

Nuclear scattering and reactions from *ab initio* no-core shell model with continuum

Open Quantum Systems: From atomic nuclei to ultracold atoms and quantum optics

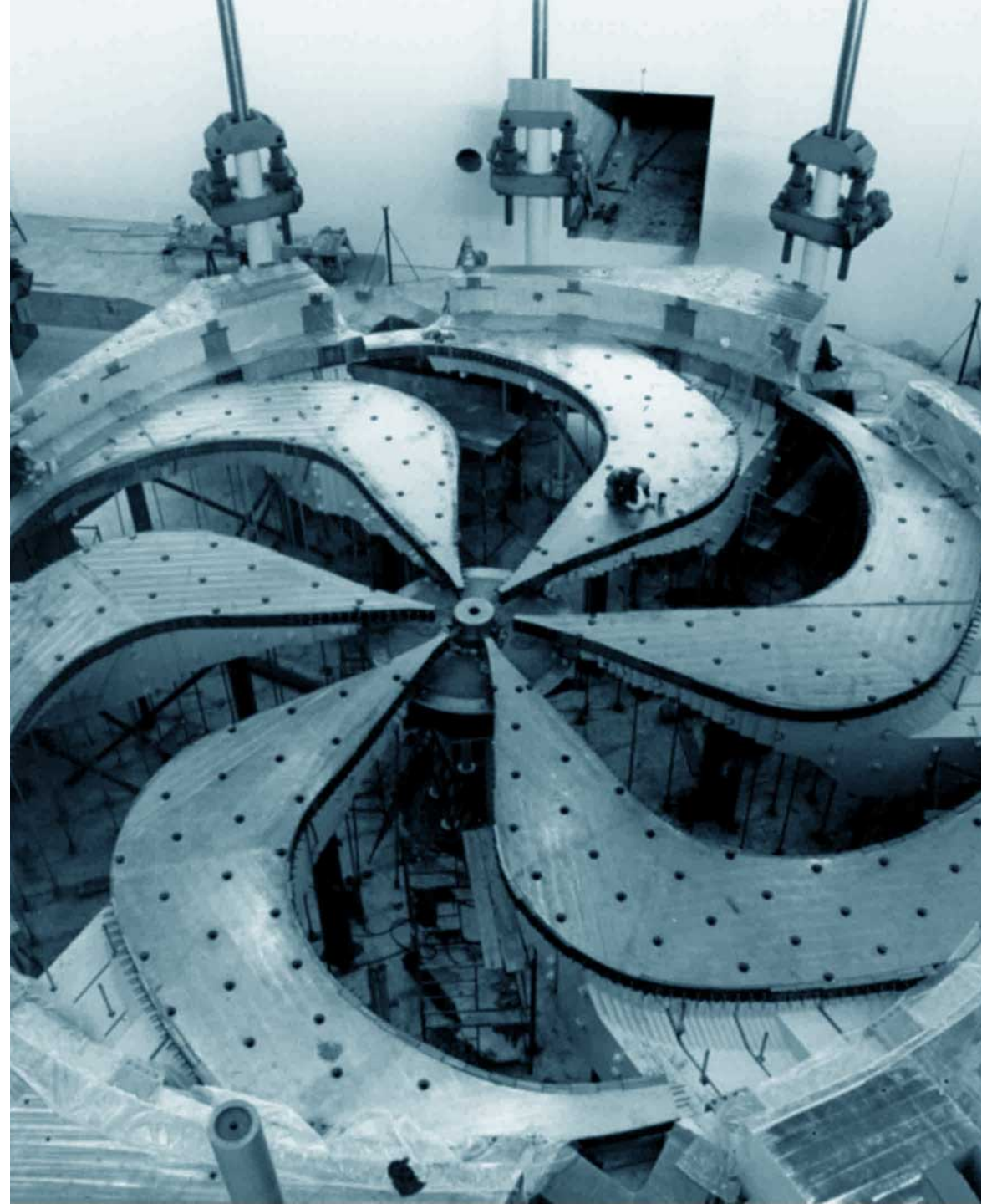
ECT* Trento, Italy, September 30 – October 4, 2019

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M. Vorabbi, A. Calci (TRIUMF), P. Gysbers (UBC/TRIUMF),
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2019-10-04



Outline

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- Introduction to *ab initio* No-Core Shell Model with Continuum (NCSMC)
- Polarized ${}^3\text{H}(\text{d},\text{n}){}^4\text{He}$ fusion
- Structure of ${}^7\text{Be}$ and ${}^7\text{Li}$ from different binary-mass partitions
- ${}^{11}\text{C}(\text{p},\gamma){}^{12}\text{N}$ capture
- Structure of the halo *sd*-shell nucleus ${}^{15}\text{C}$

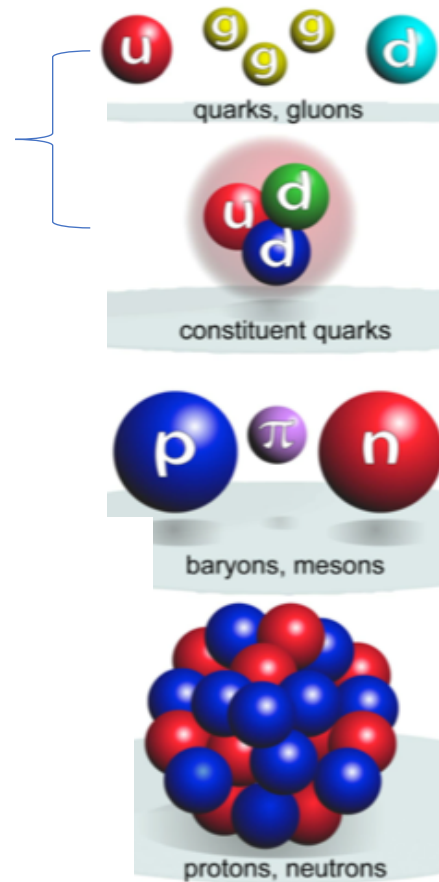
First principles or *ab initio* nuclear theory

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Quantum Chromodynamics
(QCD)

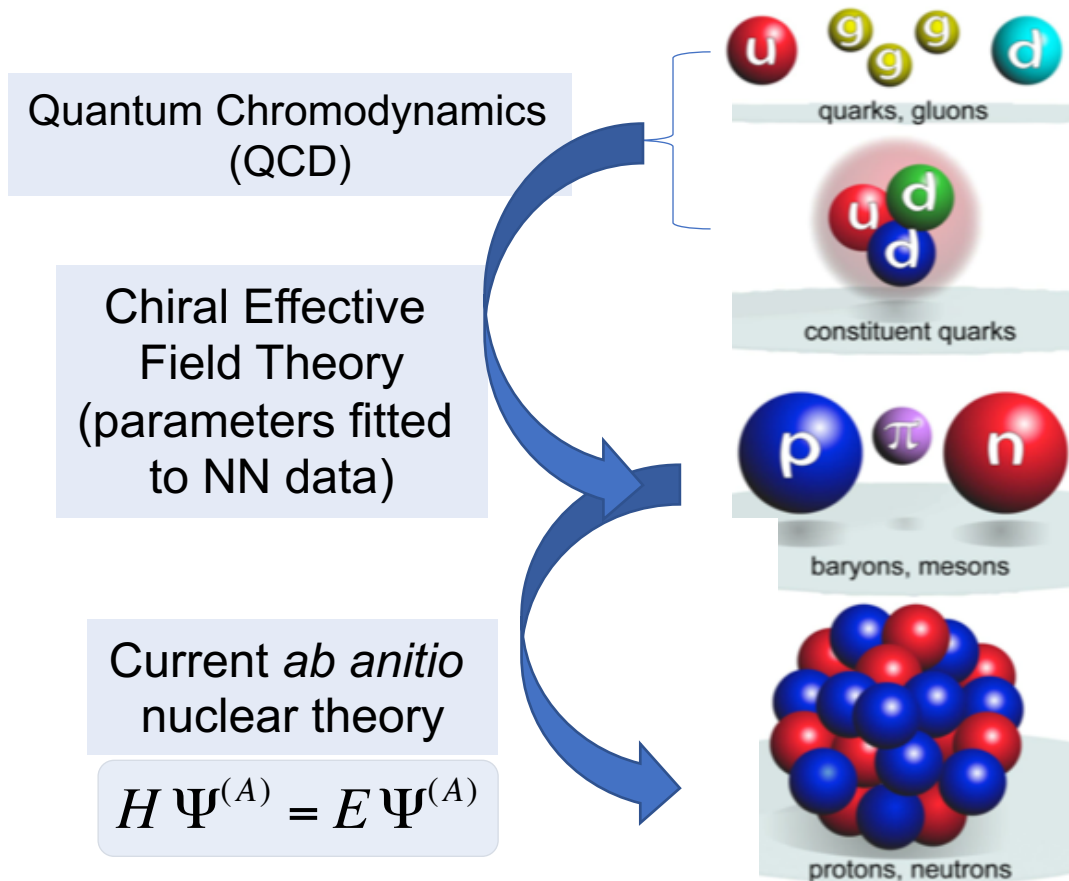


Genuine *Ab Initio*



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

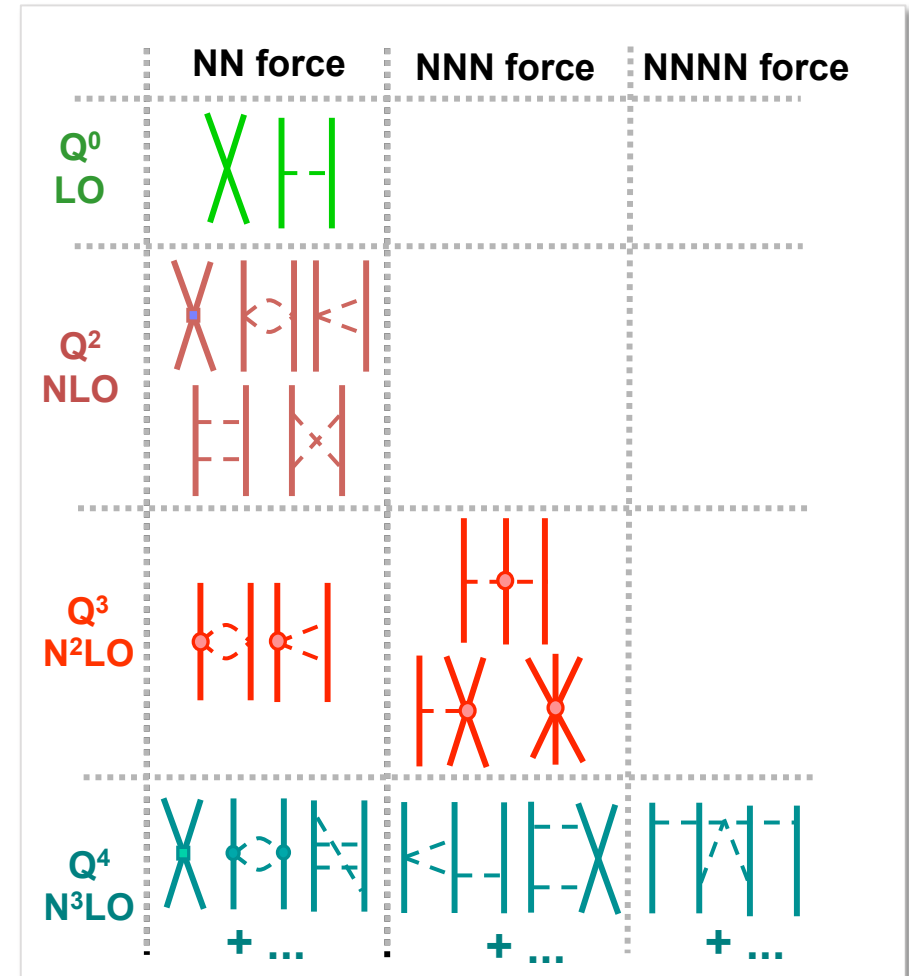
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- *Ab initio*
 - ✧ Degrees of freedom: Nucleons
 - ✧ All nucleons are active
 - ✧ Exact Pauli principle
 - ✧ Realistic inter-nucleon interactions
 - ✧ Accurate description of NN (and 3N) data
 - ✧ Controllable approximations

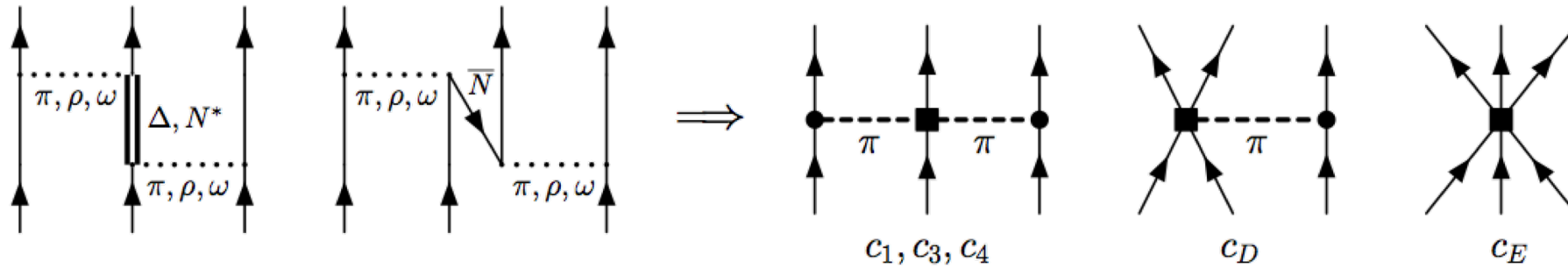
Chiral Effective Field Theory

- 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

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?

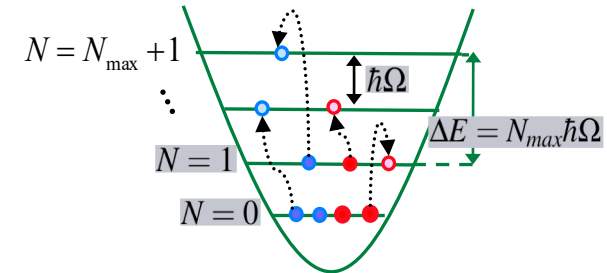
Conceptually simplest *ab initio* method: No-Core Shell Model (NCSM)

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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



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

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

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



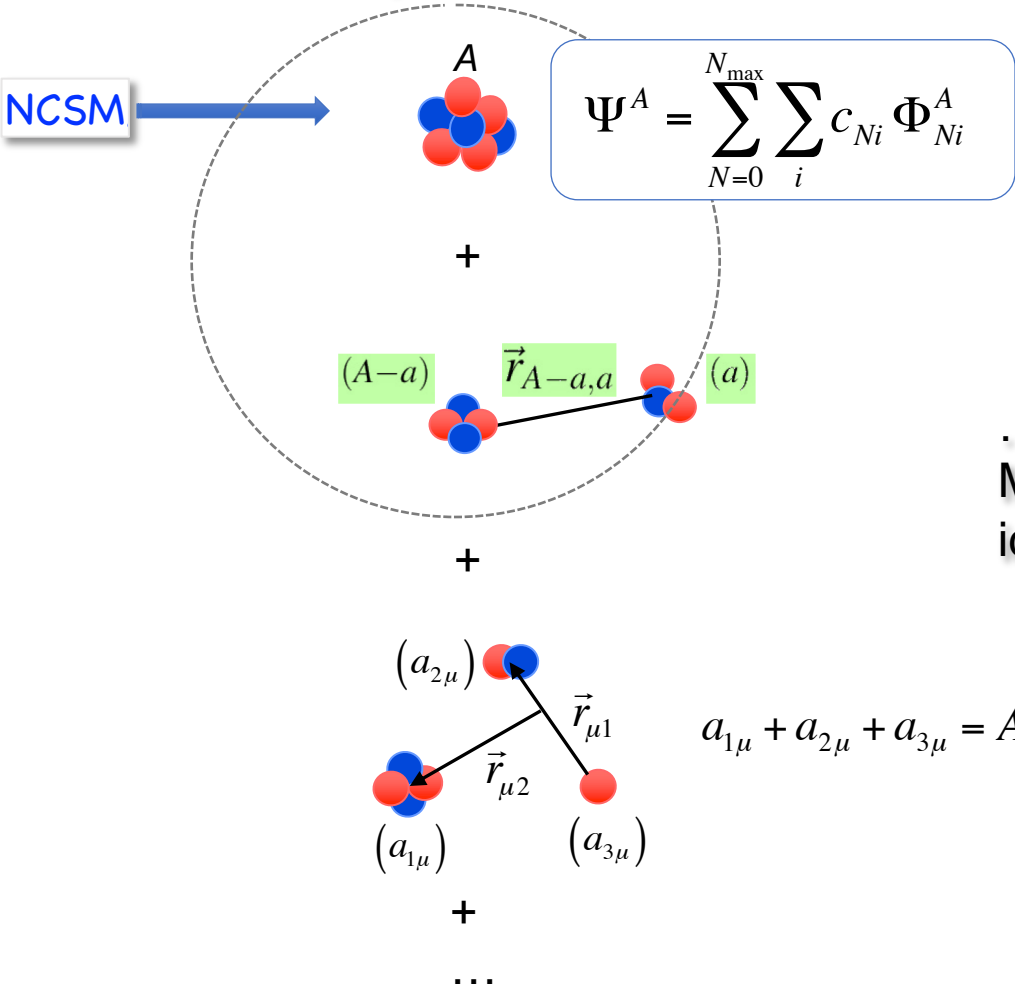
Review

Ab initio no core shell model

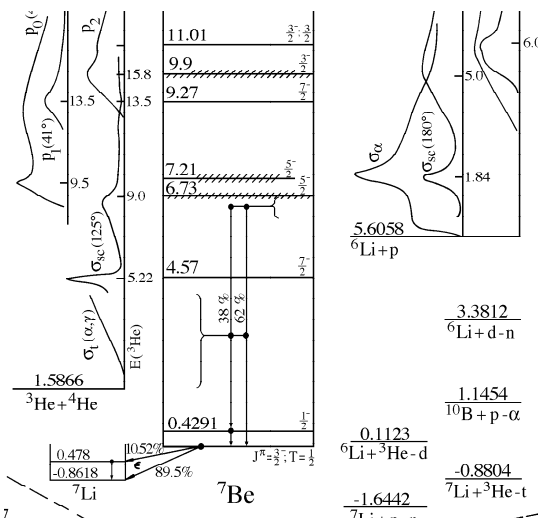
Bruce R. Barrett^a, Petr Navrátil^b, James P. Vary^{c,*}

Extending no-core shell model beyond bound states

Include more many nucleon correlations...



