

Nuclear reactions important for astrophysics from *ab initio* theory

Theory Canada 14

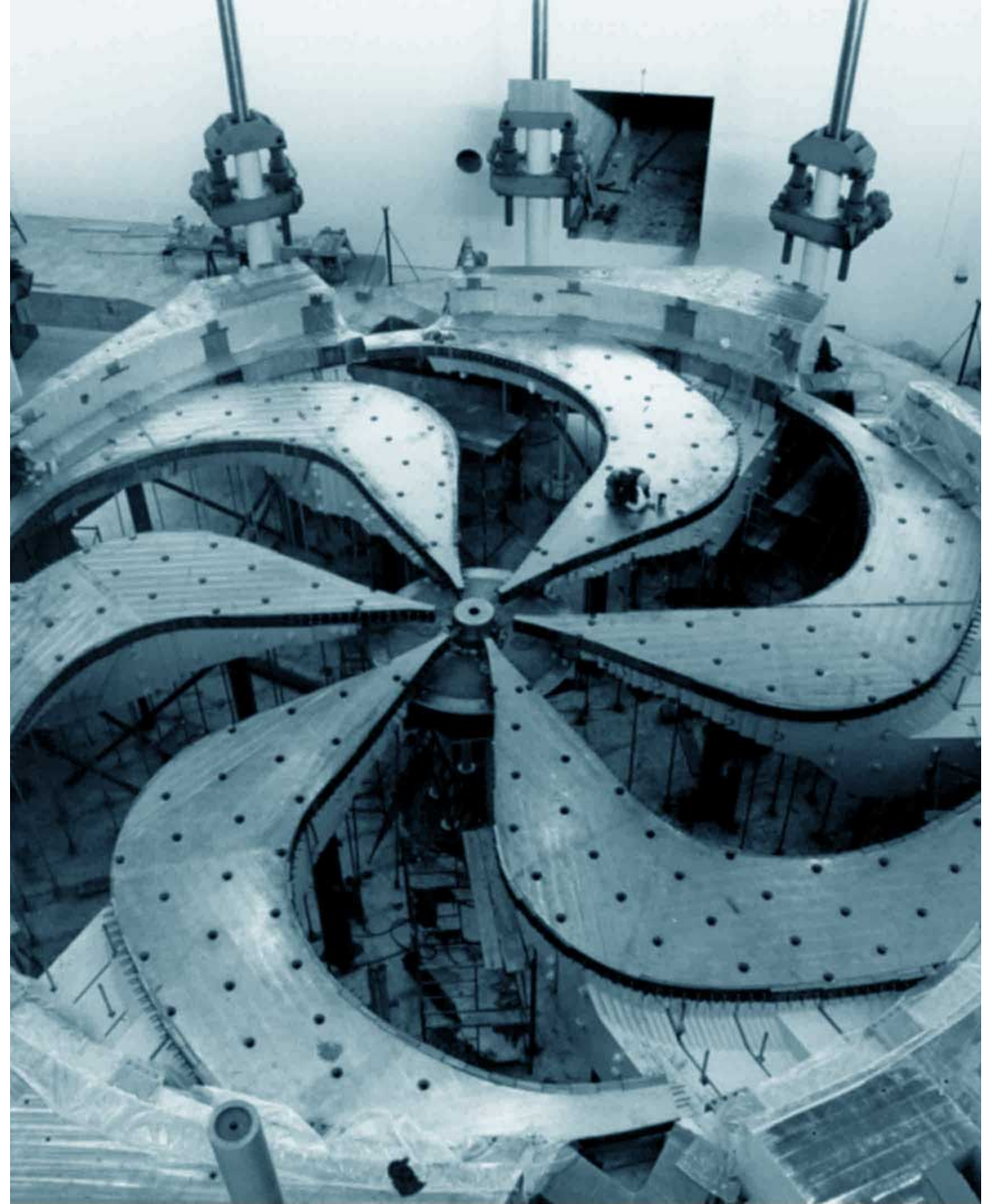
UBC, Vancouver, BC May 31 - June 1, 2019

Petr Navratil

TRIUMF

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M. Vorabbi, A. Calci (TRIUMF), P. Gysbers (UBC/TRIUMF),
M. Gennari (Waterloo), J. Dohet-Eraly (ULB),
R. Roth (Darmstadt)

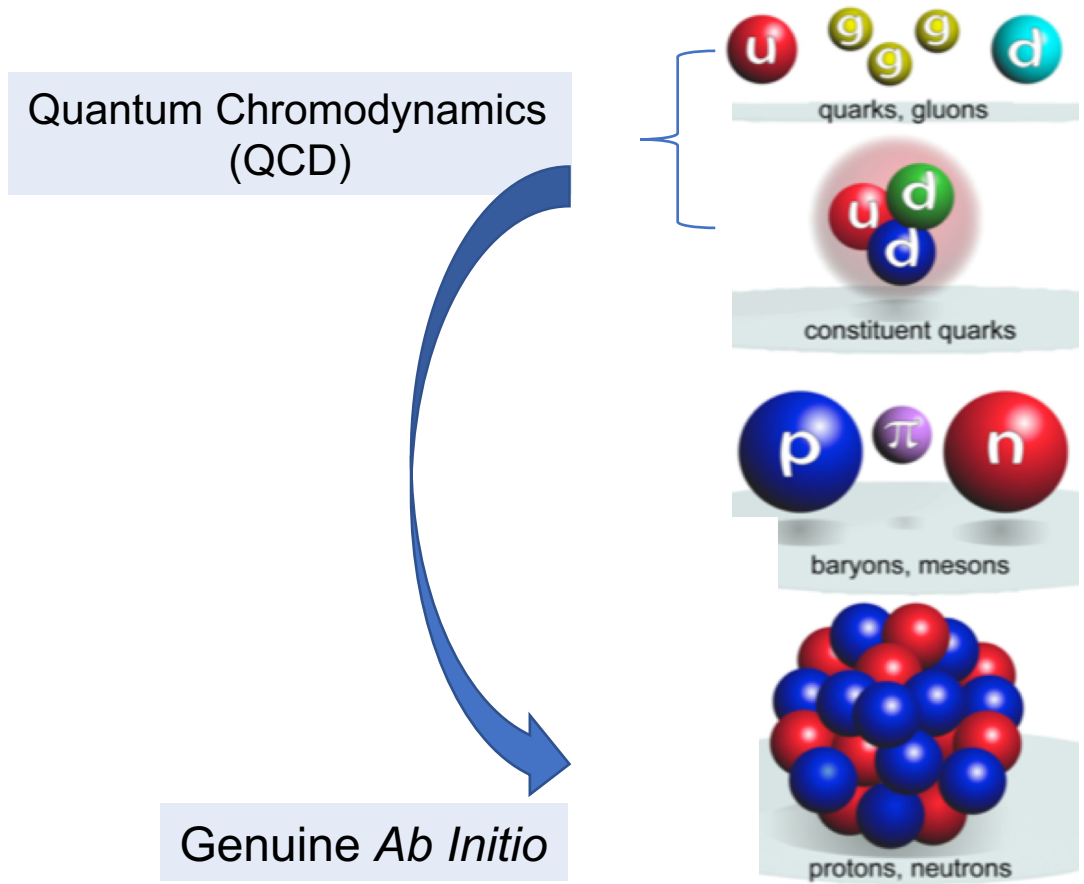
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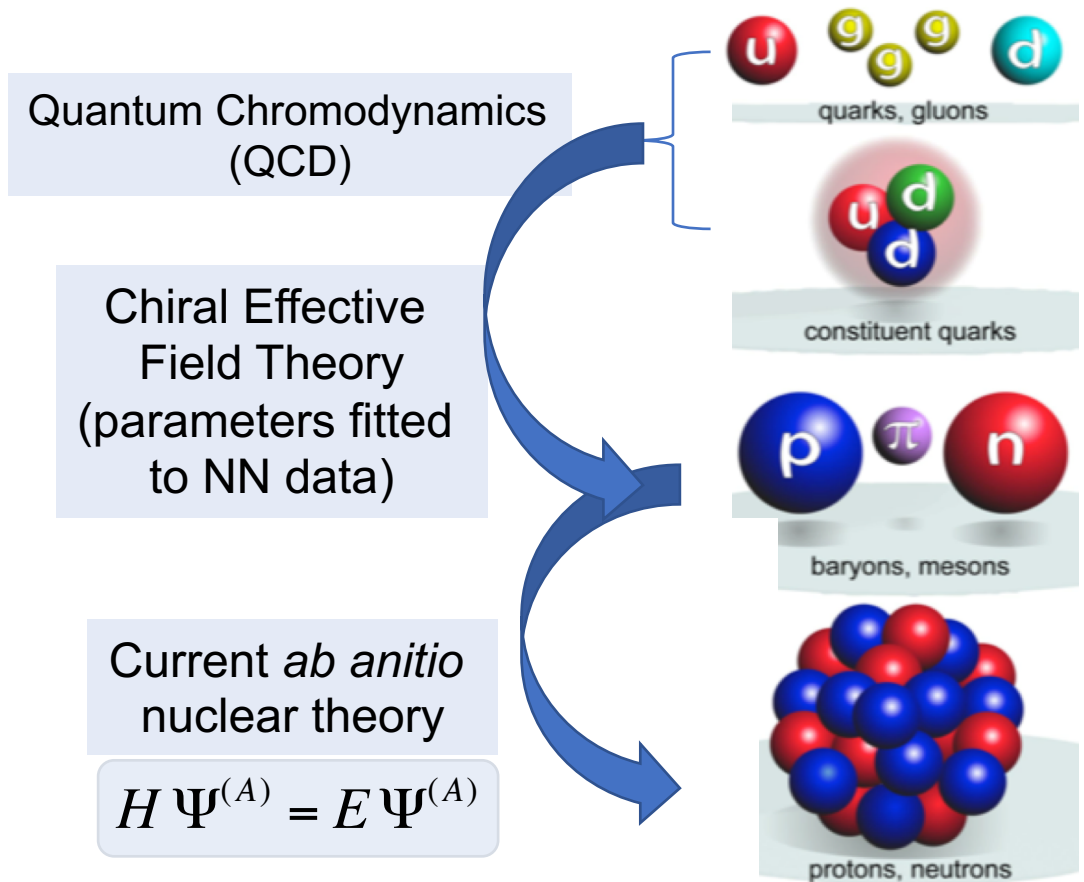
Outline

- Introduction to *ab initio* No-Core Shell Model with Continuum (NCSMC)
- Polarized ${}^3\text{H}(\text{d},\text{n}){}^4\text{He}$ fusion
- ${}^3\text{He}(\alpha,\gamma){}^7\text{Be}$ & ${}^3\text{H}(\alpha,\gamma){}^7\text{Li}$ capture reactions
- ${}^{11}\text{C}(\text{p}, \gamma){}^{12}\text{N}$
- ${}^{14}\text{C}(\text{n}, \gamma){}^{15}\text{C}$

