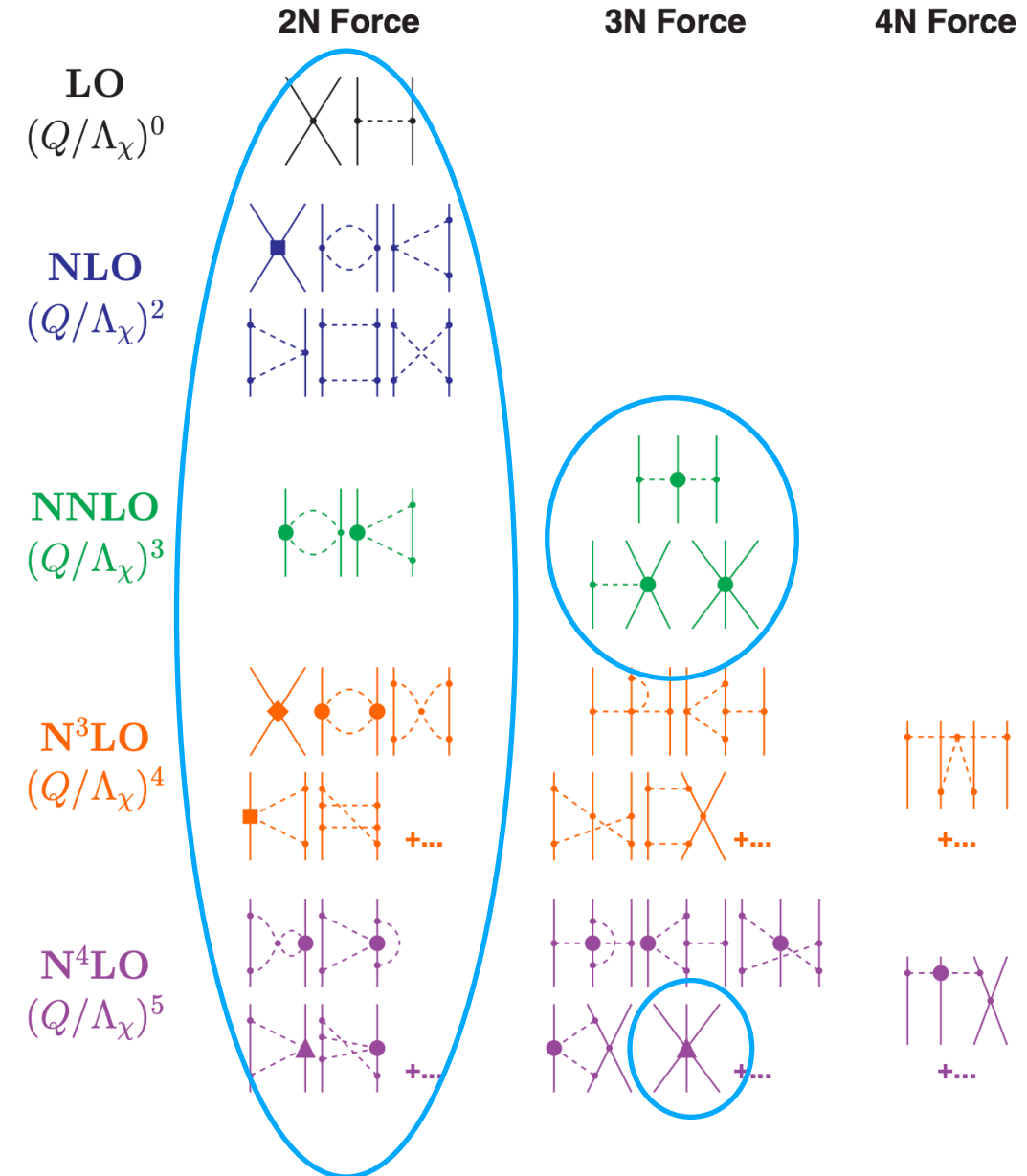
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Precision chiral EFT Hamiltonian with a sub-leading 3N interaction term

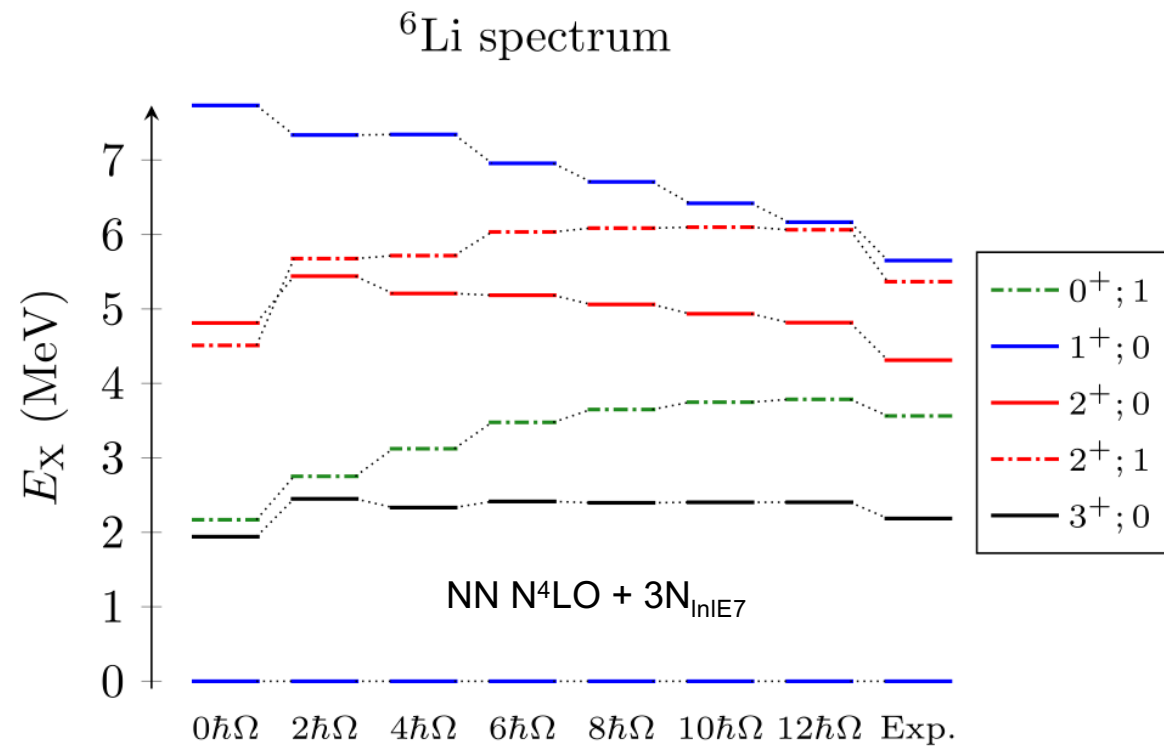
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Precision chiral EFT Hamiltonian with a sub-leading 3N interaction term

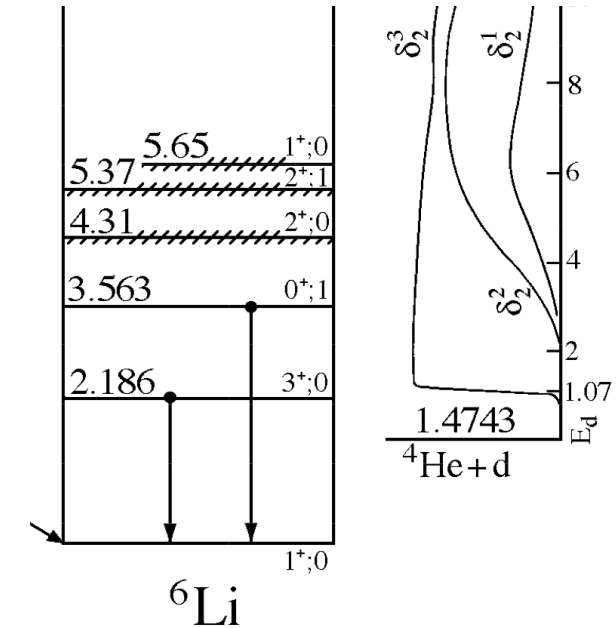
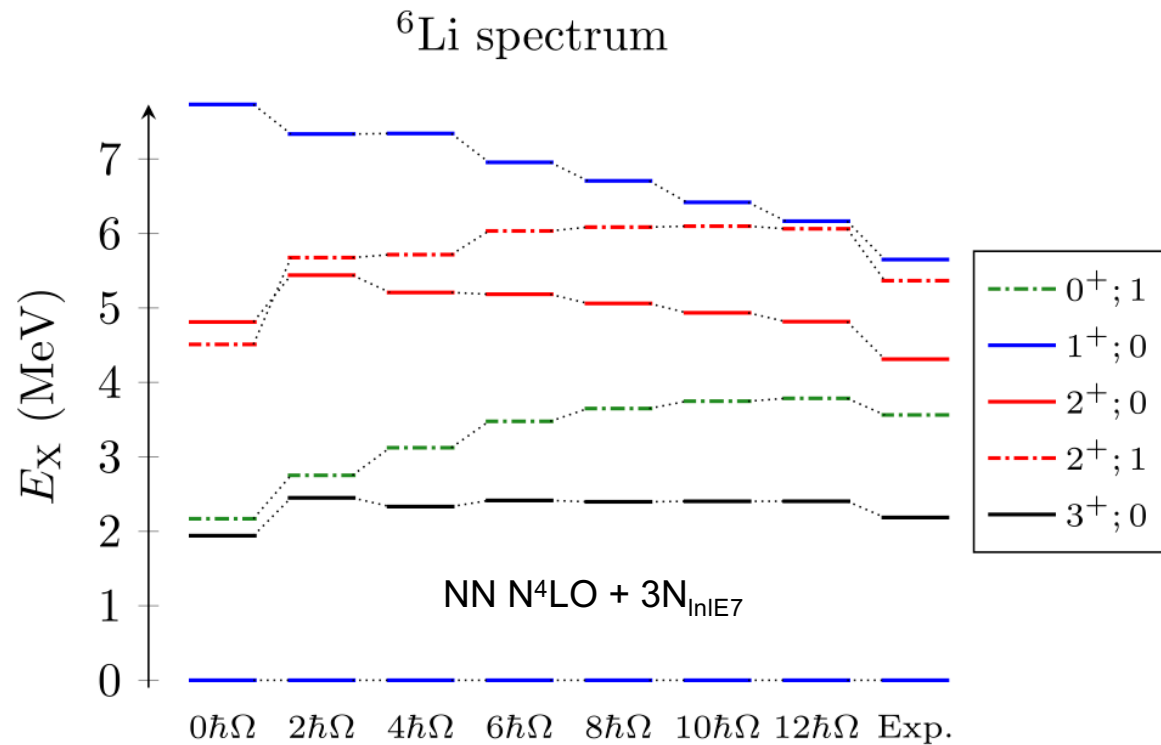
- Excitation energies of light nuclei – NCSM (HO basis)

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Precision chiral EFT Hamiltonian with a sub-leading 3N interaction term

- Excitation energies of light nuclei – NCSM (HO basis)



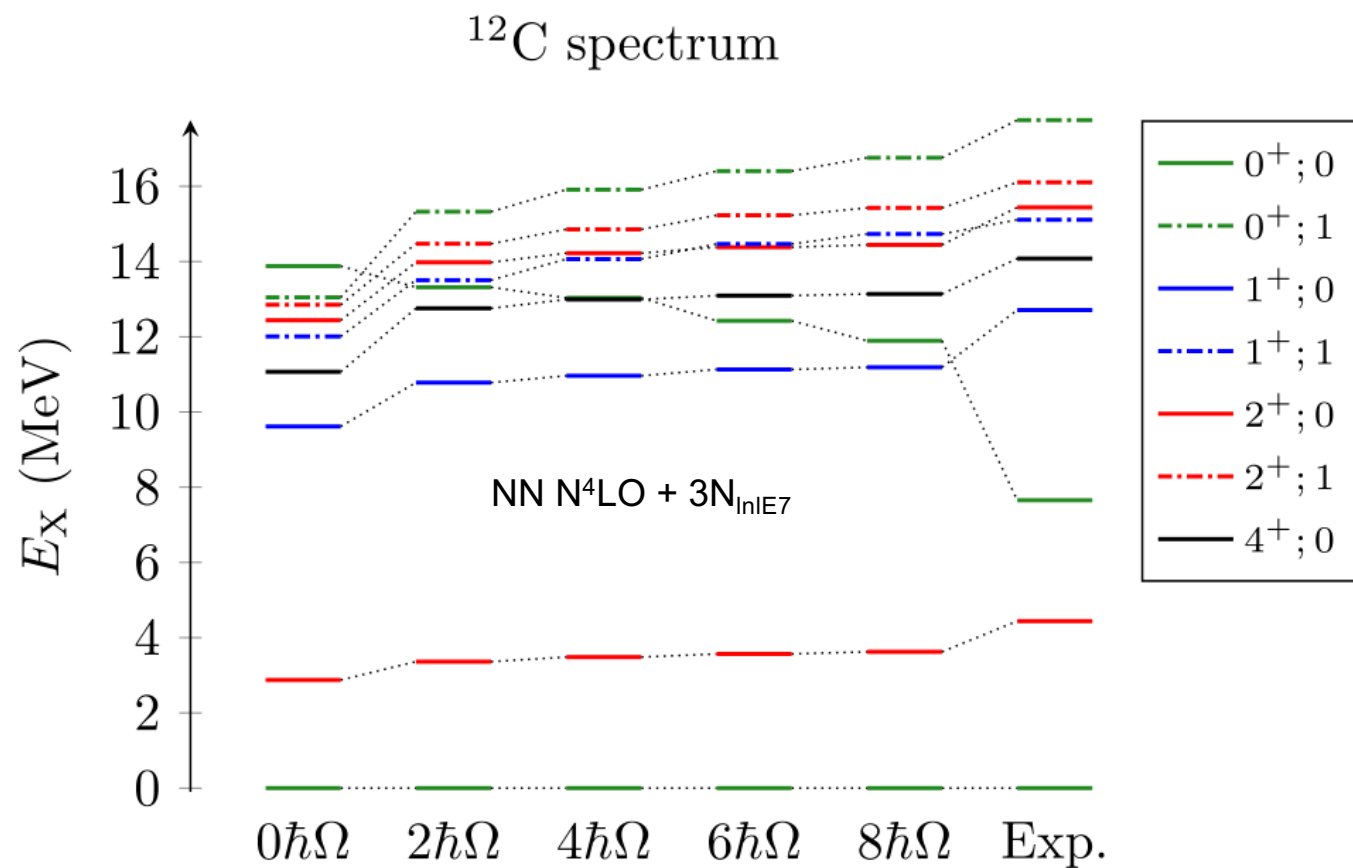
All excited states are resonances
 $2^+ 0$ and $1^+ 0$ are broad

NCSMC calculation shown later

Precision chiral EFT Hamiltonian with a sub-leading 3N interaction term

- Excitation energies of light nuclei – NCSM (HO basis)

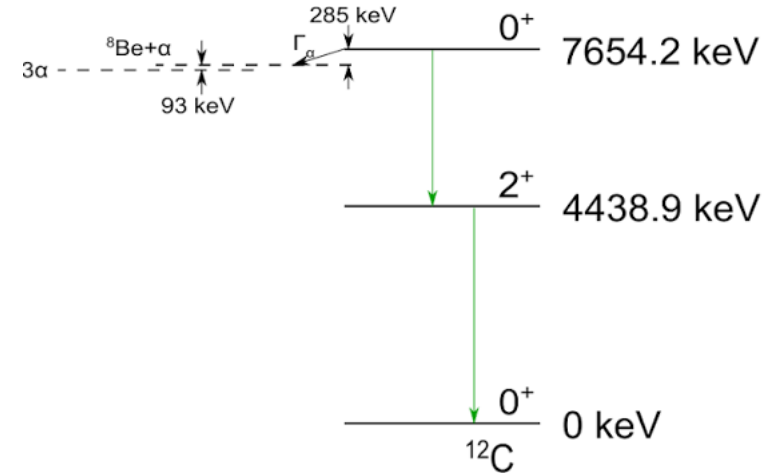
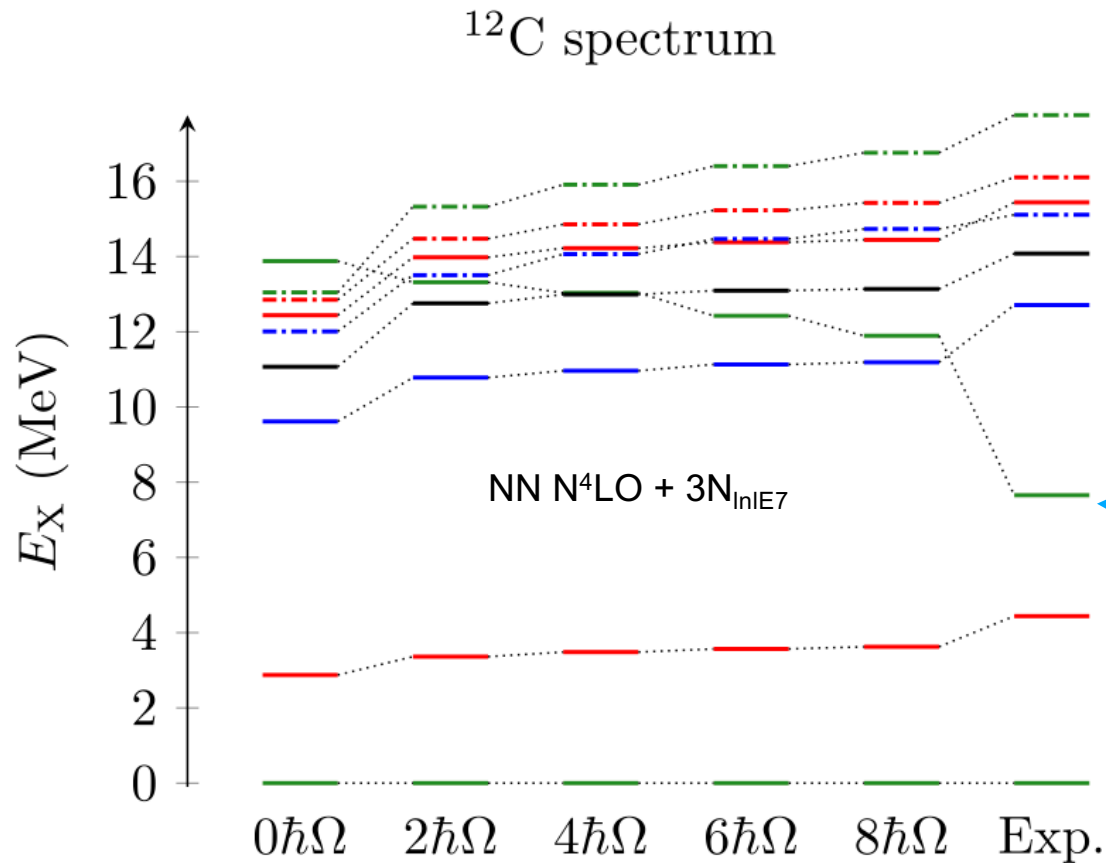
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Precision chiral EFT Hamiltonian with a sub-leading 3N interaction term

22

- Excitation energies of light nuclei – NCSM (HO basis)

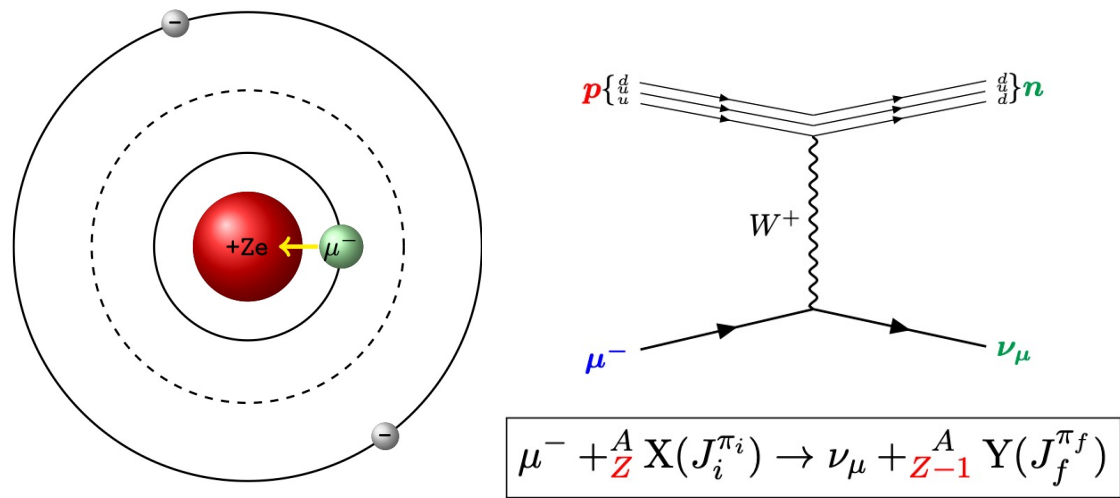


Hoyle state – ${}^8\text{Be} + \alpha$ cluster structure

Difficult (impossible) to describe
in harmonic oscillator basis

Precision chiral EFT Hamiltonian with a sub-leading 3N interaction term

- Muon capture rate on ^{12}C – NCSM (HO basis)

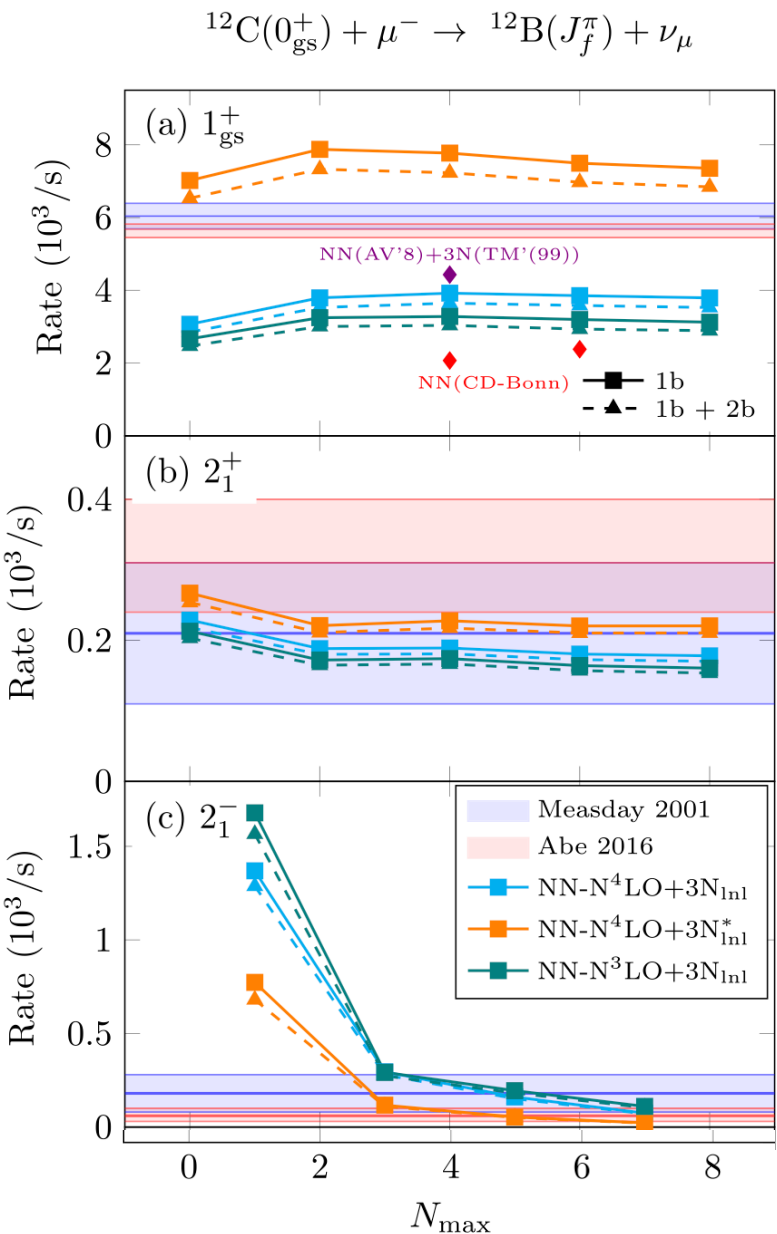


Improvement for ^{12}C muon capture rate compared to other interactions

PHYSICAL REVIEW C **109**, 065501 (2024)

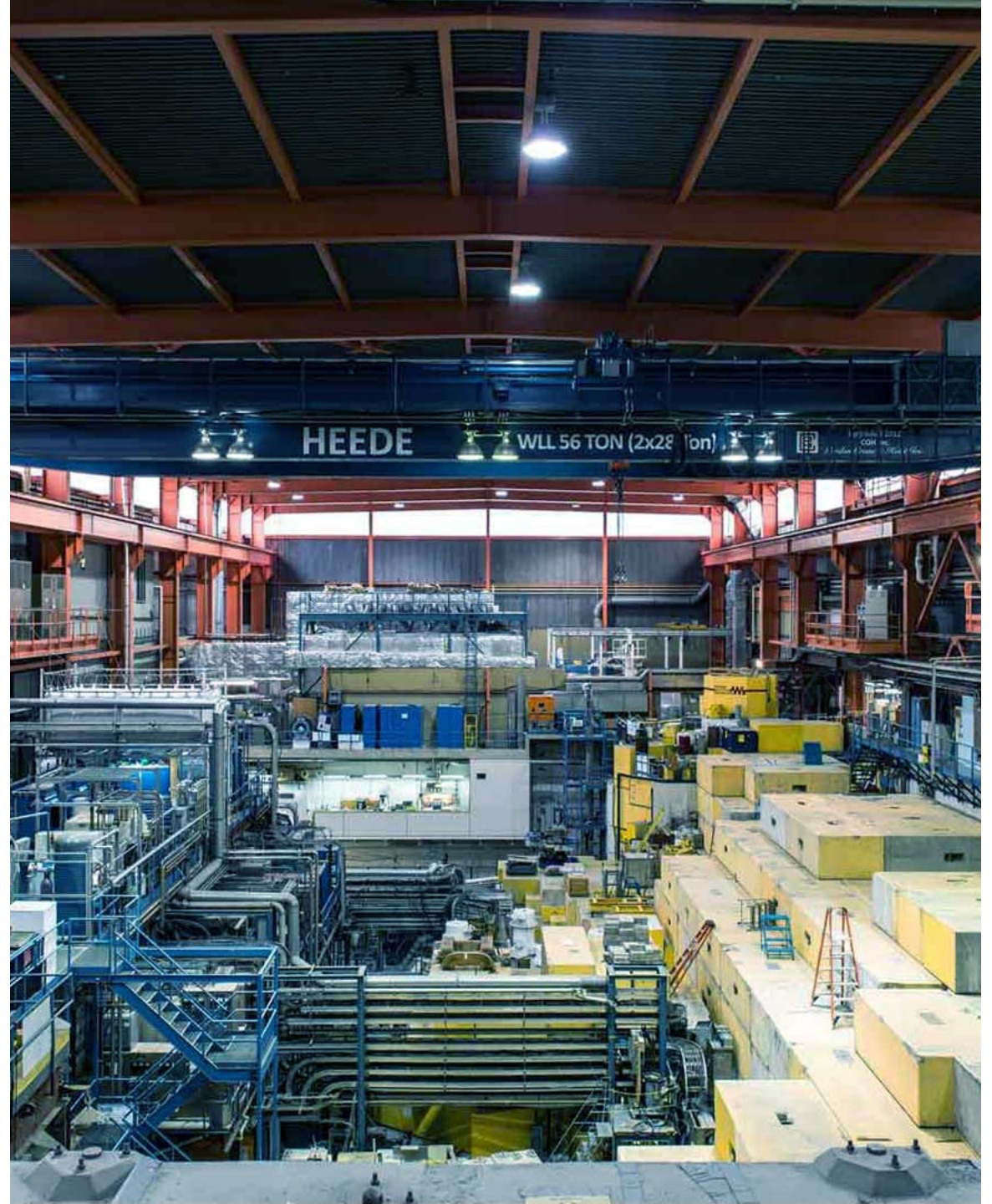
Muon capture on ^6Li , ^{12}C , and ^{16}O from *ab initio* nuclear theory

