

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

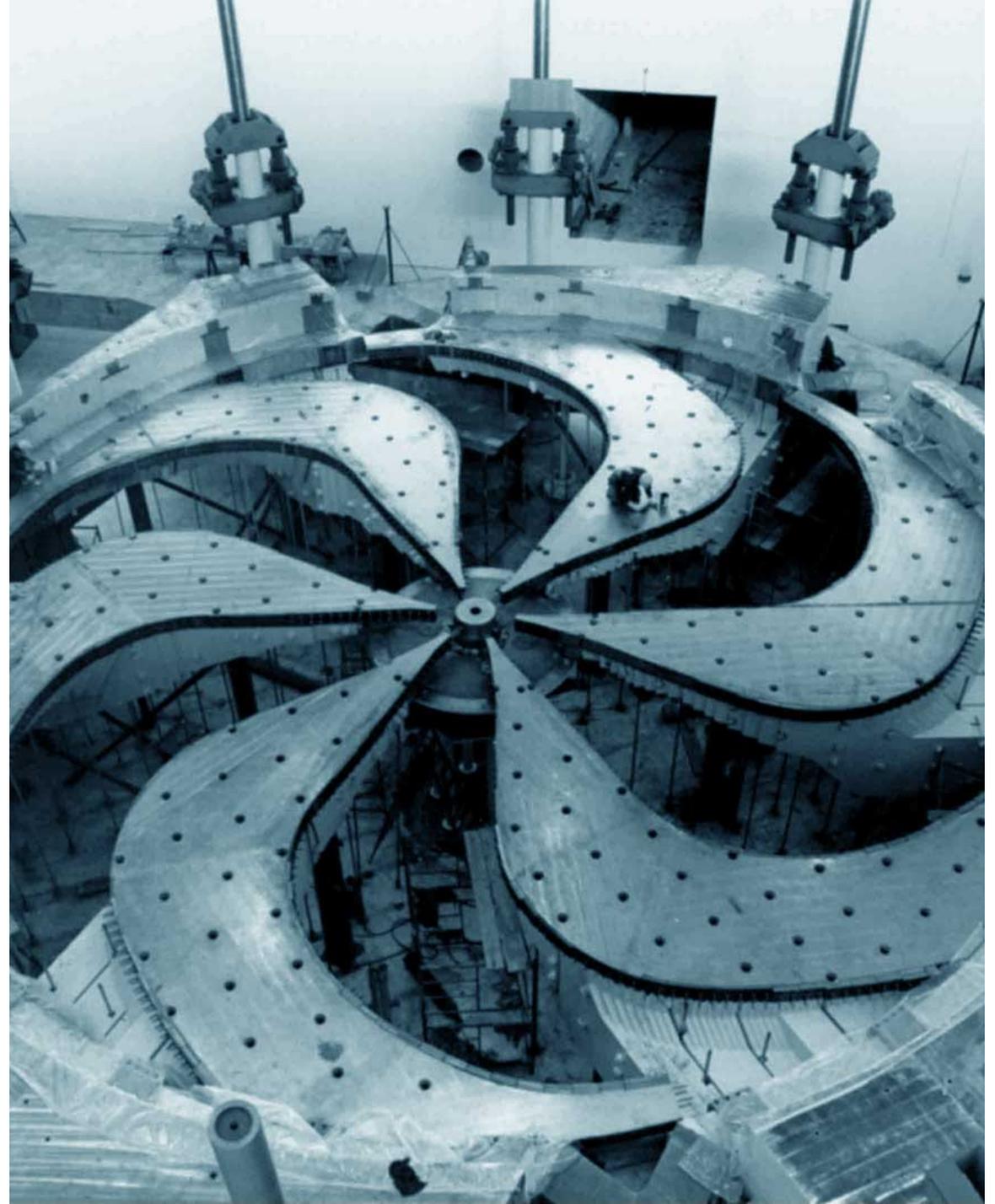
ECT* Trento, Italy, September 30 – October 4, 2019

Petr Navratil

TRIUMF

Collaborators: S. Quaglioni (LLNL), G. Hupin (Orsay),
M. Vorabbi, A. Calci (TRIUMF), P. Gysbers (UBC/TRIUMF),
M. Gennari (U Waterloo), K. Kravvaris (LLNL)

2019-10-04



Outline

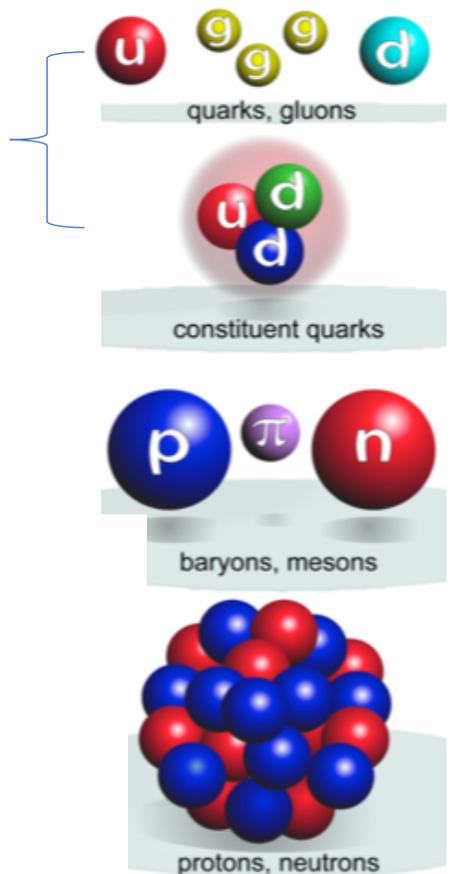
- Introduction to *ab initio* No-Core Shell Model with Continuum (NCSMC)
- Polarized ${}^3\text{H}(d,n){}^4\text{He}$ fusion
- Structure of ${}^7\text{Be}$ and ${}^7\text{Li}$ from different binary-mass partitions
- ${}^{11}\text{C}(p,\gamma){}^{12}\text{N}$ capture
- Structure of the halo *sd*-shell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

First principles or *ab initio* nuclear theory

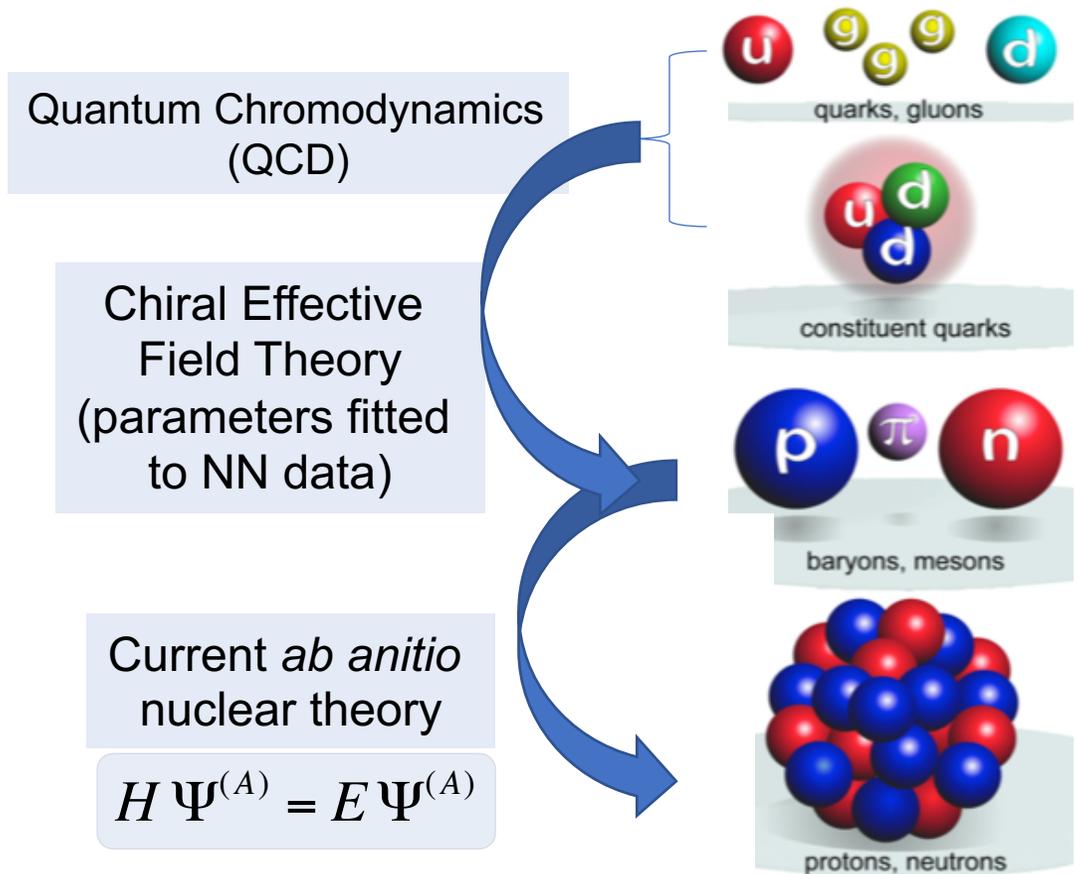
Quantum Chromodynamics
(QCD)



Genuine *Ab Initio*



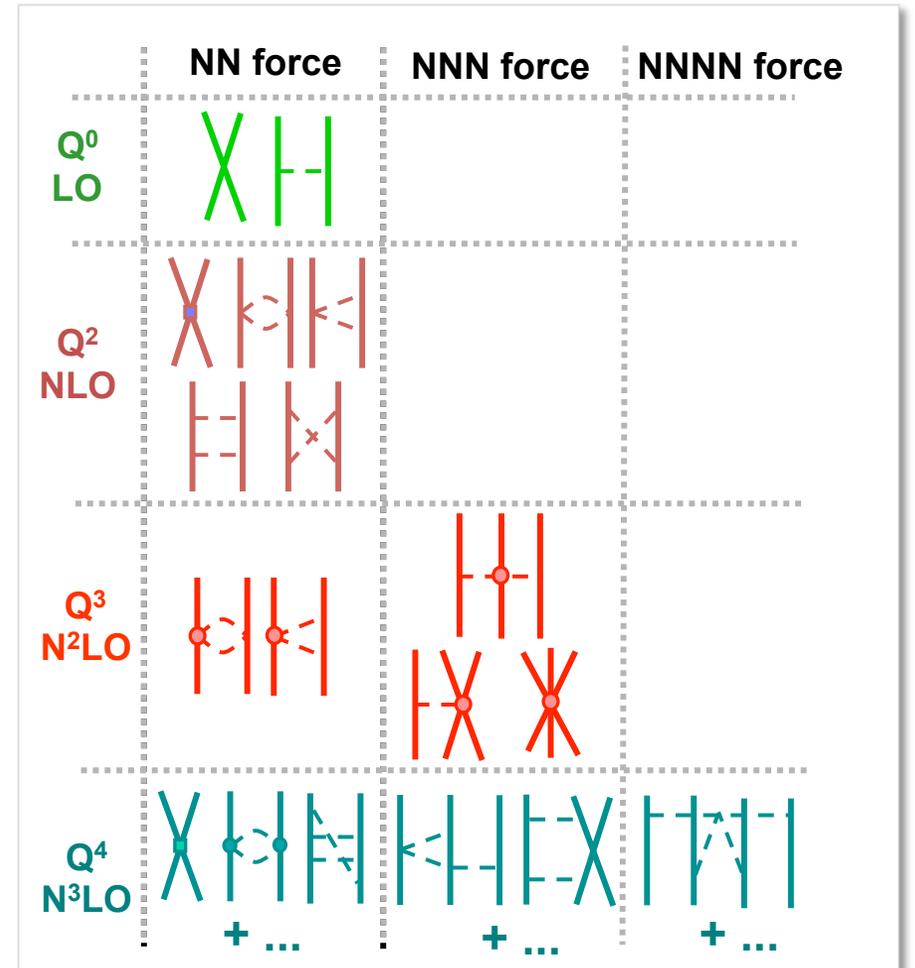
First principles or *ab initio* nuclear theory – what we do at present



- *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

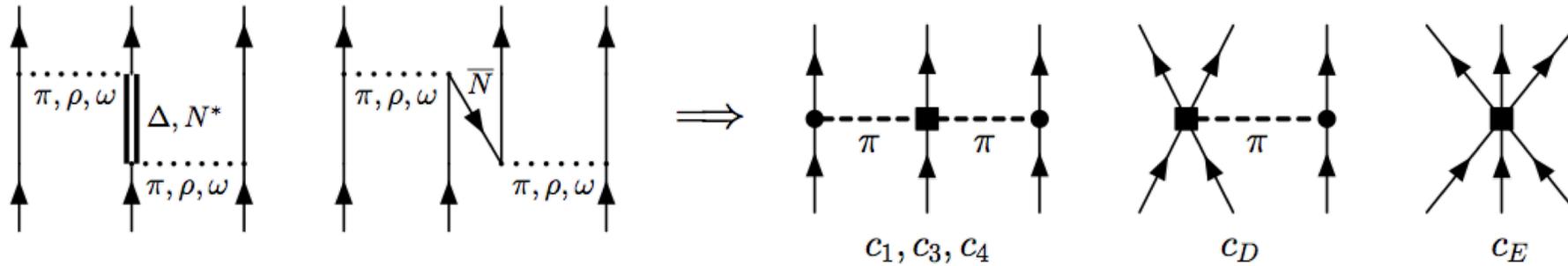
Chiral Effective Field Theory

- 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

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?

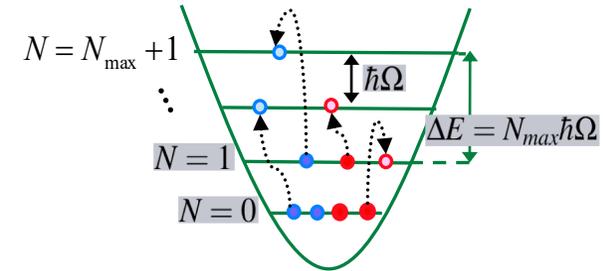
Conceptually simplest *ab initio* method: No-Core Shell Model (NCSM)

7



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



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

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

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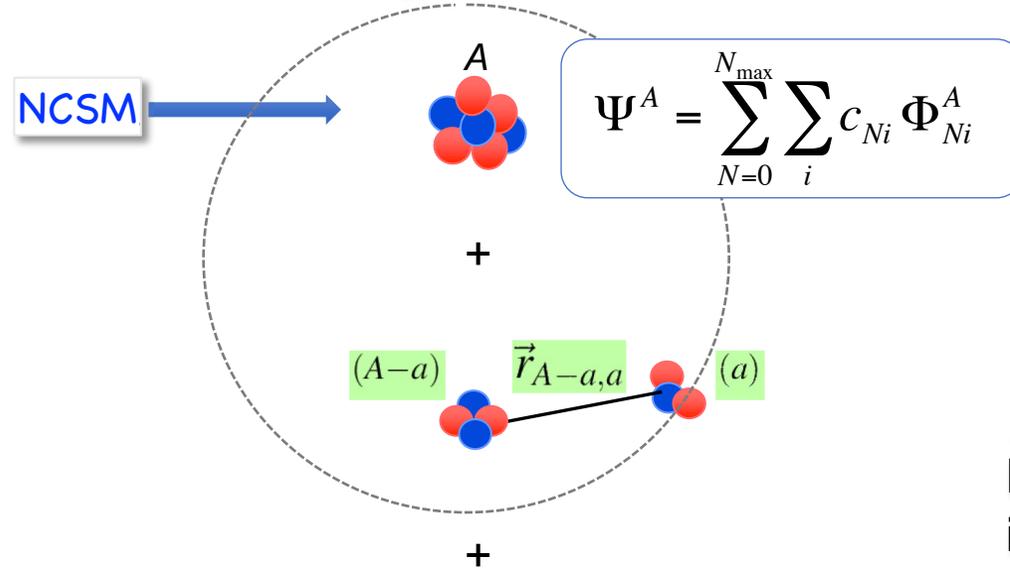
Review

Ab initio no core shell model

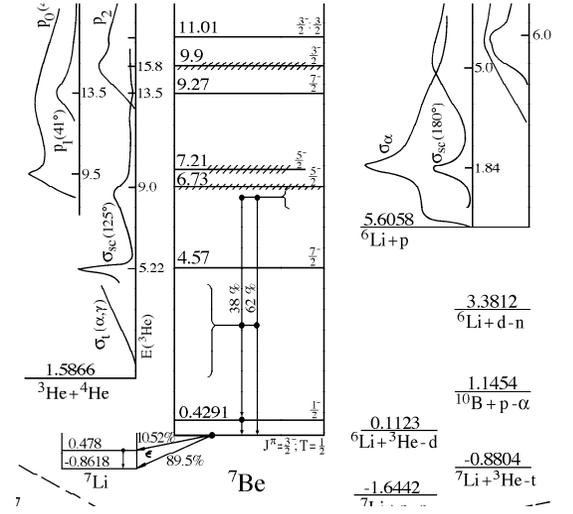
Bruce R. Barrett^a, Petr Navrátil^b, James P. Vary^{c,*}

Extending no-core shell model beyond bound states

Include more many nucleon correlations...