First principles or *ab initio* nuclear theory



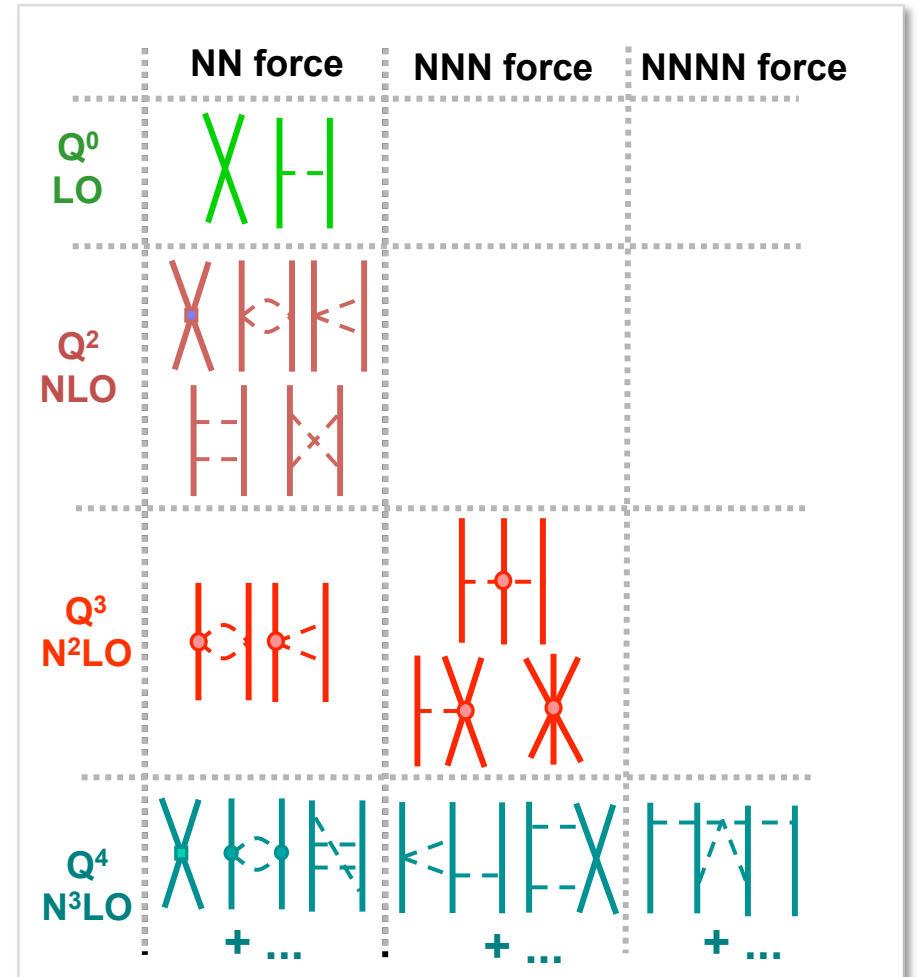
First principles or *ab initio* nuclear theory – what we do at present



- *Ab initio*
 - ✧ Degrees of freedom: Nucleons
 - ✧ All nucleons are active
 - ✧ Exact Pauli principle
 - ✧ Realistic inter-nucleon interactions
 - ✧ Accurate description of NN (and 3N) data
 - ✧ Controllable approximations

Chiral Effective Field Theory

- Inter-nucleon forces from chiral effective field theory
 - 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

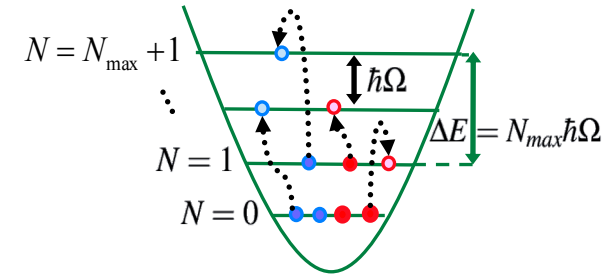
Conceptually simplest *ab initio* method: No-Core Shell Model (NCSM)

6



NCSM

- Basis expansion method
 - 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-coordinate and Slater determinant basis
- Short- and medium range correlations
- Bound-states, narrow resonances



$$(A) \quad \Psi^A = \sum_{N=0}^{N_{\max}} \sum_i c_{Ni} \Phi_{Ni}^{HO}(\vec{\eta}_1, \vec{\eta}_2, \dots, \vec{\eta}_{A-1})$$

$$(A) \quad \Psi_{SD}^A = \sum_{N=0}^{N_{\max}} \sum_j c_{Nj}^{SD} \Phi_{SDNj}^{HO}(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_A) = \Psi^A \varphi_{000}(\vec{R}_{CM})$$

Progress in Particle and Nuclear Physics 69 (2013) 131–181

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journal homepage: www.elsevier.com/locate/ppnp



Review

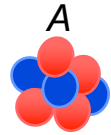
Ab initio no core shell model

Bruce R. Barrett^a, Petr Navrátil^b, James P. Vary^{c,*}

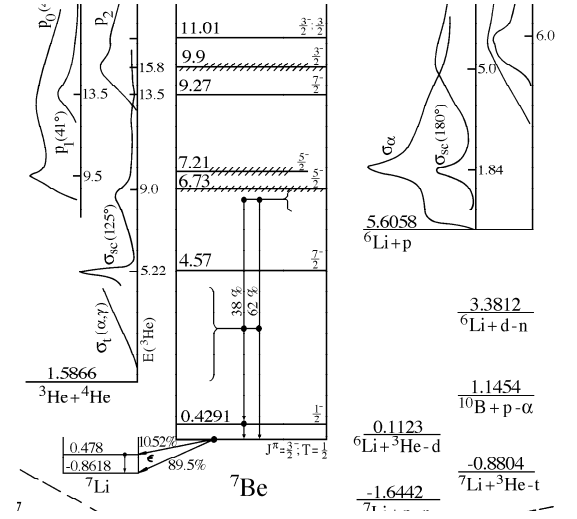
Extending no-core shell model beyond bound states

Include more many nucleon correlations...

NCSM

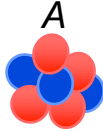


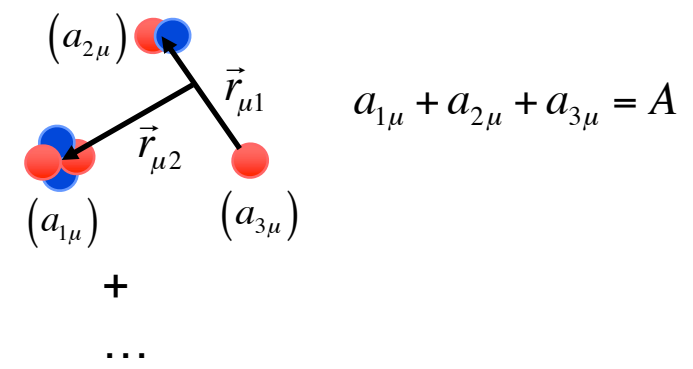
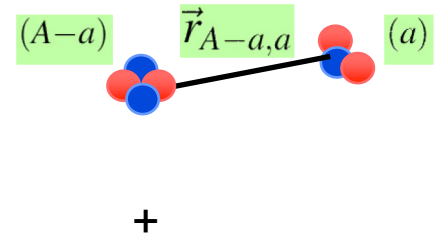
$$\Psi^A = \sum_{N=0}^{N_{\max}} \sum_i c_{Ni} \Phi_{Ni}^A$$



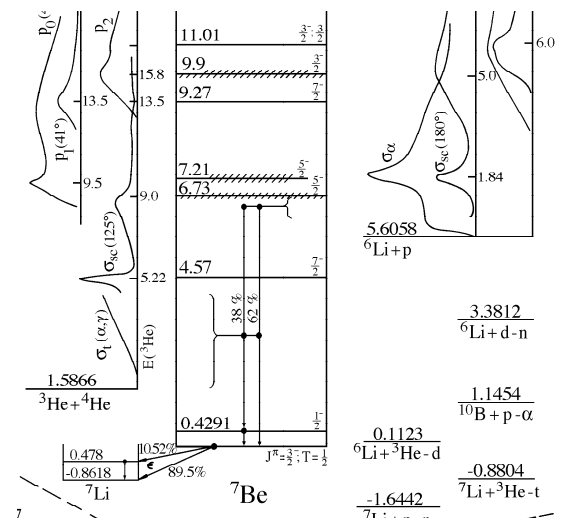
Extending no-core shell model beyond bound states

Include more many nucleon correlations...

NCSM \longrightarrow  $\Psi^A = \sum_{N=0}^{N_{\max}} \sum_i c_{Ni} \Phi_{Ni}^A$

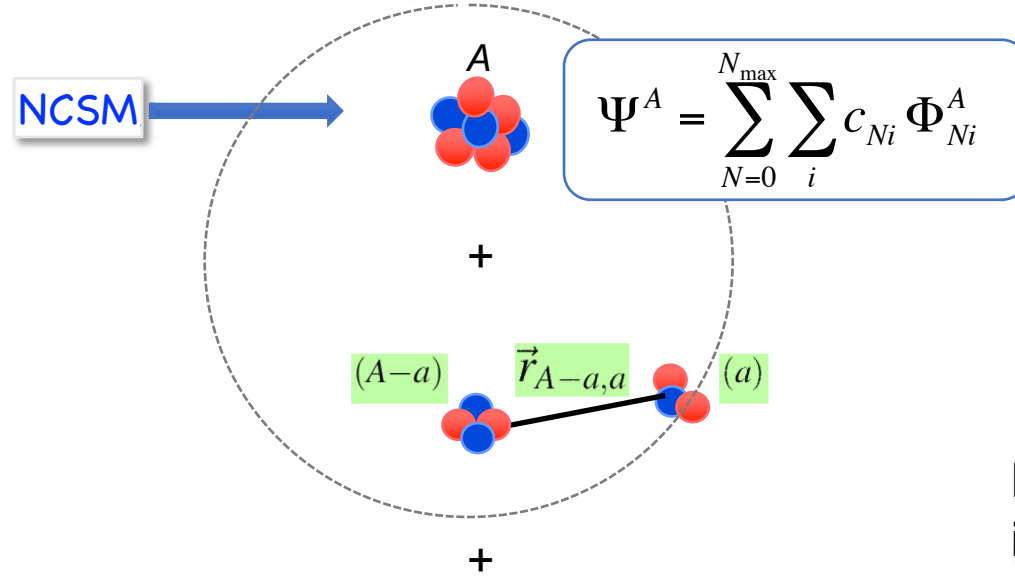


...using the Resonating Group Method (RGM) ideas

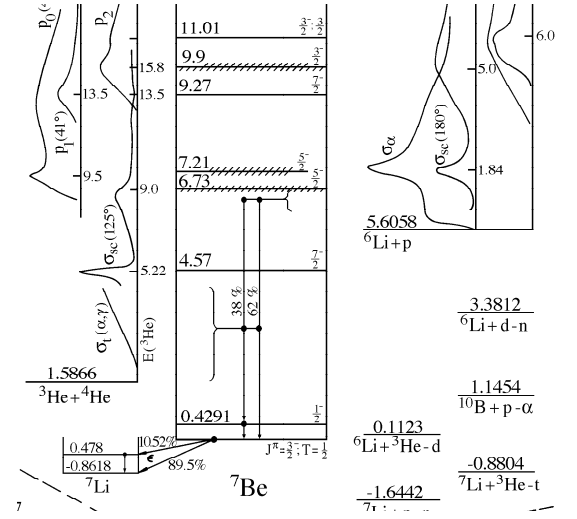


Extending no-core shell model beyond bound states

Include more many nucleon correlations...