Lotta Jokiniemi^{1,*}, Petr Navrátil^{1,2,†}, Jenni Kotila^{3,4,5,‡} and Kostas Kravvaris^{6,§}



Superaligned Fermi transitions - electroweak radiative correction δ_{NS}

2026-10-20



V_{ud} element of CKM matrix

$$\mathcal{L}_{CC} = -\frac{g}{\sqrt{2}} (\bar{u}_L, \bar{c}_L, \bar{t}_L) \gamma^\mu W_\mu^+ \underbrace{V_{CKM}} \begin{pmatrix} d_L \\ s_L \\ b_L \end{pmatrix} + h.c.$$

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- Precise V_{ud} from superallowed Fermi transitions

$$|V_{ud}|^2 = \frac{\hbar^7}{G_F^2 m_e^5 c^4} \frac{\pi^3 \ln(2)}{\mathcal{F}t(1 + \Delta_R^V)}$$

$G_F \equiv$ Fermi coupling constant
determined from muon β decay

- hadronic matrix elements modified by nuclear environment
- Fermi matrix element renormalized by isospin non-conserving forces

$$\mathcal{F}t = ft(1 + \delta'_R) \underline{(1 - \delta_C + \delta_{NS})}$$

$$\mathcal{F}t = \frac{K}{G_V^2 |M_{F0}|^2 (1 + \Delta_R^V)}$$

Δ_R^V and δ_{NS}

Leptonic current

NME of charged weak current

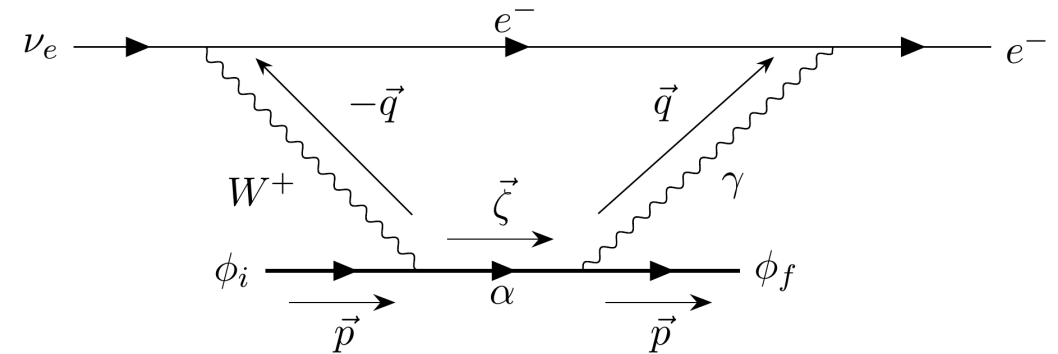
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- Tree level beta decay amplitude

$$M_{tree} = -\frac{G_F}{\sqrt{2}} L_\lambda F^\lambda(p', p)$$

- Hadronic correction in forward scattering limit

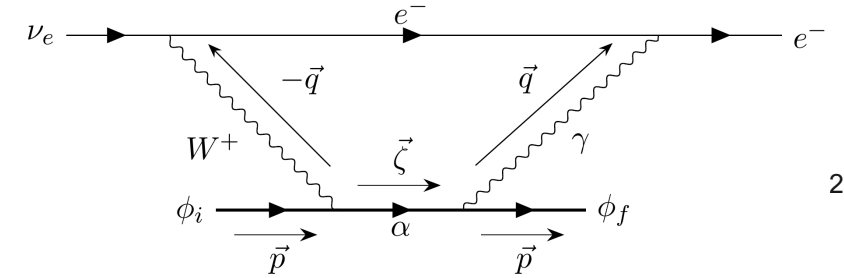
$$\delta M = \square_{\gamma W}(E_e) M_{tree}$$



$$\square_{\gamma W}^b(E_e) = \frac{e^2}{M} \int \frac{d^4 q}{(2\pi)^4} \frac{M_W^2}{M_W^2 - q^2} \frac{1}{q^2 + i\epsilon} \frac{1}{(p_e - q)^2 + i\epsilon'} \frac{M\nu\left(\frac{p_e \cdot q}{p \cdot p_e}\right) - q^2}{\nu} \frac{T_3(\nu, |\vec{q}|)}{f_+(0)}$$

Nonrelativistic Compton amplitude

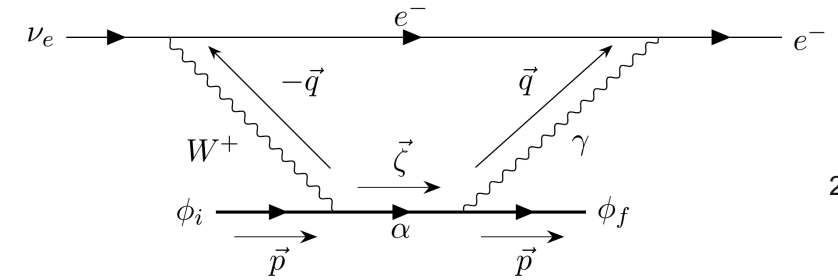
- **Goal:** Non-relativistic currents in momentum space
- Rewrite currents with A -body propagators
- Fourier transform currents into momentum space
- General multipole expansion of currents



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$$T_3(\nu, |\vec{q}|) = 4\pi i \frac{\nu}{|\vec{q}|} \sqrt{M_i M_f} \sum_{J=1}^{\infty} (2J+1) \langle \Psi_f | \left\{ T_{J0}^{\text{mag}} G(\nu + M_f + i\epsilon) T_{J0}^{5,\text{el}} + T_{J0}^{\text{el}} G(\nu + M_f + i\epsilon) T_{J0}^{5,\text{mag}} \right. \\ \left. + T_{J0}^{5,\text{mag}} G(-\nu + M_i + i\epsilon) T_{J0}^{\text{el}} + T_{J0}^{5,\text{el}} G(-\nu + M_i + i\epsilon) T_{J0}^{\text{mag}} \right\} (|\vec{q}|) | \Psi_i \rangle$$

Nonrelativistic Compton amplitude



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- **Goal:** Non-relativistic currents in momentum space
- Rewrite currents with A -body propagators
- Fourier transform currents into momentum space
- General multipole expansion of currents

*NCSM & Lanczos strength method
to compute nuclear Green's functions*

$$T_3(\nu, |\vec{q}|) = 4\pi i \frac{\nu}{|\vec{q}|} \sqrt{M_i M_f} \sum_{J=1}^{\infty} (2J+1) \langle \Psi_f | \left\{ T_{J0}^{\text{mag}} \boxed{G(\nu + M_f + i\epsilon)} T_{J0}^{5,\text{el}} + T_{J0}^{\text{el}} \boxed{G(\nu + M_f + i\epsilon)} T_{J0}^{5,\text{mag}} \right. \\ \left. + T_{J0}^{5,\text{mag}} \boxed{G(-\nu + M_i + i\epsilon)} T_{J0}^{\text{el}} + T_{J0}^{5,\text{el}} \boxed{G(-\nu + M_i + i\epsilon)} T_{J0}^{\text{mag}} \right\} (|\vec{q}|) | \Psi_i \rangle$$

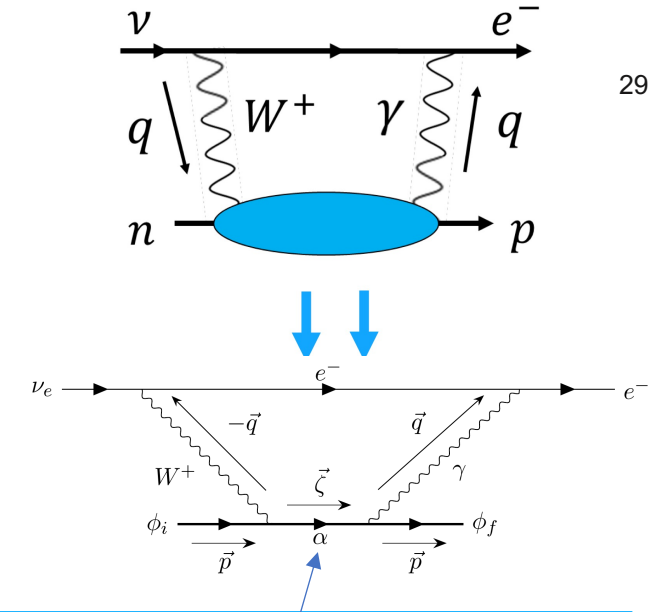
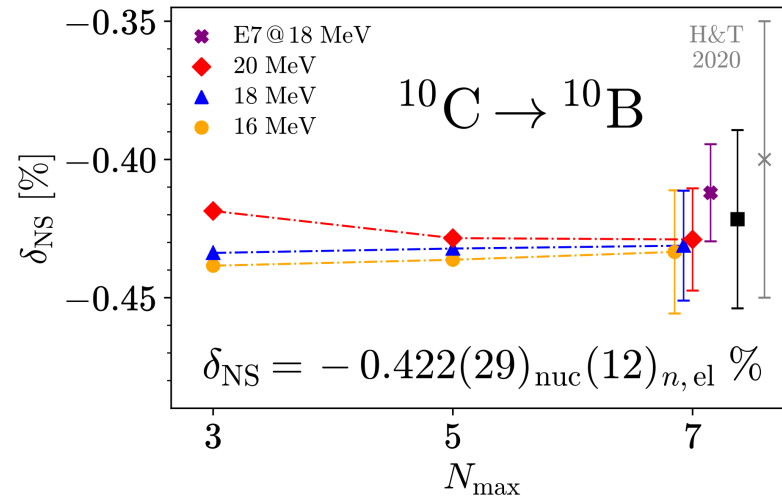
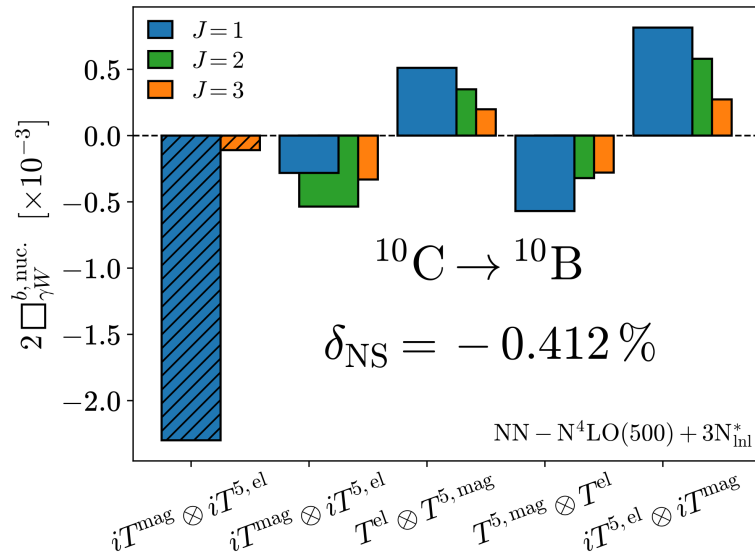
Superaligned Fermi transitions - electroweak radiative correction δ_{NS}

$^{10}\text{C} \rightarrow ^{10}\text{B}$ Fermi transition

- δ_{NS} parametrizes correction to free γW box

$$\delta_{NS} = 2[\Box_{\gamma W}^{VA, \text{nuc.}} - \Box_{\gamma W}^{VA, \text{free n}}]$$

- Ab initio* no-core shell model (NCSM)
 - A very good convergence – consistent with what used in latest evaluation with a substantially reduced theoretical uncertainties



Nuclear Green's function (propagator)
→ Lanczos strength method

PHYSICAL REVIEW LETTERS **134**, 012501 (2025)

Ab Initio Strategy for Taming the Nuclear-Structure Dependence of V_{ud} Extractions: The $^{10}\text{C} \rightarrow ^{10}\text{B}$ Superaligned Transition

Michael Gennari^{1,2}, Mehdi Drissi¹, Mikhail Gorchtein^{3,4}, Petr Navrátil^{1,2}, and Chien-Yeah Seng^{5,6}

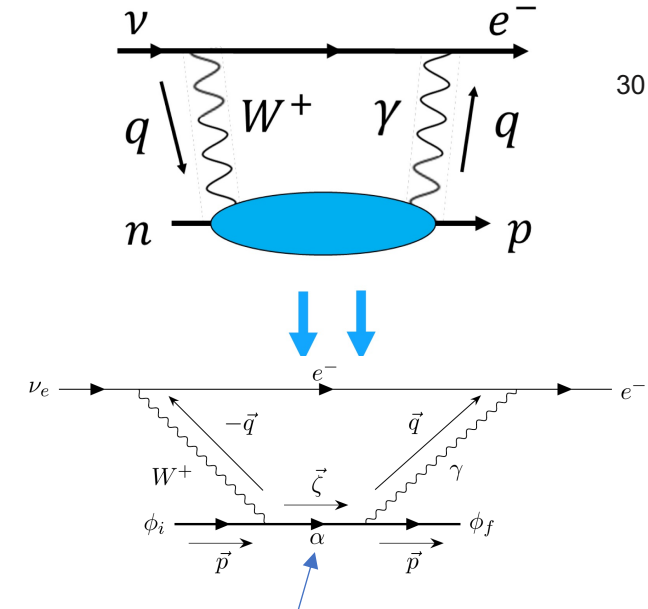
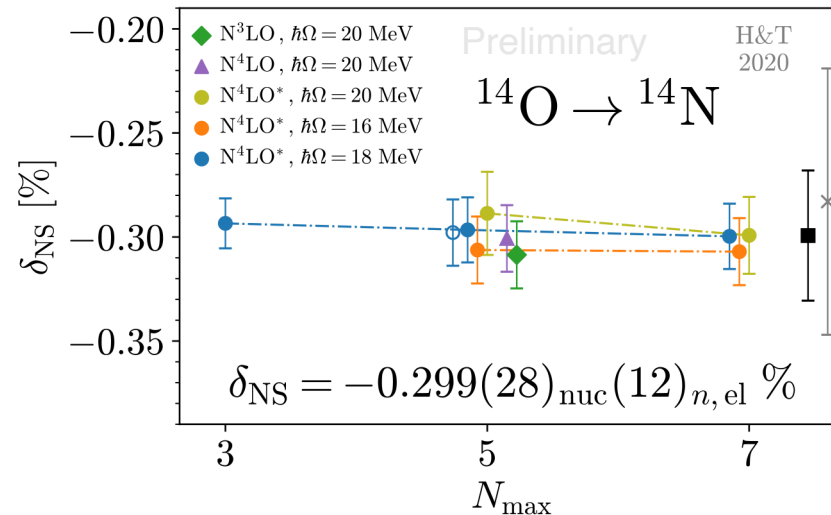
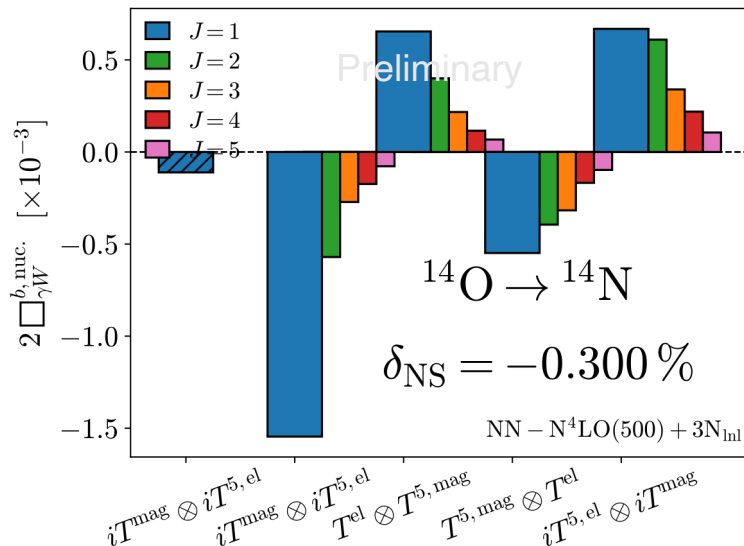
Superaligned Fermi transitions - electroweak radiative correction δ_{NS}

$^{14}\text{O} \rightarrow ^{14}\text{N}$ Fermi transition

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Nuclear Green's function (propagator)
→ Lanczos strength method

Calculations led by
Michael Gennari (Mainz)

Manuscript in preparation

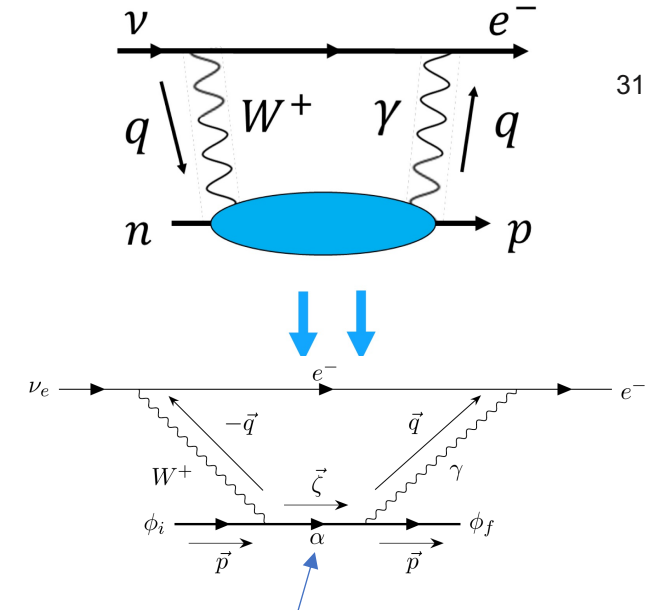
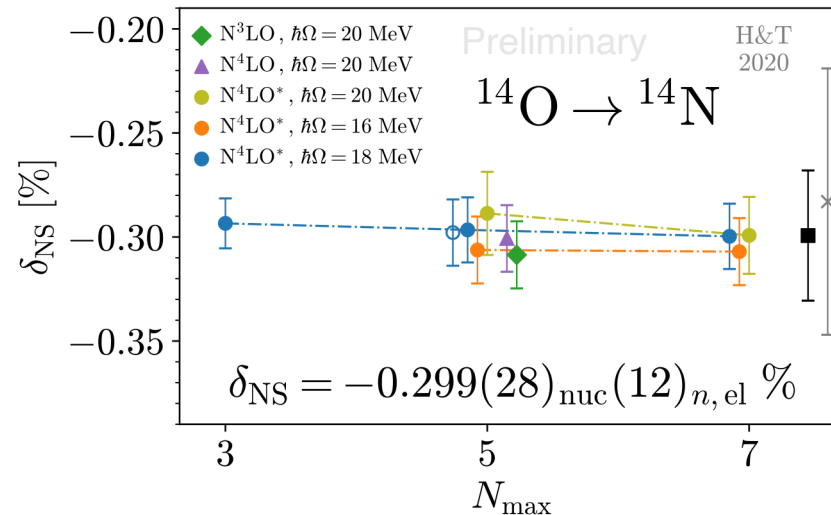
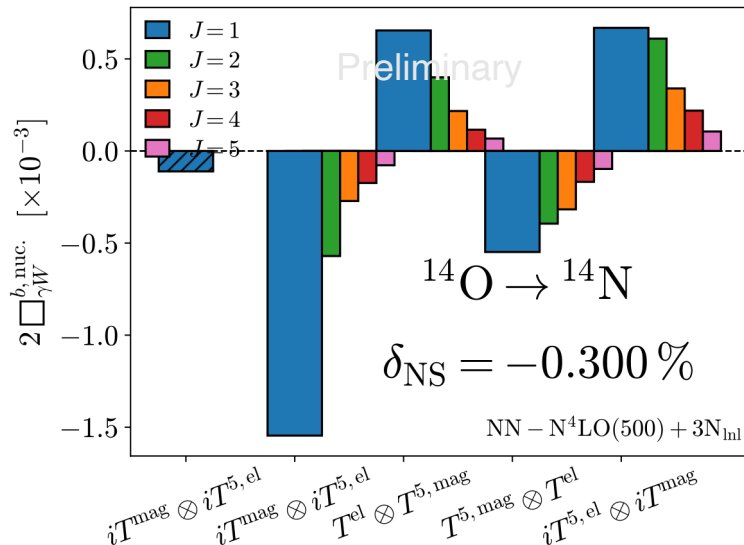
Superaligned Fermi transitions - electroweak radiative correction δ_{NS}

$^{14}\text{O} \rightarrow ^{14}\text{N}$ Fermi transition

- δ_{NS} parametrizes correction to free γW box

$$\delta_{NS} = 2[\Box_{\gamma W}^{VA, \text{nuc.}} - \Box_{\gamma W}^{VA, \text{free n}}]$$

- Ab initio* no-core shell model (NCSM)
 - A very good convergence – consistent with what used in latest evaluation with a substantially reduced theoretical uncertainties



Nuclear Green's function (propagator)
→ Lanczos strength method

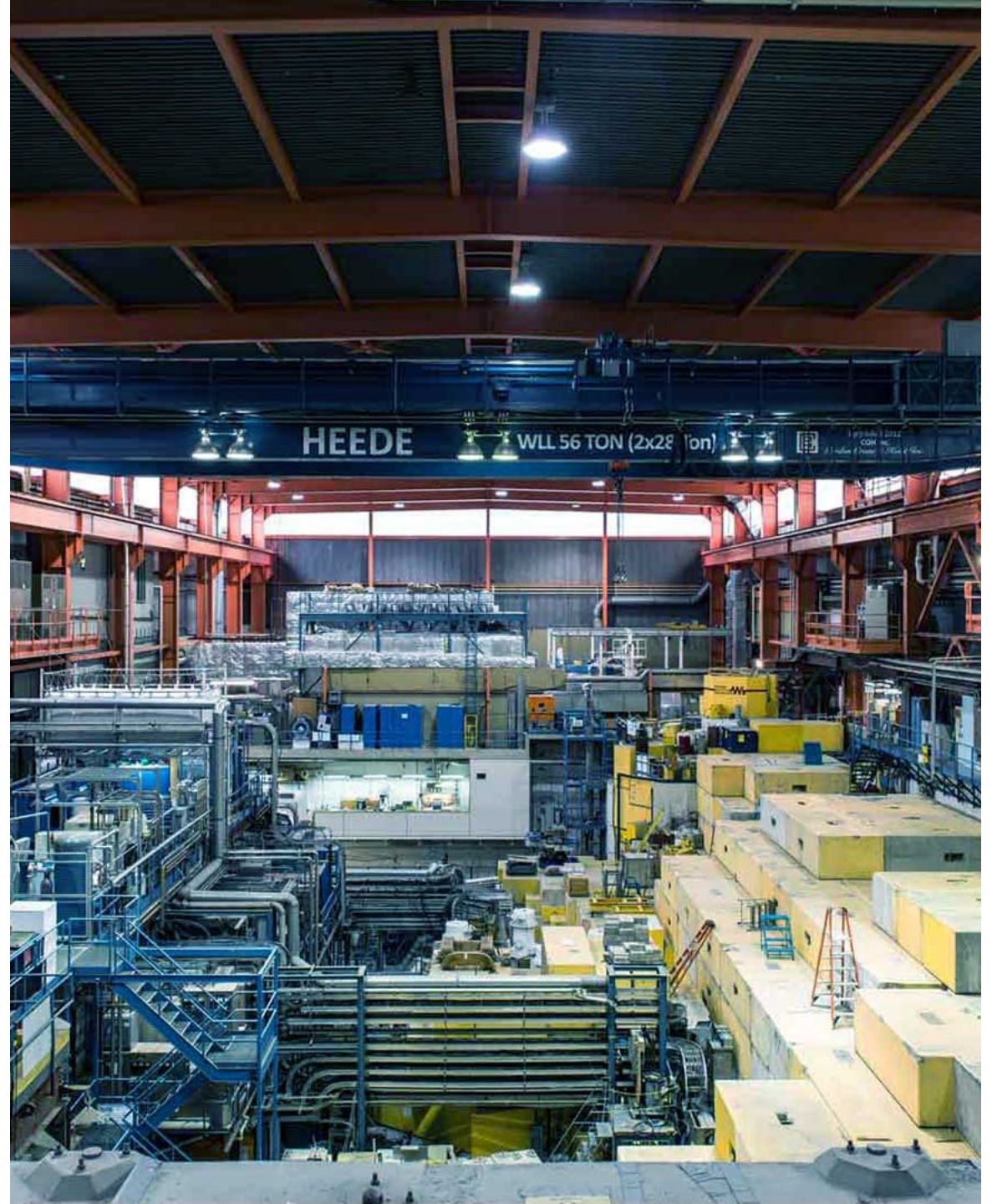
Calculations led by
Michael Gennari (Mainz)

Manuscript in preparation

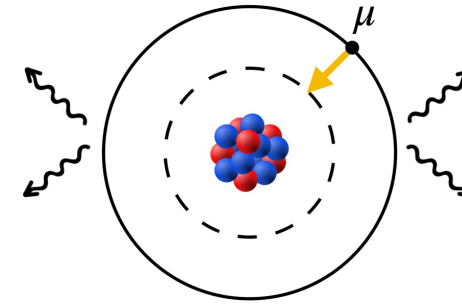
NCSM applicable also to $^{18}\text{Ne} \rightarrow ^{18}\text{F}$ and possibly $^{22}\text{Mg} \rightarrow ^{22}\text{Na}$

Muonic atoms – two-photon exchange nuclear correction

2026-10-20

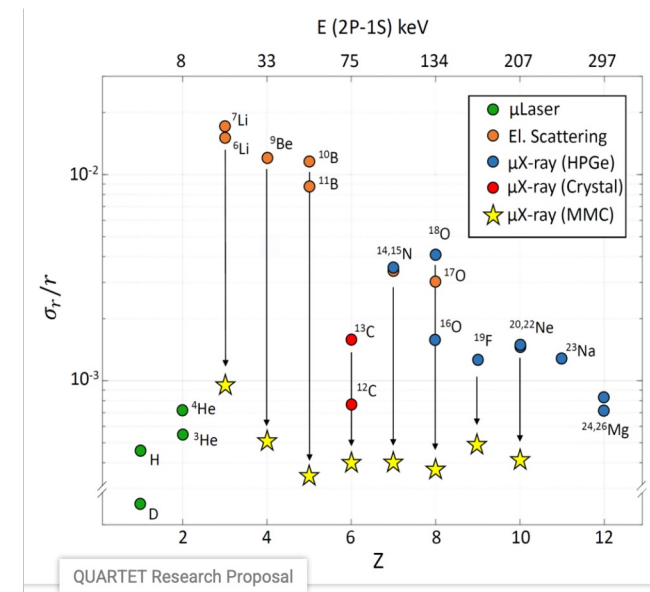


The two-photon exchange nuclear correction – X-rays in muonic atoms



Experiments at PSI by QUARTET collaboration

X-ray spectroscopy of light muonic atoms to get **charge radius** with unprecedented precision



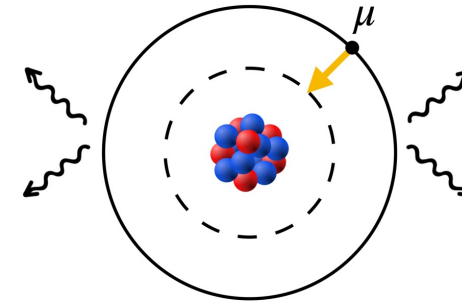
Ben Ohayon *et al.* MDPI Physics, 6(1):206–215, 2024.
Daniel Unger *et al.* J. Low Temp. Phys., 216(1-2):344–351, 2024.