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

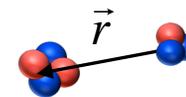


Unified approach to bound & continuum states; to nuclear structure & reactions

- 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



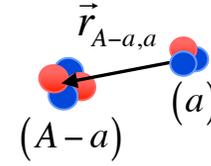
NCSM/RGM

NCSMC

$$\Psi^{(A)} = \sum_{\lambda} c_{\lambda} \left| \begin{matrix} (A) \\ \text{Nucleus} \\ \lambda \end{matrix} \right\rangle + \sum_{\nu} \int d\vec{r} \gamma_{\nu}(\vec{r}) \hat{A}_{\nu} \left| \begin{matrix} (A-a) & (a) \\ \text{Cluster 1} & \text{Cluster 2} \\ \nu \end{matrix} \right\rangle$$

Unknowns

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



Binary cluster basis

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

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

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

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

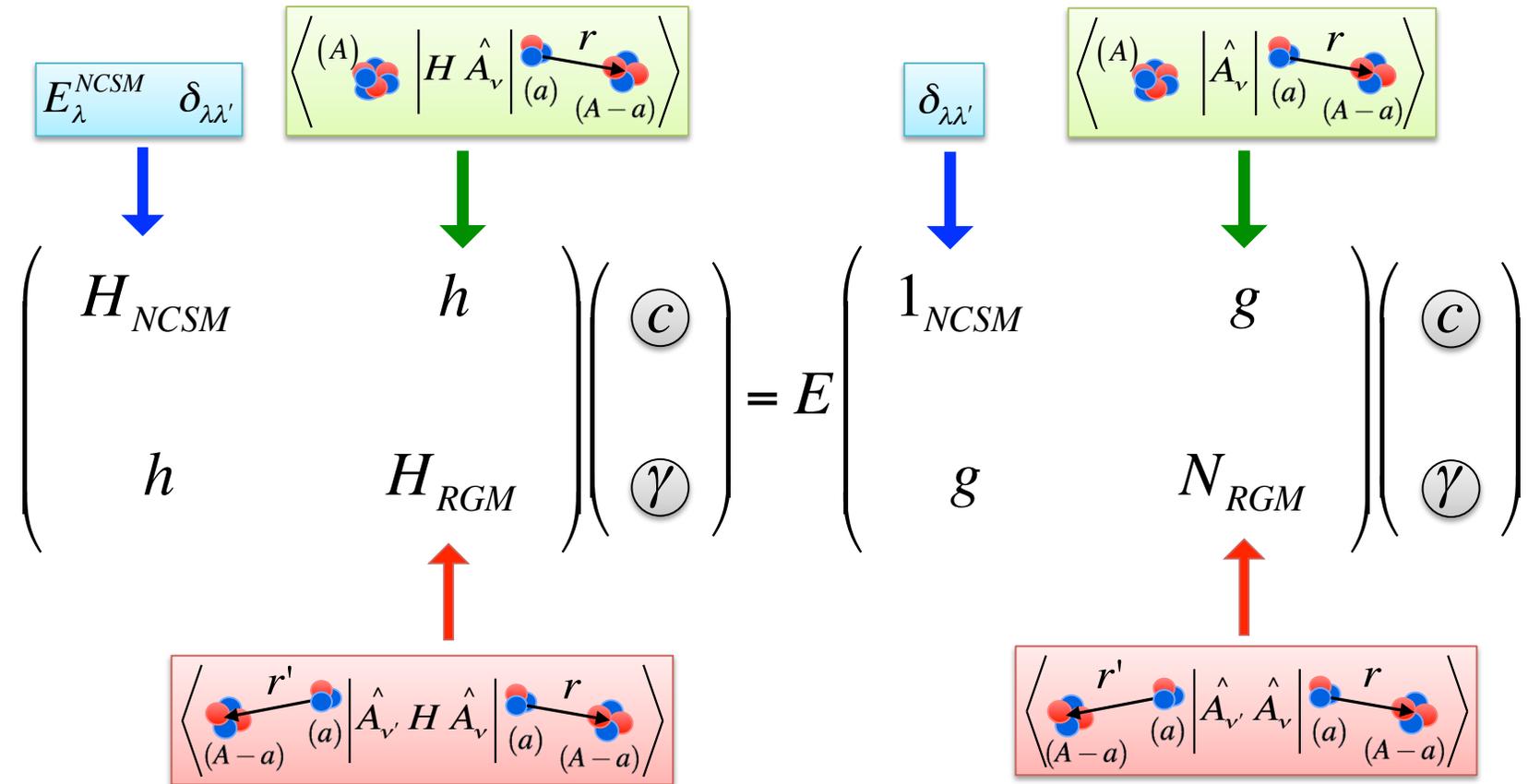
- Allows to bring the wave function of the relative motion in front of the antisymmetrizer

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

Coupled NCSMC equations

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

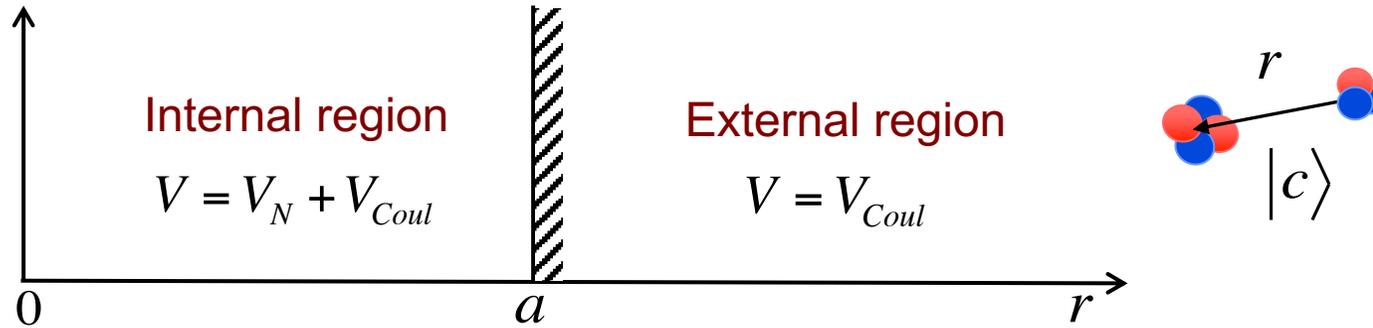
$$\Psi^{(A)} = \sum_{\lambda} c_{\lambda} \left| \begin{array}{c} (A) \\ \text{cluster} \end{array}, \lambda \right\rangle + \sum_{\nu} \int d\vec{r} \gamma_{\nu}(\vec{r}) \hat{A}_{\nu} \left| \begin{array}{c} (A-a) \\ \text{cluster} \end{array}, \nu \right\rangle$$



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

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

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

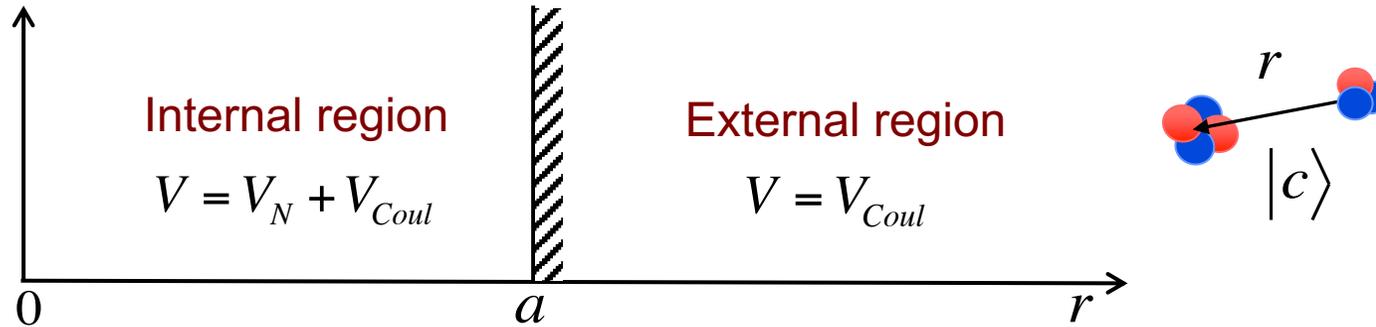


- Matching achieved through the Bloch operator: $L_c = \frac{\hbar^2}{2\mu_c} \delta(r - a) \left(\frac{d}{dr} - \frac{B_c}{r} \right)$
- System of Bloch-Schrödinger equations:

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

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

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- 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 $f_n(r)$:

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

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

- Solve for A_{cn}
- 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

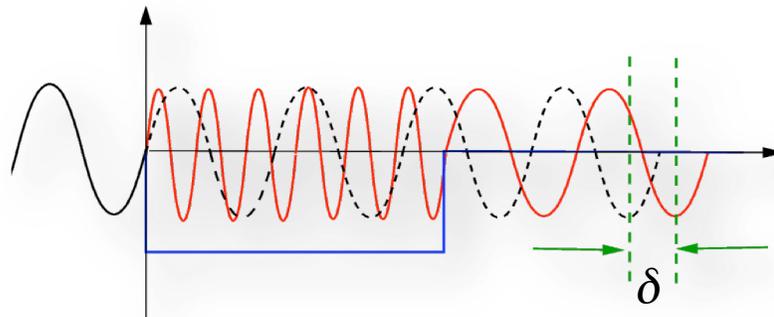
$$\sum_{c'} R_{cc'} \frac{k_{c'} a}{\sqrt{\mu_{c'} v_{c'}}} [I'_{c'}(k_{c'} a) \delta_{ci} - U_{c'i} O'_{c'}(k_{c'} a)] = \frac{1}{\sqrt{\mu_c v_c}} [I_c(k_c a) \delta_{ci} - U_{ci} O_c(k_c a)]$$

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

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



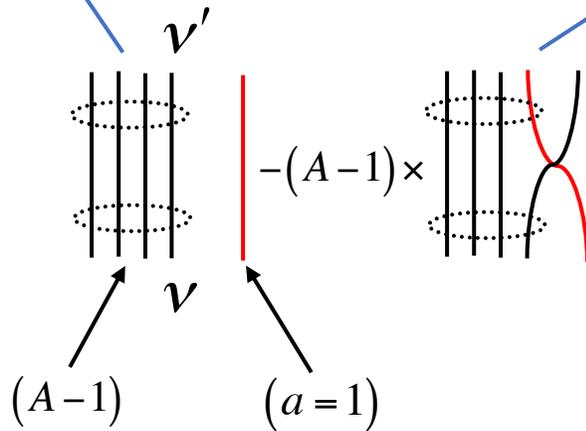
Norm kernel (Pauli principle): Single-nucleon projectile

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

$$N_{v'v}^{J^{\pi T}}(r', r) = \underbrace{\delta_{v'v} \frac{\delta(r'-r)}{r'r}}_{\text{Direct term}} - (A-1) \sum_{n'n} R_{n'l'}(r') R_{nl}(r) \underbrace{\langle \Phi_{v'n'}^{J^{\pi T}} | \hat{P}_{A-1,A} | \Phi_{vn}^{J^{\pi T}} \rangle}_{\text{Exchange term}}$$

$$\text{SD} \langle \psi_{\mu_1}^{(A-1)} | a^+ a | \psi_{\nu_1}^{(A-1)} \rangle_{\text{SD}}$$

Direct term:
Treated exactly!
(in the full space)



Exchange term:
Obtained in the model space!
(Many-body correction due to
the exchange part of the inter-
cluster antisymmetrizer)

Trick #1

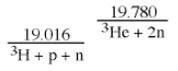
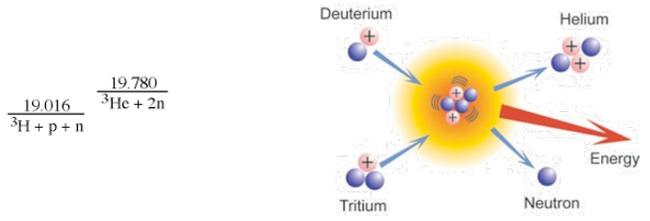
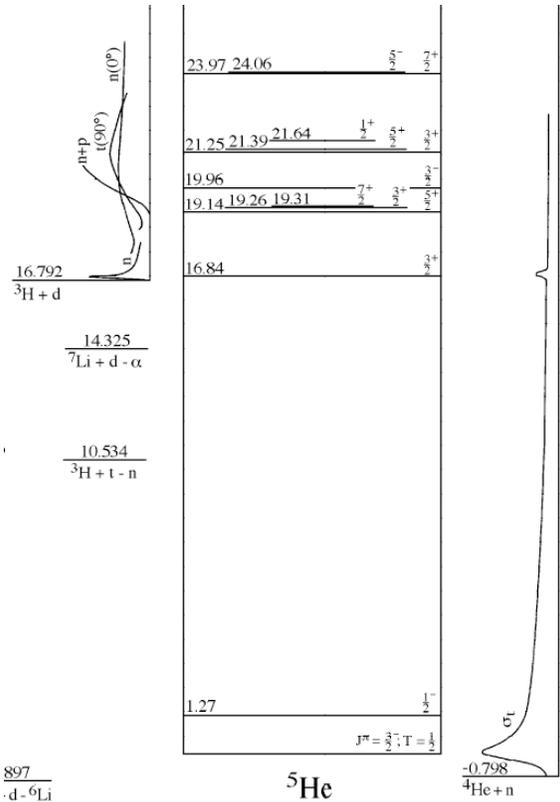
$$\frac{\delta(r - r_{A-a,a})}{r r_{A-a,a}} = \sum_n R_{nl}(r) R_{nl}(r_{A-a,a})$$

Trick #2

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

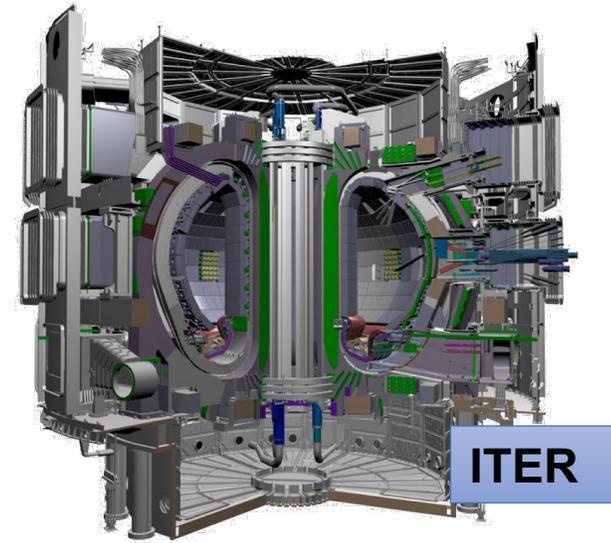
Deuterium-Tritium fusion

- 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 $E_{cm}=48$ 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-⁶Li

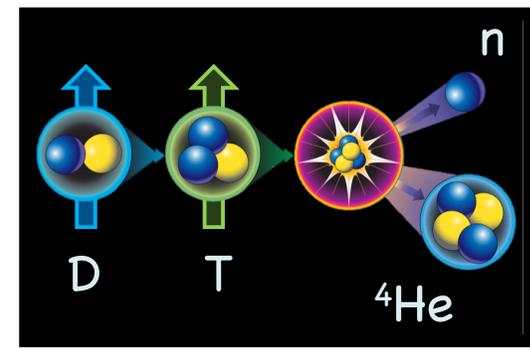
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NCSMC calculation of the DT fusion

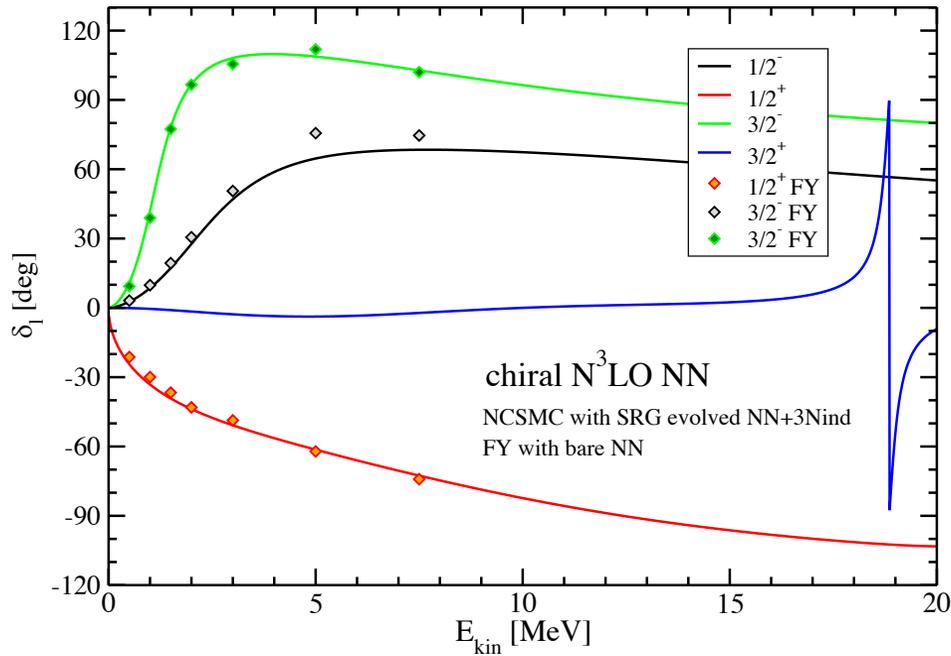
$$|\Psi\rangle = \sum_{\lambda} c_{\lambda} \left| \begin{array}{c} \text{He} \\ \text{5} \end{array}, \lambda \right\rangle + \int d\vec{r} u_{\nu_{DT}}(\vec{r}) \hat{A}_{DT} \left| \begin{array}{c} \text{D} \\ \text{T} \end{array}, \nu_{DT} \right\rangle + \int d\vec{r} u_{\nu_{n\alpha}}(\vec{r}) \hat{A}_{n\alpha}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

- 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

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

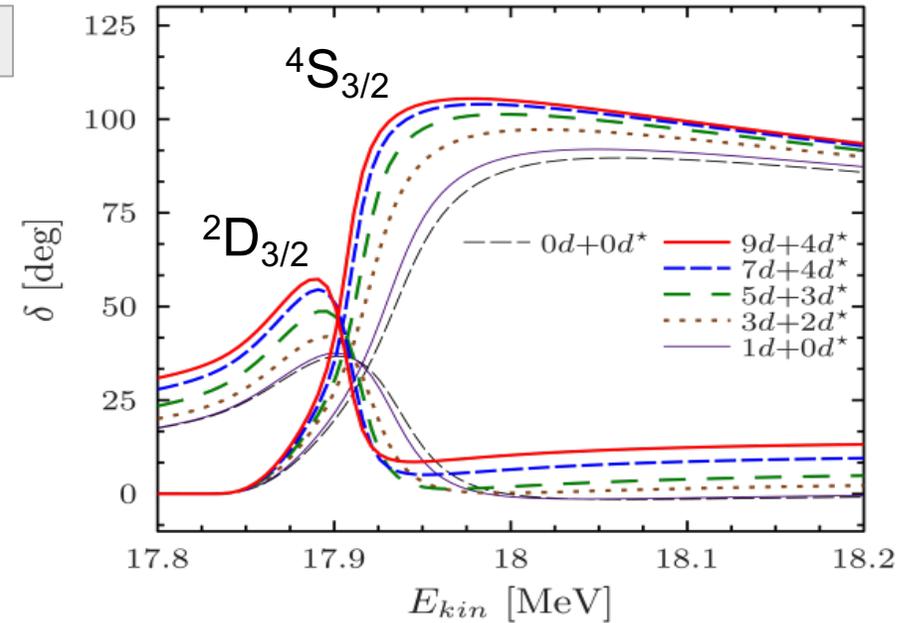


n - ^4He and d + ^3H scattering phase-shifts



$^4\text{He}+n$

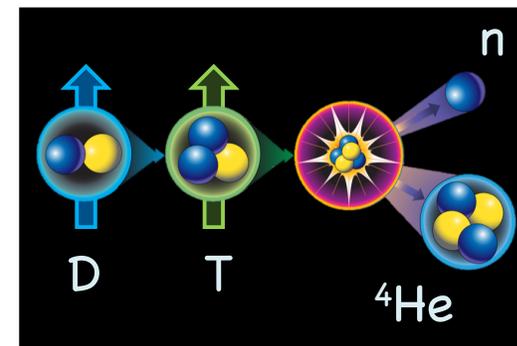
$^4\text{He}+n \rightarrow ^3\text{H}+d$