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

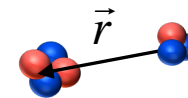


Unified approach to bound & continuum states; to nuclear structure & reactions

- No-core shell model (NCSM)
 - A -nucleon wave function expansion in the harmonic-oscillator (HO) basis
 - short- and medium range correlations
 - Bound-states, narrow resonances
- NCSM with Resonating Group Method (NCSM/RGM)
 - cluster expansion, clusters described by NCSM
 - proper asymptotic behavior
 - long-range correlations
- Most efficient: *ab initio* no-core shell model with continuum (NCSMC)



NCSM



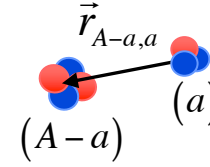
NCSM/RGM

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

Unknowns

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

Binary cluster basis



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- Working in partial waves ($\nu \equiv \{A-a \alpha_1 I_1^{\pi_1} T_1; a \alpha_2 I_2^{\pi_2} T_2; s\ell\}$)

$$|\psi^{J^{\pi T}}\rangle = \sum_{\nu} \hat{A}_{\nu} \left[\underbrace{\left(|A-a \alpha_1 I_1^{\pi_1} T_1\rangle \right)}_{\text{Target}} \underbrace{\left(|a \alpha_2 I_2^{\pi_2} T_2\rangle \right)}_{\text{Projectile}} \right]^{(sT)} Y_{\ell}(\hat{r}_{A-a,a}) \frac{g_{\nu}^{J^{\pi T}}(r_{A-a,a})}{r_{A-a,a}}$$

- Introduce a dummy variable \vec{r} with the help of the delta function

$$|\psi^{J^{\pi T}}\rangle = \sum_{\nu} \int \frac{g_{\nu}^{J^{\pi T}}(r)}{r} \hat{A}_{\nu} \left[\left(|A-a \alpha_1 I_1^{\pi_1} T_1\rangle \right) \left(|a \alpha_2 I_2^{\pi_2} T_2\rangle \right) \right]^{(sT)} Y_{\ell}(\hat{r}) \delta(\vec{r} - \vec{r}_{A-a,a}) r^2 dr d\hat{r}$$

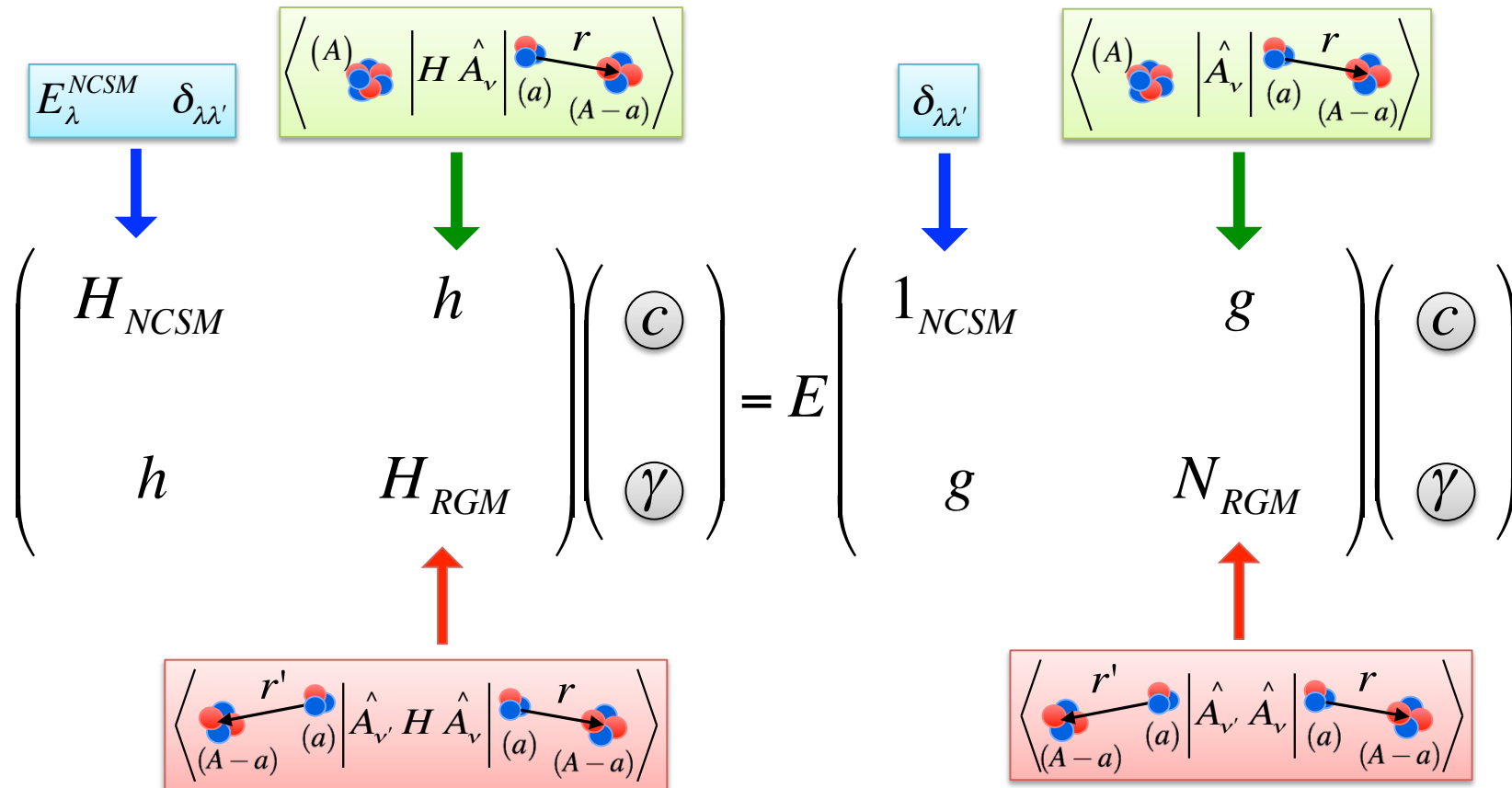
- Allows to bring the wave function of the relative motion in front of the antisymmetrizer

$$\sum_{\nu} \int d\vec{r} \gamma_{\nu}(\vec{r}) \hat{A}_{\nu} \left| \begin{array}{c} \vec{r} \\ (A-a) \quad (a) \end{array}, \nu \right\rangle$$

Coupled NCSMC equations

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$$H \Psi^{(A)} = E \Psi^{(A)} \quad \Psi^{(A)} = \sum_{\lambda} c_{\lambda} \left| \begin{matrix} (A) \\ \text{cluster} \end{matrix}, \lambda \right\rangle + \sum_v \int d\vec{r} \gamma_v(\vec{r}) \hat{A}_v \left| \begin{matrix} \text{cluster} \\ (A-a) \end{matrix}, v \right\rangle$$

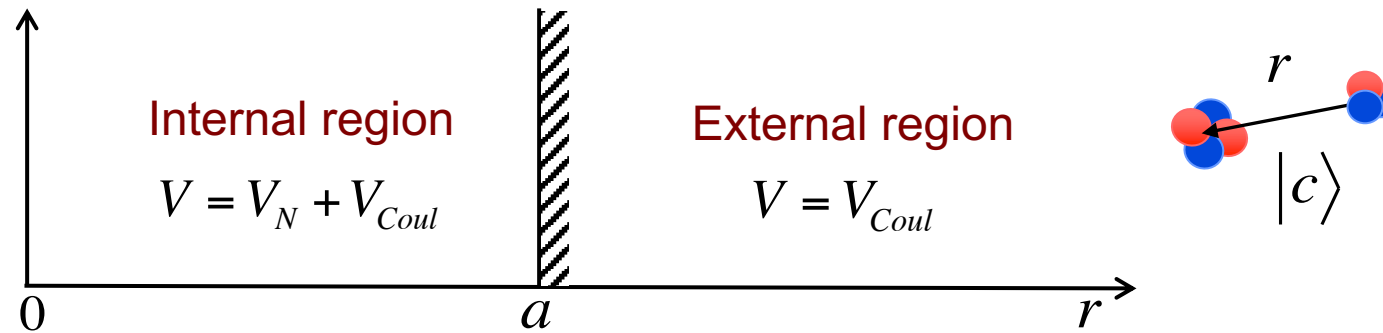


Solved by Microscopic R-matrix theory on a Lagrange mesh – efficient for **coupled channels**

Microscopic R-matrix theory on a Lagrange mesh – Coupled channels

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- Separation into “internal” and “external” regions at the channel radius a

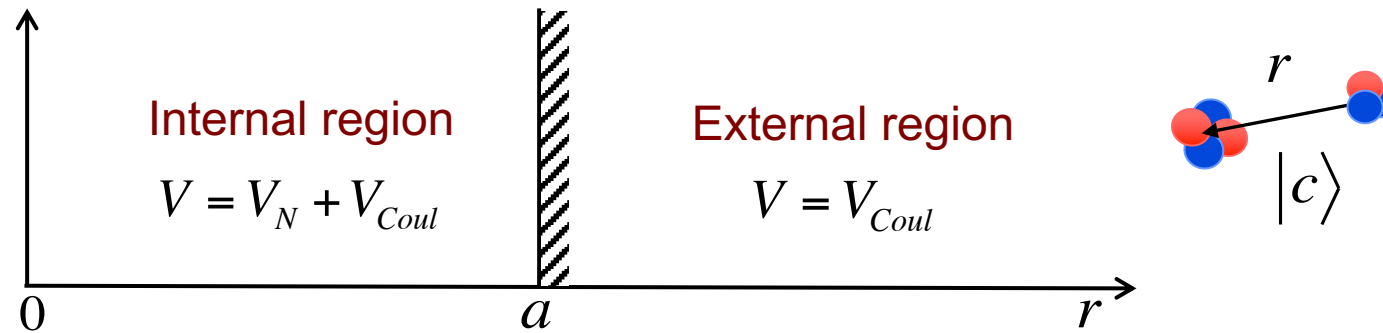


- Matching achieved through the Bloch operator: $L_c = \frac{\hbar^2}{2\mu_c} \delta(r - a) \left(\frac{d}{dr} - \frac{B_c}{r} \right)$
- System of Bloch-Schrödinger equations:

$$\left[\hat{T}_{rel}(r) + L_c + \bar{V}_{Coul}(r) - (E - E_c) \right] u_c(r) + \sum_{c'} \int dr' r' W_{cc'}(r, r') u_{c'}(r') = L_c u_c(r)$$

Microscopic R-matrix theory on a Lagrange mesh – Coupled channels

- Separation into “internal” and “external” regions at the channel radius a



- Matching achieved through the Bloch operator: $L_c = \frac{\hbar^2}{2\mu_c} \delta(r - a) \left(\frac{d}{dr} - \frac{B_c}{r} \right)$
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$$\left[\hat{T}_{rel}(r) + L_c + \bar{V}_{Coul}(r) - (E - E_c) \right] u_c(r) + \sum_{c'} \int dr' r' W_{cc'}(r, r') u_{c'}(r') = L_c u_c(r)$$

- Internal region: expansion on square-integrable basis $u_c(r) = \sum_n A_{cn} f_n(r)$
- External region: asymptotic form for large r

Bound state $u_c(r) \sim C_c W(k_c r)$

Scattering state $u_c(r) \sim v_c^{-\frac{1}{2}} \left[\delta_{ci} I_c(k_c r) - U_{ci} O_c(k_c r) \right]$

Scattering matrix

To find the Scattering matrix – Coupled channels

- After projection on the basis $f_n(r)$:

$$\sum_{c'n'} [C_{cn,c'n'} - (E - E_c)\delta_{cn,c'n'}] A_{c'n'} = \frac{\hbar^2 k_c}{2\mu_c v_c^{1/2}} \langle f_n | L_c | I_c \delta_{ci} - U_{ci} O_c \rangle$$

$$\langle f_n | \hat{T}_{rel}(r) + L_c + \bar{V}_{Coul}(r) | f_{n'} \rangle \delta_{cc'} + \langle f_n | W_{cc'}(r, r') | f_{n'} \rangle$$

1. Solve for A_{cn}
2. Match internal and external solutions at channel radius, a

$$\sum_{c'} R_{cc'} \frac{k_{c'} a}{\sqrt{\mu_{c'} v_{c'}}} [I'_{c'}(k_{c'} a) \delta_{ci} - U_{c'i} O'_{c'}(k_{c'} a)] = \frac{1}{\sqrt{\mu_c v_c}} [I_c(k_c a) \delta_{ci} - U_{ci} O_c(k_c a)]$$

- In the process introduce R -matrix, projection of the Green's function operator on the channel-surface functions

$$R_{cc'} = \sum_{nn'} \frac{\hbar}{\sqrt{2\mu_c a}} f_n(a) [C - EI]_{cn,c'n'}^{-1} \frac{\hbar}{\sqrt{2\mu_{c'} a}} f_{n'}(a)$$

Lagrange basis associated with Lagrange mesh:

$$\{ax_n \in [0, a]\}$$

$$\int_0^1 g(x) dx \approx \sum_{n=1}^N \lambda_n g(x_n)$$

$$\int_0^a f_n(r) f_{n'}(r) dr \approx \delta_{nn'}$$

To find the Scattering matrix – Coupled channels

3. Solve equation with respect to the scattering matrix U

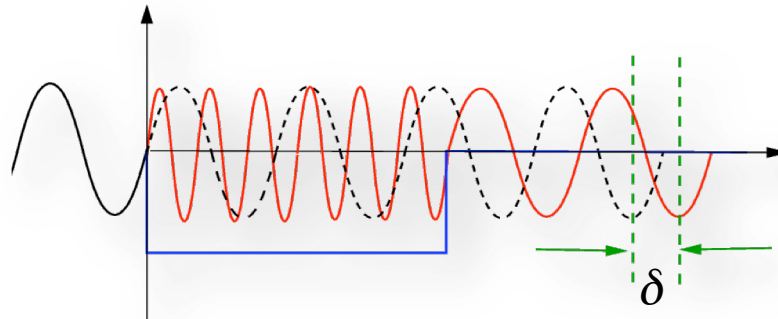
$$\sum_{c'} R_{cc'} \frac{k_{c'} a}{\sqrt{\mu_{c'} v_{c'}}} [I'_{c'}(k_{c'} a) \delta_{ci} - U_{c'i} O'_{c'}(k_{c'} a)] = \frac{1}{\sqrt{\mu_c v_c}} [I_c(k_c a) \delta_{ci} - U_{ci} O_c(k_c a)]$$

4. You can demonstrate that the solution is given by:

$$U = Z^{-1} Z^*, \quad Z_{cc'} = (k_{c'} a)^{-1} [O_c(k_c a) \delta_{cc'} - k_{c'} a R_{cc'} O'_{c'}(k_{c'} a)]$$

- Scattering phase shifts are extracted from the scattering matrix elements

$$U = \exp(2i\delta)$$



Norm kernel (Pauli principle): Single-nucleon projectile

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$$\langle \Phi_{v'r'}^{J\pi T} | \hat{A}_{v'} \hat{A}_v | \Phi_{vr}^{J\pi T} \rangle = \left\langle \begin{array}{c} (A-1) \\ \text{red and blue dots} \\ r' \end{array} \begin{array}{c} (a'=1) \\ \text{red dot} \end{array} \left| 1 - \sum_{i=1}^{A-1} \hat{P}_{iA} \right| \begin{array}{c} (A-1) \\ \text{red and blue dots} \\ r \end{array} \begin{array}{c} (a=1) \\ \text{red dot} \end{array} \right\rangle$$

$$N_{v'v}^{J\pi T}(r', r) = \underbrace{\delta_{v'v} \frac{\delta(r' - r)}{r'r}}_{\text{Direct term: Treated exactly! (in the full space)}} - (A-1) \sum_{n'n} R_{n'\ell'}(r') R_{n\ell}(r) \underbrace{\langle \Phi_{v'n'}^{J\pi T} | \hat{P}_{A-1,A} | \Phi_{vn}^{J\pi T} \rangle}_{\text{Exchange term: Obtained in the model space! (Many-body correction due to the exchange part of the inter-cluster antisymmetrizer)}}$$

$$\text{SD} \langle \psi_{\mu_1}^{(A-1)} | a^+ a | \psi_{v_1}^{(A-1)} \rangle_{\text{SD}}$$

Trick #1

$$\frac{\delta(r - r_{A-a,a})}{r r_{A-a,a}} = \sum_n R_{n\ell}(r) R_{n\ell}(r_{A-a,a})$$

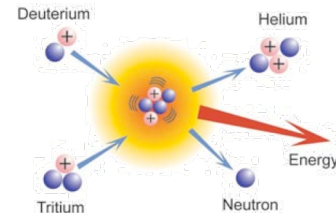
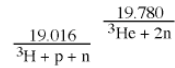
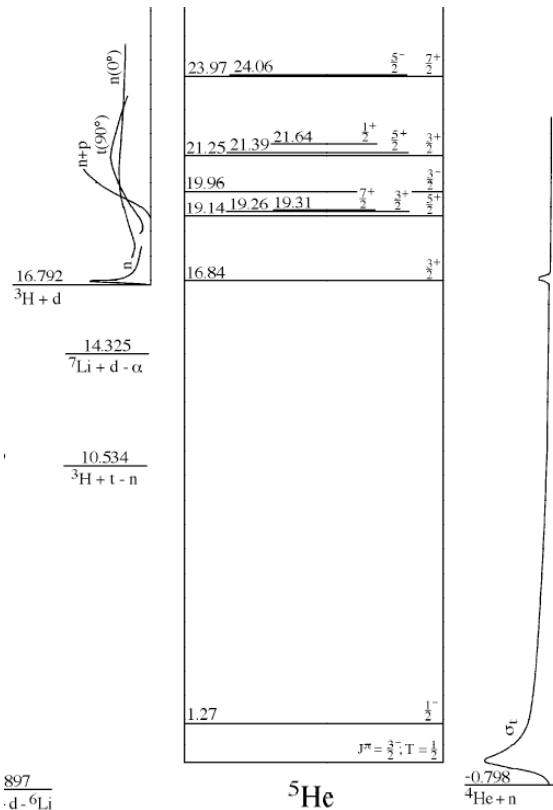
Trick #2

Target wave functions expanded in the SD basis, the CM motion exactly removed

Deuterium-Tritium fusion

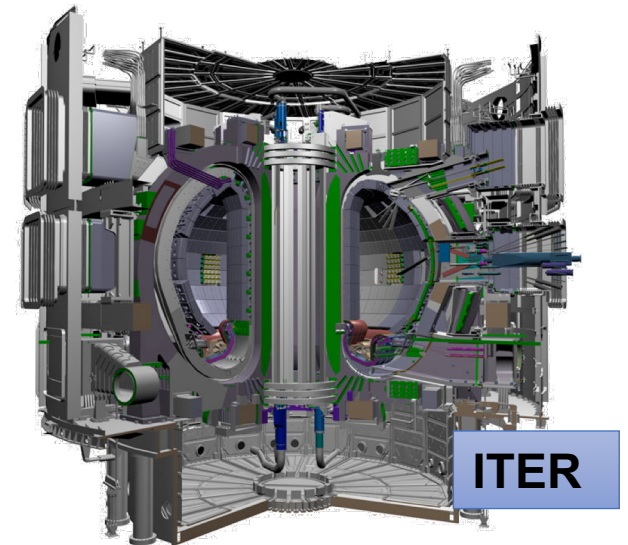
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- The $d+{}^3\text{H}\rightarrow n+{}^4\text{He}$ reaction
 - The most promising for the production of fusion energy in the near future
 - Used to achieve inertial-confinement (laser-induced) fusion at NIF, and magnetic-confinement fusion at ITER
 - 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

NCSMC calculation of the DT fusion

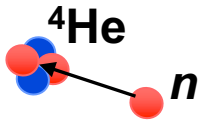
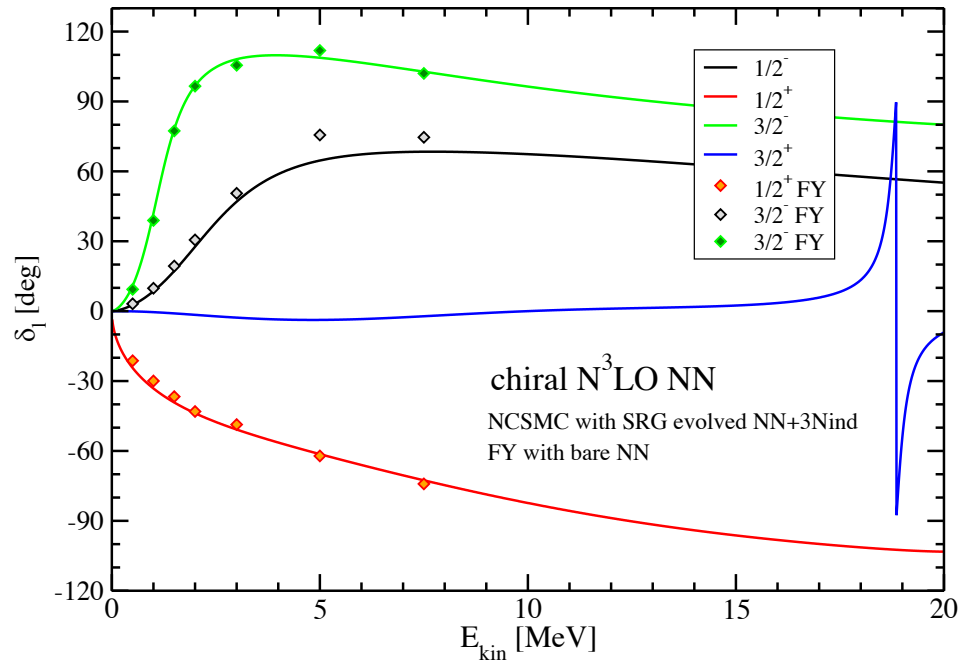
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$$|\Psi\rangle = \sum_{\lambda} c_{\lambda} \left| \begin{array}{c} \text{He} \\ \text{5} \end{array}, \lambda \right\rangle + \int d\vec{r} u_{\nu_{DT}}(\vec{r}) \hat{A}_{DT} \left| \begin{array}{c} \text{D} \\ \text{T} \end{array}, \nu_{DT} \right\rangle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

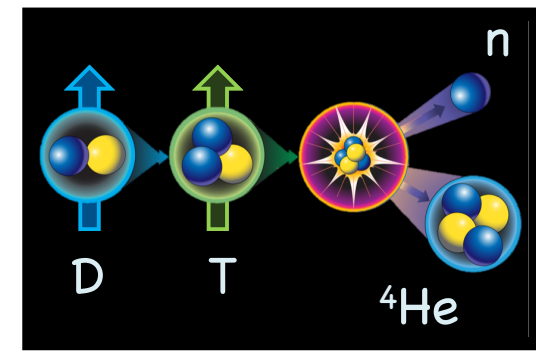
- 2x7 static ^5He eigenstates computed with the NCSM
- Continuous D-T(g.s.) cluster states (entrance channel)
 - Including positive-energy eigenstates of D to account for distortion
- Continuous n- ^4He (g.s.) cluster states (exit channel)
- Chiral NN+3N(500) interaction