The two-photon exchange nuclear correction – X-rays in muonic atoms

Radius extraction master formula

$$\delta_E = \delta_{\text{QED}} + \mathcal{C} r_c^2 + \delta_{\text{NS}}$$

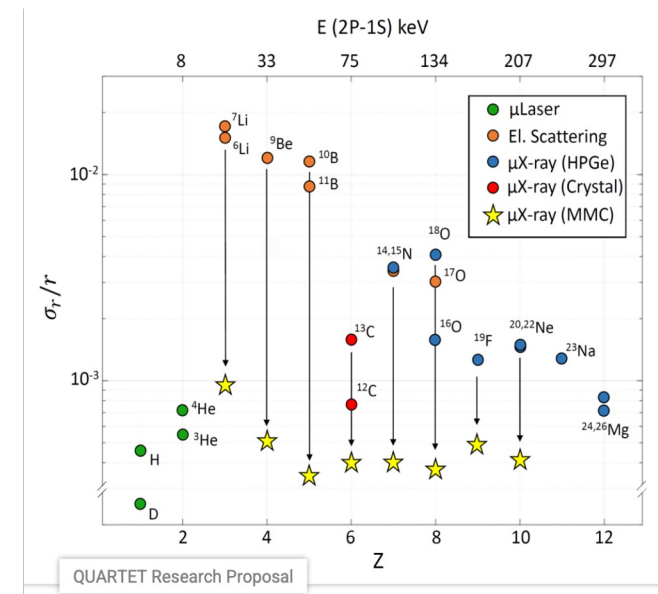
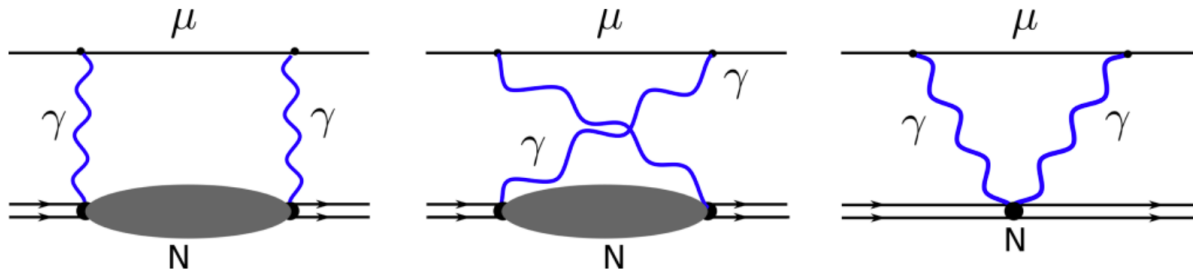
NS correction: $\delta_{\text{NS}} = \delta_{\text{TPE}} + \delta_{\text{3PE}} + \dots$



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Two photon polarizability contributions

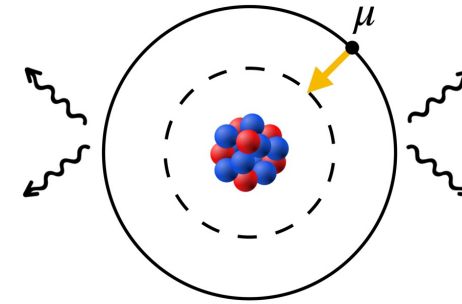


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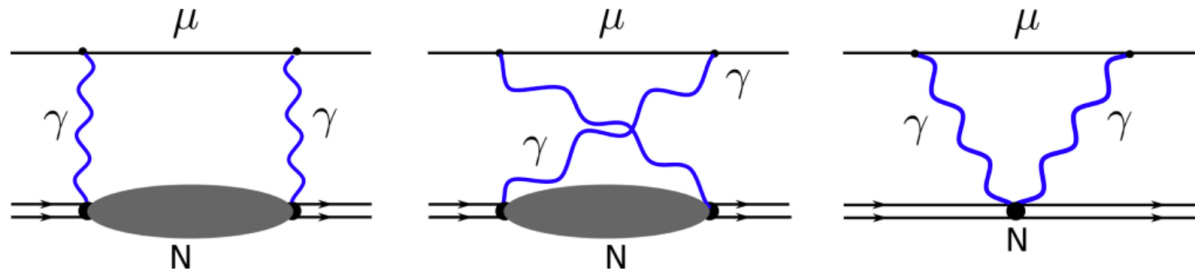
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Experiments at PSI by QUARTET collaboration

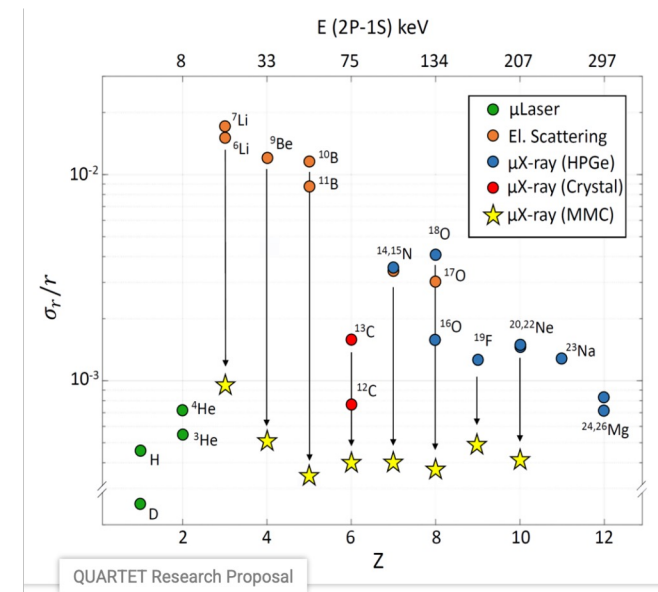
X-ray spectroscopy of light muonic atoms to get **charge radius** with unprecedented precision

Two photon polarizability contributions



$$\Delta E_{nS} = -\frac{(4\pi Z\alpha)}{m_r} |\phi_{nS}(0)|^2 \text{Im} \int \frac{d^4 q}{(2\pi)^4} D^{\mu\rho}(q) D^{\nu\tau}(-q) t_{\mu\nu}(q, k) T_{\rho\tau}(q, -q)$$

[Bernabeu et al, Nuclear Physics A (1974)] [Rosenfelder Nuclear Physics A (1983)]



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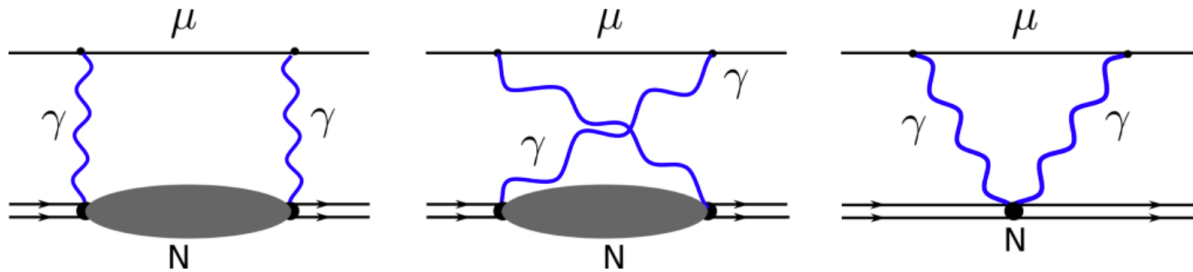
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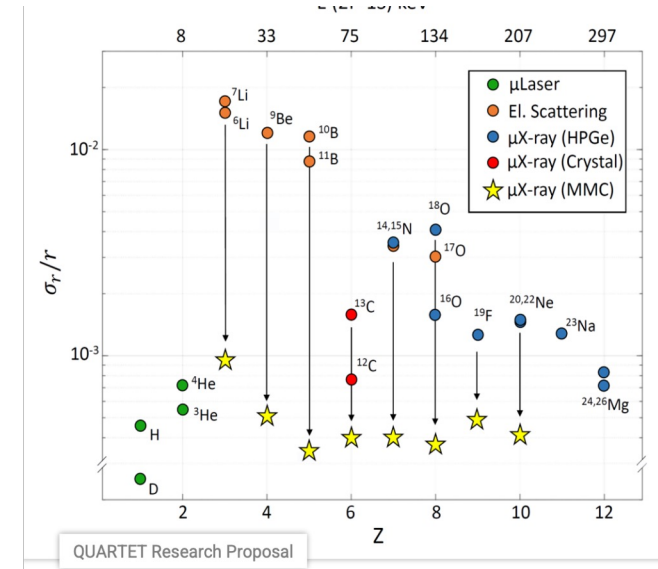


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[Bernabeu et al, Nuclear Physics A (1974)] [Rosenfelder Nuclear Physics A (1983)]

Hadronic tensor [Friar, Annals of Physics (1976)]

$$T_{\mu\nu}(q) = \delta_{\mu\nu} \left\langle \Psi \left| \int d^3 x e^{iq \cdot x} f_{SG}(x, 0) \right| \Psi \right\rangle + \sum_{N \neq 0} \left[\frac{\langle \Psi | J_\mu(0) | N \vec{q} \rangle \langle N \vec{q} | J_\nu(0) | \Psi \rangle}{E_0 - E_N + q_0 + i\epsilon} + \frac{\langle \Psi | J_\nu(0) | N - \vec{q} \rangle \langle N - \vec{q} | J_\mu(0) | \Psi \rangle}{E_0 - E_N - q_0 + i\epsilon} \right]$$



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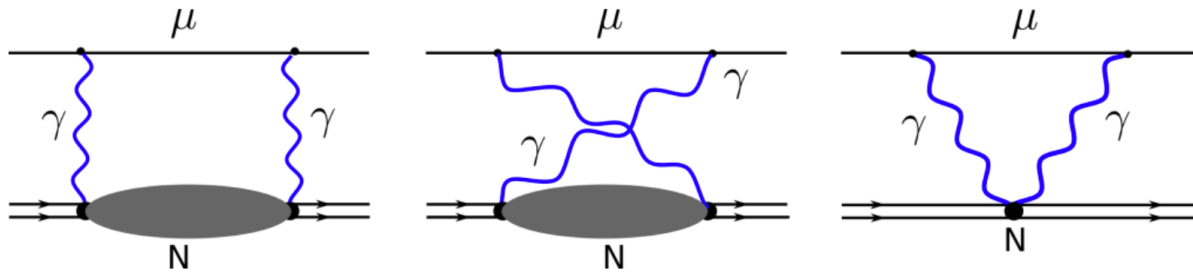
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Nuclear polarizability [Hernandez et al. PRC (2019)]

• TPE decomposition: $\delta_{\text{TPE}} = \delta_{\text{pol}}^A + \delta_{\text{pol}}^N + \delta_{\text{el}}$

• Multipole decomposition: $\delta_{\text{pol}}^A = \Delta_C + \Delta_{T,E} + \Delta_{T,M}$

$$\rightarrow \Delta_X \equiv \int d^3 q \int d\omega K_X(\omega, q) S_X(\omega, q)$$

• Response functions:

$$\rightarrow S_X(\omega, q) \equiv \sum_{J \geq 0} \sum_{N \neq 0} |\langle N | O_{X,J}(q) | \Psi \rangle|^2 \delta(E_N - E_0 - \omega)$$

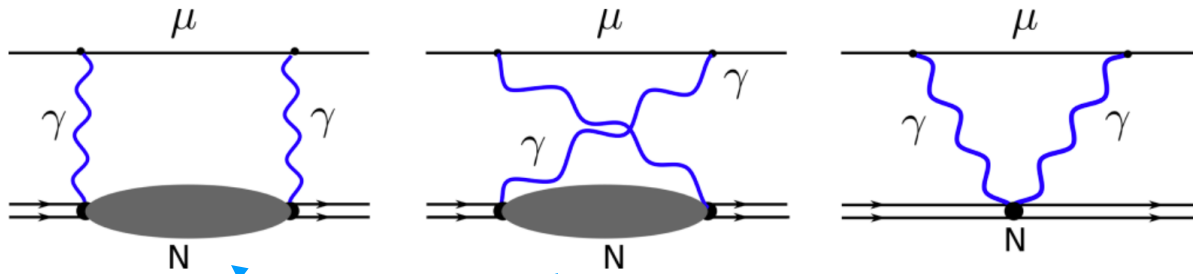
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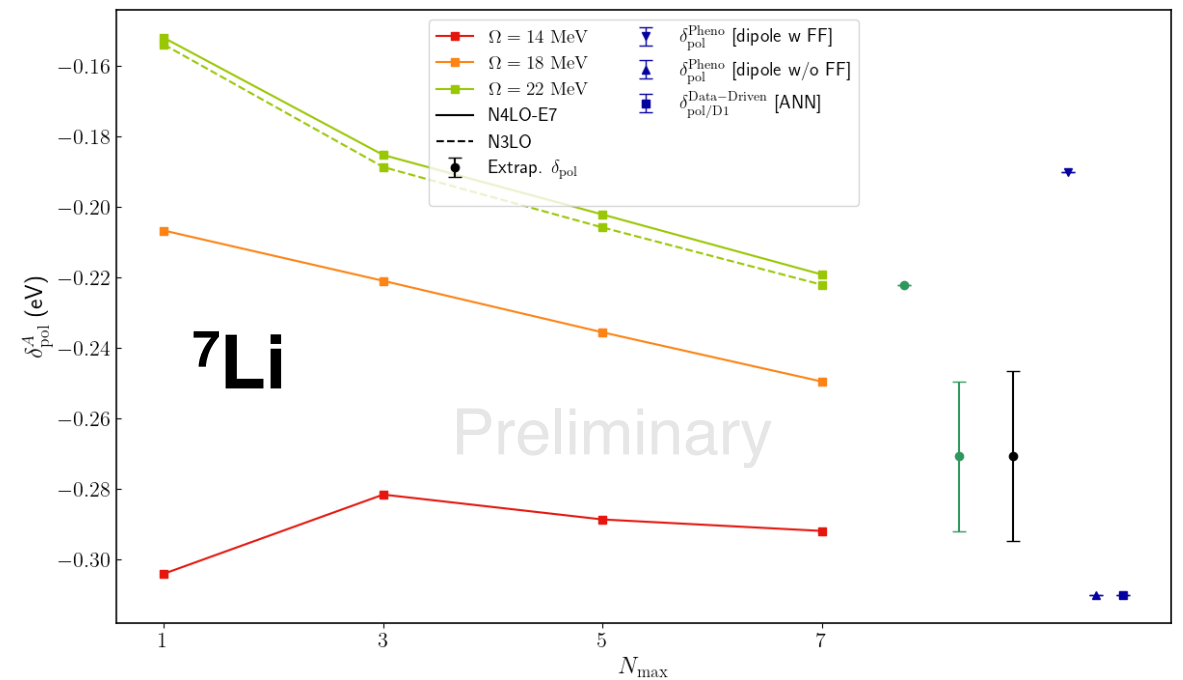
Two photon polarizability contributions



Nuclear Green's function (propagator)
→ Lanczos strength method

NCSM with Lanczos strength method
Input – chiral NN+3N forces

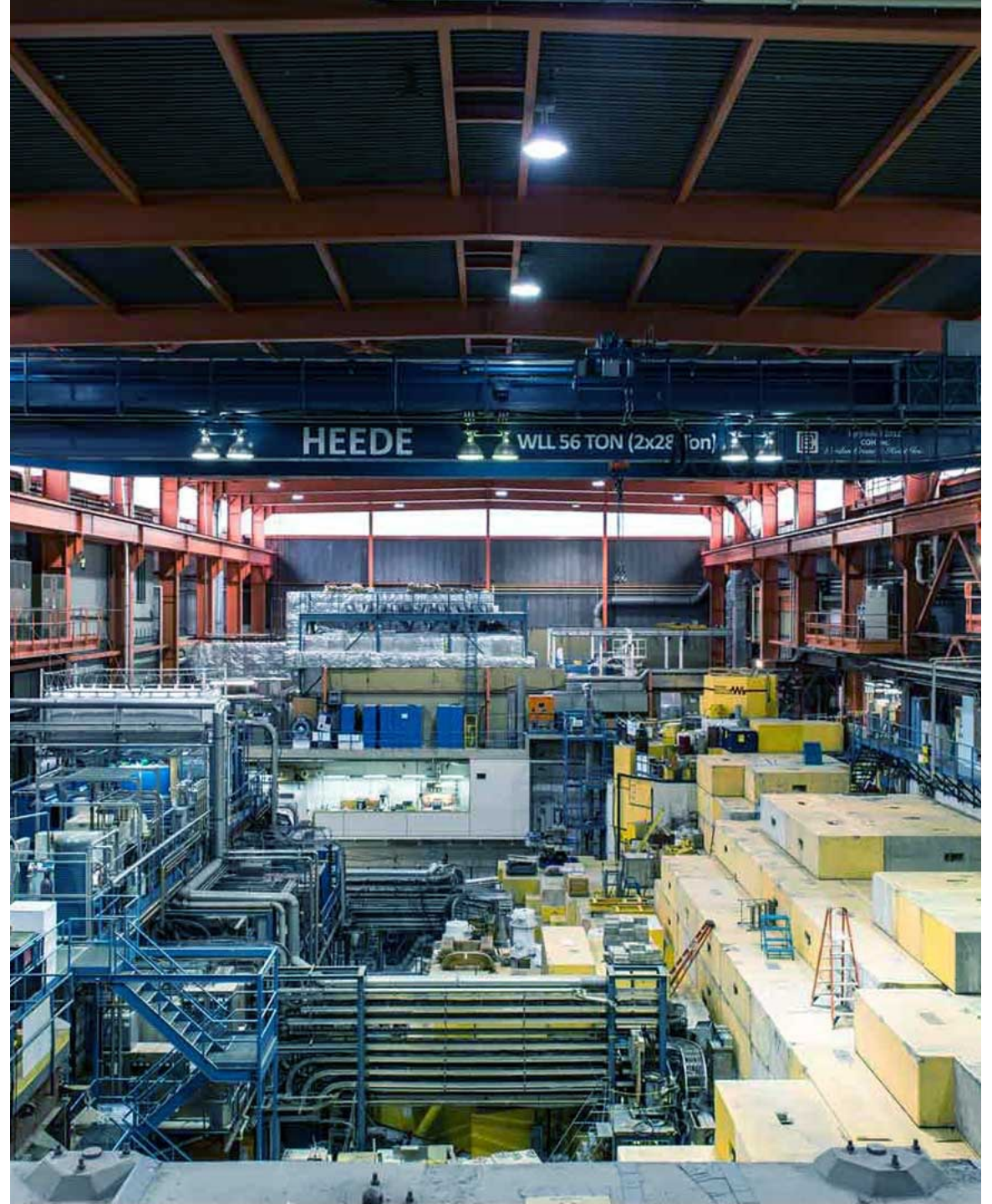
^7Li calculations led by Mehdi Drissi (TU Darmstadt)



Challenging calculations – δ_{pol}^A for ^6Li , ^9Be , $^{10,11}\text{B}$ in progress

Ab initio nuclear theory -
no-core shell model with
continuum (NCSMC)

2026-10-20



Ab initio calculations of structure including weakly bound halo states, scattering, reactions

Unified approach to bound & continuum states

40

No-Core Shell Model with Continuum (NCSMC)

$$\Psi^{(A)} = \sum_{\lambda} c_{\lambda} \left| \begin{array}{c} (A) \\ \text{cluster} \end{array}, \lambda \right\rangle + \sum_{\nu} \int d\vec{r} \gamma_{\nu}(\vec{r}) \hat{A}_{\nu} \left| \begin{array}{c} (A-a) \\ \text{cluster} \end{array}, \nu \right\rangle$$

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Phys. Scr. 91 (2016) 063002 (3pp) Physics Scripta
doi:10.1088/0031-8949/91/6/063002

Invited Comment

Unified *ab initio* approaches to nuclear structure and reactions

Petr Navrátil¹, Sofia Quaglioni², Guillaume Hupin^{3,4},
Carolina Romero-Redondo² and Angelo Calci¹

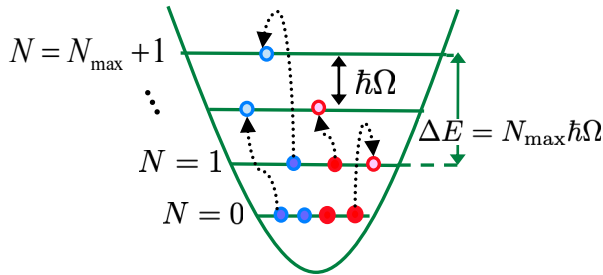
S. Baroni, P. Navratil, and S. Quaglioni,
PRL **110**, 022505 (2013); PRC **87**, 034326 (2013).

Ab initio calculations of structure including weakly bound halo states, scattering, reactions

Unified approach to bound & continuum states

41

No-Core Shell Model with Continuum (NCSMC)

$$\Psi^{(A)} = \underbrace{\sum_{\lambda} c_{\lambda} \left| \begin{matrix} (A) \\ \text{cluster} \end{matrix}, \lambda \right\rangle}_{\text{bound states}} + \sum_{\nu} \int d\vec{r} \gamma_{\nu}(\vec{r}) \hat{A}_{\nu} \left| \begin{matrix} (A-a) & (a) \\ \text{cluster} & \text{particle} \end{matrix}, \nu \right\rangle$$


Static solutions for aggregate system,
describe all nucleons close together

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Phys. Scr. 91 (2016) 063002 (3pp) doi:10.1088/0031-8949/91/6/063002

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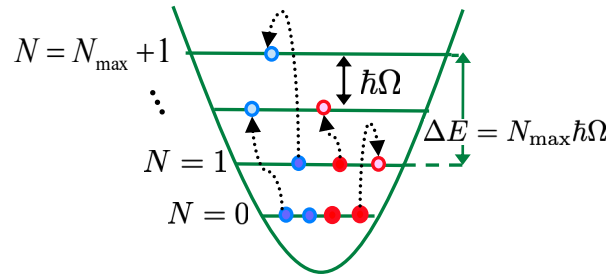
Ab initio calculations of structure including weakly bound halo states, scattering, reactions

Unified approach to bound & continuum states

42

No-Core Shell Model with Continuum (NCSMC)

$$\Psi^{(A)} = \underbrace{\sum_{\lambda} c_{\lambda} \left| \begin{array}{c} (A) \\ \text{cluster} \end{array}, \lambda \right\rangle}_{\text{Static solutions for aggregate system, describe all nucleons close together}} + \underbrace{\sum_{\nu} \int d\vec{r} \gamma_{\nu}(\vec{r}) \hat{A}_{\nu} \left| \begin{array}{c} (A-a) \\ \text{cluster} \end{array}, \nu \right\rangle}_{\text{Continuous microscopic cluster states, describe long-range projectile-target}}$$



Static solutions for aggregate system,
describe all nucleons close together

Continuous microscopic cluster states,
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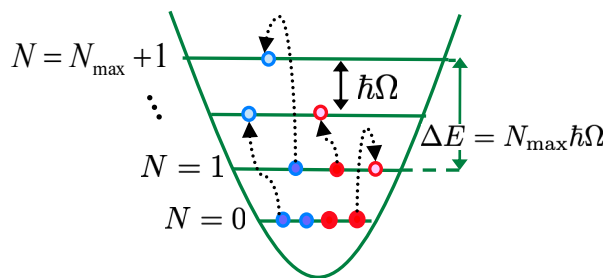
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Unified approach to bound & continuum states

43

No-Core Shell Model with Continuum (NCSMC)

$$\Psi^{(A)} = \underbrace{\sum_{\lambda} c_{\lambda} \left| \begin{array}{c} (A) \\ \text{NCSM} \end{array}, \lambda \right\rangle}_{\text{Static solutions for aggregate system, describe all nucleons close together}} + \underbrace{\sum_{\nu} \int d\vec{r} \gamma_{\nu}(\vec{r}) \hat{A}_{\nu} \left| \begin{array}{c} \text{NCSM} \\ (A-a) \quad (a) \end{array}, \nu \right\rangle}_{\text{Continuous microscopic cluster states, describe long-range projectile-target}}$$



Static solutions for aggregate system, describe all nucleons close together

Continuous microscopic cluster states, describe long-range projectile-target

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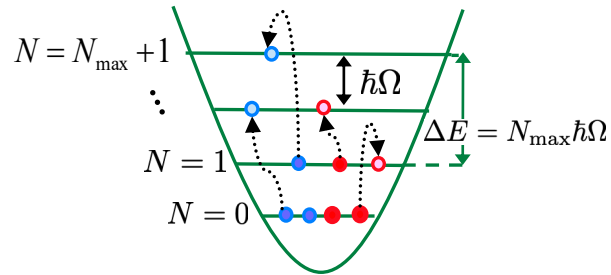
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44

No-Core Shell Model with Continuum (NCSMC)

$$\Psi^{(A)} = \underbrace{\sum_{\lambda} c_{\lambda} \left| \begin{array}{c} (A) \\ \text{cluster} \end{array}, \lambda \right\rangle}_{\text{Unknowns}} + \underbrace{\sum_{\nu} \int d\vec{r} \gamma_{\nu}(\vec{r}) \hat{A}_{\nu} \left| \begin{array}{c} (A-a) \\ \text{cluster} \end{array}, \nu \right\rangle}_{\text{Unknowns}}$$



Continuous microscopic cluster states, describe long-range projectile-target

Static solutions for aggregate system, describe all nucleons close together

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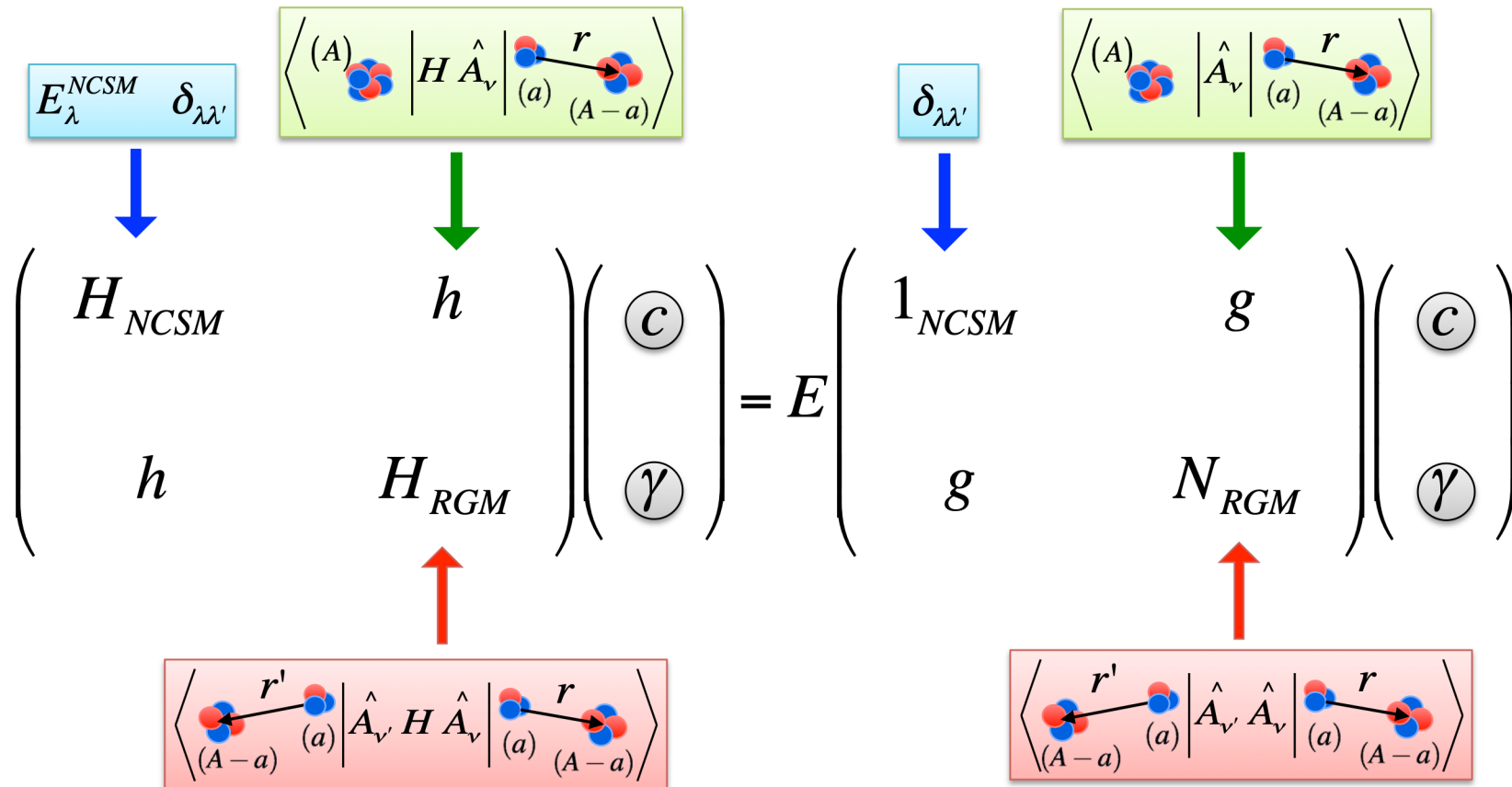
S. Baroni, P. Navratil, and S. Quaglioni,
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Coupled NCSMC equations