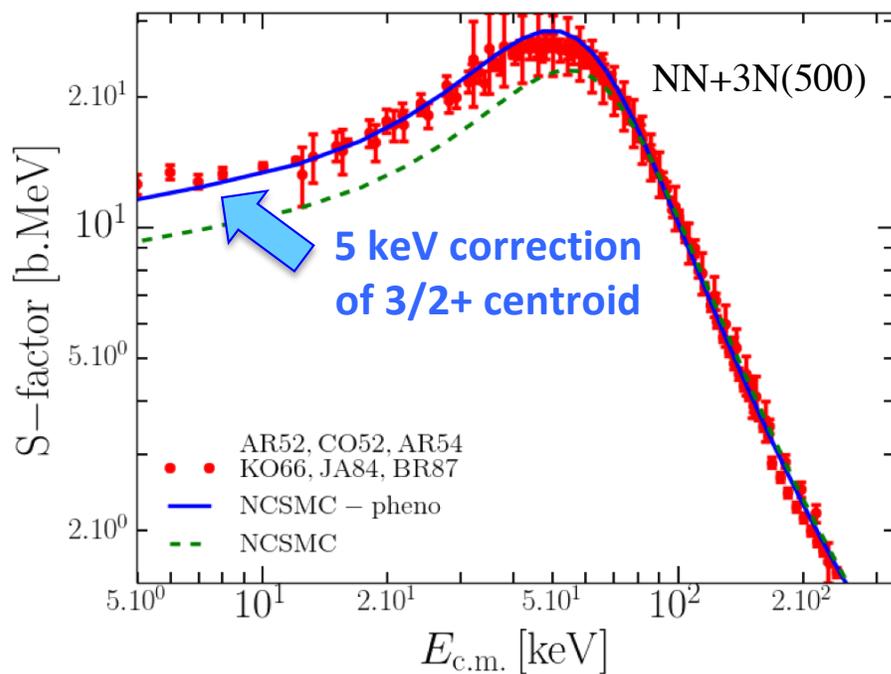
FY: Faddeev-Yakubovsky method - Rimantas Lazauskas

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



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

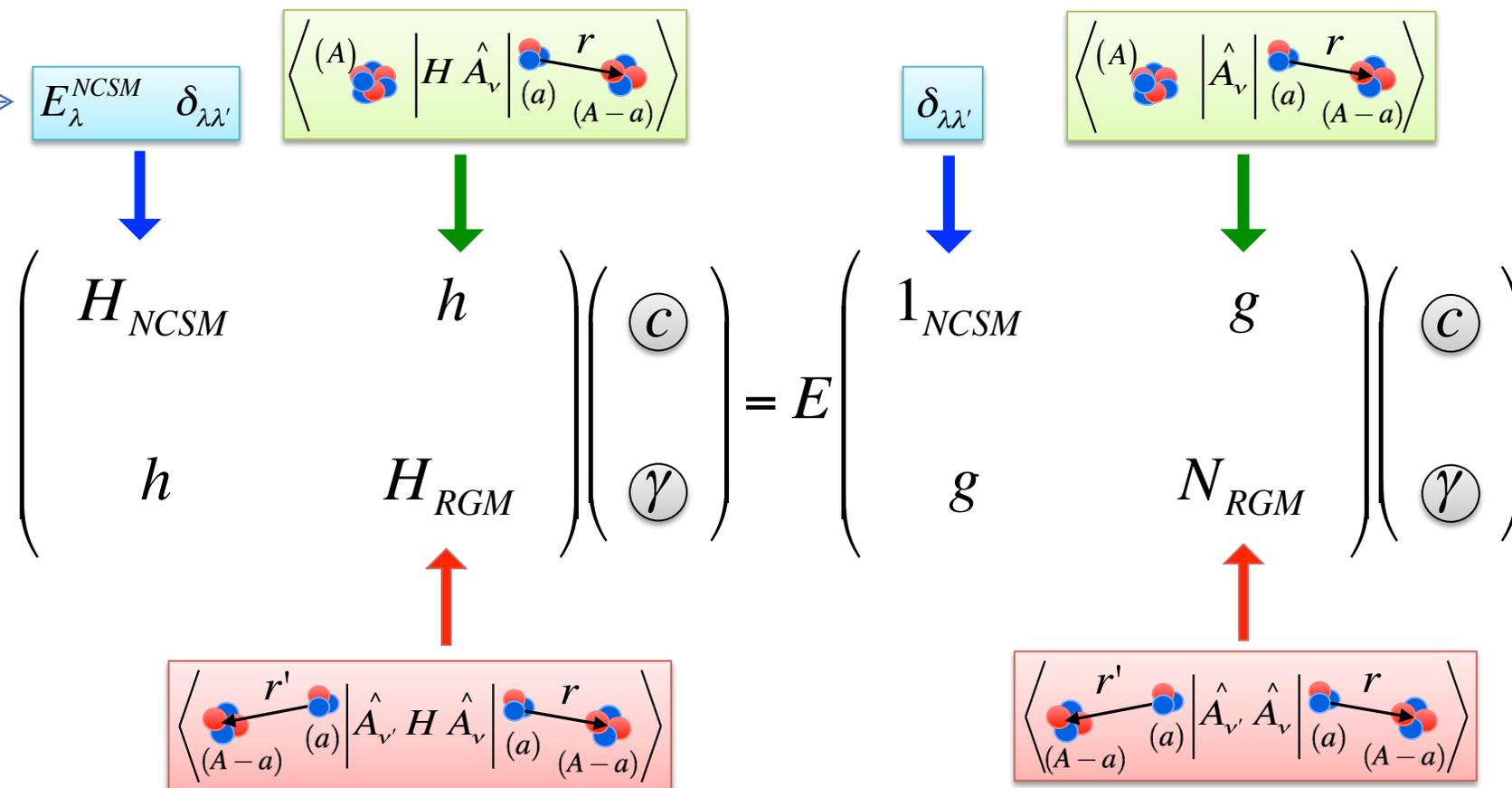
'Coulomb' Contribution (tunneling)

NCSMC phenomenology

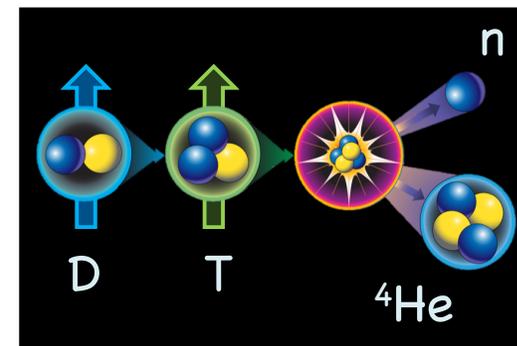
$$H \Psi^{(A)} = E \Psi^{(A)}$$

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

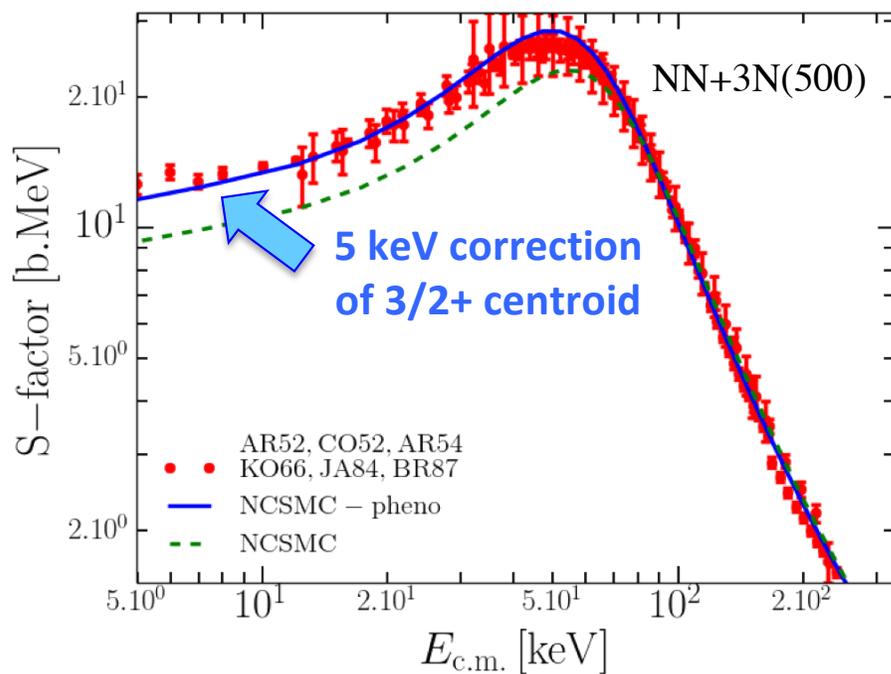
E_{λ}^{NCSM} energies treated as adjustable parameters



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



Astrophysical S-factor



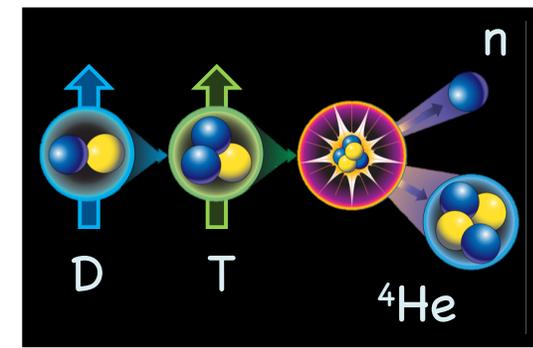
Fusion cross section

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

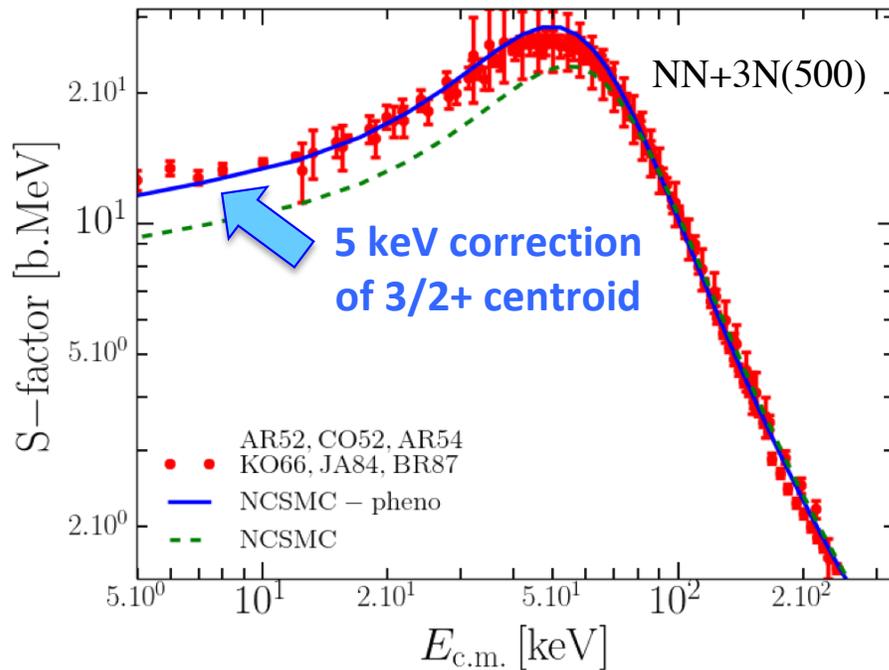
Astrophysical S-factor: nuclear contribution

'Coulomb' Contribution (tunneling)

${}^3\text{H}(d,n){}^4\text{He}$ 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

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

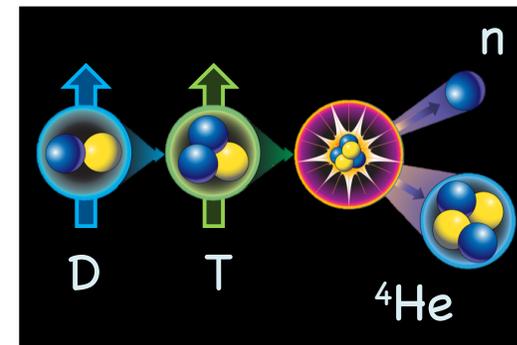
$$\approx \frac{1}{3} \sigma_{\frac{1}{2}} + \frac{2}{3} \sigma_{\frac{3}{2}}$$



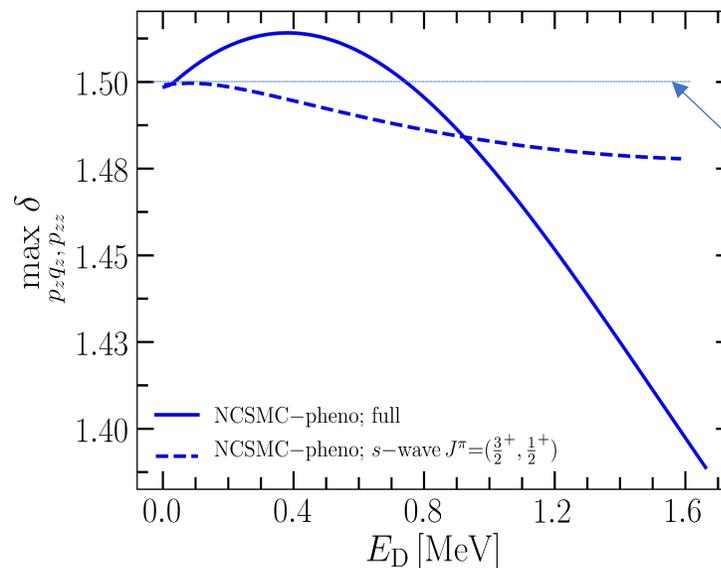
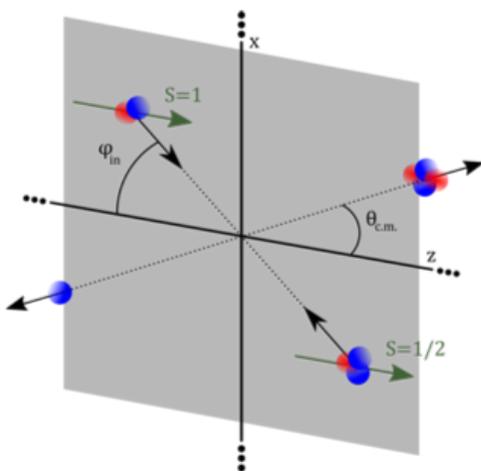
$$\sigma_{pol} \approx 1.5 \sigma_{unpol}$$

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

Polarized fusion



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



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

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

↓

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



ARTICLE

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

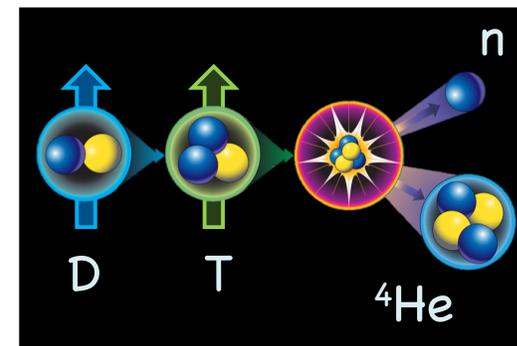
Ab initio predictions for polarized deuterium-tritium thermonuclear fusion

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

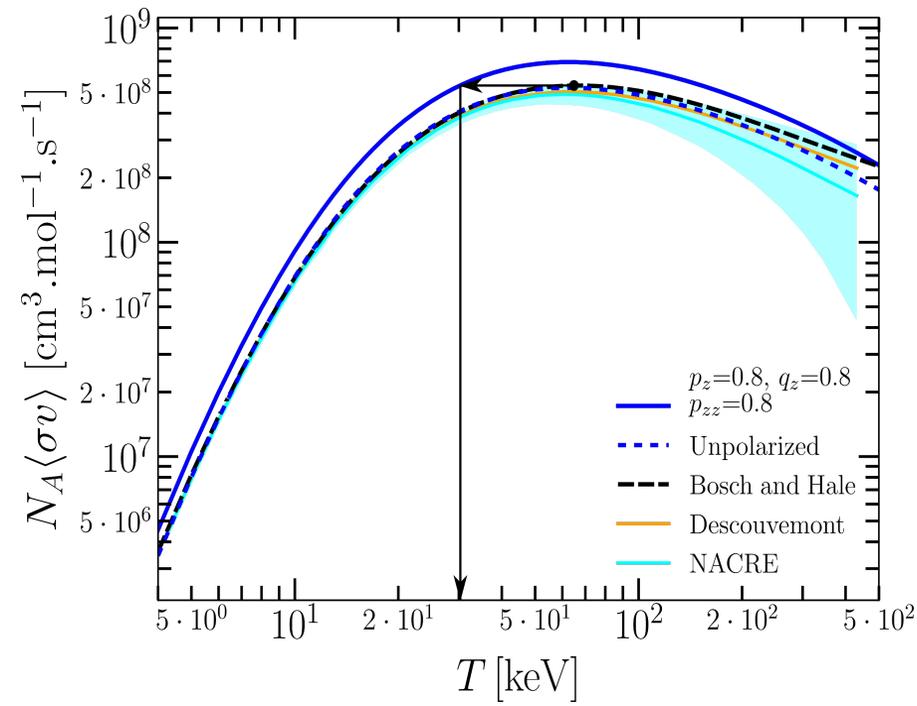
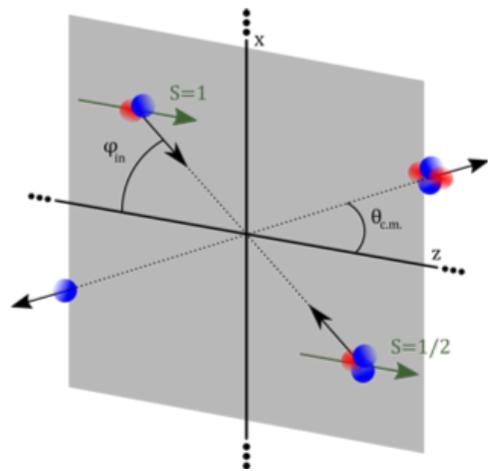
NCSMC calculation demonstrates impact of partial waves with $l > 0$ as well as the contribution of $l = 0$ $J^\pi = \frac{1}{2}^+$ channel

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

Polarized fusion



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



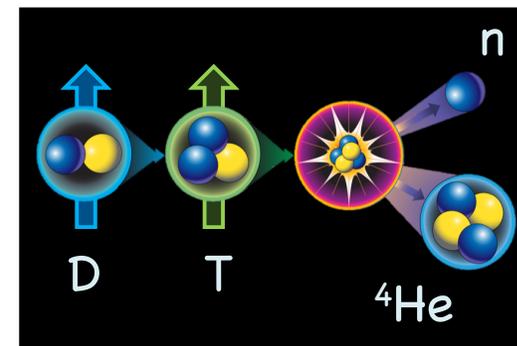
$$\langle\sigma v\rangle = \sqrt{\frac{8}{\pi\mu(k_b T)^3}} \int_0^\infty S(E) \exp\left(-\frac{E}{k_b T} - \sqrt{\frac{E_g}{E}}\right) dE,$$

