

Ab initio calculations for exotic nuclei

Understanding Nuclei from Different Theoretical Approaches

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Outline

1. No-core shell model with continuum

- a. Structure of the exotic ${}^9\text{He}$ system
- b. Study of $A=7$ systems

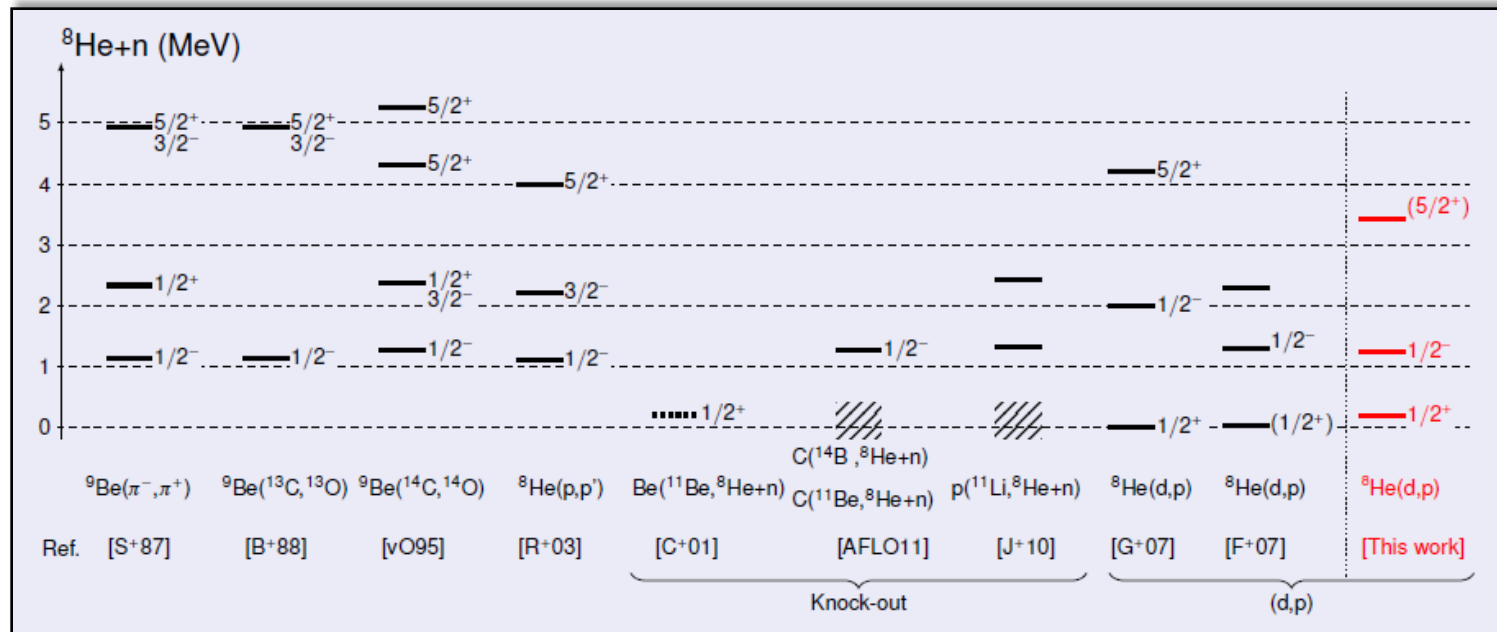
2. Microscopic optical potentials for intermediate energies with nonlocal *ab initio* densities

- Results for stable nuclei
- Results for ${}^6\text{He}$ and ${}^8\text{He}$

1a.

Structure of the exotic ${}^9\text{He}$

Experimental history of ${}^8\text{He}$

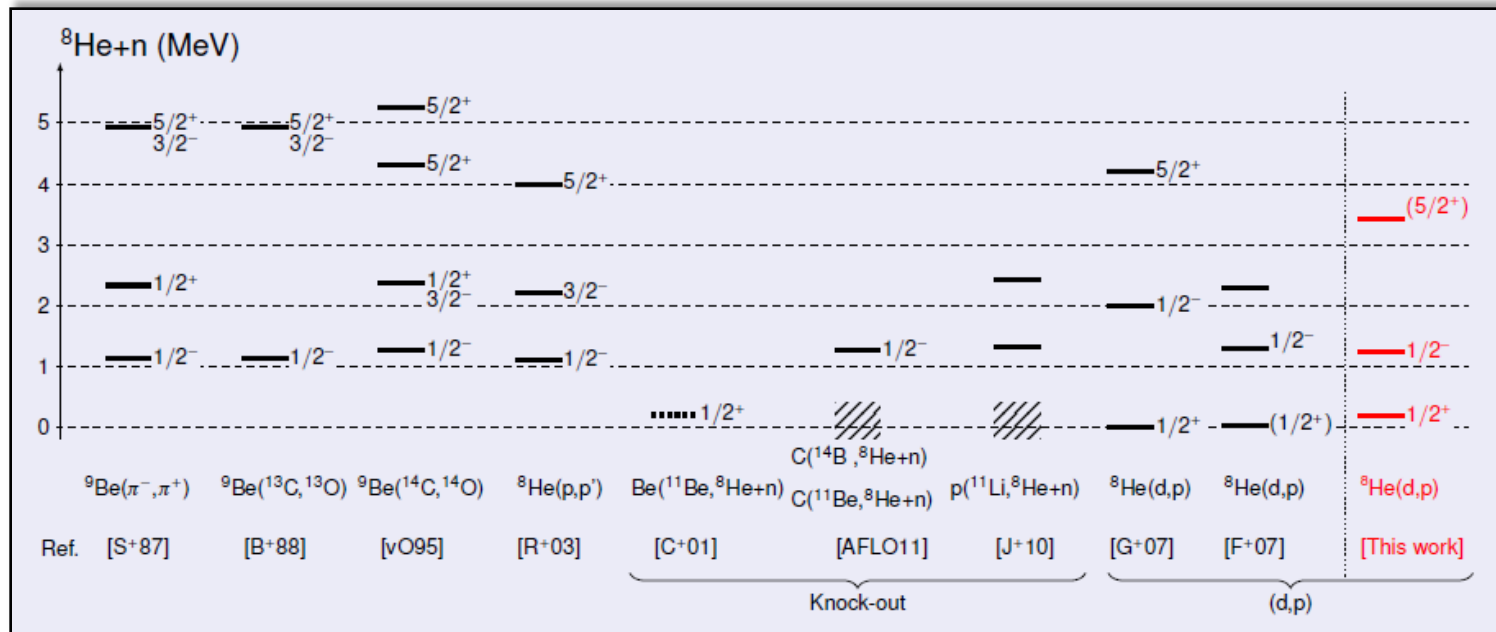


From talk by Nigel Orr at ECT* (2013)

Controversial experimental situation

- No bound state
- Most experiments see a $1/2^-$ resonance at ~ 1 MeV
- Is there a $1/2^+$ resonance? Is the ground state $1/2^+$ or $1/2^-$?
 - $a_0 \sim -10$ fm (Chen et al.)
 - $a_0 \sim -3$ fm (Al Falou et al.)
- Any higher-lying resonances?
- Recent ${}^8\text{He}(p, p)$ measurement at TRIUMF by Rogachev
Found no $T = 5/2$ resonances [PLB **754** (2016) 323]

Experimental history of ${}^9\text{He}$

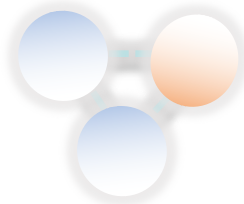
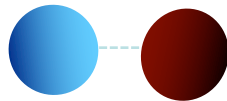
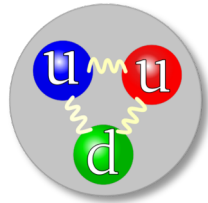


From talk by Nigel Orr at ECT* (2013)

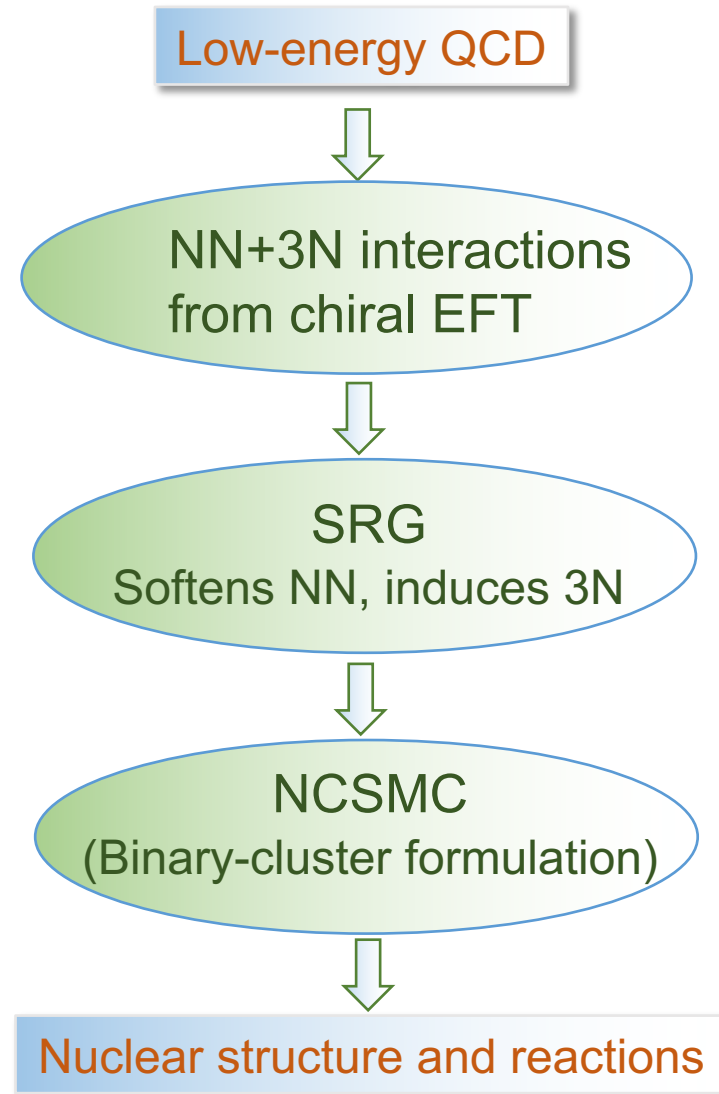
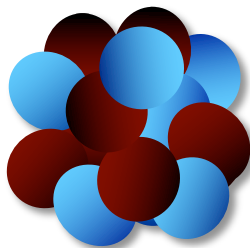
Two longstanding problems affect the physics of the ${}^9\text{He}$ system

1. The existence of the $1/2^+$ resonance
2. The width of the $1/2^-$ resonance
 - Experimentally ~ 0.1 MeV
 - Theoretically ~ 1 MeV

From QCD to nuclei

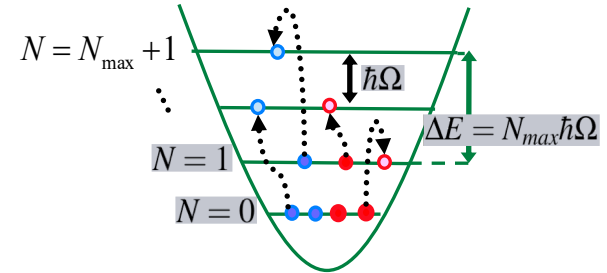


$$H|\Psi\rangle = E|\Psi\rangle$$



No-core shell model

- 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



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

$$\Psi^{(A)} = \sum_{\lambda} c_{\lambda} \left| \begin{matrix} (A) \\ \text{Nucleon Cluster} \end{matrix}, \lambda \right\rangle$$

Unknowns

No-core shell model with RGM

- NCSM with Resonating Group Method (NCSM/RGM)
 - Cluster expansion, clusters described by NCSM
 - Proper asymptotic behavior
 - Long-range correlations

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

Unknowns

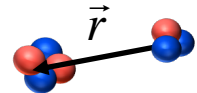
Unified approach to bound & continuum states; to nuclear structure and reactions

- 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

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

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

Unknowns

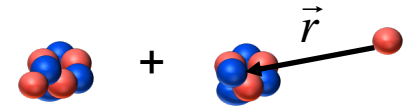
NCSMC ${}^9\text{He}$ calculations

- NCSMC calculations with several interactions

- $N^2\text{LO}_{\text{sat}}$ NN + 3N
- NN $N^3\text{LO}$ + 3N $N^2\text{LO}$
- **NN SRG- $N^4\text{LO}500$**

- Calculations with NN SRG- $N^4\text{LO}500$

- ${}^9\text{He} \sim ({}^9\text{He})_{\text{NCSM}} + (n-{}^8\text{He})_{\text{NCSM/RGM}}$
 - ${}^8\text{He}$: 0^+ and 2^+ NCSM eigenstates
 - ${}^9\text{He}$: 4 negative-parity NCSM eigenstates
6 positive-parity NCSM eigenstates

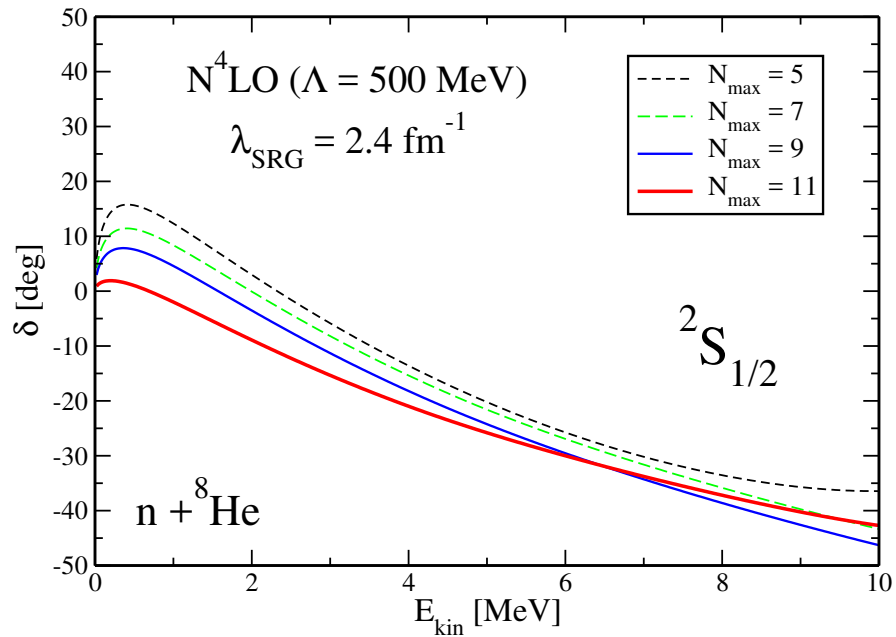


- Importance of large N_{max} basis:
 - NN SRG- $N^4\text{LO}500$ with $\lambda = 2.4 \text{ fm}^{-1}$
up to $N_{\text{max}} = 11$ with ${}^9\text{He}$ NCSM (m-scheme basis of 350 million)

Structure of unbound ${}^9\text{He}$

Phase shift convergence with
NN SRG- $N^4\text{LO}500$
 $\lambda=2.4 \text{ fm}^{-1}$

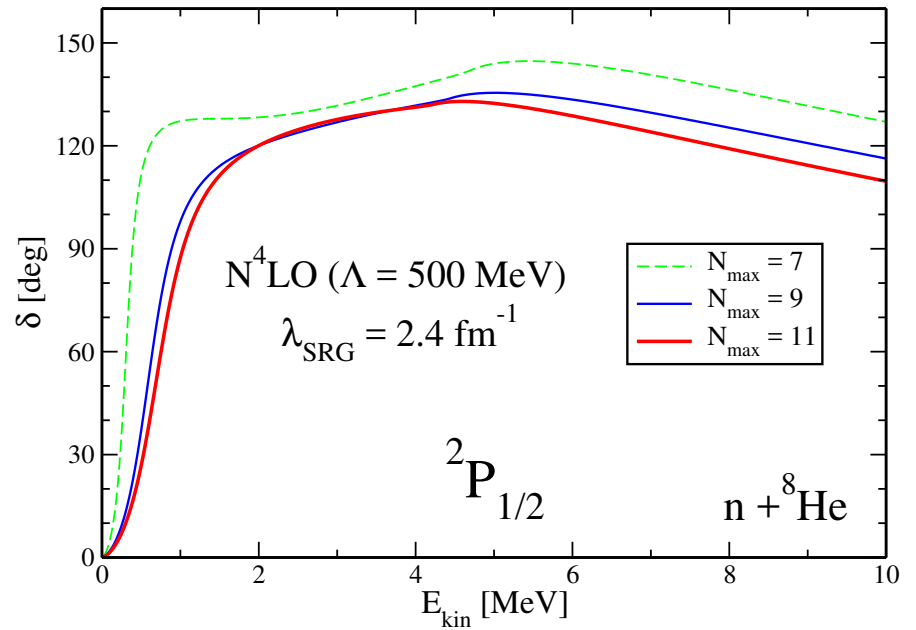
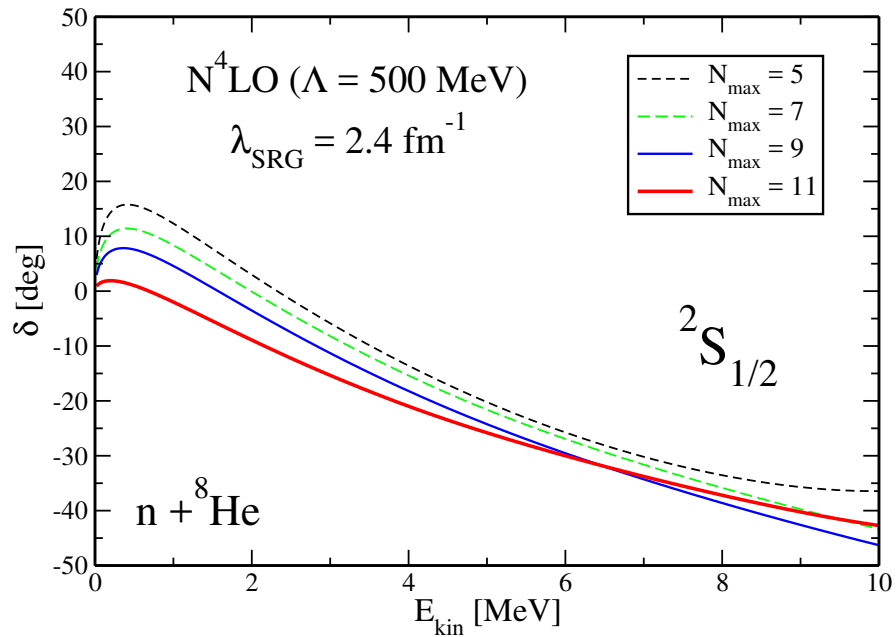
Vorabbi, Calci, Navratil, Kruse, Quaglioni, Hupin,
PRC **97**, 034314 (2018)



Structure of unbound ${}^9\text{He}$

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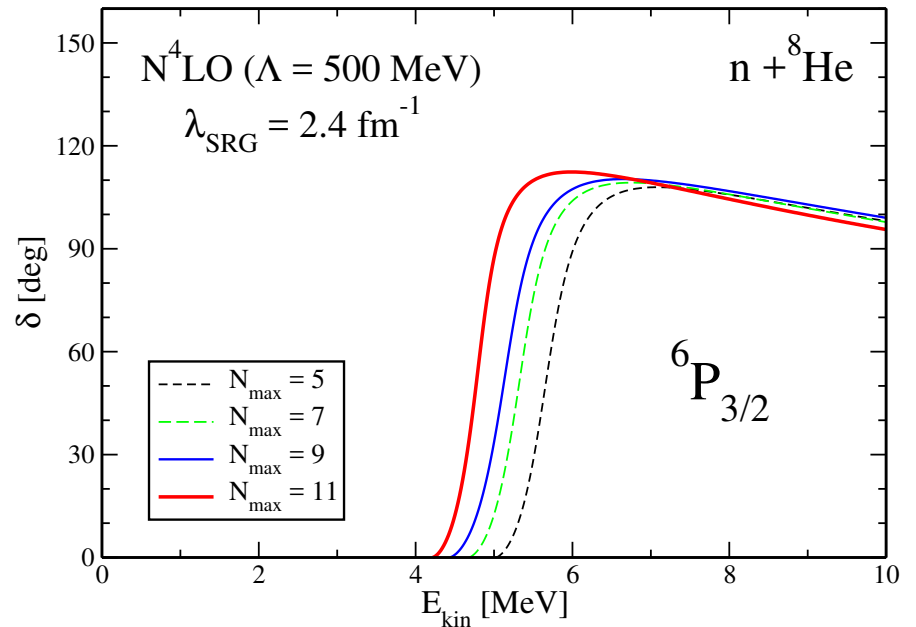
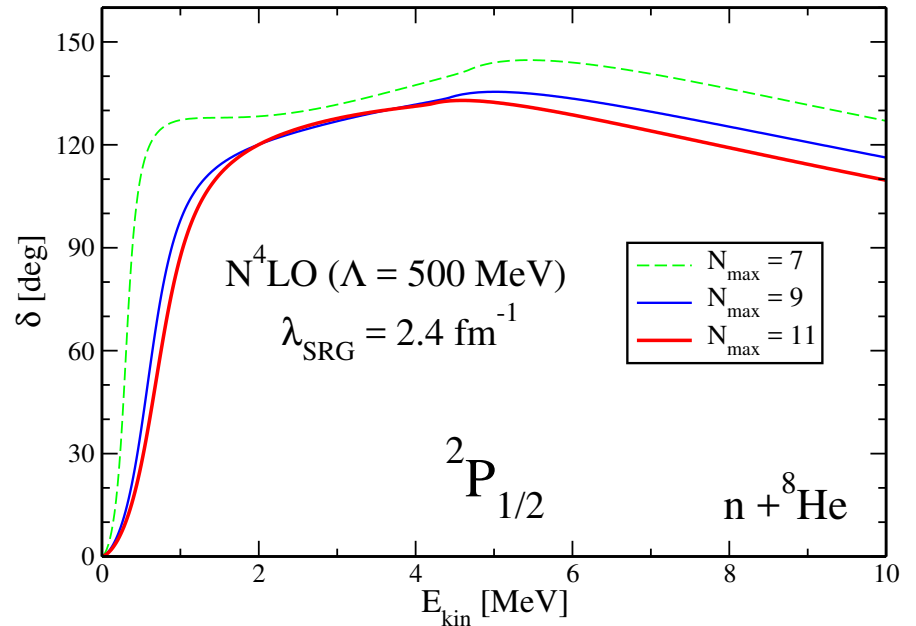
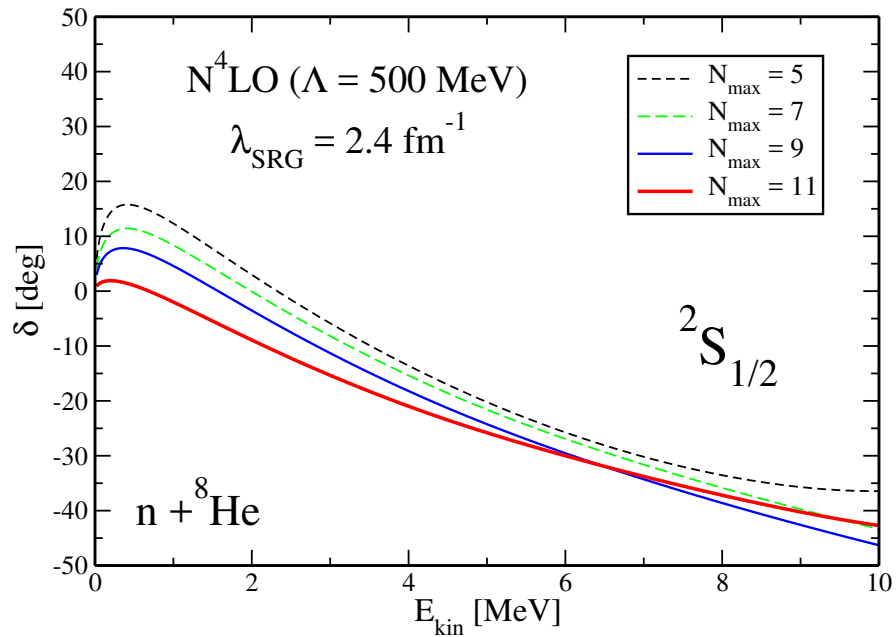
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Structure of unbound ${}^9\text{He}$