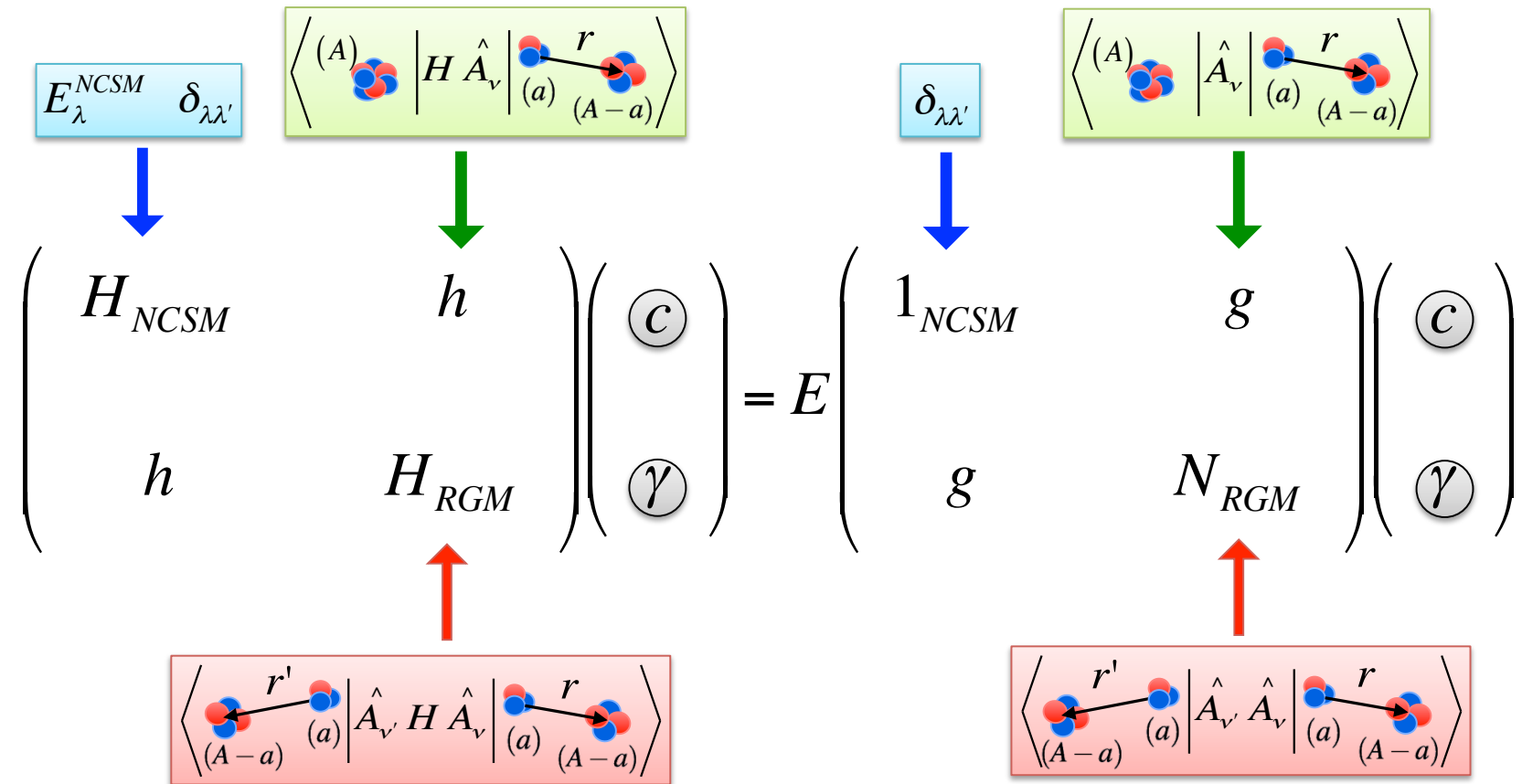
...using the Resonating Group Method (RGM) ideas



Coupled NCSMC equations

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

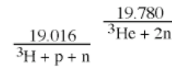
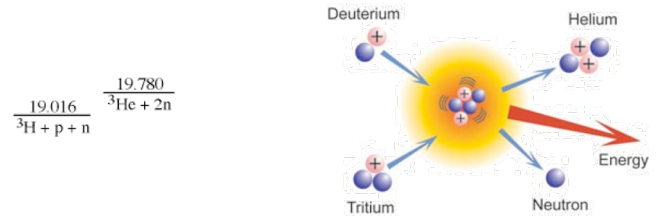
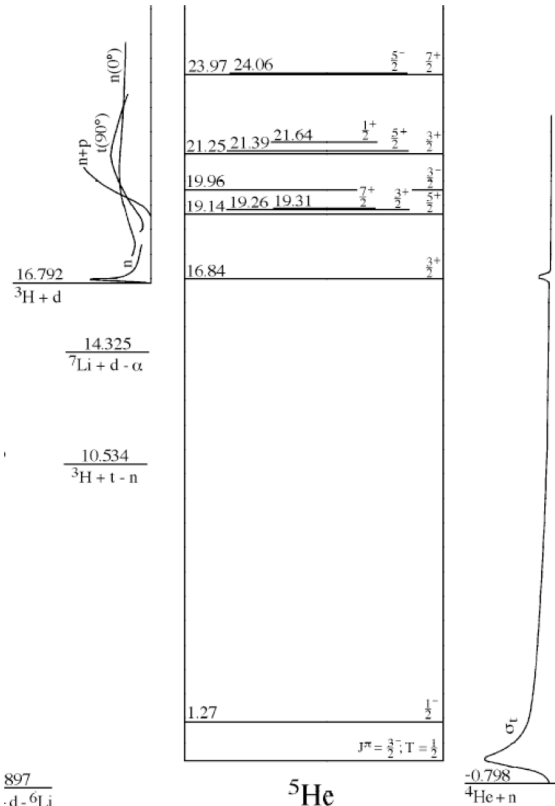
$$\Psi^{(A)} = \sum_{\lambda} c_{\lambda} \left| \begin{matrix} (A) \\ \text{cluster} \end{matrix}, \lambda \right\rangle + \sum_{\nu} \int d\vec{r} \gamma_{\nu}(\vec{r}) \hat{A}_{\nu} \left| \begin{matrix} (A-a) & (a) \\ \text{cluster} & \text{cluster} \end{matrix}, \nu \right\rangle$$



Solved by Microscopic R-matrix theory on a Lagrange mesh – efficient for **coupled channels**

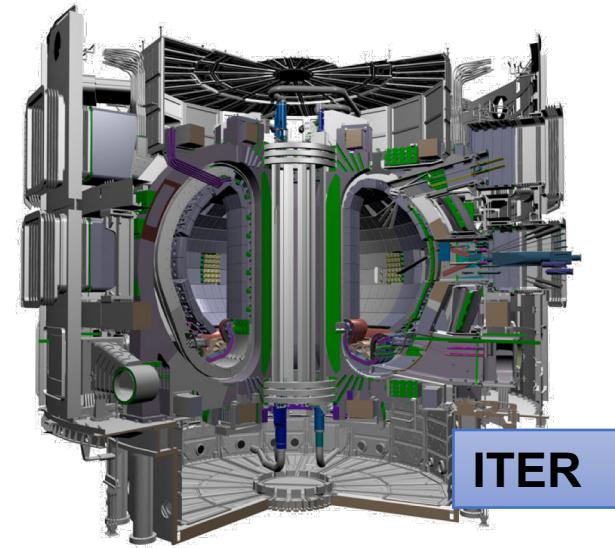
Deuterium-Tritium fusion

- The $d+{}^3\text{H}\rightarrow n+{}^4\text{He}$ reaction
 - The most promising for the production of 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

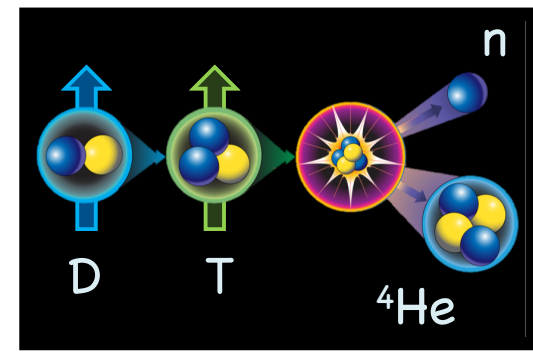


ITER

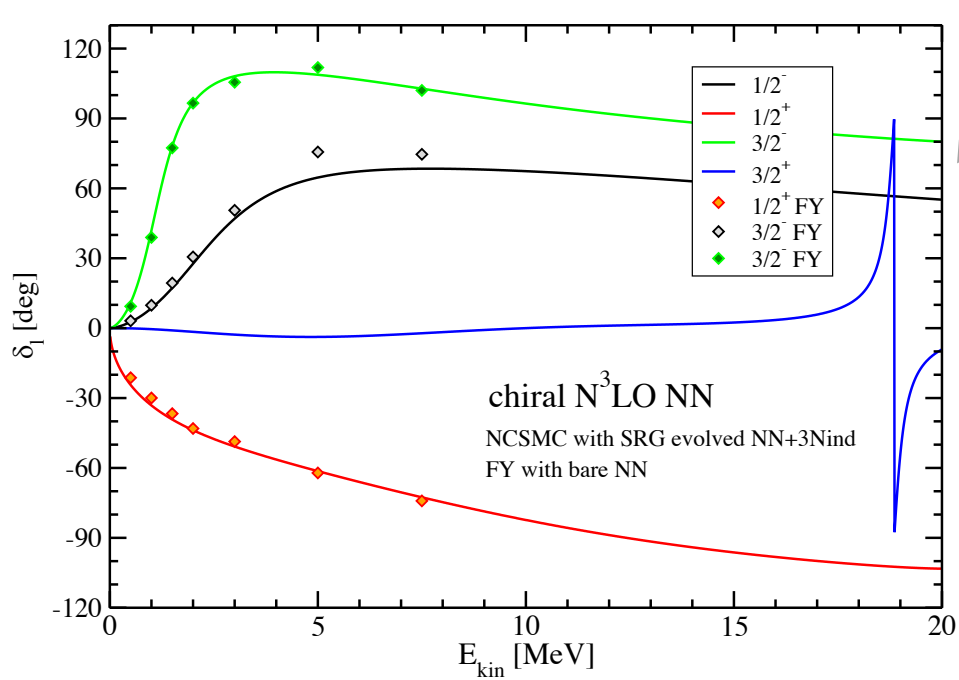
897
d - ${}^6\text{Li}$

-1 877

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

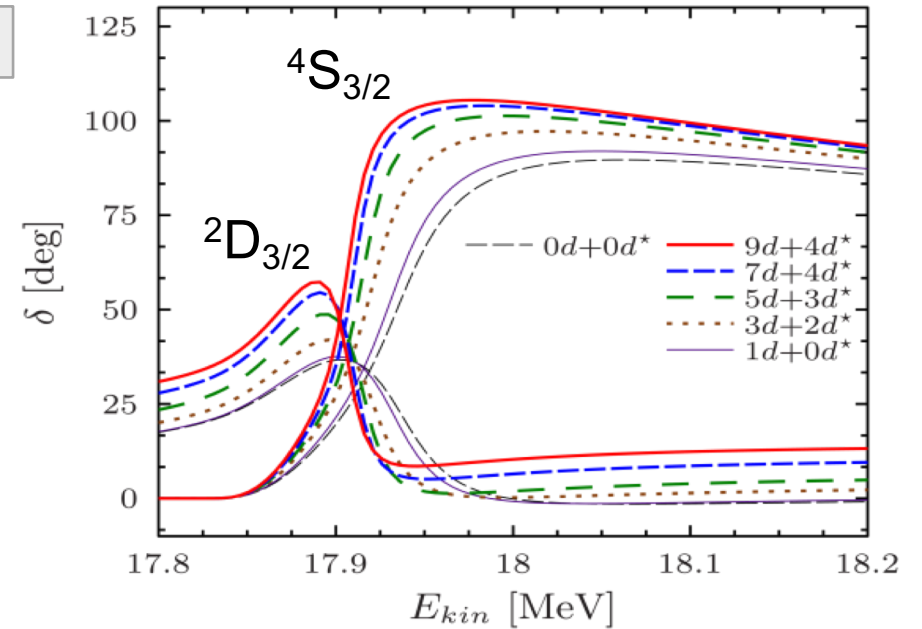


n - ^4He and d + ^3H scattering phase-shifts



$^4\text{He}+n$

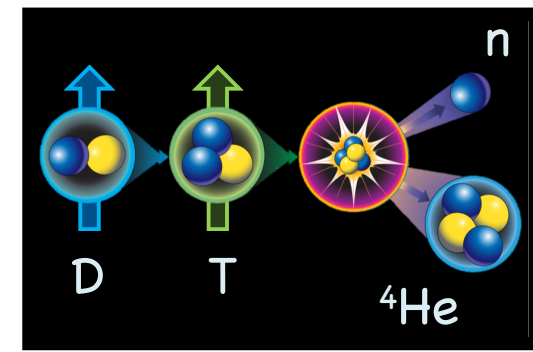
$^4\text{He}+n \rightarrow ^3\text{H}+d$



