

Ab initio calculations for low and intermediate energies nuclear reactions

Progress in *Ab Initio* Techniques in Nuclear Physics

Feb 27, 2019

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Paolo Finelli (Bologna University)

Carlotta Giusti (Pavia University)

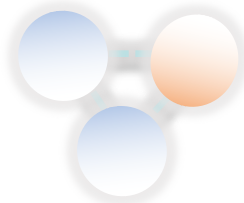
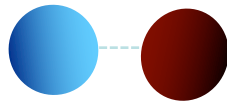
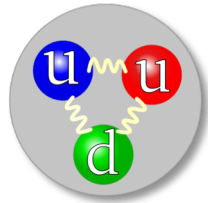
Outline

1. Study of $A=7$ systems within the No-Core Shell Model with Continuum (NCSMC)
2. Microscopic optical potentials for intermediate energies with nonlocal *ab initio* densities
 - New chiral $\bar{N}N$ interaction at N^3LO
 - Application to antiproton elastic scattering

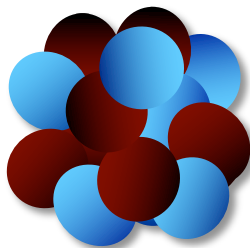
1.

Study of $A=7$ systems

From QCD to nuclei



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



Low-energy QCD



NN+3N interactions
from chiral EFT



SRG
Softens NN, induces 3N



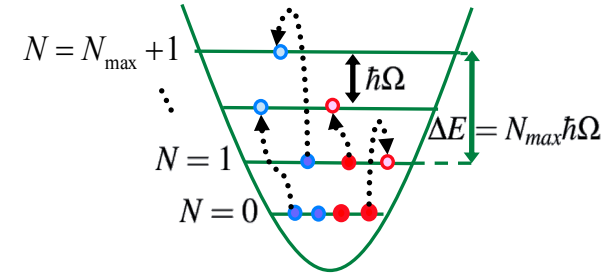
NCSMC
(Binary-cluster formulation)



Nuclear structure and reactions

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



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

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

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

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

Unknowns

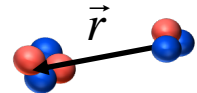
Unified approach to bound & continuum states; to nuclear structure and reactions

- 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).

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

Unknowns

Motivations

**A=7 systems
(⁷Be and ⁷Li)**

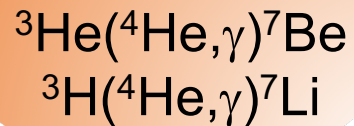
Motivations

Primordial ${}^7\text{Li}$
abundance in the
early universe

PLB **757** (2016) 430

Fraction of pp-chain
branches resulting
in ${}^7\text{Be}$ versus ${}^8\text{B}$
neutrinos

Nuclear Astrophysics



A=7 systems (${}^7\text{Be}$ and ${}^7\text{Li}$)

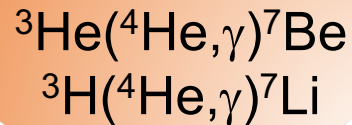
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A=7 systems (${}^7\text{Be}$ and ${}^7\text{Li}$)

New experiment in progress at LUNA

Lanzhou Experiment



Possible resonant enhancement near the threshold

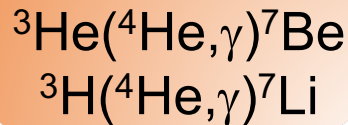
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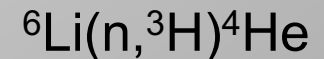
Lanzhou Experiment



Possible resonant enhancement near the threshold

A=7 systems (${}^7\text{Be}$ and ${}^7\text{Li}$)

Tritium breeding



Fusion energy generation (ITER)

Motivations

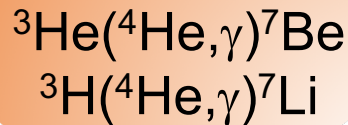
Primordial ${}^7\text{Li}$ abundance in the early universe

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Fraction of pp-chain branches resulting in ${}^7\text{Be}$ versus ${}^8\text{B}$ neutrinos

New experiment in progress at LUNA

Nuclear Astrophysics



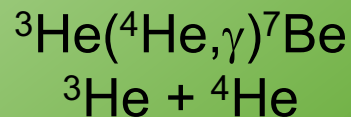
Lanzhou Experiment



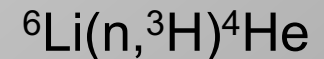
Possible resonant enhancement near the threshold

A=7 systems (${}^7\text{Be}$ and ${}^7\text{Li}$)

TRIUMF



Tritium breeding



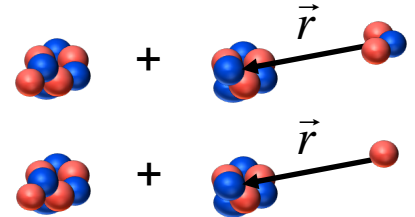
Fusion energy generation (ITER)

NCSMC calculations of A=7 systems

- NN SRG-N³LO [Entem, Machleidt, Phys. Rev. C, **68** 041001 (2003)]

- Calculations with NN SRG-N³LO

- ${}^7\text{Be} \sim ({}^7\text{Be})_{\text{NCSM}} + ({}^3\text{He} + {}^4\text{He})_{\text{NCSM/RGM}}$
 $\sim ({}^7\text{Be})_{\text{NCSM}} + (p + {}^6\text{Li})_{\text{NCSM/RGM}}$



- ${}^7\text{Li} \sim ({}^7\text{Li})_{\text{NCSM}} + ({}^3\text{H} + {}^4\text{He})_{\text{NCSM/RGM}}$
 $\sim ({}^7\text{Li})_{\text{NCSM}} + (n + {}^6\text{Li})_{\text{NCSM/RGM}}$
 $\sim ({}^7\text{Li})_{\text{NCSM}} + (p + {}^6\text{He})_{\text{NCSM/RGM}}$

- NCSM eigenstates

- ${}^3\text{He}$ and ${}^3\text{H}$: $(J^\pi, T) = (1/2^+, 1/2)$ eigenstate
 - ${}^4\text{He}$: $(J^\pi, T) = (0^+, 0)$ eigenstate
 - ${}^6\text{Li}$: $(J^\pi, T) = (1^+, 0), (3^+, 0), (0^+, 1), (2^+, 1)$ eigenstates
 - ${}^6\text{He}$: $(J^\pi, T) = (0^+, 1), (2^+, 1)$ eigenstates
 - ${}^7\text{Be}$ and ${}^7\text{Li}$: 8 negative- and 6 positive-parity eigenstates