45

$$H \Psi^{(A)} = E \Psi^{(A)}$$

$$\Psi^{(A)} = \sum_{\lambda} c_{\lambda} \left| \begin{array}{c} (A) \\ \text{cluster} \end{array}, \lambda \right\rangle + \sum_{\nu} \int d\vec{r} \gamma_{\nu}(\vec{r}) \hat{A}_{\nu} \left| \begin{array}{c} (A-a) \\ \text{cluster} \end{array}, \nu \right\rangle$$



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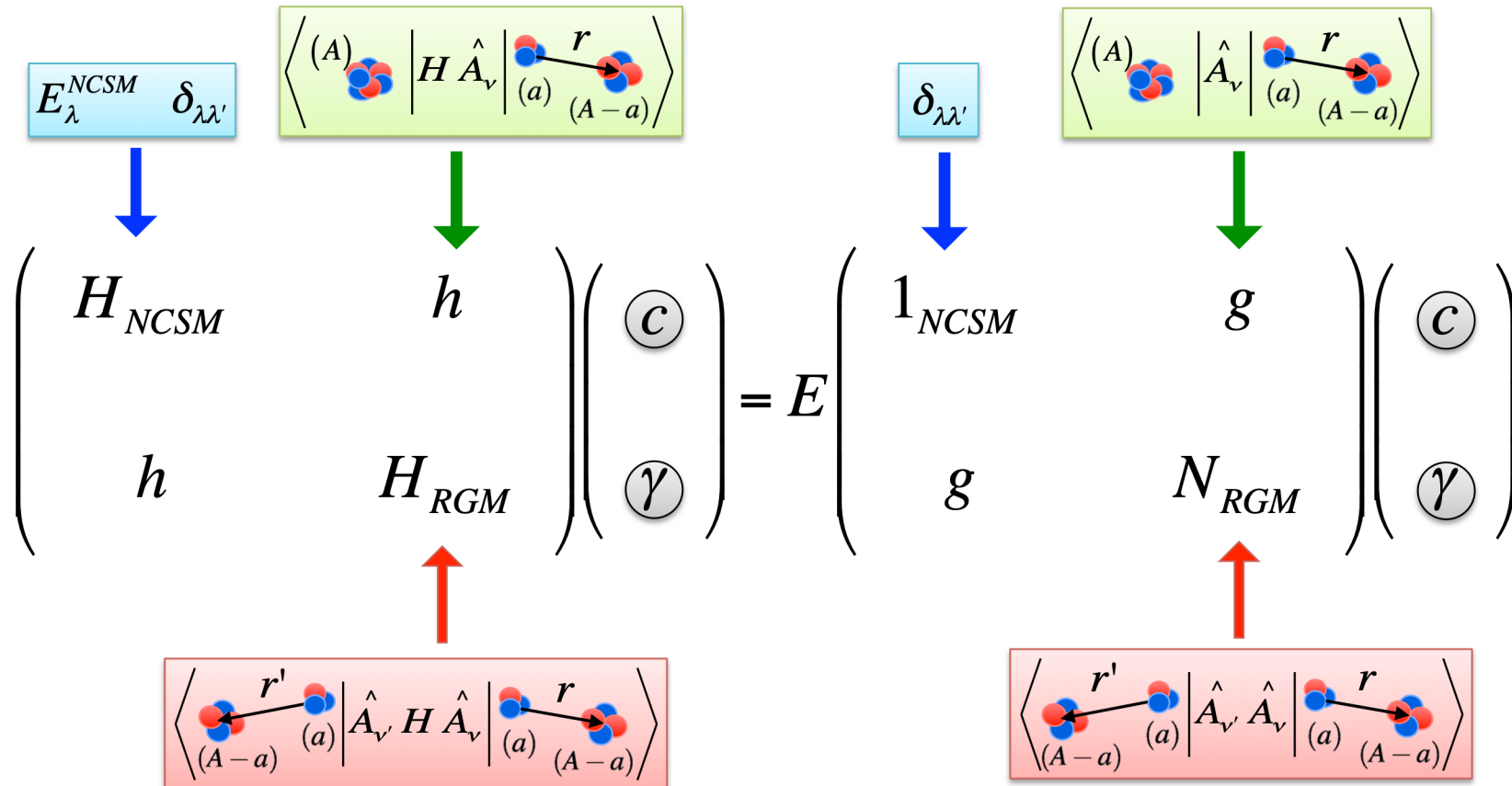
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Bound state $\gamma_{\nu}(r) \sim C_{\nu} W(k_{\nu}r)$

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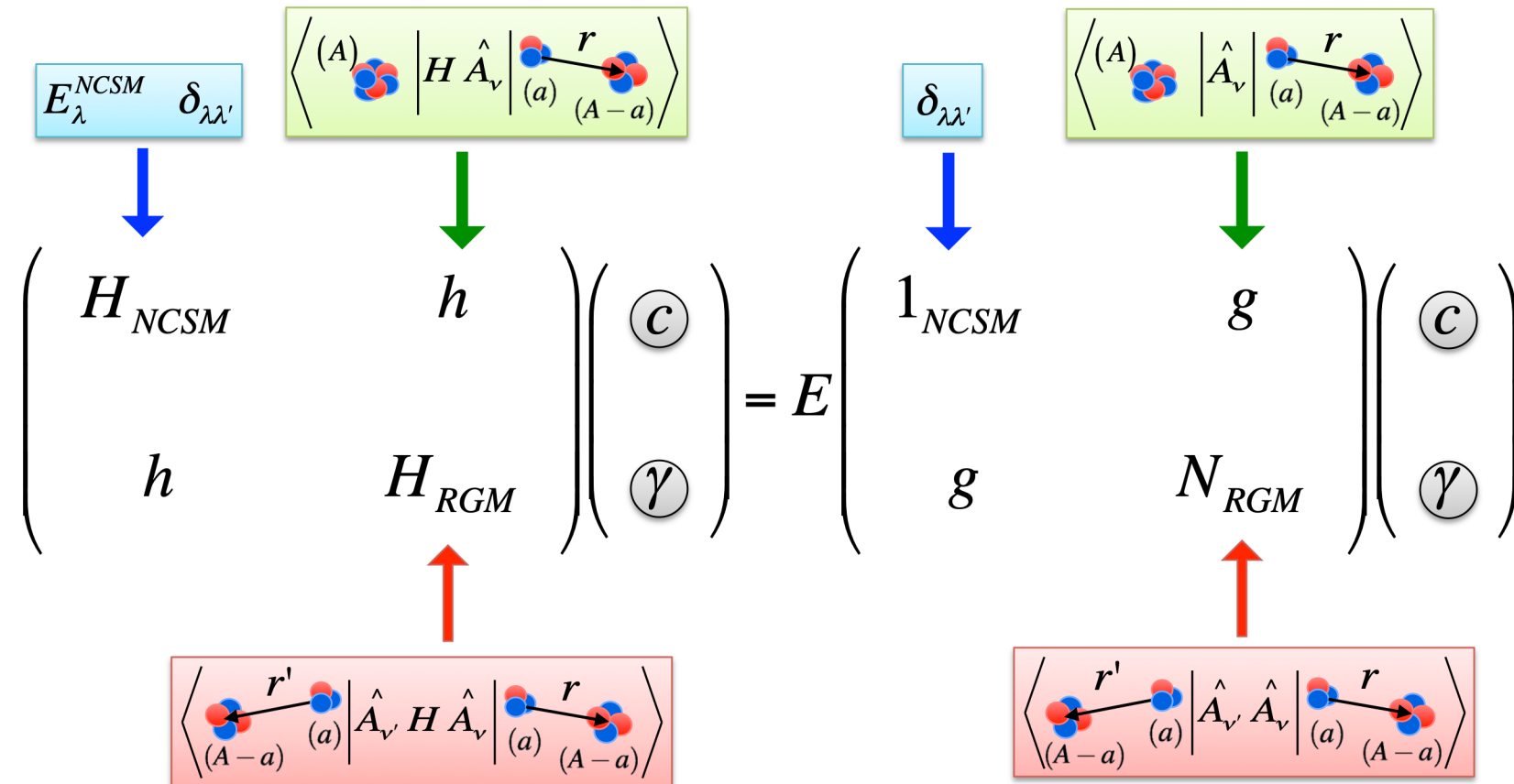
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Scattering state $\gamma_{\nu}(r) \sim \delta_{\nu i} I(k_{\nu} r) - S_{\nu i} O(k_{\nu} r)$

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Unified *ab initio* approaches to nuclear structure and reactions

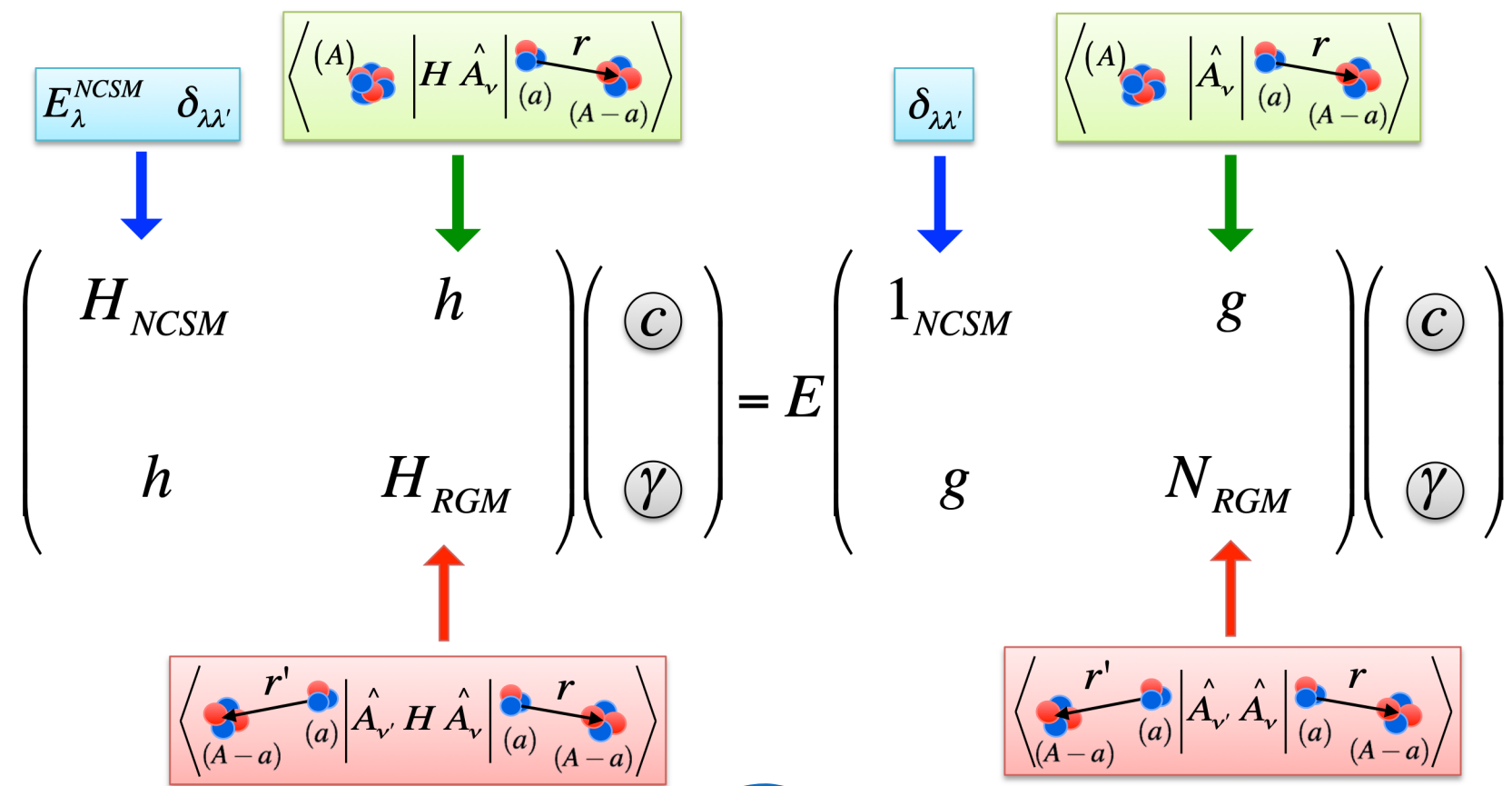
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Scattering state $\gamma_{\nu}(r) \sim \delta_{\nu i} I(k_{\nu} r) - S_{\nu i} O(k_{\nu} r)$ Scattering matrix

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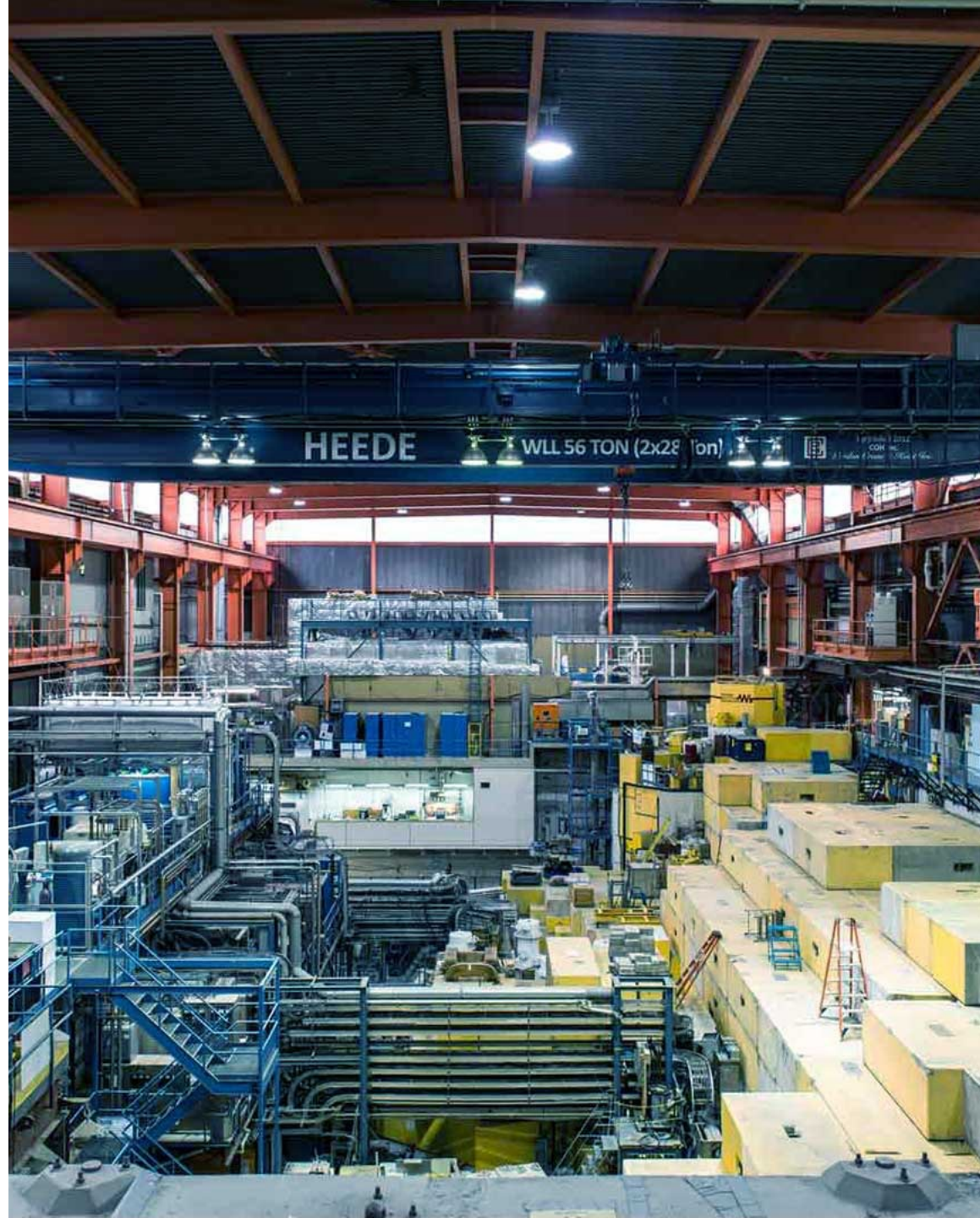
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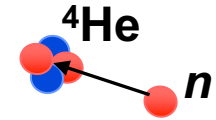
S. Baroni, P. Navratil, and S. Quaglioni,
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Nucleon- ^4He scattering

2026-10-20

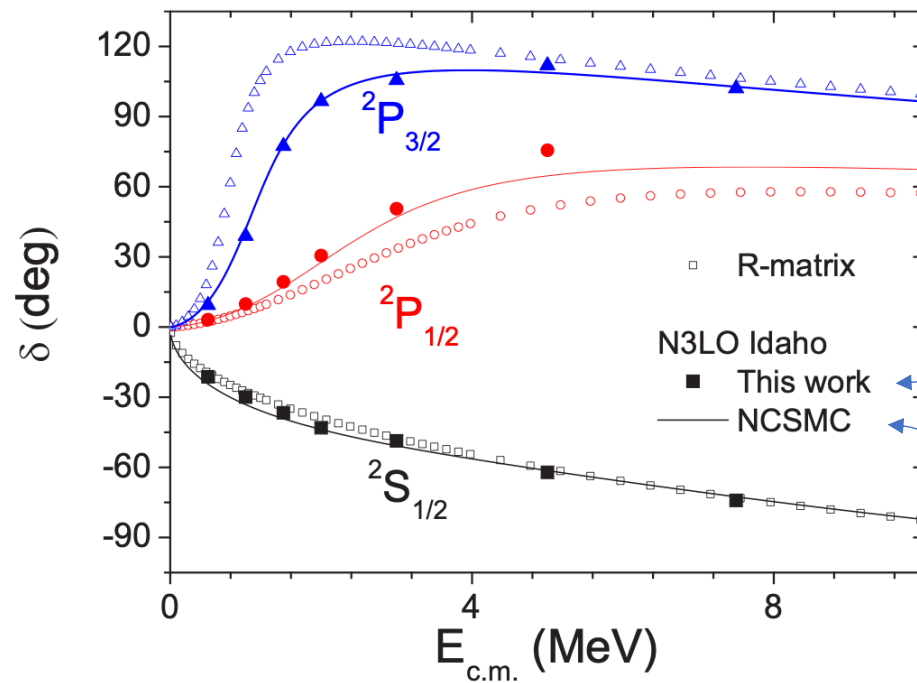


n - ^4He scattering within NCSMC



50

n - ^4He scattering phase shifts from chiral N^3LO NN interaction



Benchmark:
NCSMC vs. Faddeev-Yakubovsky method - Rimantas Lazauskas

PHYSICAL REVIEW C **97**, 044002 (2018)

Editors' Suggestion

Solution of the n - ^4He elastic scattering problem using the Faddeev-Yakubovsky equations

Rimantas Lazauskas*

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Phys. Scr. **00** (2016) 000000 (37pp)

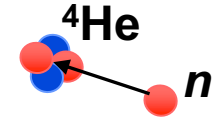
Physica Scripta

Invited Comment

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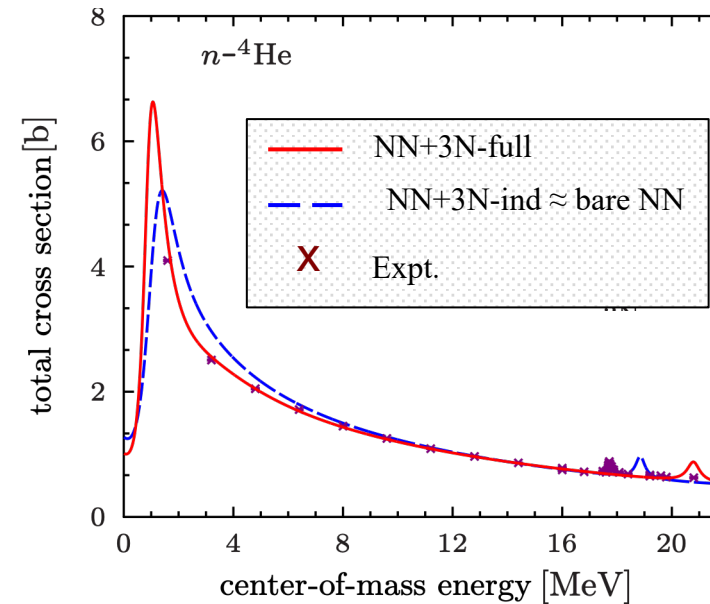
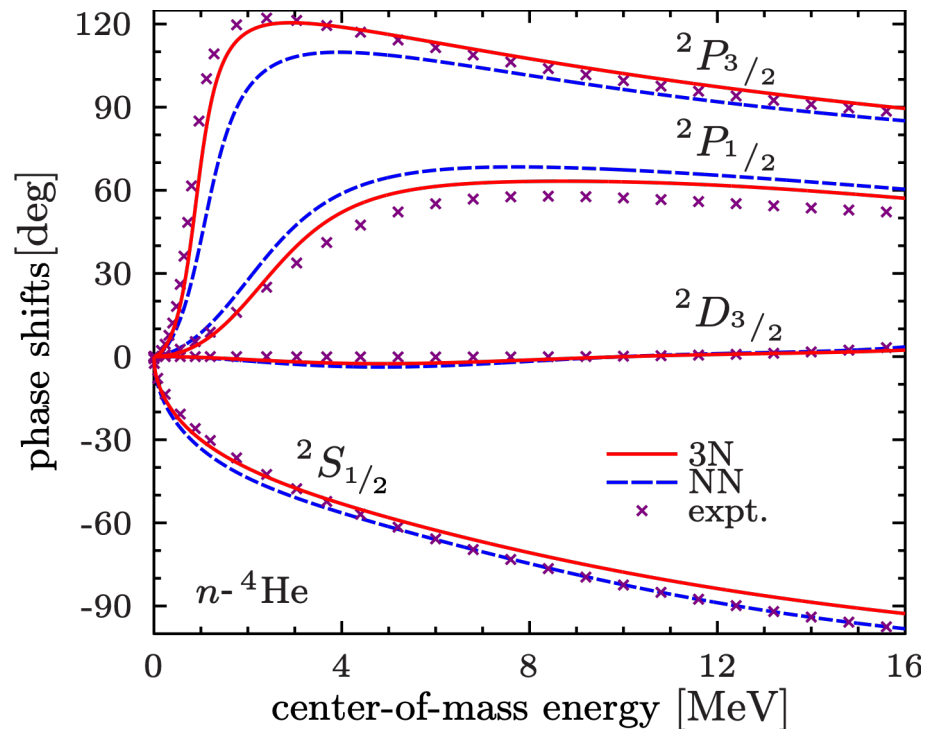
n - ^4He scattering within NCSMC



51

n - ^4He scattering phase shifts from
chiral NN and NN+3N500 potential

Total n - ^4He cross section with NN and NN+3N potentials



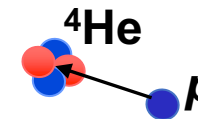
3N force enhances
 $1/2^- \leftrightarrow 3/2^-$
splitting: Essential at
low energies!