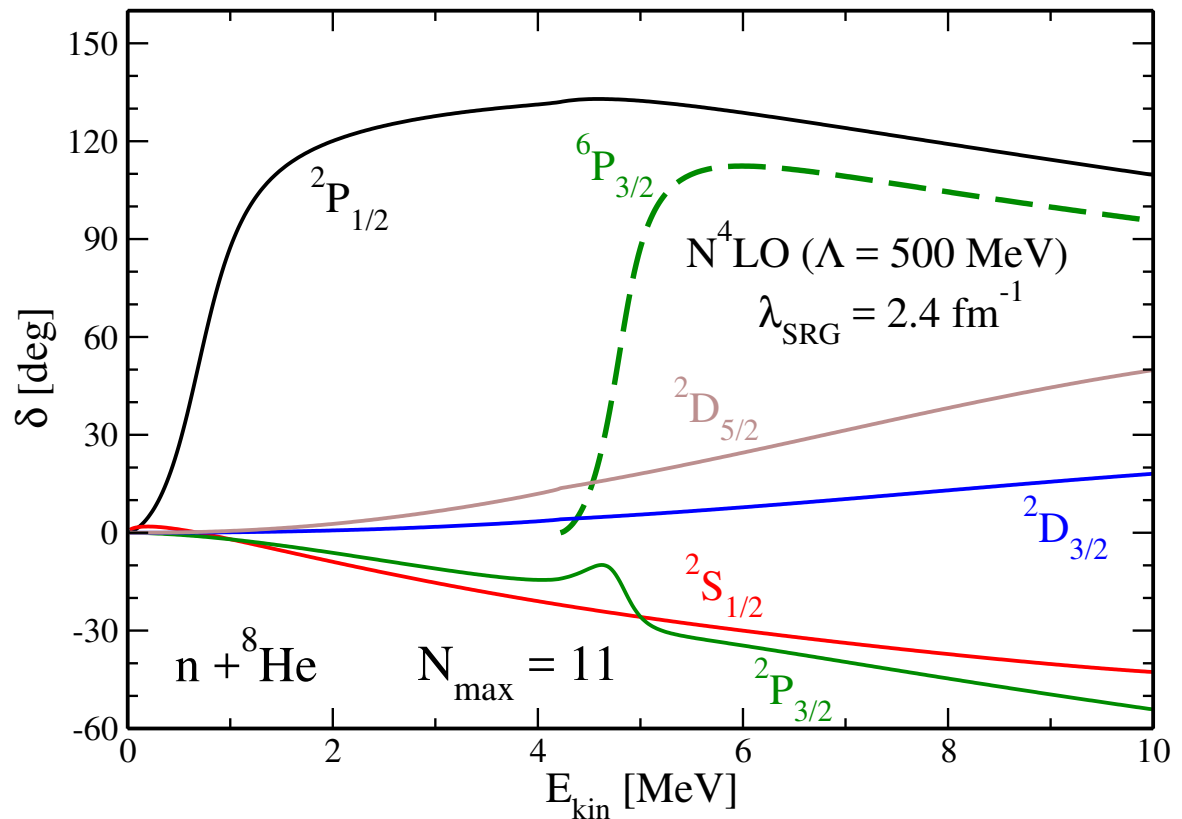
Phase shifts with NN SRG- $N^4\text{LO}500$ $\lambda=2.4 \text{ fm}^{-1}$

Energy spectrum

No bound state

Two resonances in the $2P_{1/2}$ and ${}^6P_{3/2}$ channels

No resonance in the ${}^2S_{1/2}$ state



Structure of unbound ${}^9\text{He}$

Eigenphase shifts with NN SRG- $N^4\text{LO}500$ $\lambda=2.4$ fm $^{-1}$

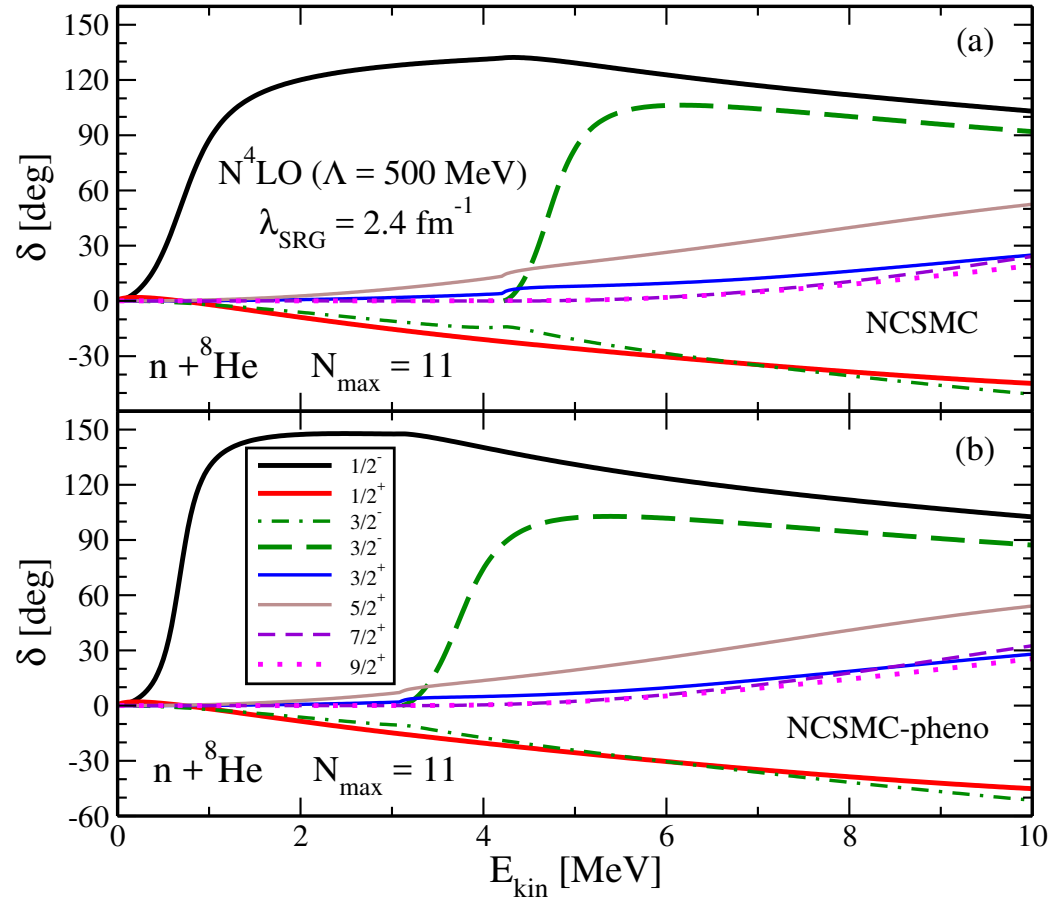
Vorabbi, Calci, Navratil, Kruse, Quaglioni, Hupin,
PRC **97**, 034314 (2018)

Summary

Robust results for $1/2^-$ (~ 1 MeV) and $3/2^-$ (~ 4 MeV) **P-wave** resonances ($3/2^-$ resonance in n - ${}^8\text{He}(2^+)$ channel)

$1/2^+$ **S-wave** with vanishing scattering length: $a_s = 0 \sim -1$ fm

No evidence for other higher lying resonances



J^π	NCSMC		NCSMC-pheno	
$1/2^-$	$E_R = 0.69$	$\Gamma = 0.83$	$E_R = 0.68$	$\Gamma = 0.37$
$3/2^-$	$E_R = 4.70$	$\Gamma = 0.74$	$E_R = 3.72$	$\Gamma = 0.95$

1b.

Study of $A=7$ systems

${}^7\text{Be}$ system

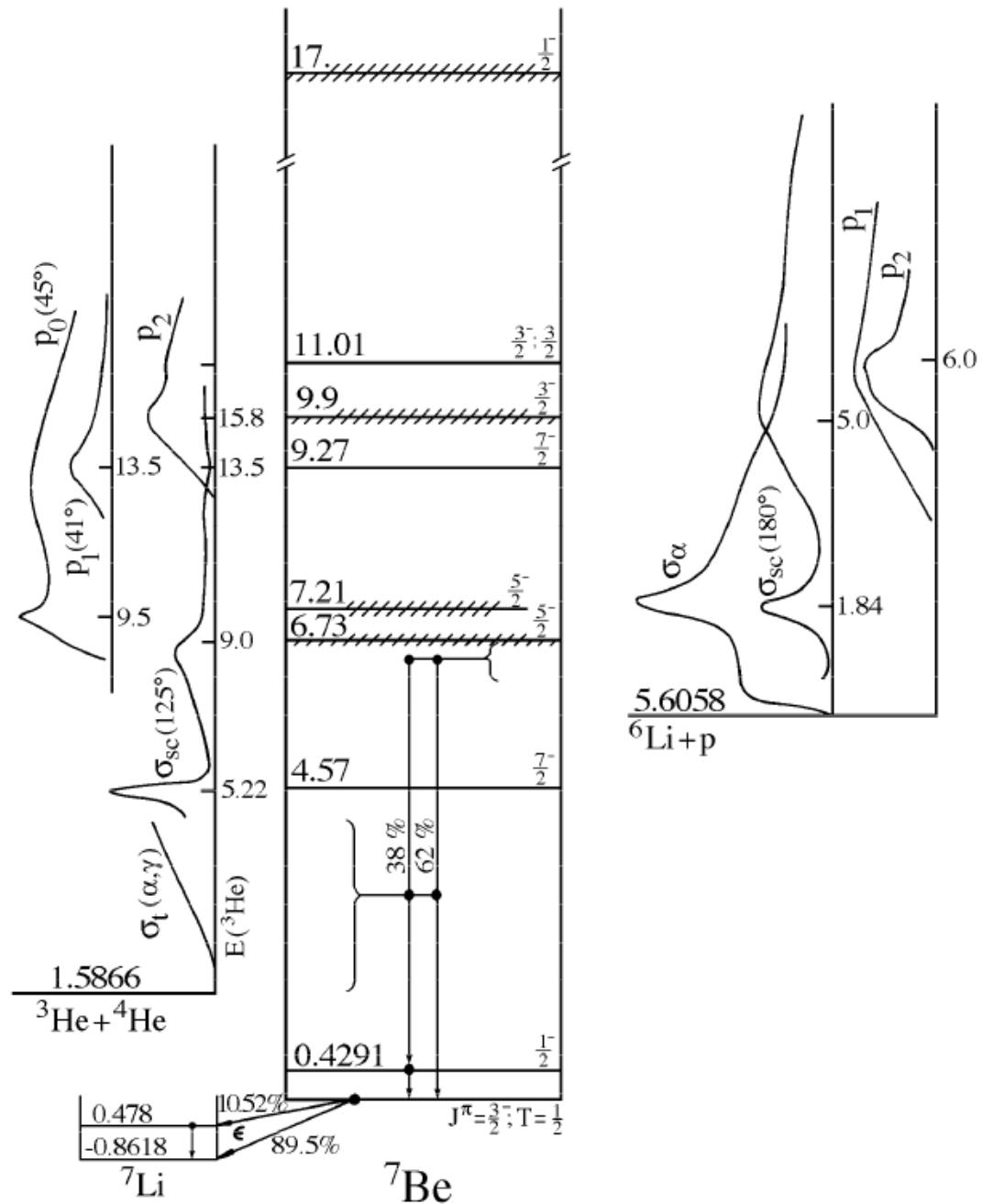
Analyzed mass partitions

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

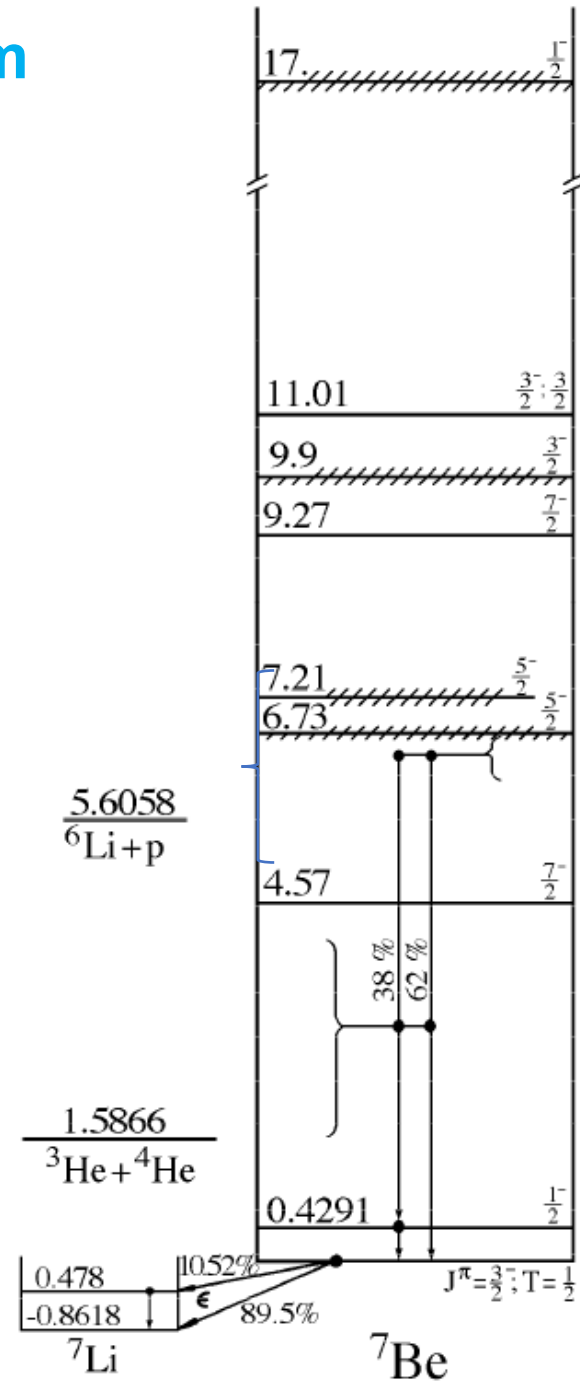
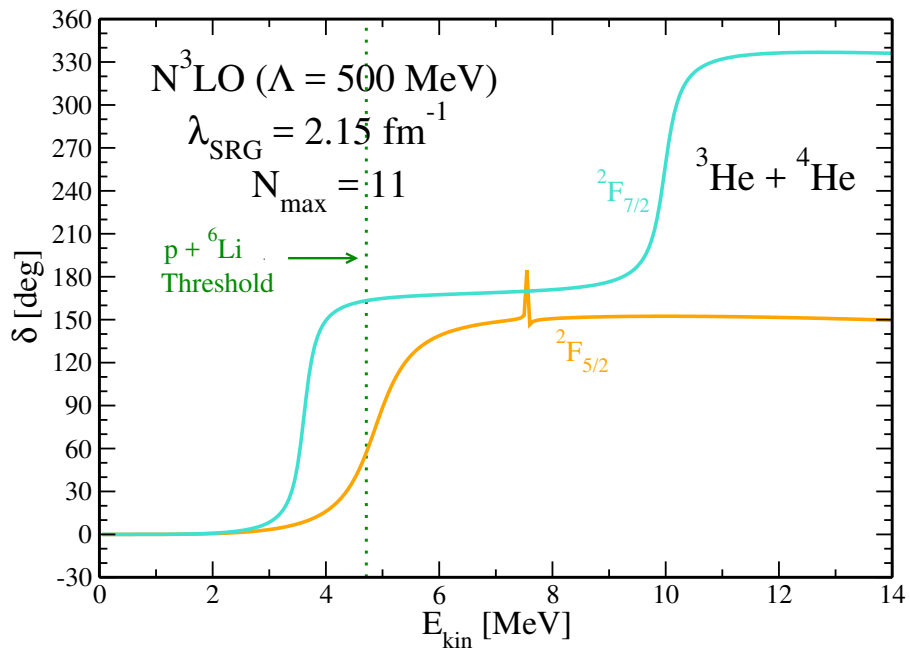
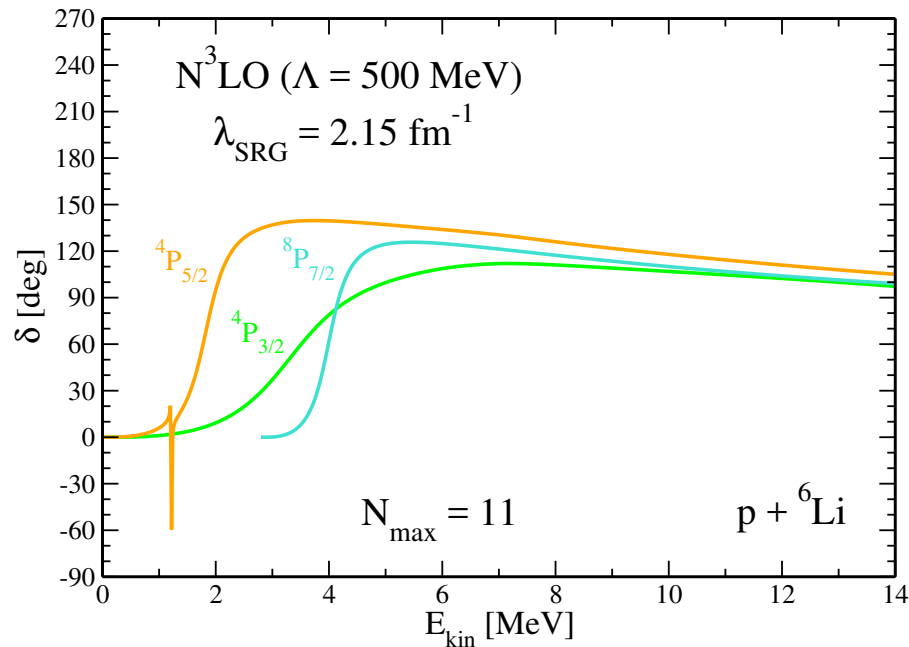
Exp.	$J^\pi = 3/2^-$
E [MeV]	-37.60

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

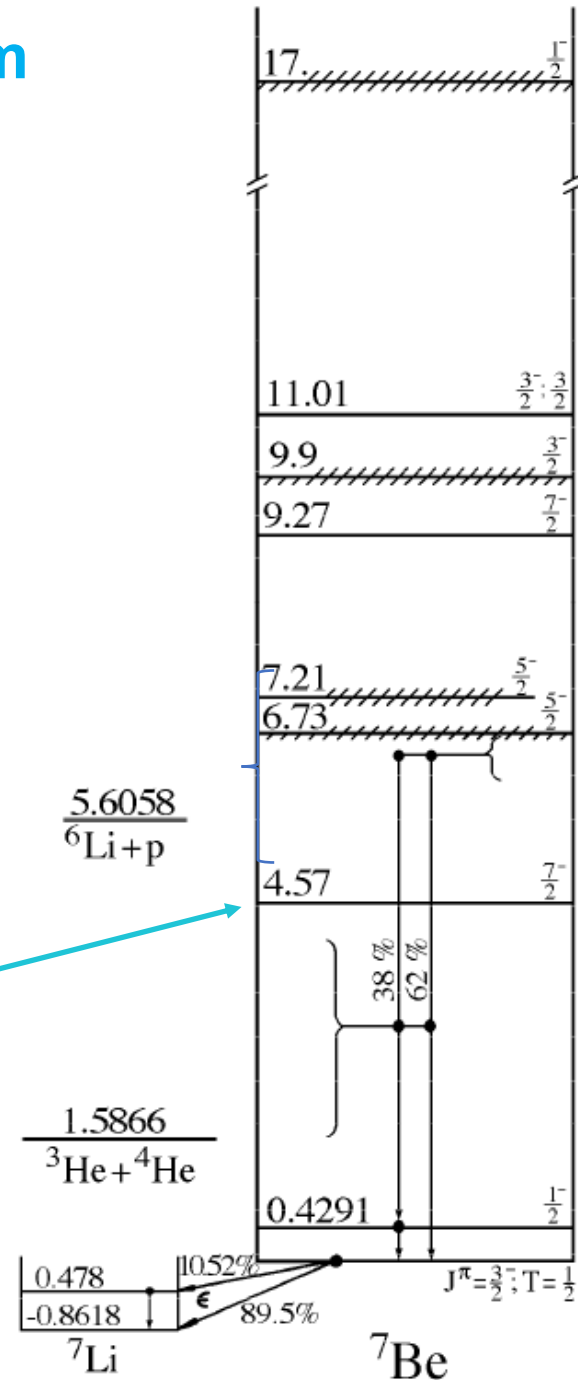
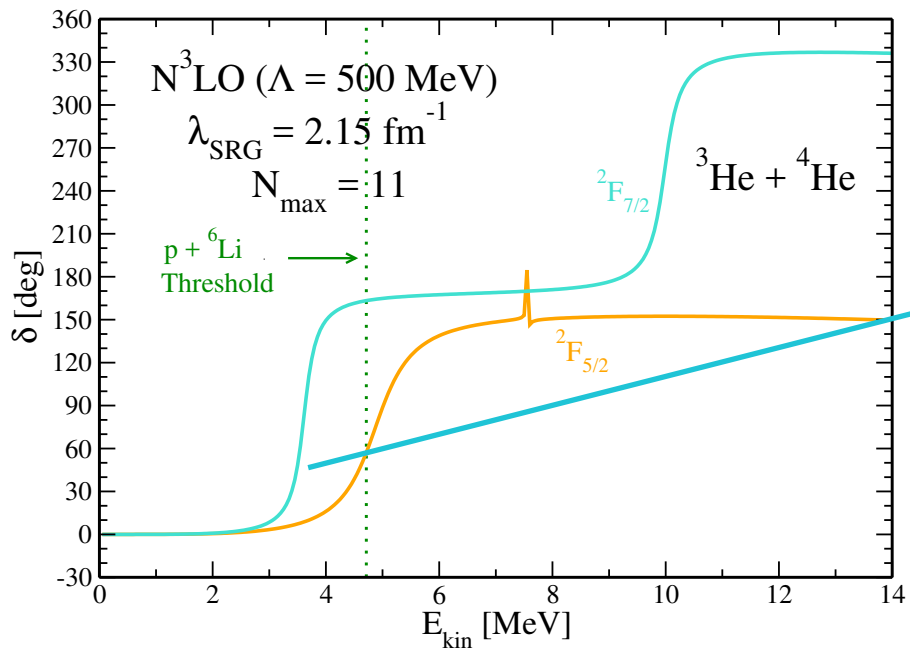
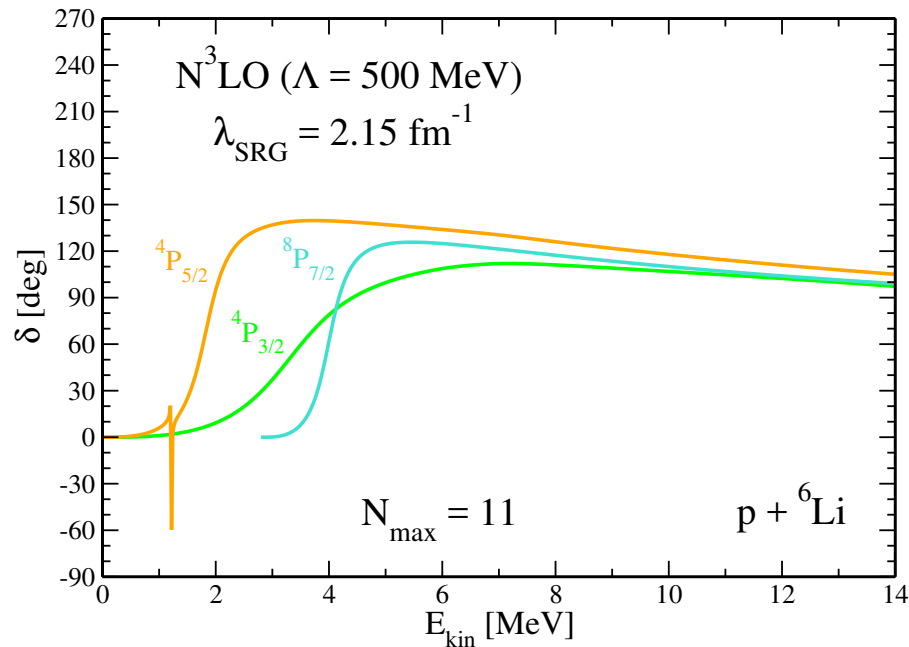
$p + {}^6\text{Li}$	$J^\pi = 3/2^-$	$J^\pi = 1/2^-$
E_{bound}	-5.729	-5.389
E [MeV]	-36.47	-36.13