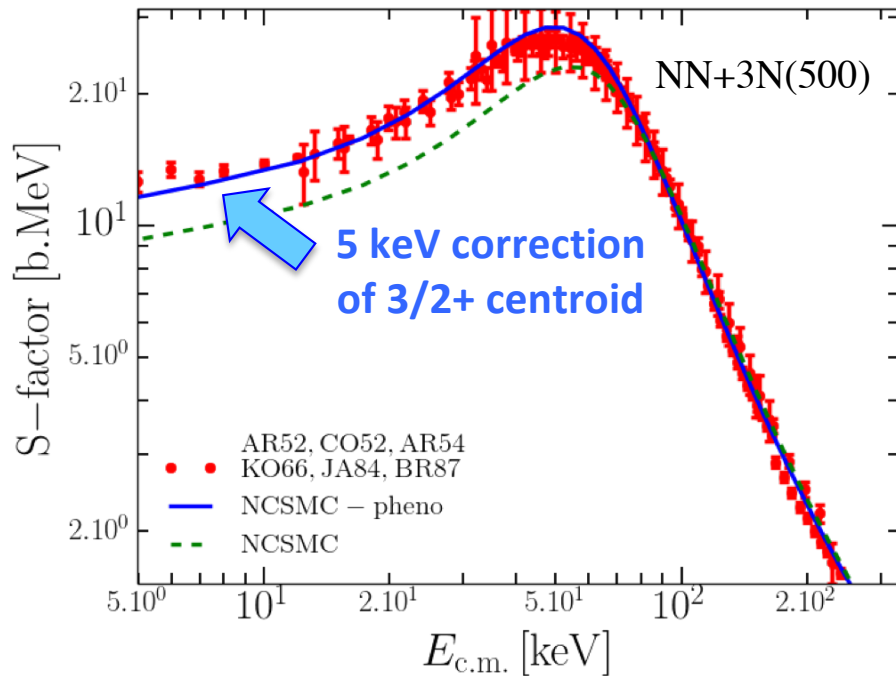
The d - ^3H fusion takes place through a transition of d + ^3H is S-wave to n + ^4He in D-wave: Importance of the **tensor** and **3N** force

FY: Faddeev-Yakubovsky method - Rimantas Lazauskas

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



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

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

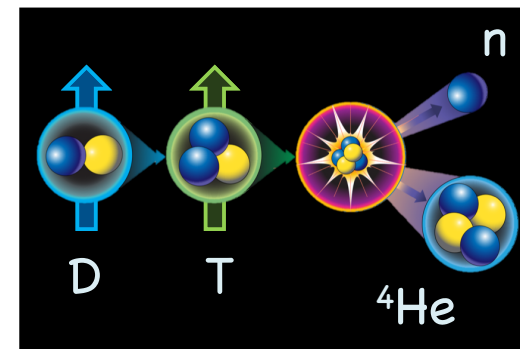
$$\approx \frac{1}{3} \sigma_{\frac{1}{2}} + \frac{2}{3} \sigma_{\frac{3}{2}}$$



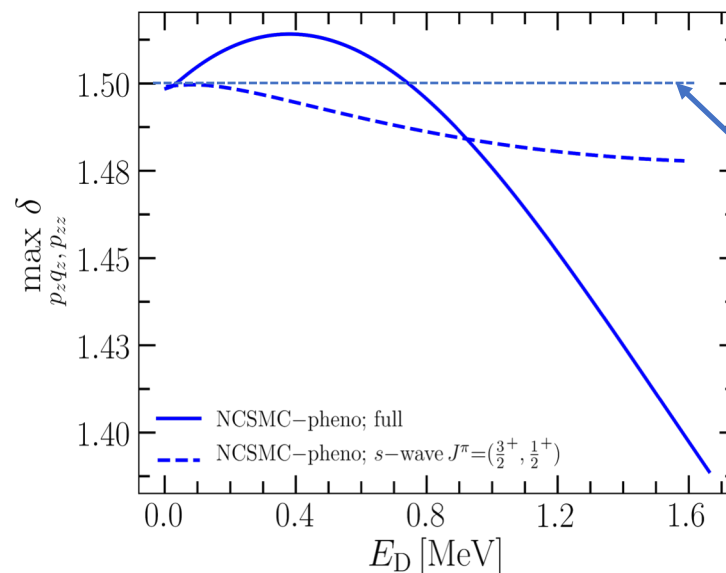
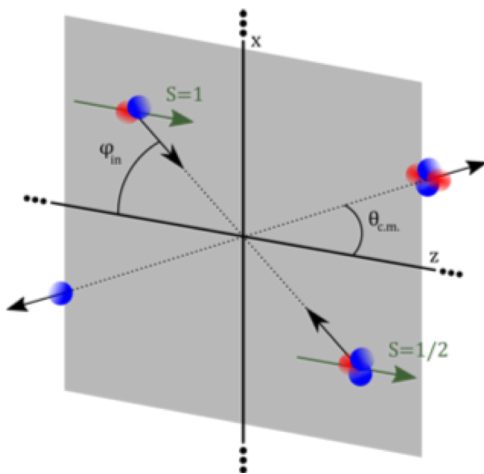
$$\sigma_{pol} \approx 1.5 \sigma_{unpol}$$

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

Polarized fusion



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

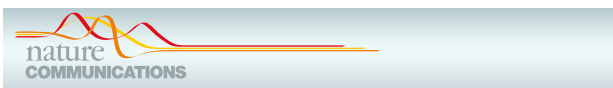


$$\sigma_{unpol} = \sum_J \frac{2J+1}{(2I_D+1)(2I_T+1)} \sigma_J$$

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

↓

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



ARTICLE

<https://doi.org/10.1038/s41467-018-08052-8> OPEN

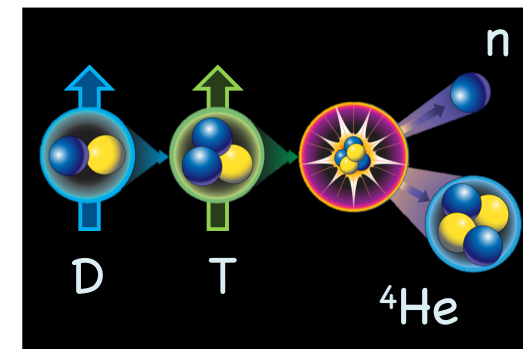
Ab initio predictions for polarized deuterium-tritium thermonuclear fusion

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

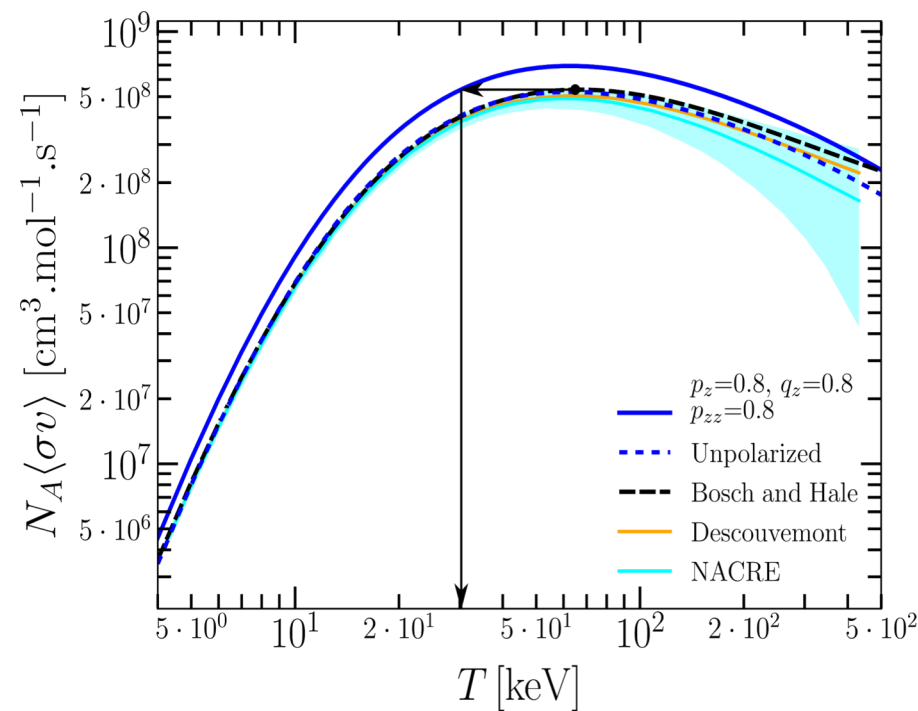
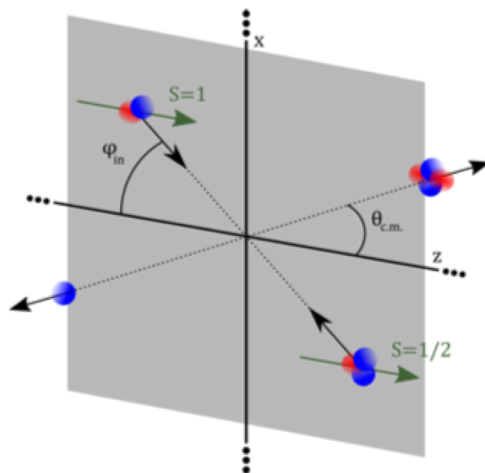
NCSMC calculation demonstrates impact of partial waves with $l > 0$ as well as the contribution of $l = 0$ $J^\pi = 1/2^+$ channel

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

Polarized fusion

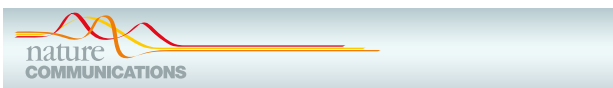


$$\frac{\partial \sigma_{pol}}{\partial \Omega_{c.m.}}(\theta_{c.m.}) = \frac{\partial \sigma_{unpol}}{\partial \Omega_{c.m.}}(\theta_{c.m.}) \left(1 + \frac{1}{2} p_{zz} A_{zz}^{(b)}(\theta_{c.m.}) + \frac{3}{2} p_z q_z C_{z,z}(\theta_{c.m.}) \right)$$

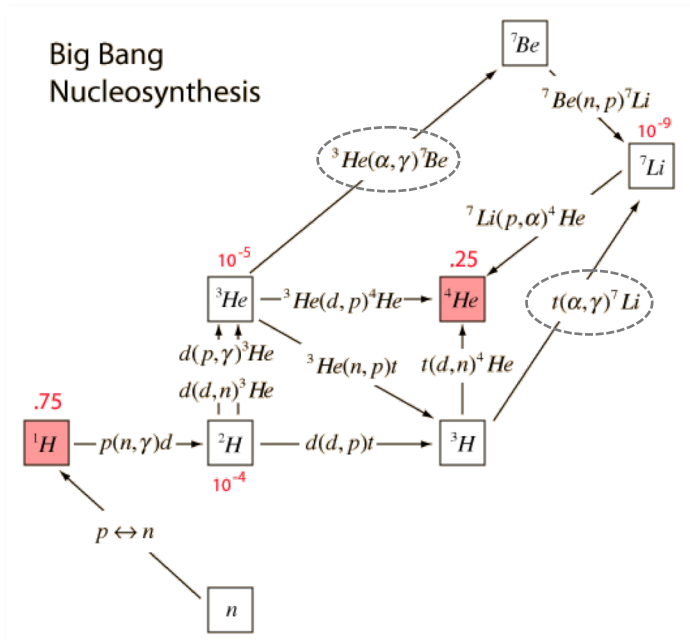
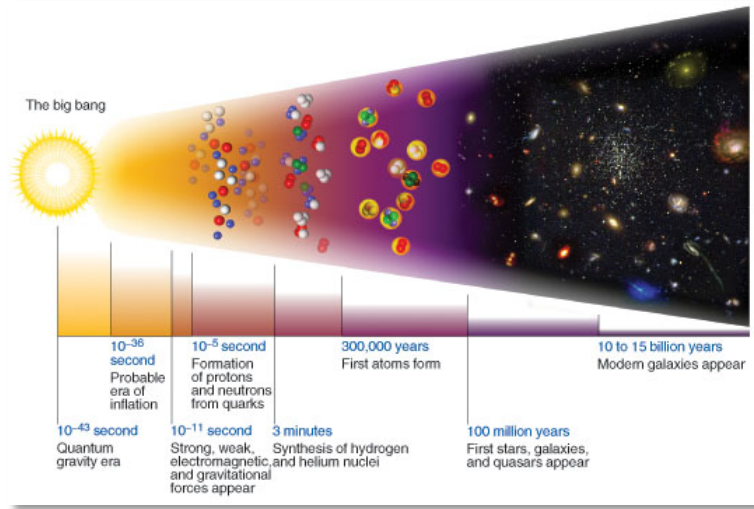


$$\langle \sigma v \rangle = \sqrt{\frac{8}{\pi \mu (k_b T)^3}} \int_0^\infty S(E) \exp\left(-\frac{E}{k_b T} - \sqrt{\frac{E_g}{E}}\right) dE,$$