PHYSICAL REVIEW C **88**, 054622 (2013)

Ab initio many-body calculations of nucleon- ^4He scattering with three-nucleon forces

Guillaume Hupin,^{1,*} Joachim Langhammer,^{2,†} Petr Navrátil,^{3,‡} Sofia Quaglioni,^{1,§} Angelo Calci,^{2,||} and Robert Roth^{2,¶}

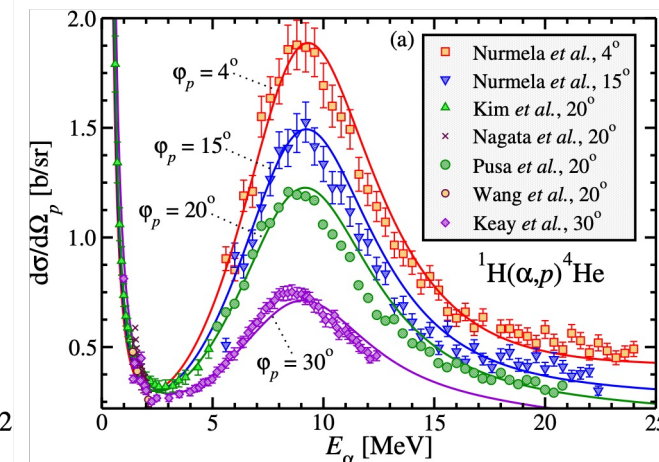
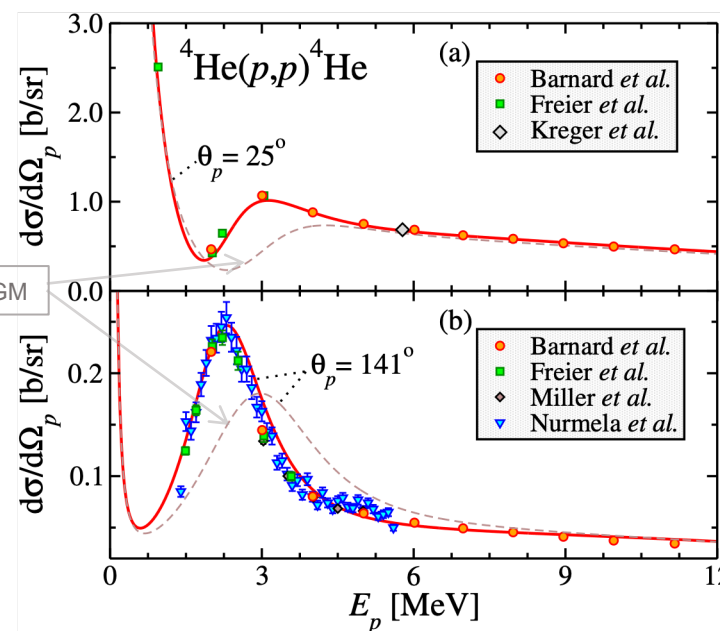
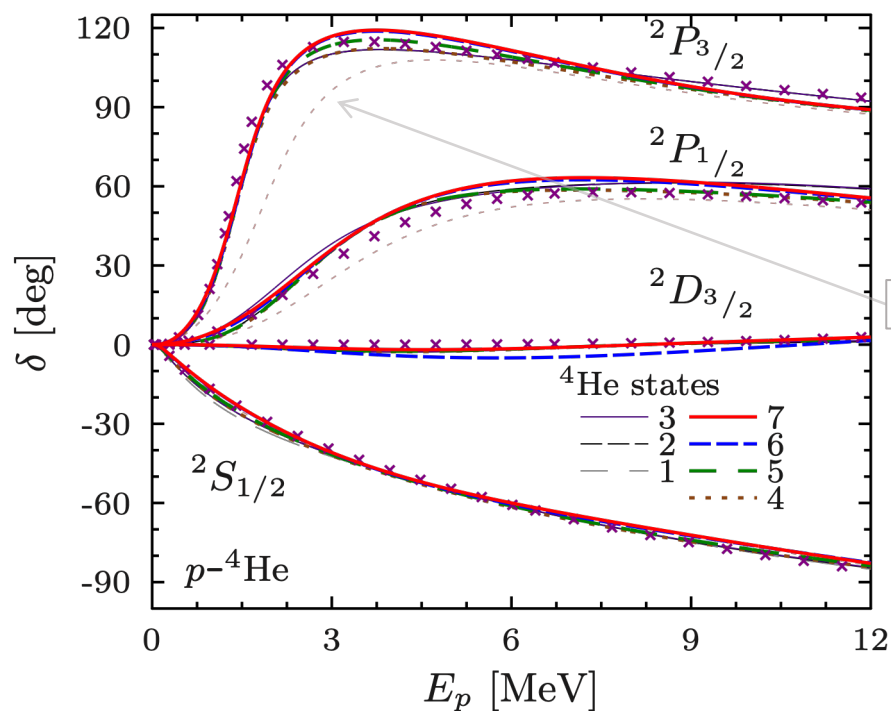
p-⁴He scattering within NCSMC



52

p-⁴He scattering phase shifts from NN+3N500 potential:
Convergence

Differential p-⁴He cross section with NN+3N potentials



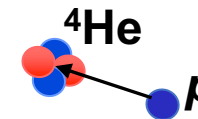
PHYSICAL REVIEW C **90**, 061601(R) (2014)

Predictive theory for elastic scattering and recoil of protons from ⁴He

Guillaume Hupin,^{1,*} Sofia Quaglioni,^{1,†} and Petr Navrátil^{2,‡}

Predictive power in the 3/2⁻ resonance region:
Applications to material science

p-⁴He scattering within NCSMC



53

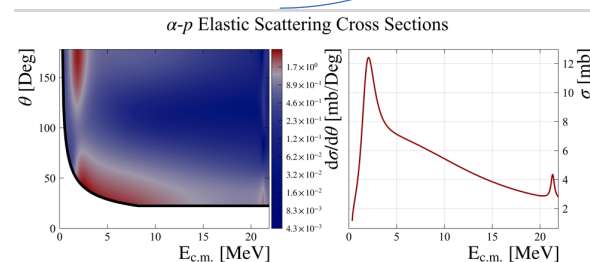
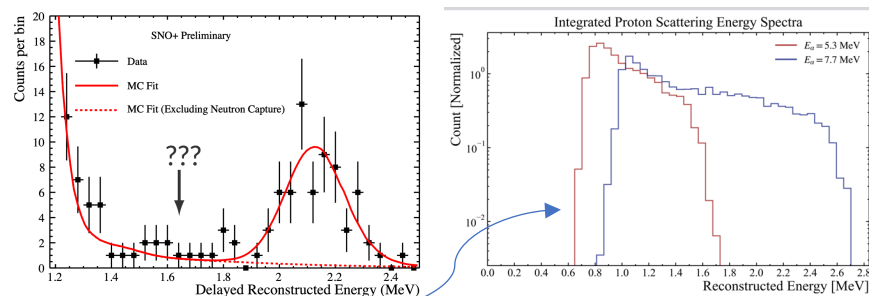
The NCSMC ⁴He(p,p) differential cross sections used by SNO+ collaboration for their background model

Differential p-⁴He cross section with NN+3N potentials

An Alpha-Proton Scattering Model for SNO+ Background Characterization

David Drobner^{1,2}, Joshua Klein¹, Serena Riccetto² and Alexander Wright² (for the SNO+ Collaboration)

¹University of Pennsylvania, ²Queen's University

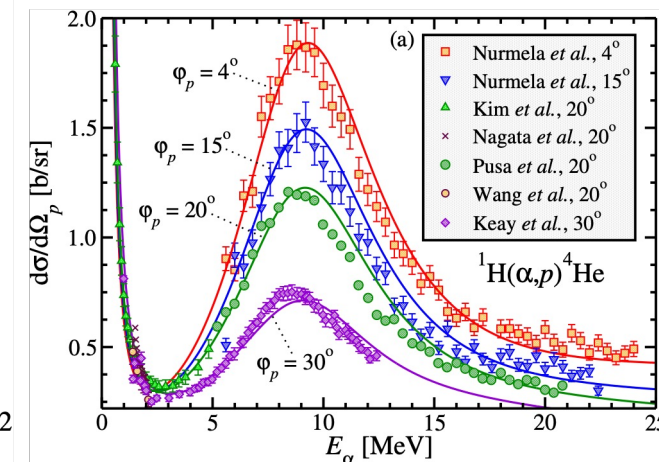
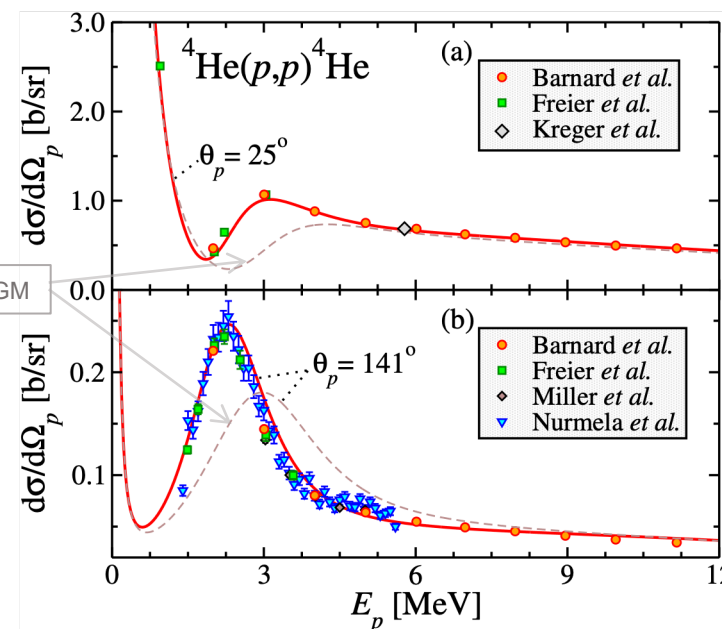


When incorporated into the background model, these spectra improve the agreement of the model with detector data.

PHYSICAL REVIEW C **90**, 061601(R) (2014)

Predictive theory for elastic scattering and recoil of protons from ⁴He

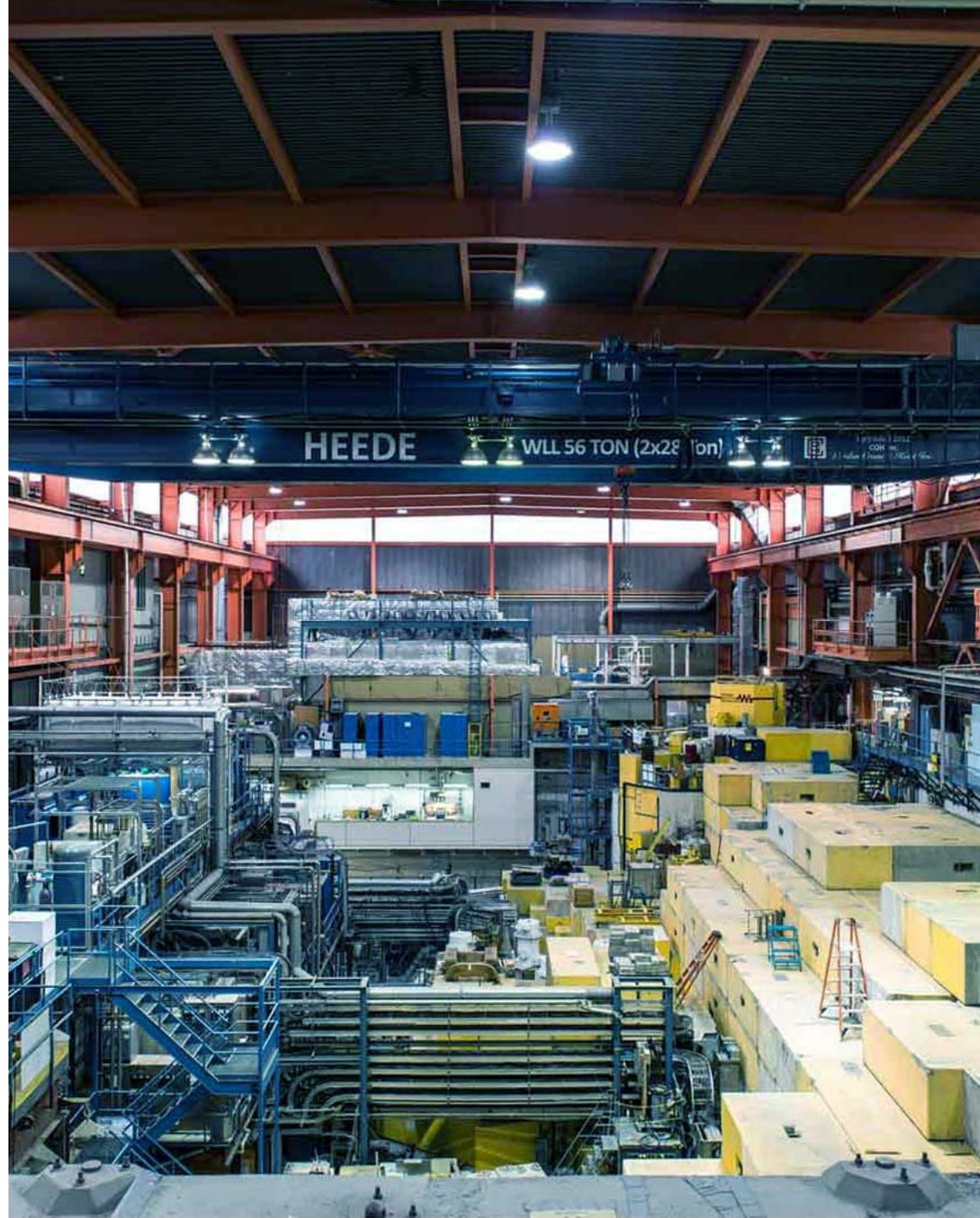
Guillaume Hupin,^{1,*} Sofia Quaglioni,^{1,†} and Petr Navrátil^{2,‡}



Predictive power in the 3/2⁻ resonance region:
Applications to material science

DT fusion

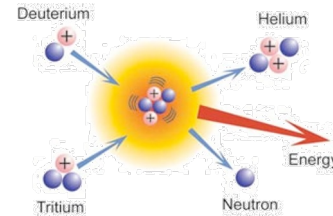
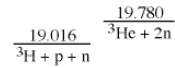
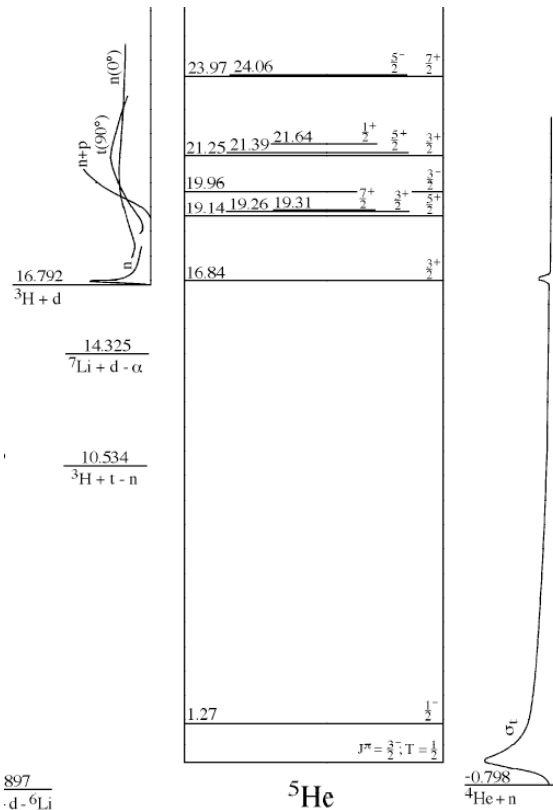
2026-10-20



Deuterium-Tritium fusion

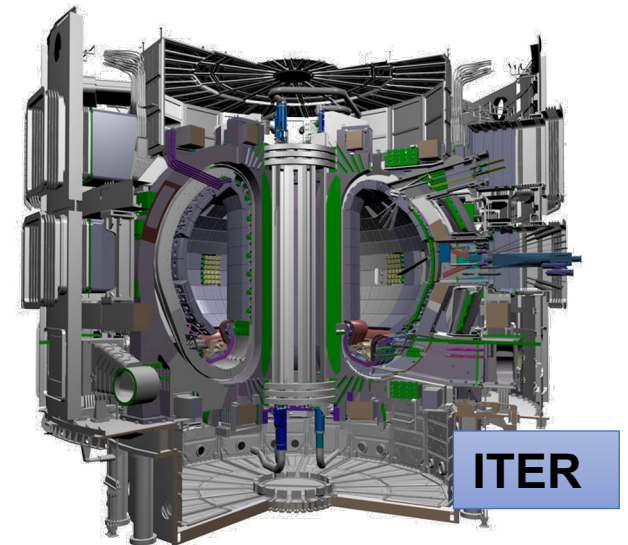
55

- The $d+{}^3\text{H}\rightarrow n+{}^4\text{He}$ reaction
 - The most promising to produce fusion energy in the near future
 - Used to achieve inertial-confinement (laser-induced) fusion at NIF, and magnetic-confinement fusion at ITER
 - With its mirror reaction, ${}^3\text{He}(d,p){}^4\text{He}$, important for Big Bang nucleosynthesis



Resonance at $E_{\text{cm}}=48$ keV ($E_d=105$ keV)
in the $J=3/2^+$ channel
Cross section at the peak: 4.88 b

17.64 MeV energy released:
14.1 MeV neutron and 3.5 MeV alpha



ITER

NCSMC calculation of the DT fusion

$$|\Psi\rangle = \sum_{\lambda} c_{\lambda} \left| \begin{array}{c} \text{He} \\ \text{5} \end{array}, \lambda \right\rangle + \int d\vec{r} u_{\nu_{DT}}(\vec{r}) \hat{A}_{DT} \left| \begin{array}{c} \text{D} \\ \text{T} \end{array}, \nu_{DT} \right\rangle + \int d\vec{r} u_{\nu_{n\alpha}}(\vec{r}) \hat{A}_{n\alpha} \left| \begin{array}{c} n \\ \alpha \end{array}, \nu_{n\alpha} \right\rangle$$

- 2x7 static ^5He eigenstates computed with the NCSM
- Continuous D-T(g.s.) cluster states (entrance channel)
 - Including positive-energy eigenstates of D to account for distortion
- Continuous n- ^4He (g.s.) cluster states (exit channel)
- Chiral NN $\text{N}^3\text{LO} + 3\text{N}(500)$ interaction



ARTICLE

<https://doi.org/10.1038/s41467-019-08052-6> OPEN

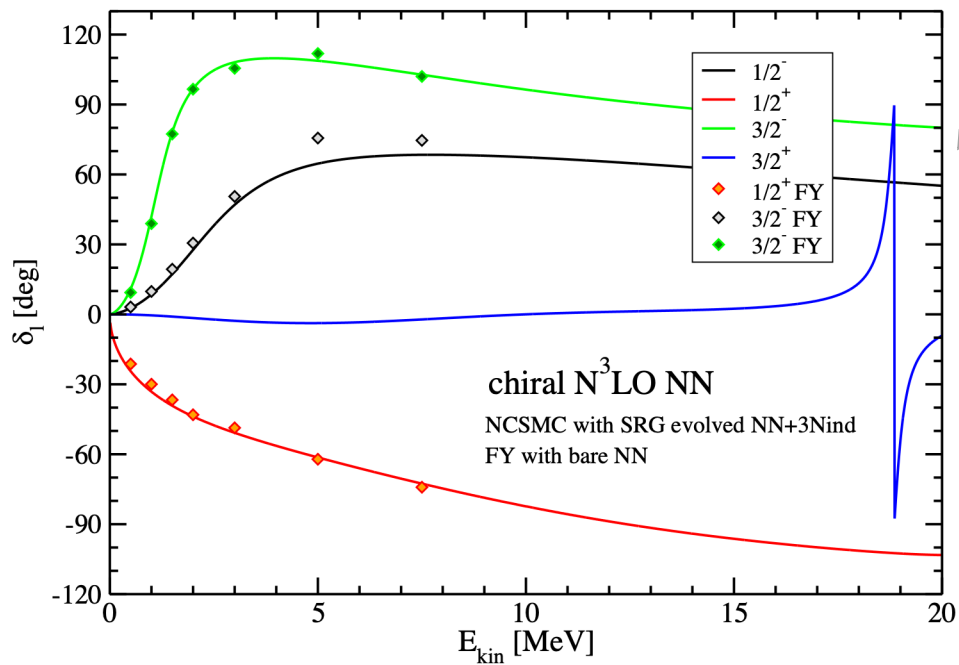
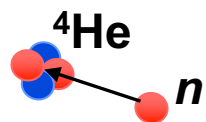
Ab initio predictions for polarized deuterium-tritium thermonuclear fusion

Guillaume Hupin^{1,2,3}, Sofia Quaglioni³ & Petr Navrátil⁴

n - ^4He scattering and $^3\text{H}+d$ fusion within NCSMC

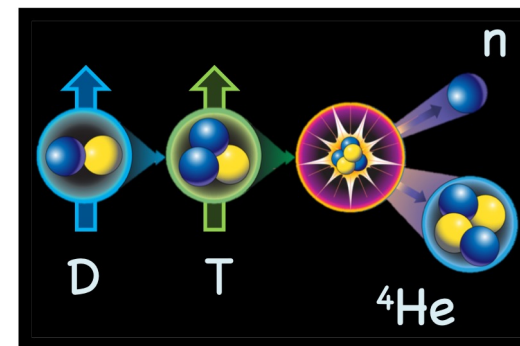
57

n - ^4He and $d+^3\text{H}$ scattering phase-shifts

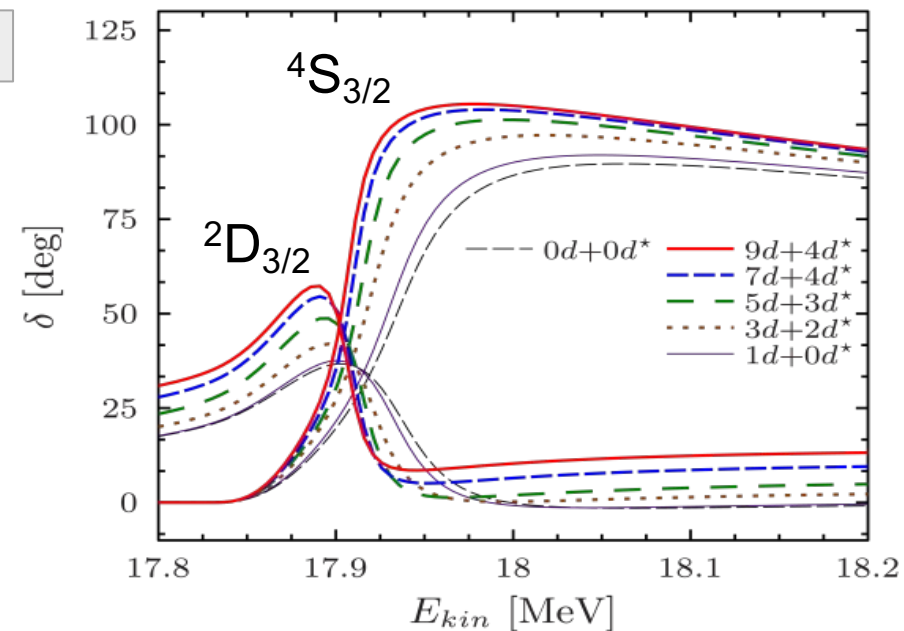


FY: Faddeev-Yakubovsky method - Rimantas Lazauskas

$^4\text{He}+n$

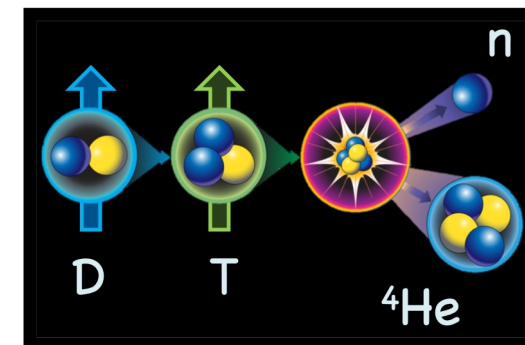


$^4\text{He}+n \leftrightarrow ^3\text{H}+d$



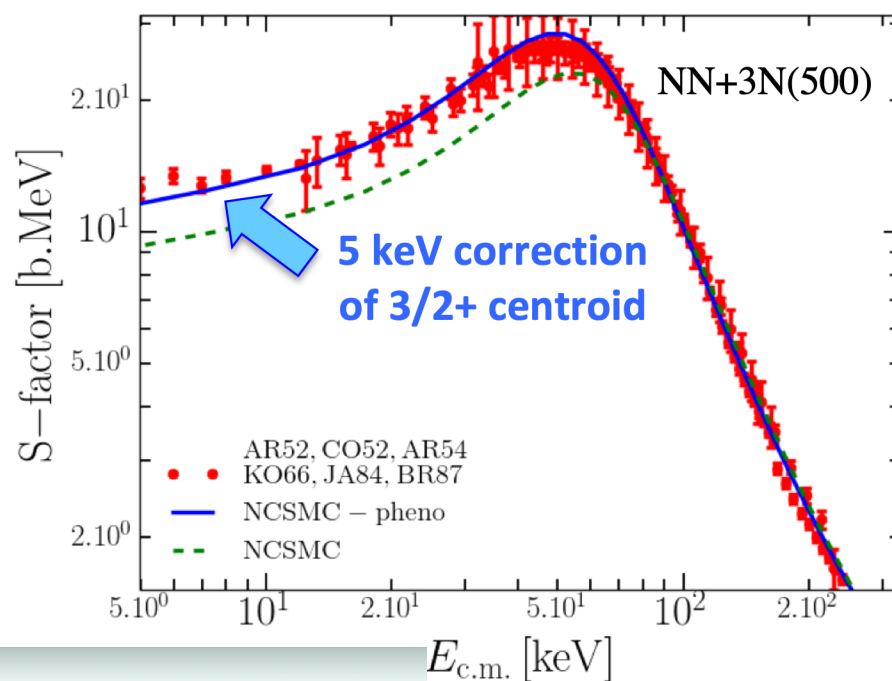
The d - ^3H fusion takes place through a transition of $d+^3\text{H}$ is S -wave to $n+^4\text{He}$ in D -wave: Importance of the **tensor** and **3N** force

$^3\text{H}(d,n)^4\text{He}$ with chiral NN $\text{N}^3\text{LO} + 3\text{N}(500)$ interaction



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Astrophysical S-factor



Fusion cross section

$$\sigma(E) = \frac{S(E)}{E} \exp\left(-\frac{2\pi Z_1 Z_2 e^2}{\hbar \sqrt{2E/m}}\right)$$

Astrophysical S-factor: nuclear contribution

'Coulomb' Contribution (tunneling)



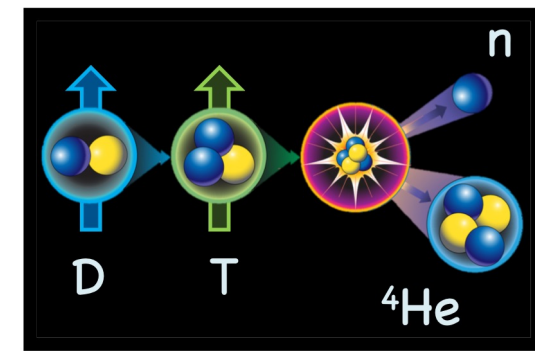
ARTICLE

<https://doi.org/10.1038/s41467-018-08052-6> OPEN

Ab initio predictions for polarized deuterium-tritium thermonuclear fusion

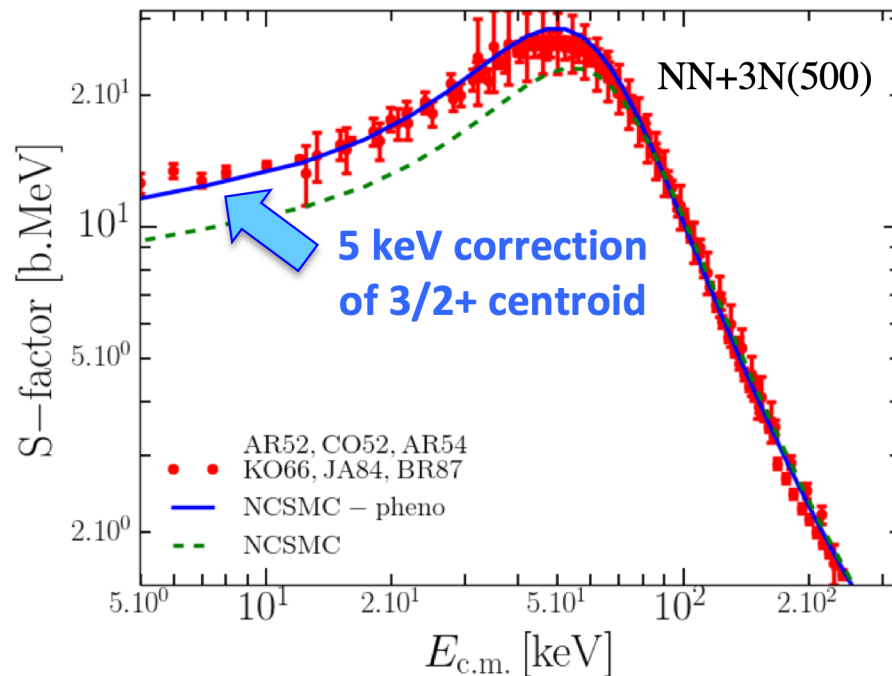
Guillaume Hupin^{1,2,3}, Sofia Quaglioni³ & Petr Navrátil⁴

$^3\text{H}(d,n)^4\text{He}$ with chiral NN $\text{N}^3\text{LO} + 3\text{N}(500)$ interaction



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Astrophysical S-factor



Assuming the fusion proceeds only in S-wave
with spins of D and T completely aligned:
Polarized cross section 50% higher than unpolarized