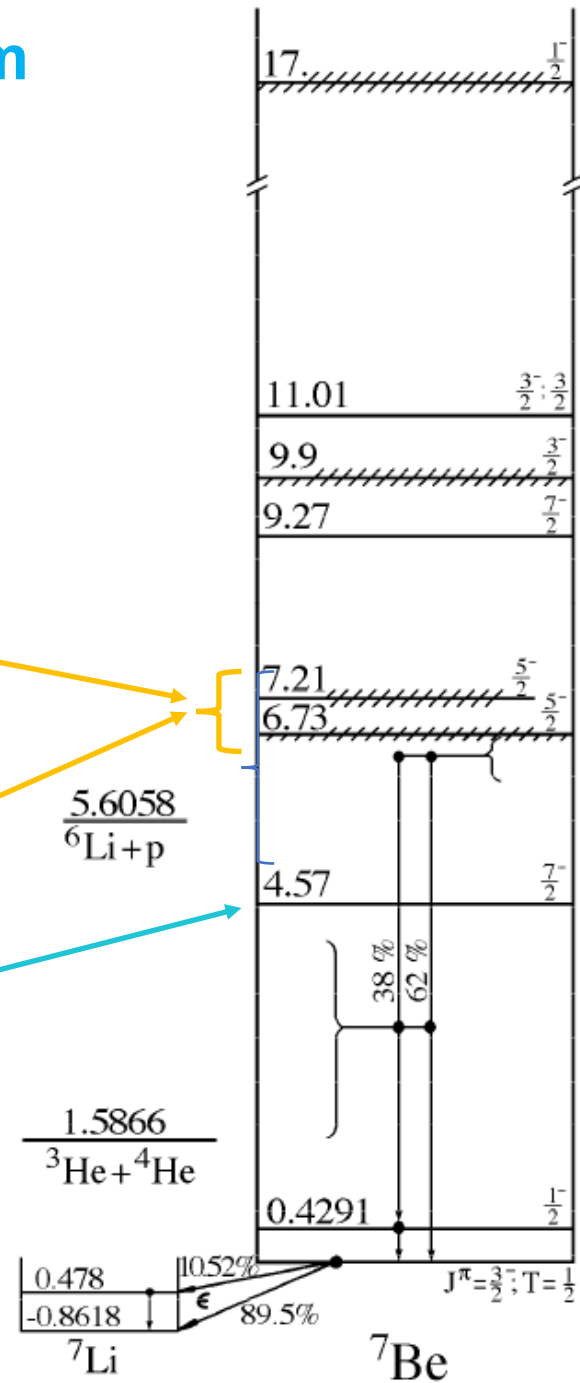
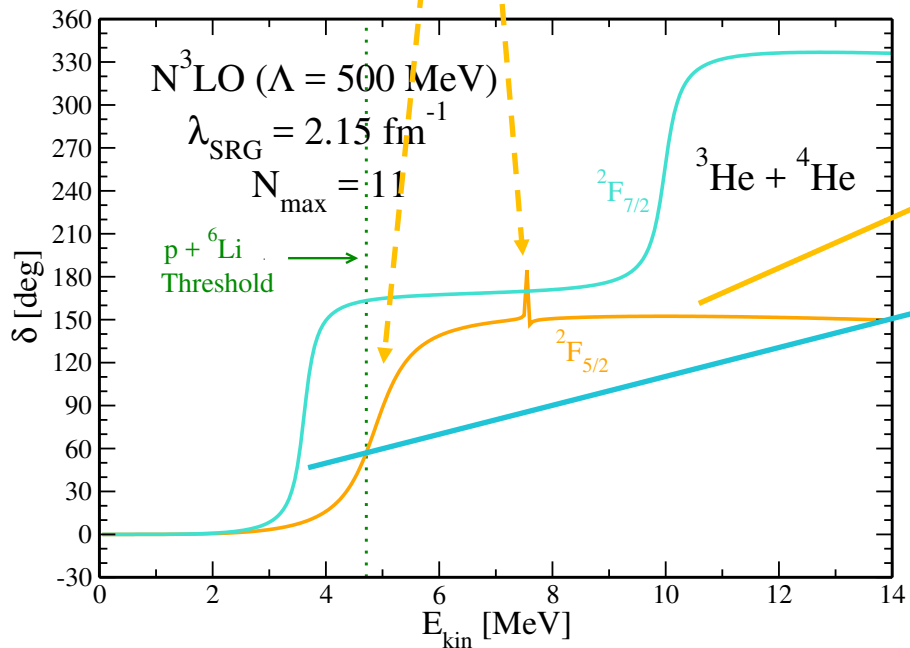
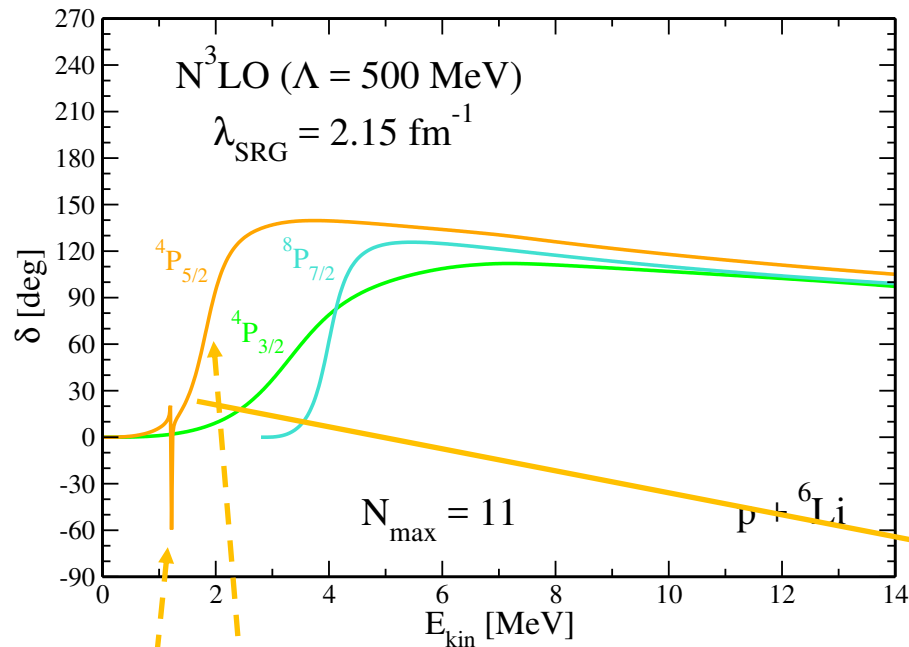
${}^7\text{Be}$ – Reproducing the energy spectrum



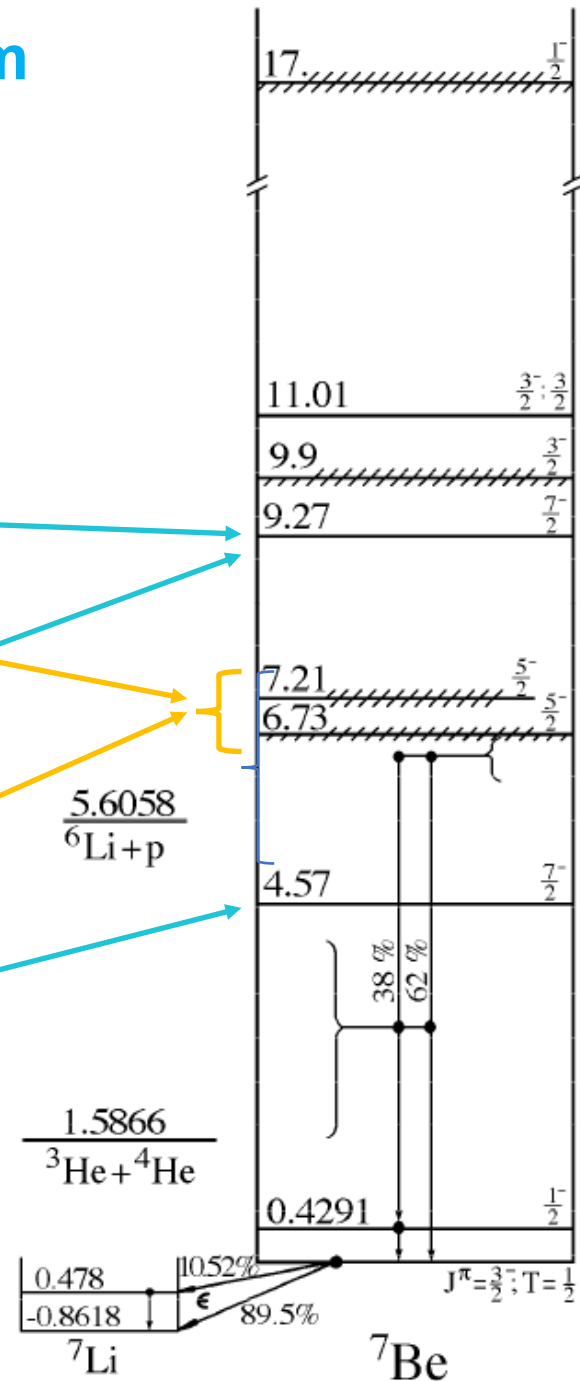
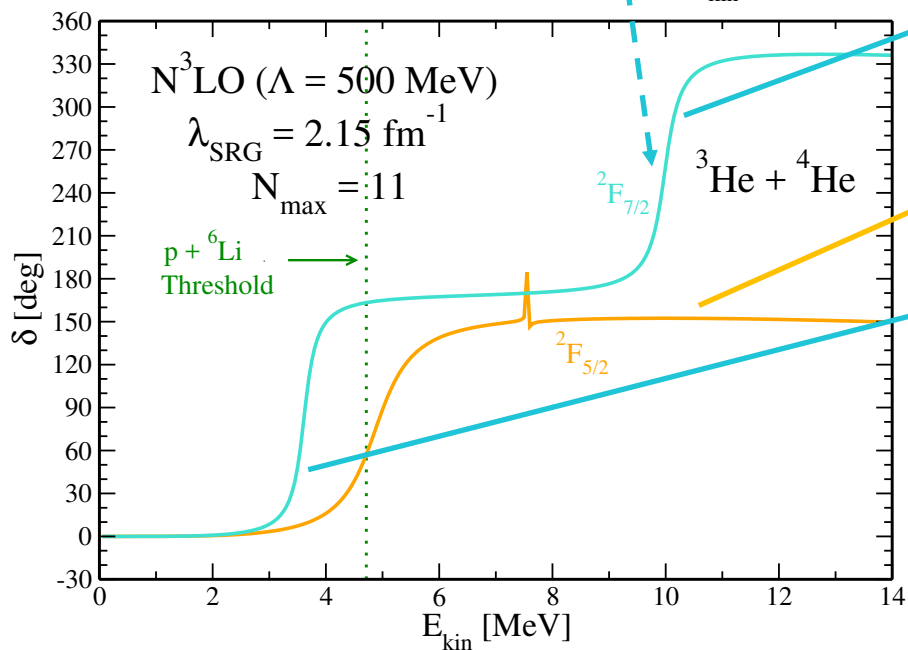
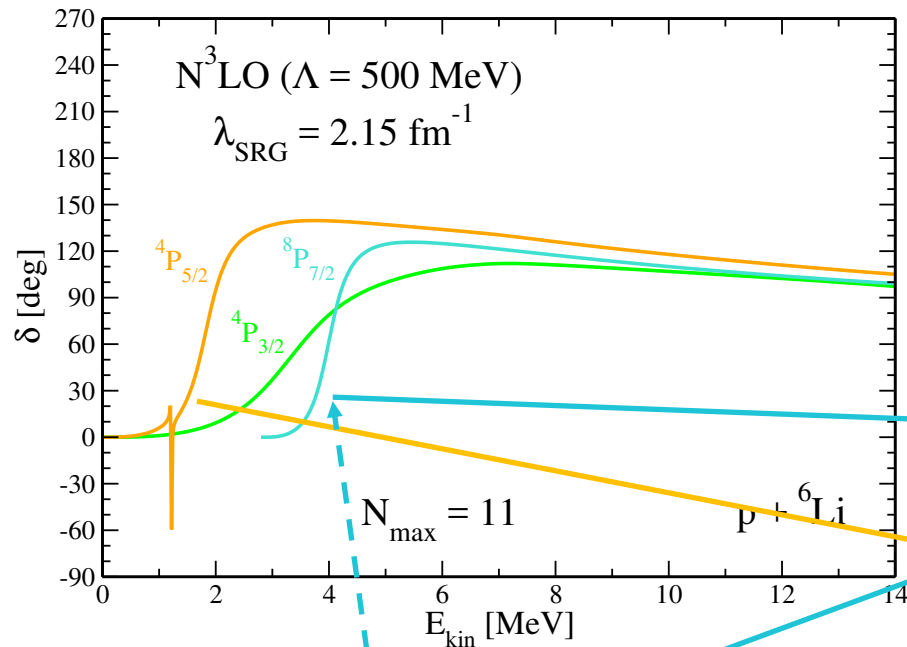
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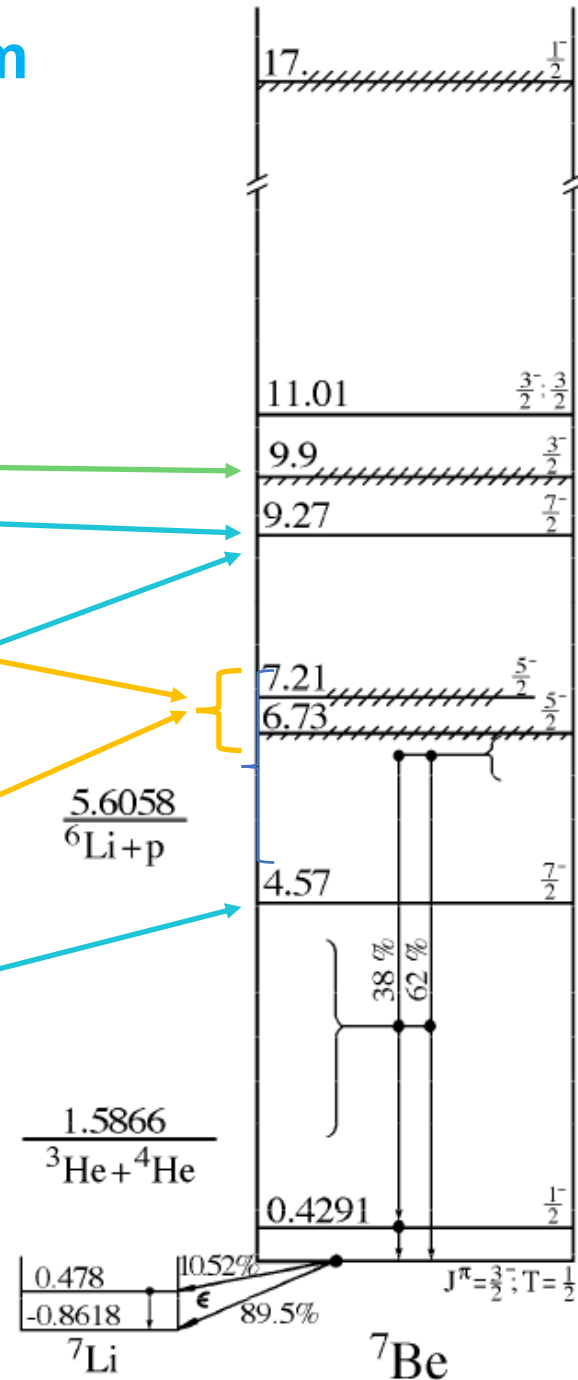
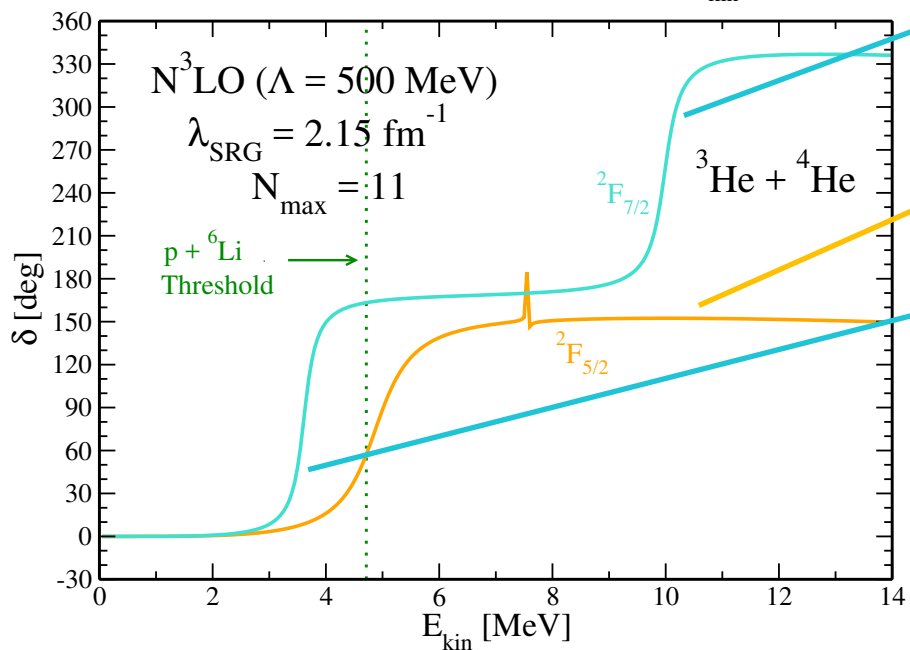
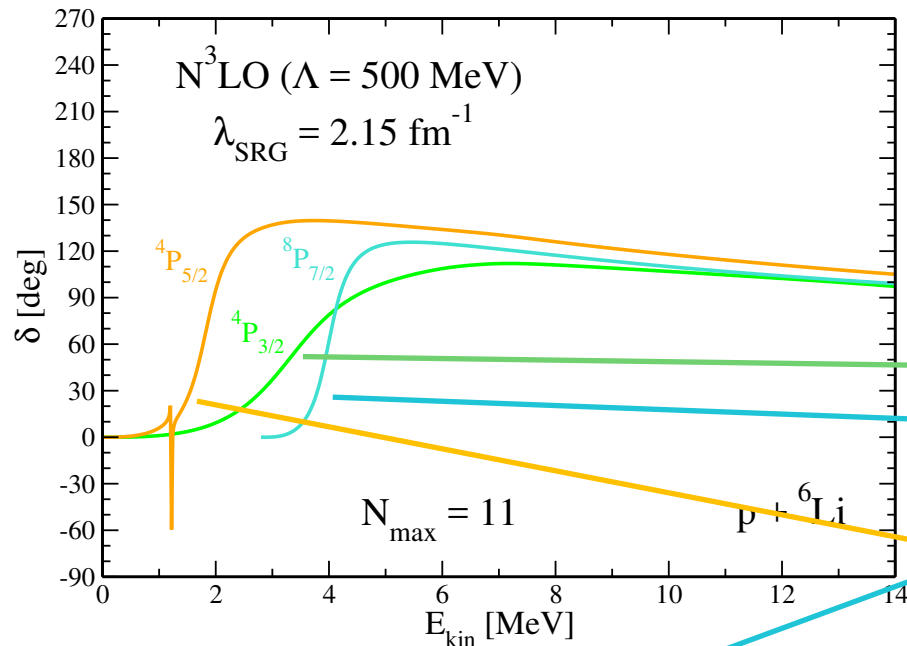
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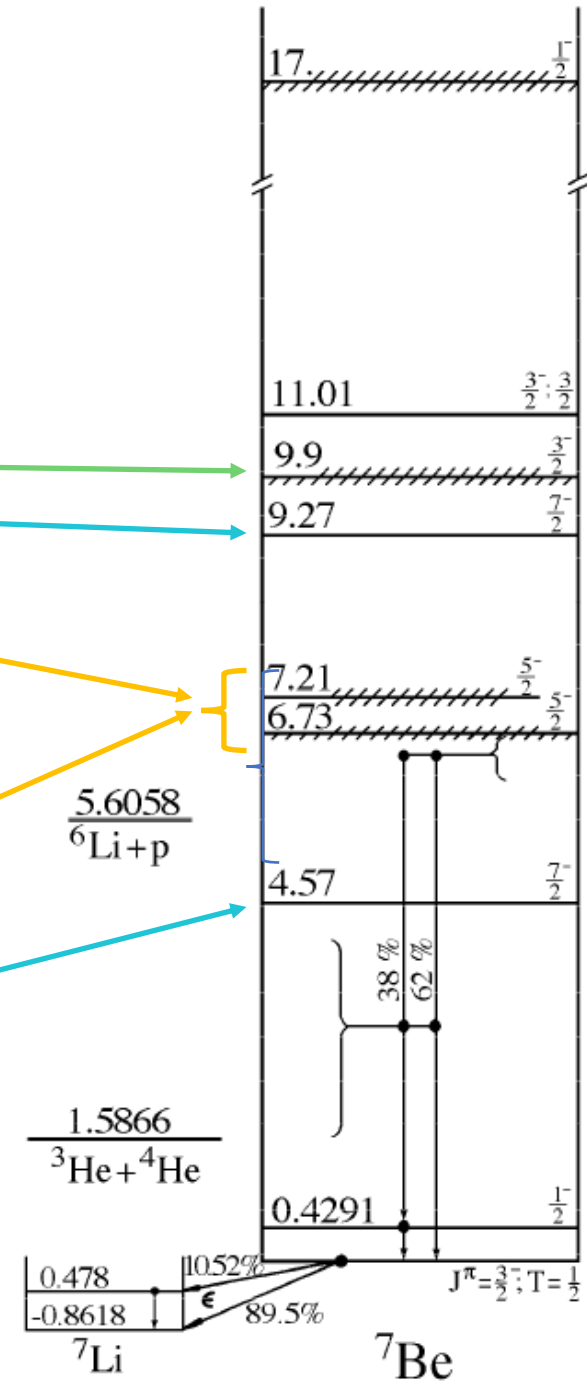
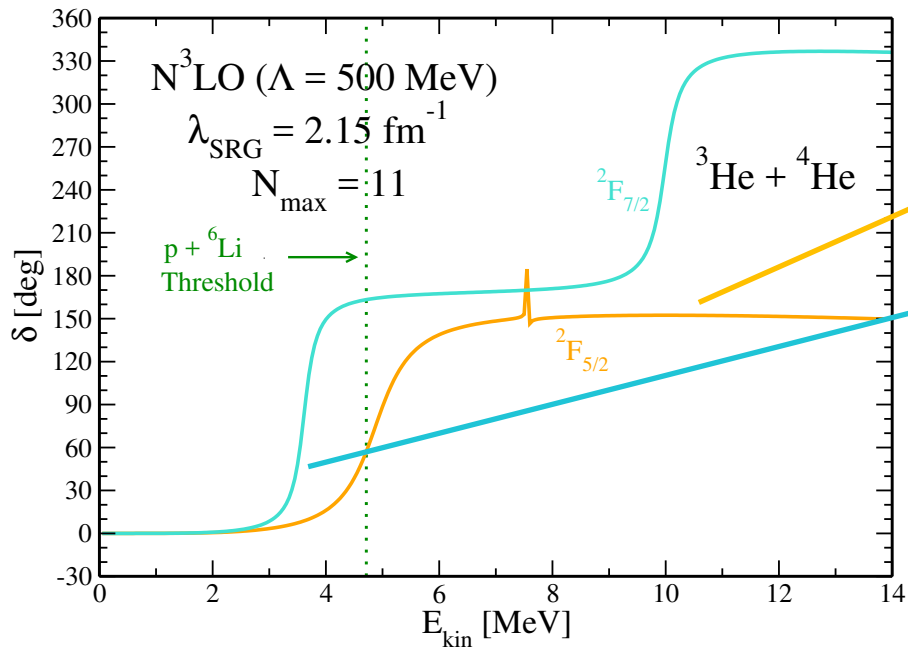
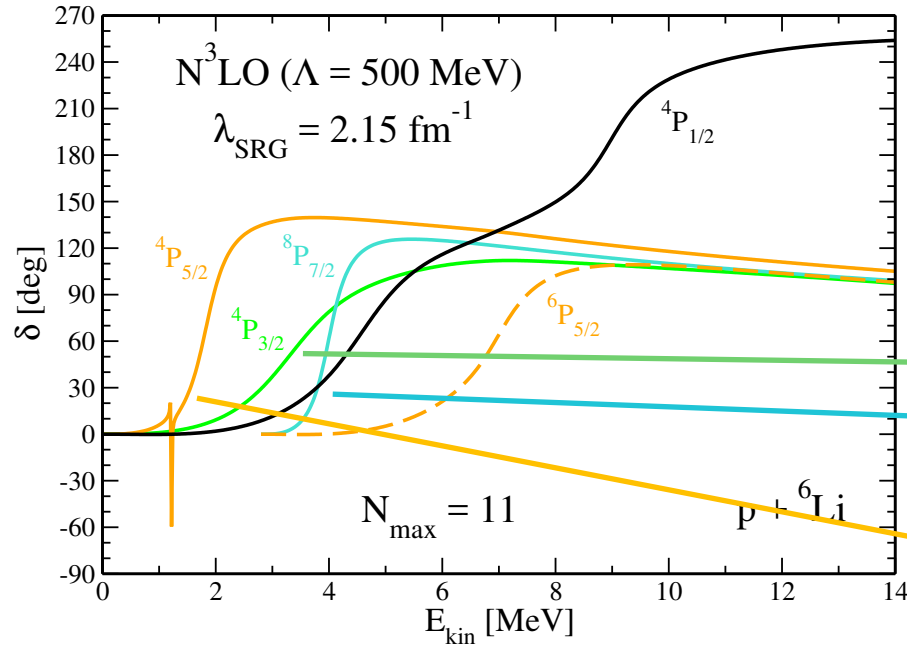
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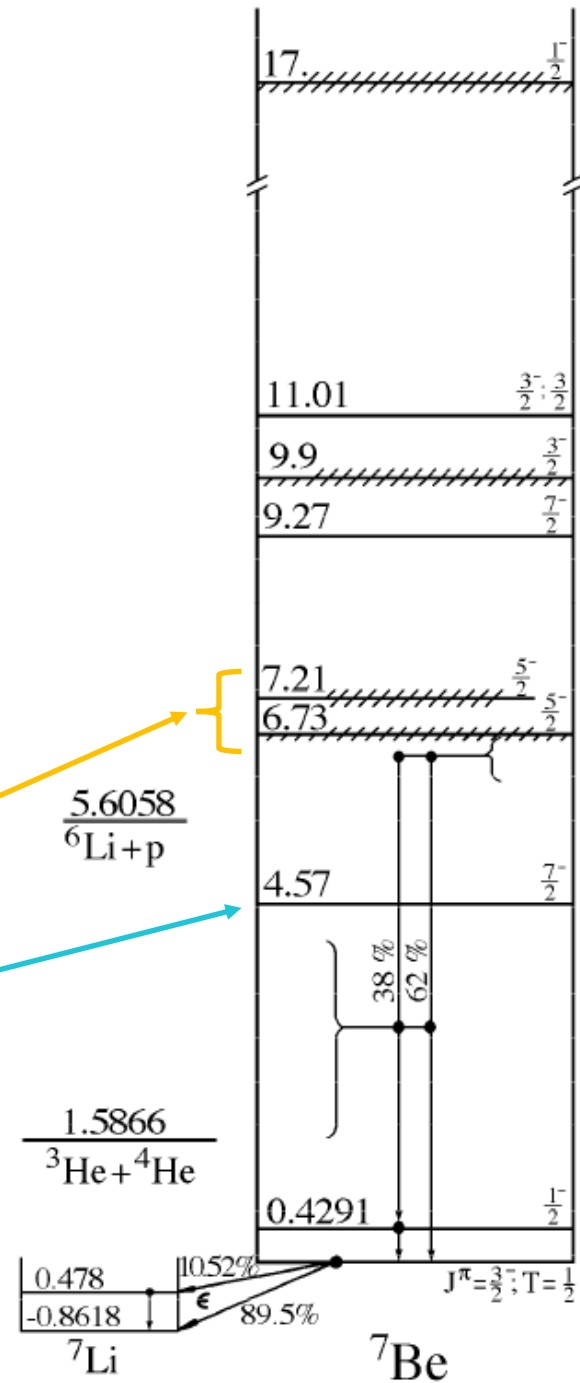
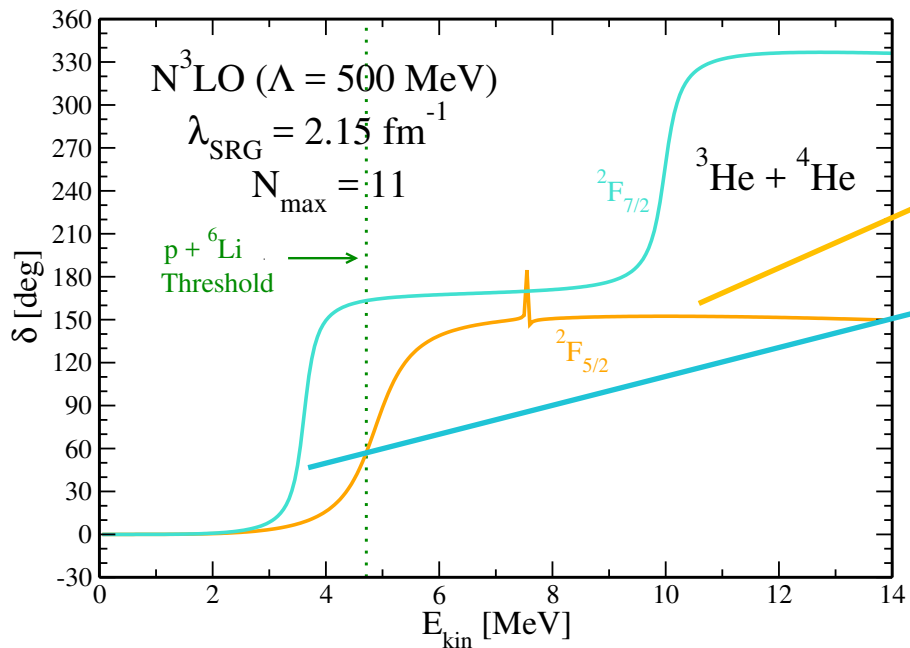
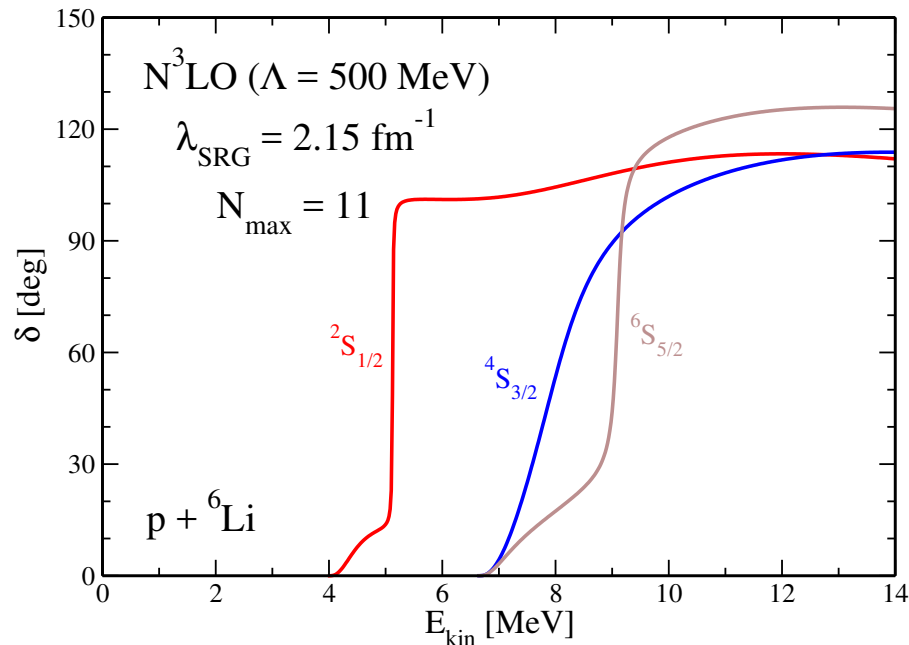
${}^7\text{Be}$ – Reproducing the energy spectrum