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

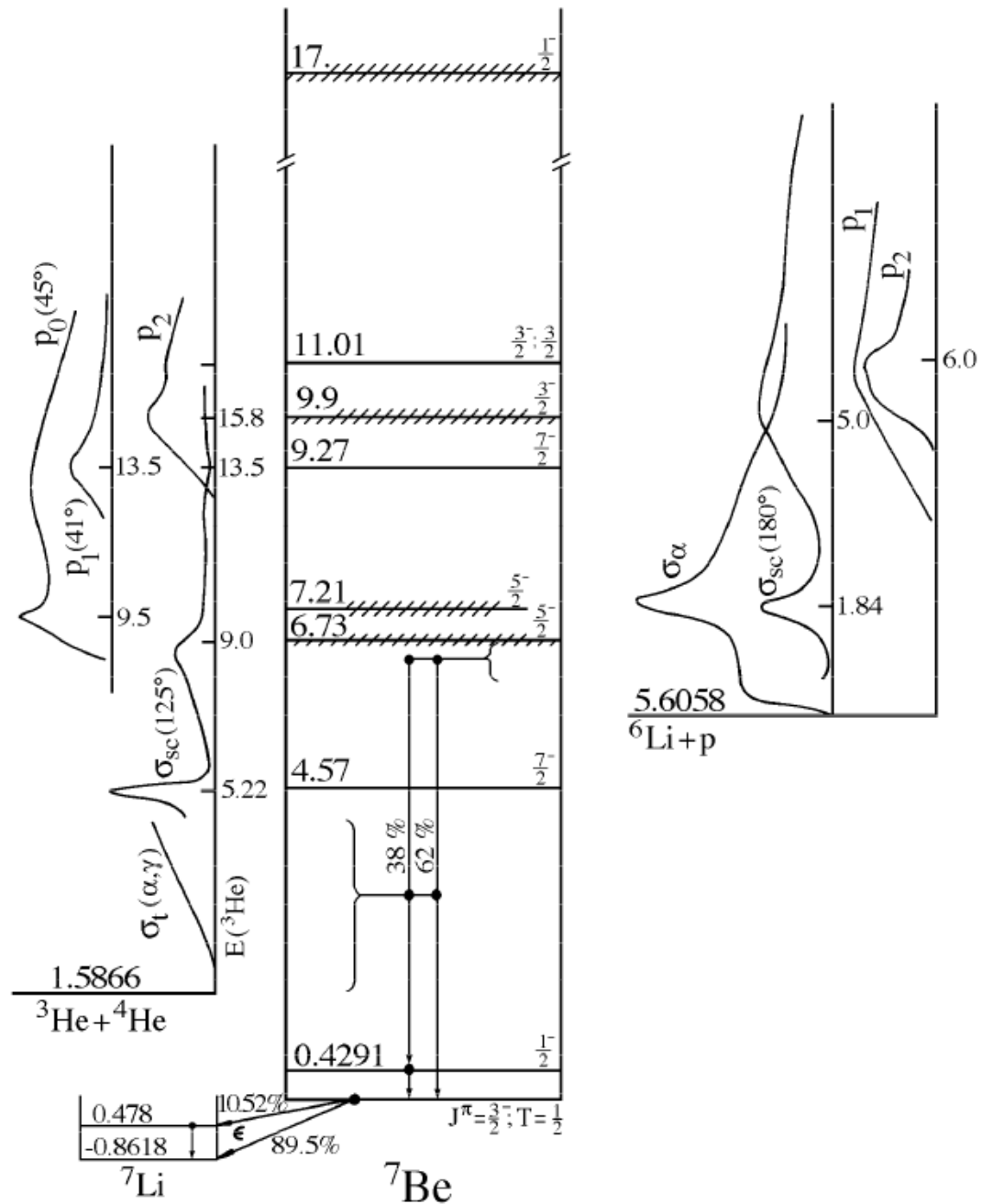
Analyzed mass partitions

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

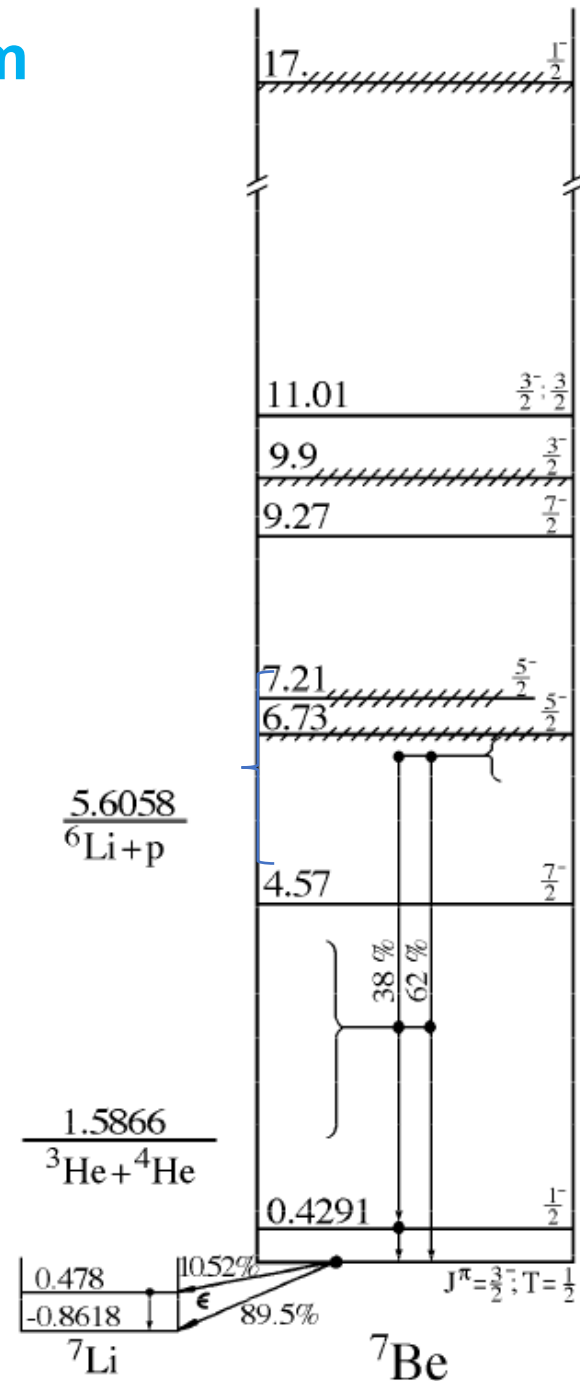
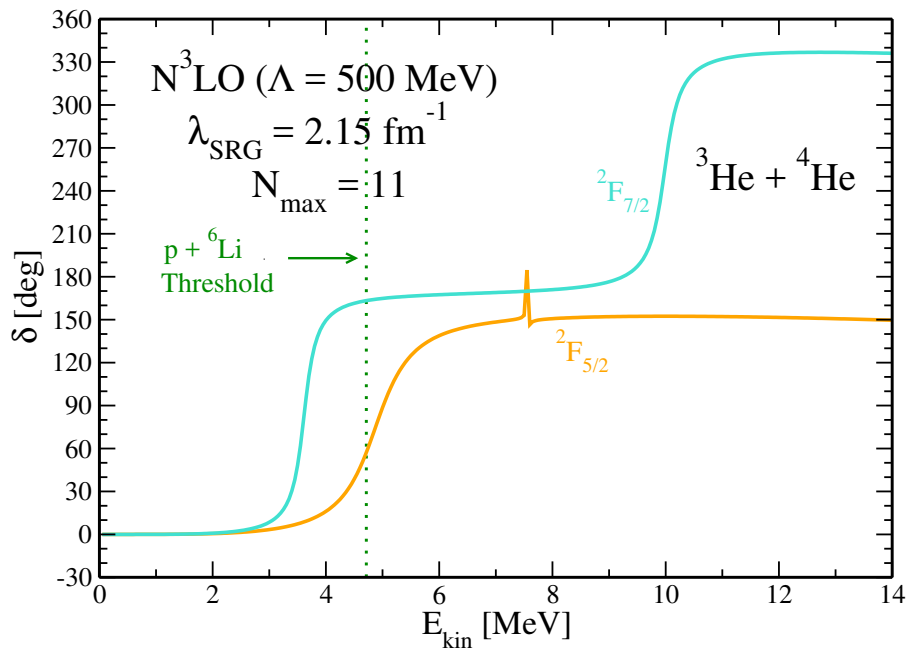
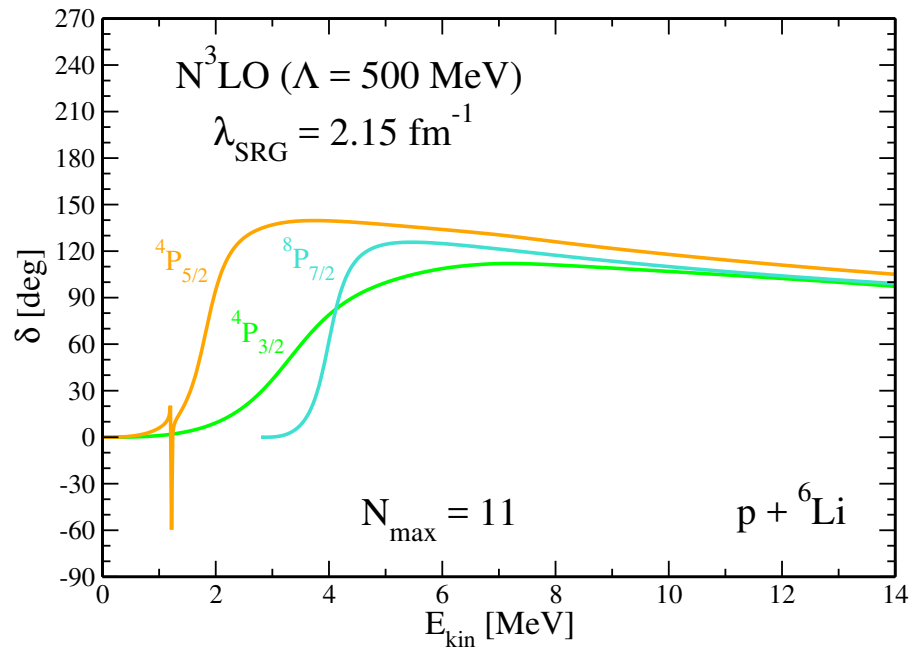
Exp.	$J^\pi = 3/2^-$
E [MeV]	-37.60