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

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

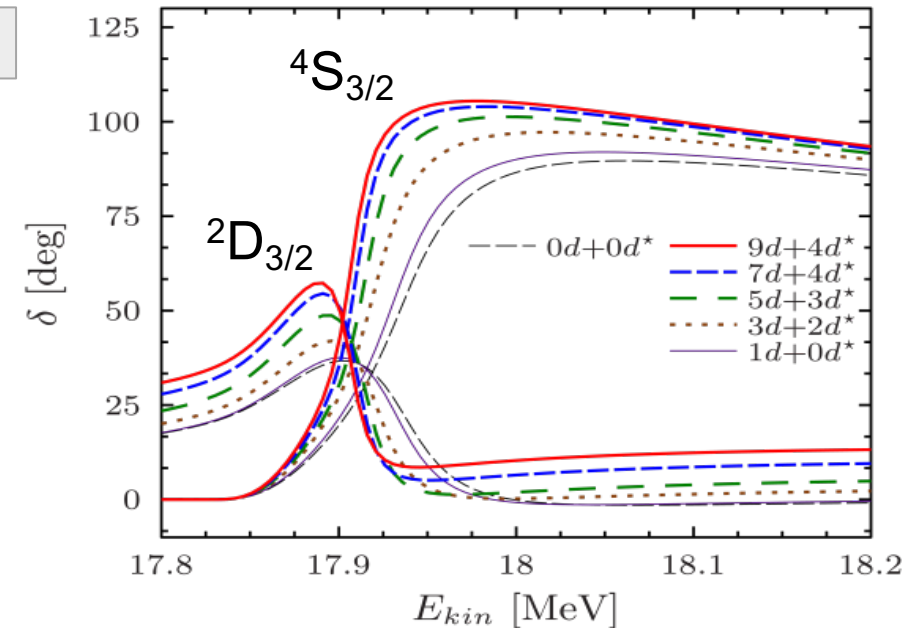


FY: Faddeev-Yakubovsky method - Rimantas Lazauskas



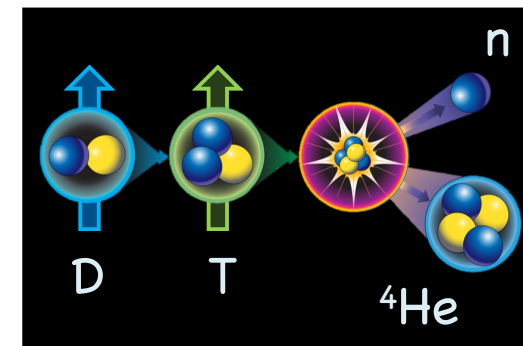
$^4\text{He}+n \rightarrow ^3\text{H}+d$

$^4\text{He}+n$



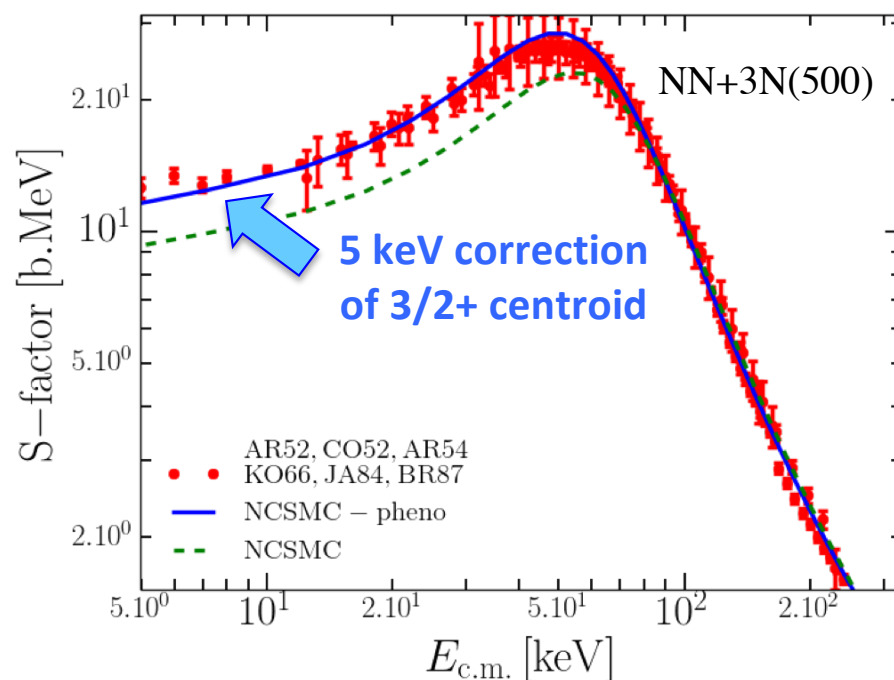
The d - ^3H fusion takes place through a transition of d + ^3H is S -wave to n + ^4He in D -wave: Importance of the **tensor** and **3N** force

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

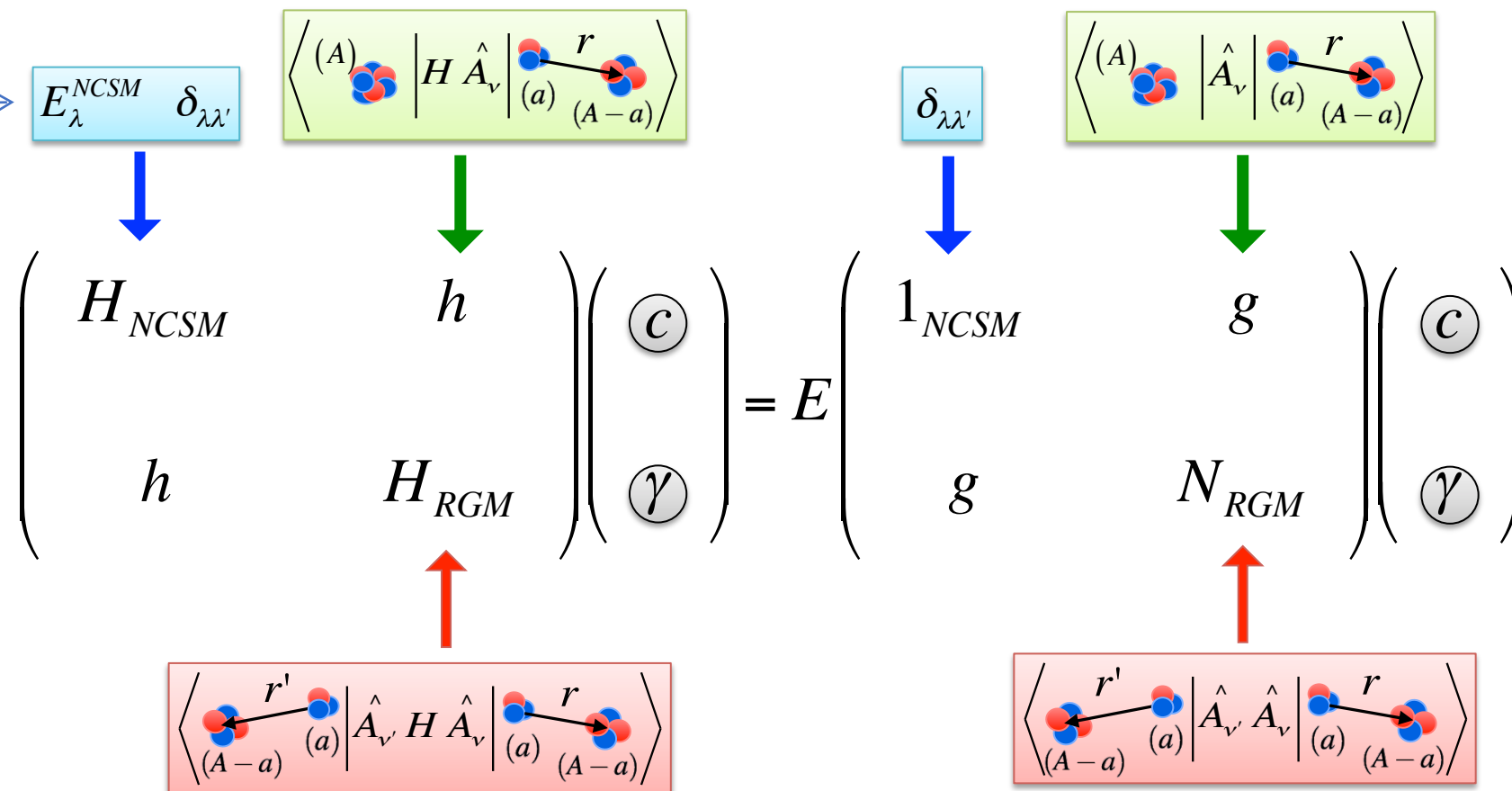
NCSMC phenomenology

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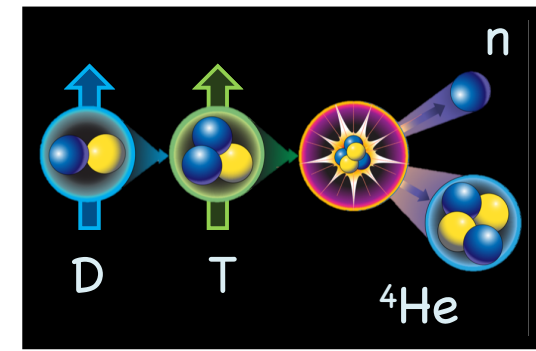
$$H \Psi^{(A)} = E \Psi^{(A)}$$

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

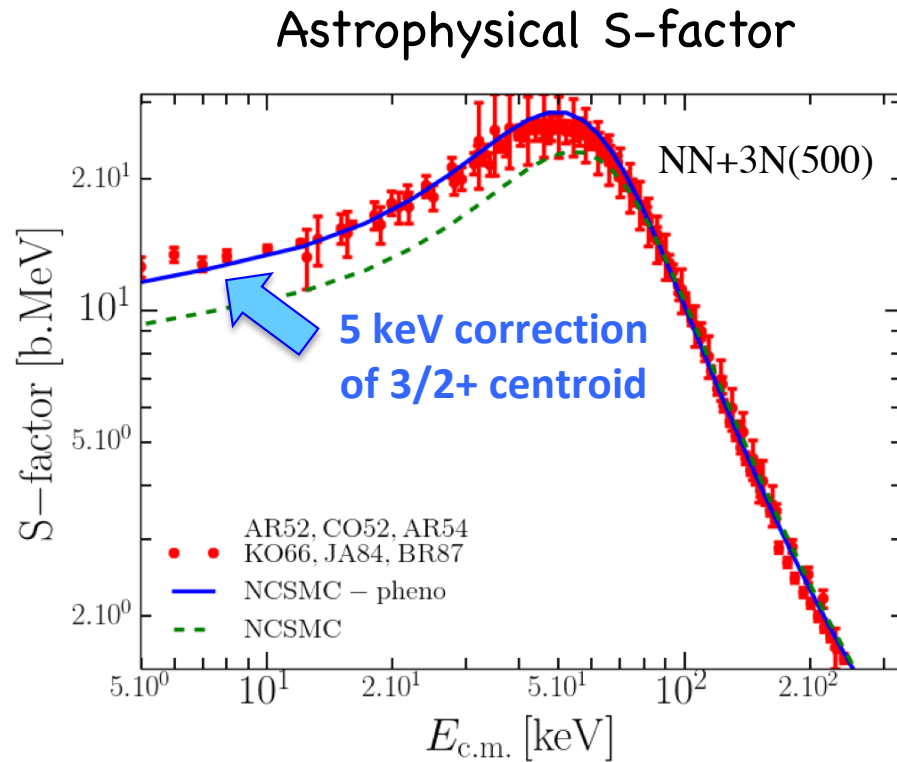
$E_{\lambda}^{\text{NCSM}}$ energies treated as adjustable parameters



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



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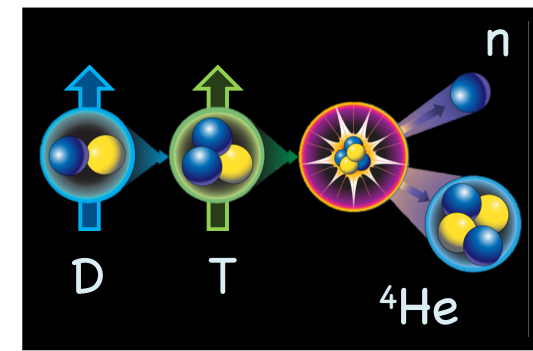
Fusion cross section

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

Astrophysical S-factor: nuclear contribution

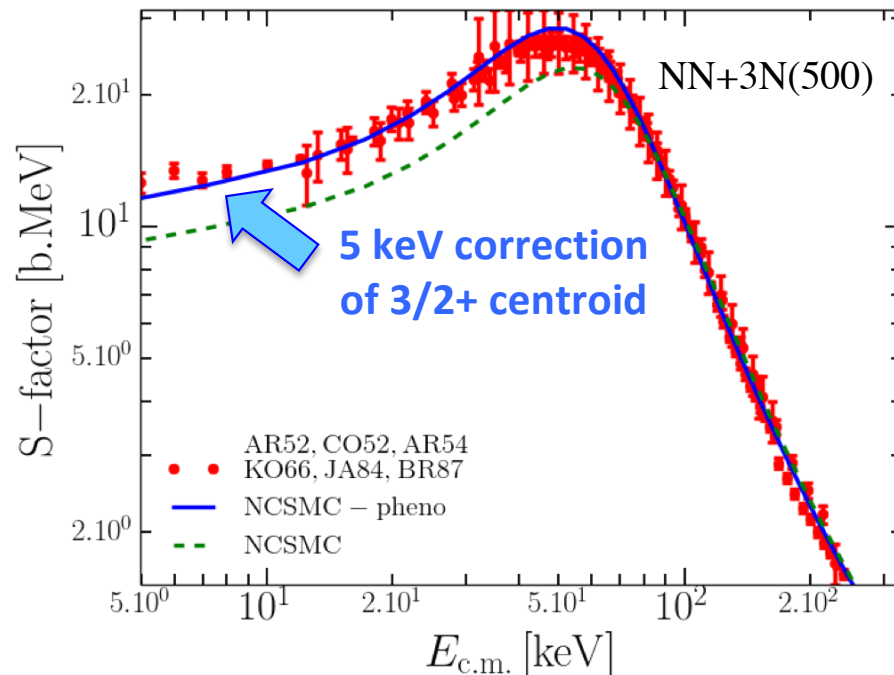
‘Coulomb’ Contribution (tunneling)

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

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

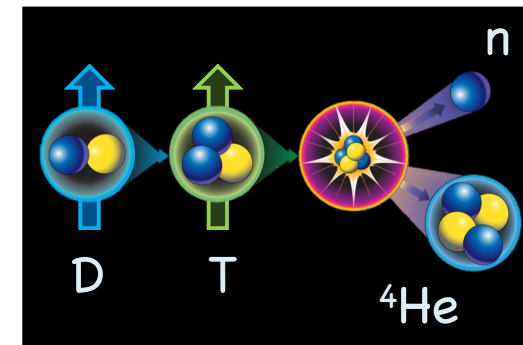
$$\approx \frac{1}{3} \cancel{\sigma_{\frac{1}{2}}} + \frac{2}{3} \sigma_{\frac{3}{2}}$$



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

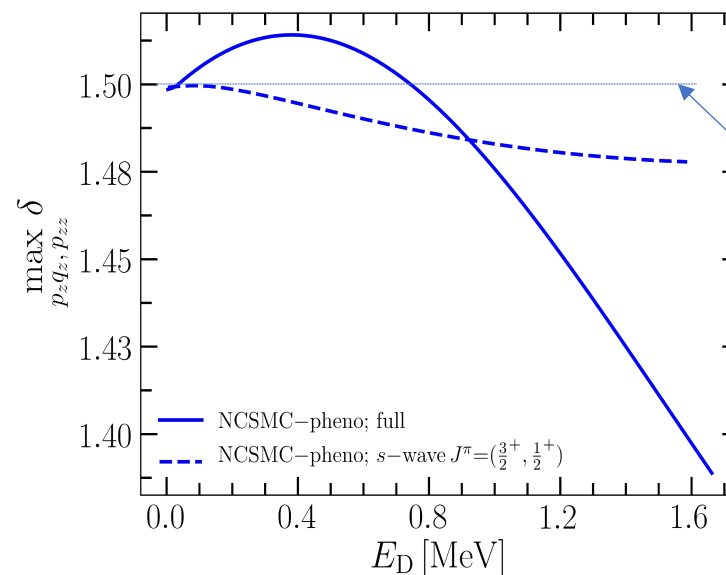
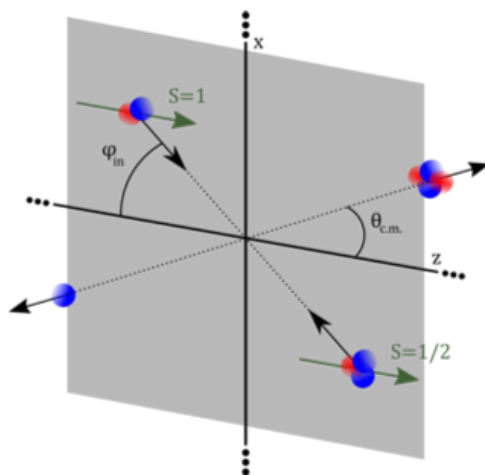
$^3\text{H}(d,n)^4\text{He}$ with chiral NN+3N(500) interaction

Polarized fusion



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



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

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

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



ARTICLE

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

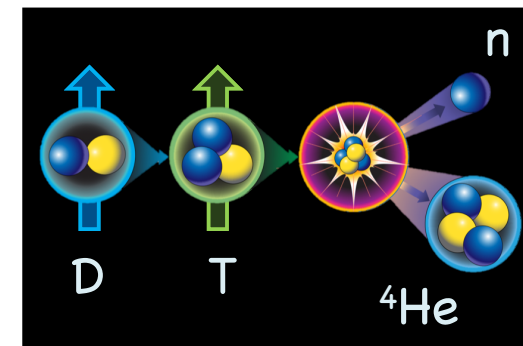
Ab initio predictions for polarized deuterium-tritium thermonuclear fusion

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

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

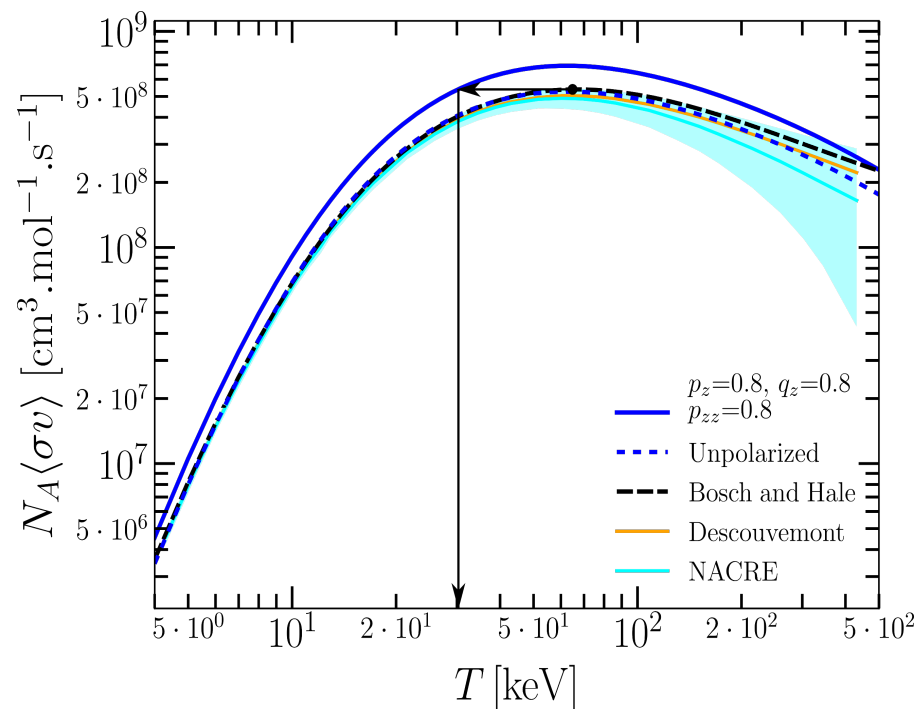
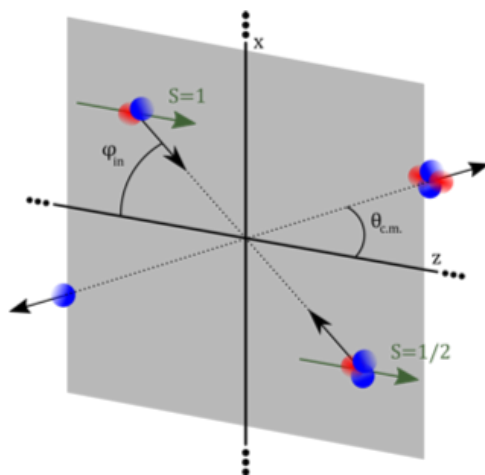
$^3\text{H}(d,n)^4\text{He}$ with chiral NN+3N(500) interaction