For a realistic 80% polarization, reaction rate increases by ~32% or the same rate at ~45% lower temperature

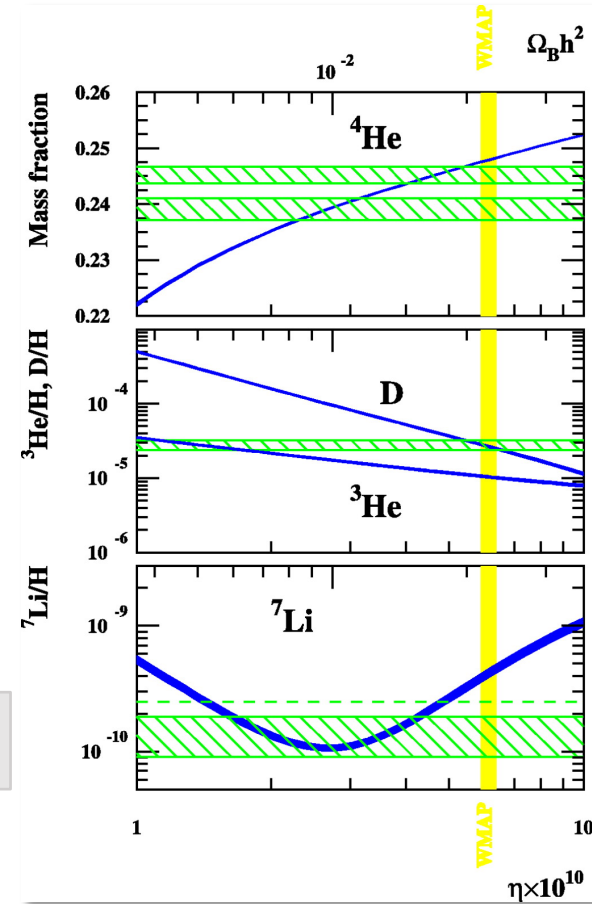


Big Bang nucleosynthesis



Key reactions

⁷Li puzzle



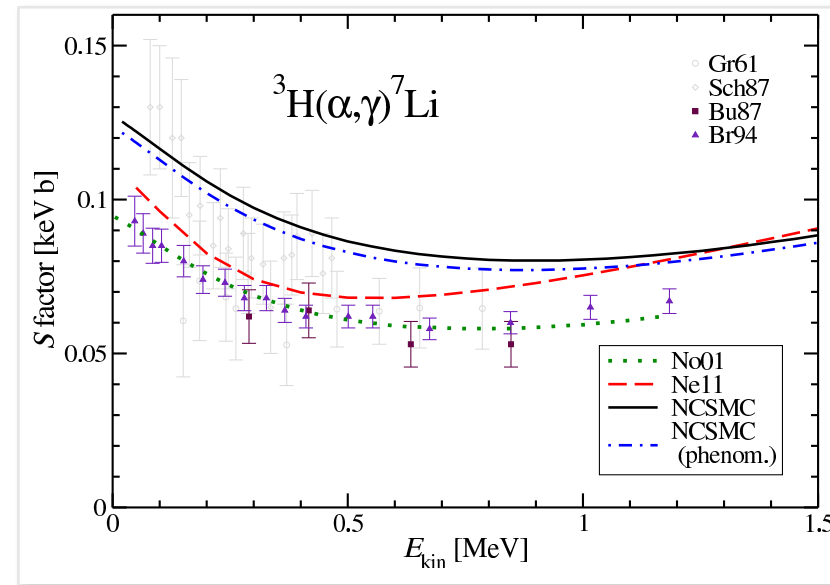
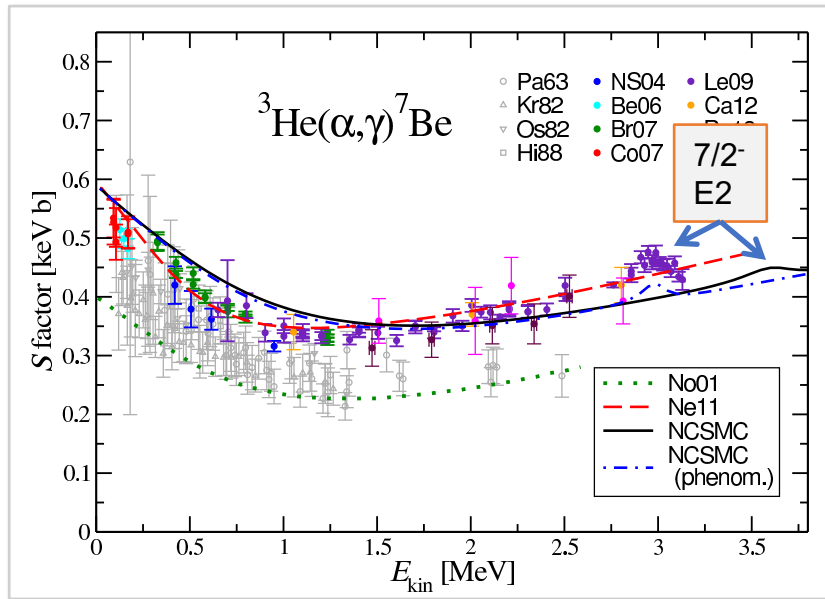
^3He - ^4He and ^3H - ^4He radiative capture

$^3\text{He}(\alpha, \gamma)^7\text{Be}$ and $^3\text{H}(\alpha, \gamma)^7\text{Li}$ astrophysical S factors from the no-core shell model with continuum



Jérémy Dohet-Eraly^{a,*}, Petr Navrátil^a, Sofia Quaglioni^b, Wataru Horiuchi^c,
Guillaume Hupin^{b,d,1}, Francesco Raimondi^{a,2}

E1 radiative capture with small E2 contribution at $7/2^-$ resonance



Theoretical calculations suggest that the most recent and precise ^7Be and ^7Li data are inconsistent

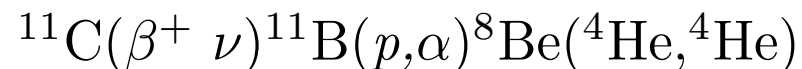
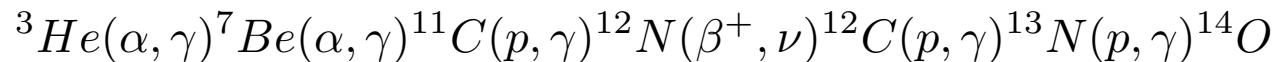
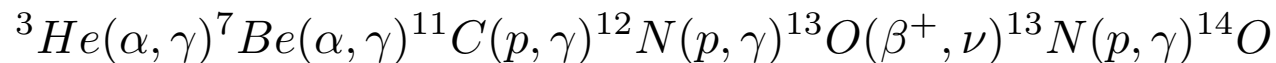
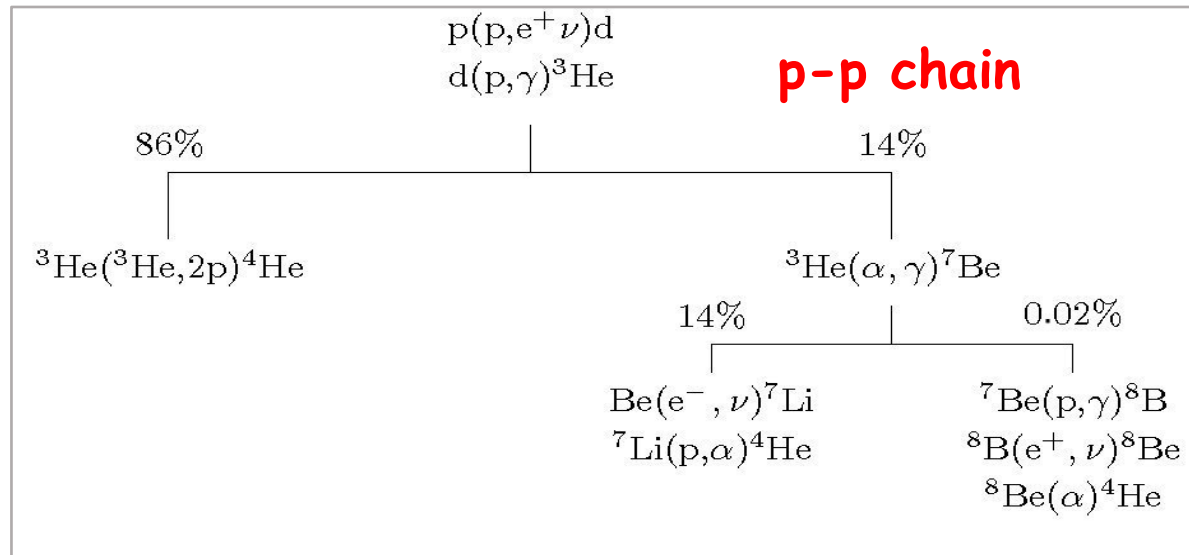
NCSMC calculations with chiral SRG- N^3LO NN potential ($\lambda=2.15 \text{ fm}^{-1}$)

^3He , ^3H , ^4He ground state, $8(\pi^-) + 6(\pi^+)$ eigenstates of ^7Be and ^7Li