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

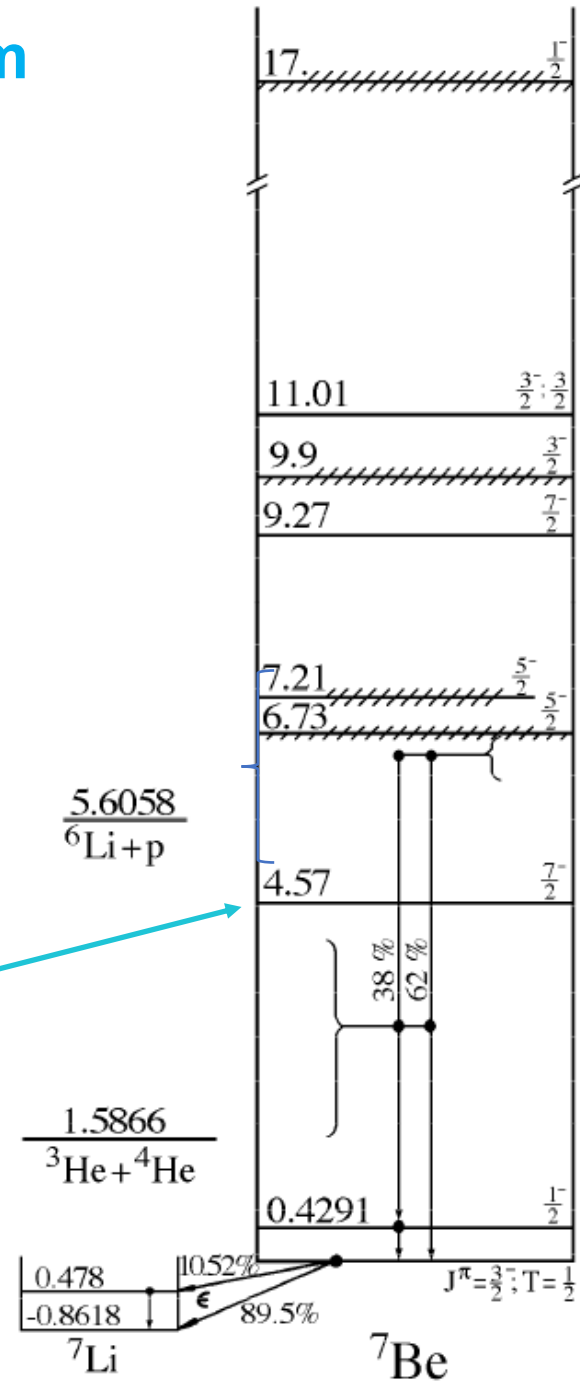
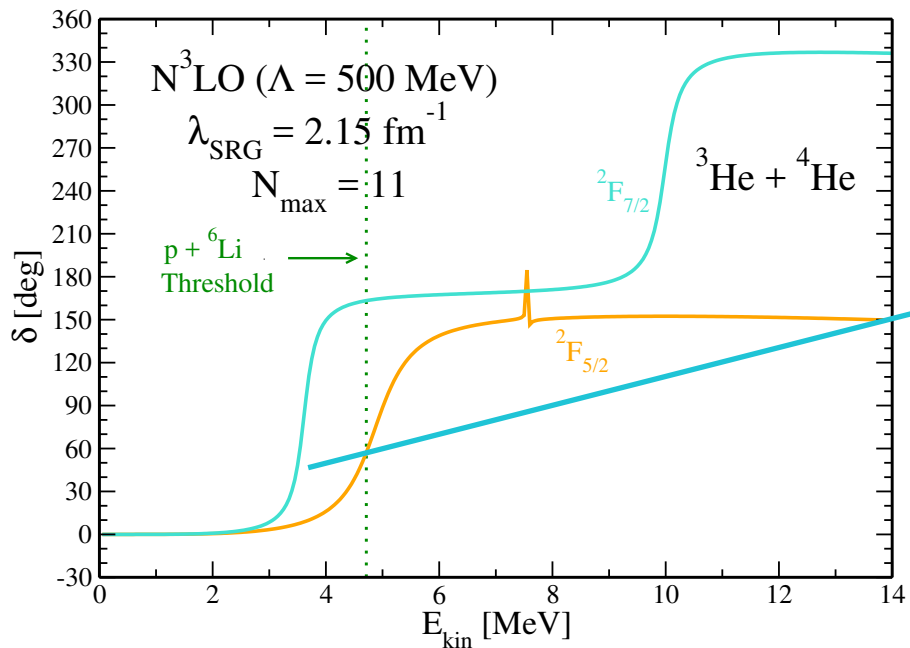
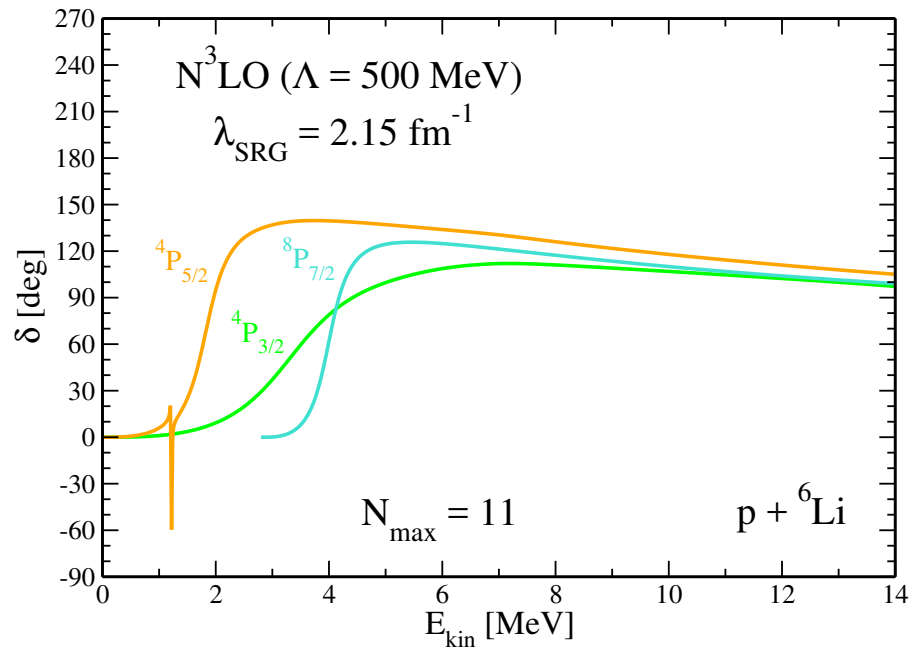
$p + {}^6\text{Li}$	$J^\pi = 3/2^-$	$J^\pi = 1/2^-$
E_{bound}	-5.729	-5.389
E [MeV]	-36.47	-36.13