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

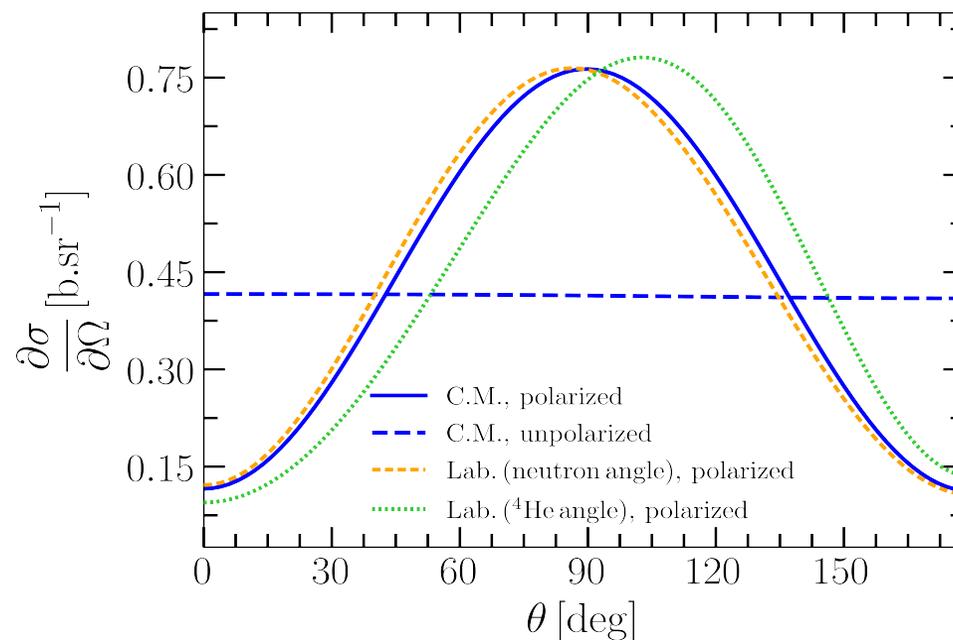
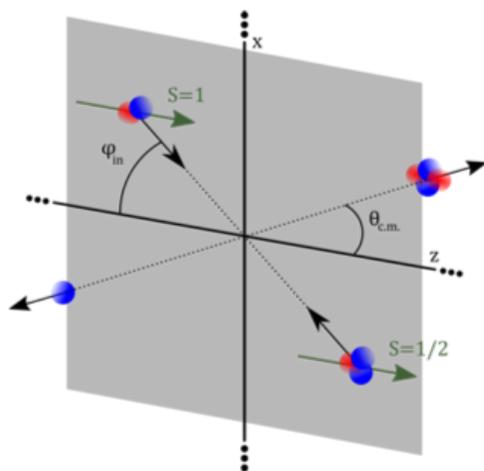


$^3\text{H}(d,n)^4\text{He}$ with chiral NN+3N(500) interaction

Polarized fusion



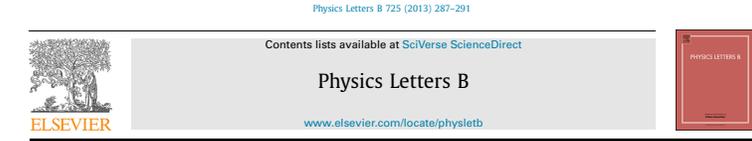
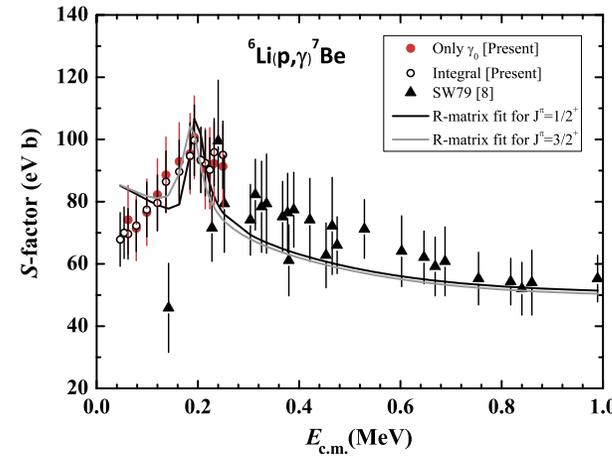
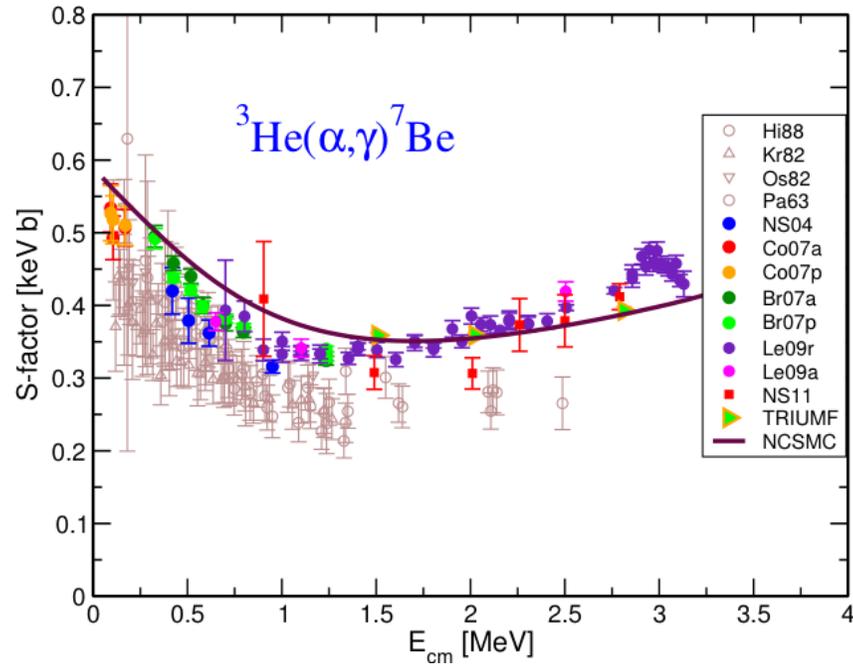
$$\frac{\partial \sigma_{pol}}{\partial \Omega_{c.m.}}(\theta_{c.m.}) = \frac{\partial \sigma_{unpol}}{\partial \Omega_{c.m.}}(\theta_{c.m.}) \left(1 + \frac{1}{2} p_{zz} A_{zz}^{(b)}(\theta_{c.m.}) + \frac{3}{2} p_z q_z C_{z,z}(\theta_{c.m.}) \right)$$



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



^7Be structure and capture reactions important for astrophysics



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



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[†]

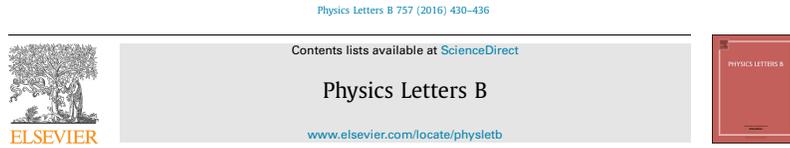
TRIUMF, 4004 Wesbrook Mall, Vancouver, British Columbia V6T 2A3, Canada

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}

${}^7\text{Be}$ structure and capture reactions important for astrophysics

NCSMC with SRG evolved chiral NN

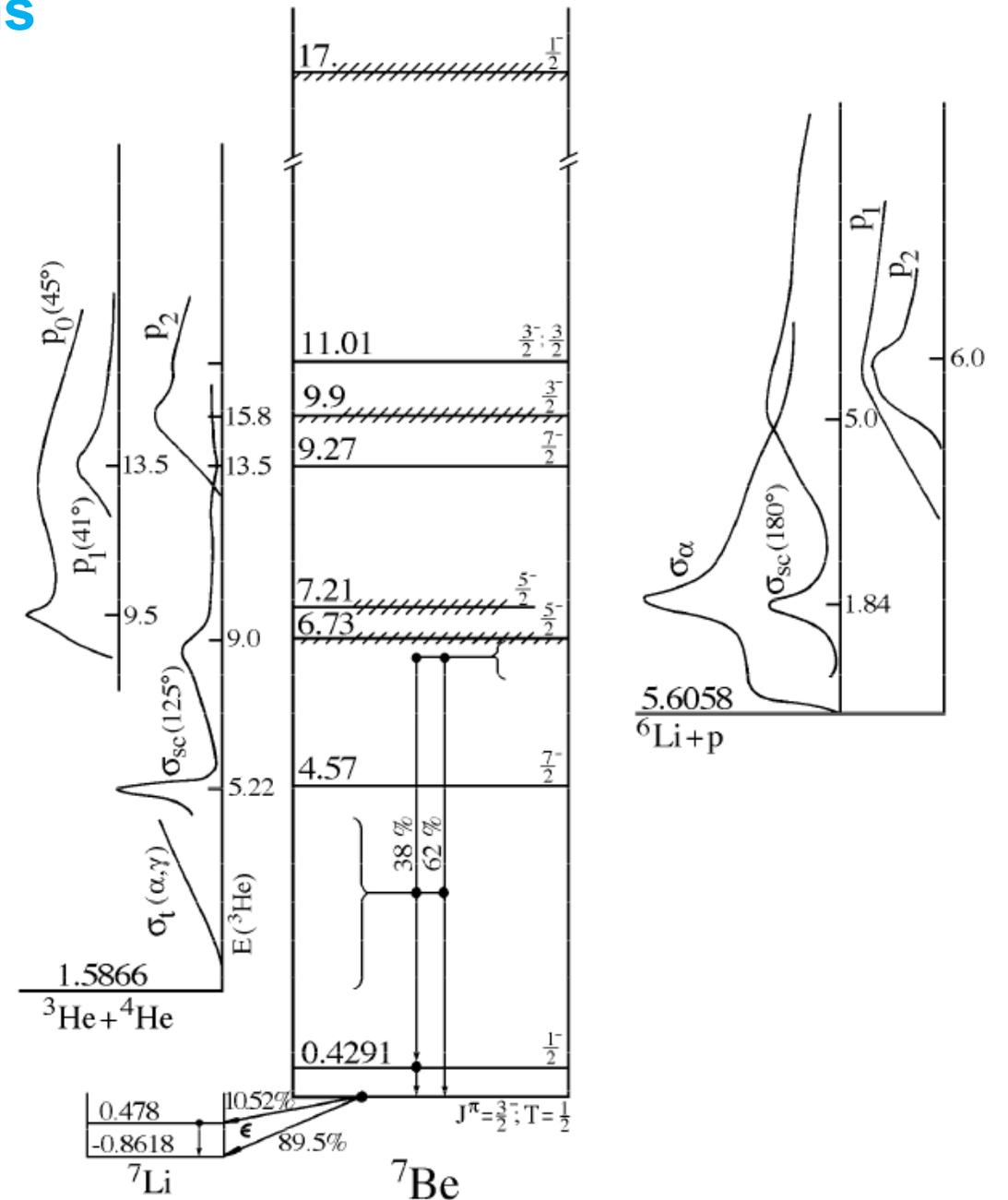
Analyzed mass partitions (no coupling yet)

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

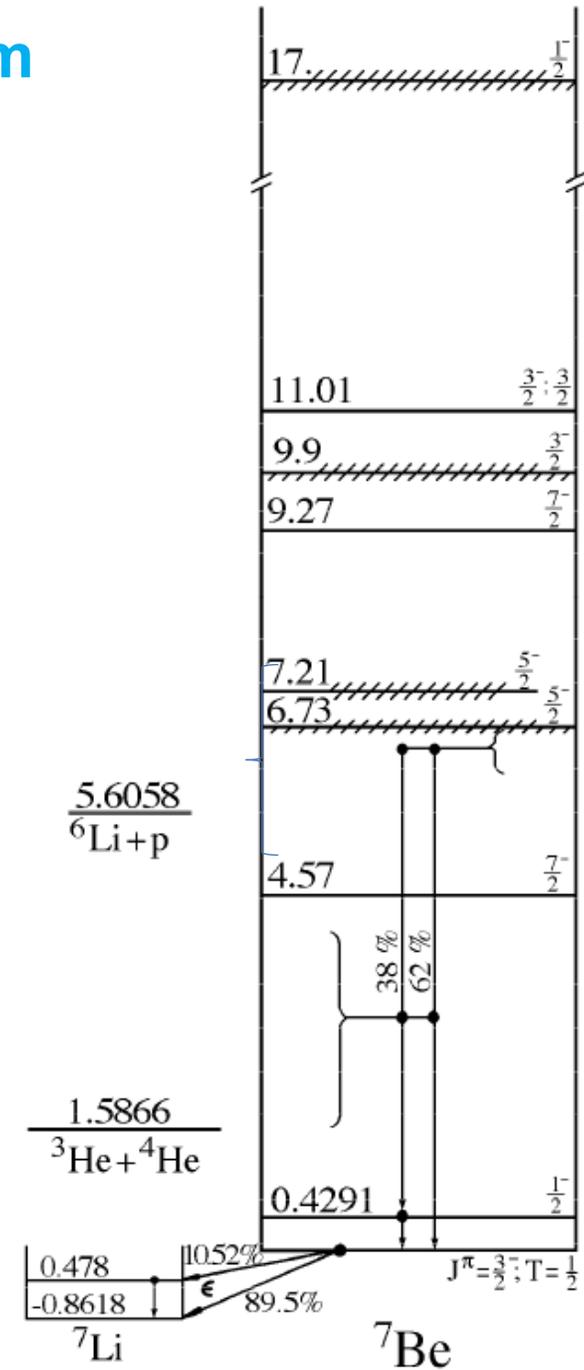
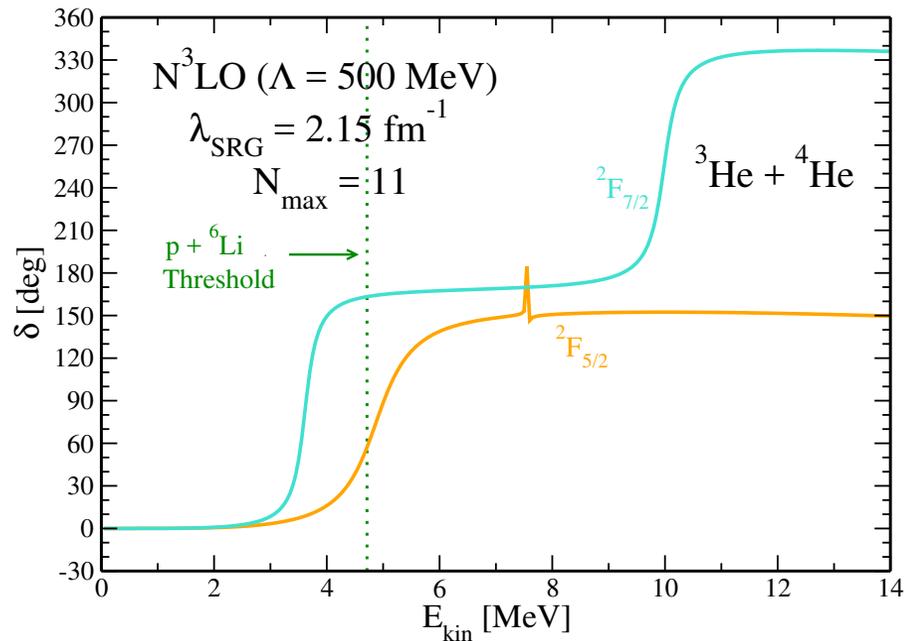
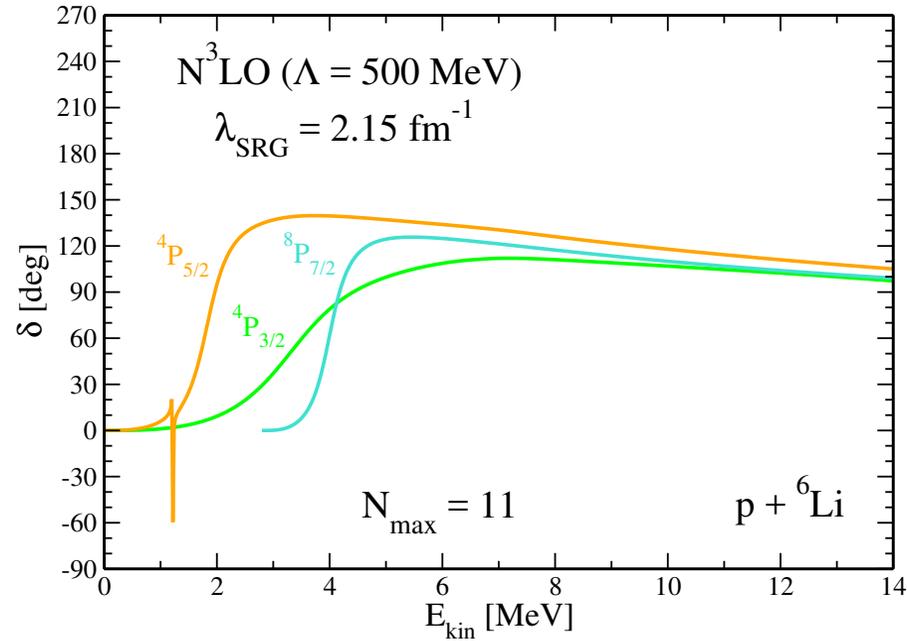
Exp.	$J^\pi = 3/2^-$
E [MeV]	-37.60