Polarized fusion



25

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



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

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



ARTICLE

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

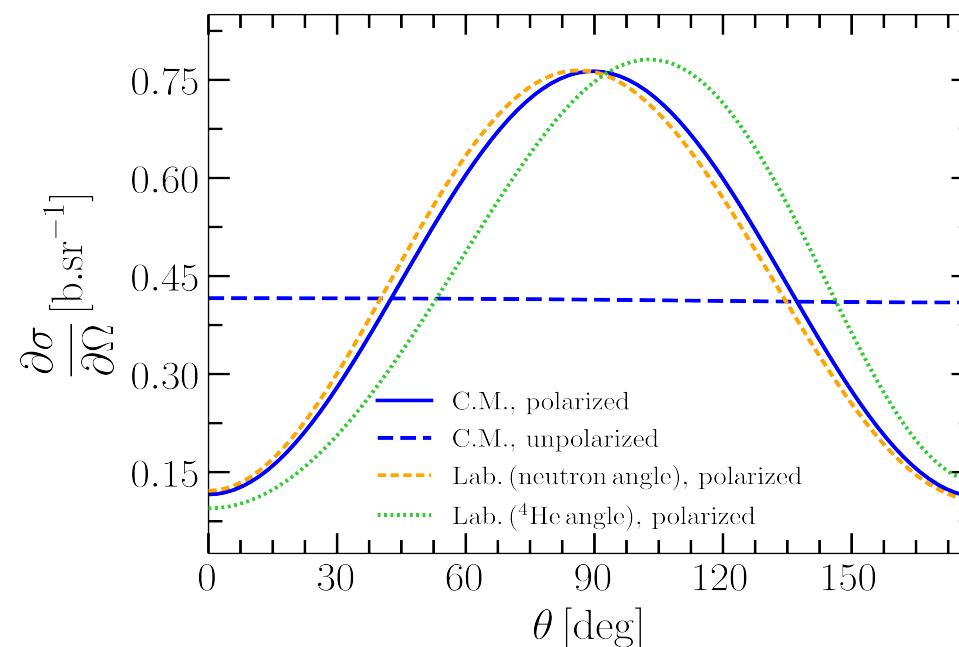
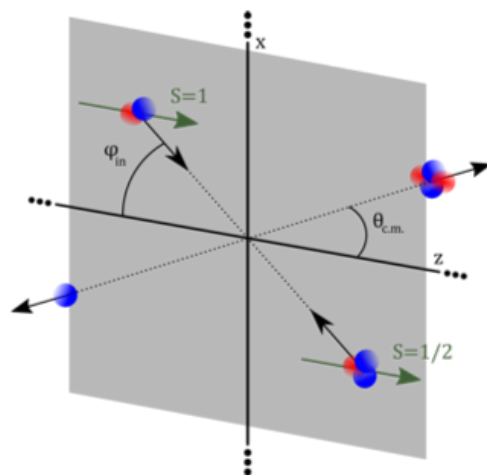
Ab initio predictions for polarized deuterium-tritium thermonuclear fusion

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

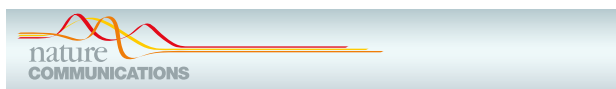
$^3\text{H}(d,n)^4\text{He}$ with chiral NN+3N(500) interaction

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



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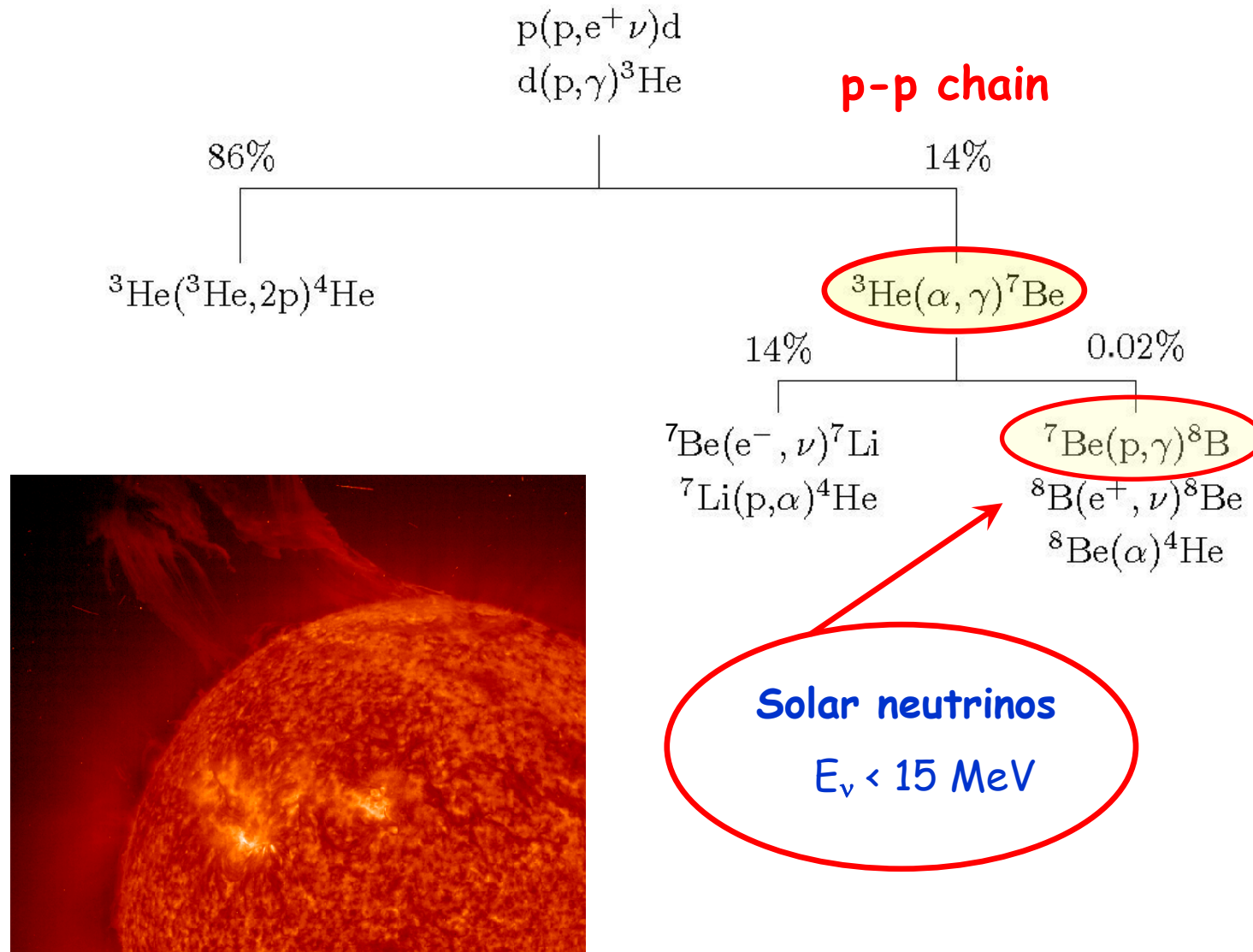
<https://doi.org/10.1038/s41467-018-08052-6> OPEN

Ab initio predictions for polarized deuterium-tritium thermonuclear fusion

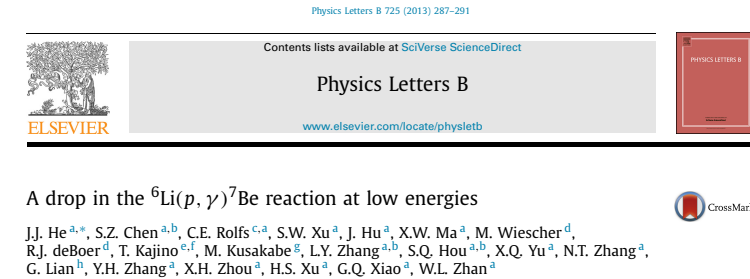
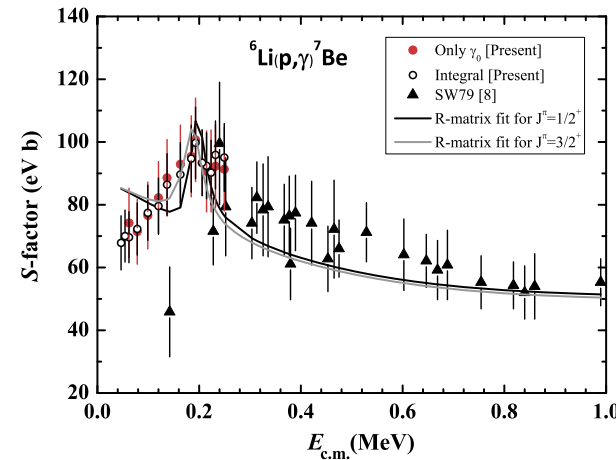
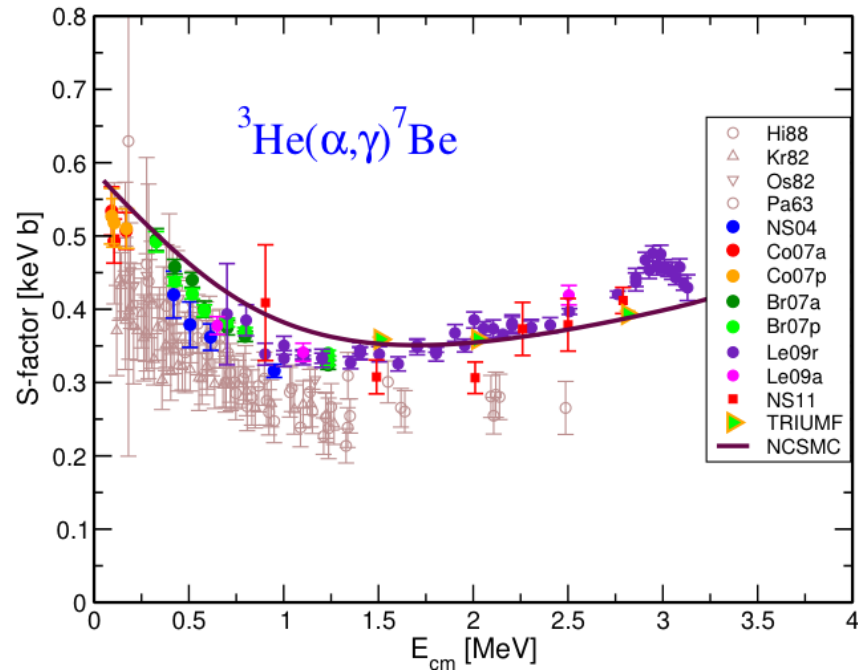
Guillaume Hupin^{1,2,3}, Sofia Quaglioni³ & Petr Navrátil⁴

Solar *p-p* chain

27



^7Be structure and capture reactions important for astrophysics



What resonances do we find in ^7Be within NCSMC?

PHYSICAL REVIEW C **100**, 024304 (2019)

^7Be and ^7Li nuclei within the no-core shell model with continuum

Matteo Vorabbi^{*} and Petr Navrátil[†]
TRIUMF, 4004 Wesbrook Mall, Vancouver, British Columbia V6T 2A3, Canada

Sofia Quaglioni
Lawrence Livermore National Laboratory, P. O. Box 808, L-414, Livermore, California 94551, USA

Guillaume Hupin[‡]
Institut de Physique Nucléaire, CNRS/IN2P3, Université Paris-Sud, Université Paris-Saclay, F-91406, Orsay, France



$^3\text{He}(\alpha, \gamma)^7\text{Be}$ 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}

^7Be structure and capture reactions important for astrophysics

NCSMC with SRG evolved chiral NN

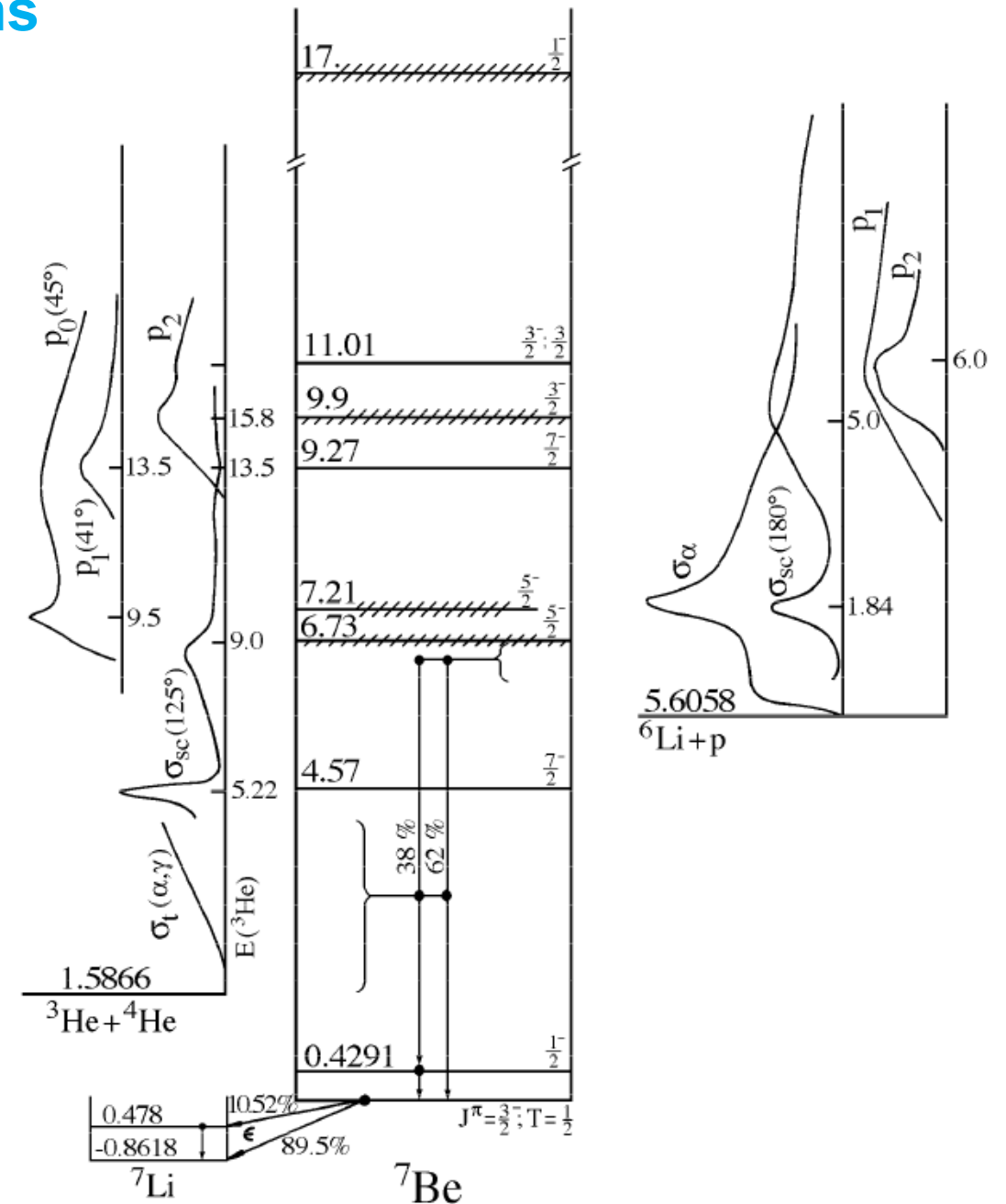
Analyzed mass partitions (no coupling yet)

- $^3\text{He} + ^4\text{He}$
- $p + ^6\text{Li}$

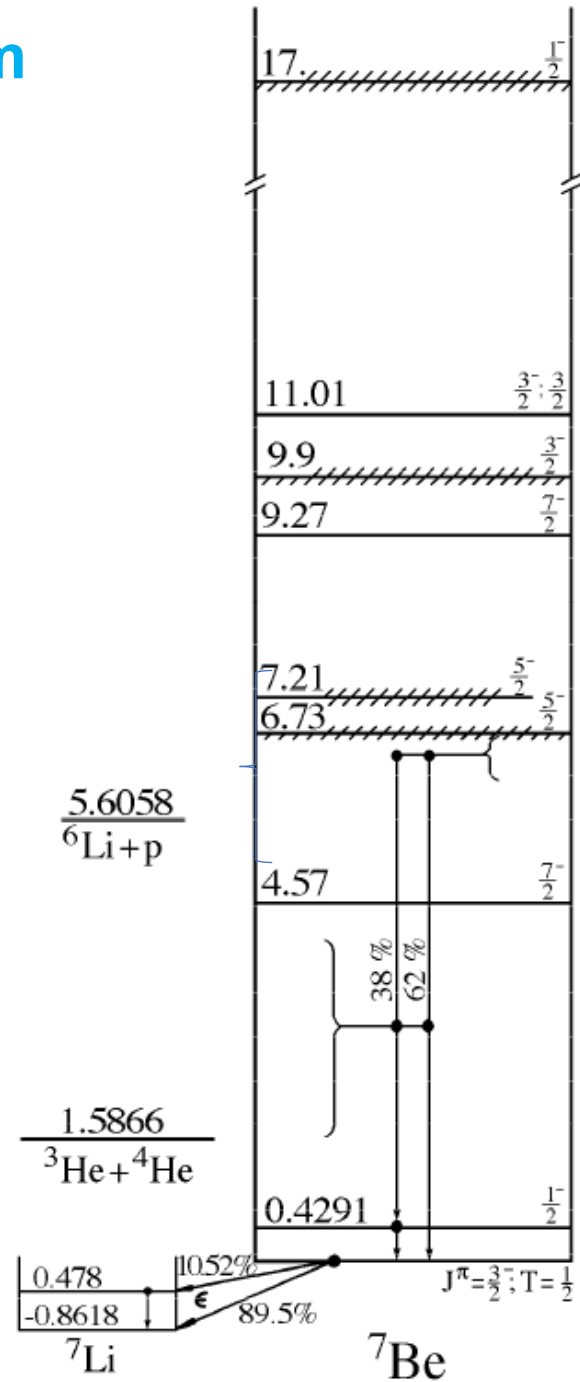
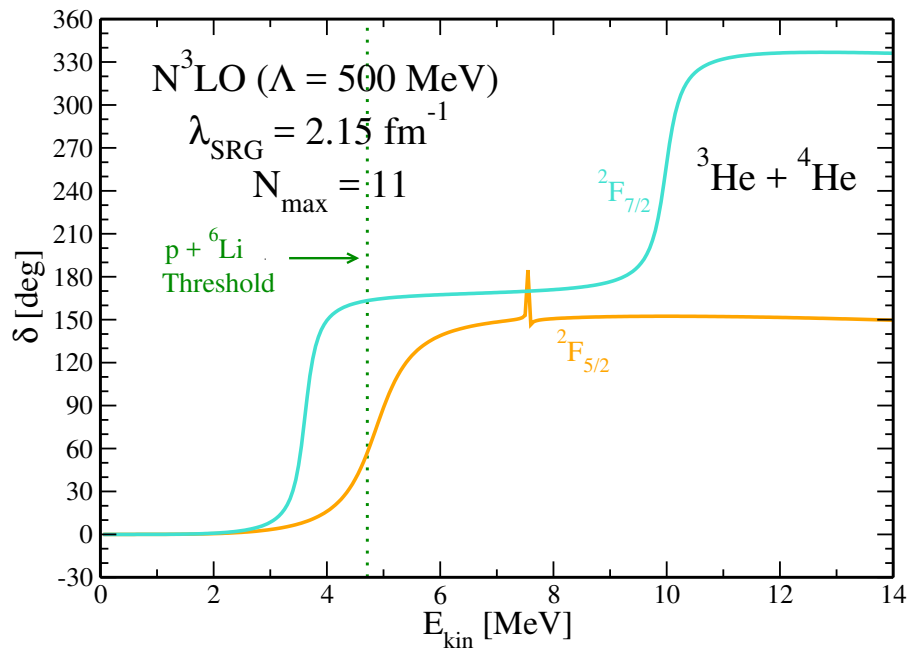
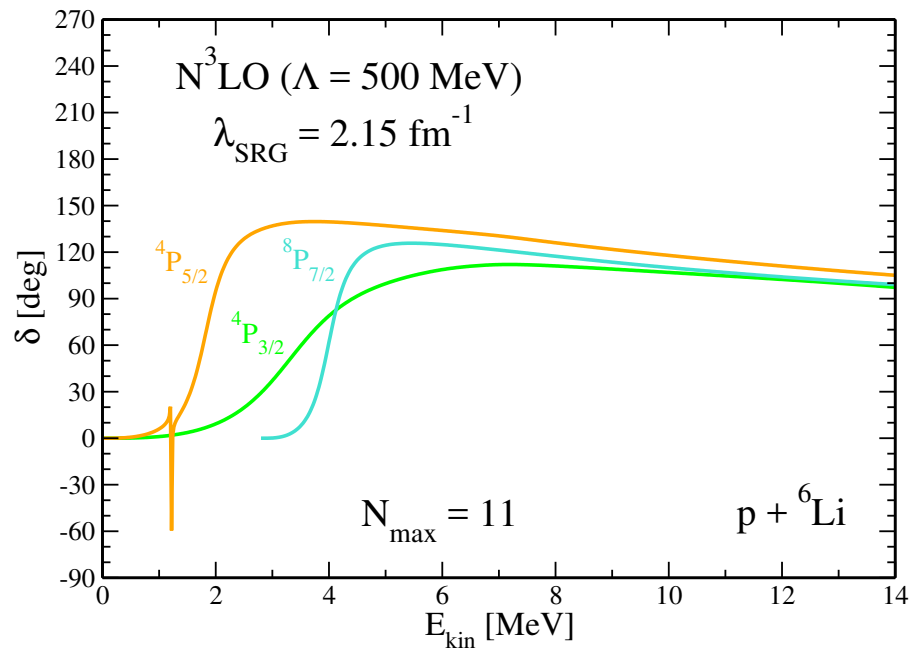
Exp.	$J^\pi = 3/2^-$
E [MeV]	-37.60