- While the DT fusion rate has been measured extensively, a fundamental understanding of the process is still missing
- Very little is known experimentally of how the polarization of the reactants' spins affects the reaction

$$\sigma_{unpol} = \sum_J \frac{2J+1}{(2I_D+1)(2I_T+1)} \sigma_J$$

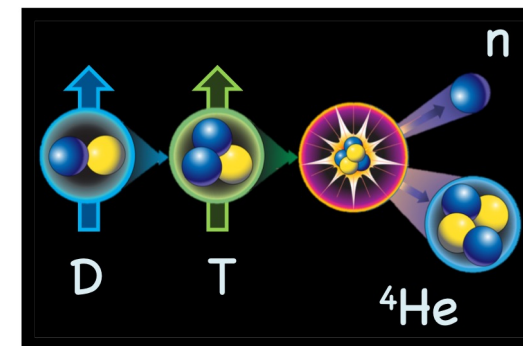
$$\approx \frac{1}{3} \cancel{\sigma_{\frac{1}{2}}} + \frac{2}{3} \sigma_{\frac{3}{2}}$$



$$\sigma_{pol} \approx 1.5 \sigma_{unpol}$$

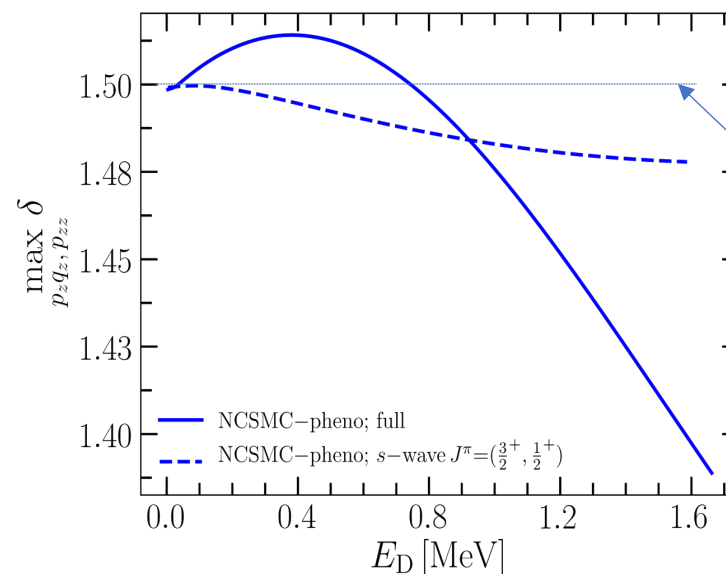
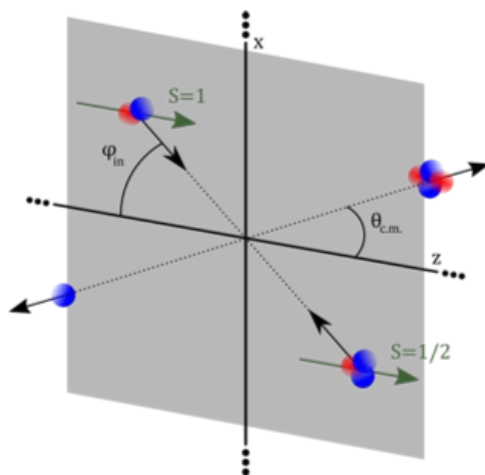
$^3\text{H}(d,n)^4\text{He}$ with chiral NN $\text{N}^3\text{LO} + 3\text{N}(500)$ interaction

Polarized fusion



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$$\frac{\partial \sigma_{pol}}{\partial \Omega_{c.m.}}(\theta_{c.m.}) = \frac{\partial \sigma_{unpol}}{\partial \Omega_{c.m.}}(\theta_{c.m.}) \left(1 + \frac{1}{2} p_{zz} A_{zz}^{(b)}(\theta_{c.m.}) + \frac{3}{2} p_z q_z C_{z,z}(\theta_{c.m.}) \right)$$

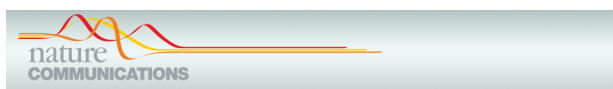


$$\sigma_{unpol} = \sum_J \frac{2J+1}{(2I_D+1)(2I_T+1)} \sigma_J$$

$$\approx \frac{1}{3} \sigma_{\frac{1}{2}} + \frac{2}{3} \sigma_{\frac{3}{2}}$$

↓

$$\sigma_{pol} \approx 1.5 \sigma_{unpol}$$



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<https://doi.org/10.1038/s41467-019-08052-6>

OPEN

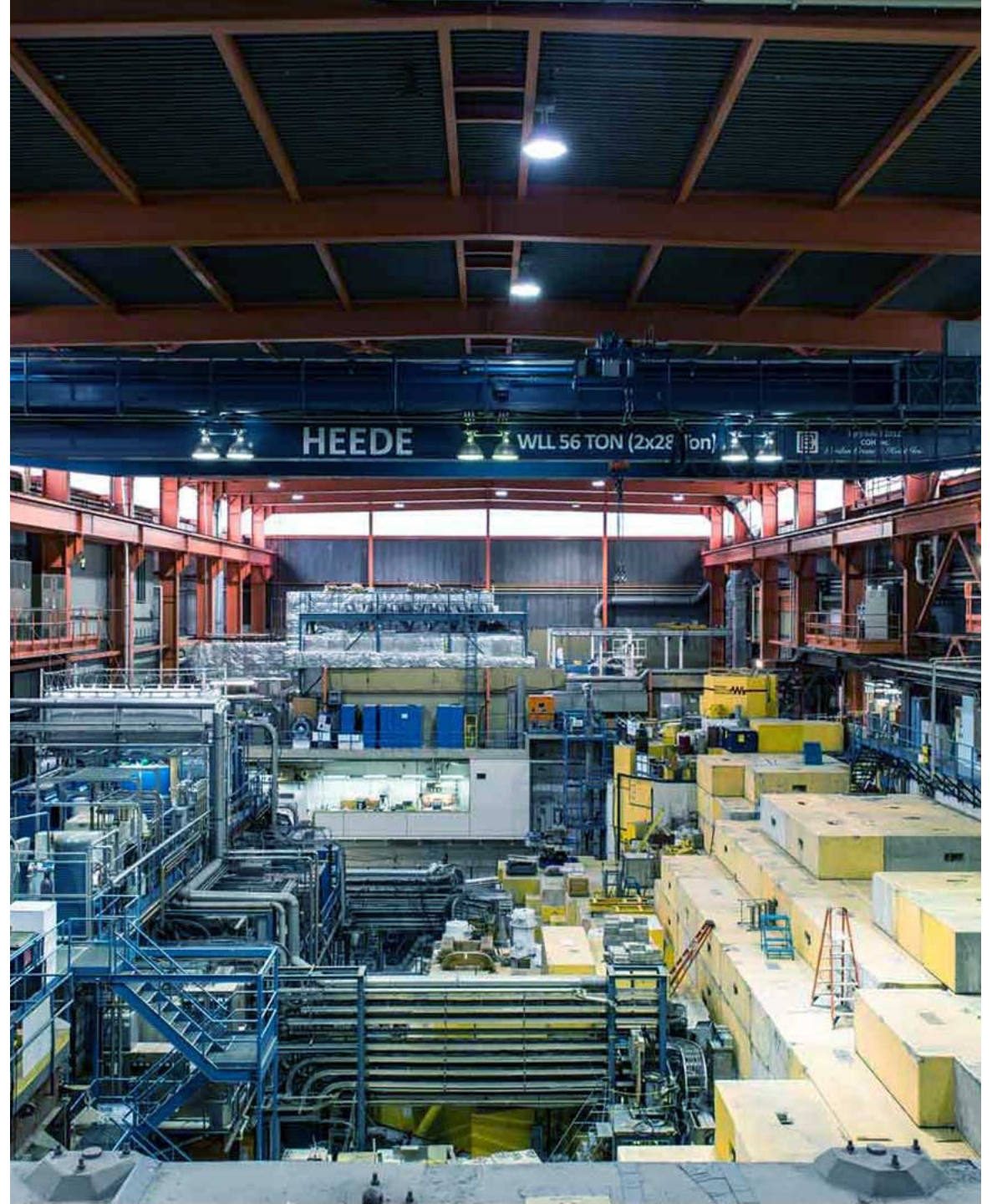
Ab initio predictions for polarized deuterium-tritium thermonuclear fusion

Guillaume Hupin^{1,2,3}, Sofia Quaglioni³ & Petr Navrátil⁴

NCSMC calculation demonstrates impact of partial waves with $l > 0$ as well as the contribution of $l = 0$ $J^\pi = \frac{1}{2}^+$ channel

Nuclear structure of ${}^6\text{Li}$ & radiative capture of deuterons on ${}^4\text{He}$

2026-10-20



Nuclear structure of ${}^6\text{Li}$

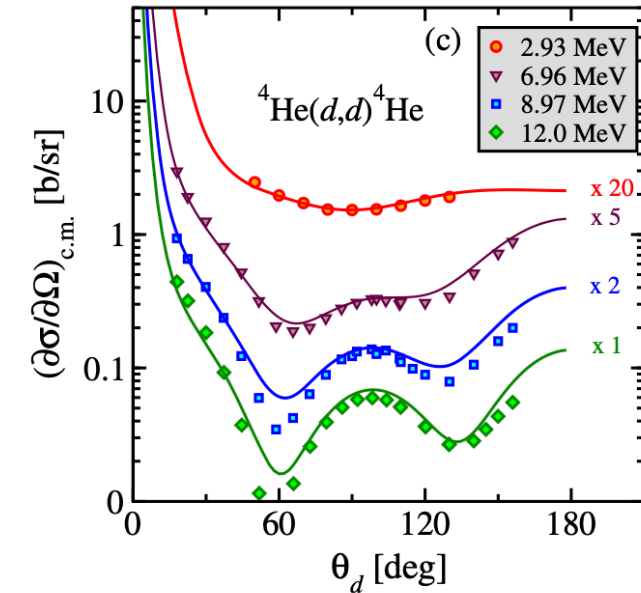
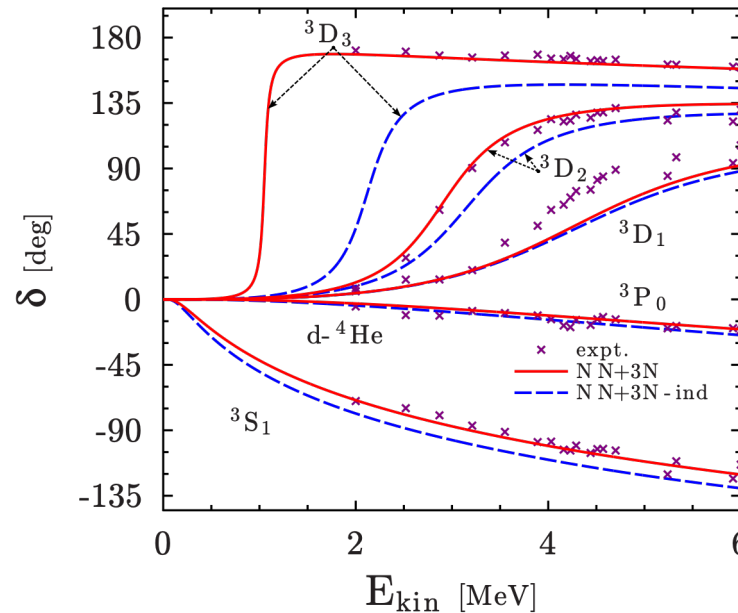
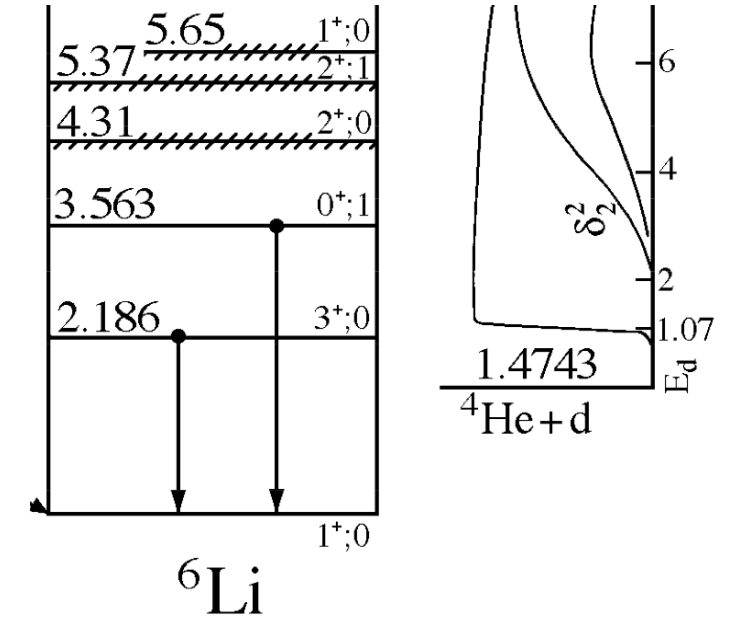
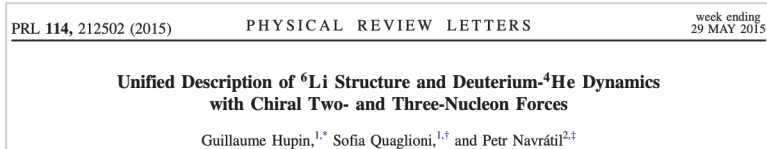
- Application of NCSMC
 - Trial wave function

$$|\Psi^{J^\pi T}\rangle = \sum_{\lambda} c_{\lambda} |{}^6\text{Li } \lambda J^\pi T\rangle + \oint_{\nu} drr^2 \frac{\gamma_{\nu}(r)}{r} \mathcal{A}_{\nu} |\Phi_{\nu r}^{J^\pi T}\rangle$$

$$|\Phi_{\nu r}^{J^\pi T}\rangle = [(|{}^4\text{He } \lambda_{\alpha} J_{\alpha}^{\pi_{\alpha}} T_{\alpha}\rangle |{}^2\text{H } \lambda_d J_d^{\pi_d} T_d\rangle)^{(sT)} Y_{\ell}(\hat{r}_{\alpha,d})]^{(J^\pi T)} \times \frac{\delta(r - r_{\alpha,d})}{rr_{\alpha,d}}$$

$$\mathcal{A}_{\nu} = \frac{1}{\sqrt{15}} \left(1 - \sum_{i=1}^4 \sum_{j=5}^6 P_{i,j} + \sum_{i<j=1}^4 P_{i,5} P_{j,6} \right)$$

${}^6\text{Li} \leftrightarrow {}^4\text{He} + d$ investigated within NCSMC in the past

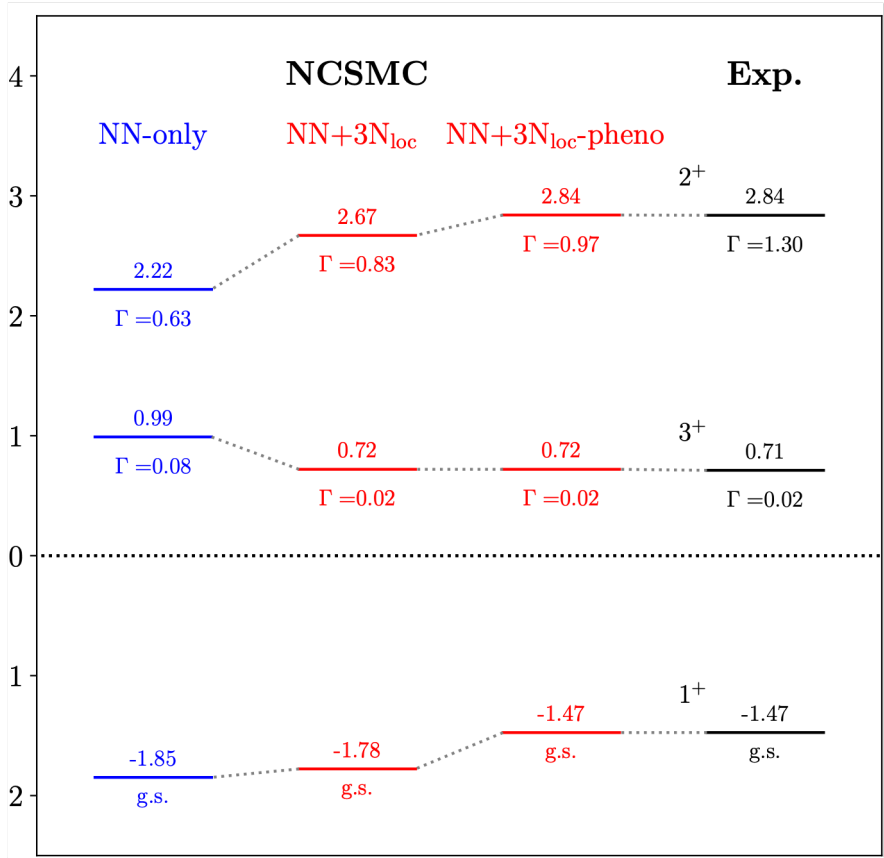


Ab Initio Prediction of the $^4\text{He}(d,\gamma)^6\text{Li}$ Big Bang Radiative Capture

C. Hebborn^{1,2,*}, G. Hupin³, K. Kravvaris², S. Quaglioni², P. Navrátil⁴, and P. Gysbers^{4,5}

Nuclear structure of ^6Li

- New NCSMC calculations with chiral NN+3N interaction – minor improvements



$^4\text{He}+d$ threshold

Ground state properties:
Energy
Asymptotic normalization constants
Magnetic moment

	NN-only	3N _{loc}	3N _{loc} -pheno	Exp. or Eval.
$E_{\text{g.s.}}$	-1.848	-1.778	-1.474	-1.4743
C_0	2.95	2.89	2.62(4)	2.28(7) 2.29(12)
C_2	-0.0369	-0.0642	-0.0554(305)	-0.077(18)
C_2/C_0	-0.013	-0.022	-0.021(11)	-0.025(6)(10)
μ	0.85	0.84	0.84(1)	0.8220473(6)

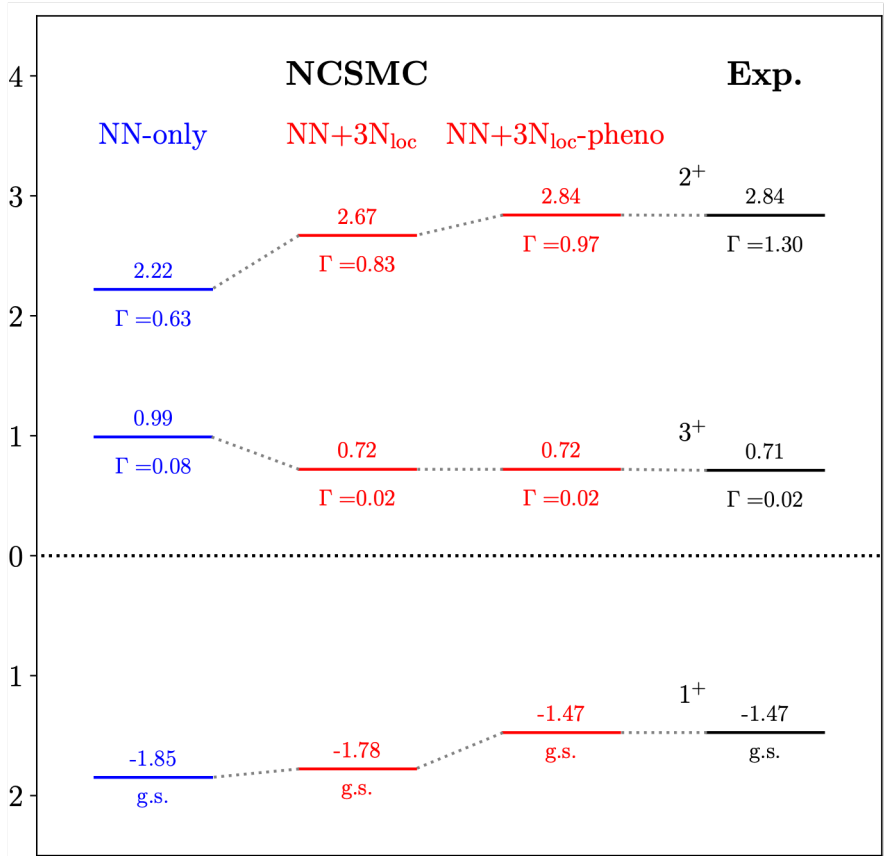
Ab Initio Prediction of the $^4\text{He}(d,\gamma)^6\text{Li}$ Big Bang Radiative Capture

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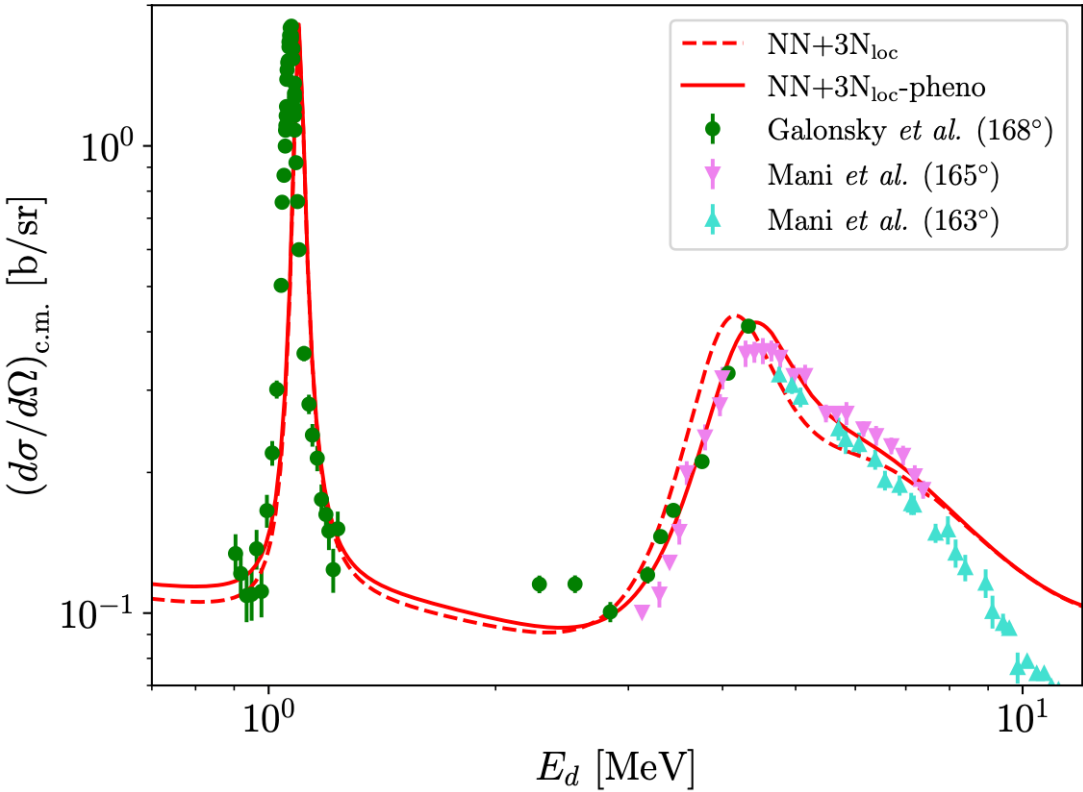
Radiative capture of deuterons on ^4He

- NCSMC calculations with chiral NN+3N interaction

Structure of ^6Li



Elastic scattering $^4\text{He}(d,d)^4\text{He}$ cross section at the deuteron back scattered angle 164°



Ab Initio Prediction of the ${}^4\text{He}(d,\gamma){}^6\text{Li}$ Big Bang Radiative CaptureC. Hebborn^{1,2,*}, G. Hupin³, K. Kravvaris², S. Quaglioni², P. Navrátil⁴, and P. Gysbers^{4,5}

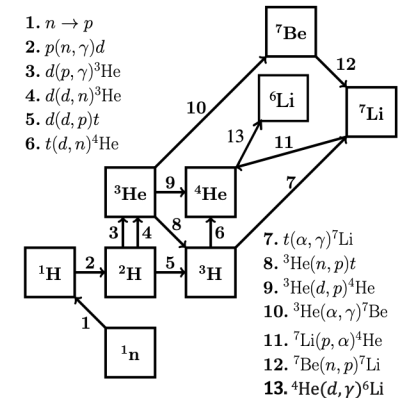
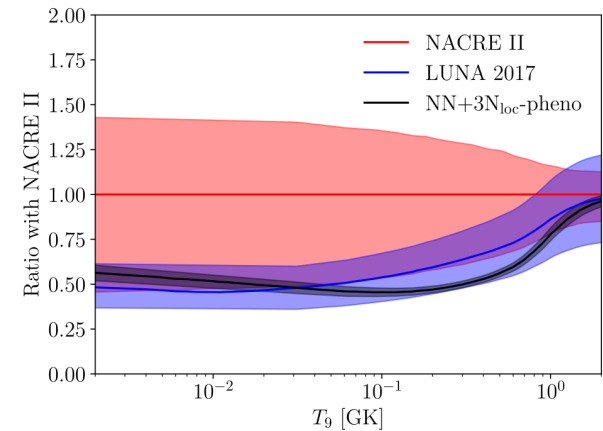
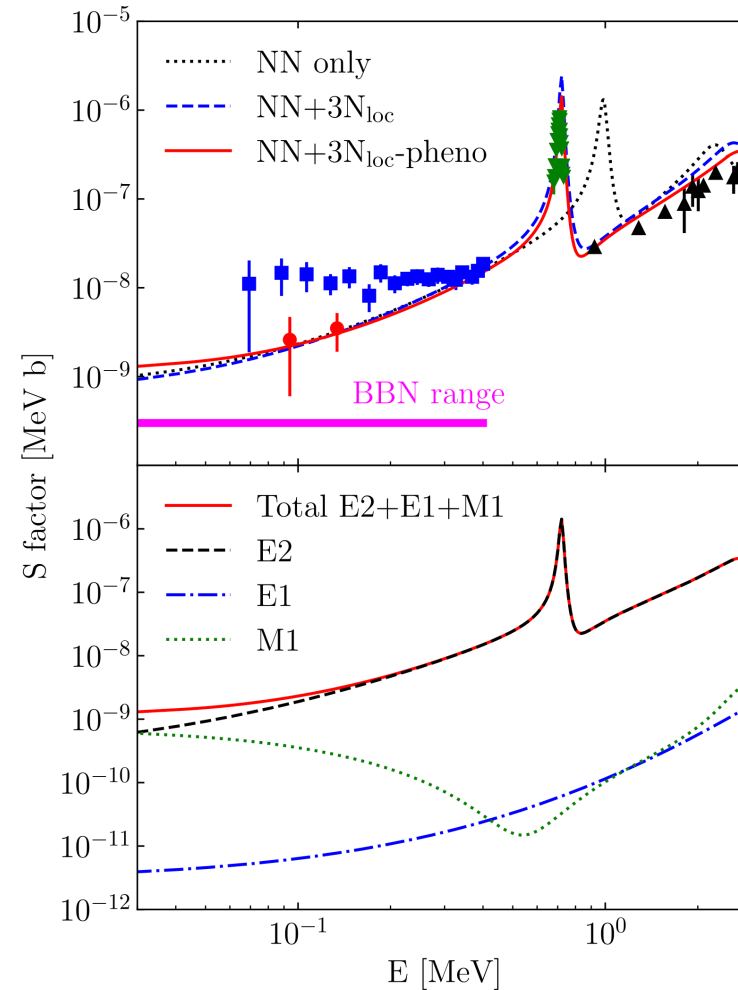
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Radiative capture of deuterons on ${}^4\text{He}$

- Three orders of magnitude discrepancy between BBN predictions and observations
 - Problem with astronomical observations?
 - Problem with our understanding of the reaction rate?
 - New physics?
- NCSMC calculations with chiral NN+3N interaction
 - Radiative capture S-factor
 - Dominated by E2
 - M1 significant at low energy
 - E1 negligible – isospin suppressed ($T=0 \rightarrow T=0$)
 - Thermonuclear reaction rate
 - Smaller than NACRE II evaluation
 - Agreement with LUNA result with reduced uncertainty