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

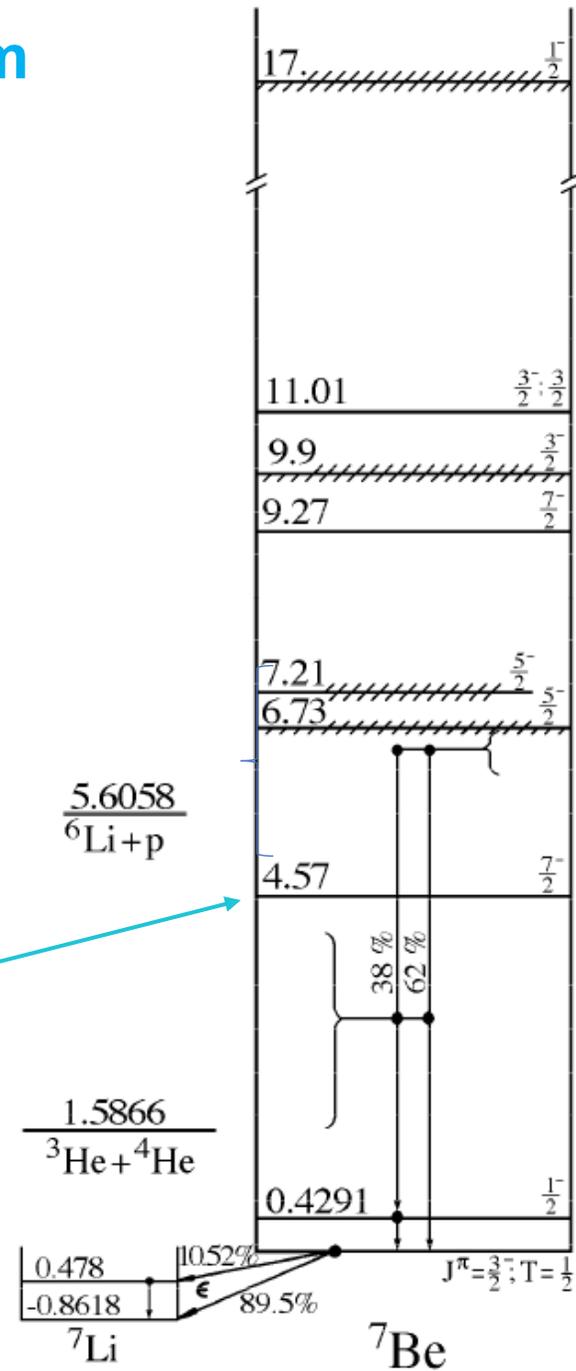
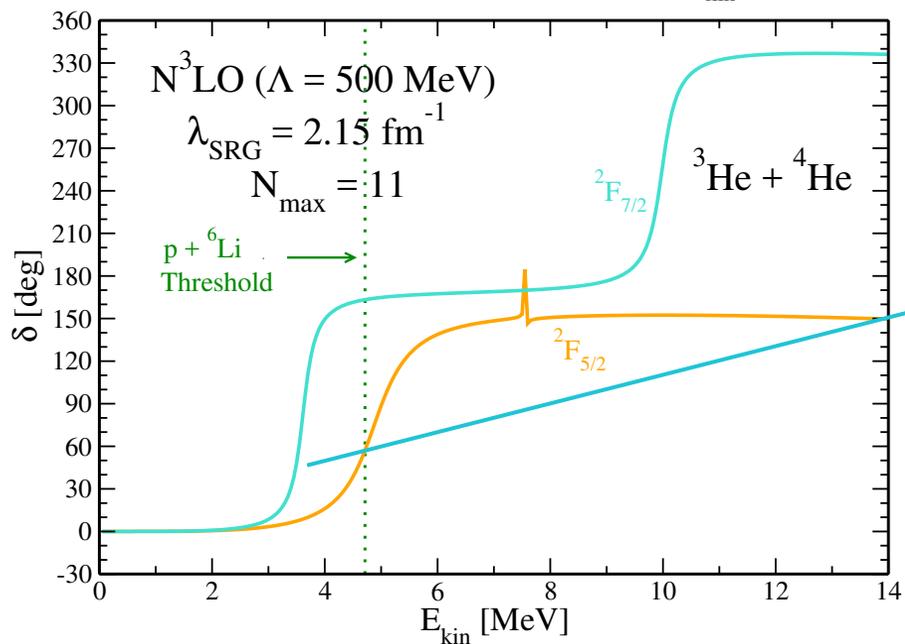
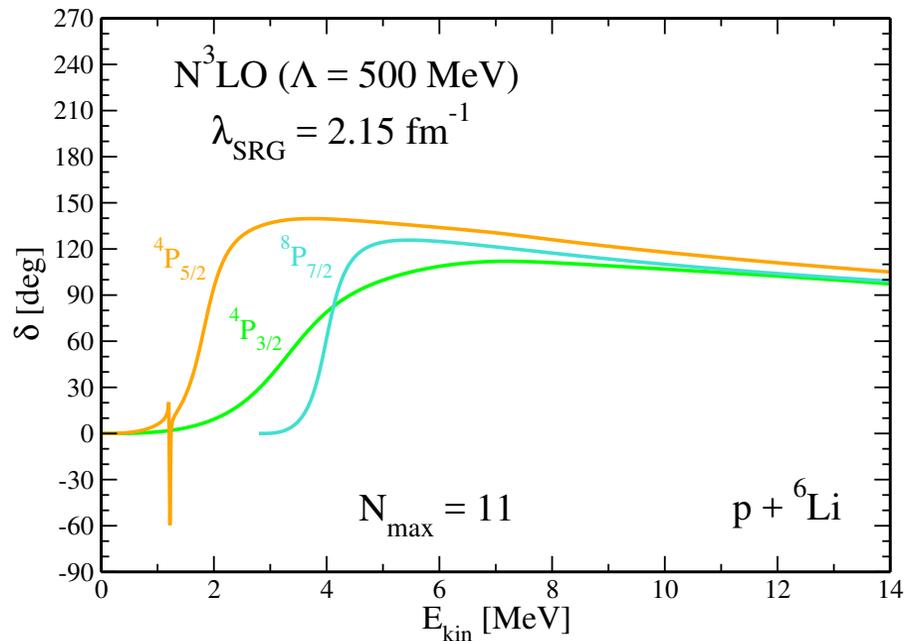
$p + {}^6\text{Li}$	$J^\pi = 3/2^-$	$J^\pi = 1/2^-$
E_{bound}	-5.729	-5.389
E [MeV]	-36.47	-36.13



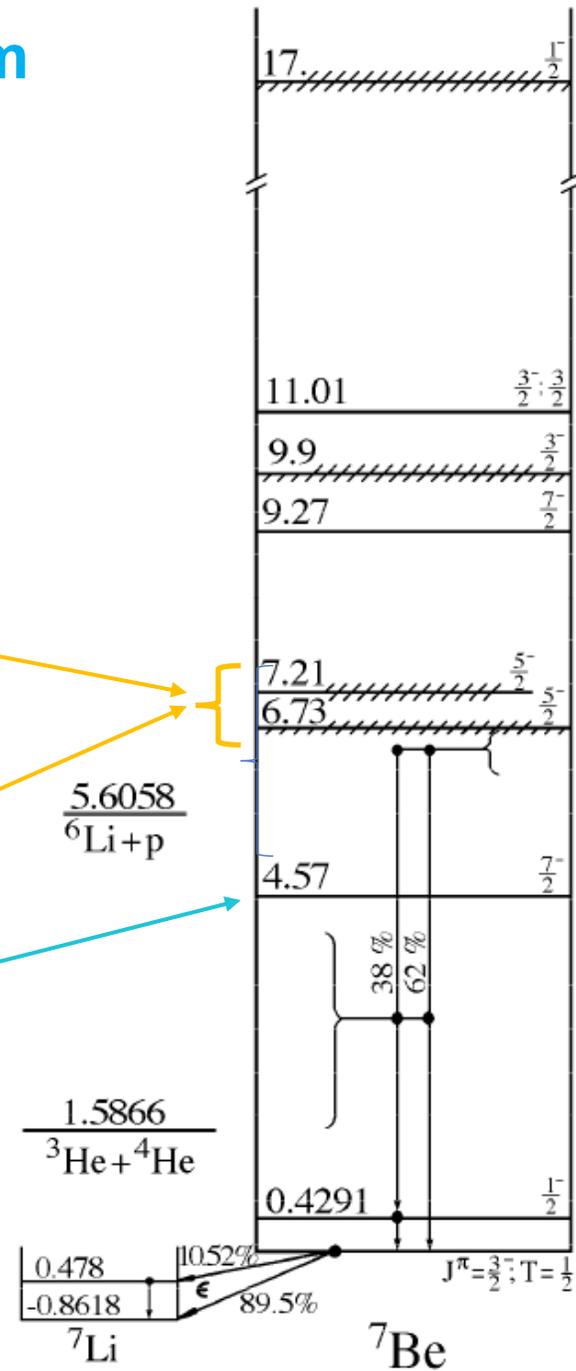
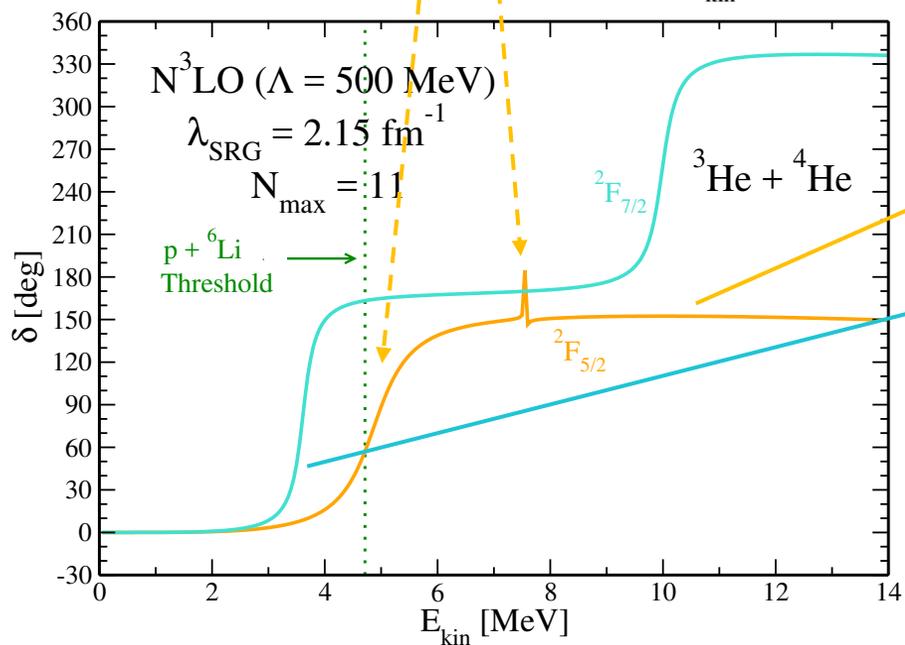
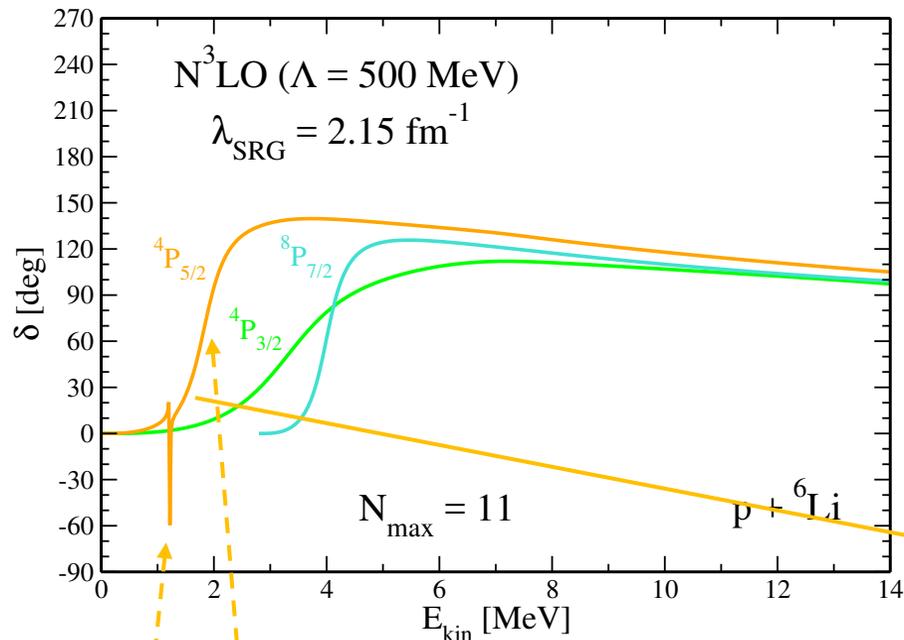
${}^7\text{Be}$ – Reproducing the energy spectrum



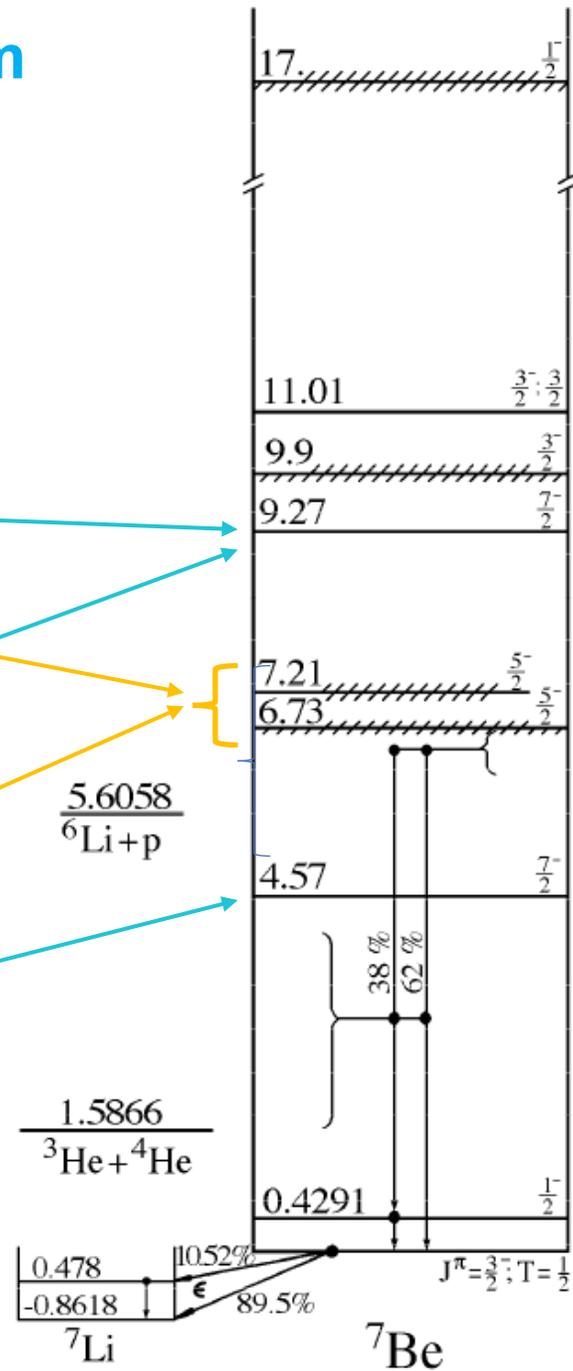
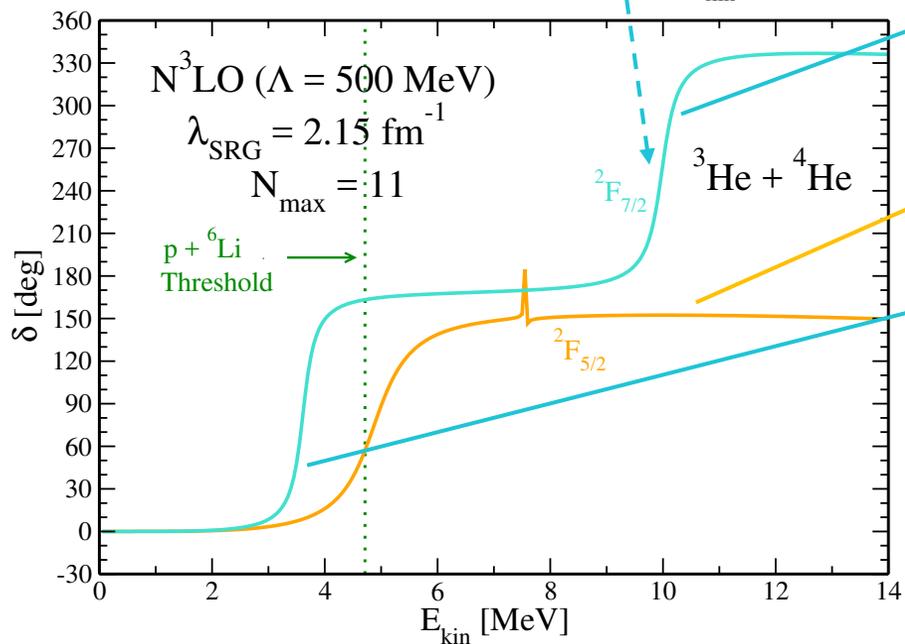
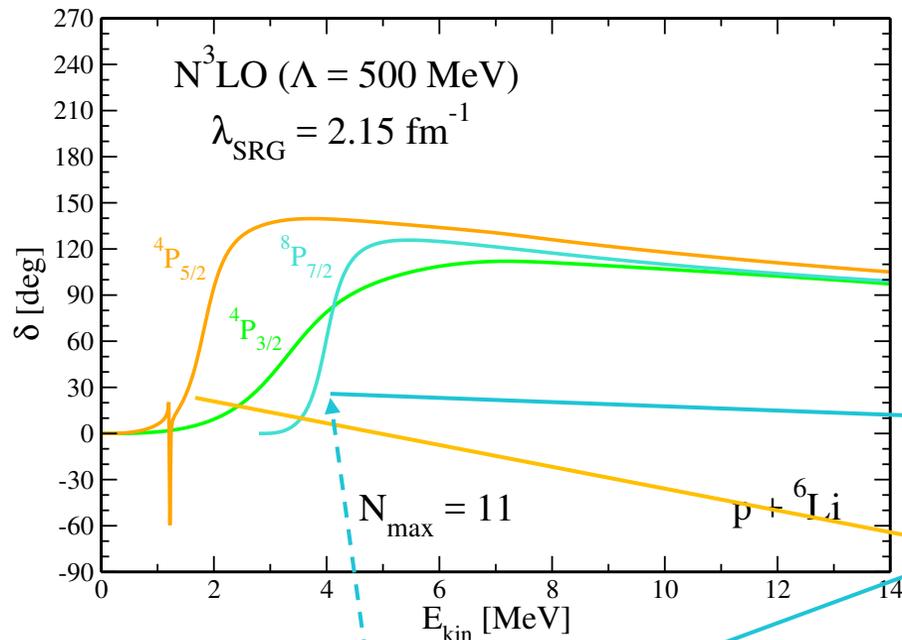
${}^7\text{Be}$ – Reproducing the energy spectrum