$^3\text{He} + ^4\text{He}$	$J^\pi = 3/2^-$	$J^\pi = 1/2^-$
E_{bound}	-1.519	-1.256
E [MeV]	-36.98	-36.71

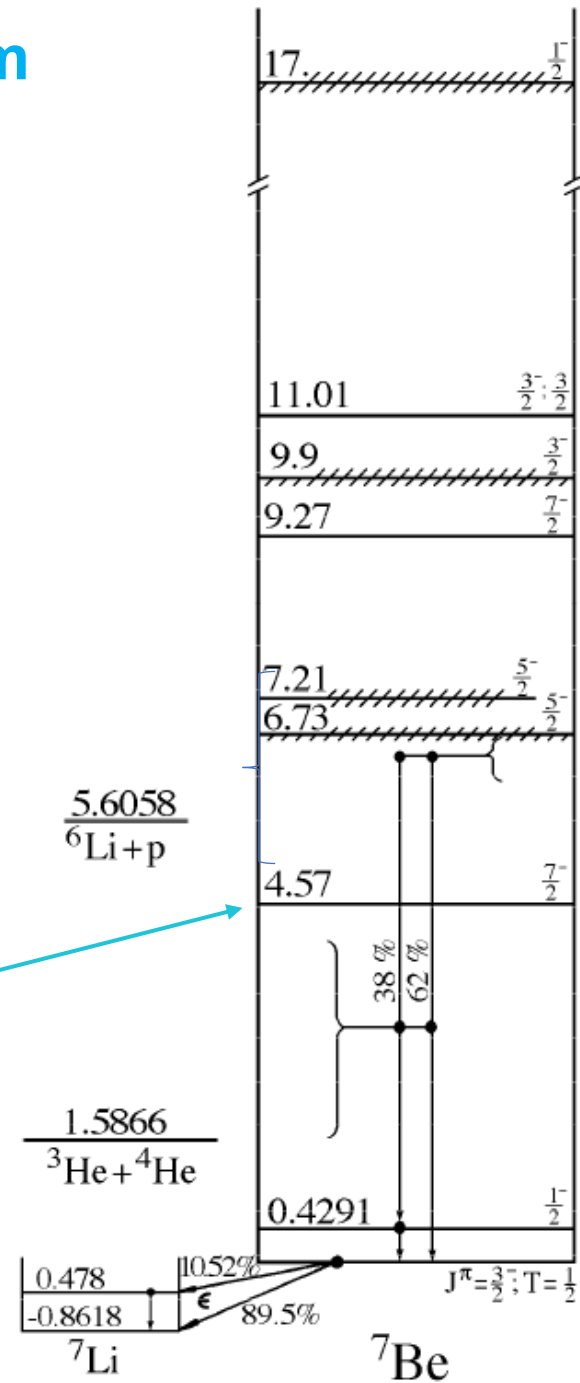
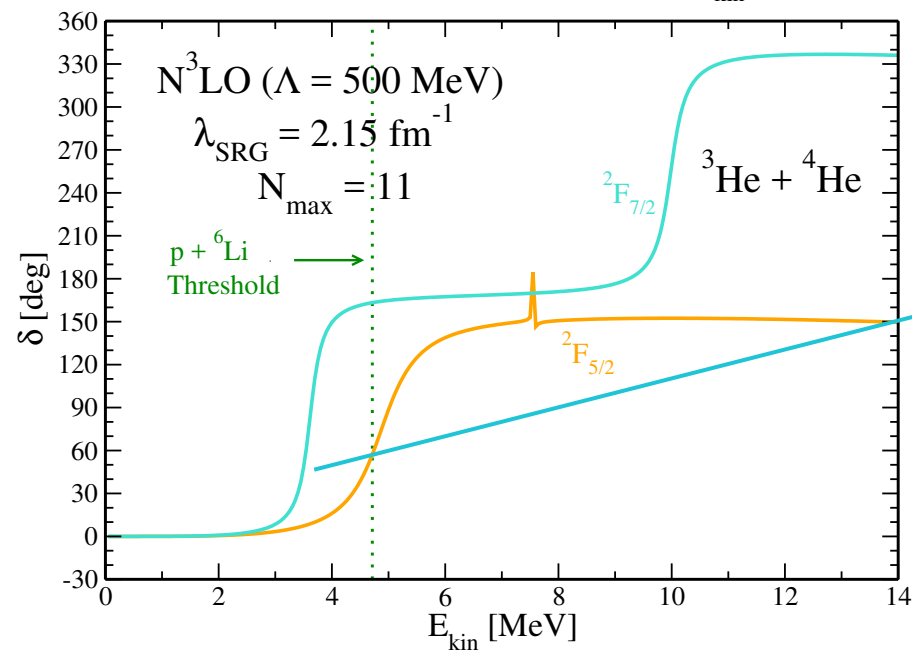
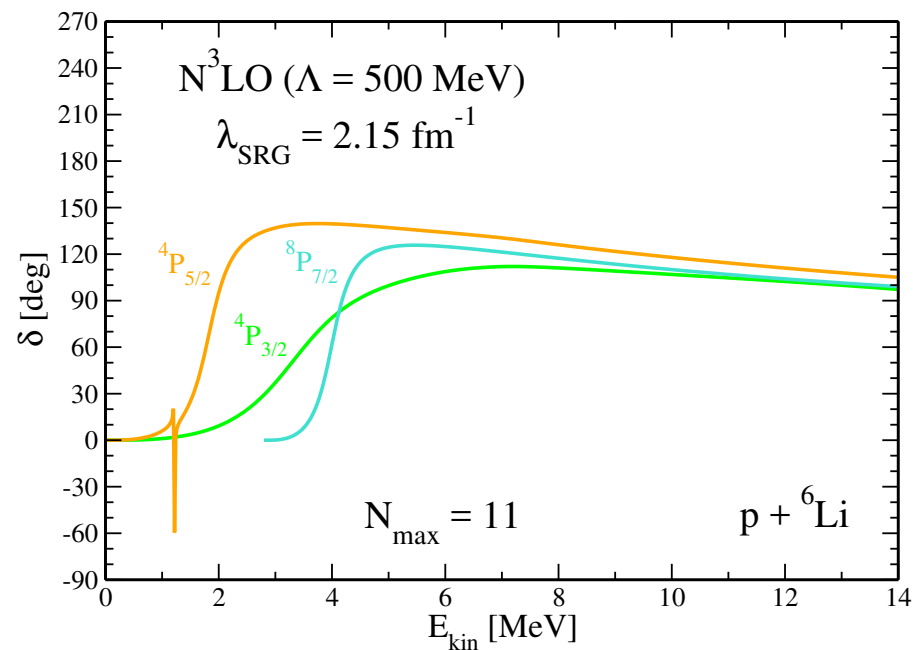
$p + ^6\text{Li}$	$J^\pi = 3/2^-$	$J^\pi = 1/2^-$
E_{bound}	-5.729	-5.389
E [MeV]	-36.47	-36.13



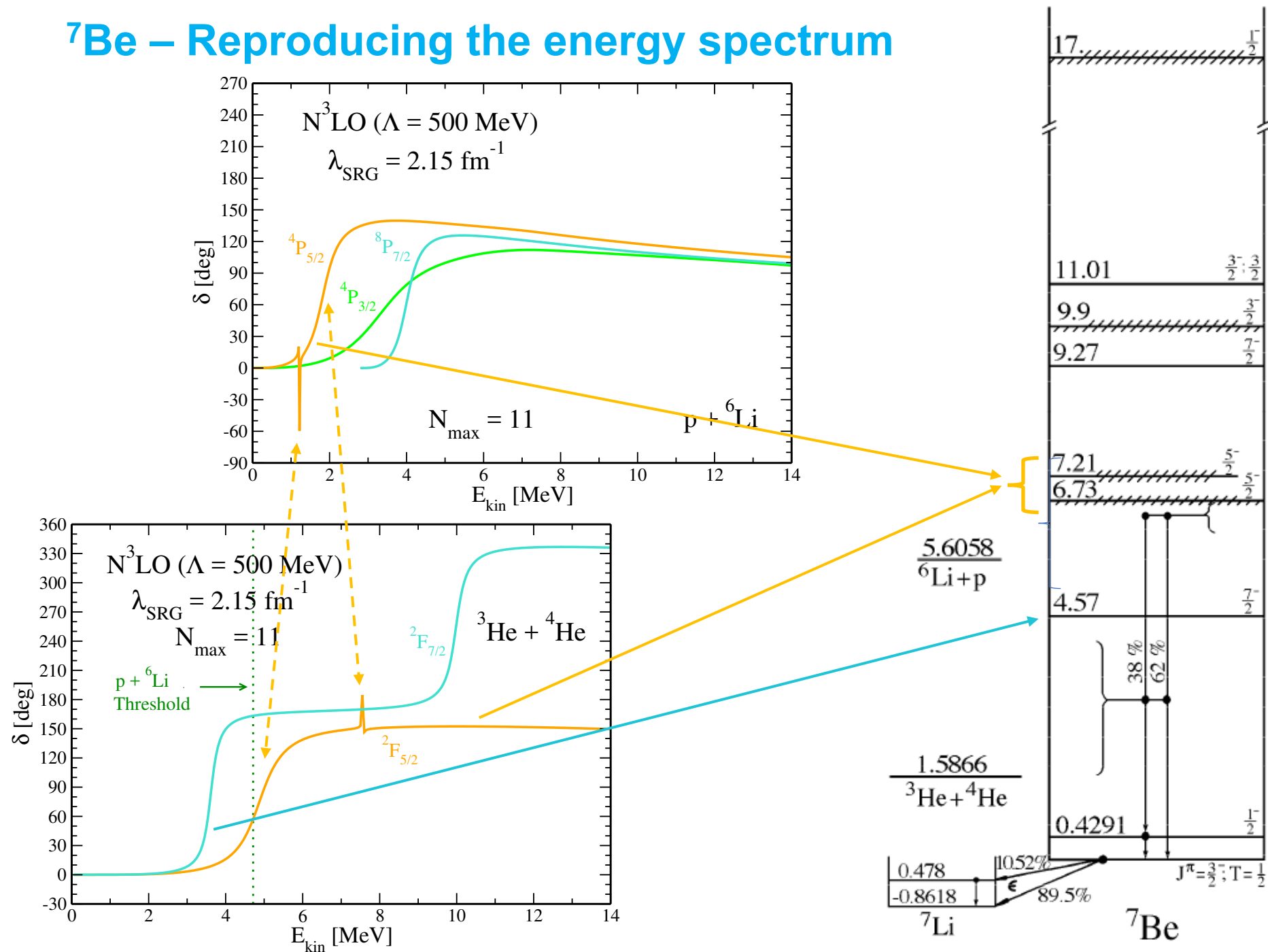
⁷Be – Reproducing the energy spectrum



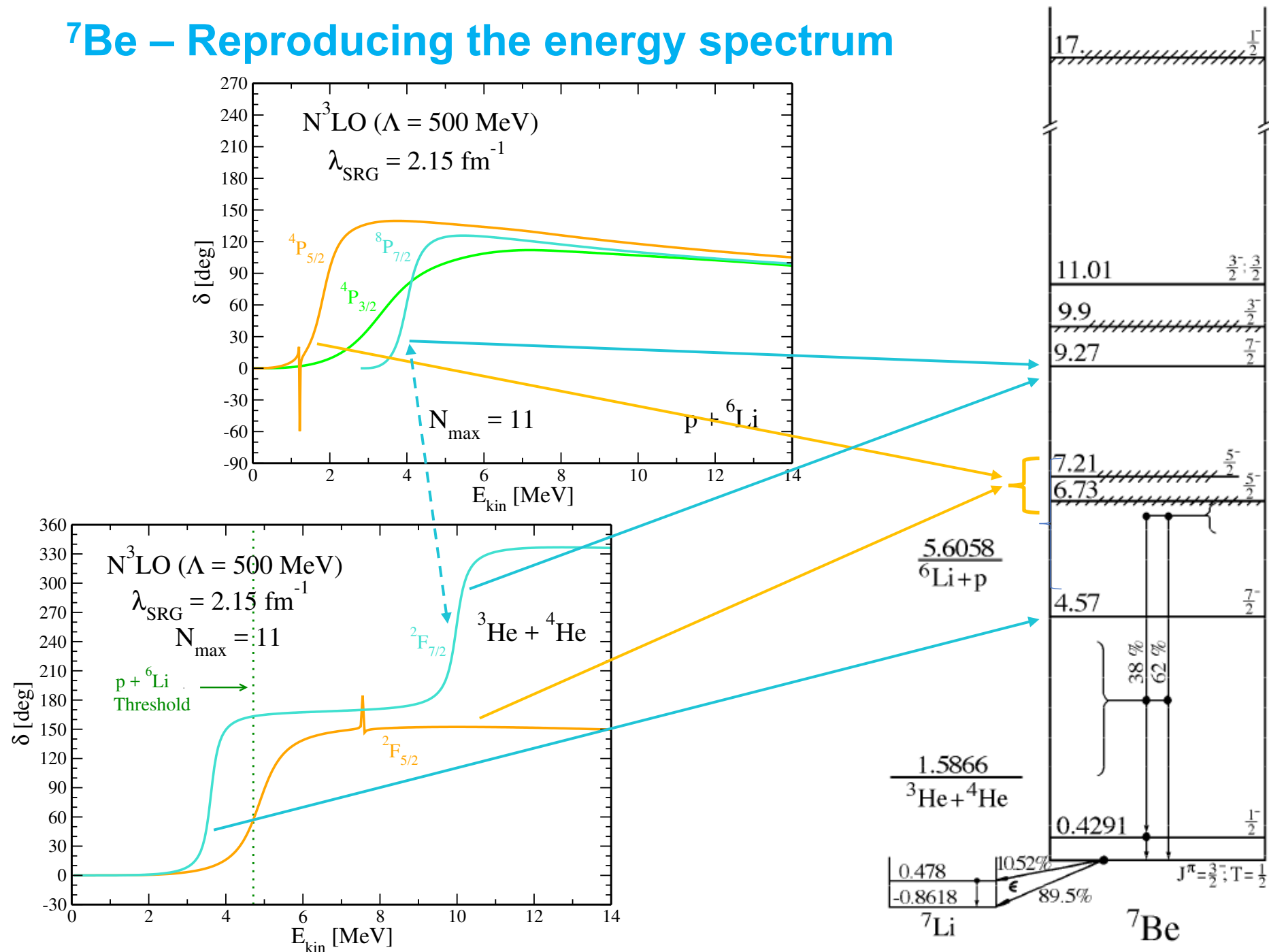
${}^7\text{Be}$ – Reproducing the energy spectrum



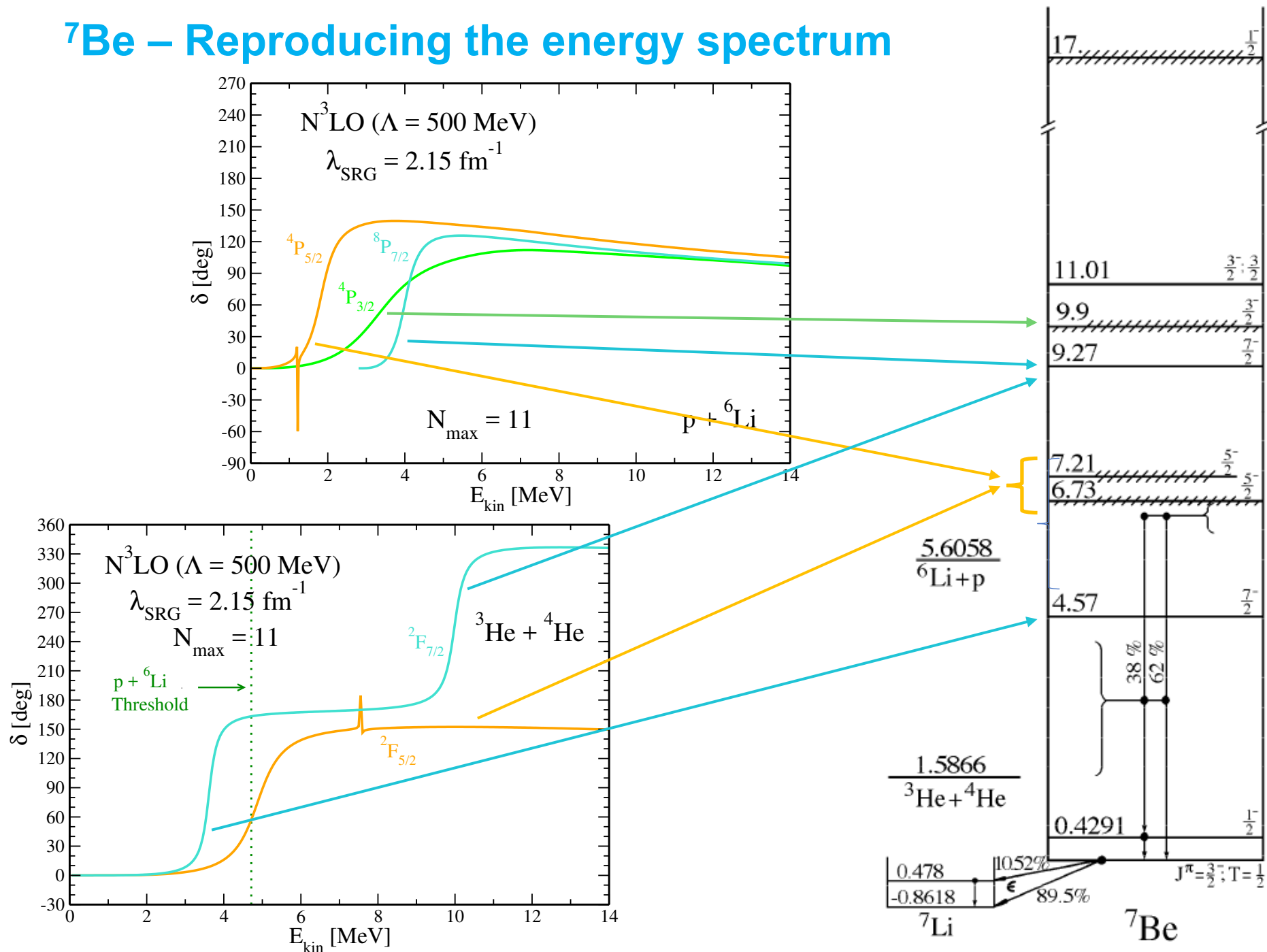
${}^7\text{Be}$ – Reproducing the energy spectrum