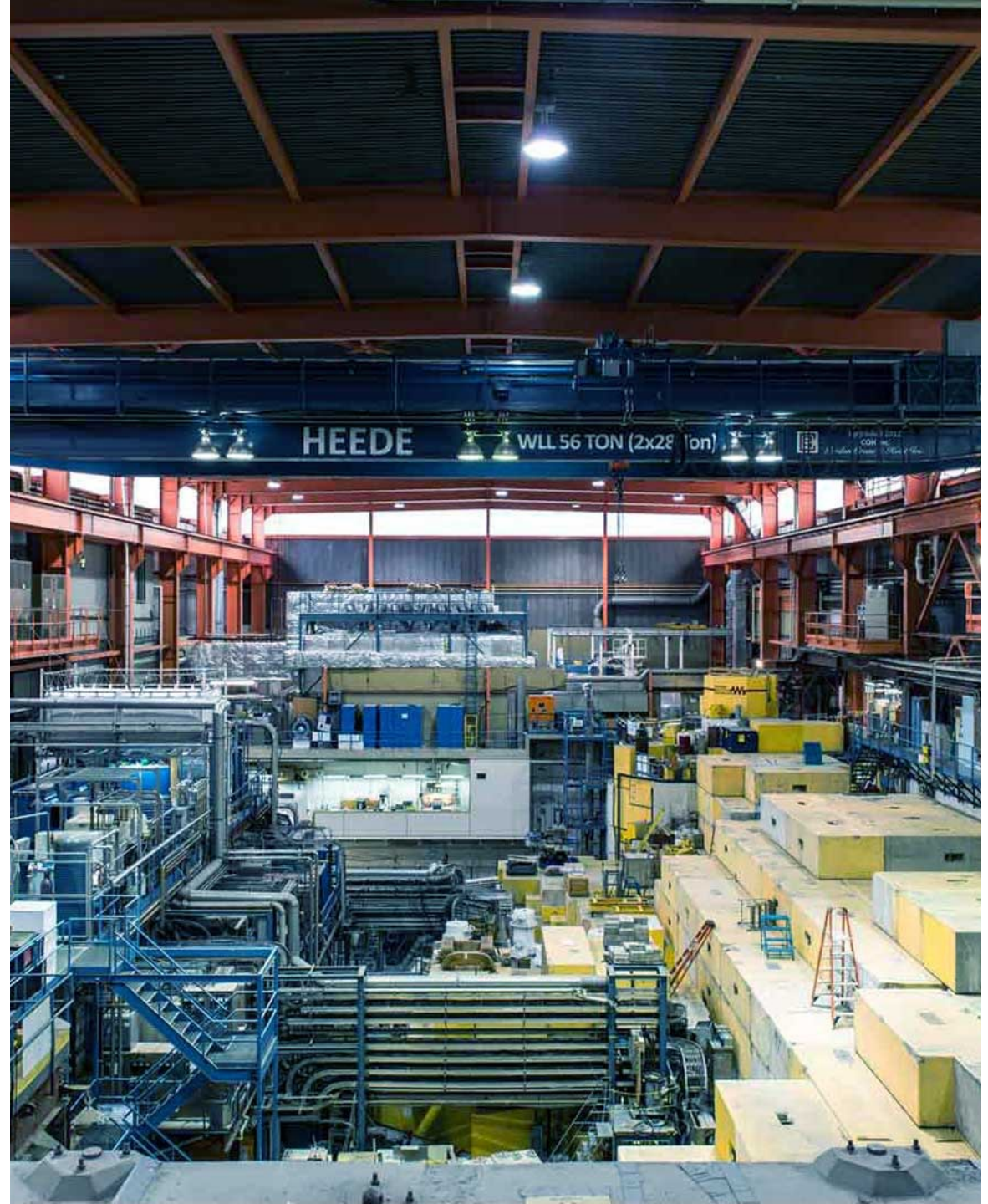
$$\mathcal{M}^{E\lambda} = e \sum_{j=1}^A \frac{1 + \tau_{jz}}{2} [\mathbf{r}_j - \mathbf{R}_{cm}^{(A)}]^\lambda$$

$$\mathcal{M}^{M1} = \frac{\mu_N}{\hbar c} \sqrt{\frac{3}{4\pi}} \sum_{j=1}^A (g_{lj} L_j + g_{sj} S_j)$$



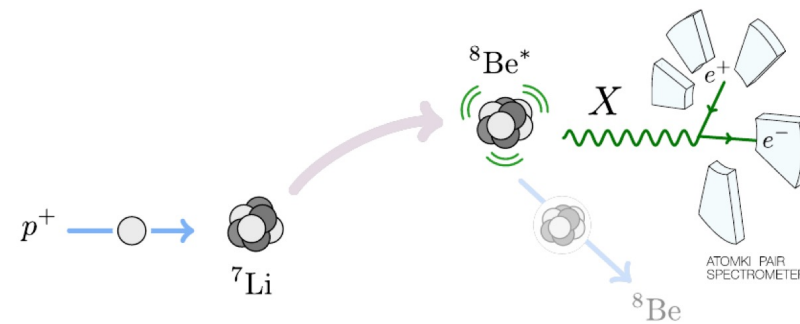
${}^7\text{Li}(p,e^+e^-){}^8\text{Be}$ internal pair creation
and the X17 anomaly

2026-10-20



X17 Anomaly

Phys. Rev. Lett. **116**, 042501 (2016) – ${}^7\text{Li}+p \rightarrow {}^8\text{Be}$
 Phys. Rev. C **104**, 044003 (2021) – ${}^3\text{H}+p \rightarrow {}^4\text{He}$
 Phys. Rev. C **106**, L061601 (2022) – ${}^{11}\text{B}+p \rightarrow {}^{12}\text{C}$

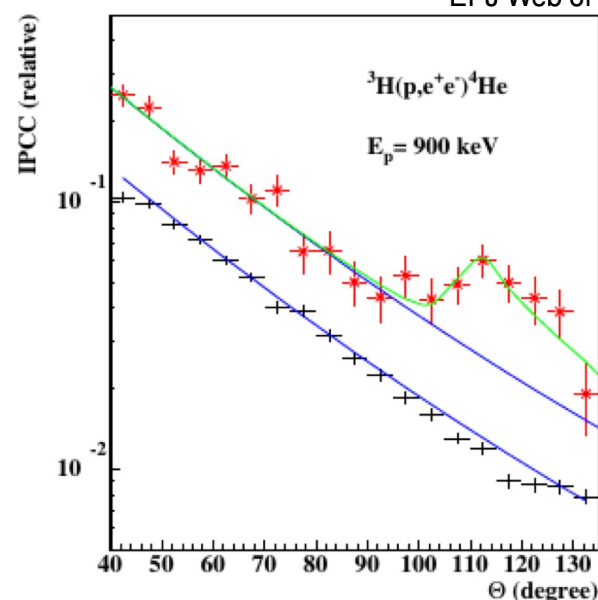
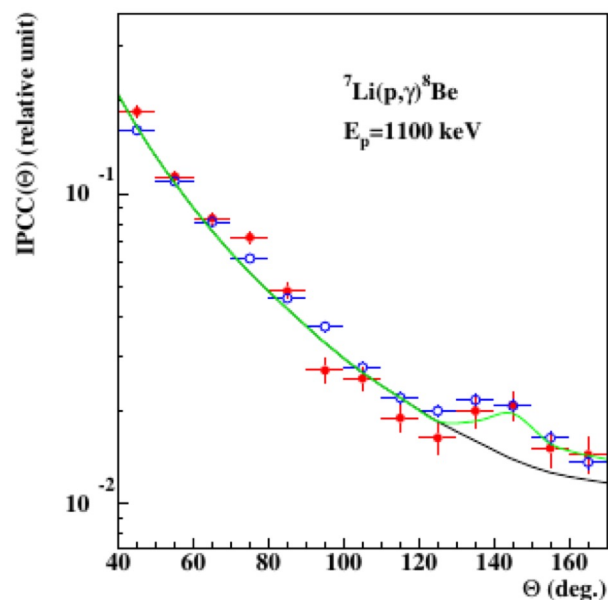


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Feng PRD **95**, 035017 (2017)

“An anomaly in the internal pair creation on the M1 transition depopulating the 18.15 MeV isoscalar 1^+ state on ${}^8\text{Be}$ was observed. This could be explained by the creation and subsequent decay of a new boson .. mass 17.01(16) MeV”

Firak, Krasznahorkay, et al
 EPJ Web of Conferences **232** 04005 (2020)



IPCC:
 Internal Pair Creation
 Angular Correlation

Angle between e^- and e^+

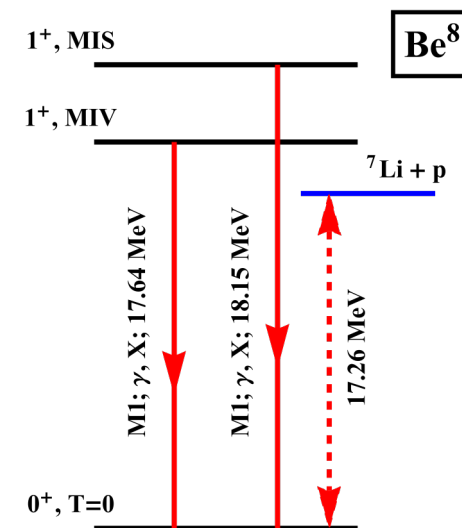
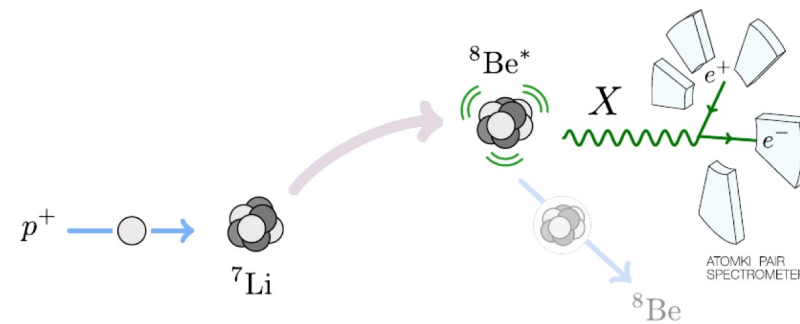


Fig. from PLB 813, 136061 (2021)

X17 Anomaly

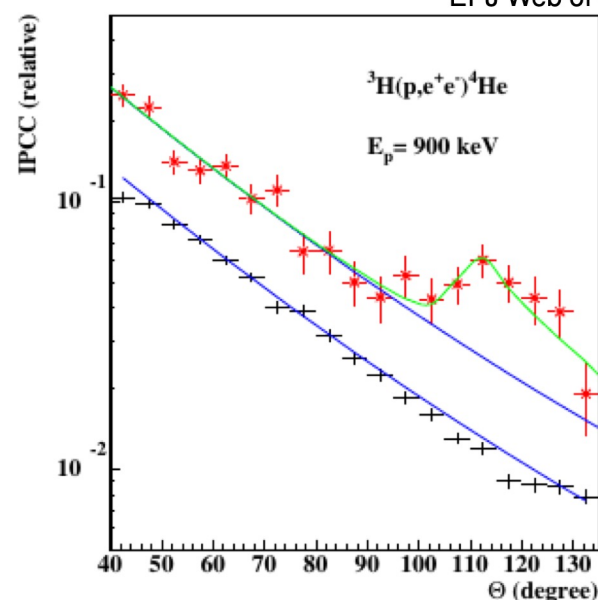
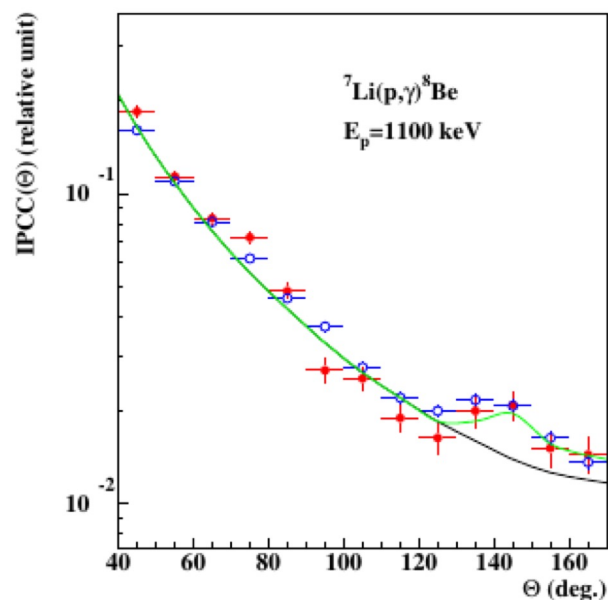
Phys. Rev. Lett. **116**, 042501 (2016) – ${}^7\text{Li}+p \rightarrow {}^8\text{Be}$
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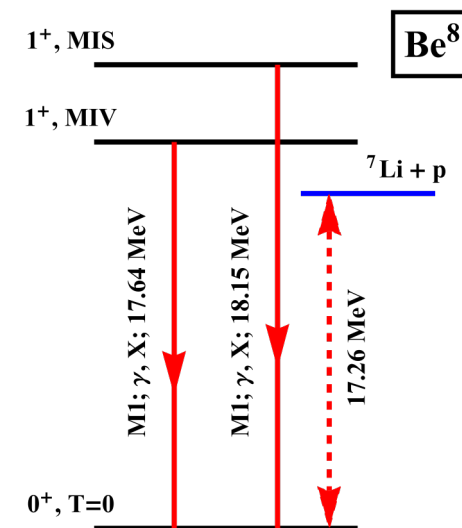
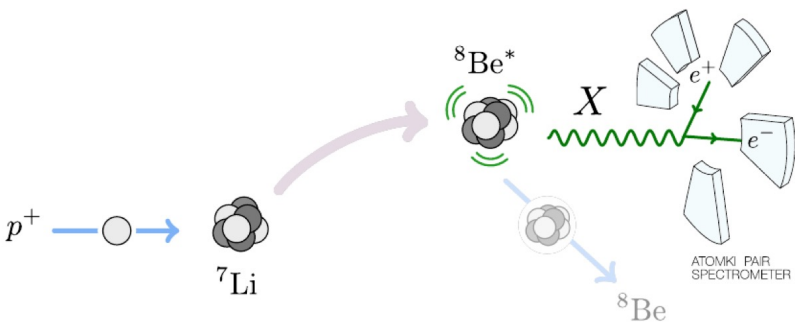


Fig. from PLB 813, 136061 (2021)

New experiments:
 MEG-II – X
 PADME – ✓

X17 Anomaly

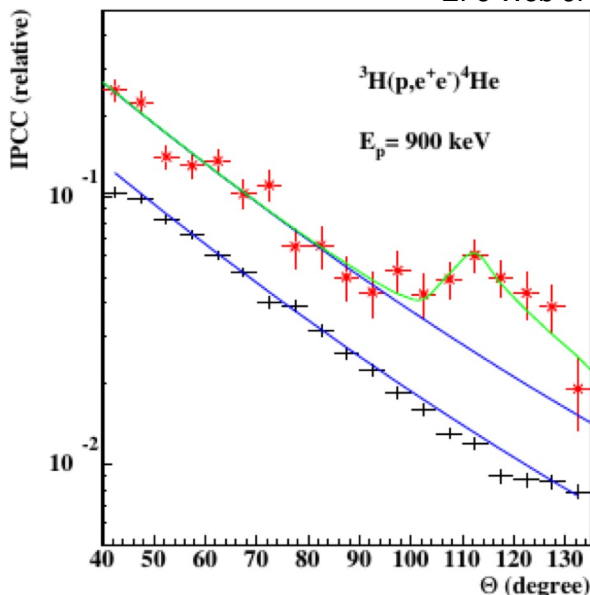
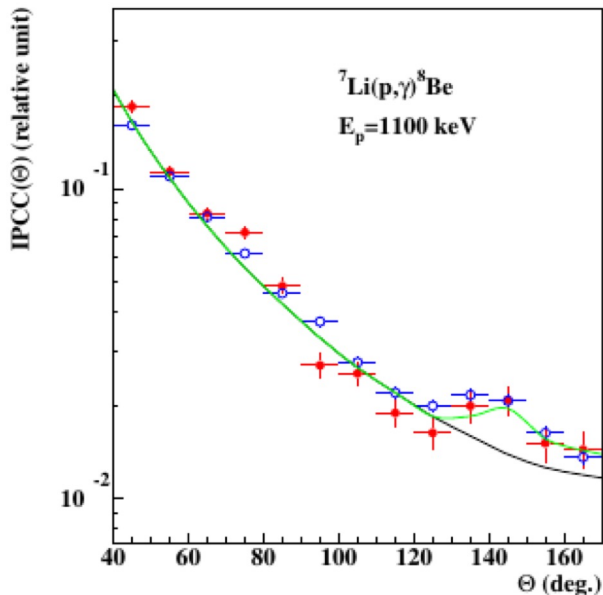
Phys. Rev. Lett. **116**, 042501 (2016) – ${}^7\text{Li}+p \rightarrow {}^8\text{Be}$
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Feng PRD **95**, 035017 (2017)

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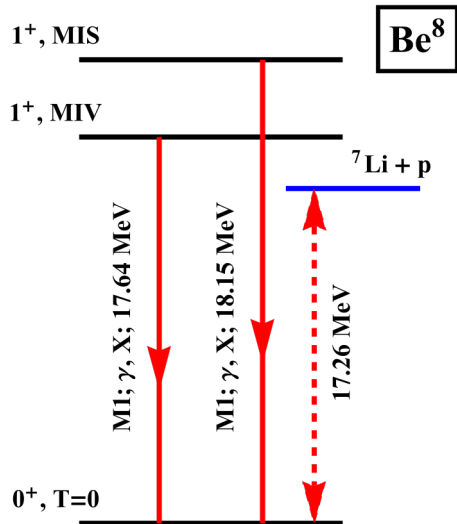


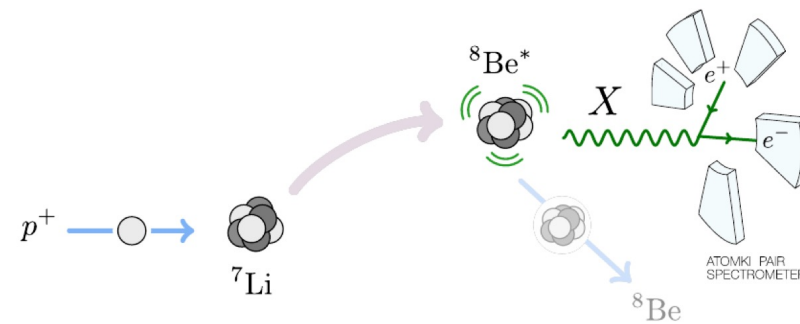
Fig. from PLB 813, 136061 (2021)

New experiments:
 MEG-II – X
 PADME – ✓

Analogous to
 DarkLight @ TRIUMF , MAGIX @ Mainz

X17 Anomaly

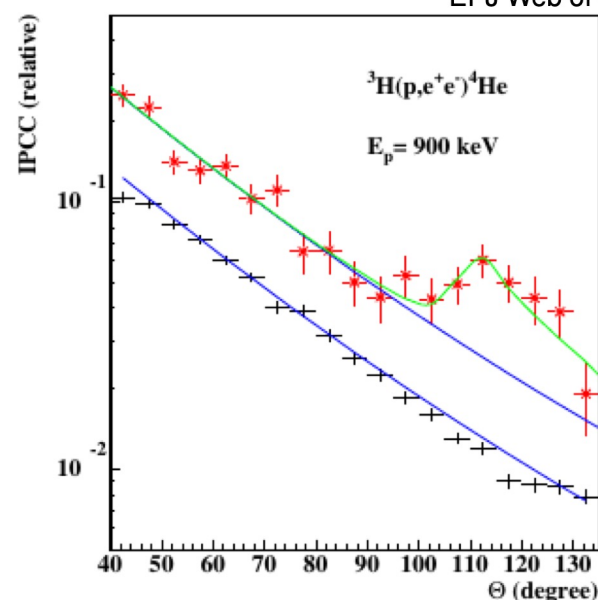
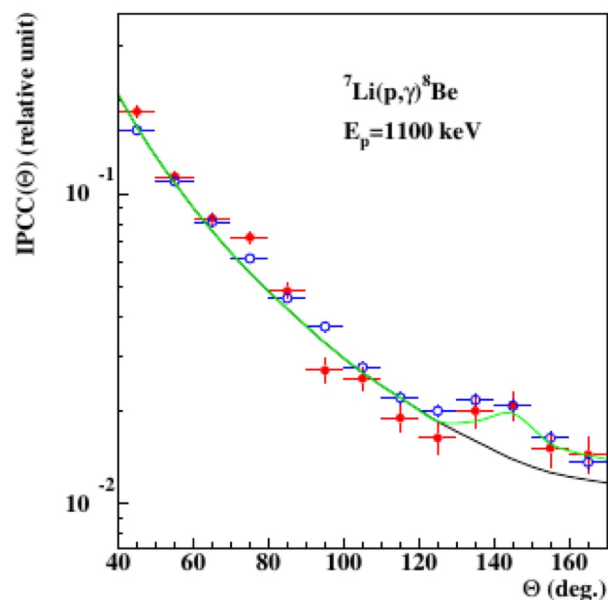
Phys. Rev. Lett. **116**, 042501 (2016) – ${}^7\text{Li}+p \rightarrow {}^8\text{Be}$
 Phys. Rev. C **104**, 044003 (2021) – ${}^3\text{H}+p \rightarrow {}^4\text{He}$
 Phys. Rev. C **106**, L061601 (2022) – ${}^{11}\text{B}+p \rightarrow {}^{12}\text{C}$



Feng PRD **95**, 035017 (2017)

“An anomaly in the internal pair creation on the M1 transition depopulating the 18.15 MeV isoscalar 1^+ state on ${}^8\text{Be}$ was observed. This could be explained by the creation and subsequent decay of a new boson .. mass 17.01(16) MeV”

Firak, Krasznahorkay, et al
 EPJ Web of Conferences **232** 04005 (2020)



IPCC:
 Internal Pair Creation
 Angular Correlation

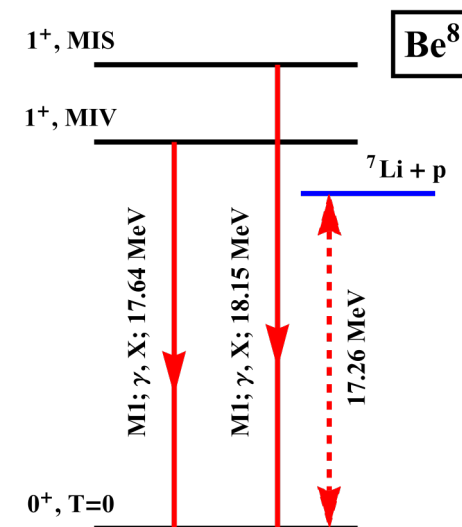


Fig. from PLB 813, 136061 (2021)

Can *ab initio* nuclear theory help interpret the anomaly?

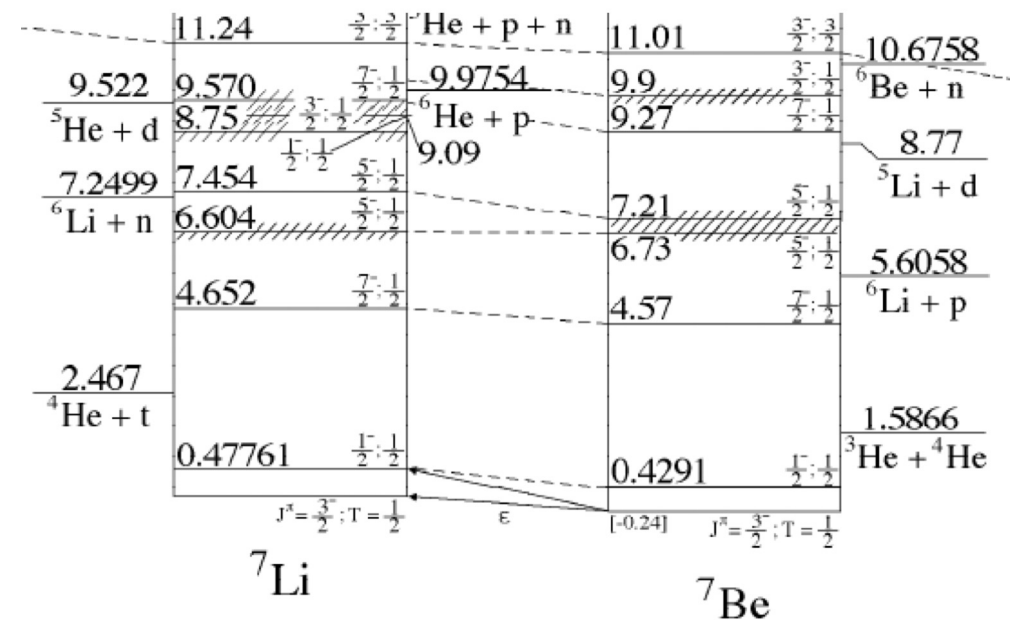
NCSMC calculations of ^8Be structure and $^7\text{Li}+p$ scattering and capture

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- Wave function ansatz

$$\Psi_{\text{NCSMC}}^{(8)} = \sum_{\lambda} c_{\lambda} |^8\text{Be}, \lambda\rangle + \sum_{\nu} \int dr \gamma_{\nu}(r) \hat{A}_{\nu} |^7\text{Li} + p, \nu\rangle + \sum_{\mu} \int dr \gamma_{\mu}(r) \hat{A}_{\mu} |^7\text{Be} + n, \mu\rangle$$

- $3/2^{-}$, $1/2^{-}$, $7/2^{-}$, $5/2^{-}$, $5/2^{-}$ ^7Li and ^7Be states in cluster basis
- 15 positive and 15 negative parity states in ^8Be composite state basis

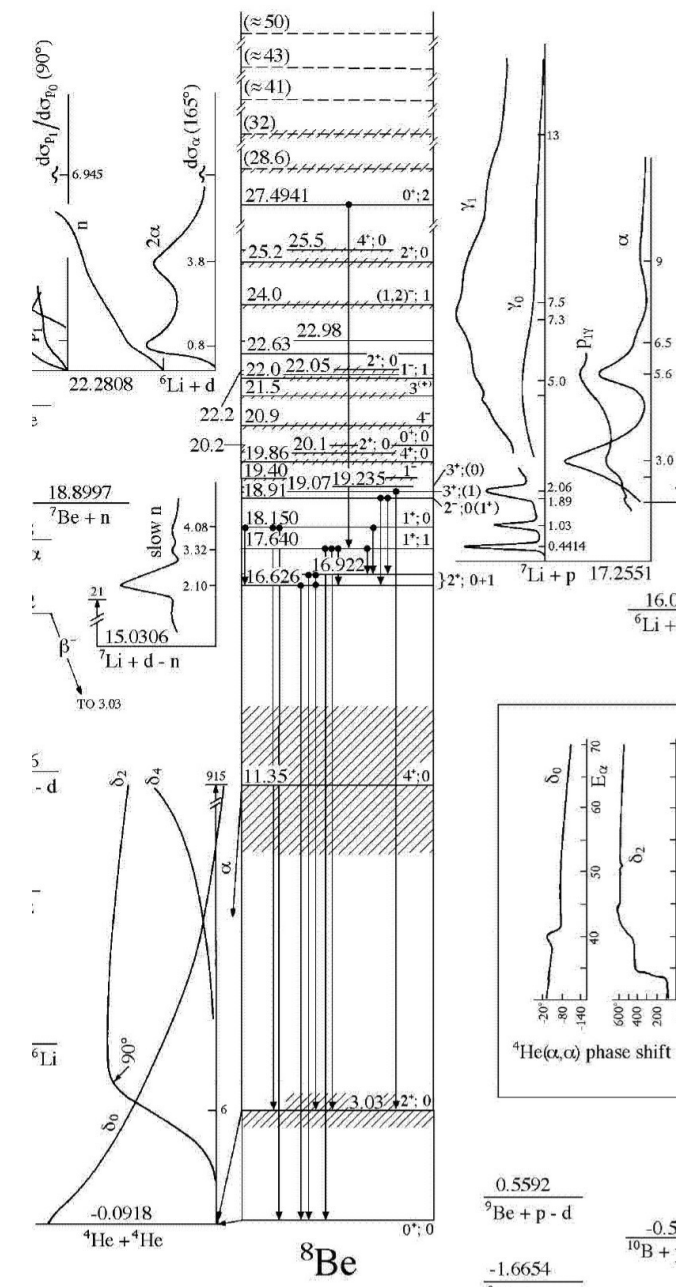


NCSMC calculations of ^8Be structure and $^7\text{Li}+p$ scattering and capture

- Wave function ansatz

$$\Psi_{\text{NCSMC}}^{(8)} = \sum_{\lambda} c_{\lambda} |^8\text{Be}, \lambda\rangle + \sum_{\nu} \int dr \gamma_{\nu}(r) \hat{A}_{\nu} |^7\text{Li} + p, \nu\rangle + \sum_{\mu} \int dr \gamma_{\mu}(r) \hat{A}_{\mu} |^7\text{Be} + n, \mu\rangle$$