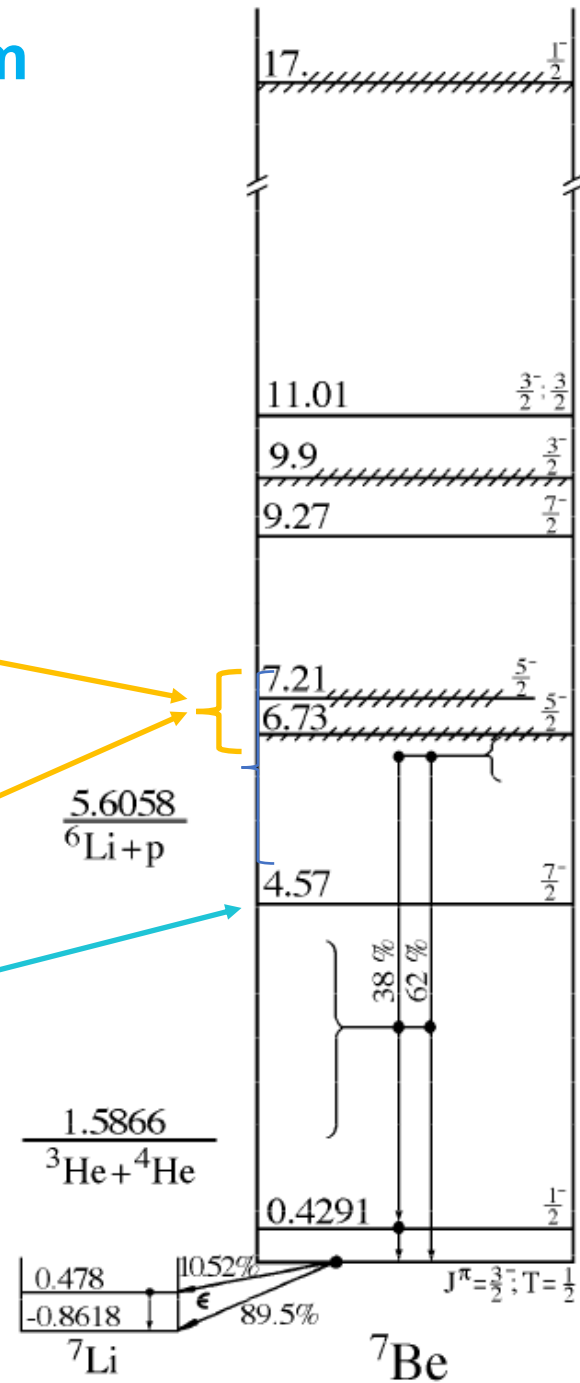
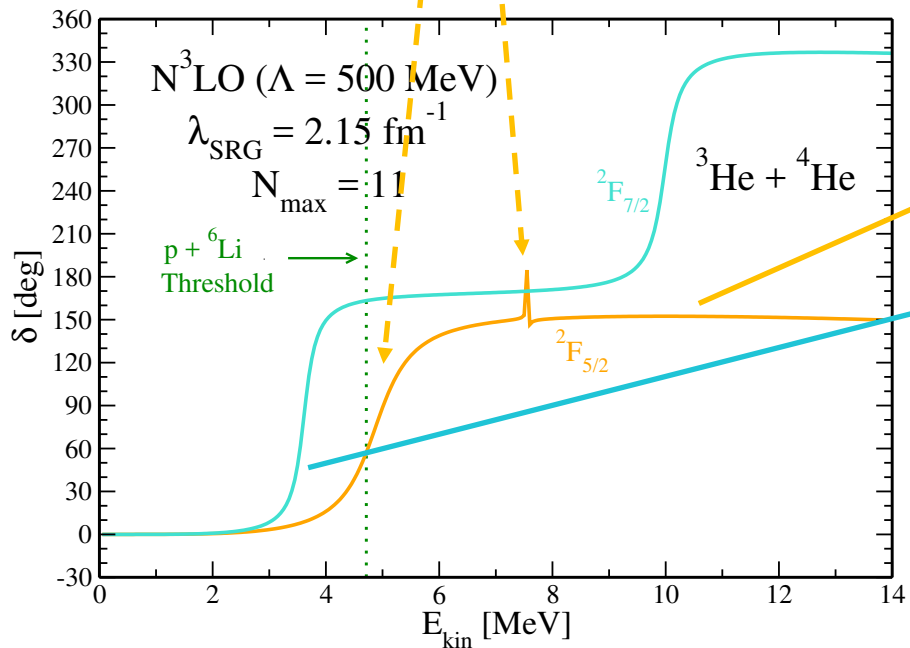
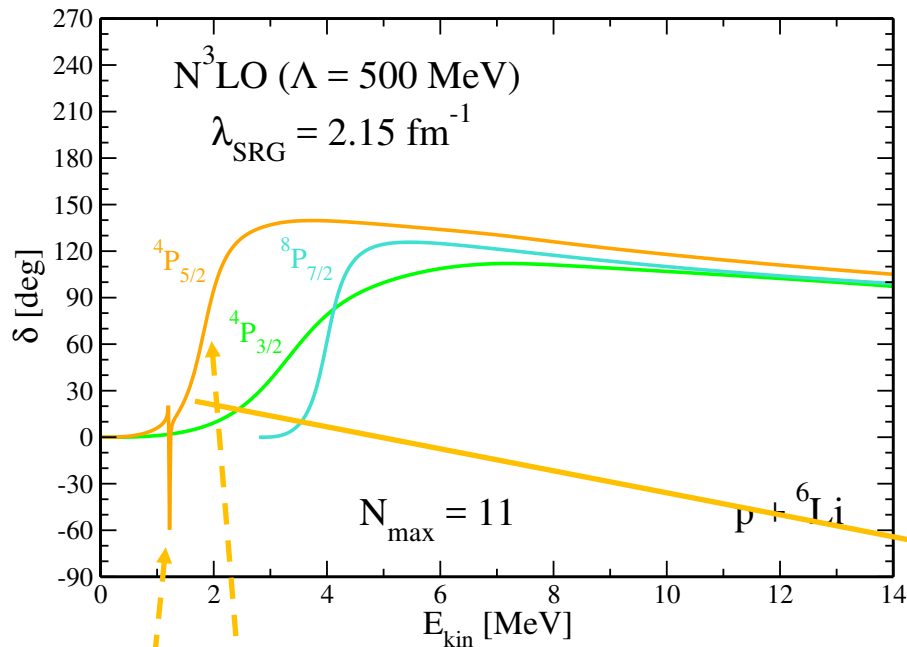
${}^7\text{Be}$ – Reproducing the energy spectrum