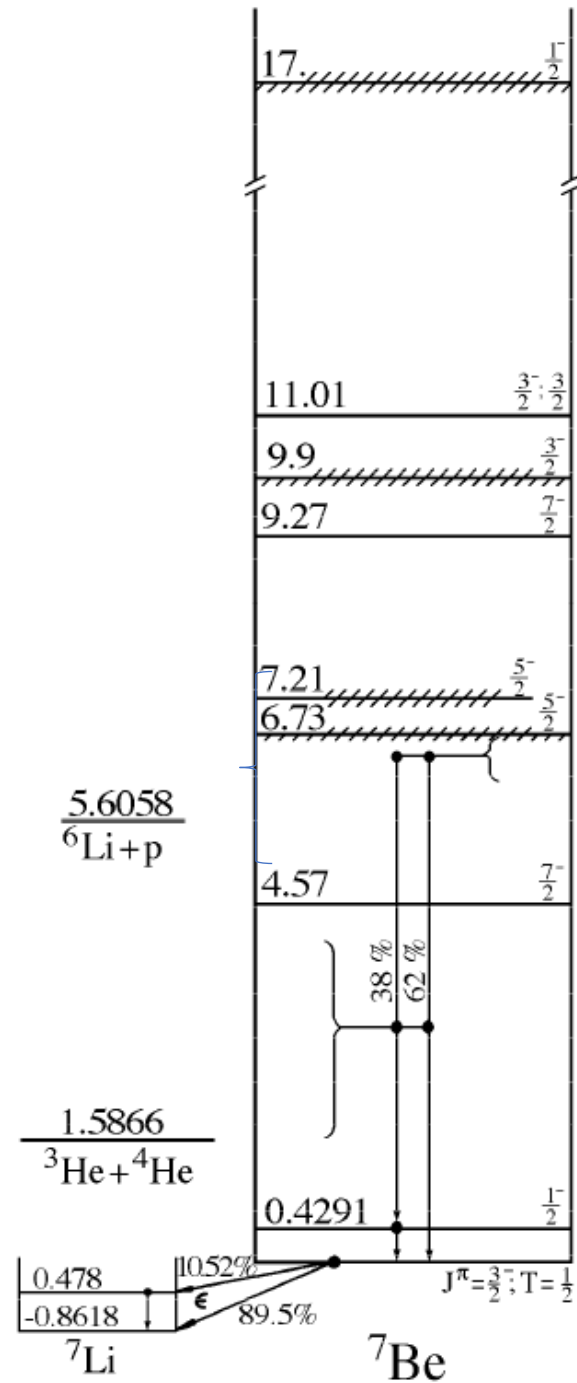
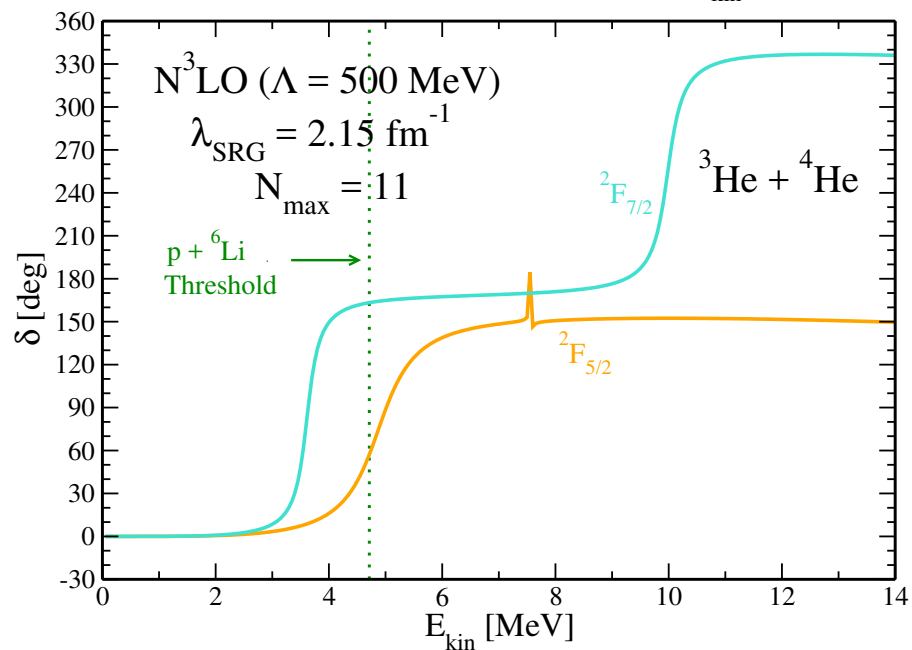
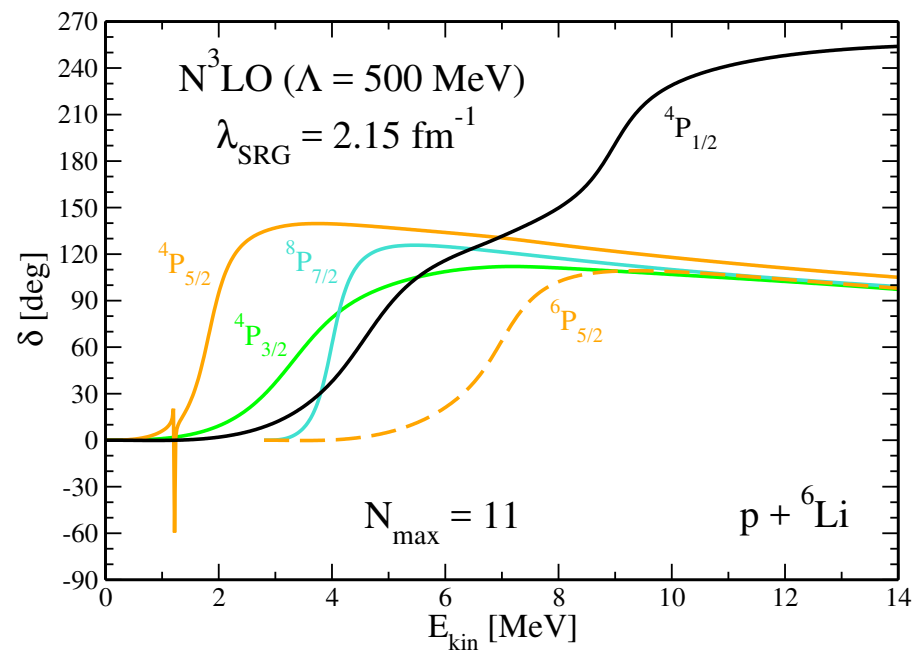
${}^7\text{Be}$ – Reproducing the energy spectrum



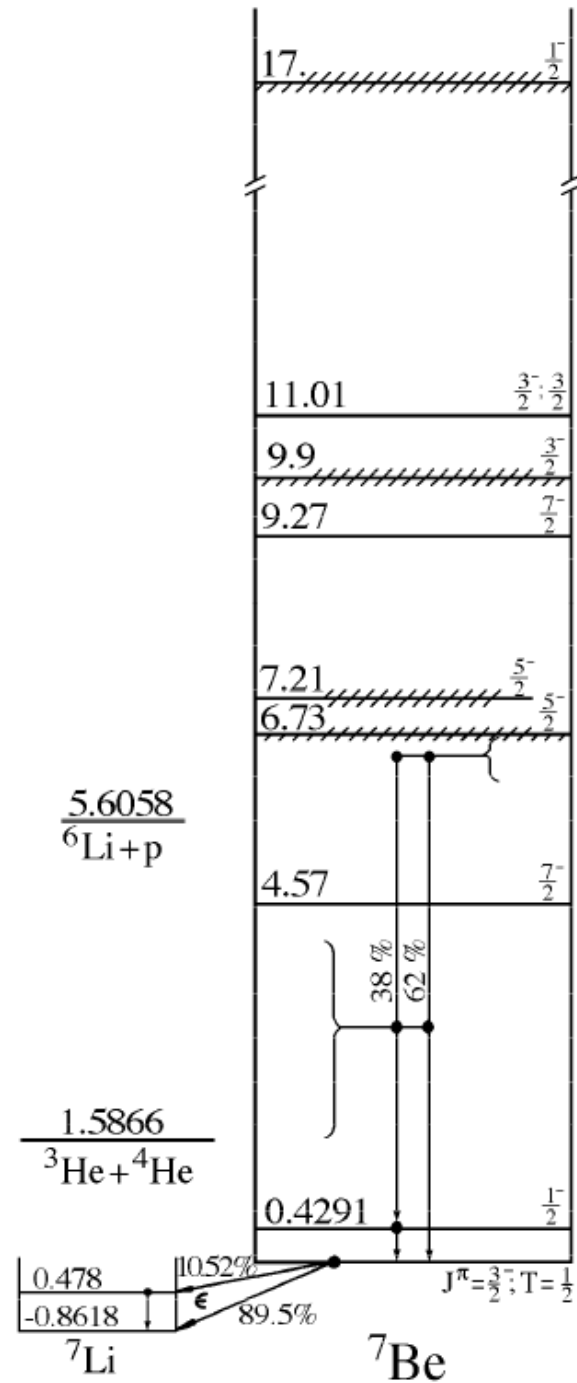
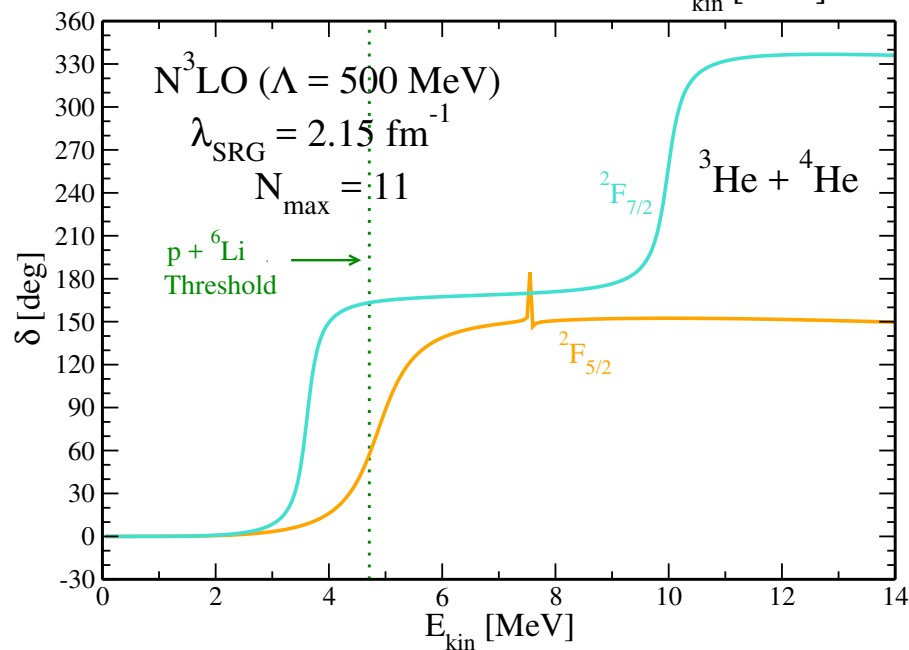
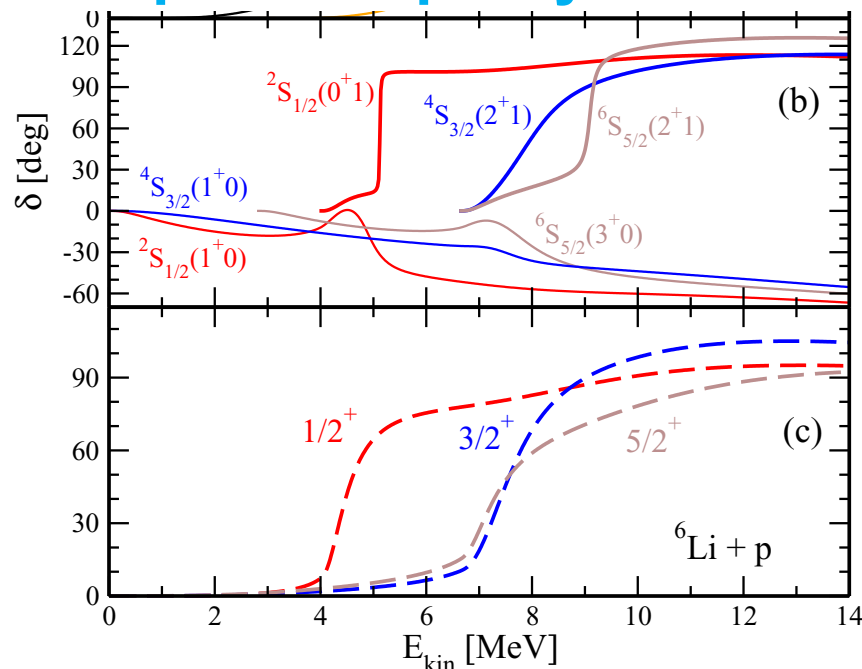
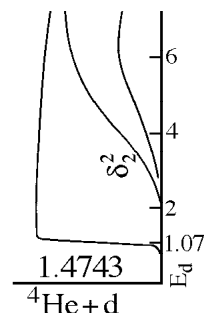
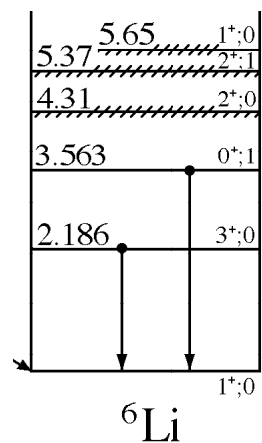
${}^7\text{Be}$ – Reproducing the energy spectrum



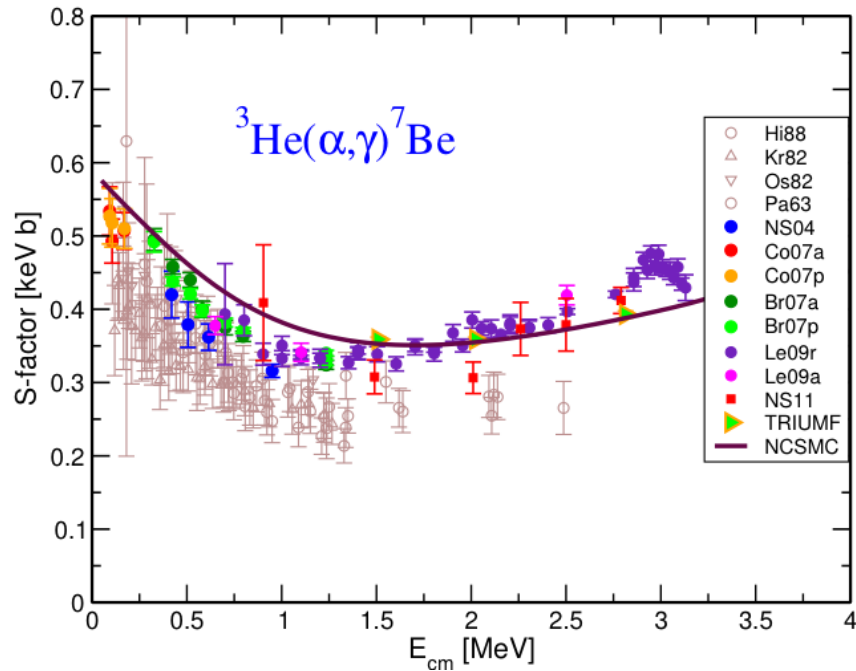
${}^7\text{Be}$ – New negative-parity states



${}^7\text{Be}$ – New positive-parity states



S-factor for ${}^3\text{He}(\alpha,\gamma){}^7\text{Be}$ and ${}^6\text{Li}(p,\gamma){}^7\text{Be}$ reaction



Physics Letters B 757 (2016) 430–436



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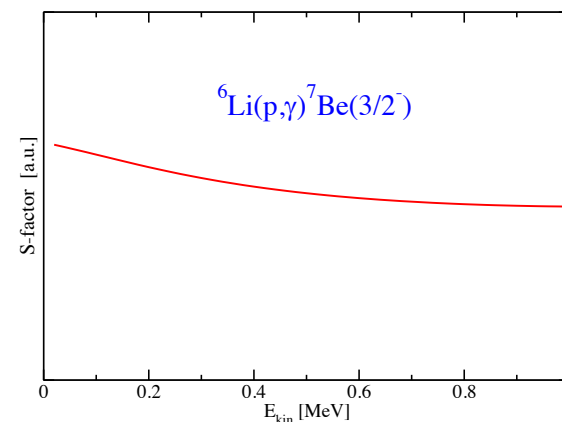
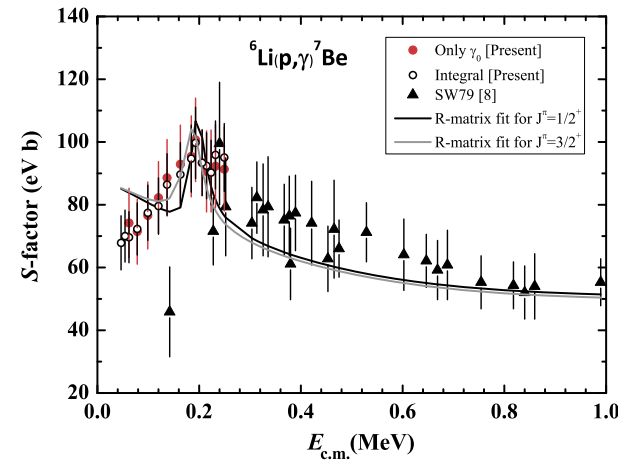
Physics Letters B

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${}^3\text{He}(\alpha,\gamma){}^7\text{Be}$ 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}



Physics Letters B 725 (2013) 287–291



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A drop in the ${}^6\text{Li}(p,\gamma){}^7\text{Be}$ reaction at low energies

J.J. He^{a,*}, S.Z. Chen^{a,b}, C.E. Rolfs^{c,a}, S.W. Xu^a, J. Hu^a, X.W. Ma^a, M. Wiescher^d, R.J. deBoer^d, T. Kajino^{e,f}, M. Kusakabe^g, L.Y. Zhang^{a,b}, S.Q. Hou^{a,b}, X.Q. Yu^a, N.T. Zhang^a, G. Lian^h, Y.H. Zhang^a, X.H. Zhou^a, H.S. Xu^a, G.Q. Xiao^a, W.L. Zhan^a



No resonance in ${}^7\text{Be}$ close to ${}^6\text{Li}+p$ threshold contrary to claim in Lanzhou experiment

PHYSICAL REVIEW C 100, 024304 (2019)

${}^7\text{Be}$ and ${}^7\text{Li}$ nuclei within the no-core shell model with continuum

Matteo Vorabbi^{a,*} and Petr Navrátil^b

TRIUMF, 4004 Wesbrook Mall, Vancouver, British Columbia V6T 2A3, Canada

Sofia Quaglioni

Lawrence Livermore National Laboratory, P. O. Box 808, L-414, Livermore, California 94551, USA

Guillaume Hupin^a

Institut de Physique Nucléaire, CNRS/IN2P3, Université Paris-Sud, Université Paris-Saclay, F-91406, Orsay, France

^7Be and ^7Li nuclei within the no-core shell model with continuumMatteo Vorabbi^{*} and Petr Navrátil[†]

TRIUMF, 4004 Wesbrook Mall, Vancouver, British Columbia V6T 2A3, Canada

Sofia Quaglioni

Lawrence Livermore National Laboratory, P. O. Box 808, L-414, Livermore, California 94551, USA

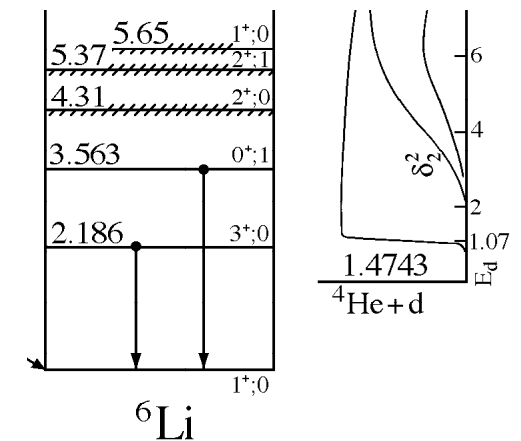
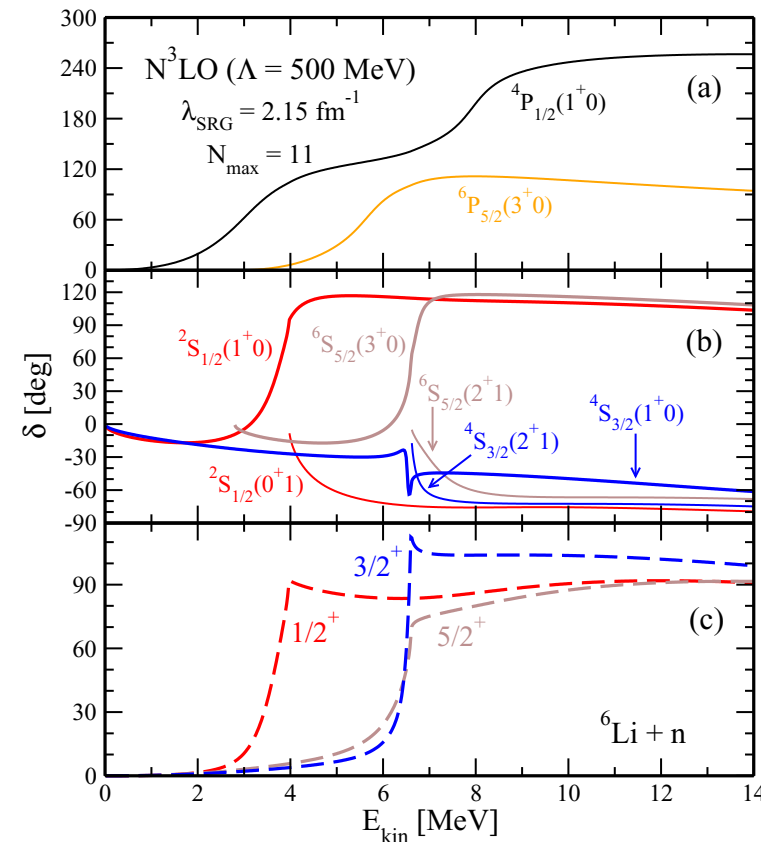
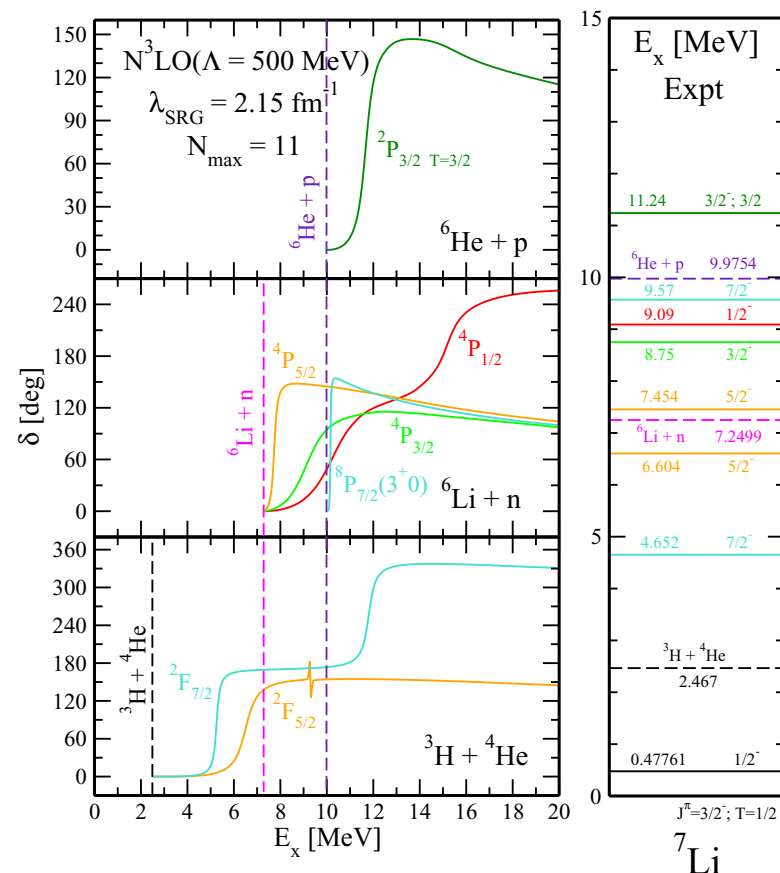
Guillaume Hupin[⊗]

Institut de Physique Nucléaire, CNRS/IN2P3, Université Paris-Sud, Université Paris-Saclay, F-91406, Orsay, France

38

S-wave resonance just above the threshold of $^6\text{He}+p$?