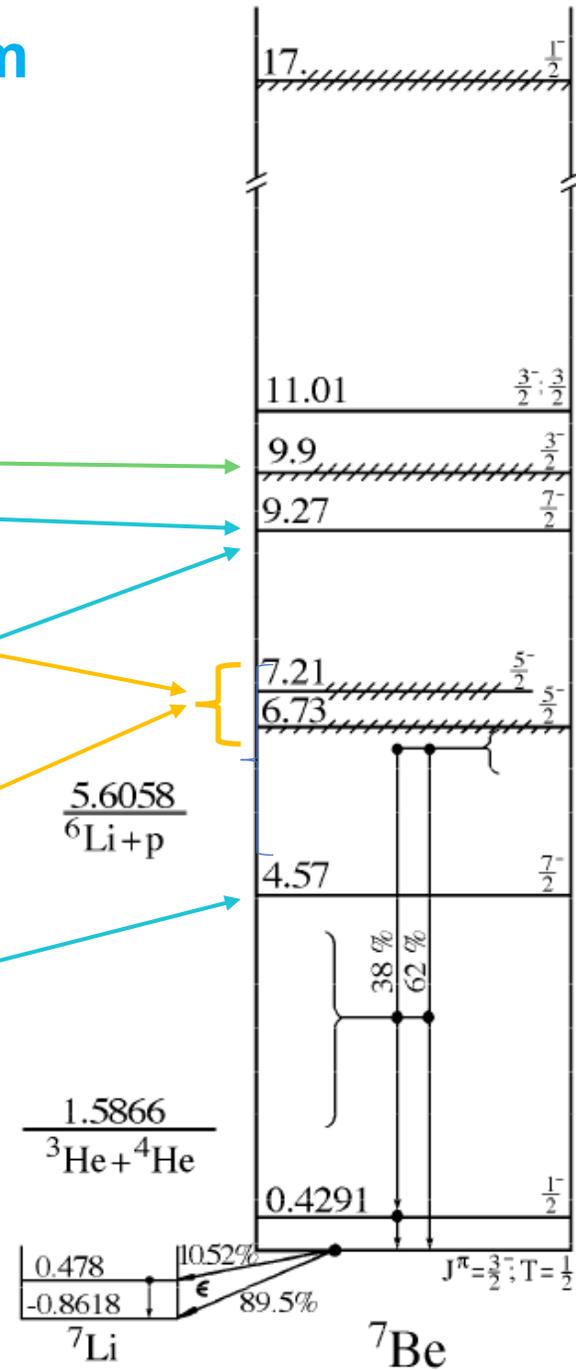
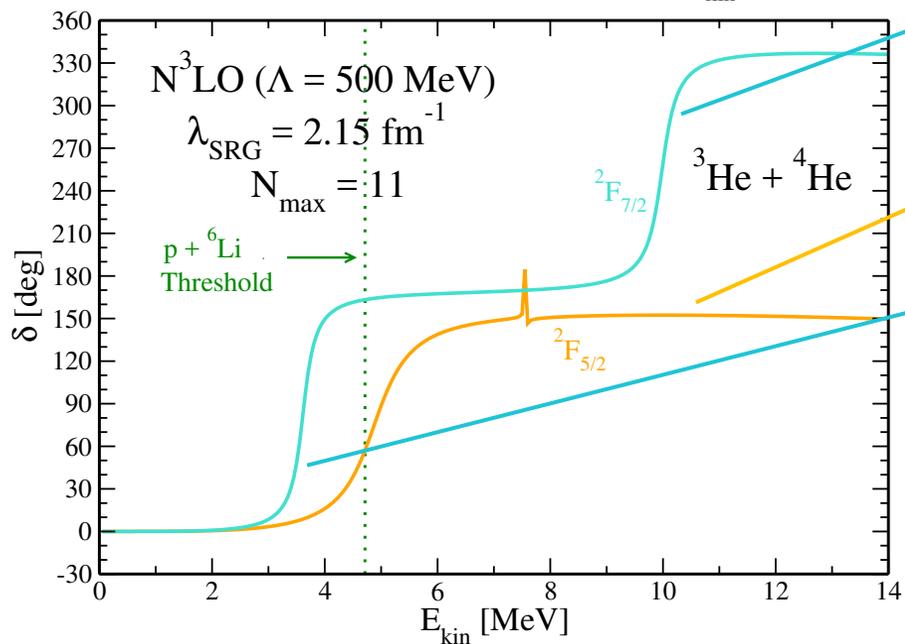
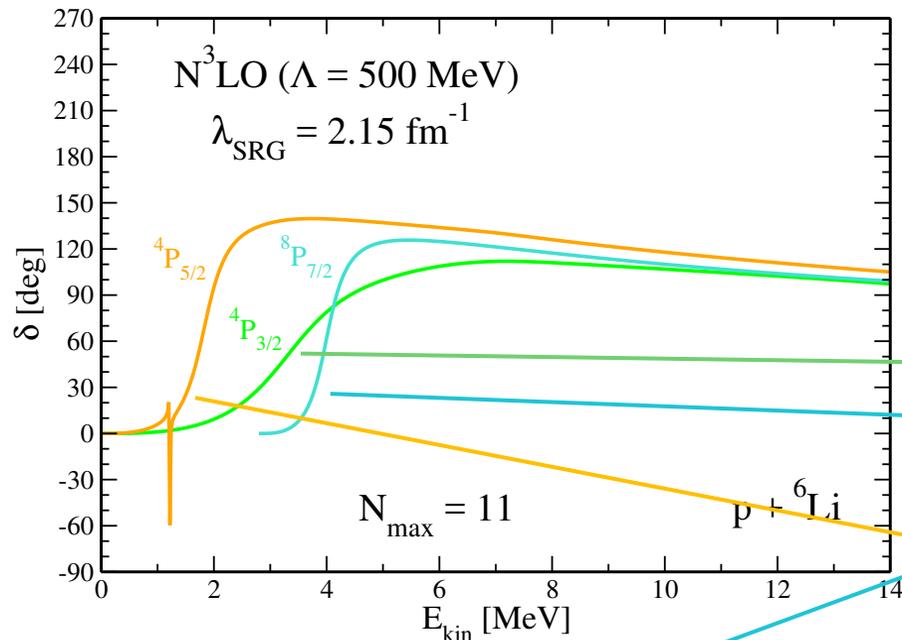
${}^7\text{Be}$ – Reproducing the energy spectrum



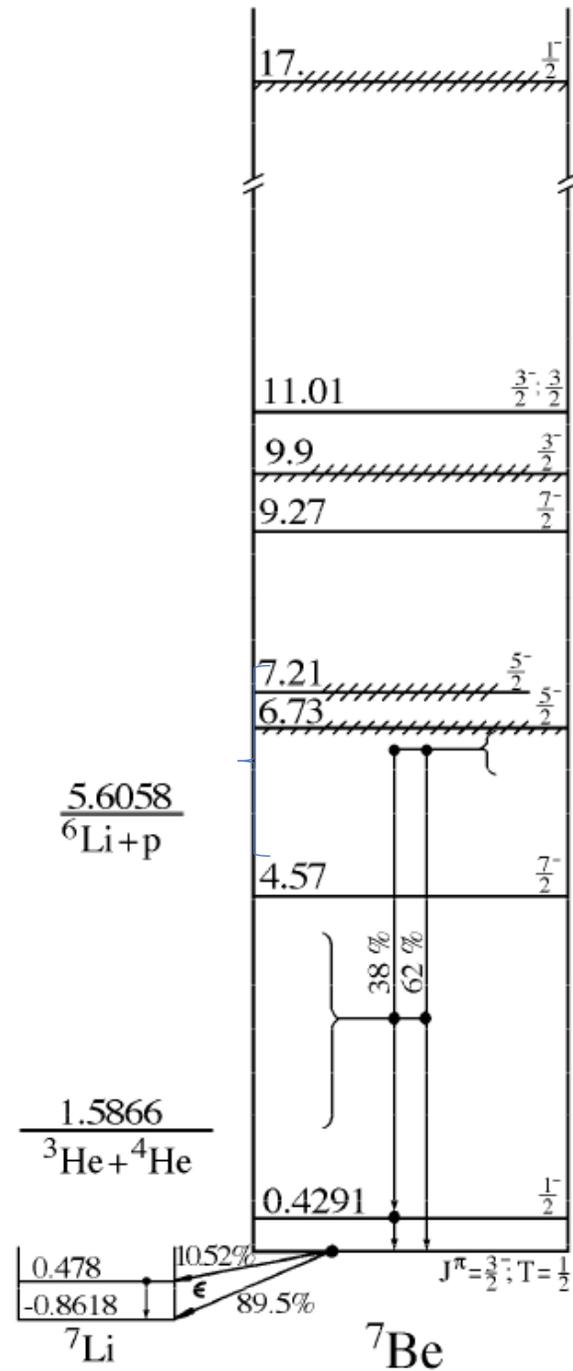
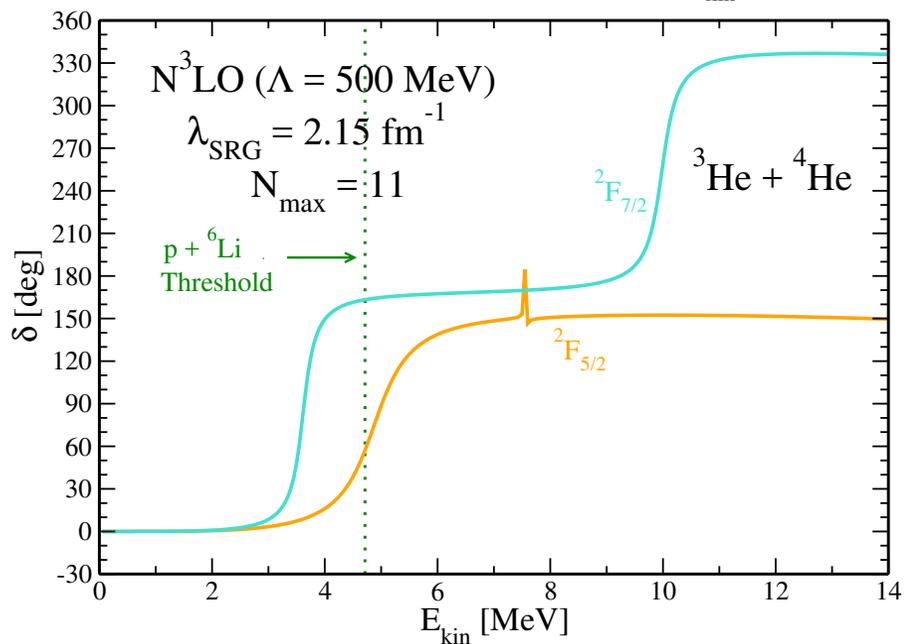
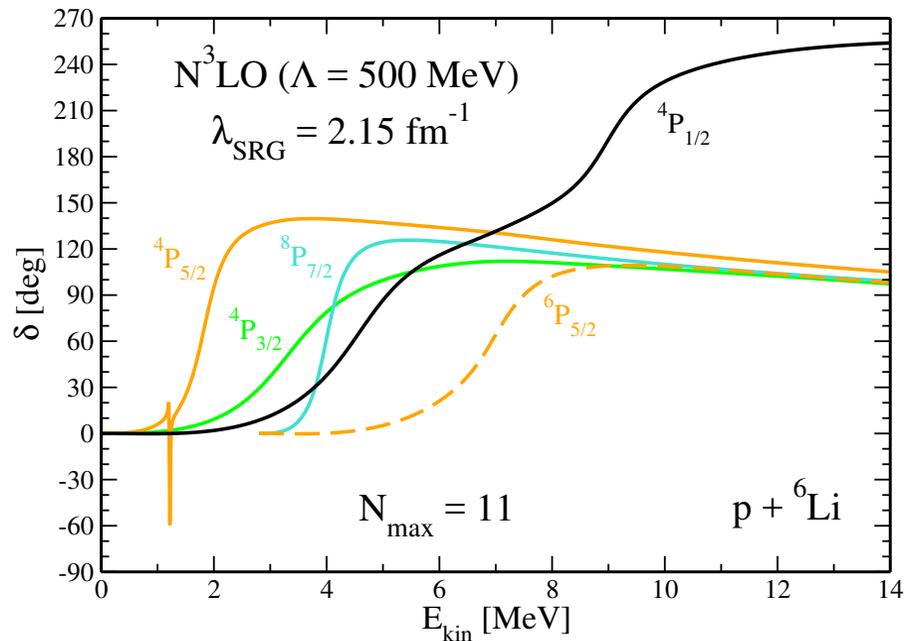
${}^7\text{Be}$ – Reproducing the energy spectrum



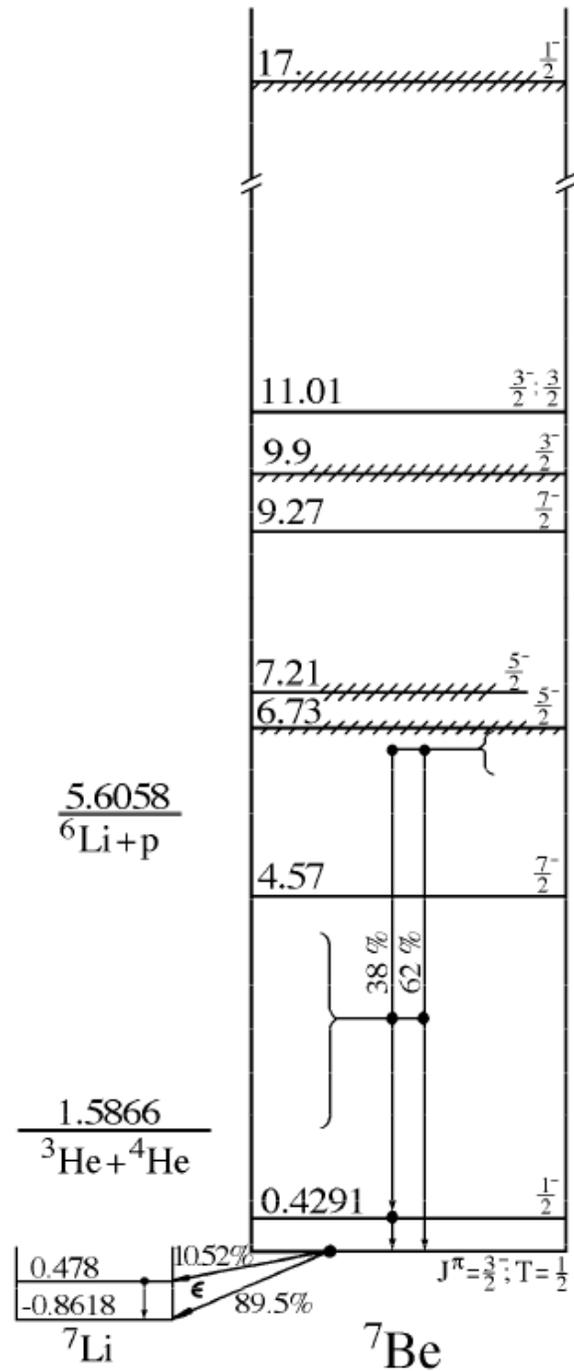
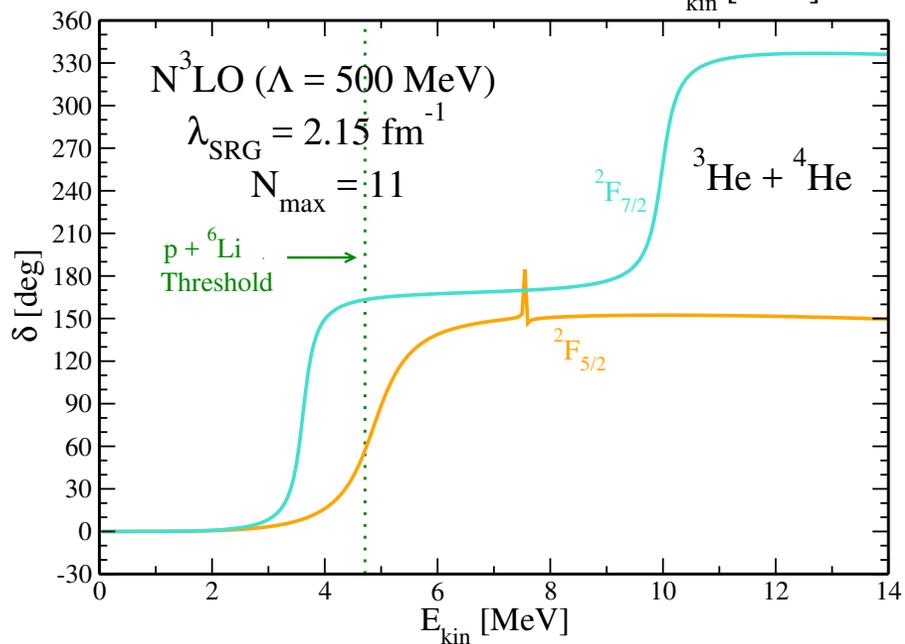
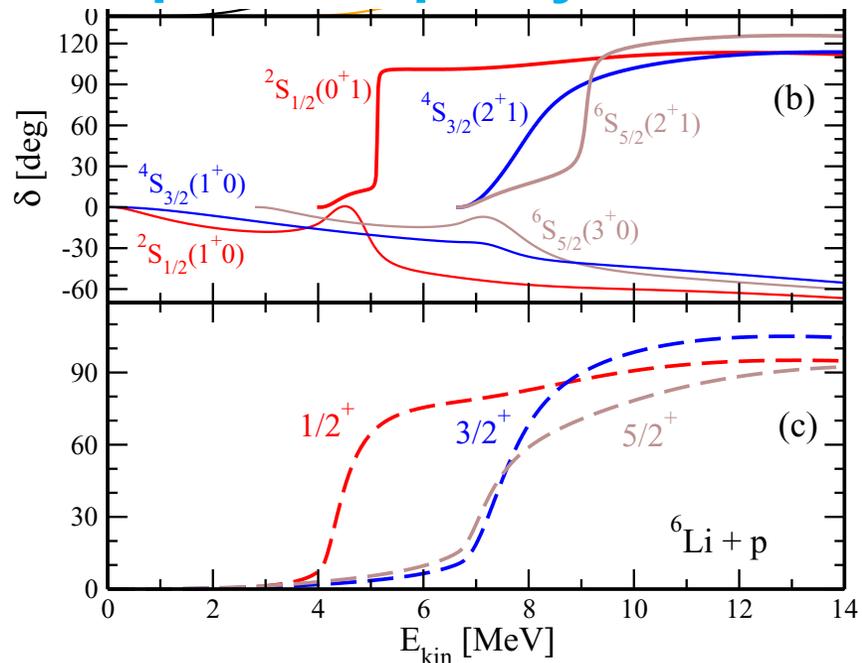
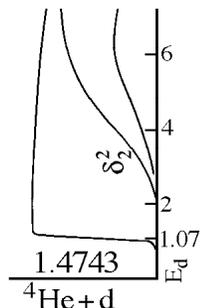
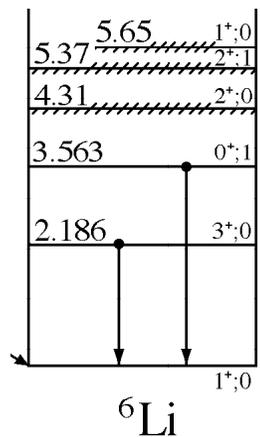
${}^7\text{Be}$ – Reproducing the energy spectrum



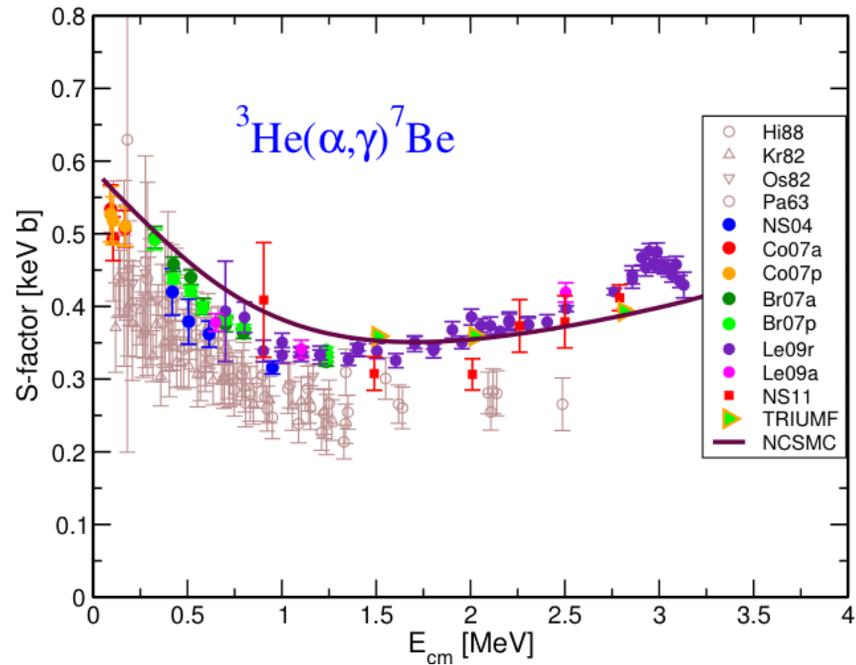
${}^7\text{Be}$ – New negative-parity states