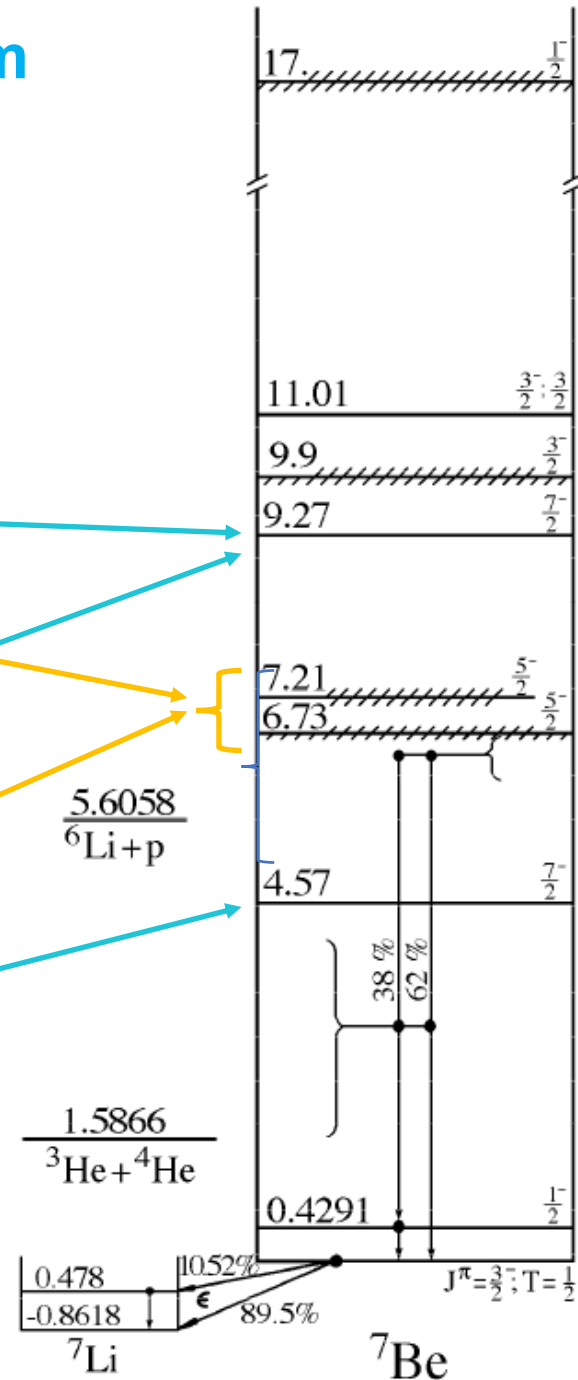
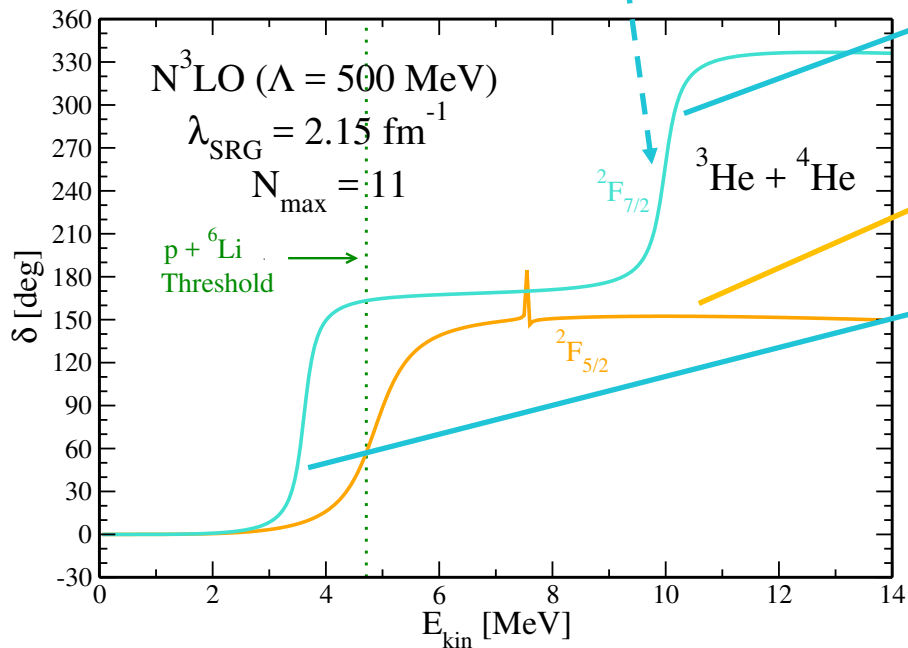
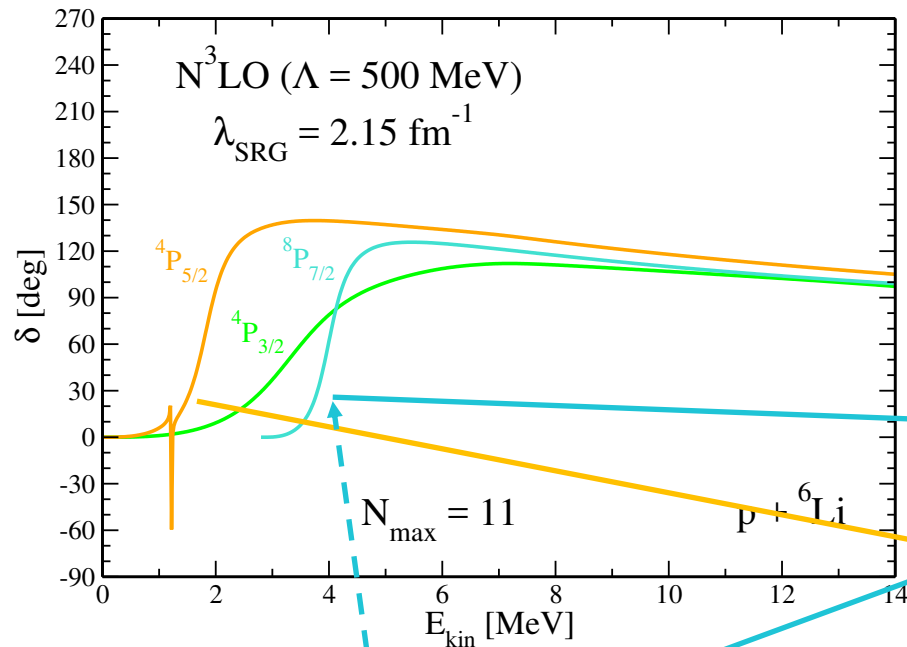
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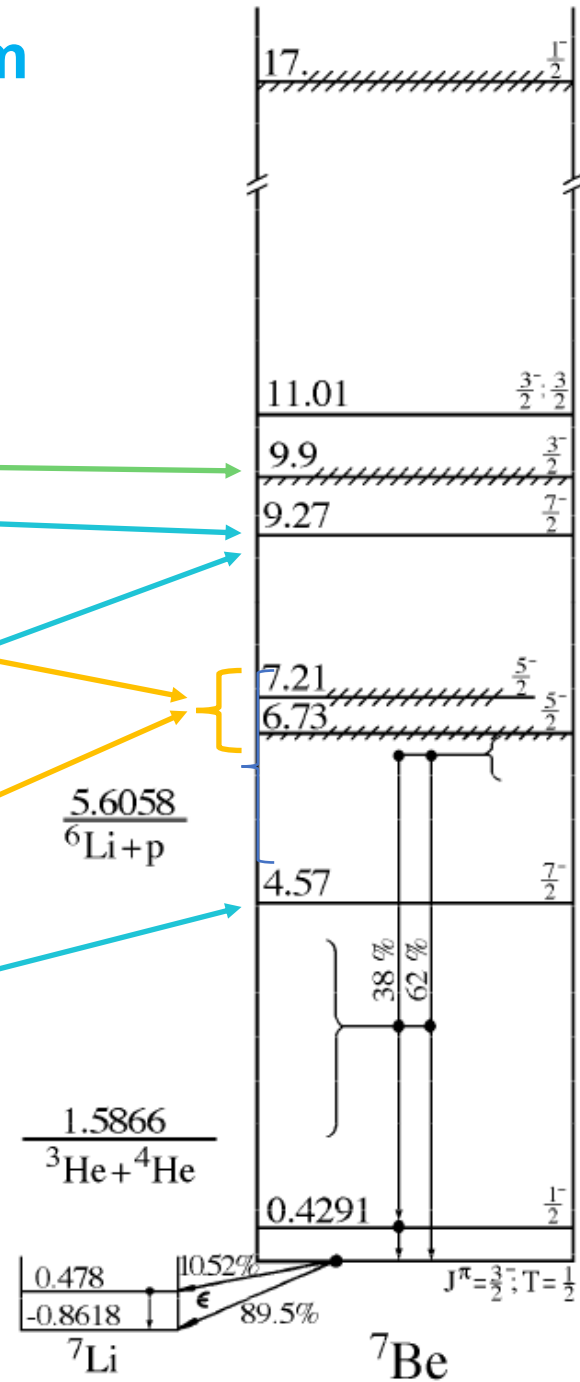
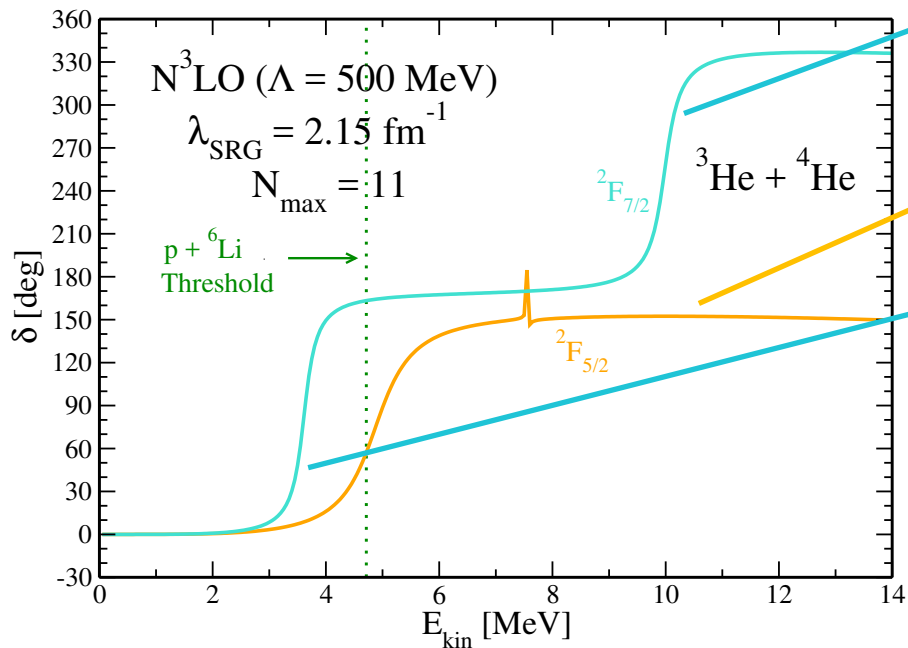
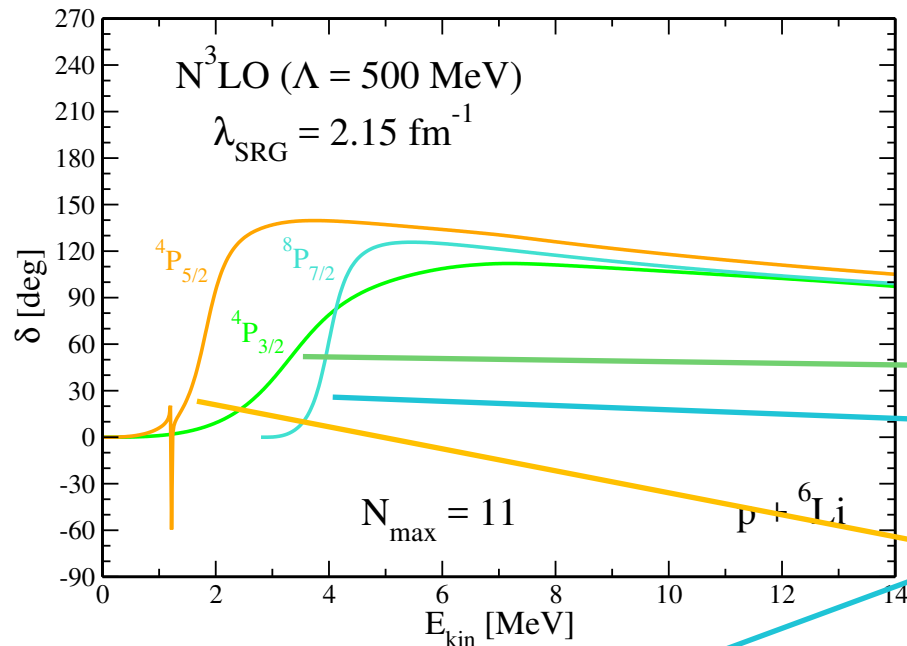