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



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



${}^7\text{Li}$ system

Analyzed mass partitions

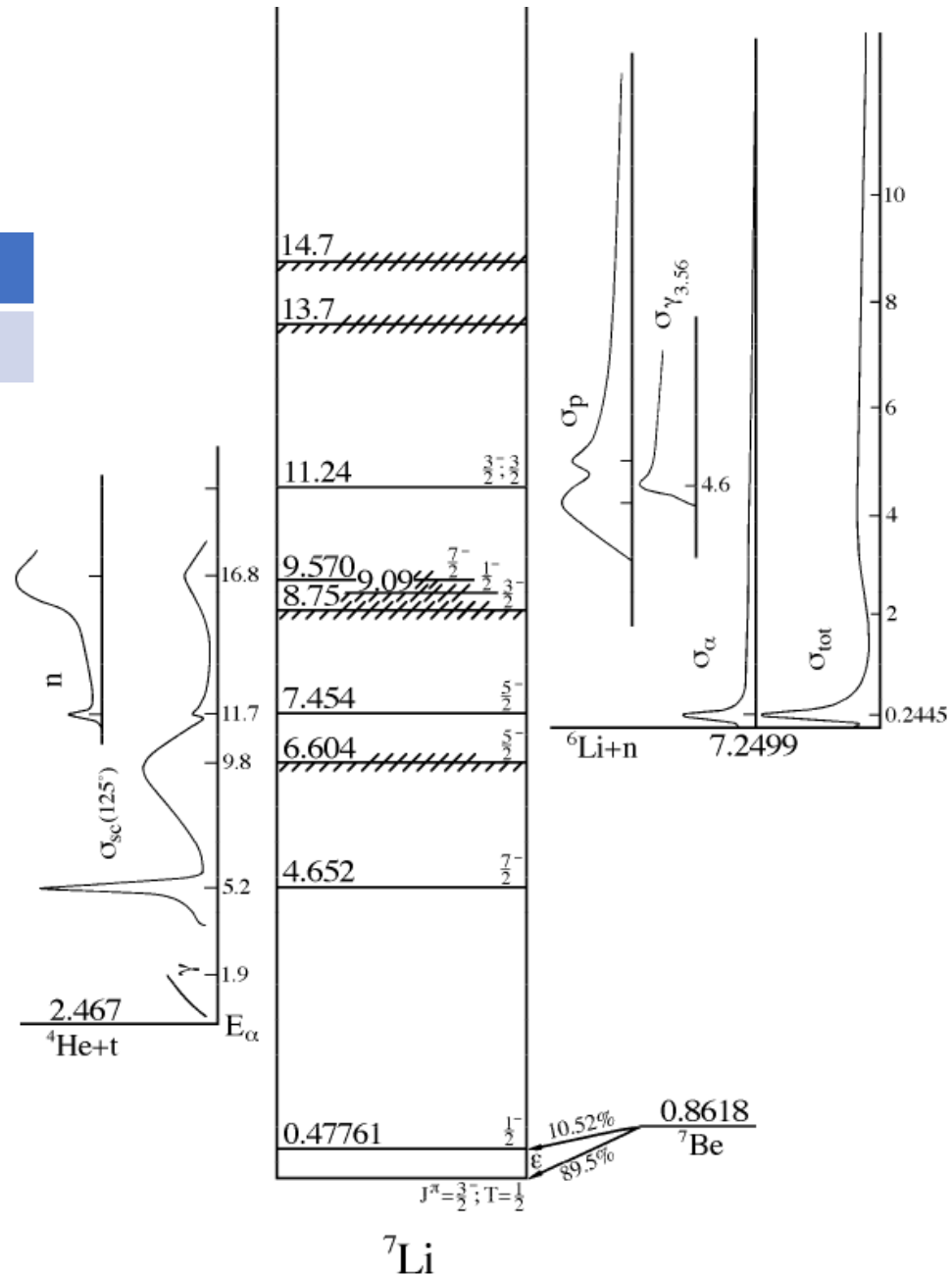
- ${}^3\text{H} + {}^4\text{He}$
- $n + {}^6\text{Li}$
- $p + {}^6\text{He}$

Exp.	$J^\pi = 3/2^-$
E [MeV]	-39.245

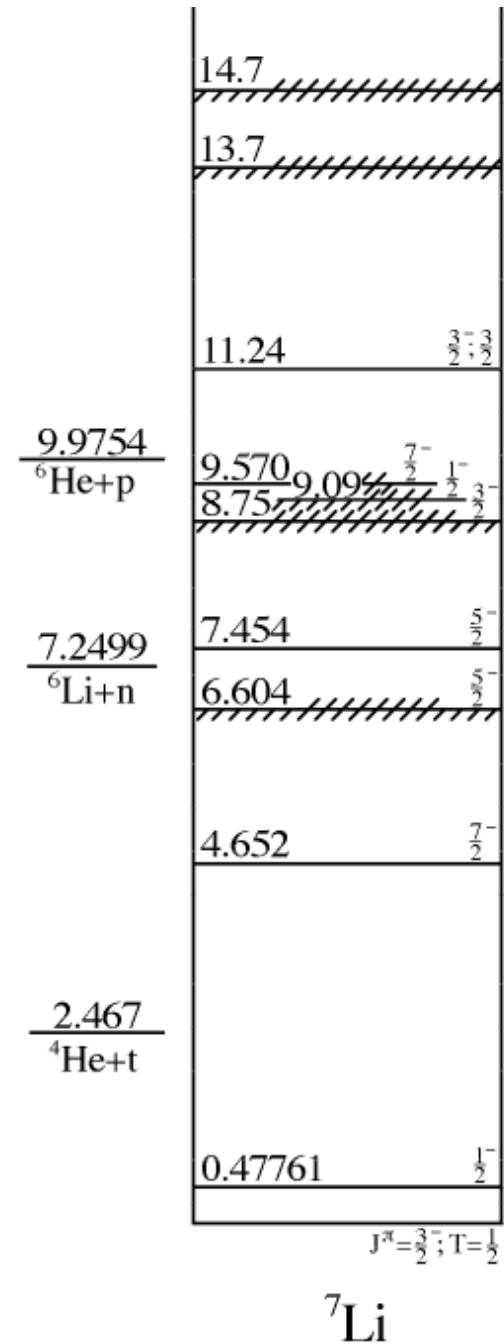
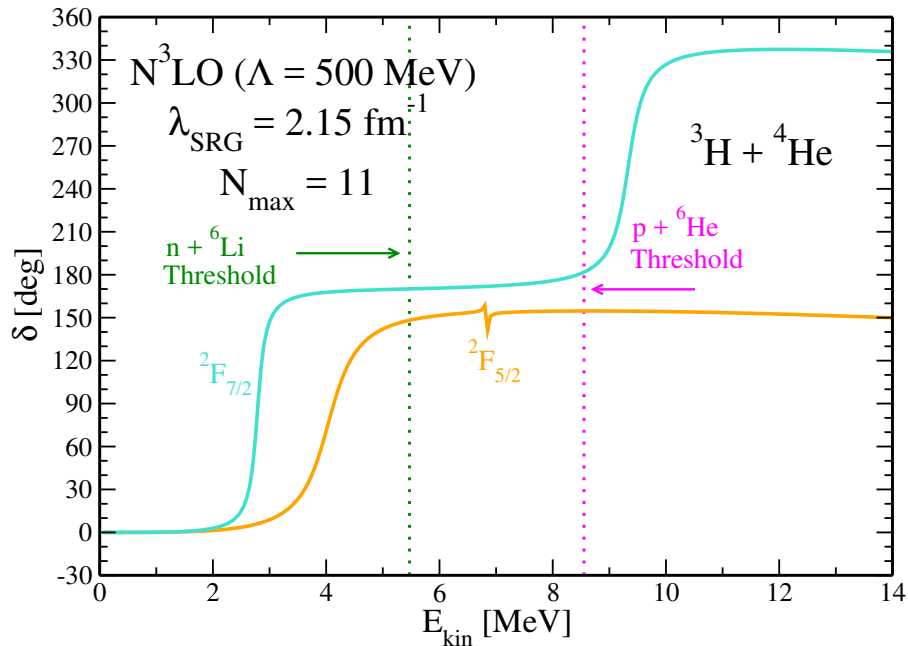
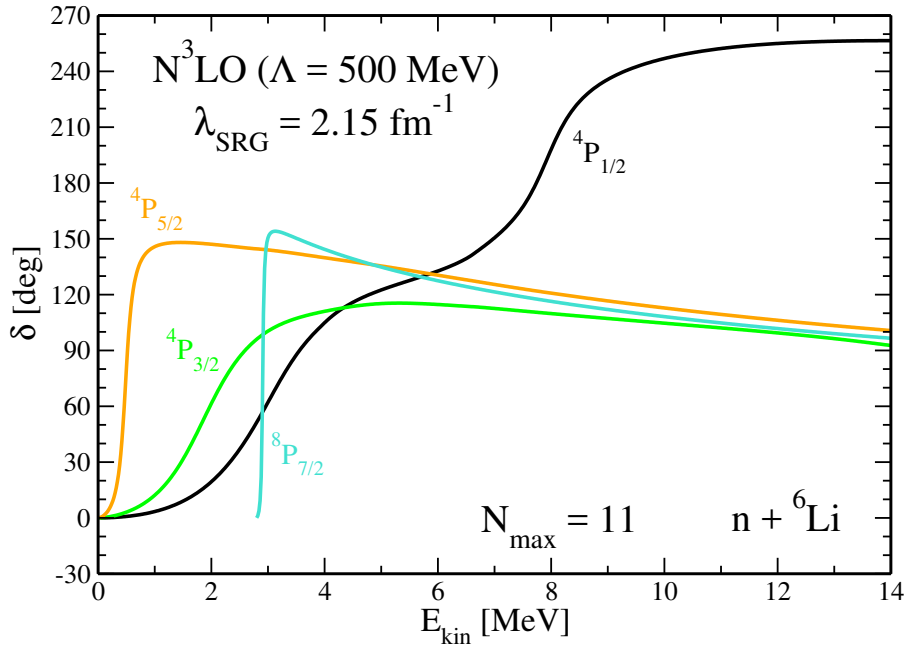
${}^3\text{H} + {}^4\text{He}$	$J^\pi = 3/2^-$	$J^\pi = 1/2^-$
E_{bound}	-2.432	-2.153
E [MeV]	-38.65	-38.37

$n + {}^6\text{Li}$	$J^\pi = 3/2^-$	$J^\pi = 1/2^-$
E_{bound}	-7.381	-7.048
E [MeV]	-38.13	-37.79

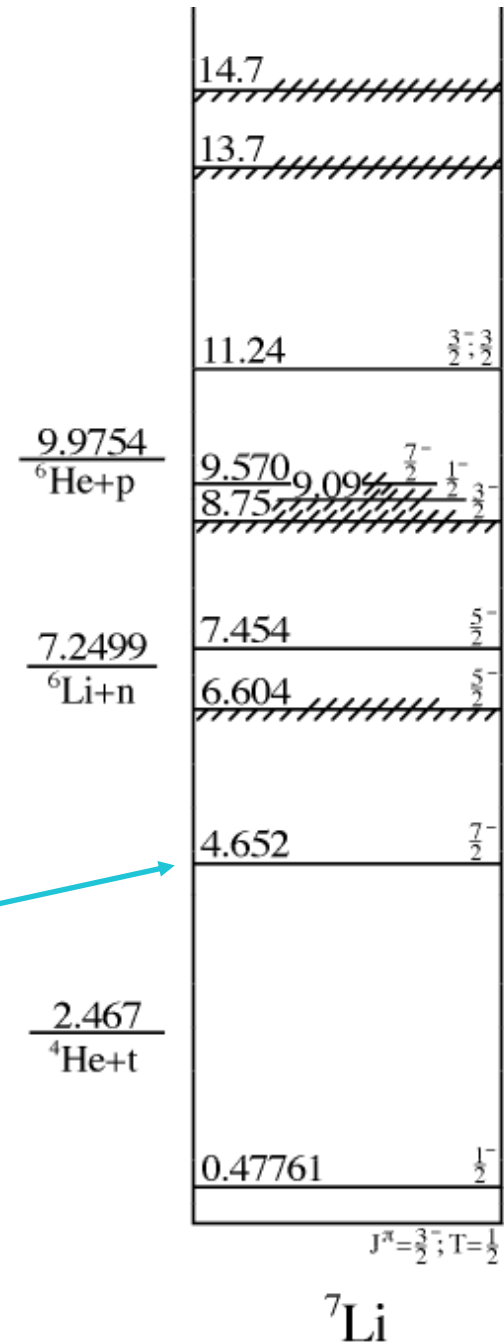
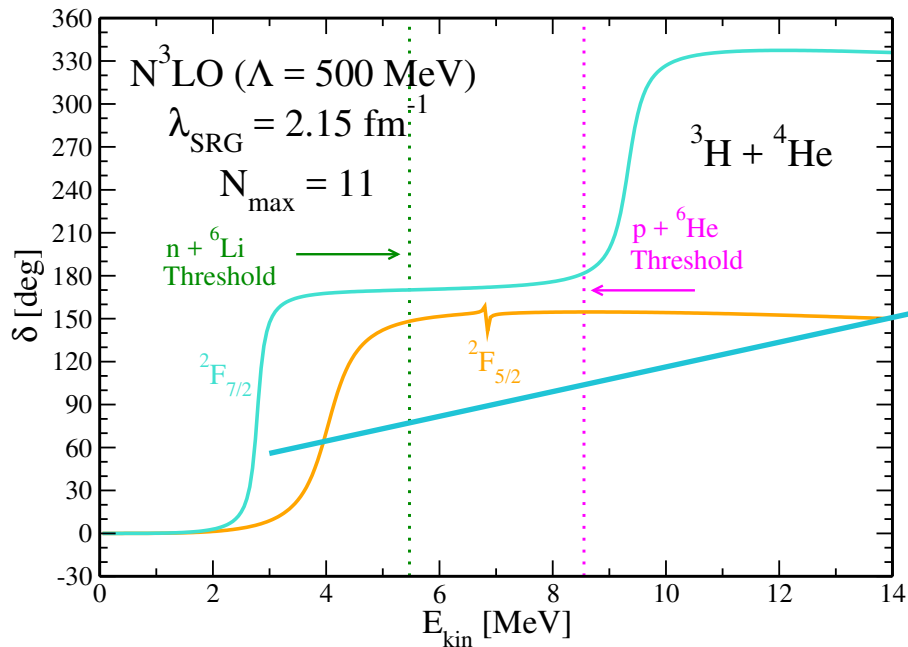
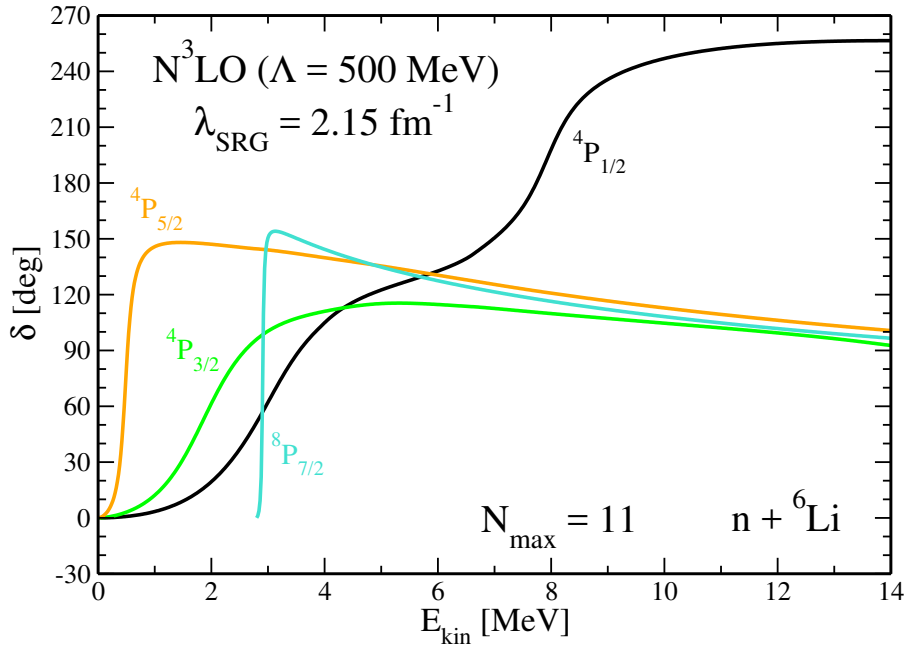
$p + {}^6\text{He}$	$J^\pi = 3/2^-$	$J^\pi = 1/2^-$
E_{bound}	-10.40	-10.06
E [MeV]	-38.06	-37.73



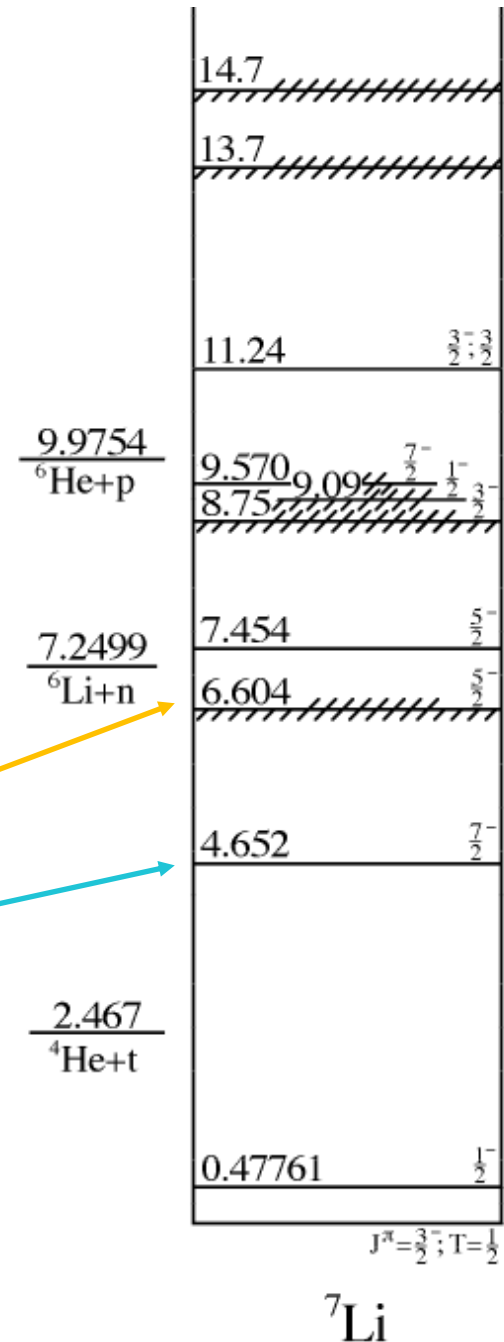
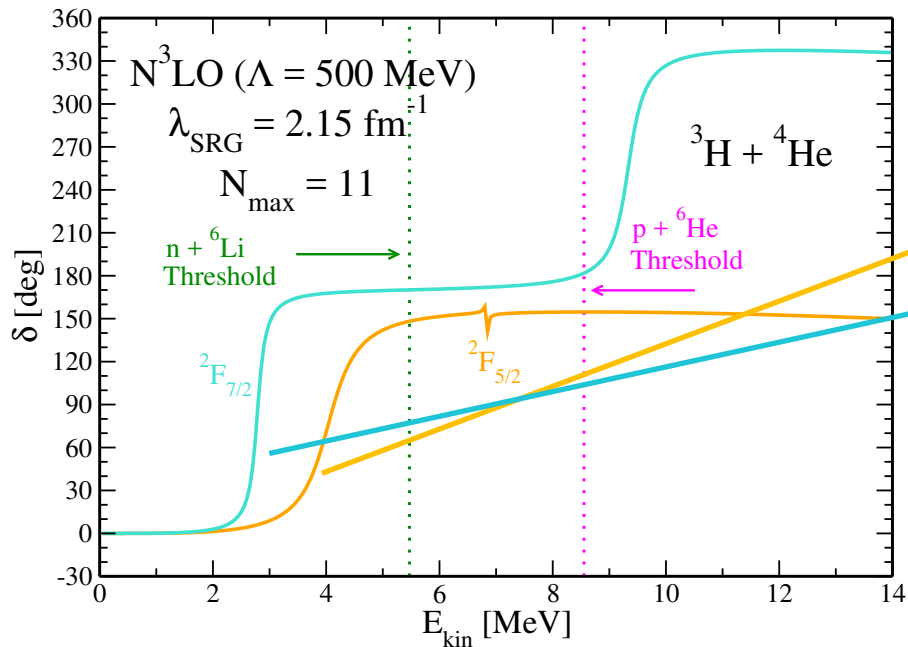
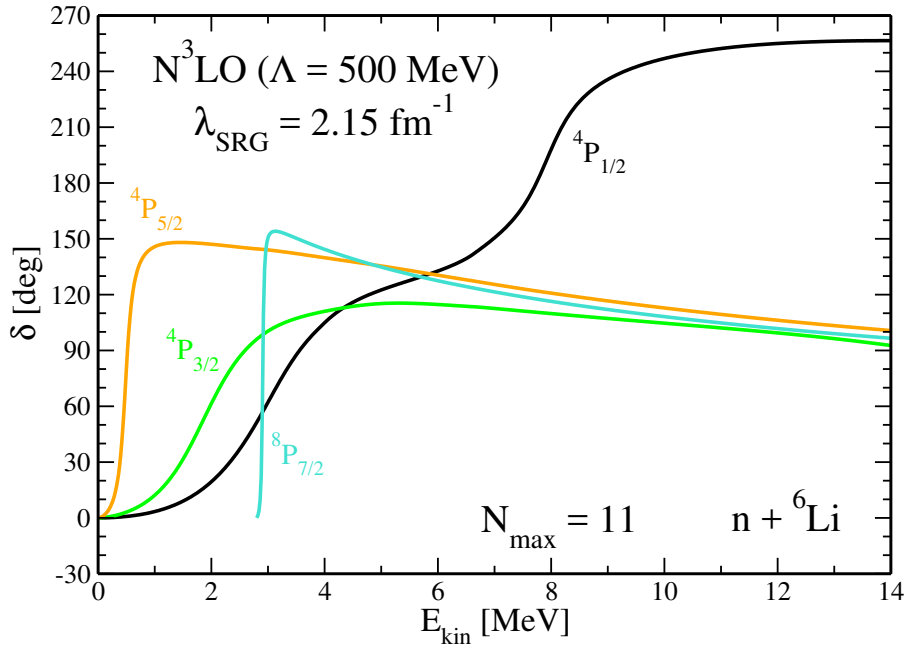
${}^7\text{Li}$ – Reproducing the energy spectrum