- NCSMC study of ^7Li and ^7Be nuclei using all binary mass partitions
 - Known resonances reproduced
 - Prediction of several new resonances of both parities



^7Be and ^7Li nuclei within the no-core shell model with continuumMatteo Vorabbi[✉] and Petr Navrátil[†]

TRIUMF, 4004 Wesbrook Mall, Vancouver, British Columbia V6T 2A3, Canada

Sofia Quaglioni

Lawrence Livermore National Laboratory, P. O. Box 808, L-414, Livermore, California 94551, USA

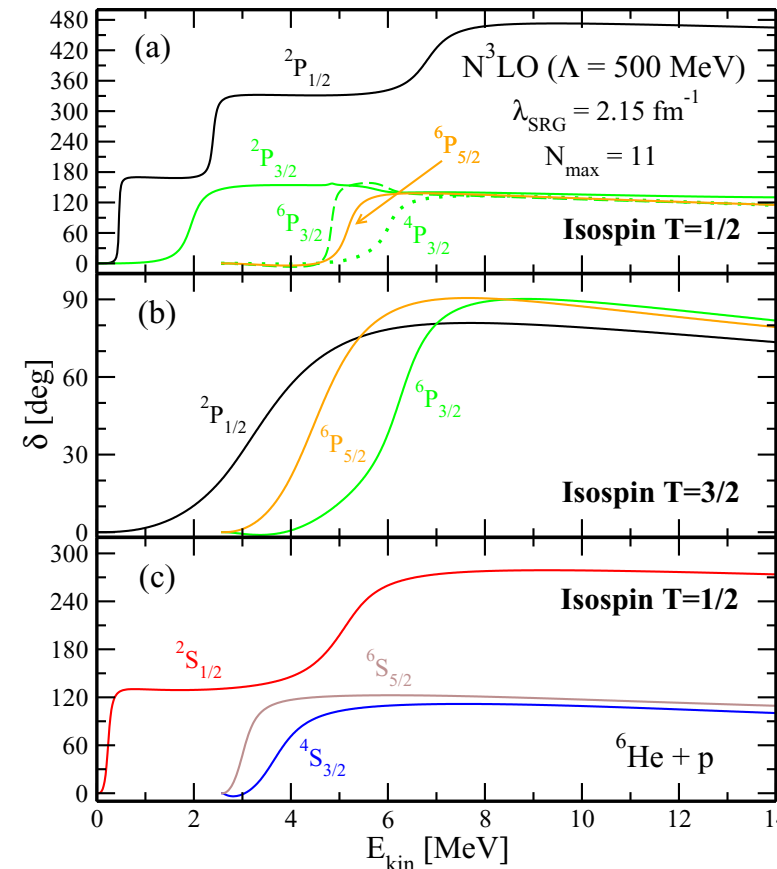
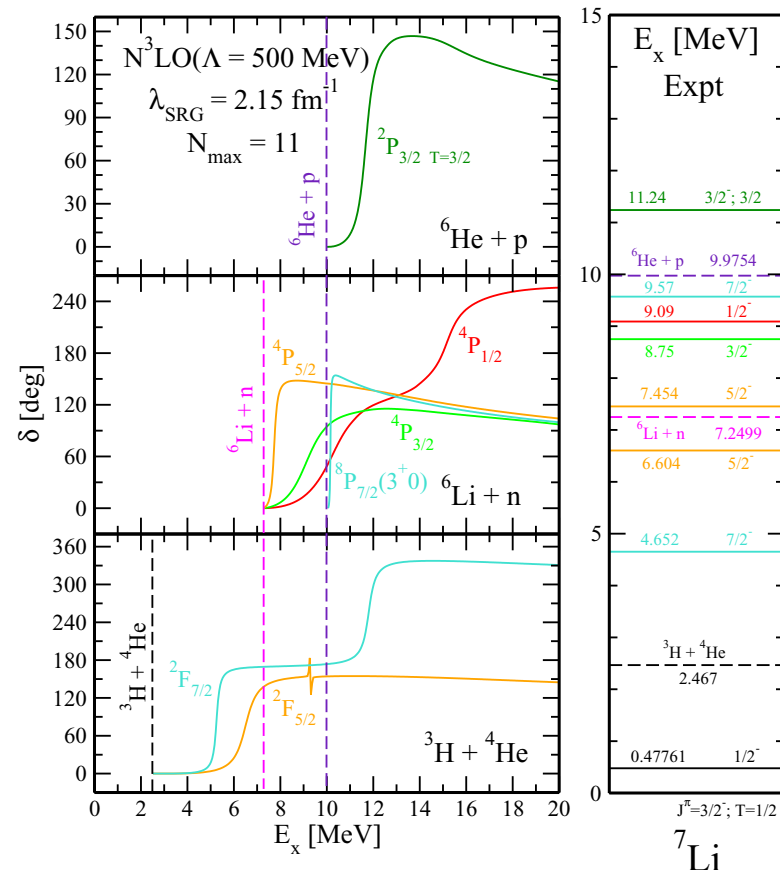
Guillaume Hupin[✉]

Institut de Physique Nucléaire, CNRS/IN2P3, Université Paris-Sud, Université Paris-Saclay, F-91406, Orsay, France

39

S-wave resonance just above the threshold of $^6\text{He}+p$?

- NCSMC study of ^7Li and ^7Be nuclei using all binary mass partitions
 - Known resonances reproduced
 - Prediction of several new resonances of both parities



S-wave resonance predicted at low energy in $^6\text{He}+p$ scattering with possible astrophysics implications.
Can this be investigated at TRIUMF or elsewhere?

Similarity to $^{10}\text{Be}+p$ system?

PHYSICAL REVIEW LETTERS **123**, 082501 (2019)

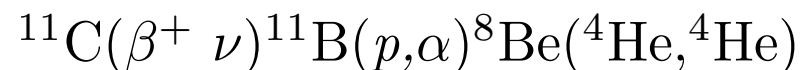
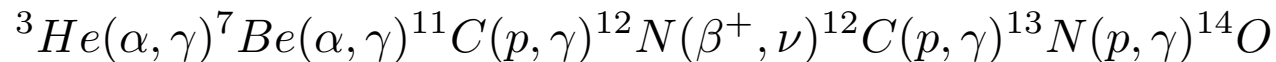
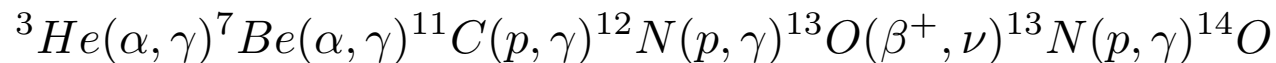
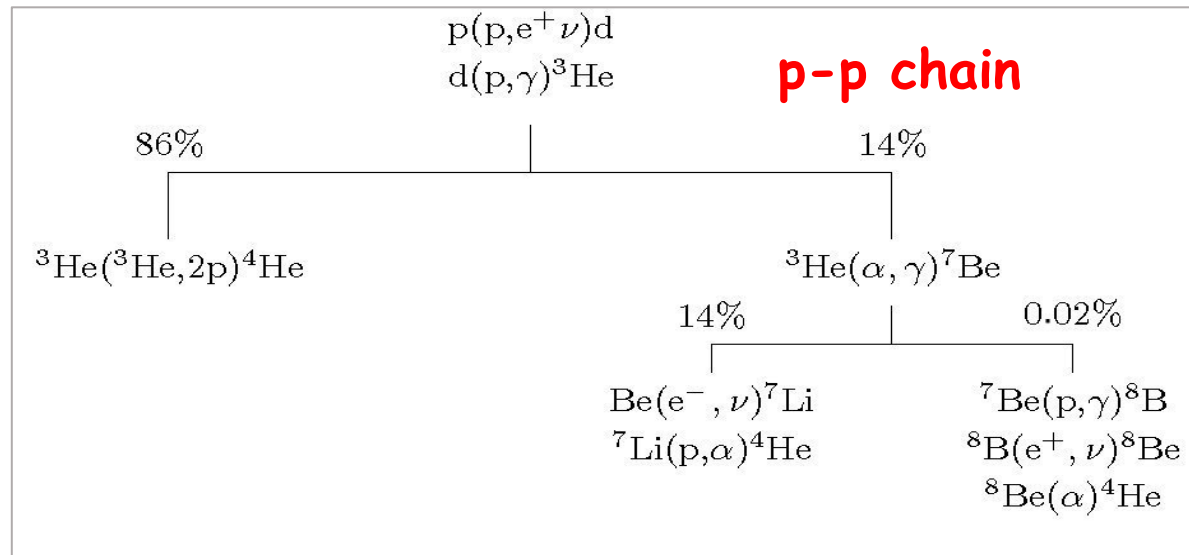
Editors' Suggestion

Direct Observation of Proton Emission in ^{11}Be

Y. Ayyad,^{1,2,*} B. Olaizola,³ W. Mittag,^{2,4} G. Potel,¹ V. Zelevinsky,^{1,2,4} M. Horoi,⁵ S. Beceiro-Novo,⁴ M. Alcorta,³ C. Andreoiu,⁶ T. Ahn,⁷ M. Anholm,^{3,8} L. Atar,⁹ A. Babu,³ D. Bazin,^{2,4} N. Bernier,^{3,10} S. S. Bhattacharjee,³ M. Bowry,³ R. Caballero-Folch,³ M. Cortesi,² C. Dalitz,¹¹ E. Dunlavy,^{3,12} A. B. Garnsworthy,³ M. Holl,^{3,13} B. Kootte,^{3,8} K. G. Leach,¹⁴ J. S. Randhawa,² Y. Saito,^{3,10} C. Santamaria,¹⁵ P. Siu,^{3,16} C. E. Svensson,⁹ R. Umashankar,³ N. Watwood,² and D. Yates^{3,10}

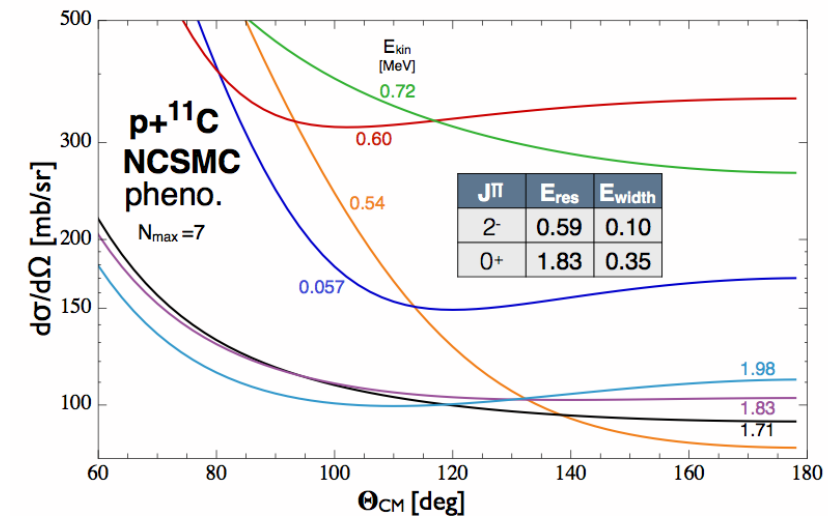
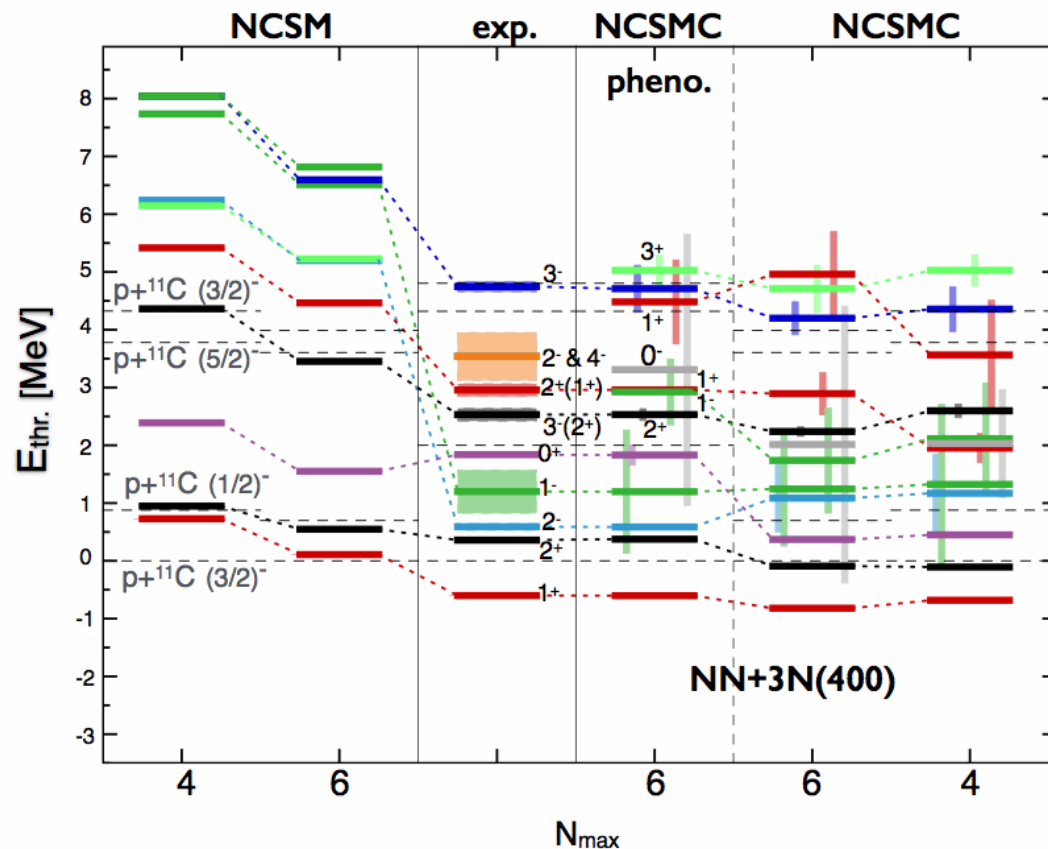
$p+^{11}\text{C}$ scattering and $^{11}\text{C}(p,\gamma)^{12}\text{N}$ capture

- $^{11}\text{C}(p,\gamma)^{12}\text{N}$ capture relevant in hot p - p chain: Link between pp chain and the CNO cycle - bypass of slow triple alpha capture $^4\text{He}(\alpha\alpha,\gamma)^{12}\text{C}$



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

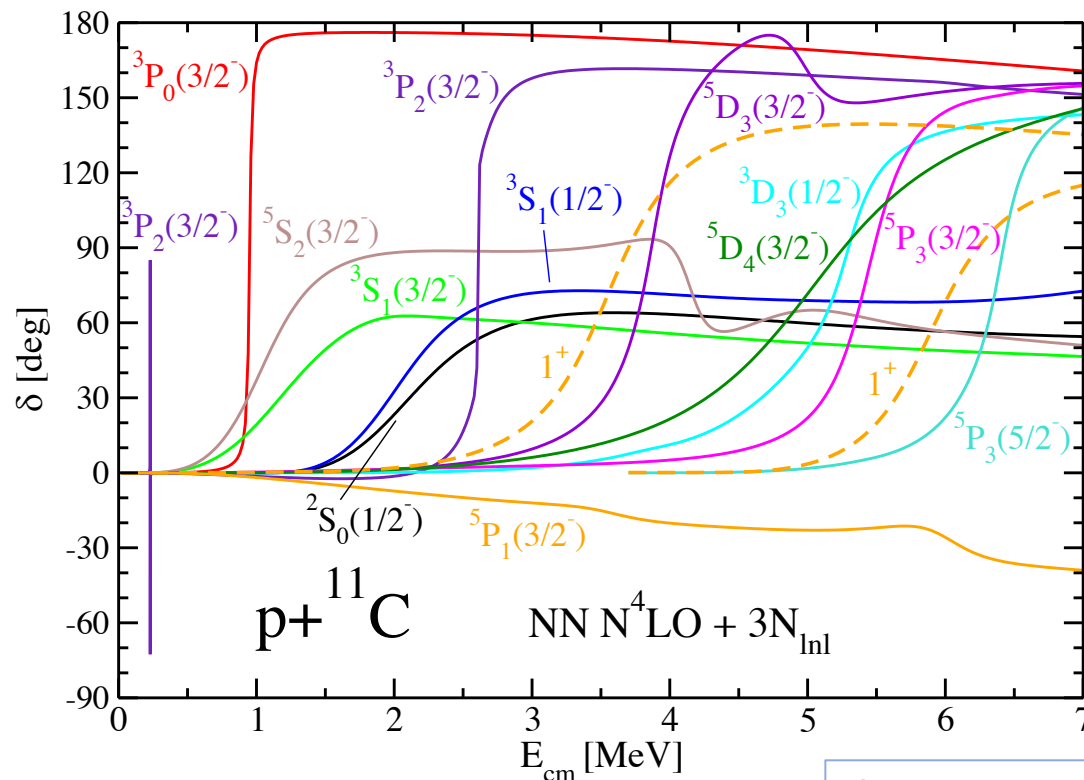
- NCSMC calculations of $^{11}\text{C}(p,p)$ with chiral NN+3N under way
 - ^{11}C : $3/2^-$, $1/2^-$, $5/2^-$, $3/2^-$ NCSM eigenstates
 - ^{12}N : ≥ 6 $\pi = +1$ and ≥ 4 $\pi = -1$ NCSM eigenstates



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

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

- NCSM with continuum calculations of $^{11}\text{C}(\text{p},\text{p})$ with higher-precision chiral NN+3N under way
 - ^{11}C and ^{12}N NCSM eigenstates calculated with NCSD code on Summit using GPU acceleration
 - 1024 nodes, 6144 MPI tasks with 1 GPU/task and 7 OpenMP threads/task
 - Largest matrix dimensions: 131 million for ^{11}C and 167 million for ^{12}N (~7 hours to get 9 eigenstates)