Preliminary: $N_{\text{max}}=12$, $h\Omega=20 \text{ MeV}$

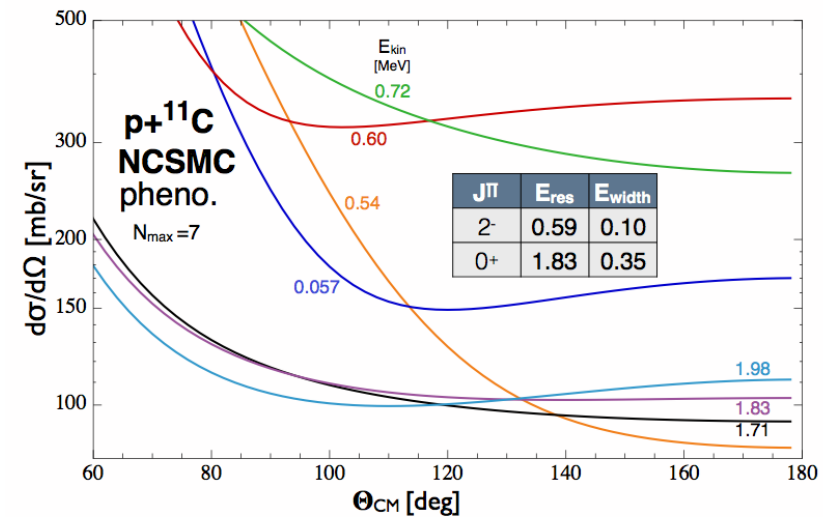
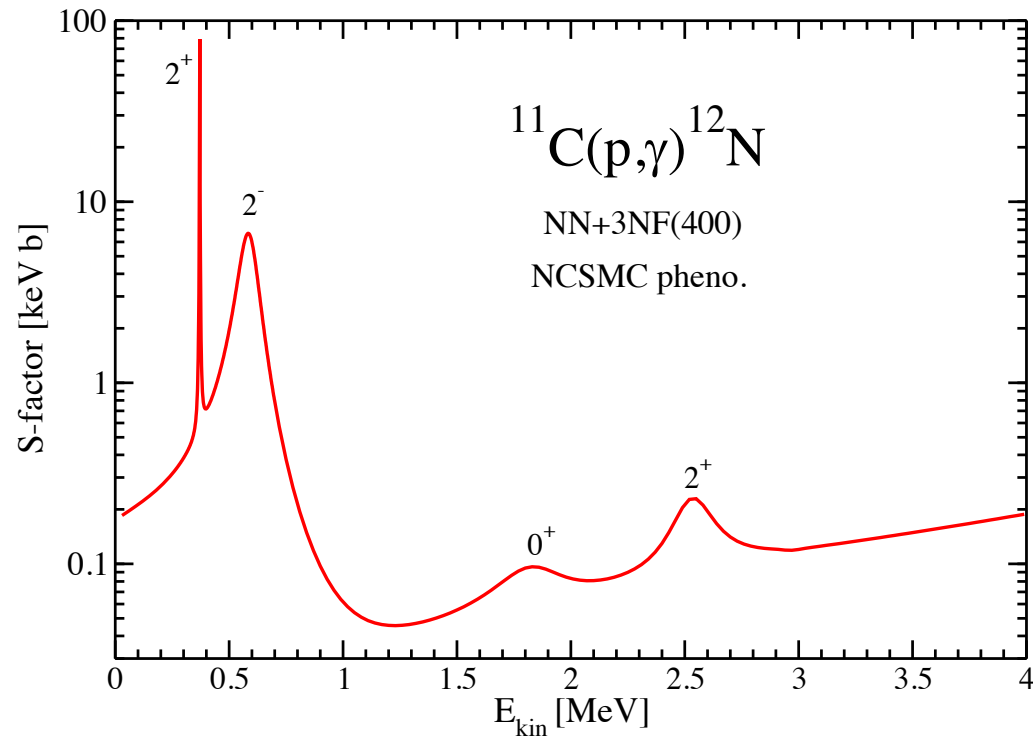
p+¹¹C scattering and ¹¹C(p,γ)¹²N capture

- ¹¹C(p,γ)¹²N capture relevant in hot *p-p* chain: Link between pp chain and the CNO cycle - bypass of slow triple alpha capture ⁴He(αα,γ)¹²C



$p+^{11}\text{C}$ scattering and $^{11}\text{C}(p,\gamma)^{12}\text{N}$ capture

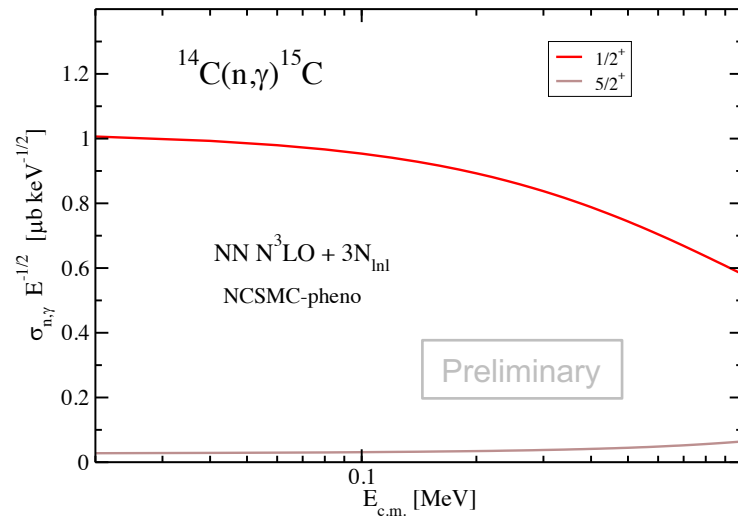
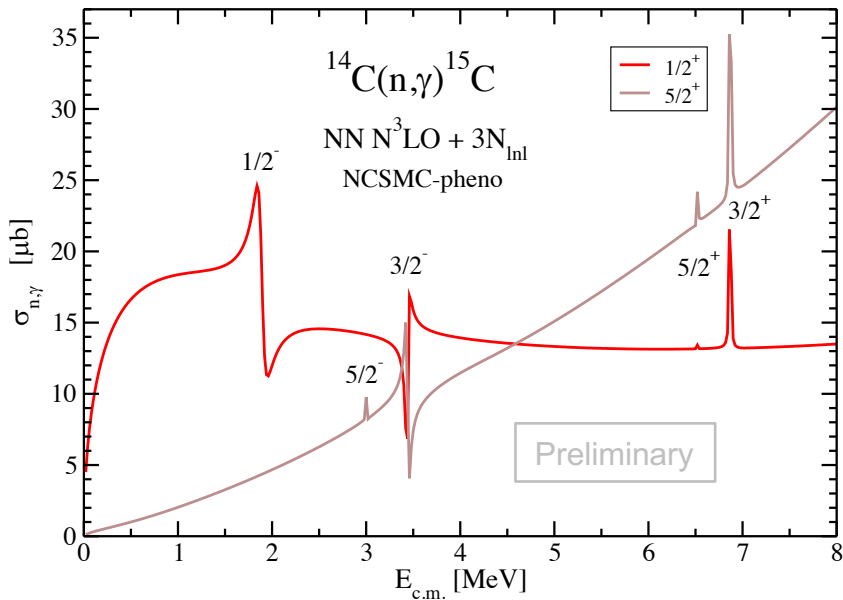
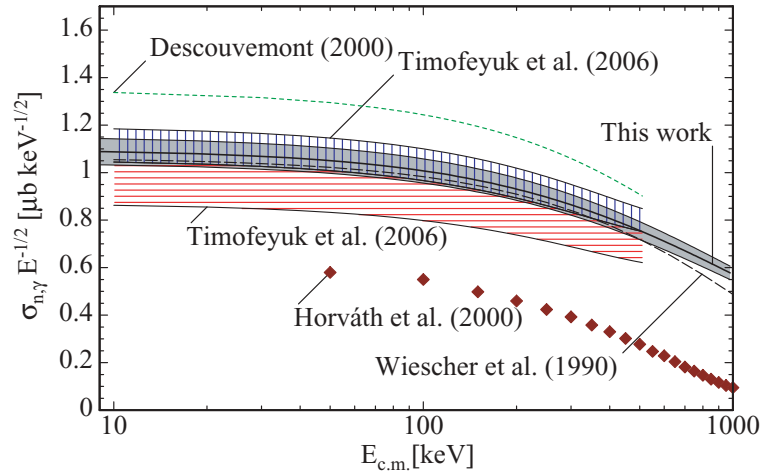
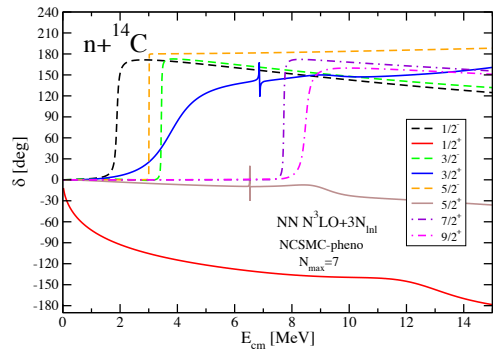
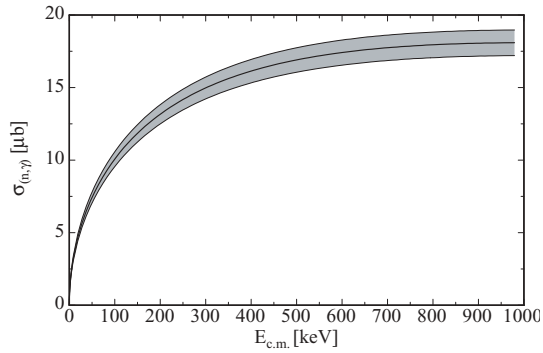
- NCSMC calculations of $^{11}\text{C}(p,p)$ with chiral NN+3N under way
 - ^{11}C : $3/2^-$, $1/2^-$, $5/2^-$, $3/2^-$ NCSM eigenstates
 - ^{12}N : ≥ 6 $\pi = +1$ and ≥ 4 $\pi = -1$ NCSM eigenstates



NCSMC calculations to be validated by TRIUMF scattering cross section measurement and applied to calculate the $^{11}\text{C}(p,\gamma)^{12}\text{N}$ capture

$^{14}\text{C}(n,\gamma)^{15}\text{C}$ capture cross section

- Comparison to Karlsruhe experiment – Phys. Rev. C 77, 015804 (2008)



- Relevant for
- Inhomogeneous Big Bang models
- Neutron induced CNO cycles
- Neutrino driven wind models for the r-process
- Validation of Coulomb dissociation method

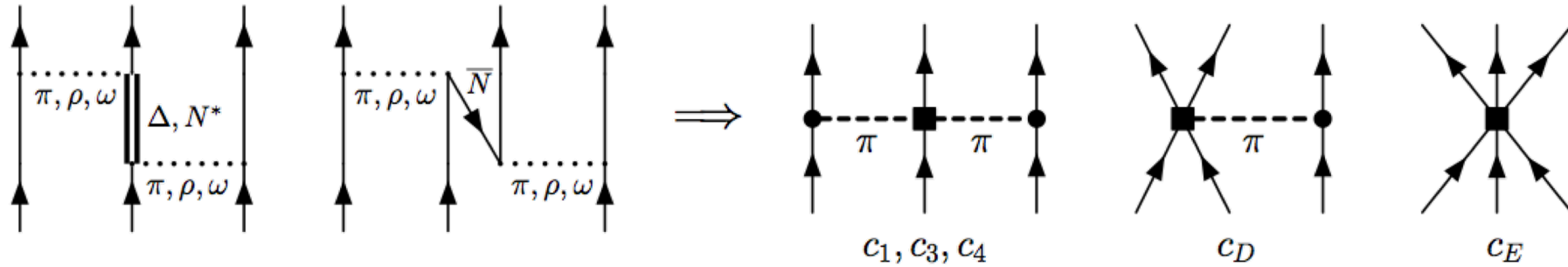
Conclusions

- *Ab initio* calculations of nuclear structure and reactions becoming feasible beyond the lightest nuclei
 - Make connections between the low-energy QCD, many-body systems, and nuclear astrophysics
- Polarized DT fusion investigated within NCSMC
 - Sheds light on importance of $l > 0$ partial waves
- Analysis of ${}^3\text{He}(\alpha, \gamma){}^7\text{Be}$ & ${}^3\text{H}(\alpha, \gamma){}^7\text{Li}$ capture reactions
 - Experimental data inconsistent
- NCSMC applied to predict for ${}^{11}\text{C}(p, \gamma){}^{12}\text{N}$ capture
 - Support for upcoming TRIUMF ${}^{11}\text{C}+p$ scattering experiment
- NCSMC calculations of ${}^{15}\text{C}$ *sd*-shell halo nucleus in progress
 - ${}^{14}\text{C}(n, \gamma){}^{15}\text{C}$ capture cross section in agreement with experiment

Thank you!
Merci!



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

The question is not: Do three-body forces enter the description?