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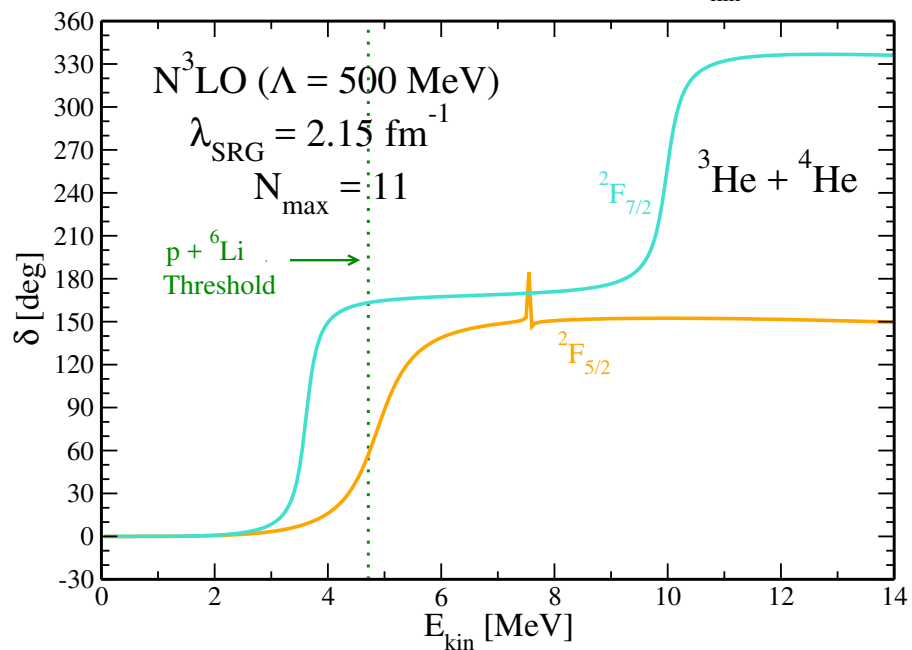
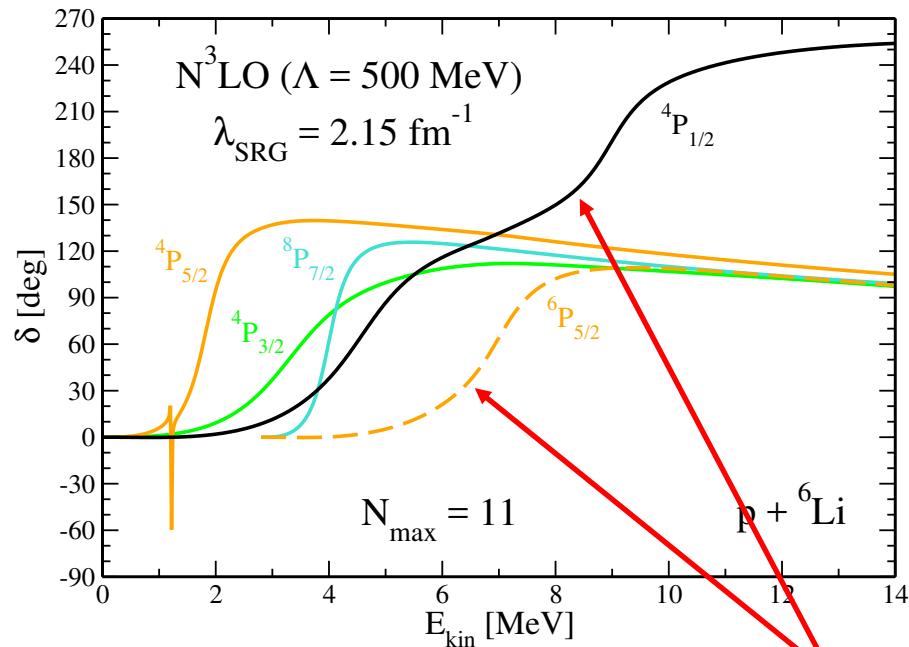
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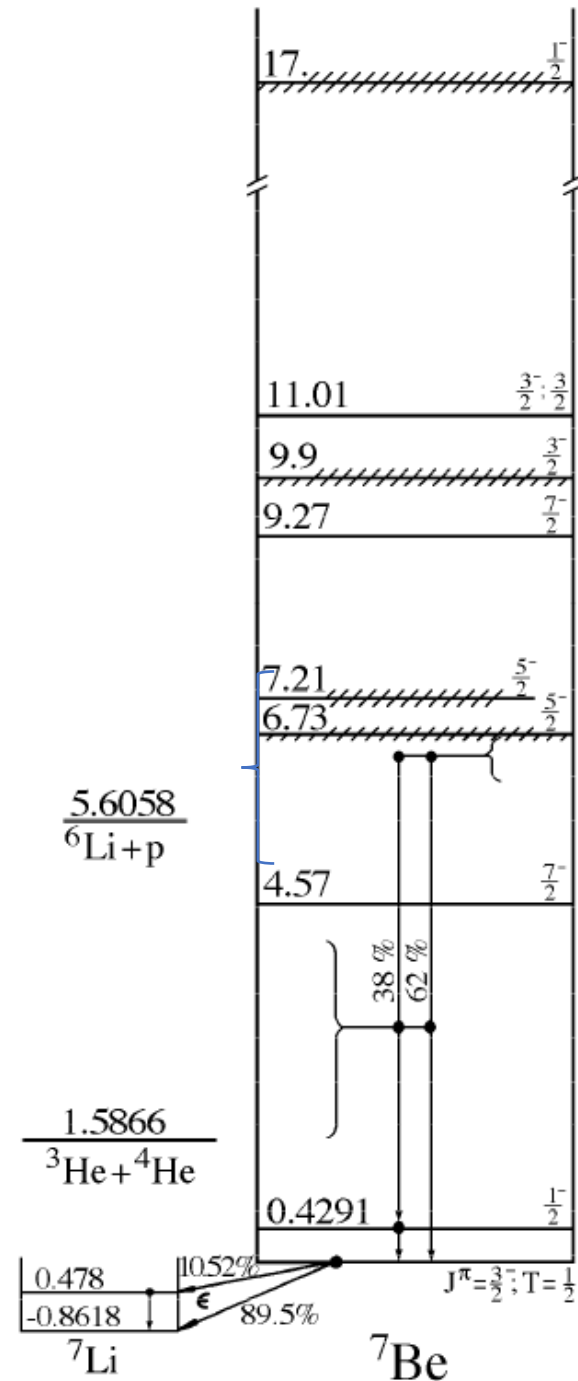
${}^7\text{Be}$ – Reproducing the energy spectrum