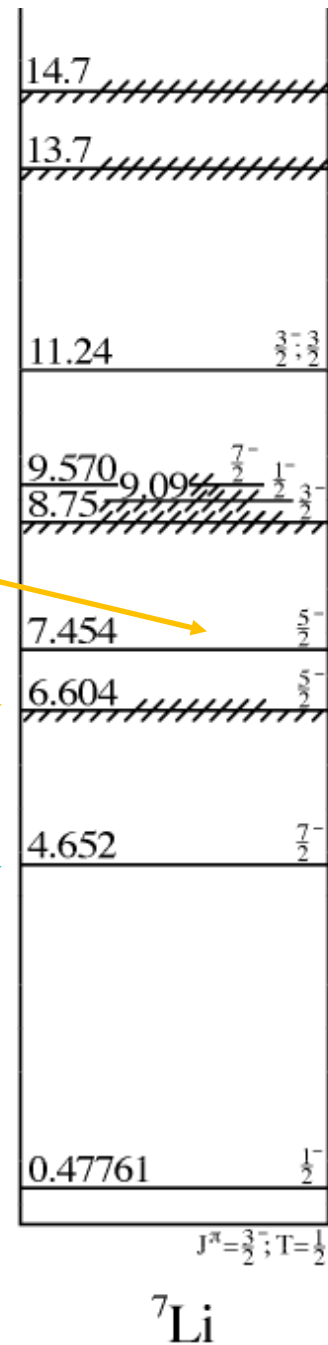
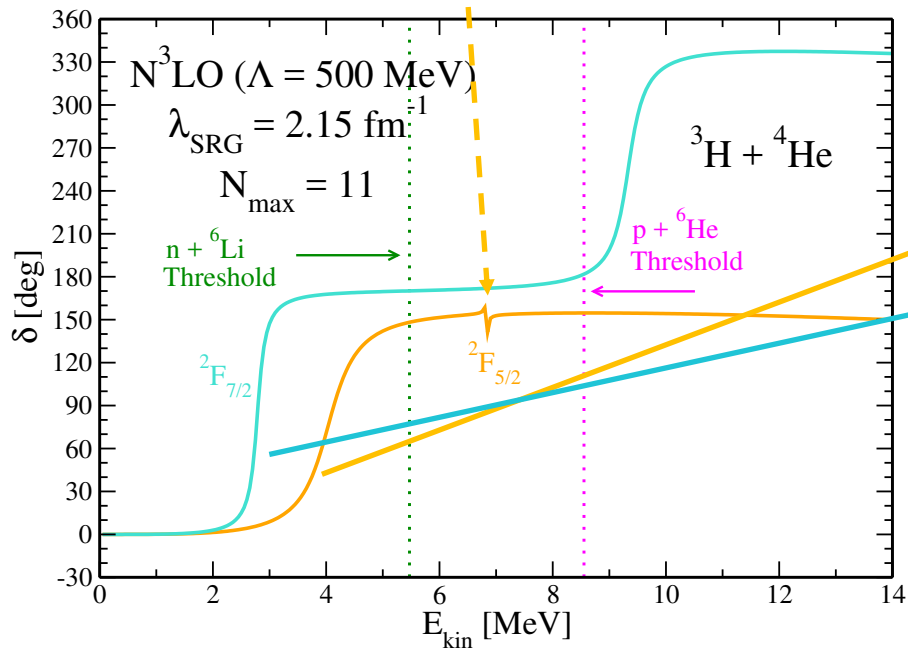
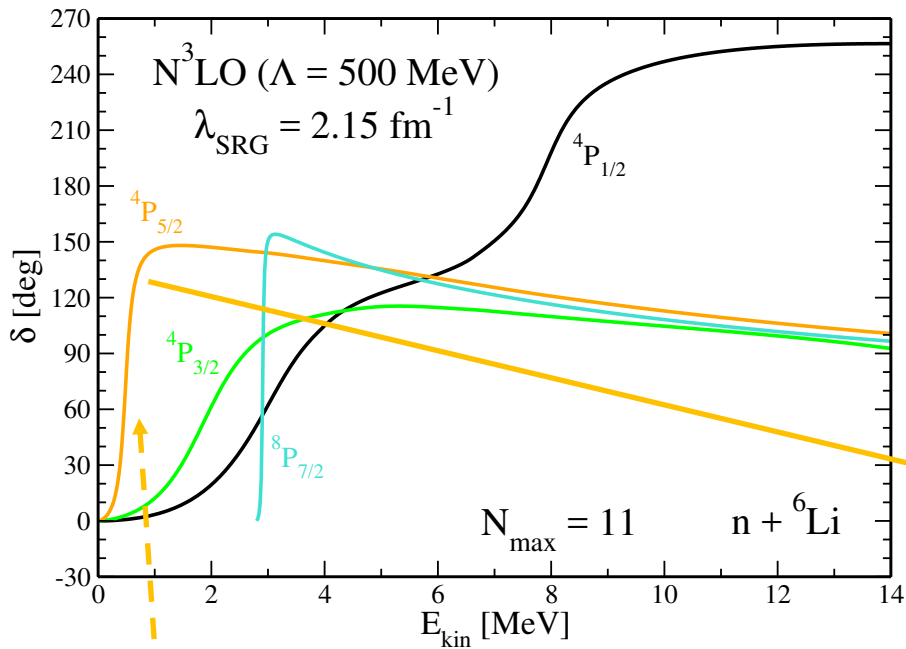
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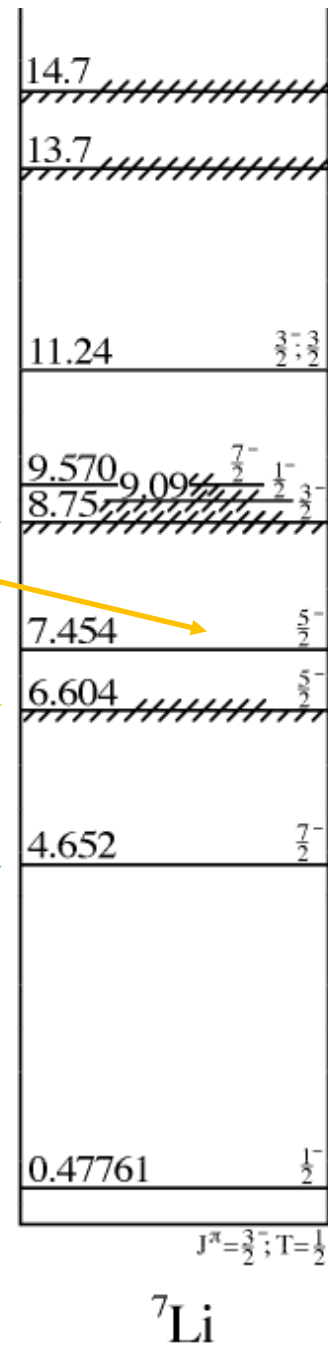
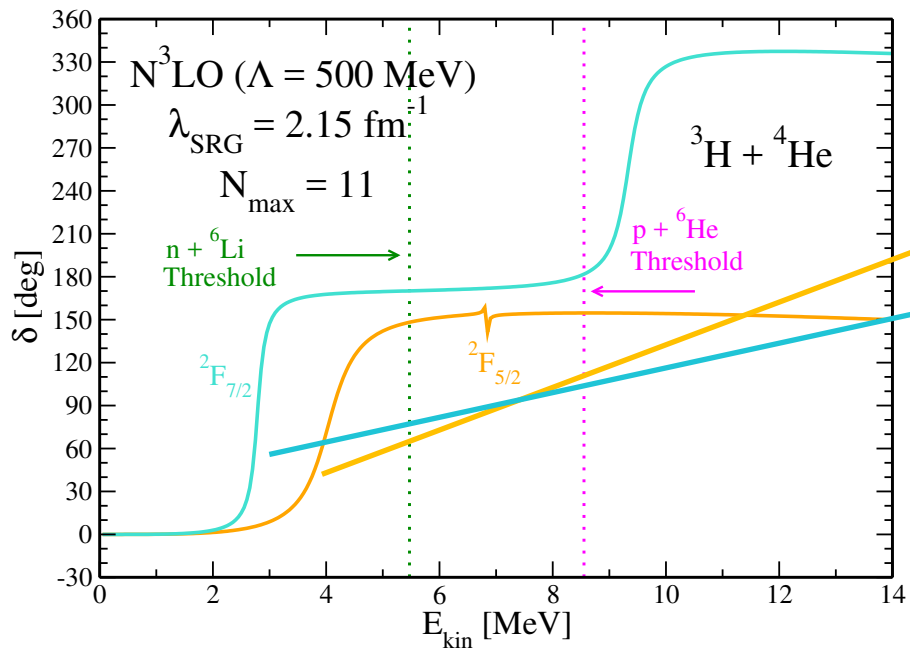
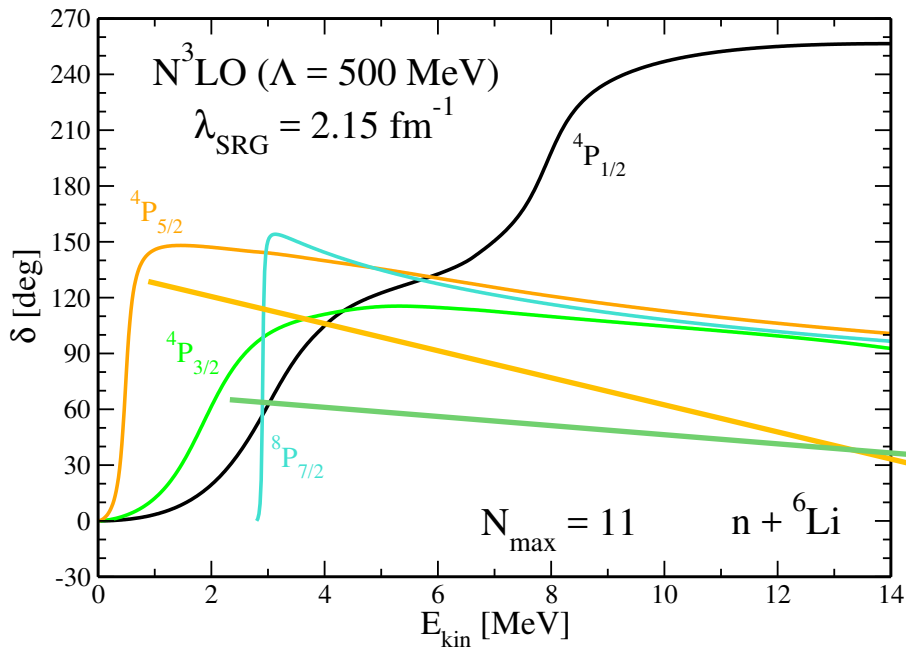
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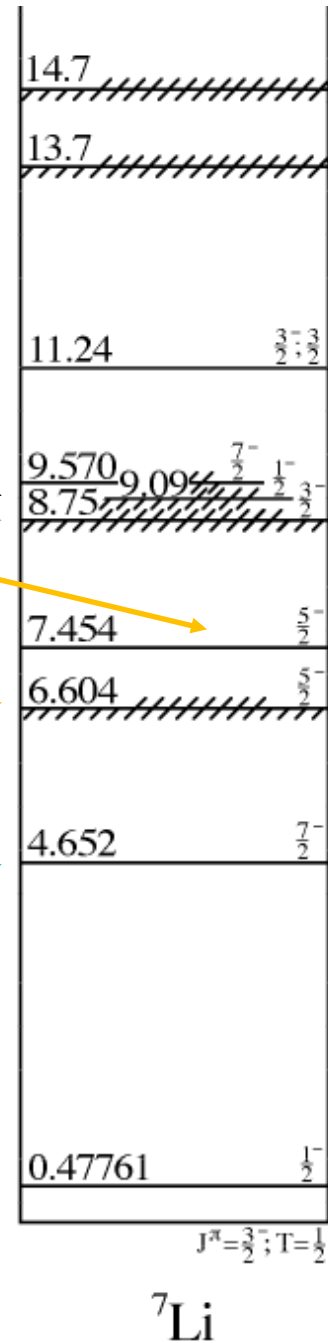
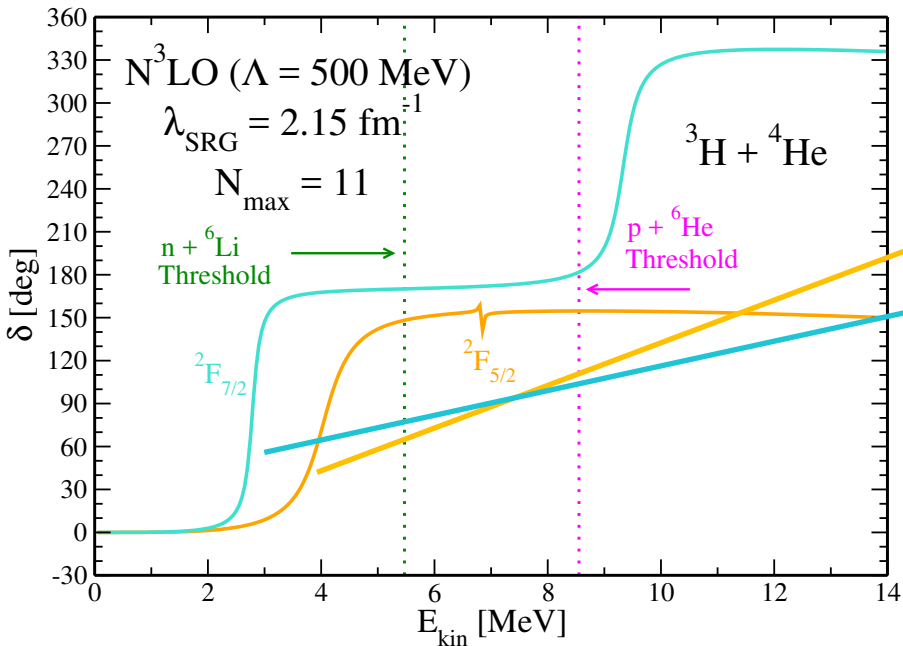
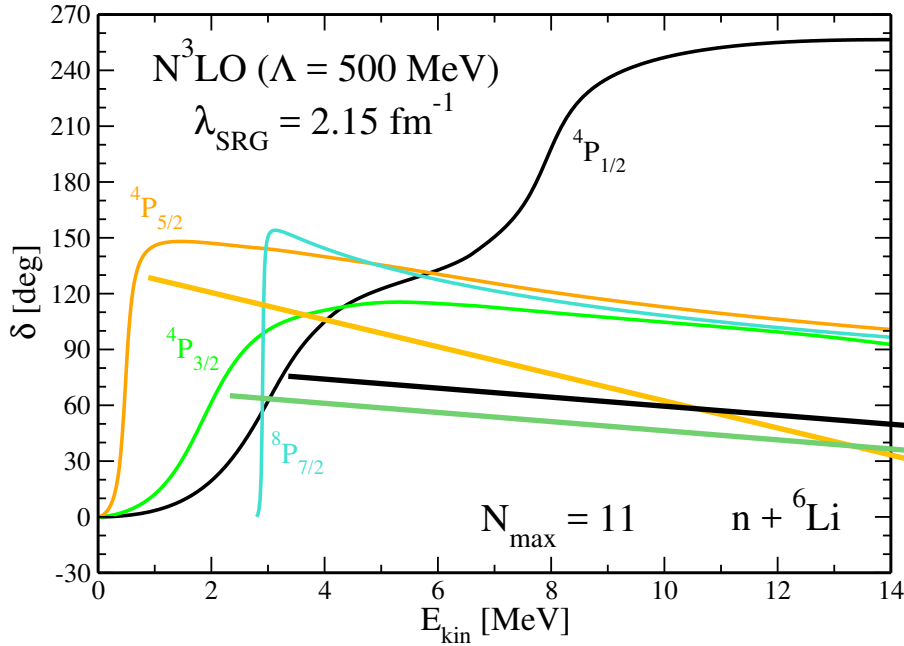
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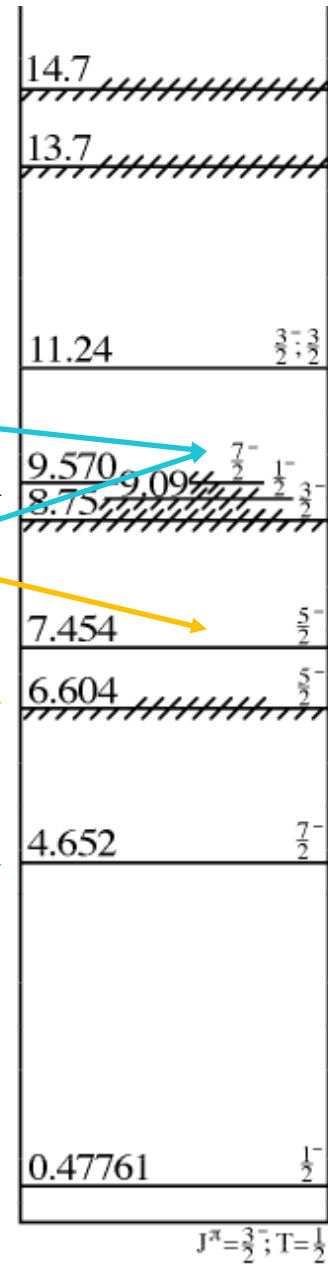
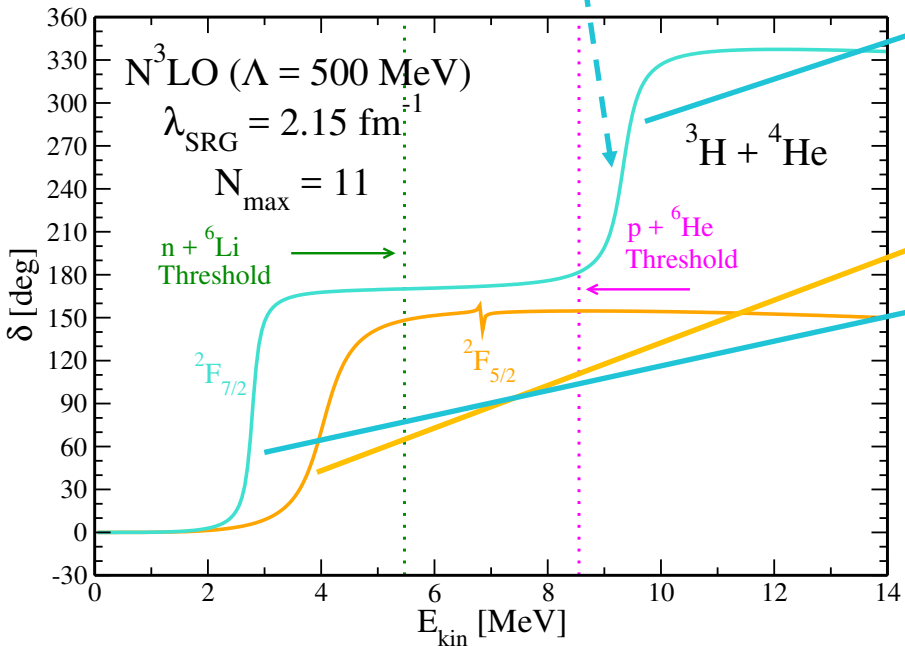
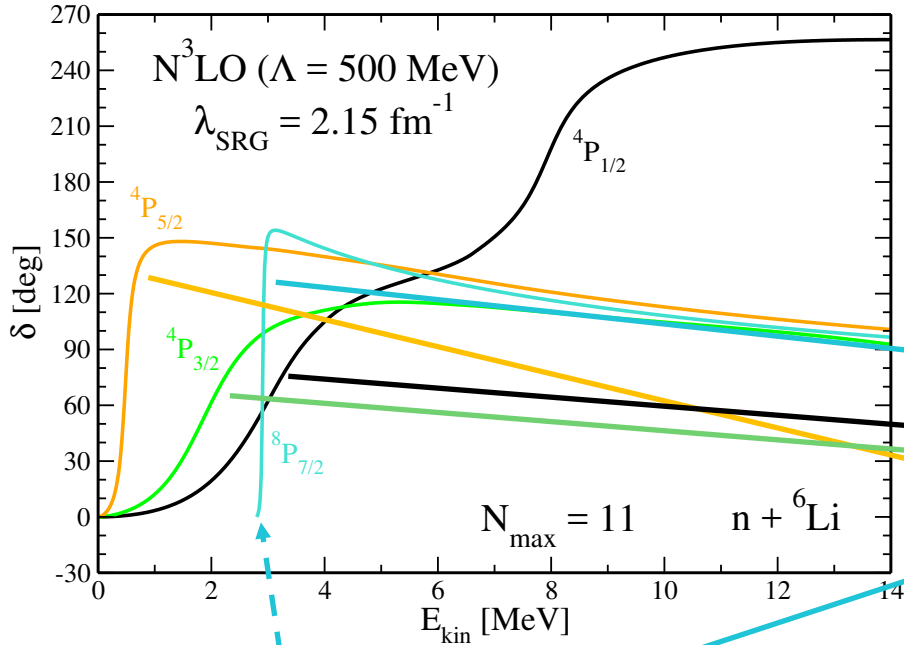
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${}^7\text{Li}$ – Reproducing the energy spectrum



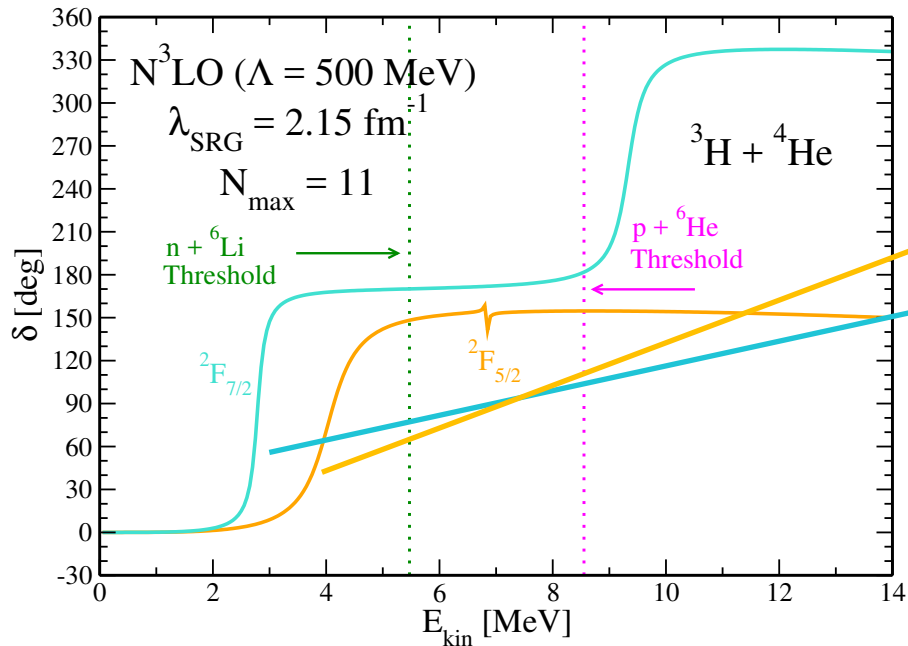
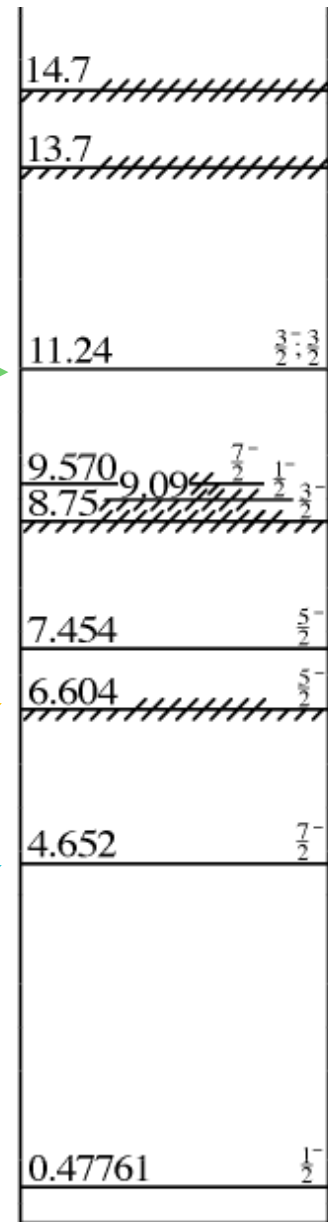
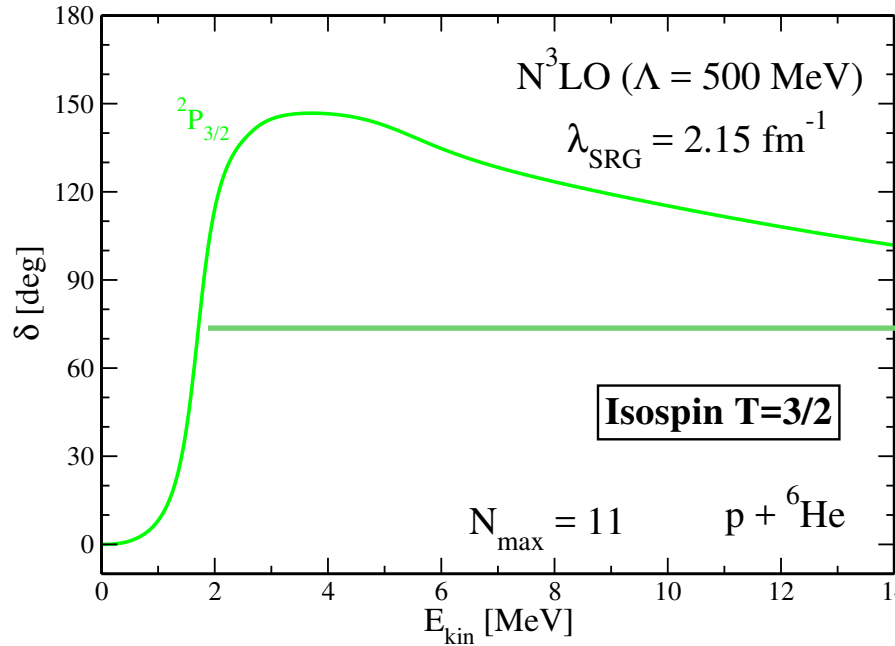
${}^7\text{Li}$ – Reproducing the energy spectrum