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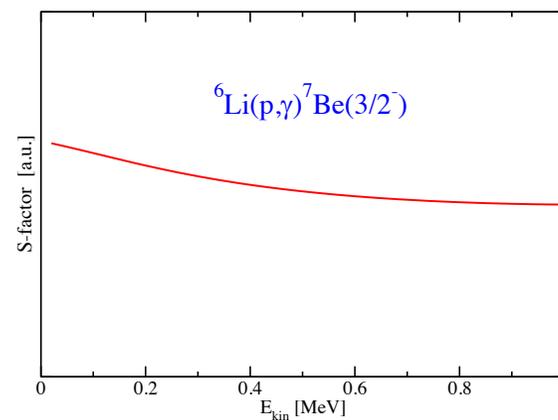
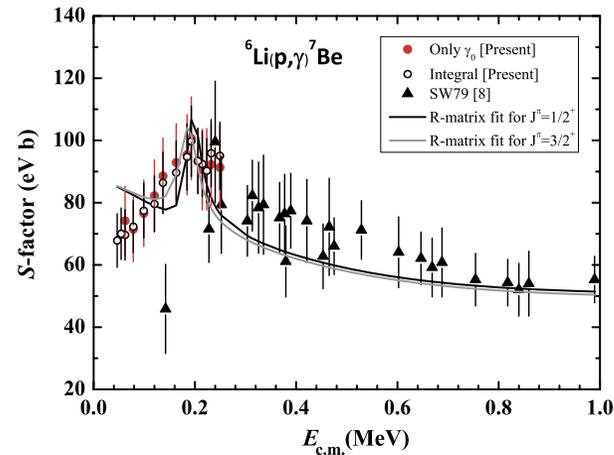
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${}^3\text{He}(\alpha,\gamma){}^7\text{Be}$ and ${}^3\text{H}(\alpha,\gamma){}^7\text{Li}$ astrophysical S factors from the no-core shell model with continuum



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^g and Petr Navrátil^h

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 Hupinⁱ

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 continuum

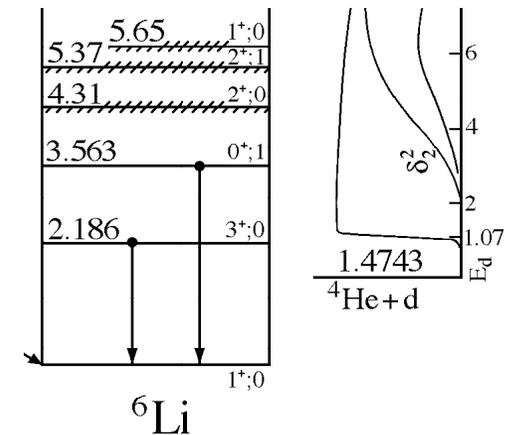
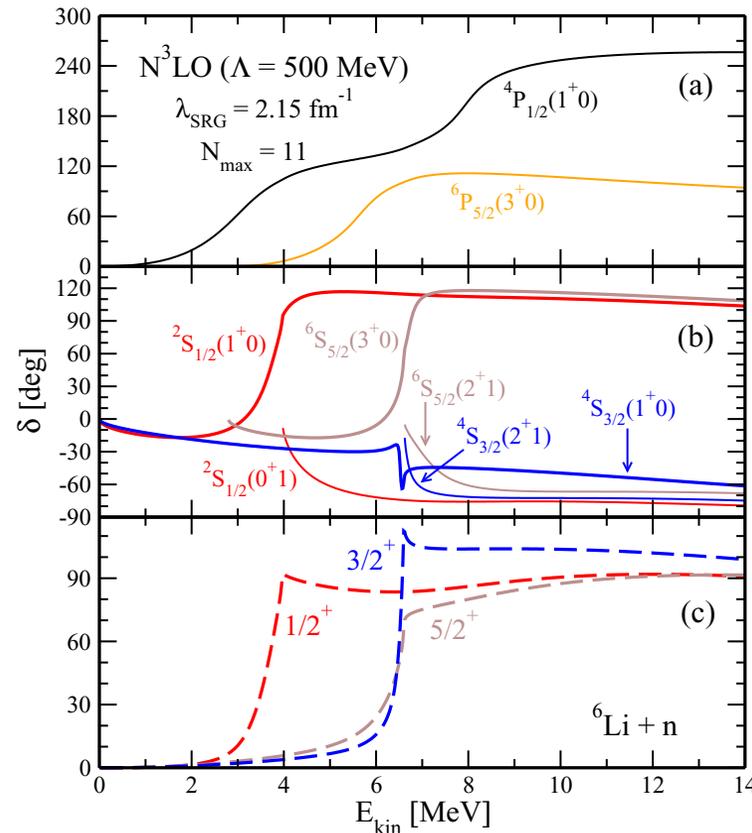
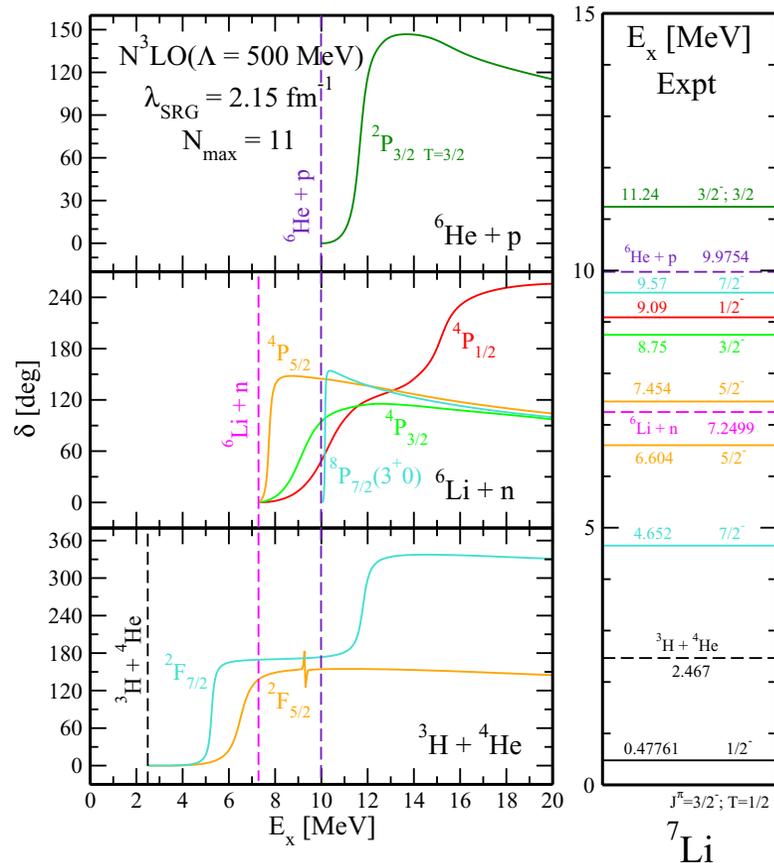
Matteo Vorabbi^{*} and Petr Navrátil[†]
 TRIUMF, 4004 Wesbrook Mall, Vancouver, British Columbia V6T 2A3, Canada

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

S-wave resonance just above the threshold of ⁶He+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 continuum

Matteo Vorabbi[✉] and Petr Navrátil[†]

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

Sofia Quaglioni

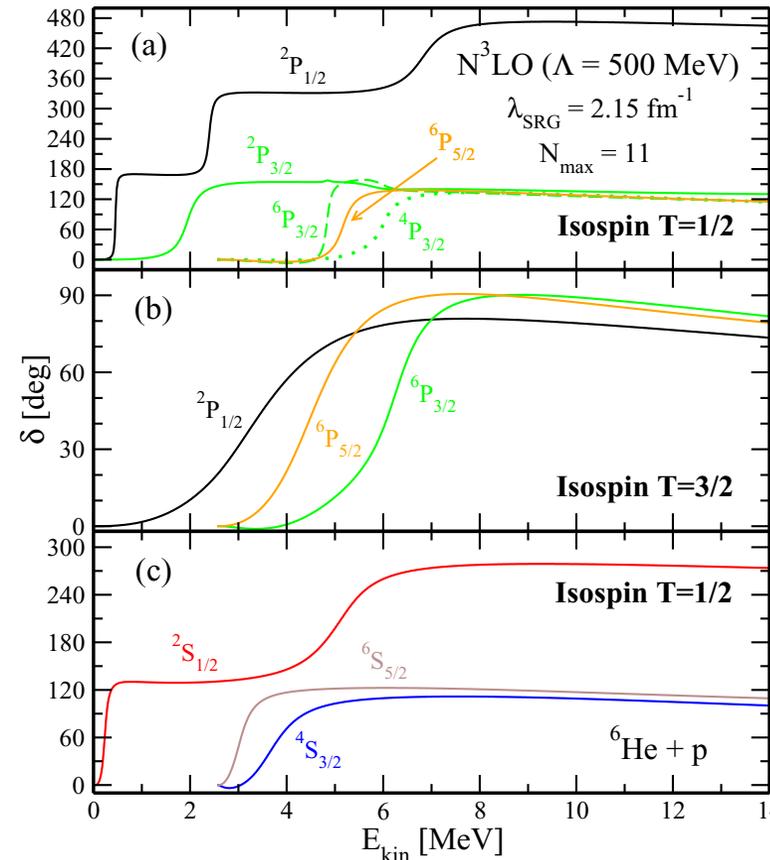
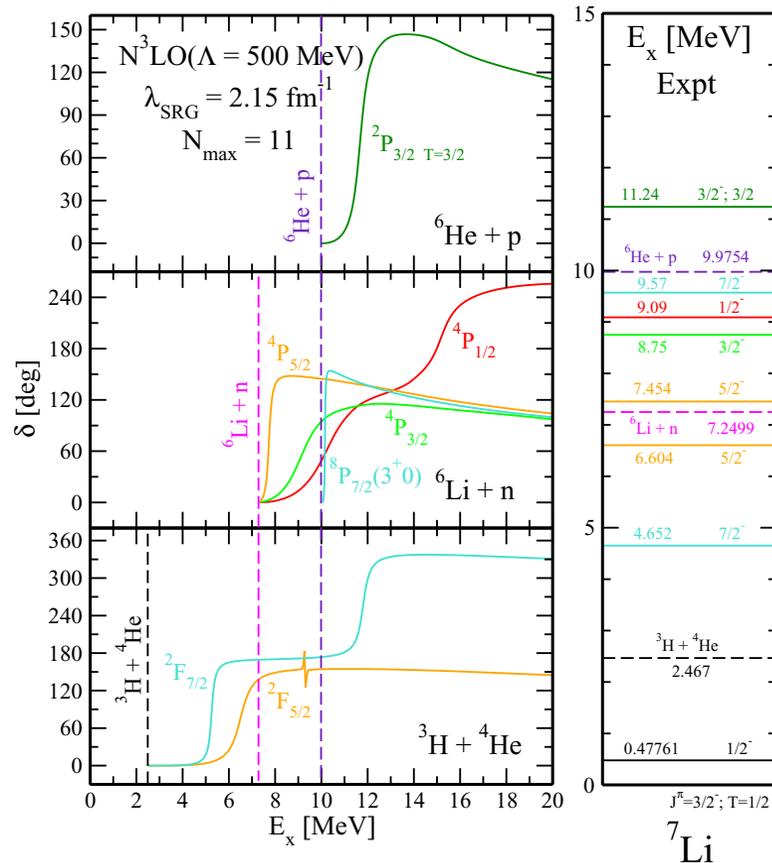
Lawrence Livermore National Laboratory, P. O. Box 808, L-414, Livermore, California 94551, USA

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

S-wave resonance just above the threshold of ⁶He+p?

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 - Known resonances reproduced
 - Prediction of several new resonances of both parities



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

Similarity to ¹⁰Be+p system?

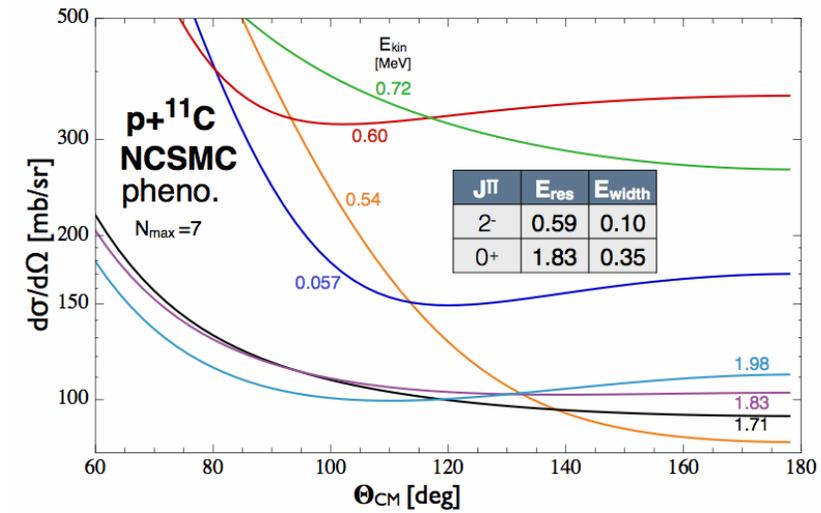
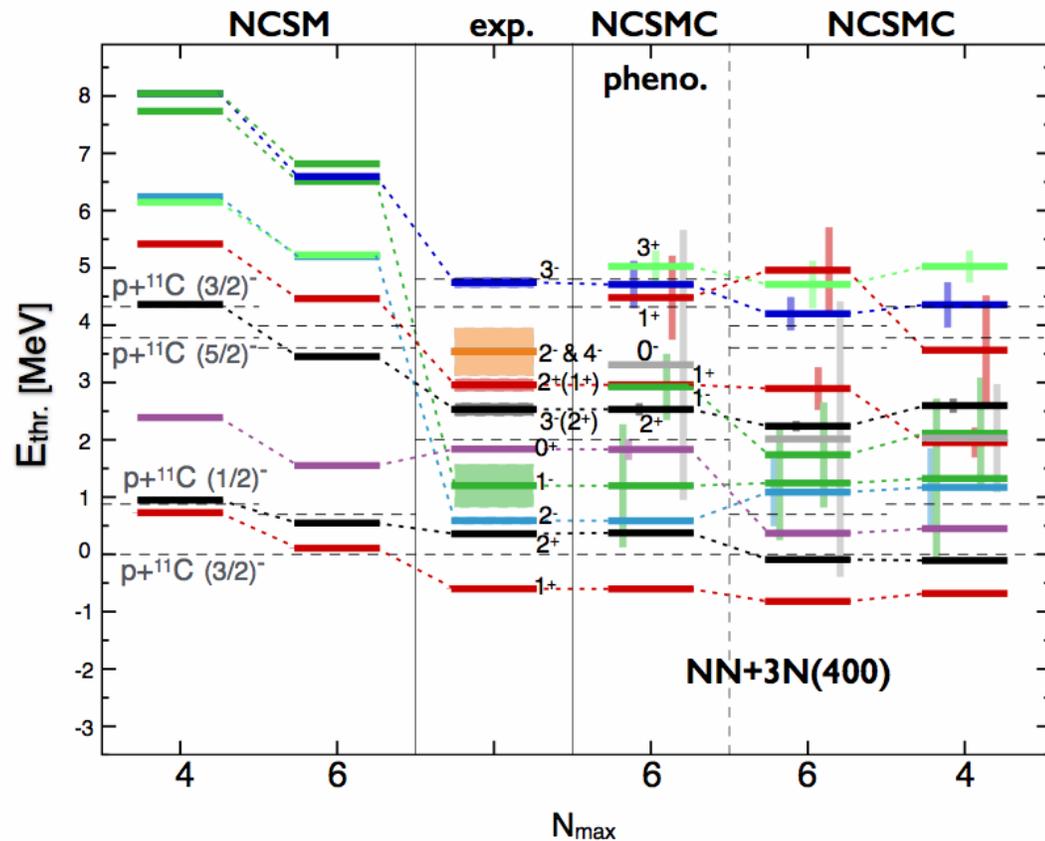
Editors' Suggestion

Direct Observation of Proton Emission in ¹¹Be

Y. Ayyad,^{1,2,*} B. Olaizola,³ W. Mittig,^{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. Koonen,^{3,8} K. G. Leach,¹⁴ J. S. Randhawa,² Y. Saito,^{3,10} C. Santamaria,¹⁵ P. Siuryte,^{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

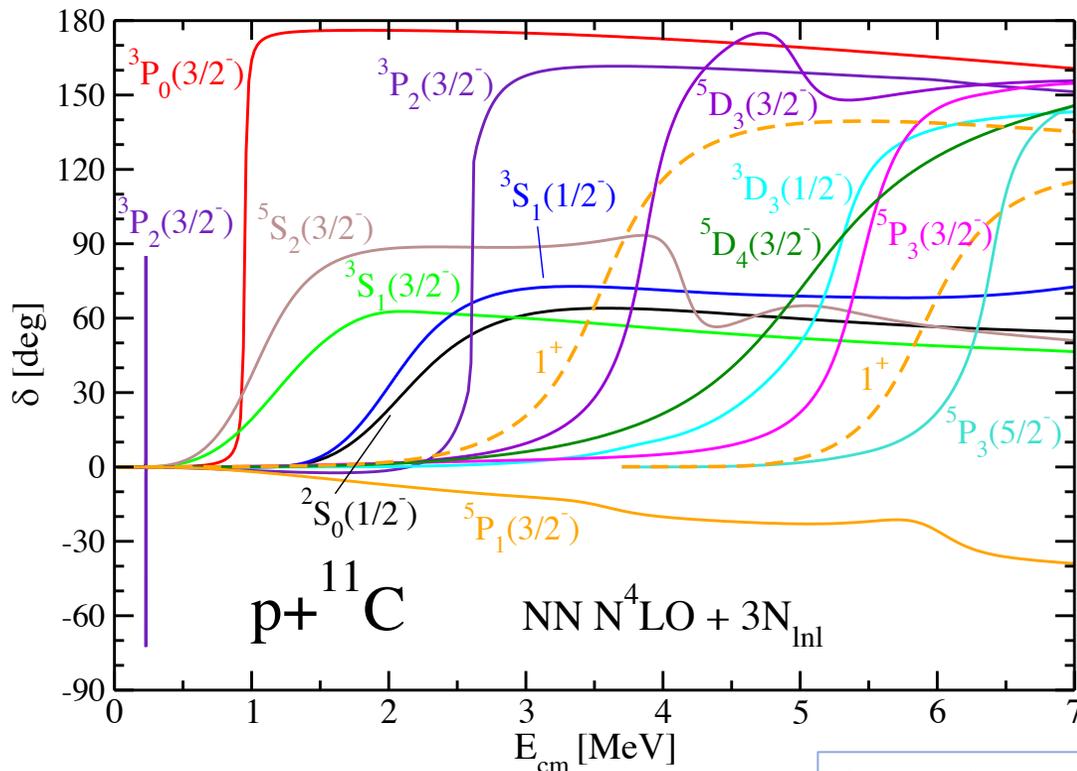
- NCSMC calculations of $^{11}\text{C}(p,p)$ with chiral NN+3N under way
 - ^{11}C : $3/2^-$, $1/2^-$, $5/2^-$, $3/2^-$ NCSM eigenstates
 - ^{12}N : $\geq 6 \pi = +1$ and $\geq 4 \pi = -1$ NCSM eigenstates