- $3/2^-$, $1/2^-$, $7/2^-$, $5/2^-$, $5/2^-$ ^7Li and ^7Be states in cluster basis
- 15 positive and 15 negative parity states in ^8Be composite state basis
- $^4\text{He}+^4\text{He}$ cluster not included for technical reasons
 - Limited importance for the proton capture on ^7Li



Ab initio calculations of ${}^7\text{Li}(p,\gamma){}^8\text{Be}$ radiative capture

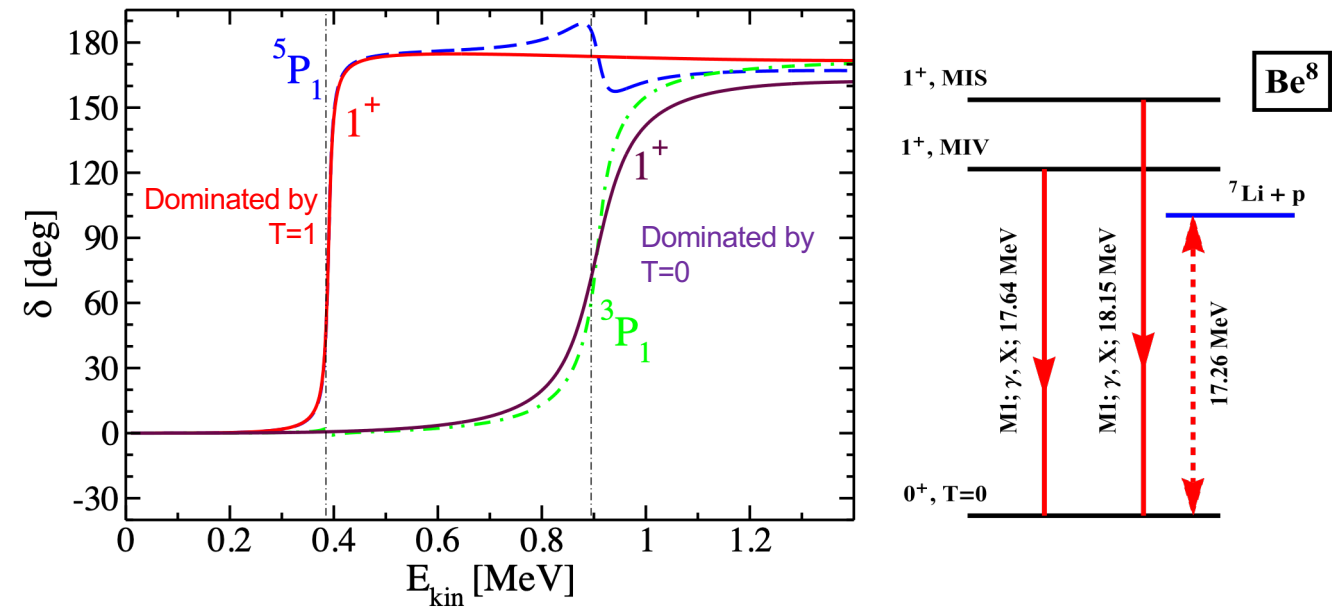
Ab initio investigation of the ${}^7\text{Li}(p, e^+e^-){}^8\text{Be}$ process and the X17 boson

P. Gysbers^{1,2,3}, P. Navrátil^{1,4}, K. Kravvaris⁵, G. Hupin⁶, and S. Quaglioni⁵

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- No-core shell model with continuum (NCSMC) with wave function ansatz

$$\Psi_{\text{NCSMC}}^{(8)} = \sum_{\lambda} c_{\lambda} |{}^8\text{Be}, \lambda\rangle + \sum_{\nu} \int dr \gamma_{\nu}(r) \hat{A}_{\nu} |{}^7\text{Li} + p, \nu\rangle + \sum_{\mu} \int dr \gamma_{\mu}(r) \hat{A}_{\mu} |{}^7\text{Be} + n, \mu\rangle$$



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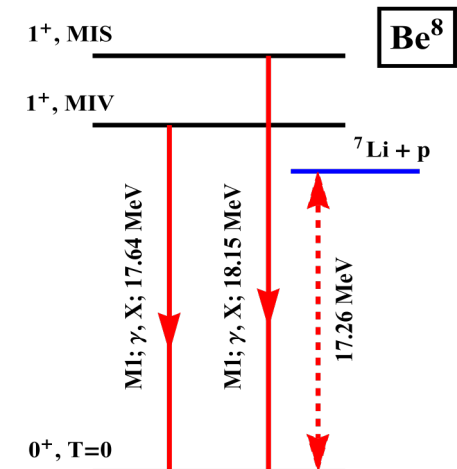
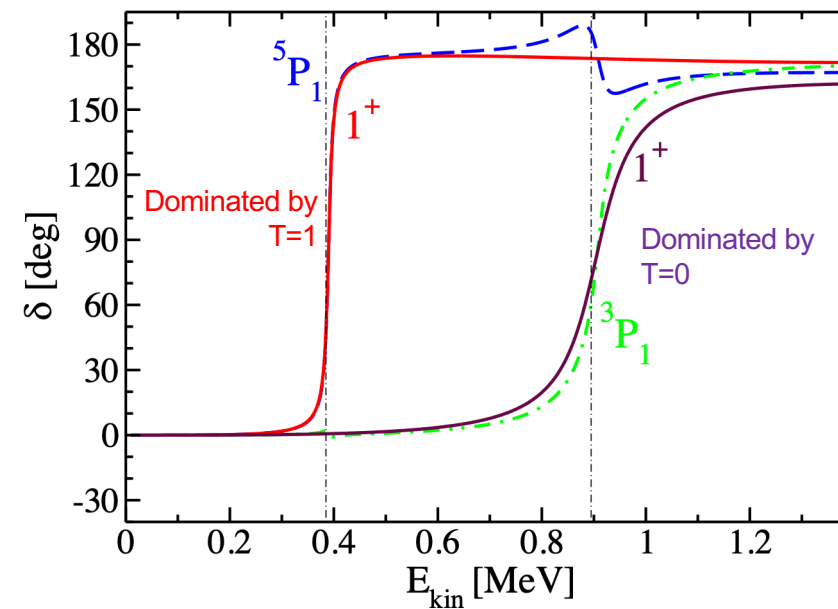
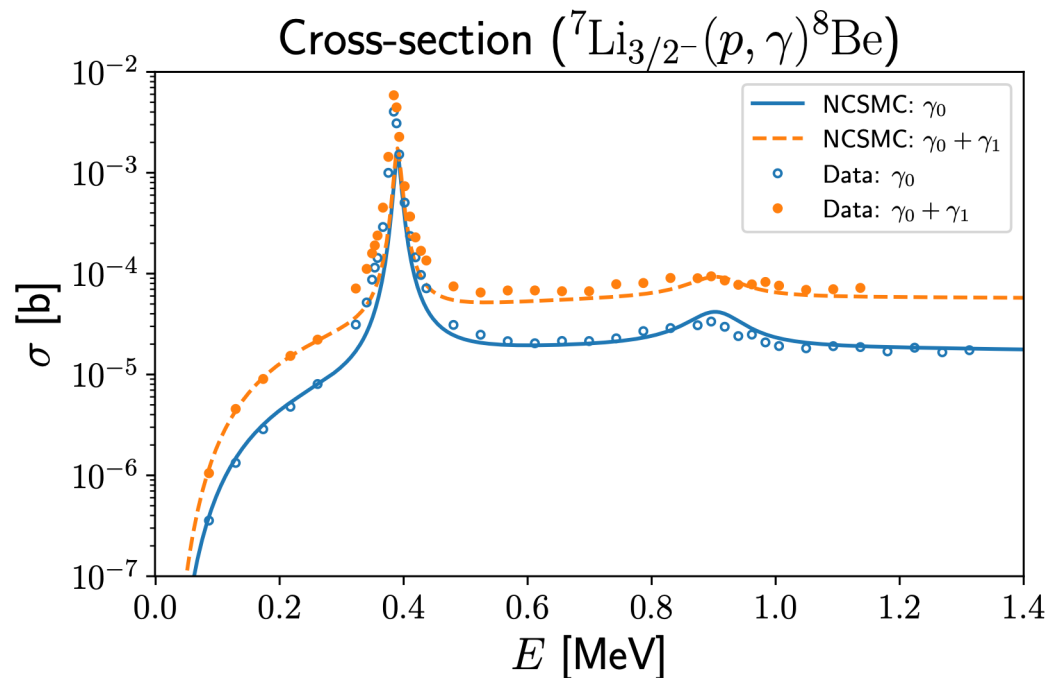
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$$\Psi_{\text{NCSMC}}^{(8)} = \sum_{\lambda} c_{\lambda} |{}^8\text{Be}, \lambda\rangle + \sum_{\nu} \int dr \gamma_{\nu}(r) \hat{A}_{\nu} |{}^7\text{Li} + p, \nu\rangle + \sum_{\mu} \int dr \gamma_{\mu}(r) \hat{A}_{\mu} |{}^7\text{Be} + n, \mu\rangle$$

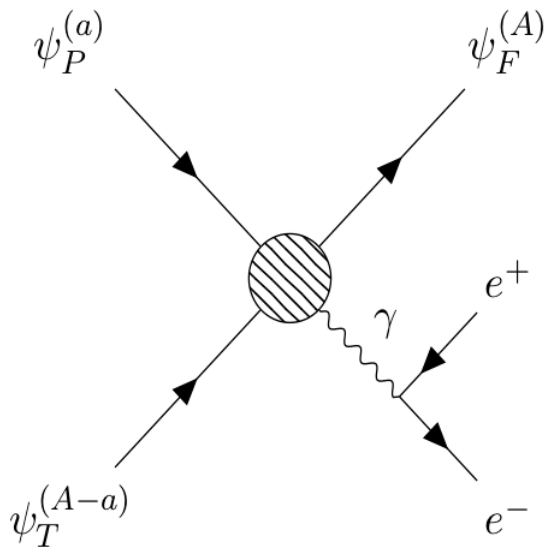


Data: Zahnow *et al.*
Z.Phys.A **351** 229-236 (1995)

γ_0 : decay to ground state (0^+)
 γ_1 : decay to first excited (2^+)

Ab initio calculations of ${}^7\text{Li}(p,e^+e^-){}^8\text{Be}$ pair production

Internal electron-positron pair conversion correlation



$$\frac{d^4\sigma}{d\Omega_+d\Omega_-}(\theta_{ee}) = \int dy \frac{2\alpha^2}{(2\pi)^3} \frac{\omega f_r}{v} \frac{p_+ p_-}{Q^4} \sum_{n \in \{1,4,5\}} v_n R_n$$

NCSMC directly predicts the relative importance of different multipoles – E1, M1 etc.

Calculating properly the pair production cross section with the interference of different multipoles improves description.

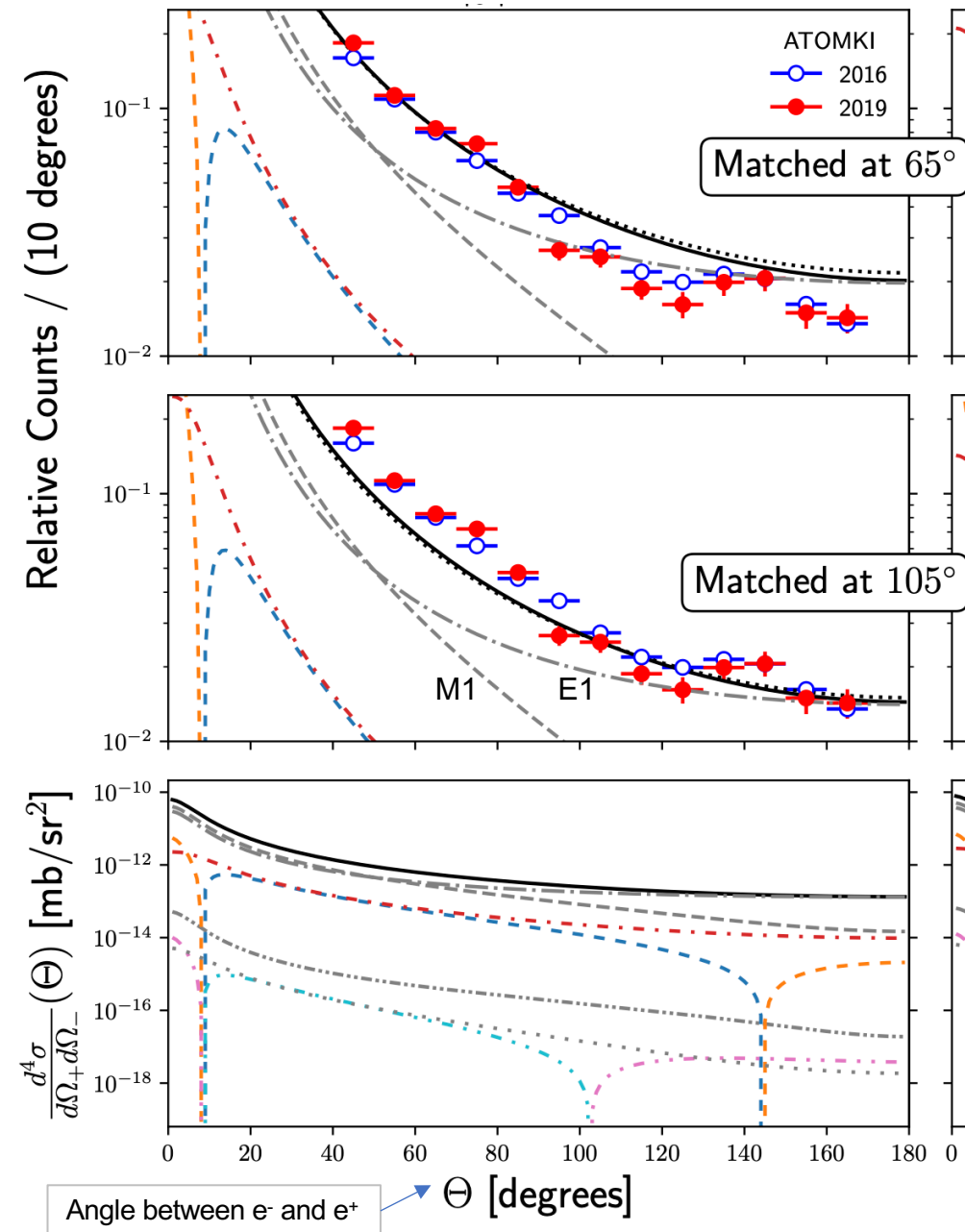
A reasonable although not perfect agreement with ATOMKI data

PHYSICAL REVIEW C **110**, 015503 (2024)

Editors' Suggestion

Ab initio investigation of the ${}^7\text{Li}(p, e^+e^-){}^8\text{Be}$ process and the X17 boson

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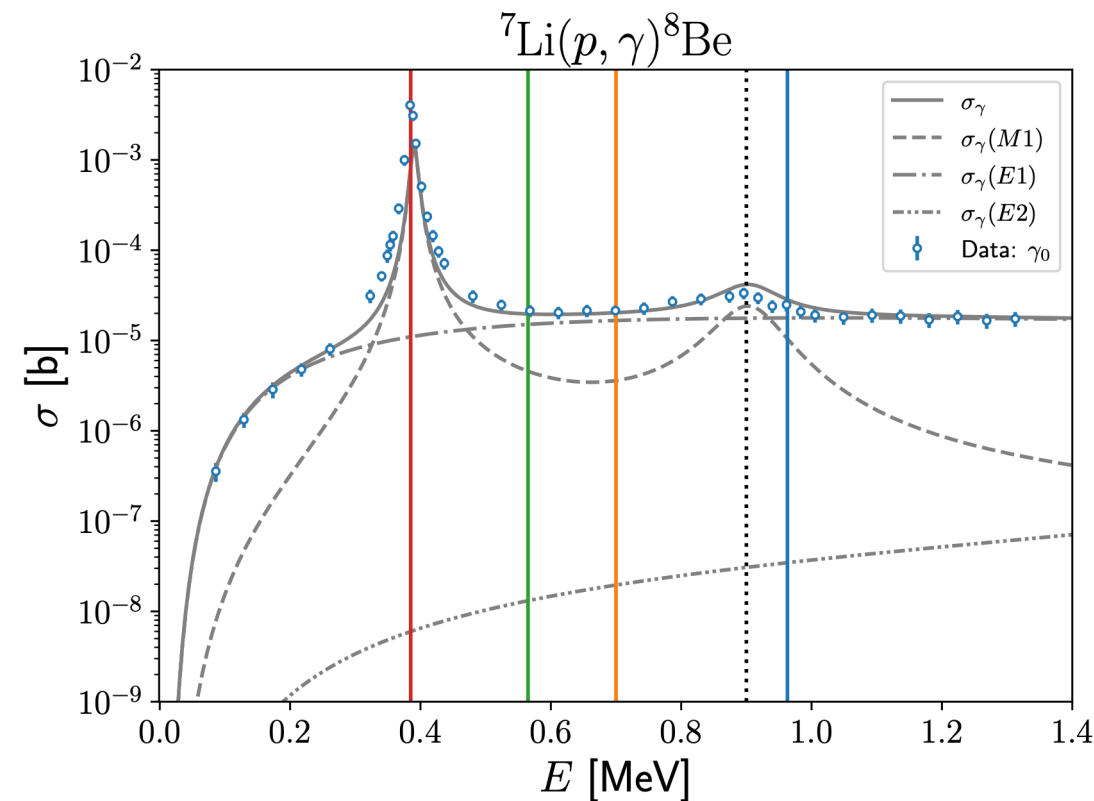


Ab initio calculations of ${}^7\text{Li}(p,\gamma){}^8\text{Be}$ radiative capture, ${}^7\text{Li}(p,e^+e^-){}^8\text{Be}$ pair production

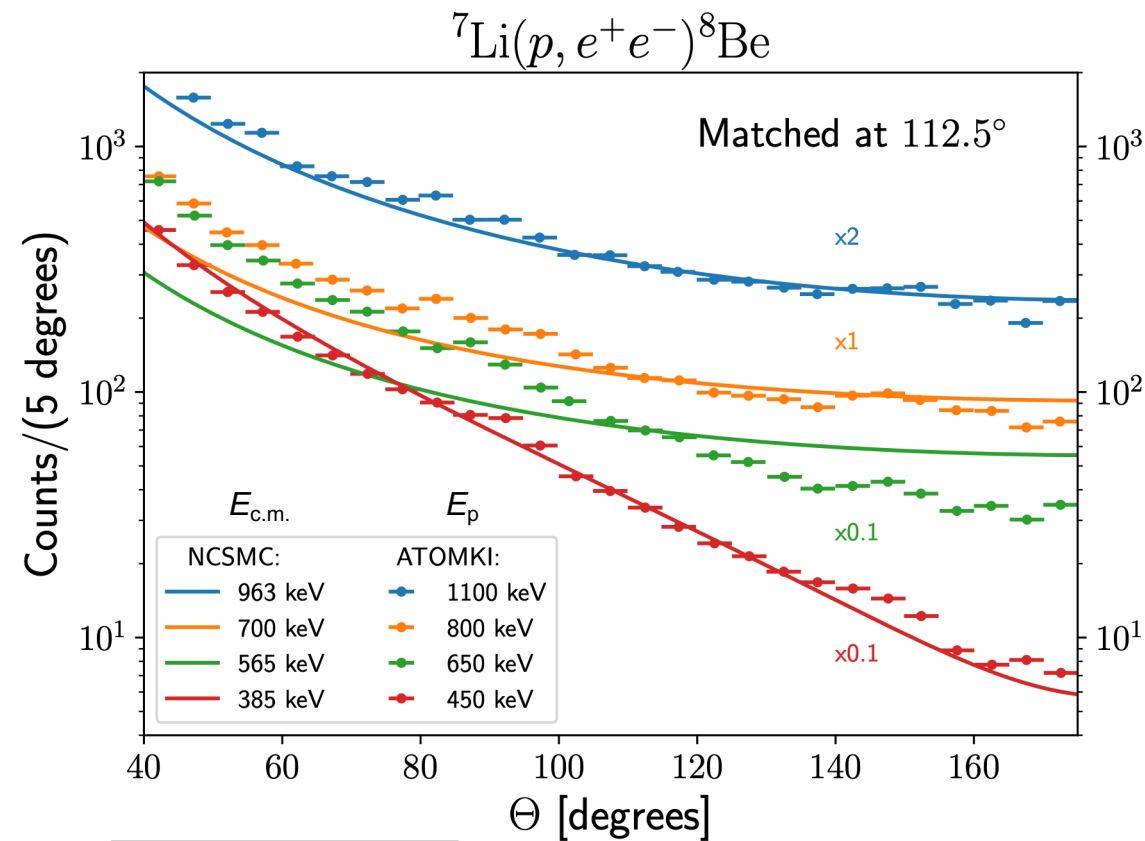
New ATOMKI measurements in-between & at resonance energies

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N. J. Sas et al., “Observation of the X17 anomaly in the ${}^7\text{Li}(p,e^+e^-){}^8\text{Be}$ direct proton-capture reaction,” arXiv:2205.07744



NCSMC calculations match well resonance data.
Disagree in-between resonances – flat E1 distribution.
Proton slow-down in the thick target?



PHYSICAL REVIEW C **110**, 015503 (2024)

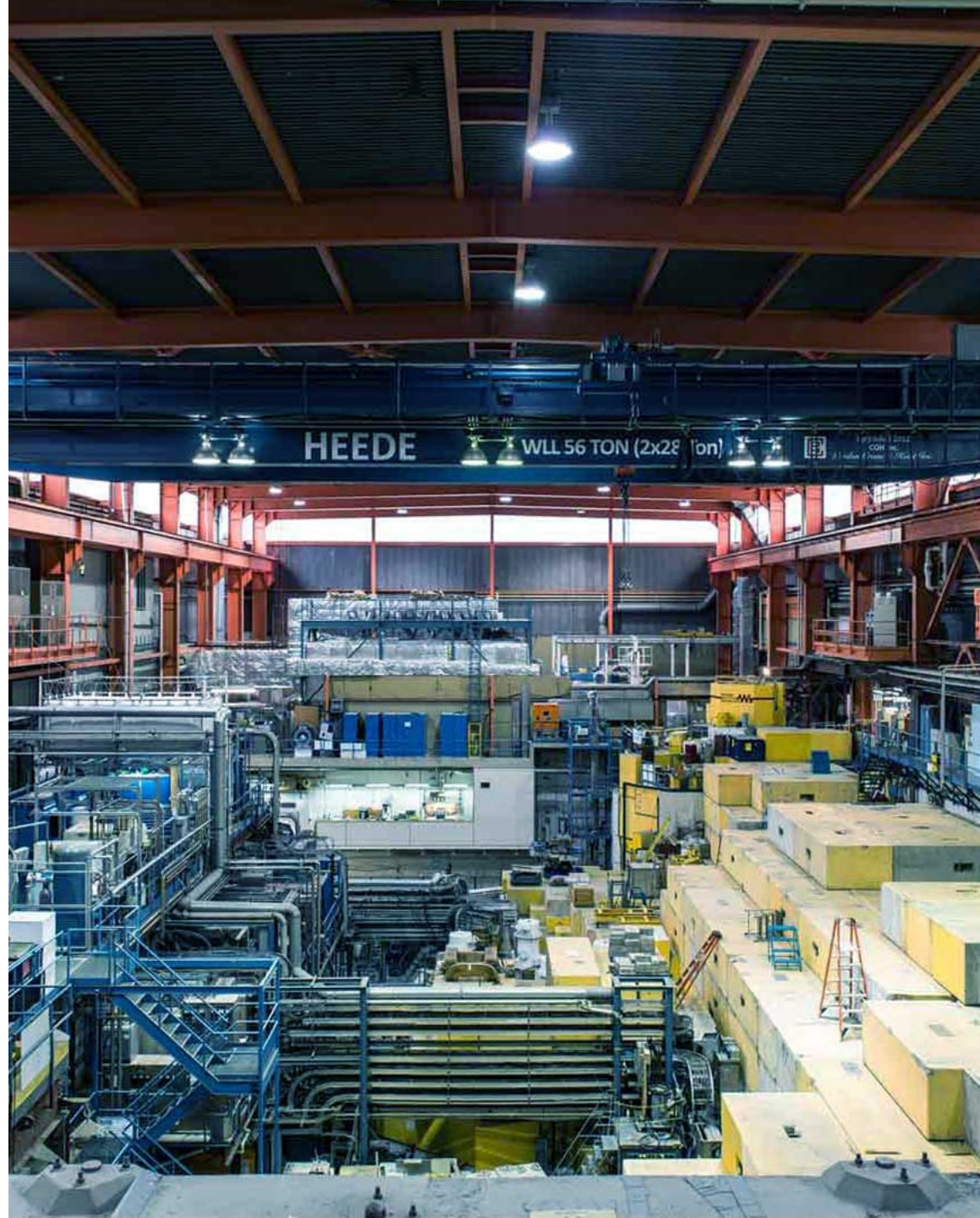
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Conclusions

2026-10-20



Conclusions

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- *Ab initio* nuclear theory
 - Makes connections between the low-energy QCD and many-nucleon systems
 - With chiral EFT based NN and 3N forces, it is a predictive theory of nuclear properties
 - Sensitivity to the details of nuclear Hamiltonian – feedback on the quality of NN+3N forces
- Applications of *ab initio* no-core shell model and the Lanczos strength method
 - Electroweak radiative correction δ_{NS} for ^{10}C and ^{14}O Fermi transitions – reduced theoretical uncertainty
 - Two-photon exchange nuclear correction to muonic X-ray transitions in Li, Be, B isotopes in progress
- Applications of *ab initio* no-core shell model with continuum to nuclear scattering and reactions
 - Nucleon - α scattering - cross section at resonance well reproduced – used by SNO+ collaboration
 - DT fusion – importance of the near threshold $3/2^+$ S-wave resonance
 - $^2\text{H}(\alpha, \gamma)^6\text{Li}$ – agreement with latest LUNA experimental data
 - Searches for new physics (X17)

EIC connection – *ab initio* calculations of electron scattering on light nuclei planned

Current NCSM & NCSMC collaborators

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Jakub Herko, Diego Araujo, Marshall Kodar, Stephan Foster, Roan Stafford (TRIUMF)

Sofia Quaglioni, Kostas Kravvaris (LLNL)

Guillaume Hupin, Chloe Hebborn (CNRS/IN2P3 Orsay)

Michael Gennari (Mainz)

Peter Gysbers (FRIB)

Mehdi Drissi, Lotta Jokiniemi (TU Darmstadt)

Matteo Vorabbi (Surrey)