${}^7\text{Li}$

$J^\pi = \frac{3^-}{2}; T = \frac{1}{2}$

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



$\frac{2.467}{{}^4\text{He}+t}$

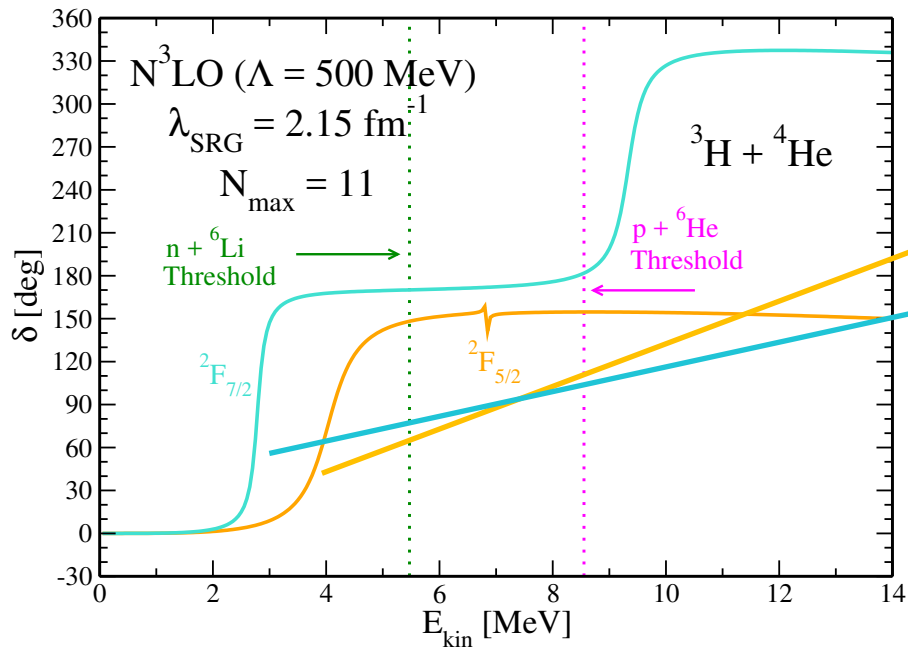
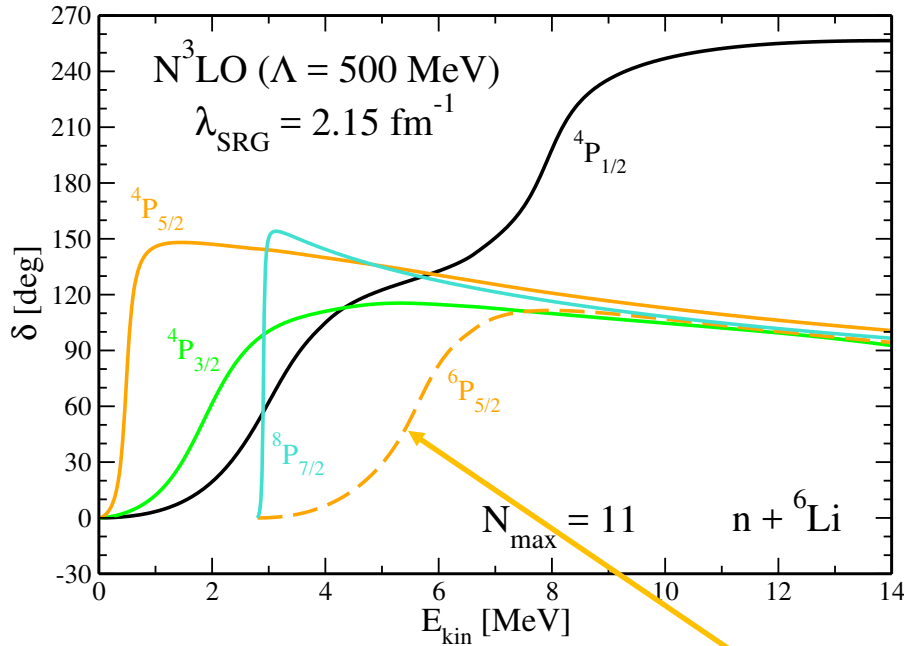
$\frac{9.9754}{{}^6\text{He}+p}$

$\frac{7.2499}{{}^6\text{Li}+n}$

$J^\pi = \frac{3}{2}^-; T = \frac{1}{2}$

${}^7\text{Li}$

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

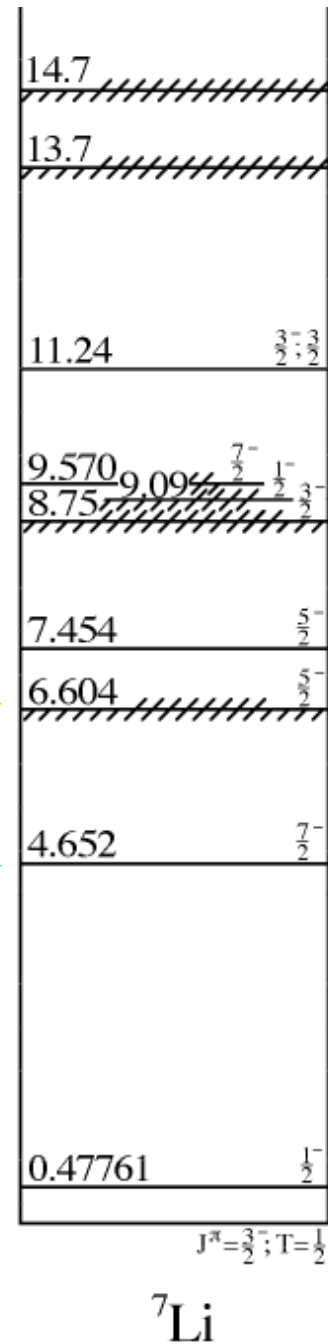


NEW

$$\frac{9.9754}{{}^6\text{He}+p}$$

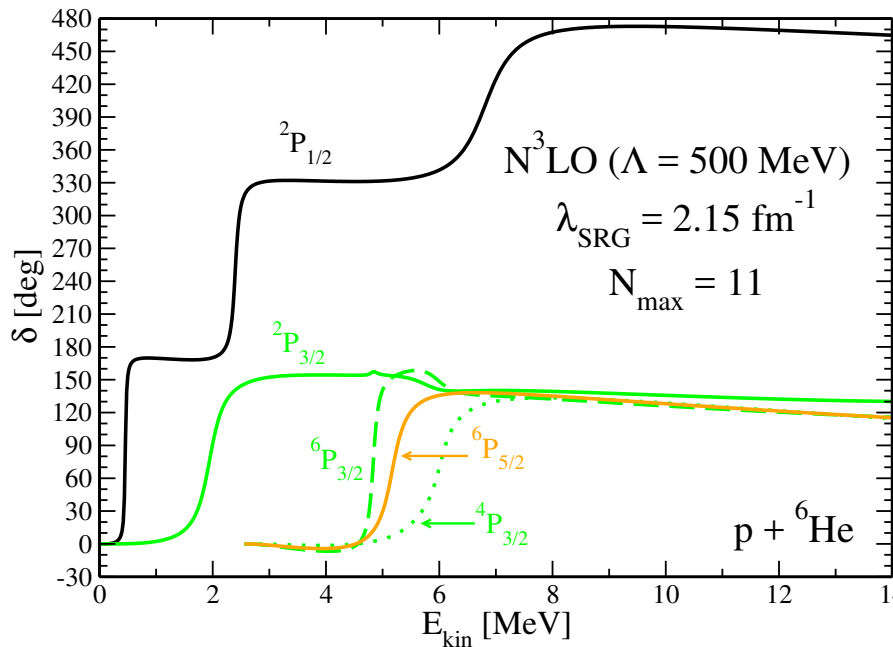
$$\frac{7.2499}{{}^6\text{Li}+n}$$

$$\frac{2.467}{{}^4\text{He}+t}$$



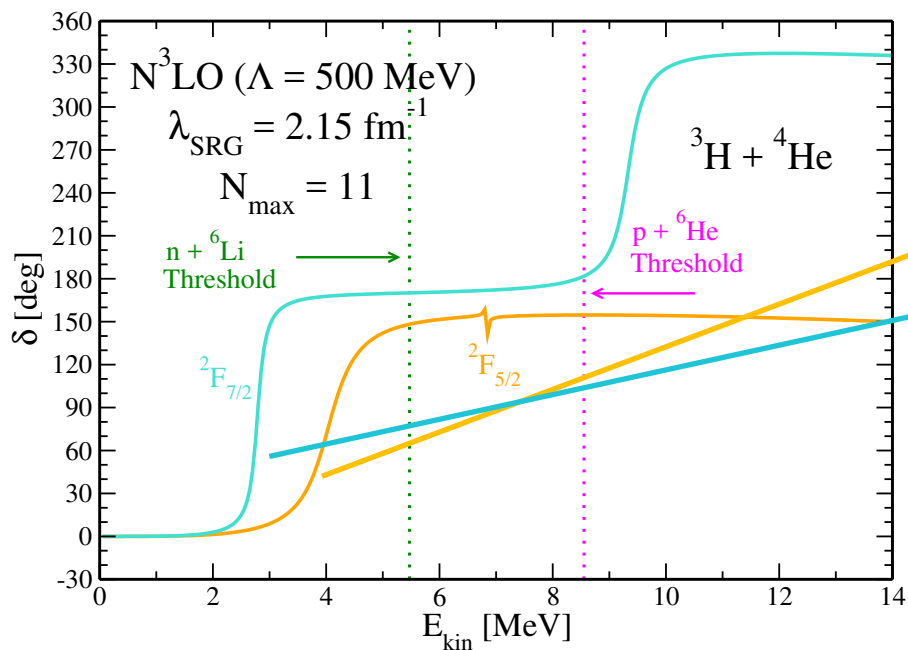
${}^7\text{Li}$ – New negative-parity states

5 new $T=1/2$ resonances

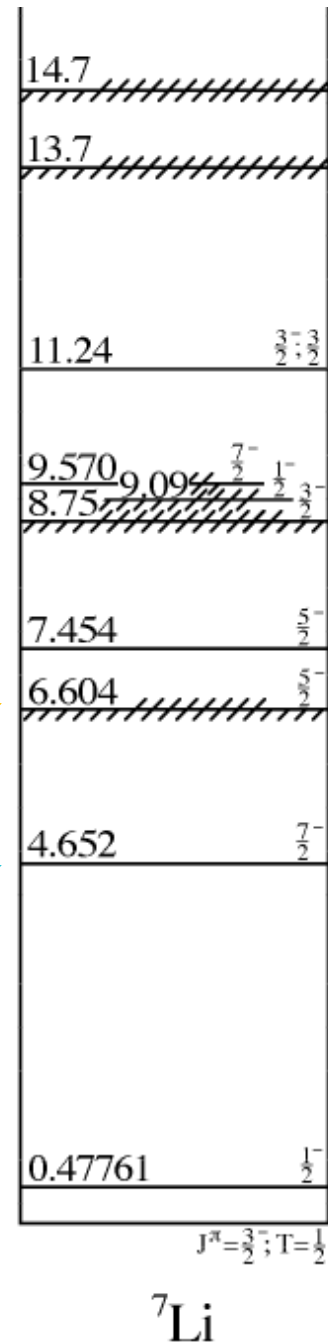


$\frac{9.9754}{{}^6\text{He}+p}$

$\frac{7.2499}{{}^6\text{Li}+n}$

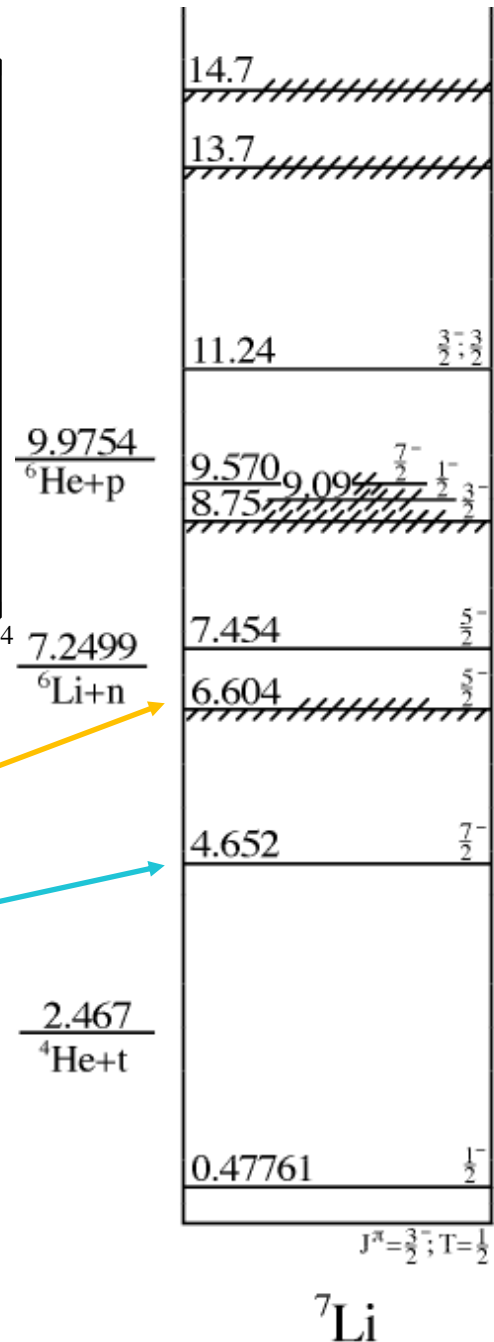
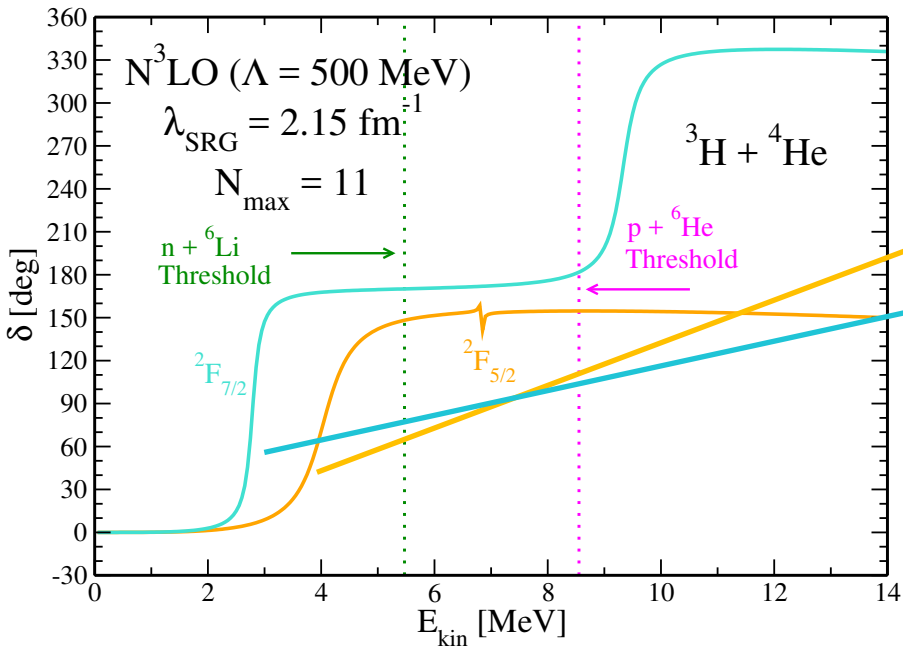
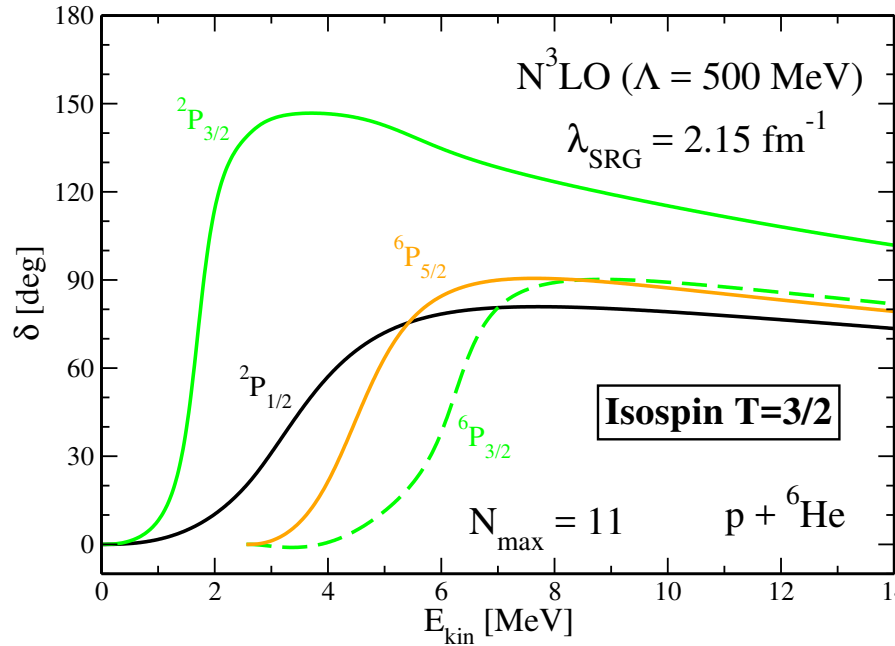


$\frac{2.467}{{}^4\text{He}+t}$

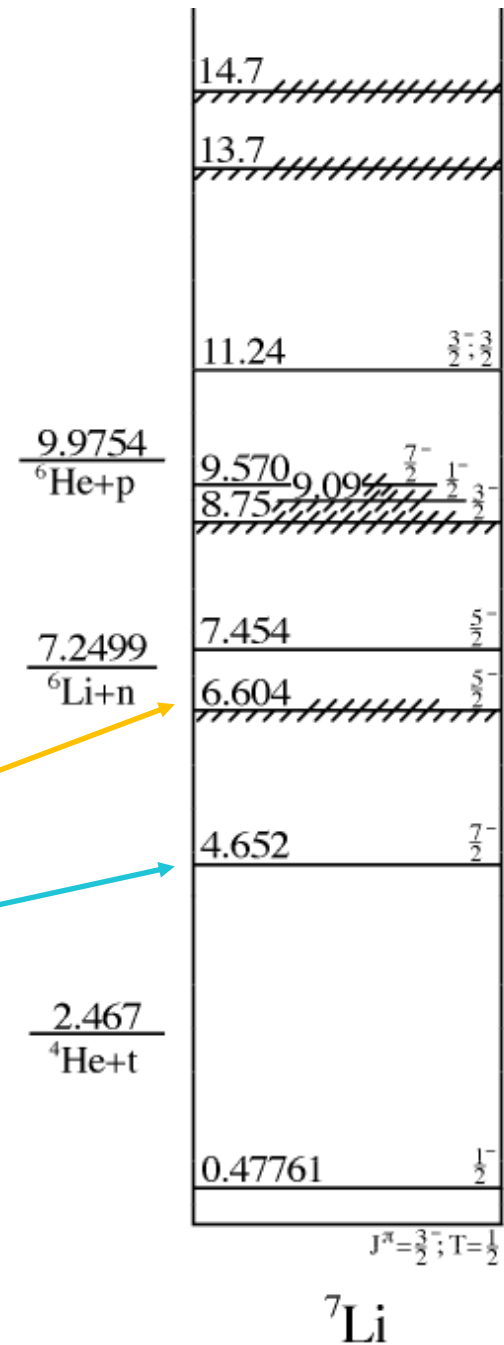
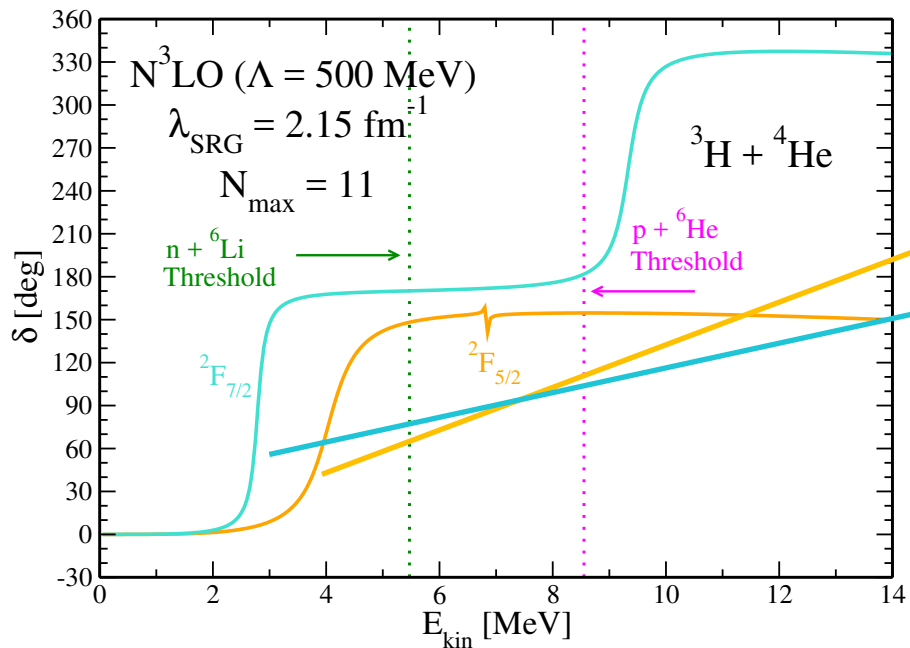
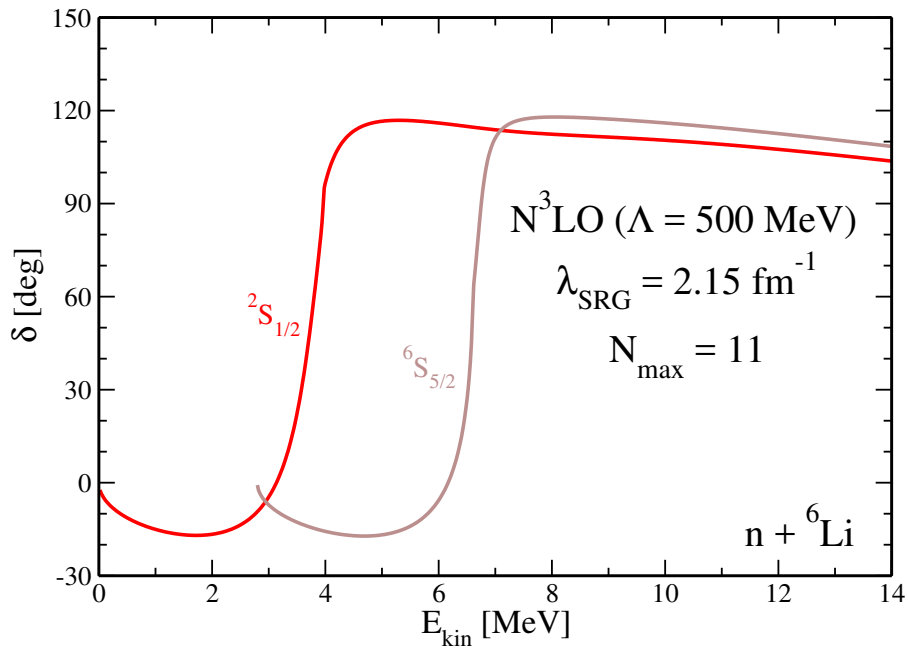