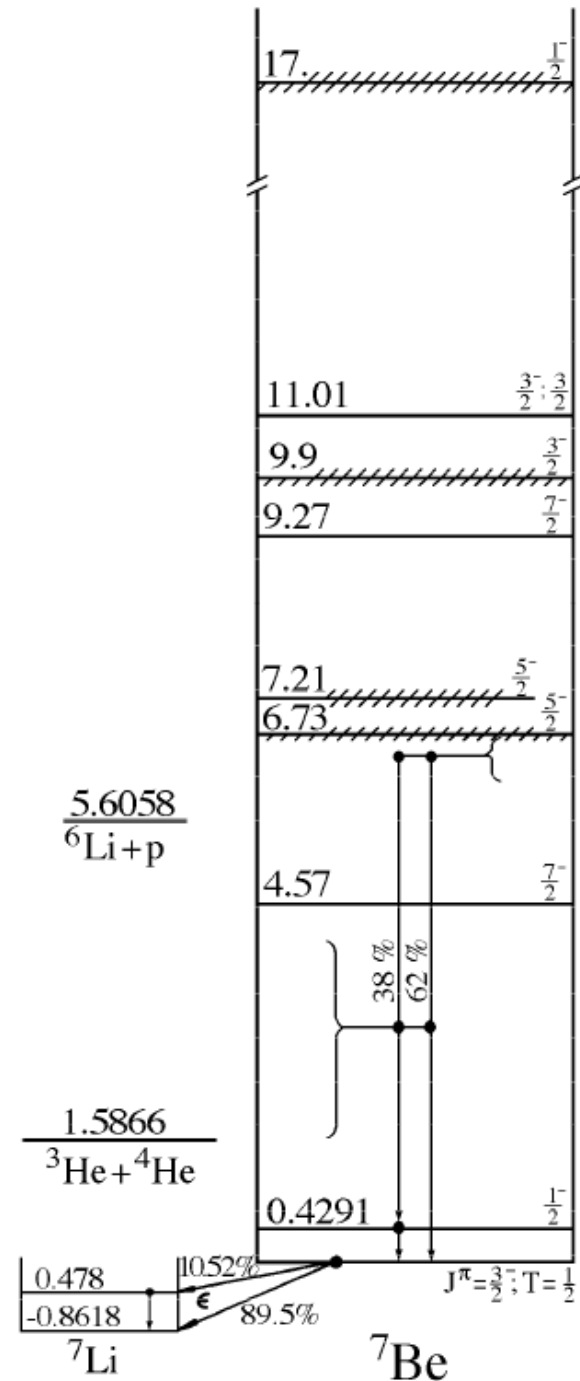
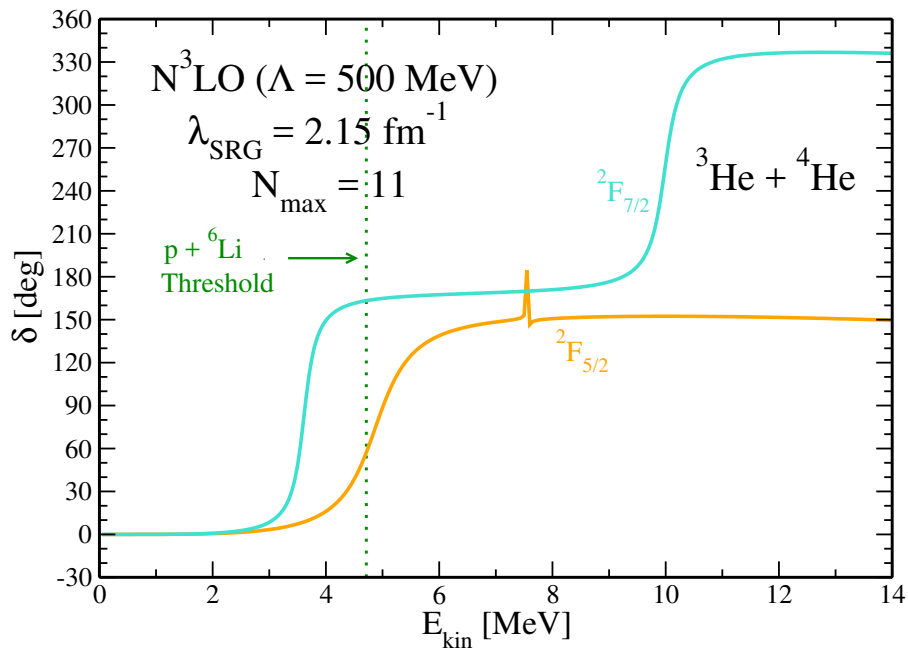
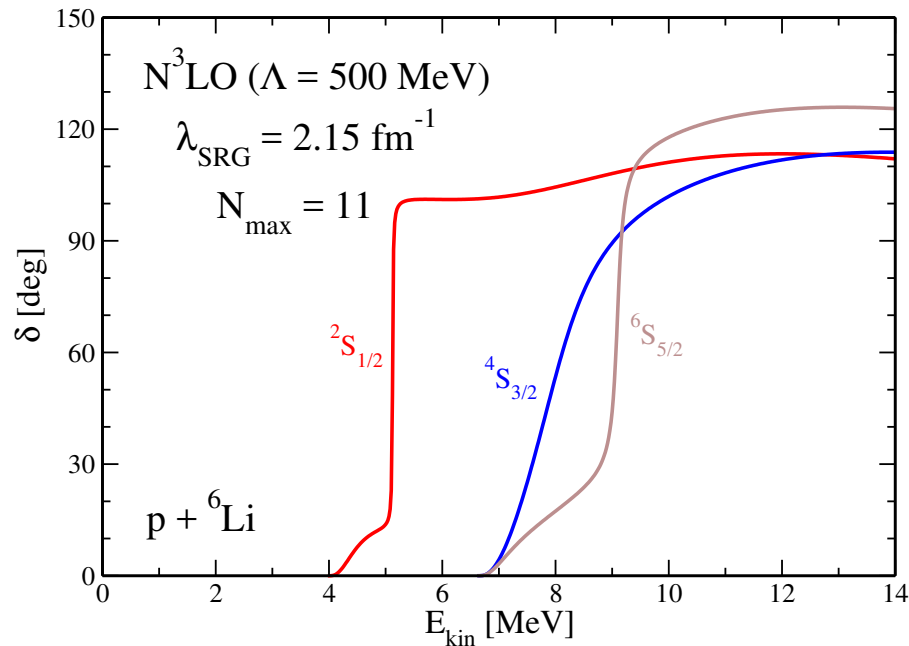
${}^7\text{Be}$ – New negative-parity states