Calculated bound-state energy $E(1^+ 1) = -0.52$ MeV

6.40	6.275	(1 ⁻ , 3 ⁺)	(1 ⁻)
5.60	5.348		3 ⁻
4.561	4.410		(1, 2) ⁺
4.142		4 ⁻	2 ⁻ + 4 ⁻
3.558			(1, 2) ⁺
3.132		(2 ⁺ , 3 ⁻)	
2.439			0 ⁺
1.800			1 ⁻
1.190	0.961	2 ⁺	2 ⁻
			1 ⁺ ; 1

Experiment

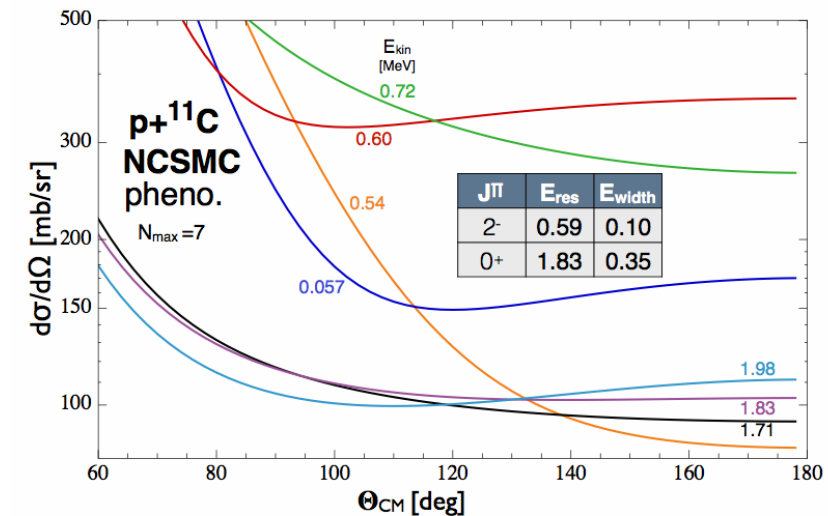
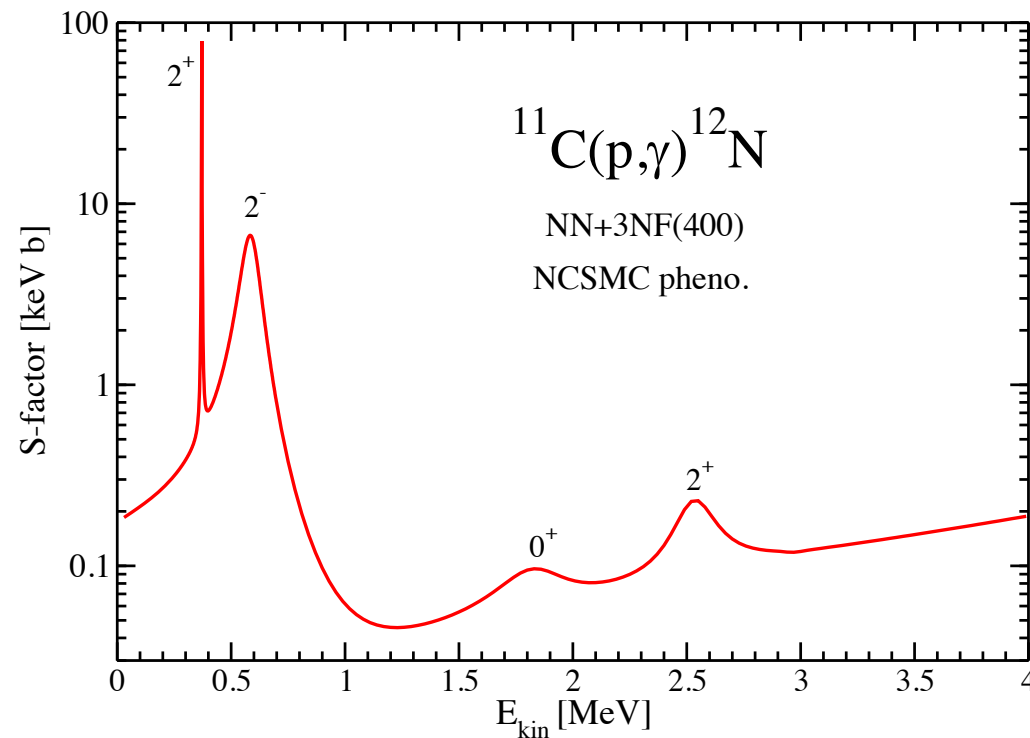
^{12}N

$2m_0c^2$

$\frac{0.601}{^{11}\text{C} + \text{p}}$

$p+^{11}\text{C}$ 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 : $\geq 6 \pi = +1$ and $\geq 4 \pi = -1$ NCSM eigenstates



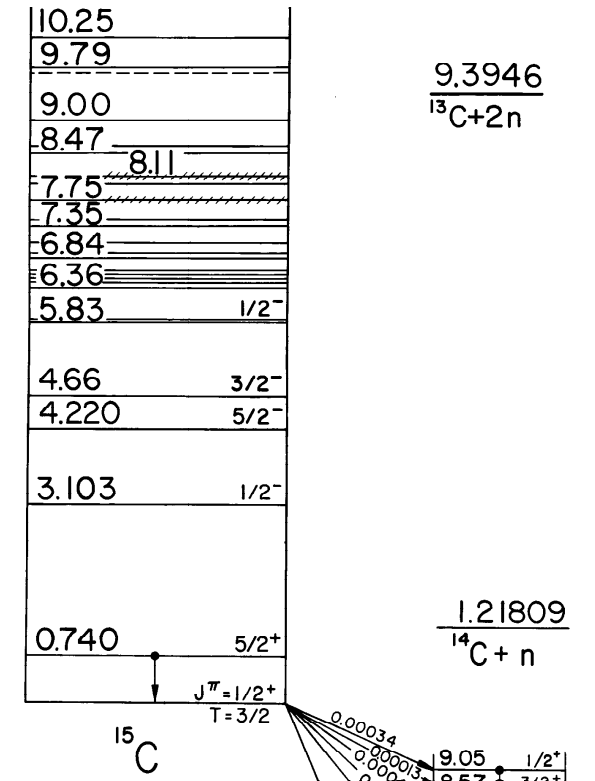
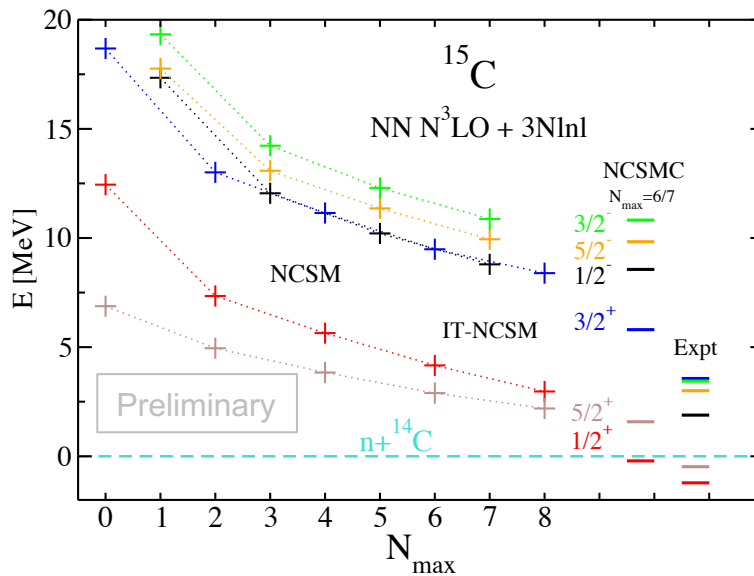
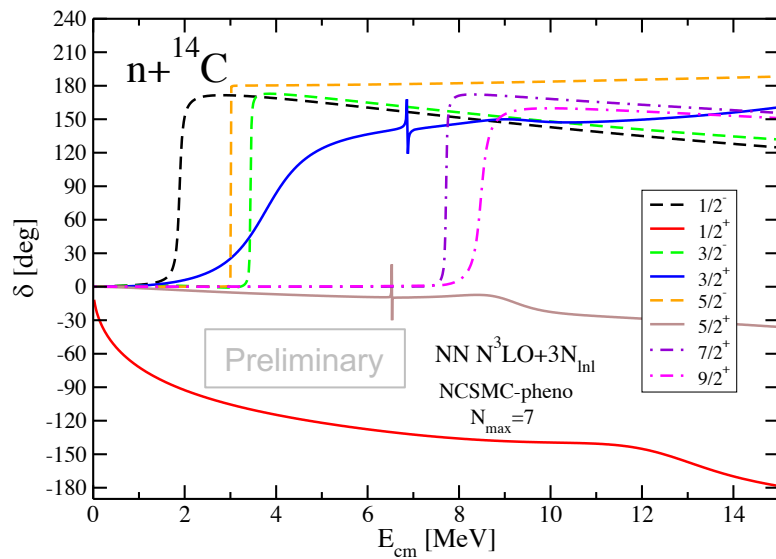
NCSMC calculations to be validated by
measured cross sections and applied to
calculate the $^{11}\text{C}(p,\gamma)^{12}\text{N}$ capture

-
- Energy level diagram for ^{15}C showing various states and transitions. The diagram includes a vertical stack of energy levels with labels such as 10.25, 9.79, 9.00, 8.47, 8.11, 7.75, 7.35, 6.84, 6.36, 5.83, 4.66, 4.220, 3.103, and 0.740. Transitions are indicated by arrows, with labels like $J^\pi = 1/2^+$ and $T = 3/2$. A detailed inset shows a transition from ^{15}C to $^{14}\text{C} + n$, with energy levels 9.05 and 9.3946, and a transition energy of 0.00034.

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

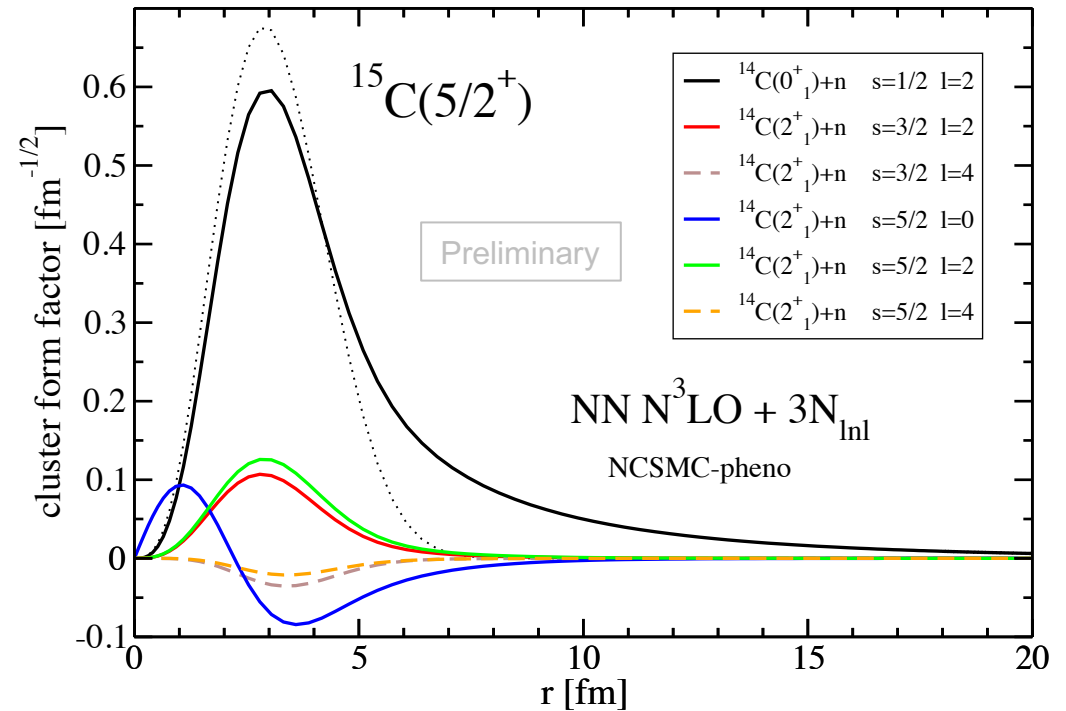
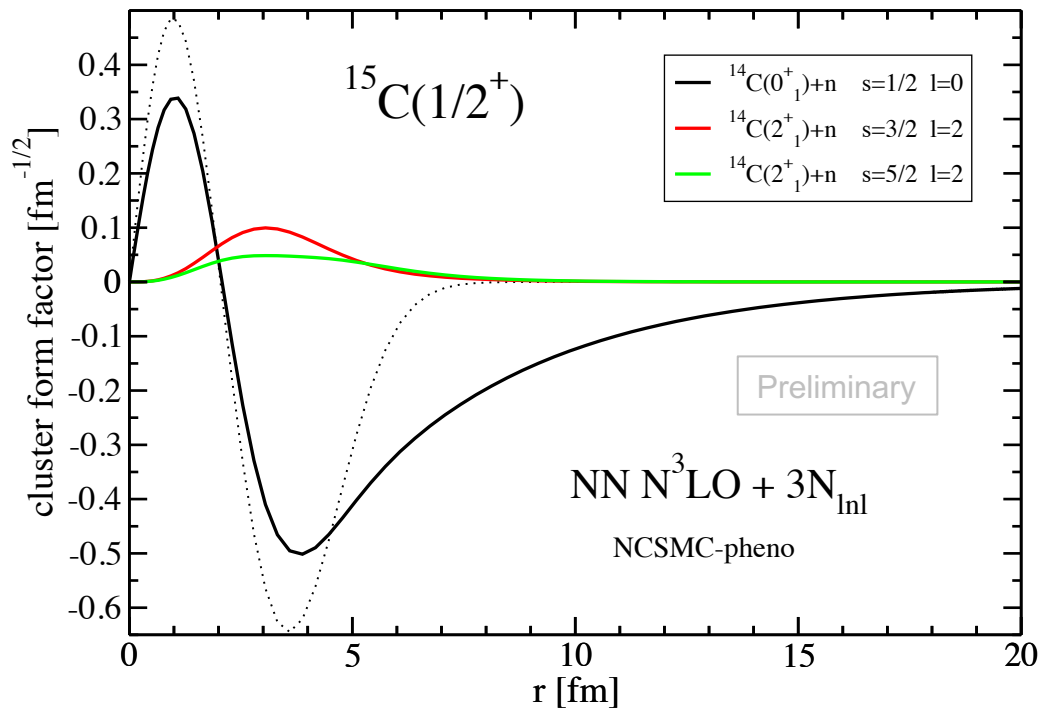
NCSMC-pheno



^{15}C cluster form factors

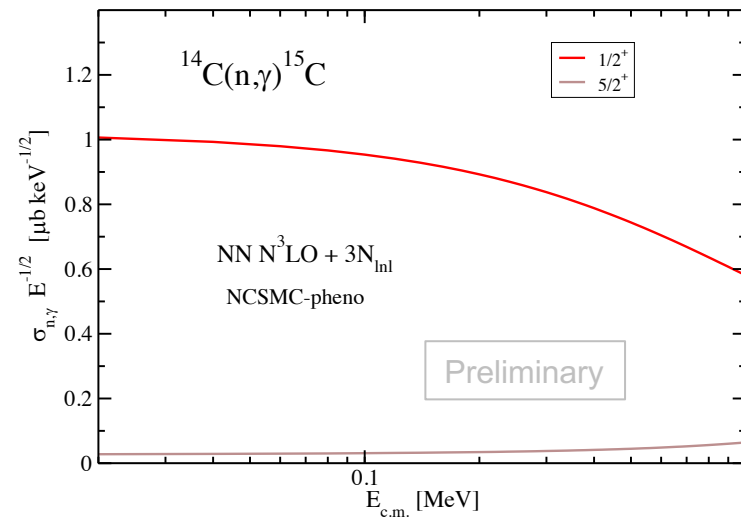
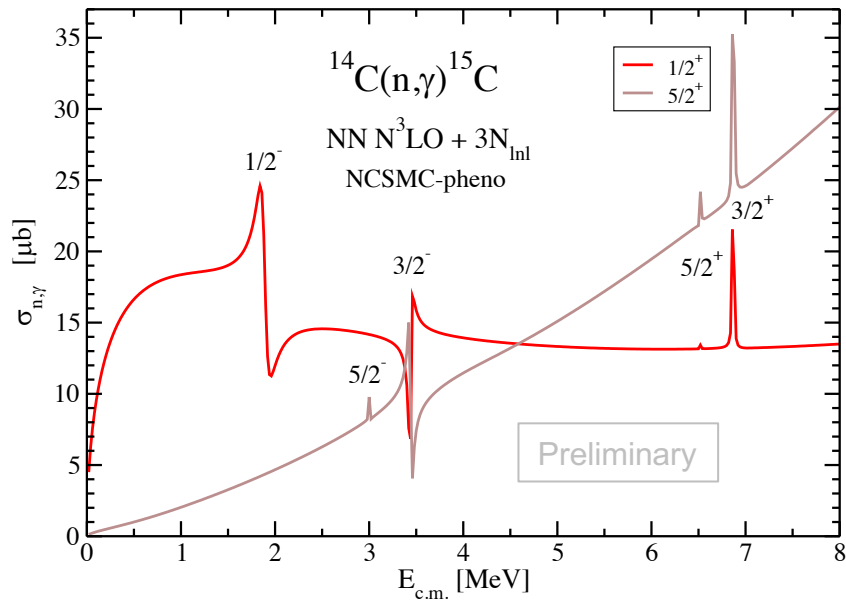
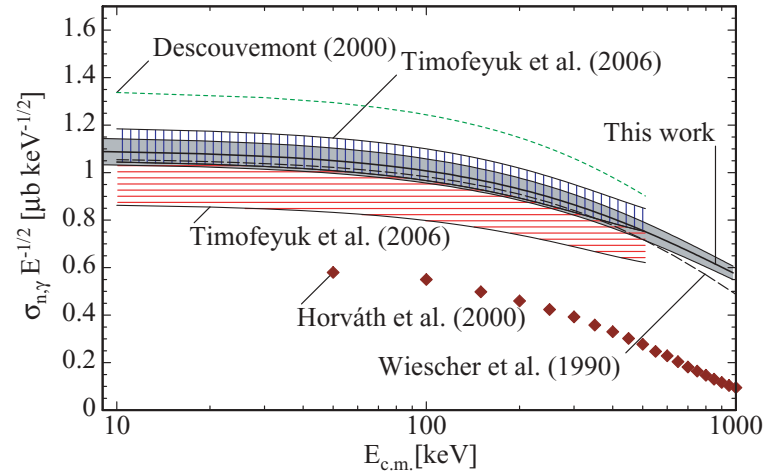
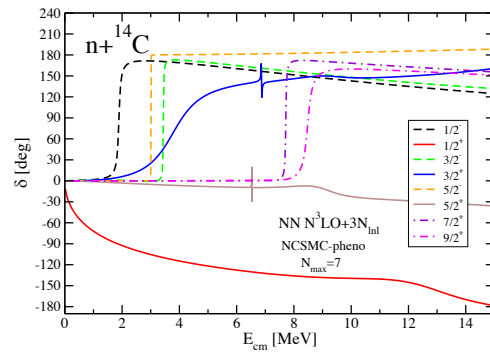
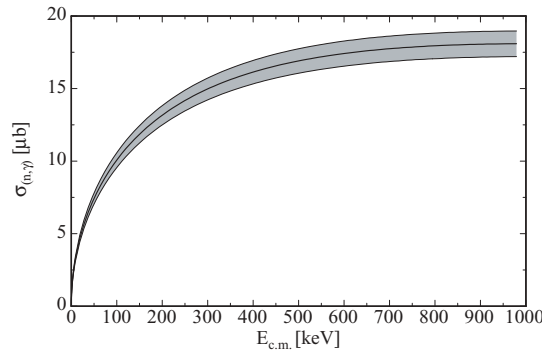
■ $1/2^+$ S-wave and $5/2^+$ D-wave ANCs

- $C_{1/2^+} = 1.282 \text{ fm}^{-1/2}$ - 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.



$^{14}\text{C}(n,\gamma)^{15}\text{C}$ 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 with predictive power becoming feasible beyond the lightest nuclei
- These calculations 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
- Structure of ${}^7\text{Be}$ and ${}^7\text{Li}$ from different binary mass partitions
 - Investigation of capture reactions relevant for astrophysics
 - Observation of a narrow S-wave resonance above $6\text{He}+p$ threshold – similarity to ${}^{10}\text{Be}+p$ system?
- ${}^{11}\text{C}(p,\gamma){}^{12}\text{N}$ NCSMC calculations with validation of the ${}^{11}\text{C}+p$ scattering by TRIUMF experiment
- ${}^{15}\text{C}$ NCSMC calculations in progress
 - Capture cross section, cluster form factor, ANCs

Thank you!
Merci!