${}^7\text{Li}$ – New negative-parity states

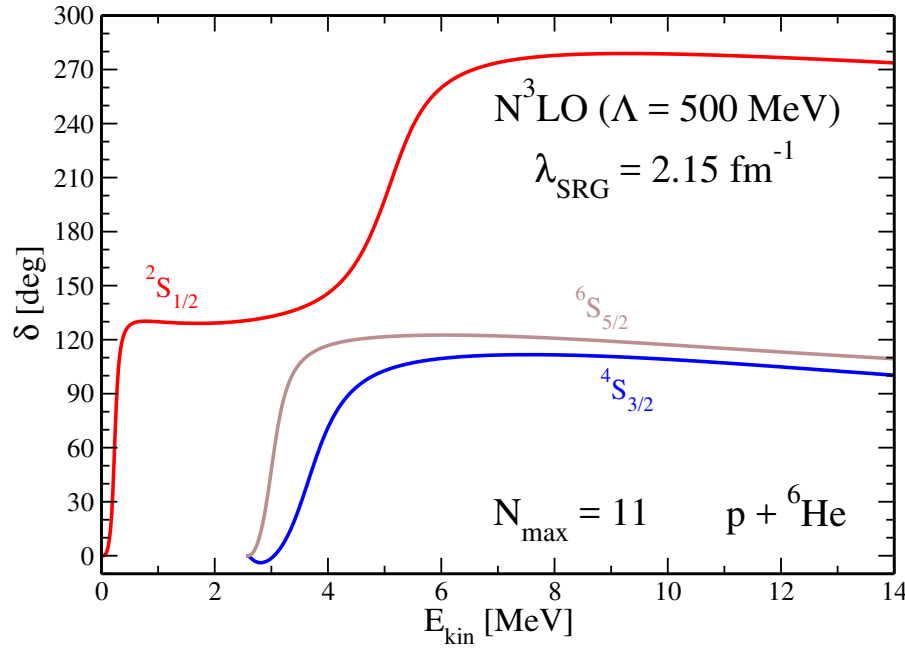
3 new $T=3/2$ resonances



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

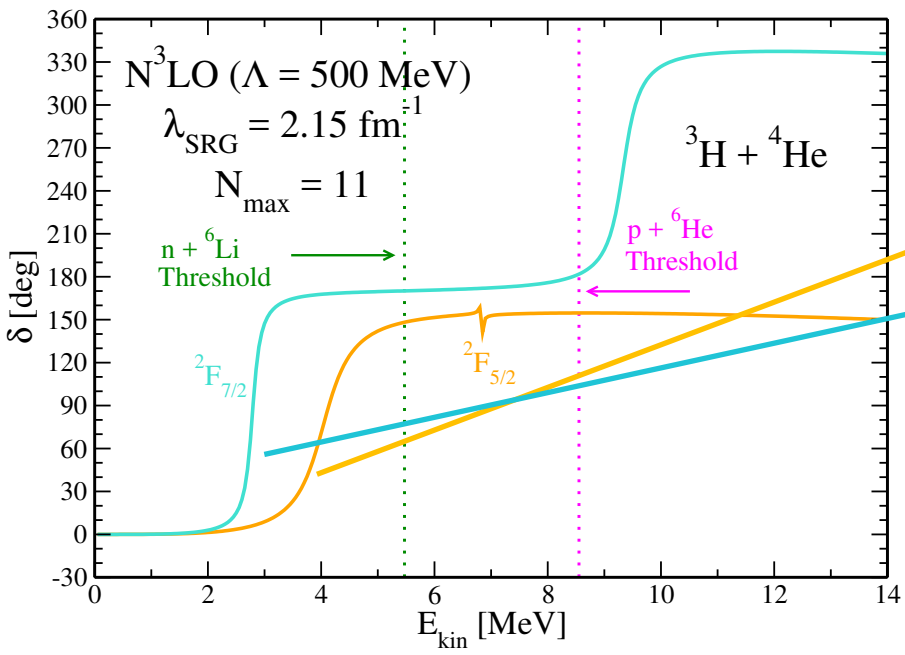


${}^7\text{Li}$ – New positive-parity states

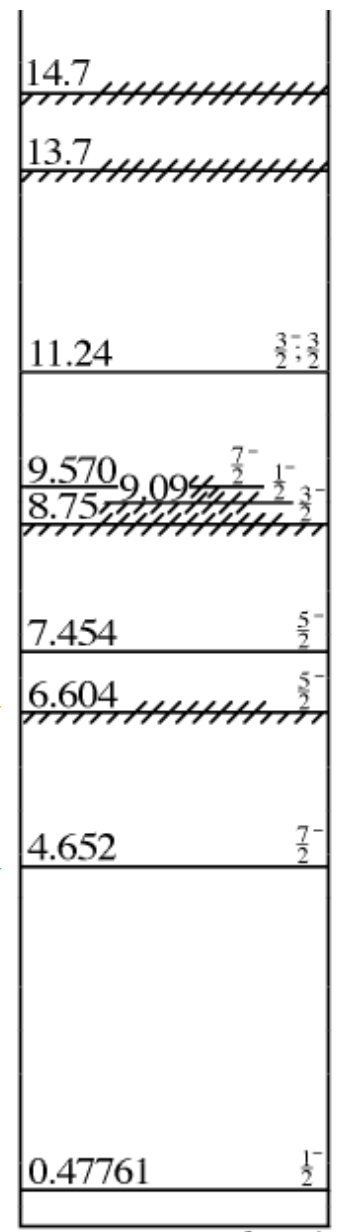


$\frac{9.9754}{{}^6\text{He}+p}$

$\frac{7.2499}{{}^6\text{Li}+n}$



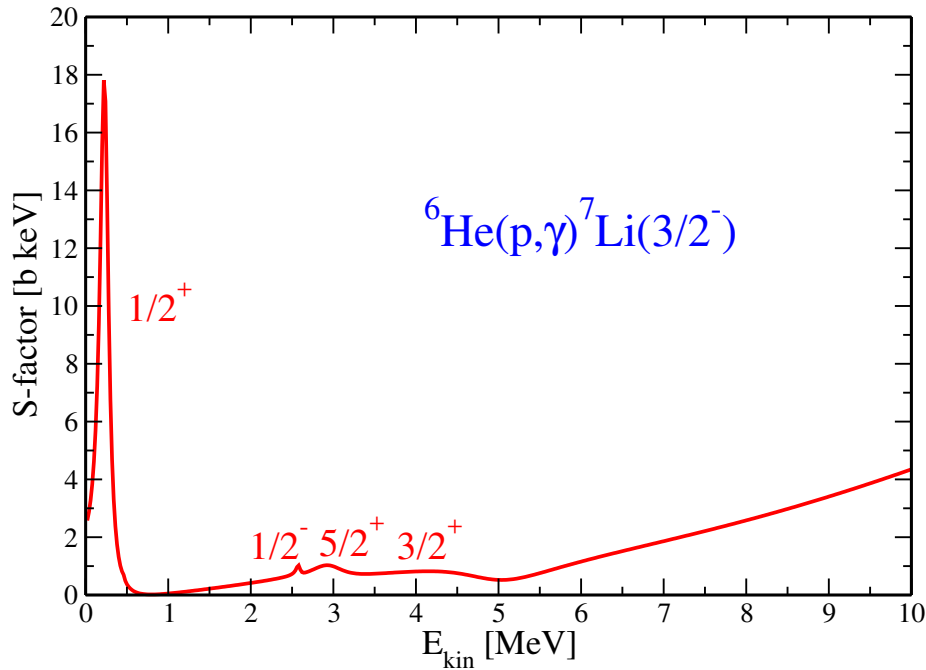
$\frac{2.467}{{}^4\text{He}+t}$



$J^\pi = \frac{3^-}{2}; T = \frac{1}{2}$

${}^7\text{Li}$

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

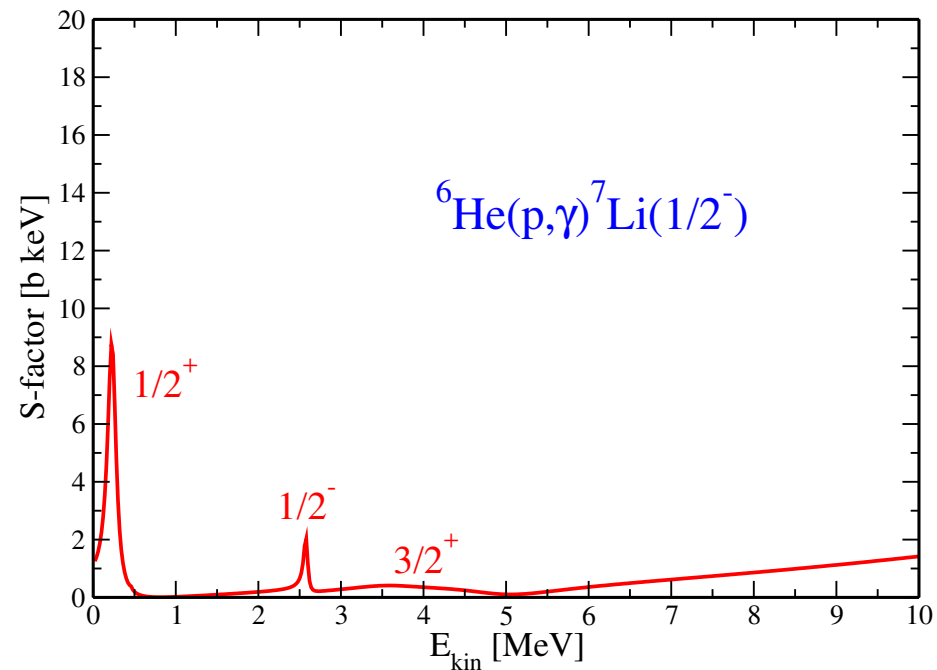


Cross section and S-factor

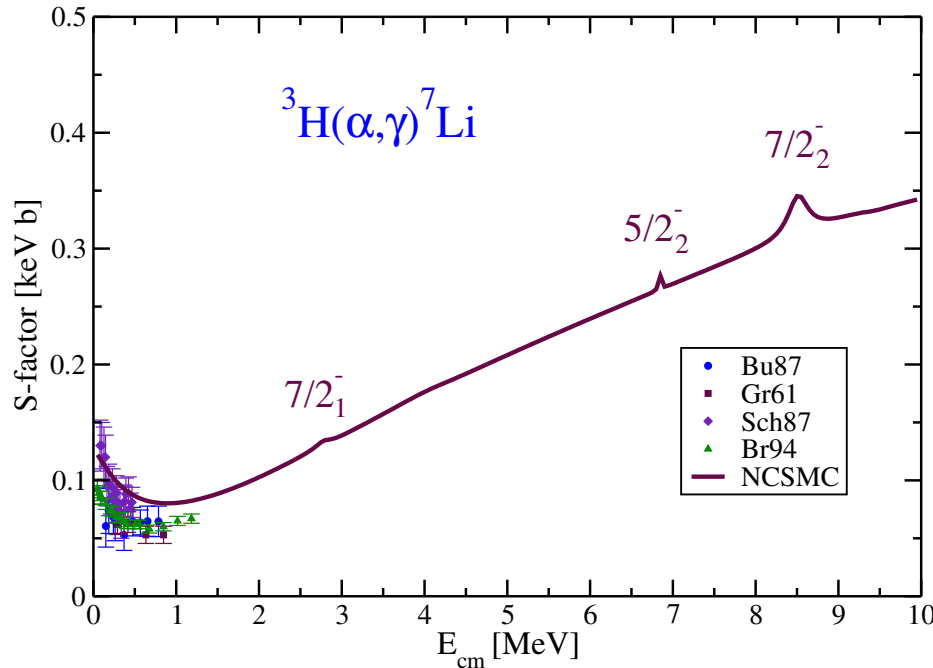
$$\sigma(E) = S(E)E^{-1} \exp[-2\pi\eta(E)]$$

Sommerfeld parameter

$$\eta(E) = \frac{Z_1 Z_2 e^2}{\hbar v}$$



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

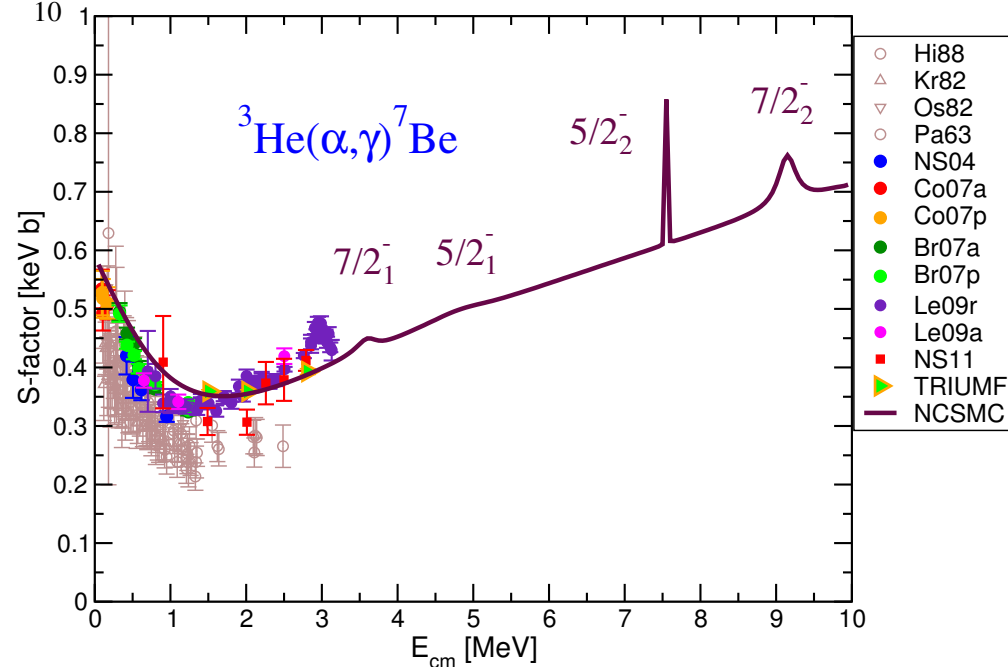


Cross section and S-factor

$$\sigma(E) = S(E)E^{-1} \exp[-2\pi\eta(E)]$$

Sommerfeld parameter

$$\eta(E) = \frac{Z_1 Z_2 e^2}{\hbar v}$$



2.

**Microscopic optical potentials for
intermediate energies**

Motivation

Nuclear reaction theory relies on reducing the many-body problem to a problem with few degrees of freedom:
optical potentials.

Phenomenological

Unfortunately, currently used optical potentials for low-energy reactions are phenomenological, and primarily constrained by elastic scattering.

Unreliable when extrapolated beyond their fitted range in energy and nuclei

Microscopical

Existing microscopic optical potentials are *usually* developed in a high-energy regime (≥ 100 MeV) and not applicable for lower energy reactions.

No fitting

Statement of the problem

Lippmann-Schwinger (LS) equation for the nucleon-nucleus transition amplitude

$$T = V + VG_0(E)T$$

All two nucleon interactions

$$V = \sum_{i=1}^A v_{0i}$$

Green function propagator

$$G_0(E) = (E - H_0 + i\epsilon)^{-1}$$

where

$$H_0 = h_0 + H_A$$

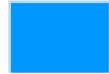
h_0 kinetic term of the projectile

$$H_A |\Phi_A\rangle = E_A |\Phi_A\rangle \quad \begin{array}{l} \text{target} \\ \text{Hamiltonian} \end{array}$$

Statement of the problem

Lippmann-Schwinger (LS) equation for the nucleon-nucleus transition amplitude

$$T = V + VG_0(E)T$$



Let's introduce the **optical potential U**



$$T = U + UG_0(E)PT$$

$$U = V + VG_0(E)QU$$

Projection operators

$$P + Q = 1$$

$$[G_0, P] = 0$$

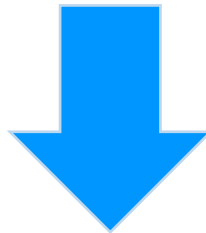
In the case of elastic scattering,
 P projects onto the elastic channel

$$P = \frac{|\Phi_A\rangle \langle \Phi_A|}{\langle \Phi_A | \Phi_A \rangle}$$

Statement of the problem

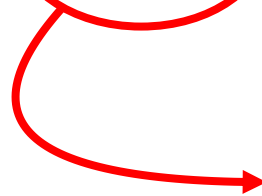
Lippmann-Schwinger (LS) equation for the nucleon-nucleus transition amplitude

$$T = V + VG_0(E)T$$



Transition amplitude T for elastic scattering

$$T_{\text{el}} \equiv PTP = PUP + PUPG_0(E)T_{\text{el}}$$

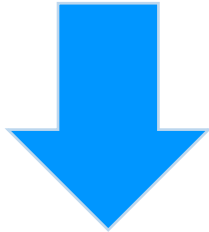


we need to calculate PUP

Statement of the problem

Lippmann-Schwinger (LS) equation for the nucleon-nucleus elastic transition amplitude

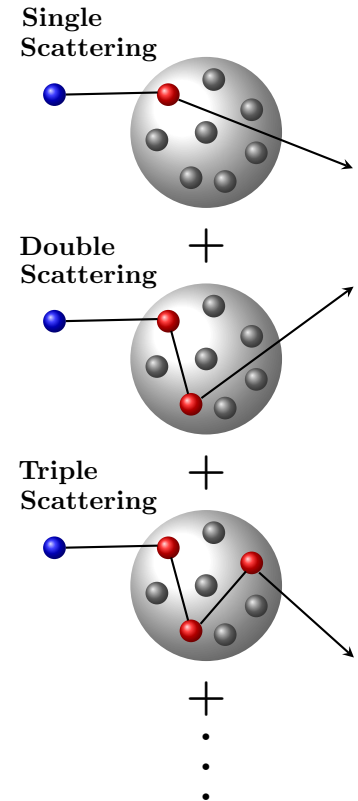
$$T_{\text{el}} = PUP + PUPG_0(E)T_{\text{el}}$$



Spectator expansion for U

Chinn, Elster, Thaler, Weppner, PRC **52**, 1992 (1995)

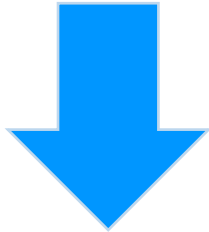
$$U = \sum_{i=1}^A \tau_i + \sum_{i,j \neq i}^A \tau_{ij} + \sum_{i,j \neq i, k \neq i,j}^A \tau_{ijk} + \dots$$



Single scattering approximation

Lippmann-Schwinger (LS) equation for the nucleon-nucleus elastic transition amplitude

$$T_{\text{el}} = PUP + PUPG_0(E)T_{\text{el}}$$

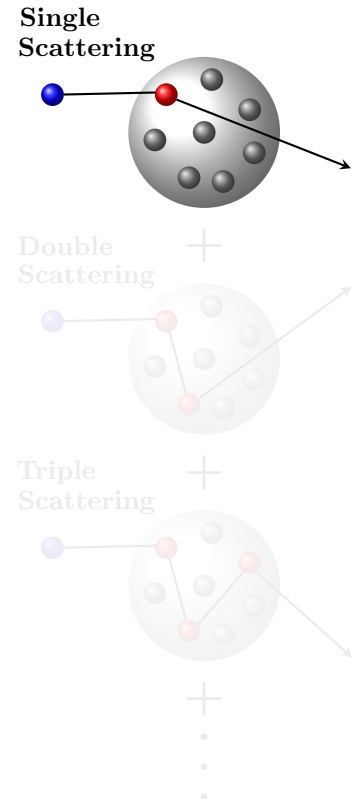


Spectator expansion for U

Chinn, Elster, Thaler, Weppner, PRC **52**, 1992 (1995)

Single scattering approximation

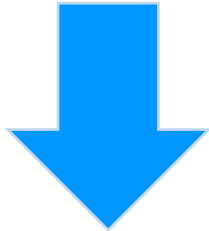
$$U = \sum_{i=1}^A \tau_i + \sum_{i,j \neq i}^A \tau_{ij} + \sum_{i,j \neq i, k \neq i,j}^A \tau_{ijk} + \dots$$



Impulse approximation

Lippmann-Schwinger (LS) equation for the nucleon-nucleus elastic transition amplitude

$$T_{\text{el}} = PUP + PUPG_0(E)T_{\text{el}}$$



Spectator expansion for U

Chinn, Elster, Thaler, Weppner, PRC **52**, 1992 (1995)

$$\tau_i \approx t_{0i}$$

Impulse approximation

$$U = \sum_{i=1}^A t_{0i} \left\{ \begin{array}{l} t_{0i} = v_{0i} + v_{0i}g_i t_{0i} \\ g_i = \frac{1}{E - h_0 - h_i + i\epsilon} \end{array} \right.$$

The interaction between the projectile and the target nucleon is considered as free

The first-order optical potential

$$U(\mathbf{q}, \mathbf{K}; E) = \sum_{\alpha=n,p} \int d^3 \mathbf{P} \eta(\mathbf{P}, \mathbf{q}, \mathbf{K}) t_{p\alpha} \left[\mathbf{q}, \frac{1}{2} \left(\frac{A+1}{A} \mathbf{K} - \mathbf{P} \right); E \right]$$

$$\times \rho_{\alpha} \left(\mathbf{P} - \frac{A-1}{2A} \mathbf{q}, \mathbf{P} + \frac{A-1}{2A} \mathbf{q} \right) \quad \mathbf{q} = \mathbf{k}' - \mathbf{k}$$

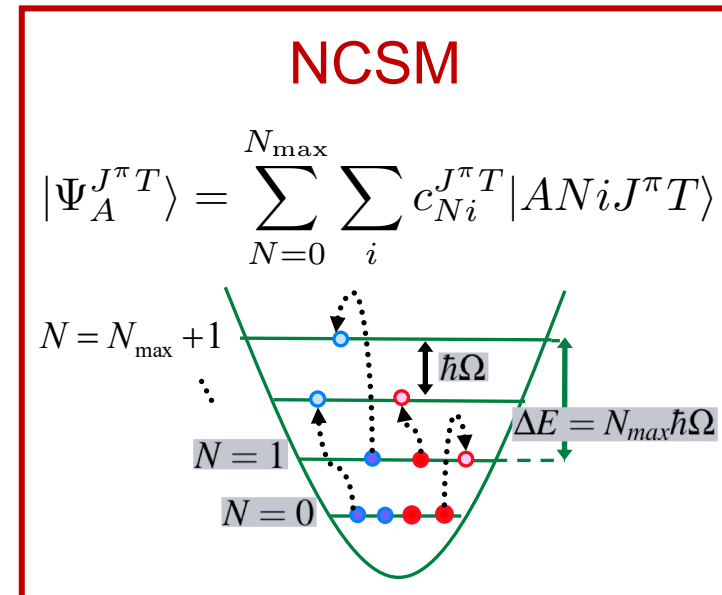
$$\mathbf{K} = \frac{1}{2} (\mathbf{k}' + \mathbf{k})$$

Basic ingredients

- Nucleon-nucleon scattering matrix t_{NN}
- Non-local nuclear densities

$$\rho_{\text{op}} = \sum_{i=1}^A \delta(\mathbf{r} - \mathbf{r}_i) \delta(\mathbf{r}' - \mathbf{r}'_i)$$

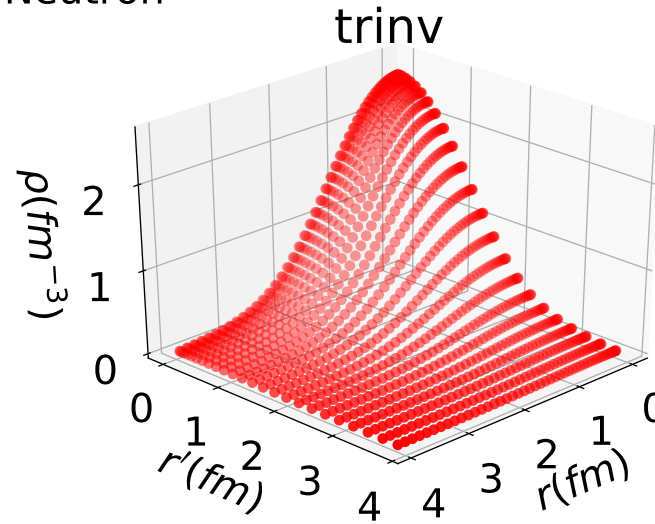
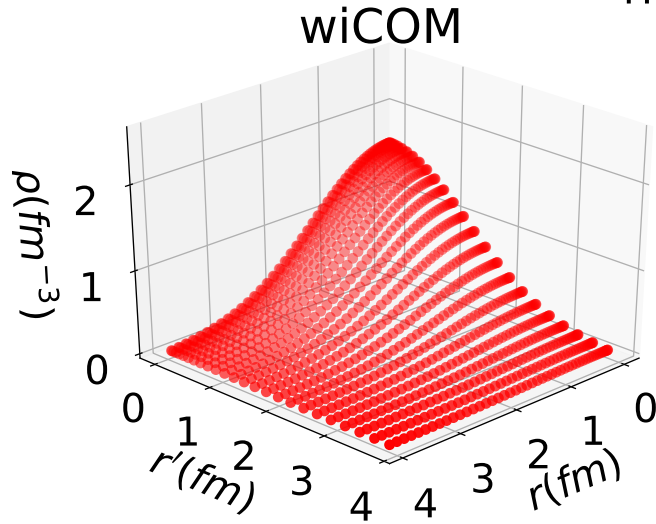
The matrix elements between a general initial and final state are obtained from the NCSM
 Extension of: Navratil, PRC **70**, 014317 (2004)