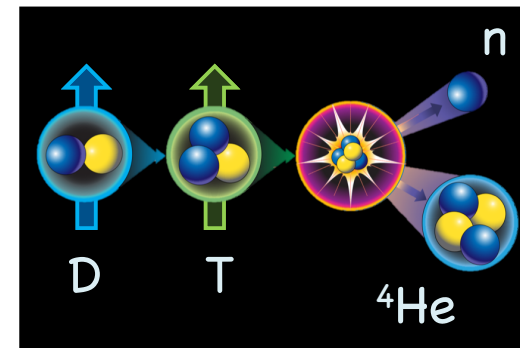
The only question is: How large are three-body forces?

NCSMC calculation of the DT fusion

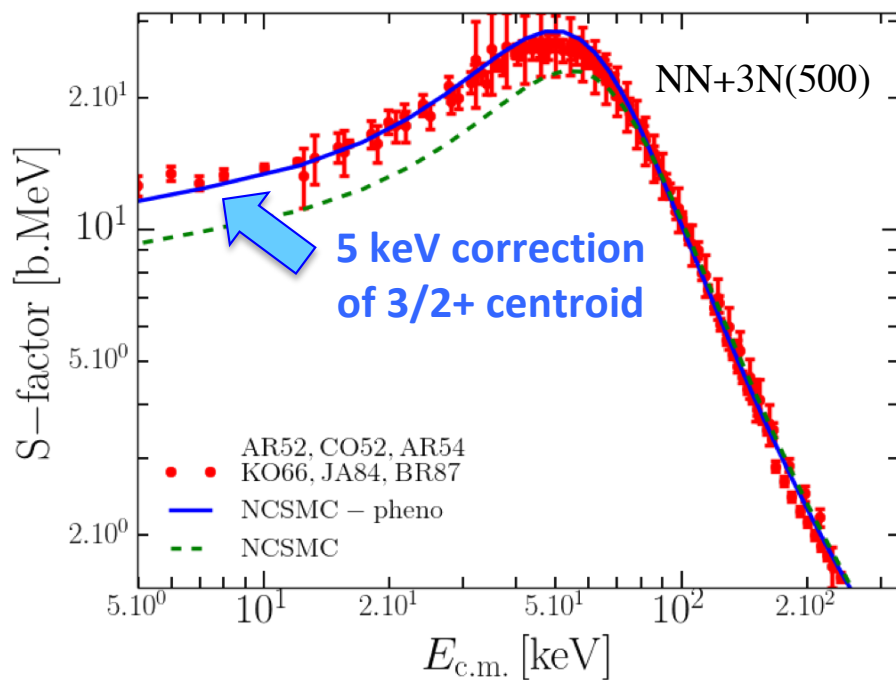
$$|\Psi\rangle = \sum_{\lambda} c_{\lambda} \left| \begin{array}{c} \text{5He} \\ \text{He} \end{array}, \lambda \right\rangle + \int d\vec{r} u_{\nu_{DT}}(\vec{r}) \hat{A}_{DT} \left| \begin{array}{c} \text{D} \\ \text{T} \end{array}, \nu_{DT} \right\rangle + \int d\vec{r} u_{\nu_{n\alpha}}(\vec{r})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

- 2x7 static ${}^5\text{He}$ 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- ${}^4\text{He}$ (g.s.) cluster states (exit channel)
- Chiral NN+3N(500) interaction

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



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

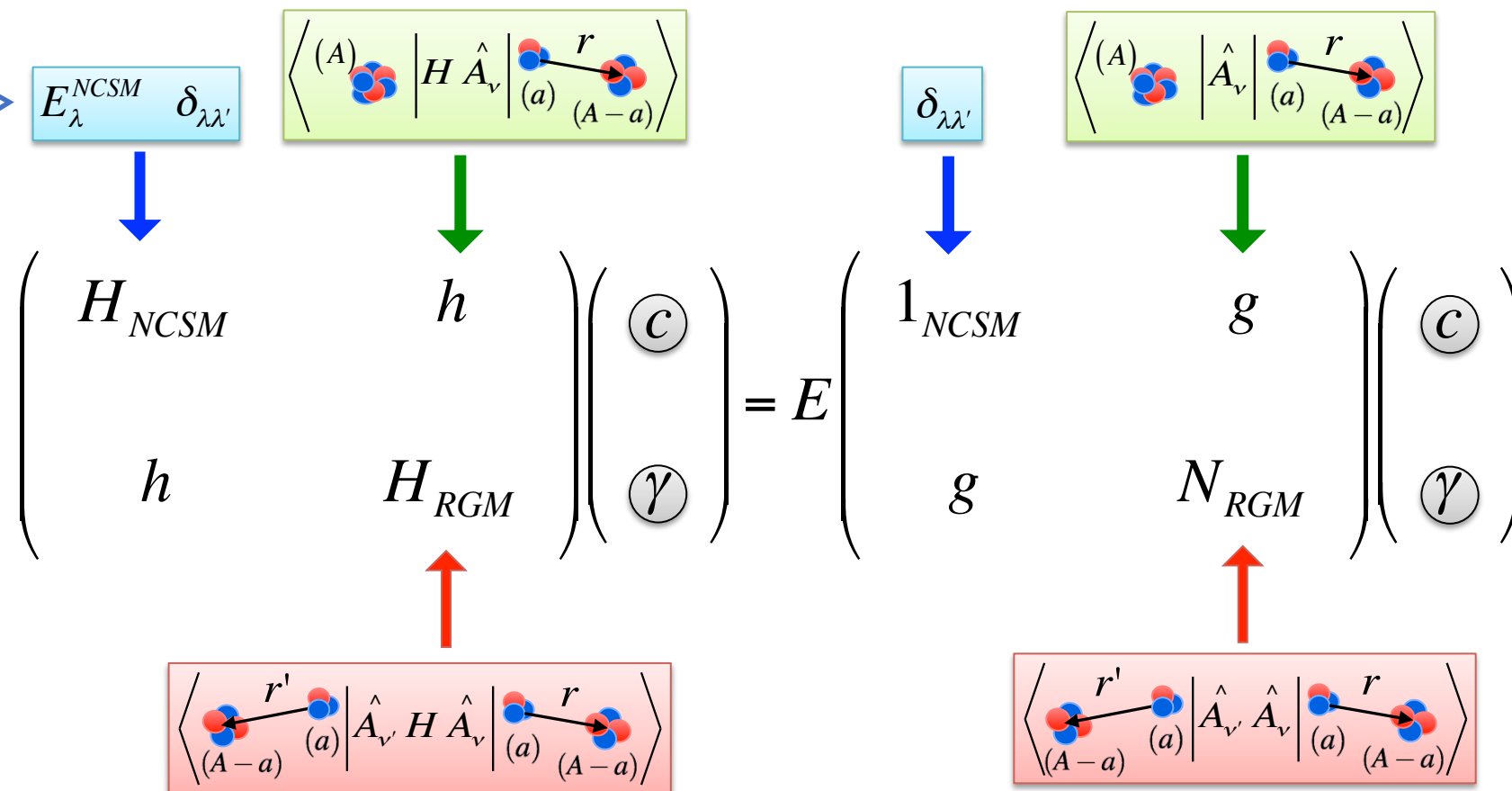
'Coulomb' Contribution (tunneling)

NCSMC phenomenology

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

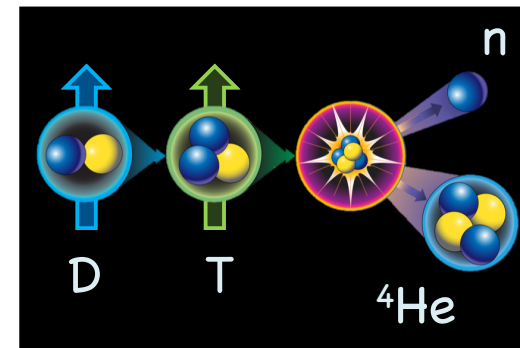
$$\Psi^{(A)} = \sum_{\lambda} c_{\lambda} \left| \begin{matrix} (A) \\ \text{cluster} \end{matrix}, \lambda \right\rangle + \sum_{\nu} \int d\vec{r} \gamma_{\nu}(\vec{r}) \hat{A}_{\nu} \left| \begin{matrix} (A-a) & (a) \\ \text{cluster} & \text{cluster} \end{matrix}, \nu \right\rangle$$

E_{λ}^{NCSM} energies treated as adjustable parameters

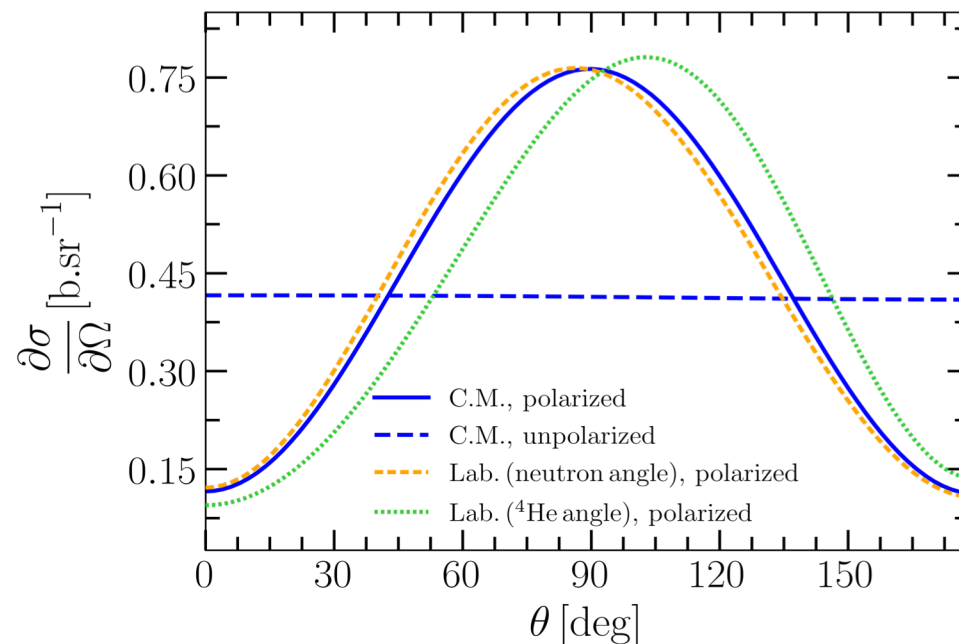
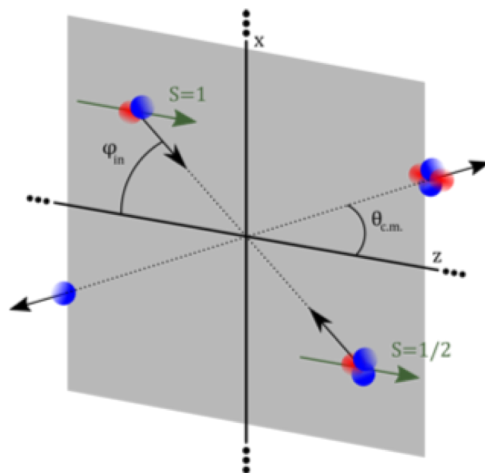


$^3\text{H}(d,n)^4\text{He}$ with chiral NN+3N(500) interaction

Polarized fusion



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



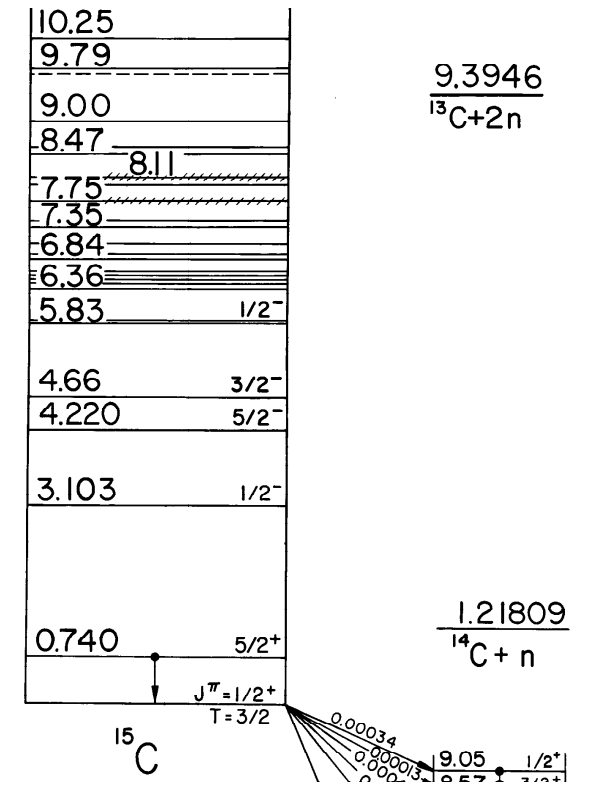
For a realistic 80% polarization, outgoing neutrons and alphas emitted dominantly in the perpendicular direction to the magnetic field