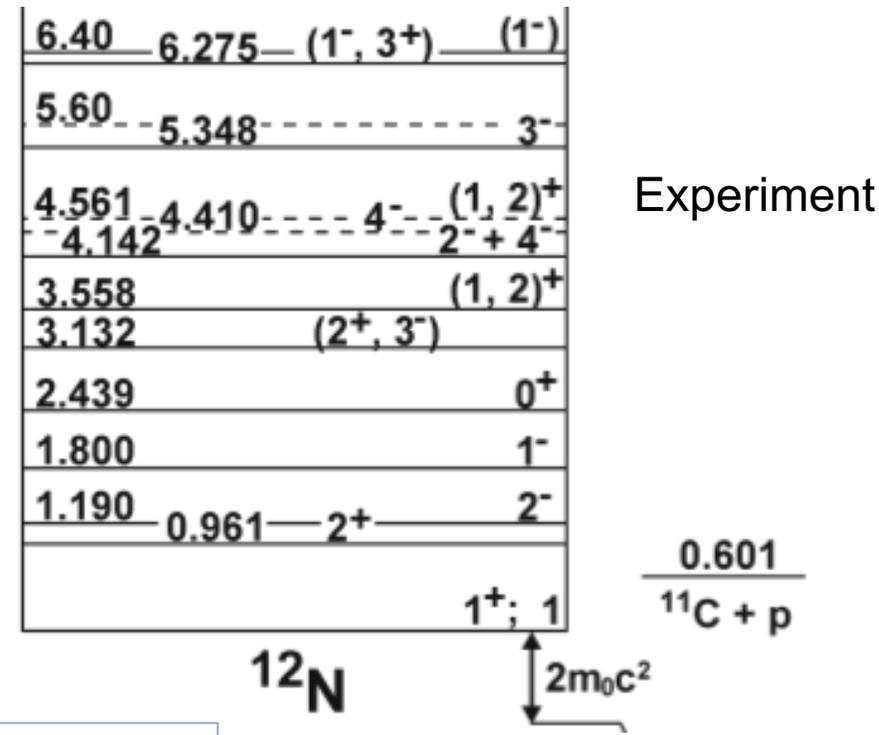
NCSMC calculations to be validated by measured cross sections and applied to calculate the $^{11}\text{C}(p,\gamma)^{12}\text{N}$ capture

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

- NCSM with continuum calculations of $^{11}\text{C}(p,p)$ 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)

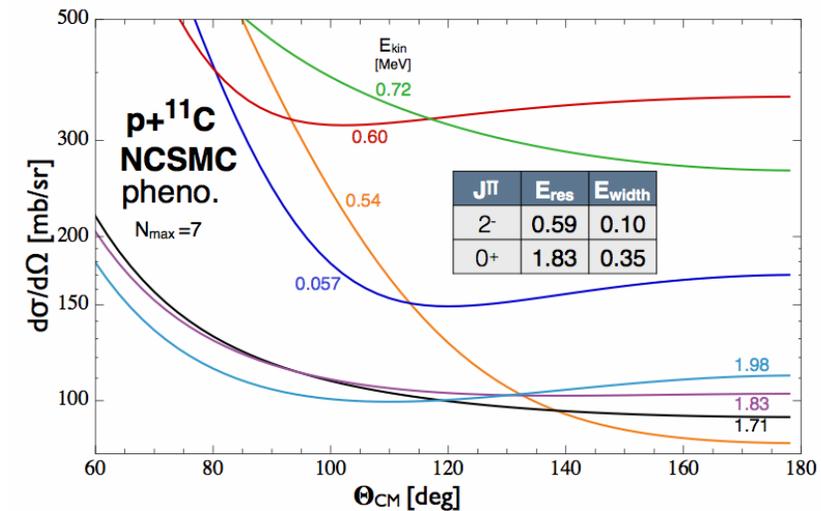
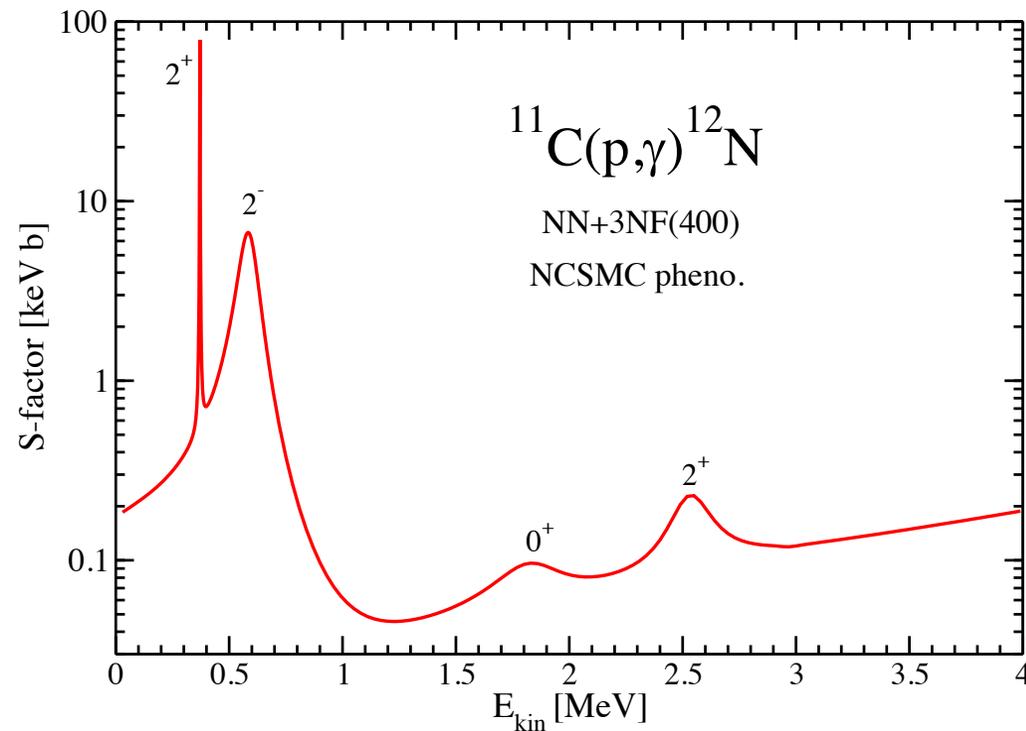


Calculated bound-state energy $E(1^+ 1) = -0.52$ MeV



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

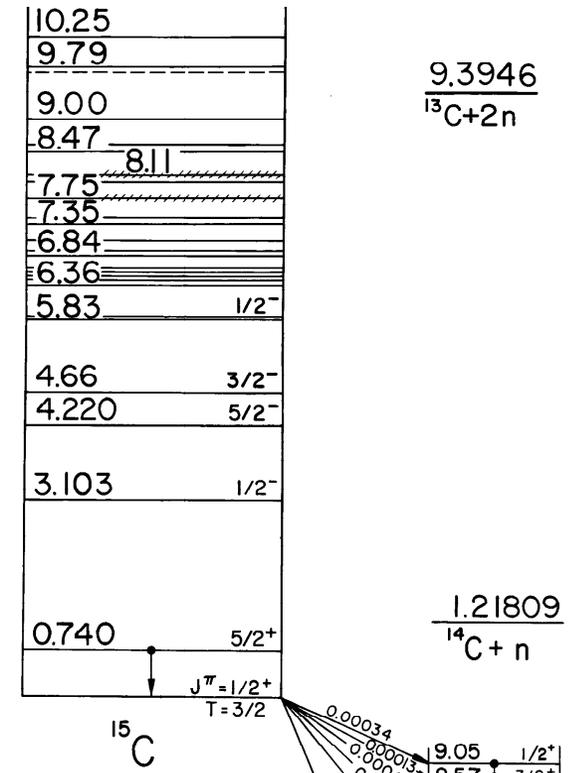


NCSMC calculations to be validated by measured cross sections and applied to calculate the $^{11}\text{C}(p,\gamma)^{12}\text{N}$ capture

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

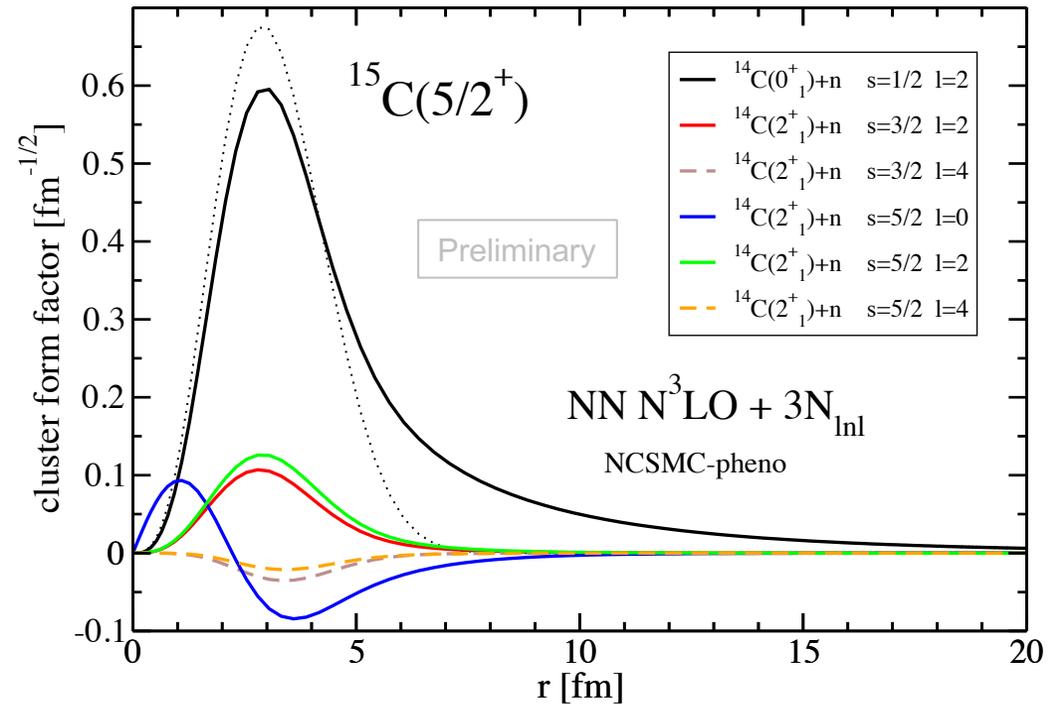
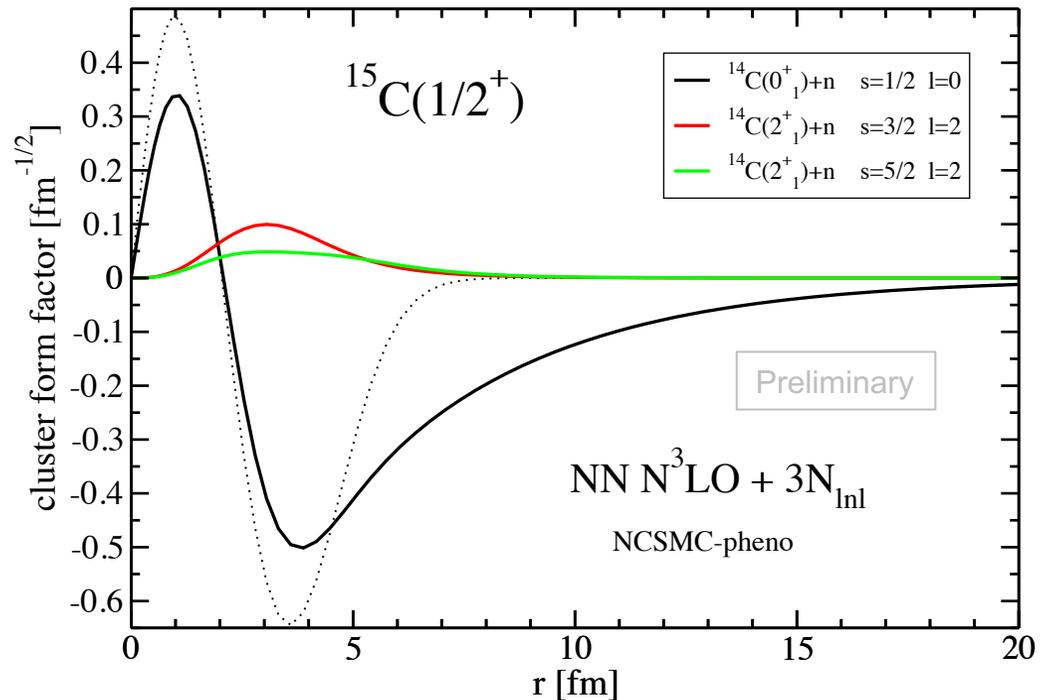
- Motivation:
 - Halo $1/2^+$ *S*-wave and $5/2^+$ *D*-wave bound states
 - $^{14}\text{C}(n,\gamma)^{15}\text{C}$ capture relevant for astrophysics

- 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 $\lambda = 2.0 \text{ fm}^{-1}$



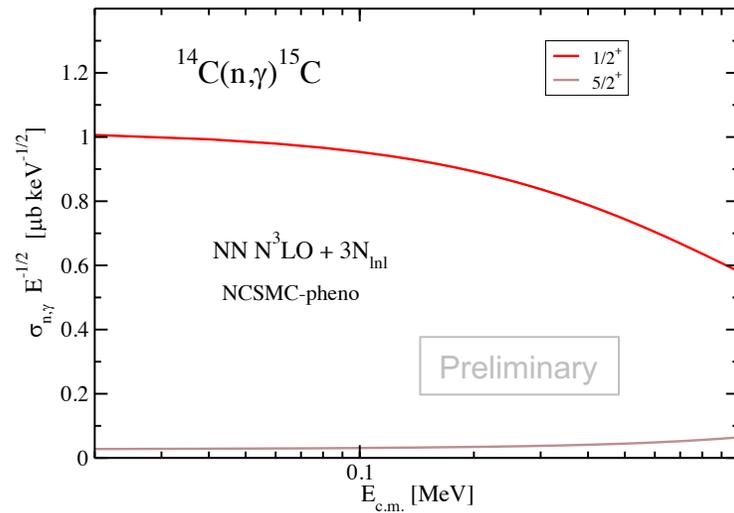
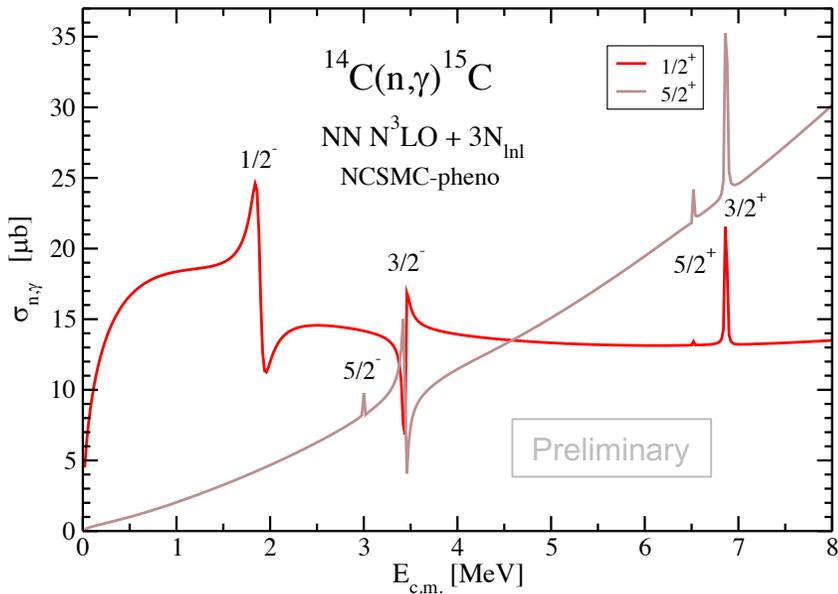
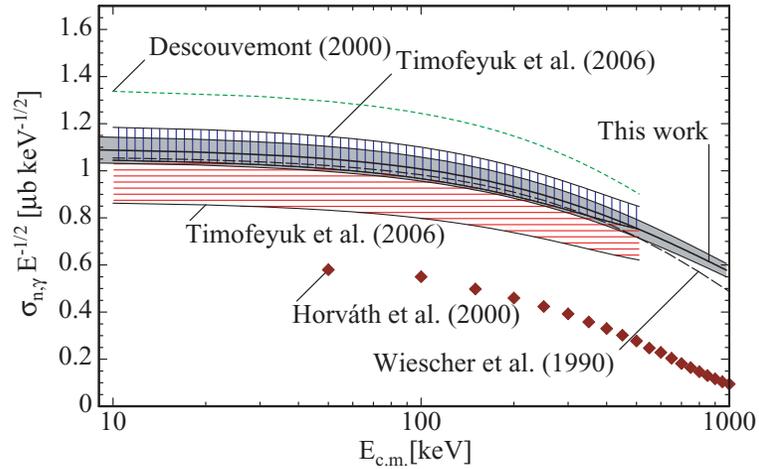
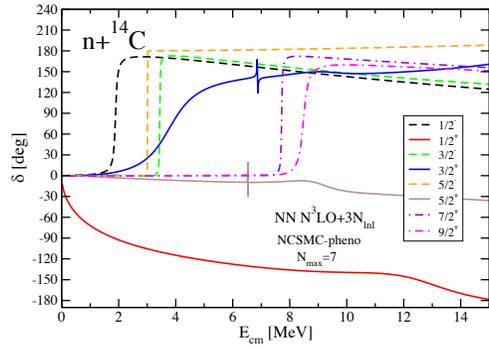
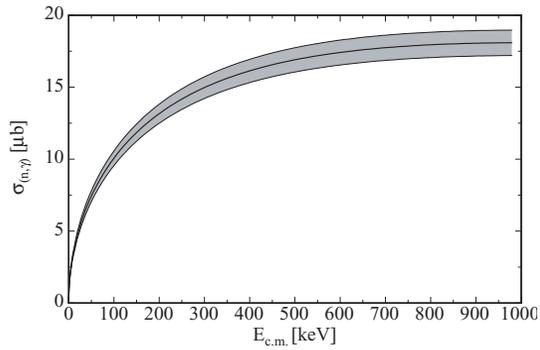
^{15}C cluster form factors

- $1/2^+$ 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!