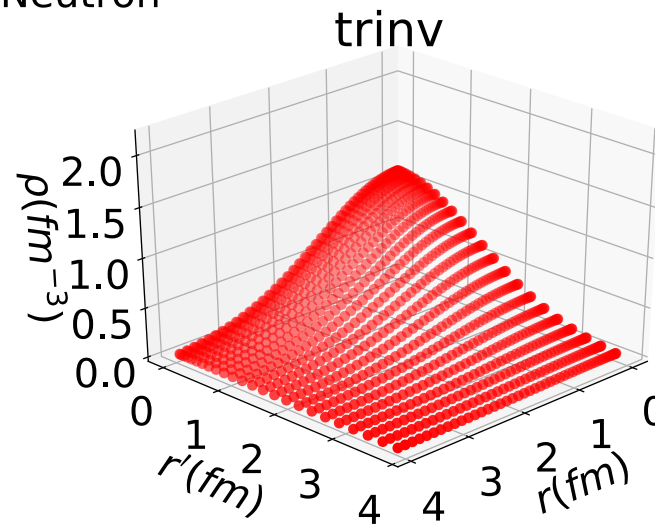
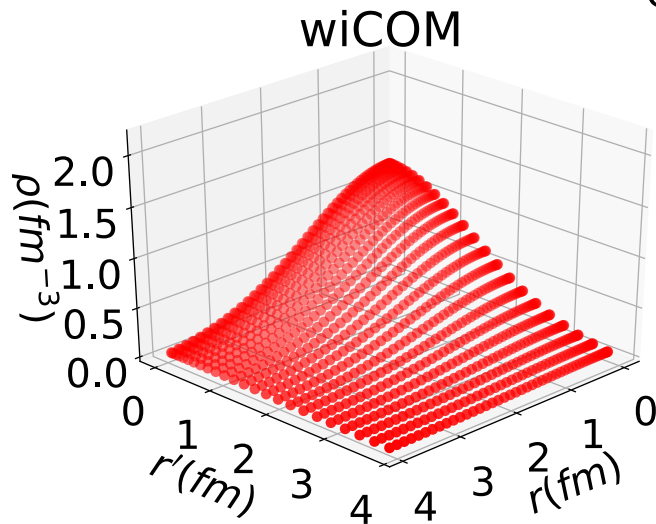
Non-local densities

Gennari, Vorabbi, Calci, Navratil, PRC **97**, 034619 (2018)

^4He Neutron

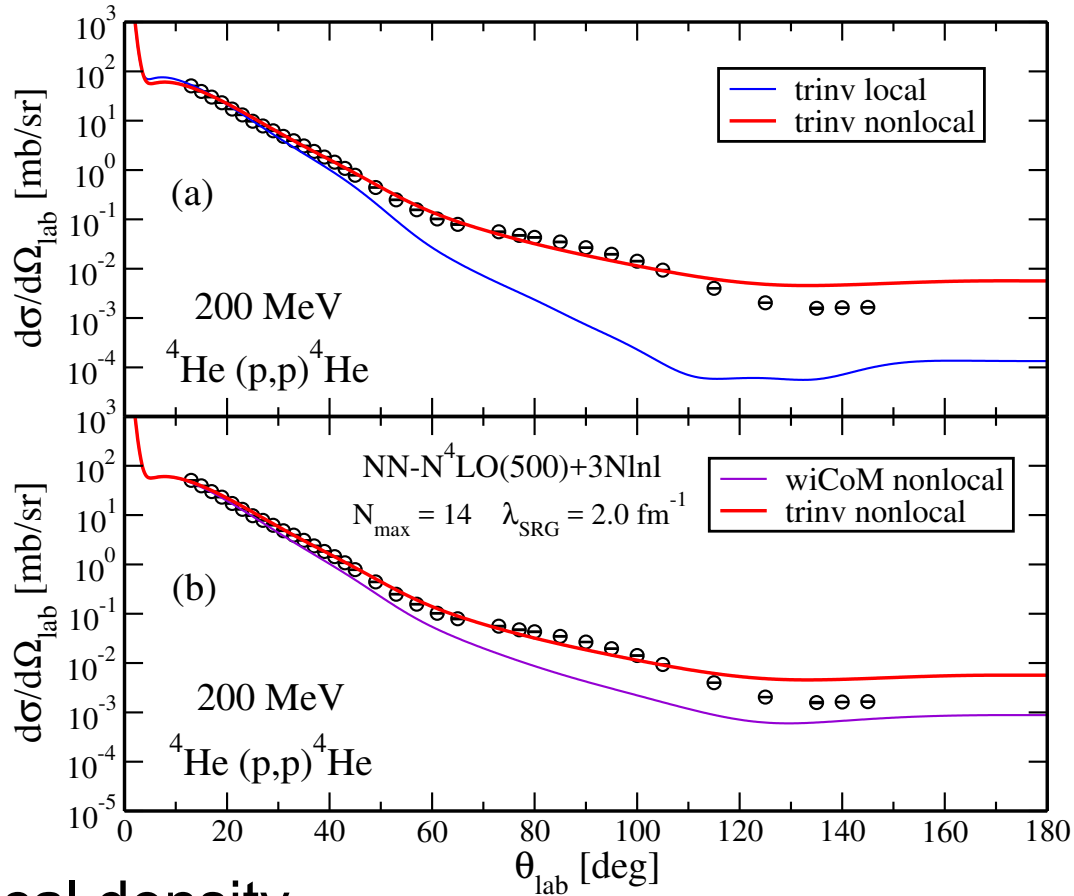


^{12}C Neutron



Scattering observables – Stable nuclei

Gennari, Vorabbi, Calci, Navratil, PRC **97**, 034619 (2018)



FF from local density

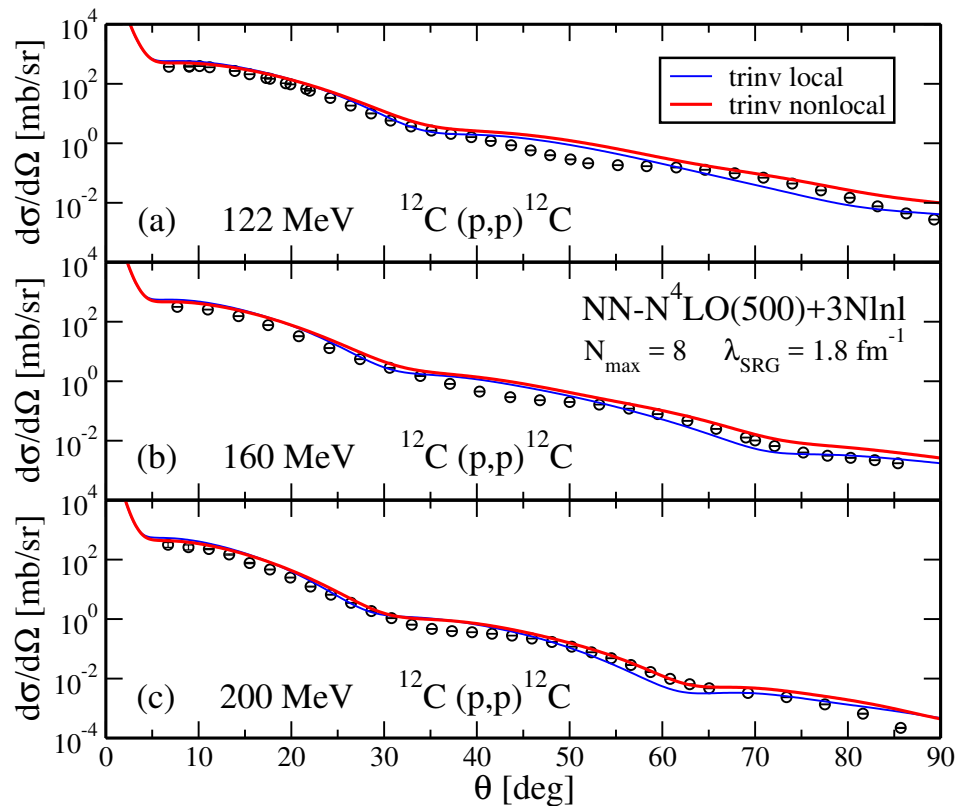
$$\rho_\alpha(q) = 4\pi \int_0^\infty dr r^2 j_0(qr) \rho_\alpha(r)$$

Navratil, PRC **70**, 014317 (2004)

Factorized optical potential

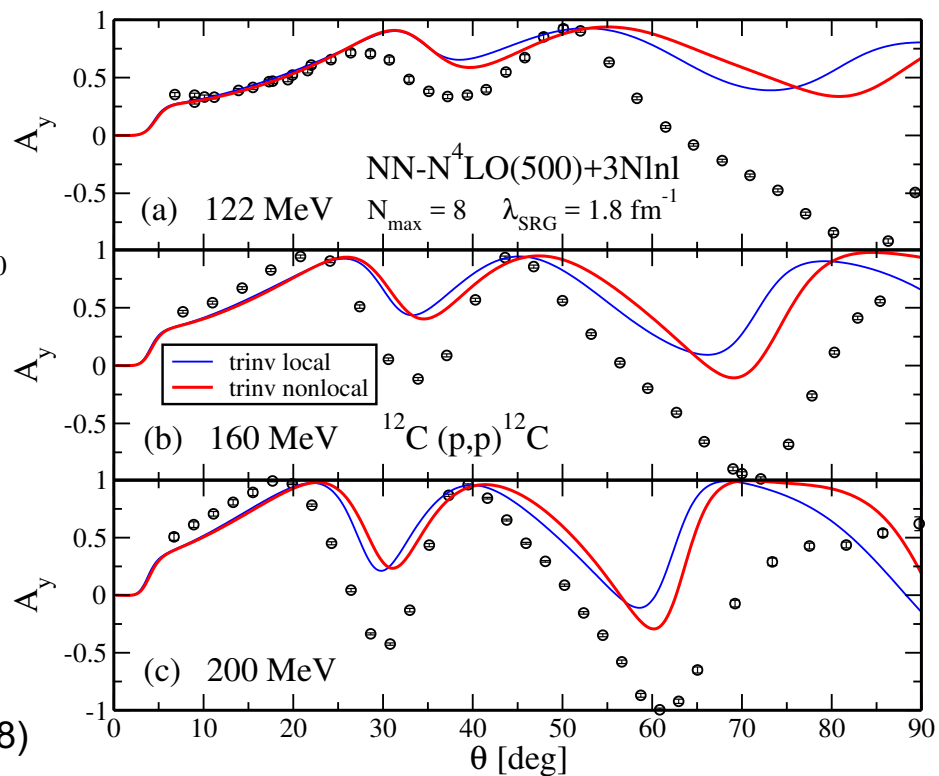
$$U(\mathbf{q}, \mathbf{K}; E) \sim \sum_{\alpha=n,p} t_{p\alpha} \left[\mathbf{q}, \frac{A+1}{2A} \mathbf{K}; E \right] \rho_\alpha(q)$$

Scattering observables – Stable nuclei

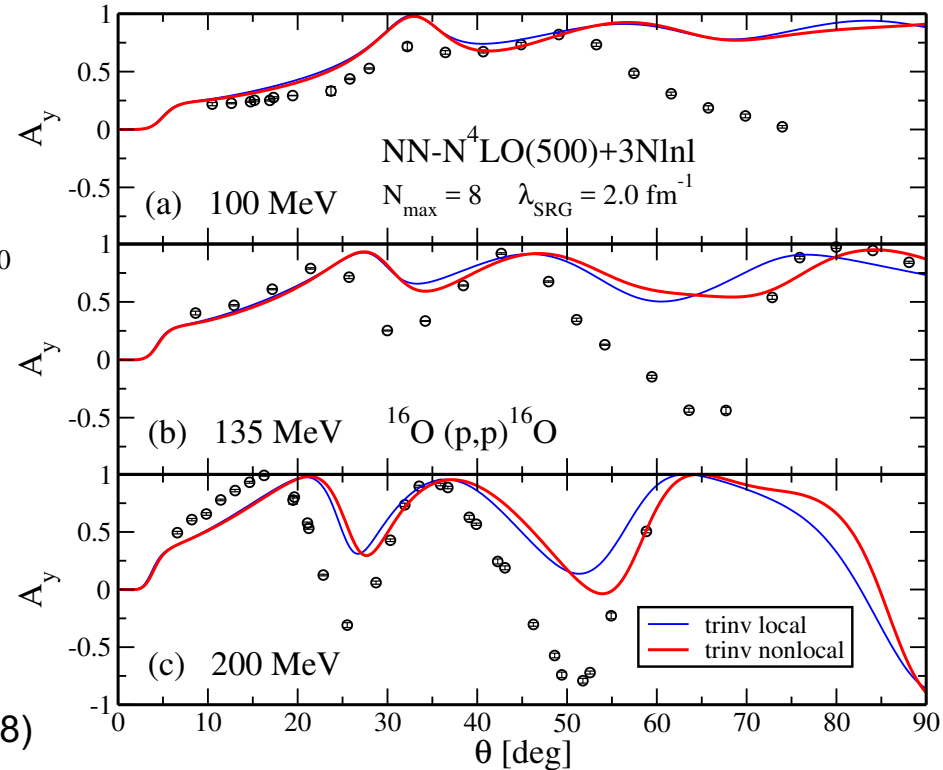
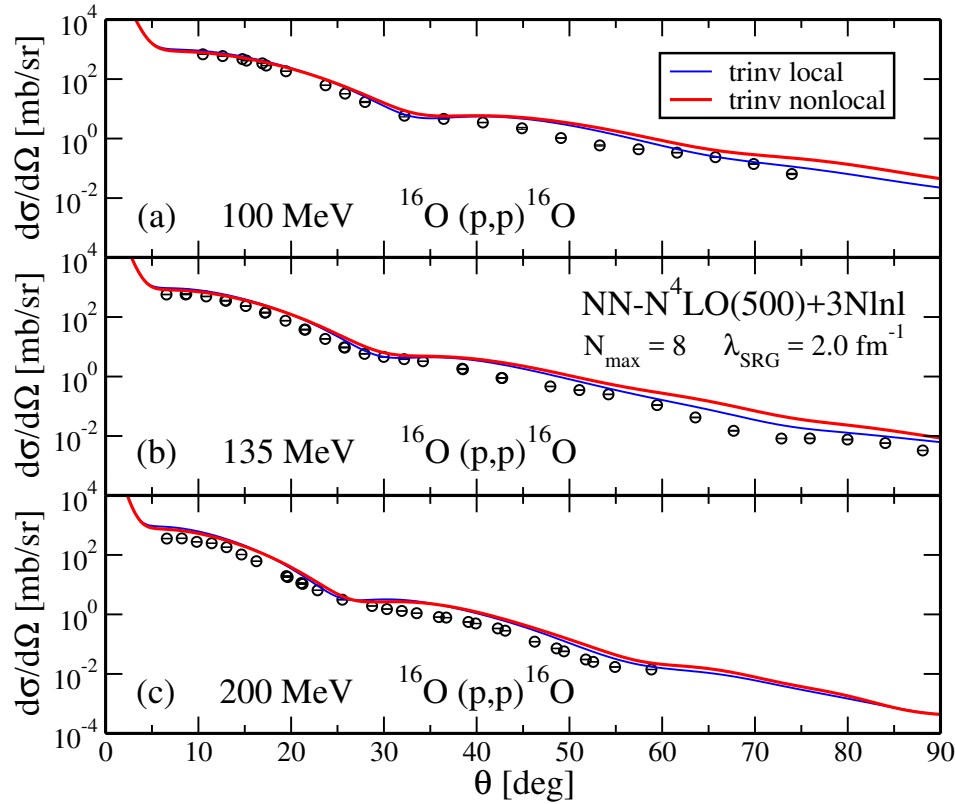


Good description of differential cross sections

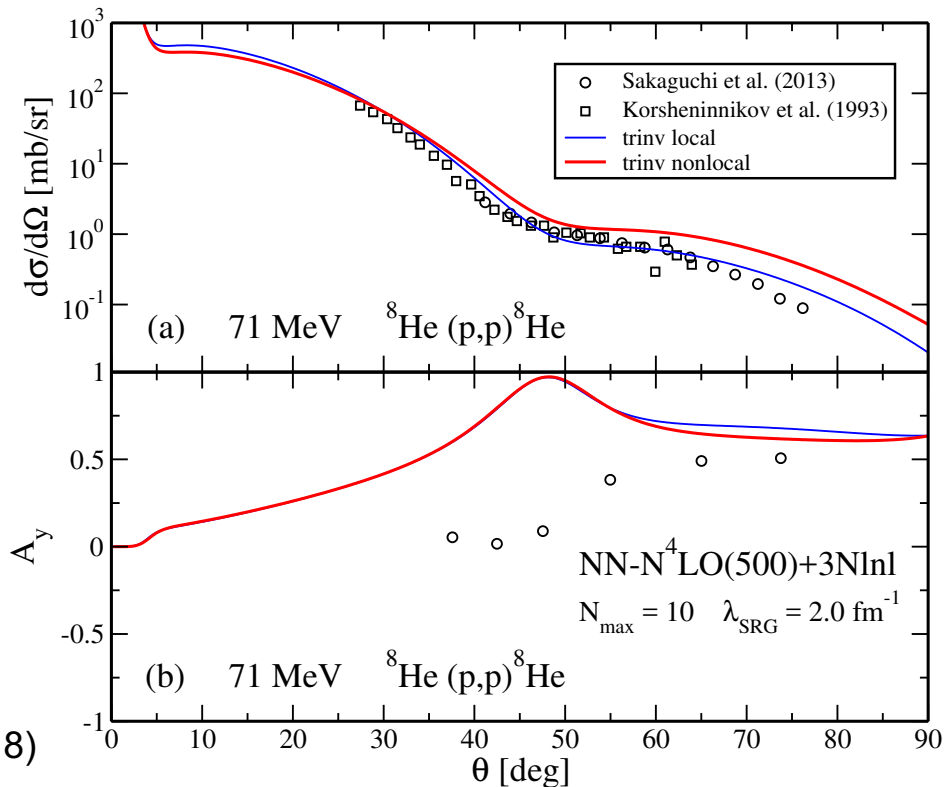
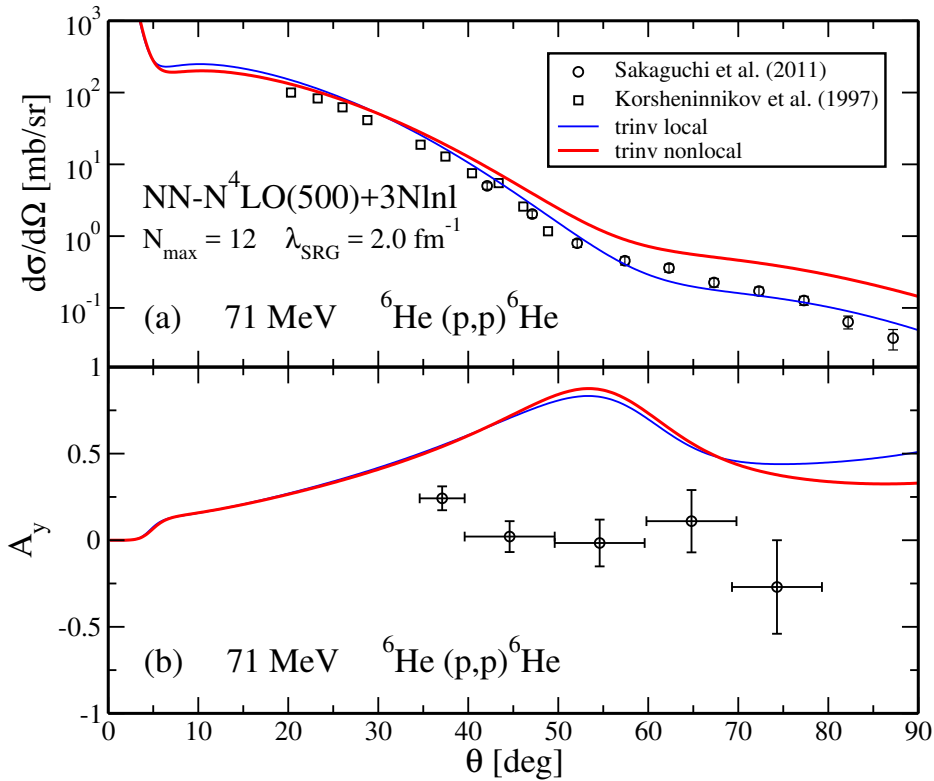
Reproduction of the general trend of the A_y



Scattering observables – Stable nuclei

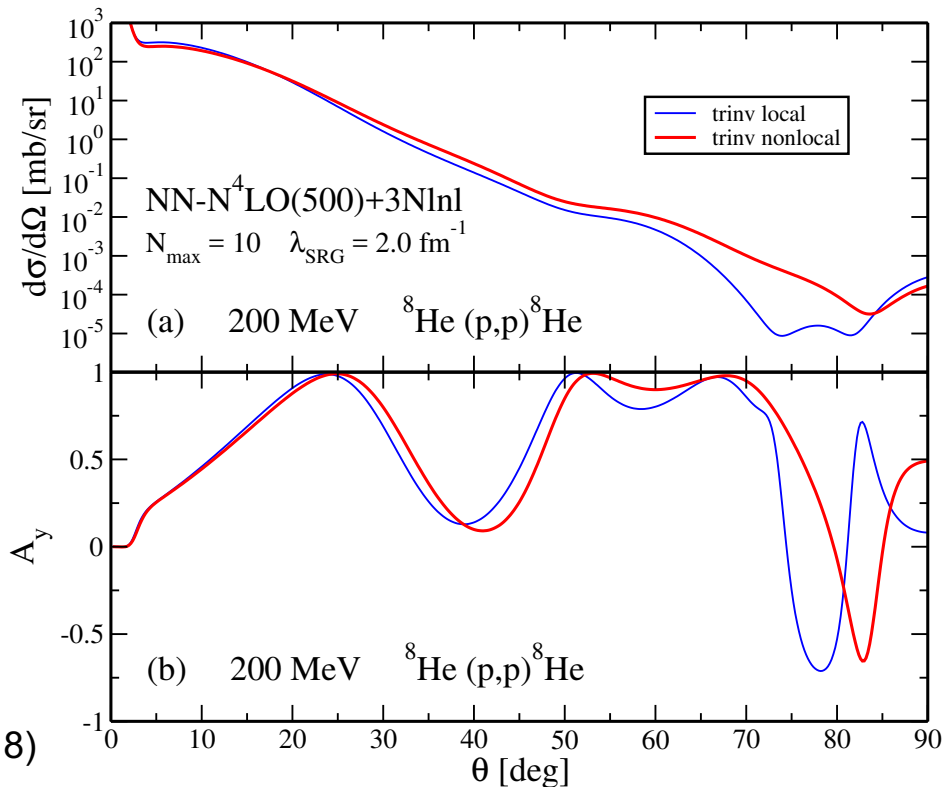
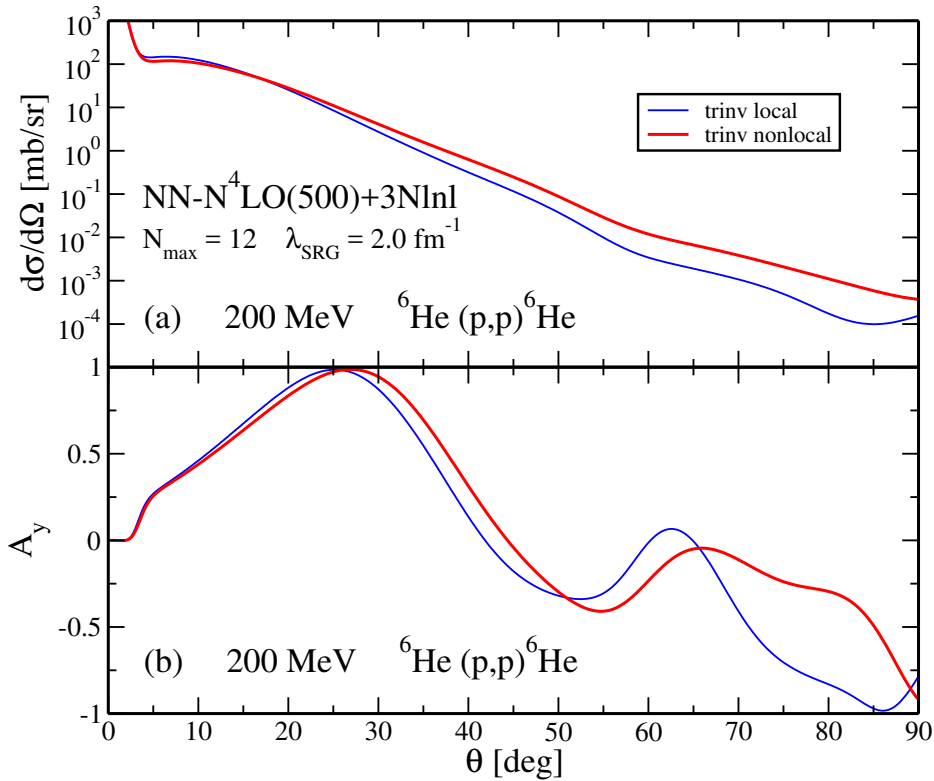


Scattering observables – Halo nuclei



Reasonable description of the differential cross section

Scattering observables – Halo nuclei



Different behavior of A_y
after 40 degrees

Outlook

- Investigation of the ${}^9\text{He}$ structure with the inclusion of the three-nucleon interaction
 - Introducing a controlled approximation for the 3N terms
- Calculation of the $p+{}^8\text{He}$ scattering process
 - New TRIUMF experiment for ${}^8\text{He}(p,p)$ reaction
- Coupling between different mass partitions for $A=7$ systems
- Improvement of the optical potential
 - Inclusion of three-nucleon interaction
 - Inclusion of medium effects