Halo *sd*-shell nucleus ^{15}C and its unbound mirror ^{15}F

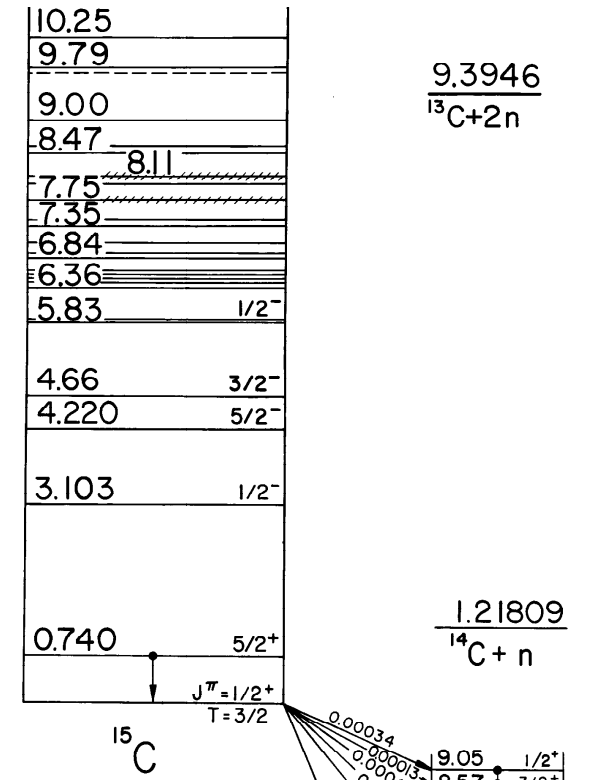
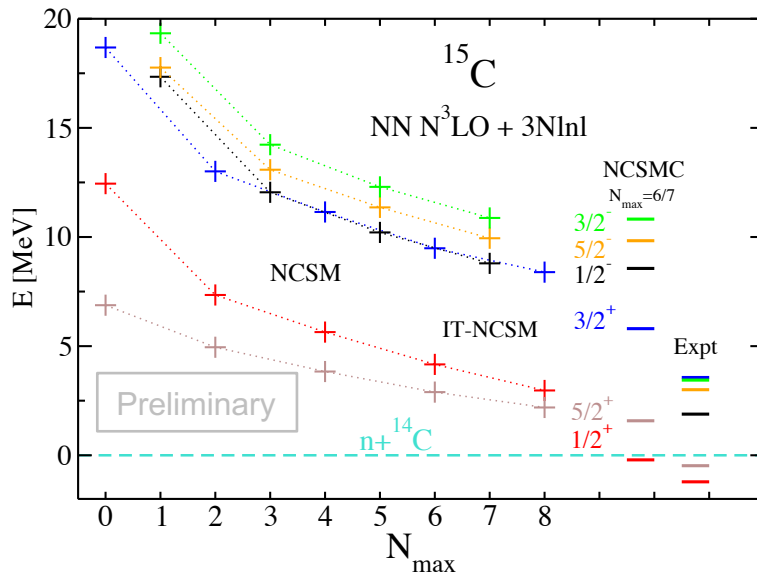
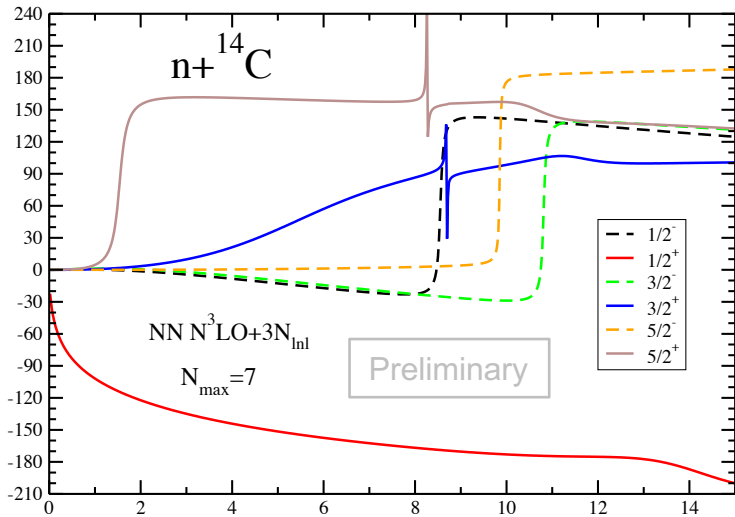
- Motivation:
 - Halo $1/2^+$ S-wave and $5/2^+$ D-wave bound states
 - $^{14}\text{C}(n,\gamma)^{15}\text{C}$ capture relevant for astrophysics
 - Unbound ^{15}F mirror – very narrow unnatural parity resonances embedded in continuum predicted in $^{14}\text{O}(p,p)^{14}\text{O}$
 - measured at GANIL

- Calculations in progress – all results preliminary
- NN chiral interaction – N³LO Entem & Machleidt 2003, SRG evolved with $\lambda = 2.0 \text{ fm}^{-1}$
- 3N chiral interaction – N²LO with local/non-local regulator, SRG evolved with $\lambda = 2.0 \text{ fm}^{-1}$



Halo *sd*-shell nucleus ^{15}C

- NCSMC
 - ^{14}C (^{14}O) 0^+ and 2^+ eigenstates
 - ^{15}C (^{15}F) lowest 7 positive and 3 negative parity eigenstates



Halo *sd*-shell nucleus ^{15}C

- NCSMC
 - ^{14}C (^{14}O) 0^+ and 2^+ eigenstates
 - ^{15}C (^{15}F) lowest 7 positive and 3 negative parity eigenstates

NCSMC-pheno

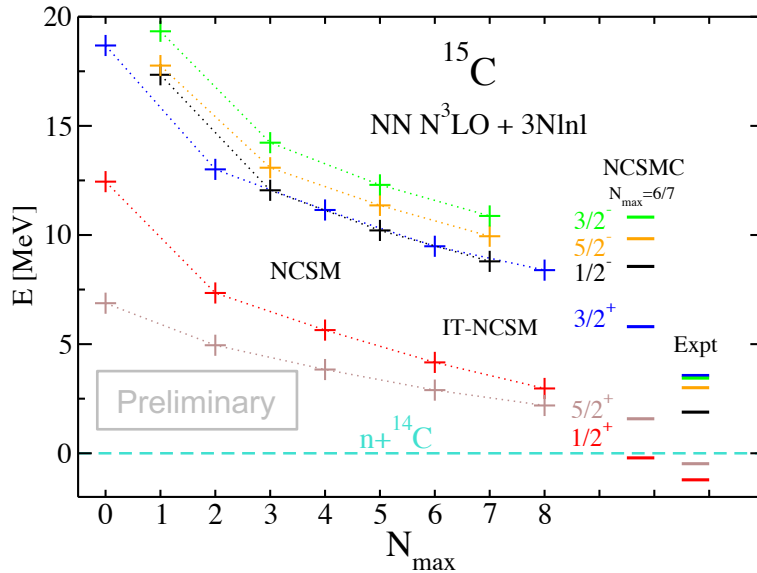
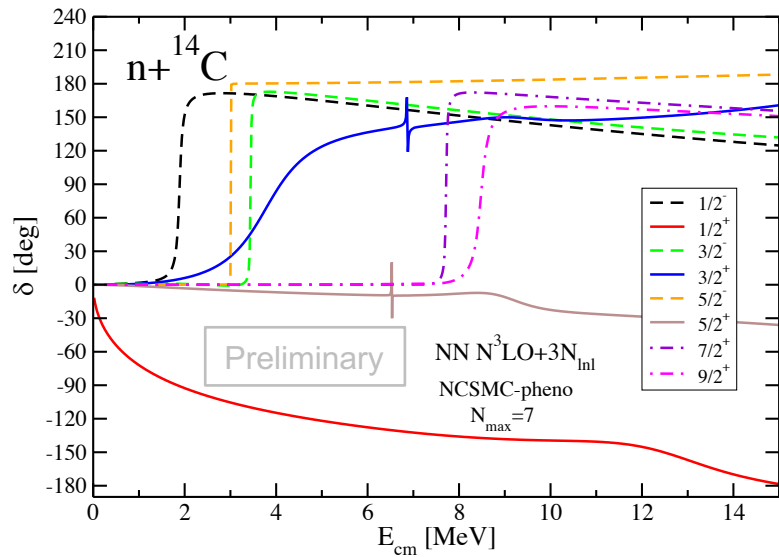


Table 15.1 from (1991AJ01): Energy levels of ^{15}C ^a

E_x (MeV \pm keV)	$J^\pi; T$	τ or $\Gamma_{\text{c.m.}}$ (keV)	Decay	Reactions
g.s.	$\frac{1}{2}^+; \frac{3}{2}$	$\tau_{1/2} = 2.449 \pm 0.005$ s $ g = 2.63 \pm 0.14$	β^-	1, 2, 3, 4, 6, 7, 9
0.7400 ± 1.5	$\frac{5}{2}^+$	$\tau_m = 3.76 \pm 0.10$ ns $g = -0.703 \pm 0.012$	γ	2, 3, 4, 7, 8
3.103 ± 4	$\frac{1}{2}^-$	$\Gamma_{\text{c.m.}} \leq 40$		2, 3, 9
4.220 ± 3	$\frac{5}{2}^-$	< 14		2, 3
4.657 ± 9	$\frac{3}{2}^-$			2, 3
4.78 ± 100	$\frac{3}{2}^+$	1740 ± 400		6
5.833 ± 20	$(\frac{3}{2}^+)$	64 ± 8		2, 6
5.866 ± 8	$\frac{1}{2}^-$			2, 3
6.358 ± 6	$(\frac{5}{2}^+, \frac{7}{2}^+, \frac{9}{2}^+)$	< 20		2, 3
6.417 ± 6	$(\frac{3}{2}^-, \frac{7}{2}^-)$	≈ 50		2, 3
6.449 ± 7	$(\frac{9}{2}^-, \frac{11}{2}^-)$	< 14		2, 3
6.536 ± 4	^a	< 14		2, 3
6.626 ± 8	$(\frac{3}{2}^-)$	20 ± 10		2, 3
6.841 ± 4	^a	< 14		2, 3
6.881 ± 4	$(\frac{9}{2}^-)$ ^a	< 20		2, 3
7.095 ± 4	$(\frac{3}{2}^-)$	< 15		2, 3
7.352 ± 6	$(\frac{9}{2}^-, \frac{11}{2}^-)$	20 ± 10		2, 4
7.414 ± 20				2
7.75 ± 30 ^b				2
8.01 ± 30				2

^{15}C cluster form factors

- $1/2^+$ S-wave and $5/2^+$ D-wave ANCs

- $C_{1/2^+} = 1.282 \text{ fm}^{-1/2}$ - compare to Moschini & Capel inferred from transfer data: $1.26(2) \text{ fm}^{-1/2}$
- $C_{5/2^+} = 0.048 \text{ fm}^{-1/2}$ $0.056(1) \text{ fm}^{-1/2}$
- Spectroscopic factors: 0.96 for $1/2^+$ and 0.90 for $5/2^+$ - experiments 0.95(5) and 0.69, resp.