NEW



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



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

Analyzed mass partitions

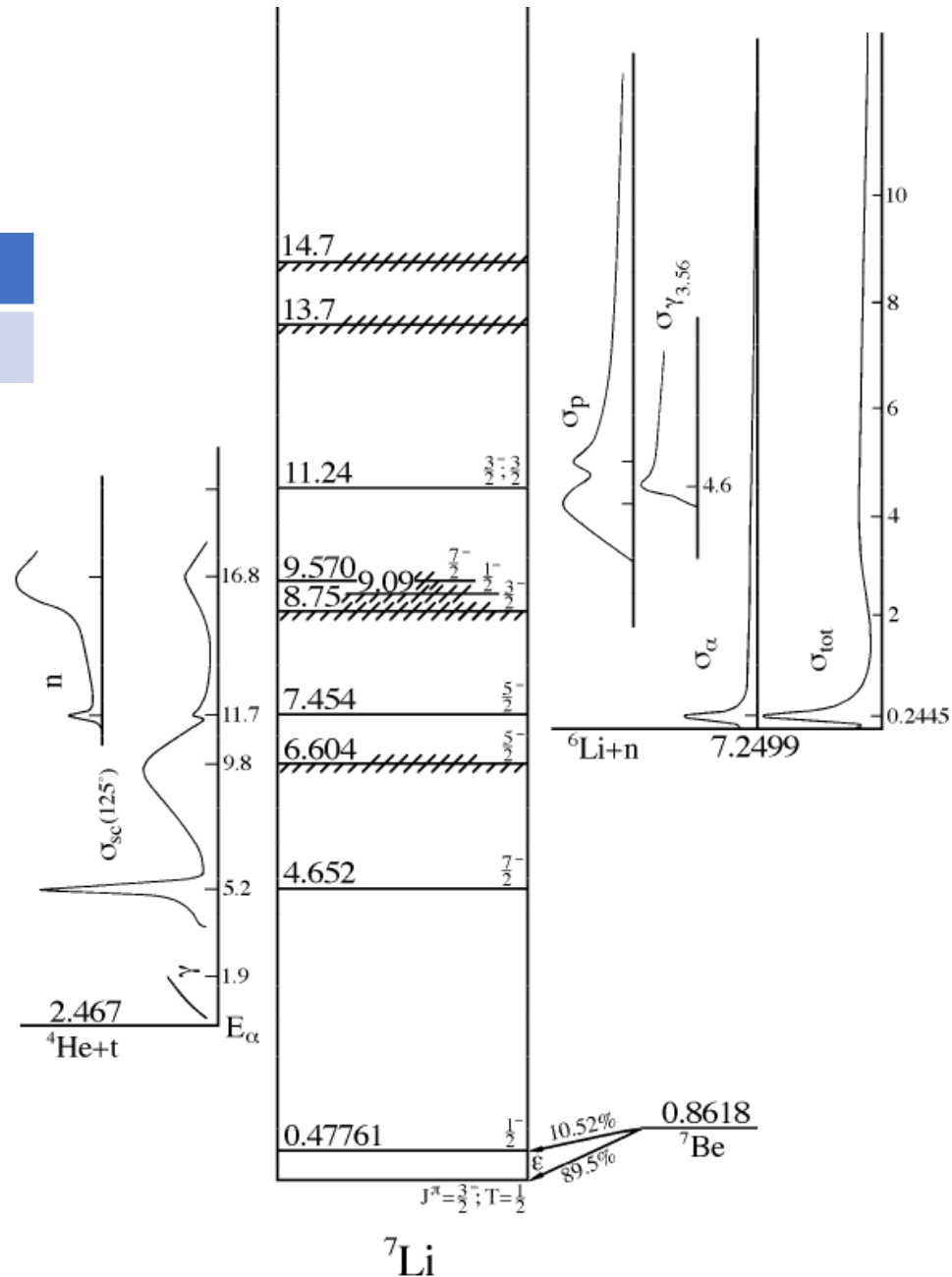
- ${}^3\text{H} + {}^4\text{He}$
- $n + {}^6\text{Li}$
- $p + {}^6\text{He}$

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

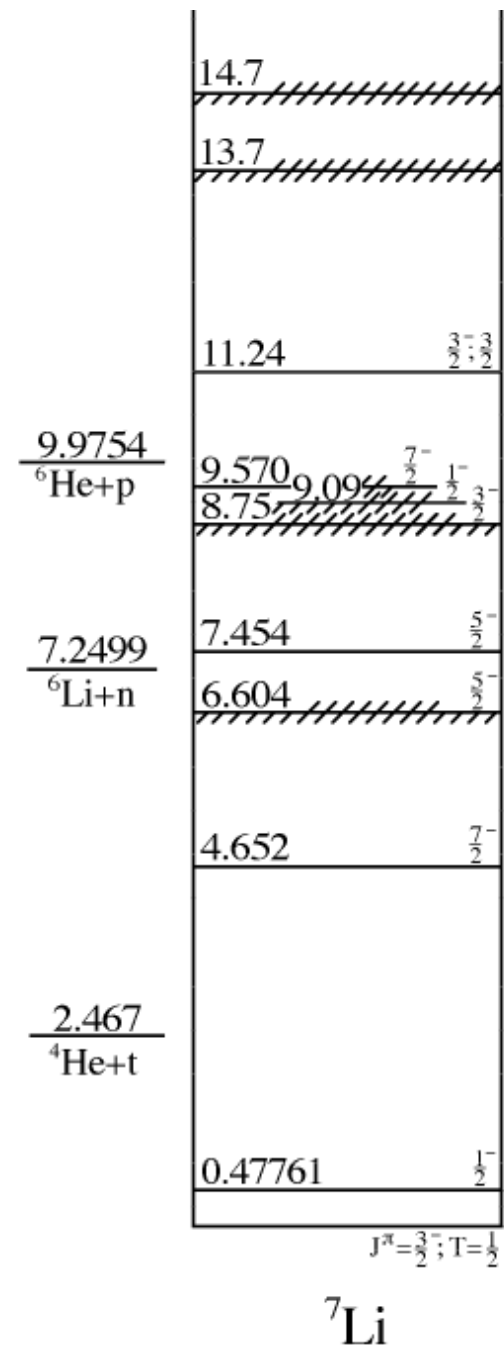
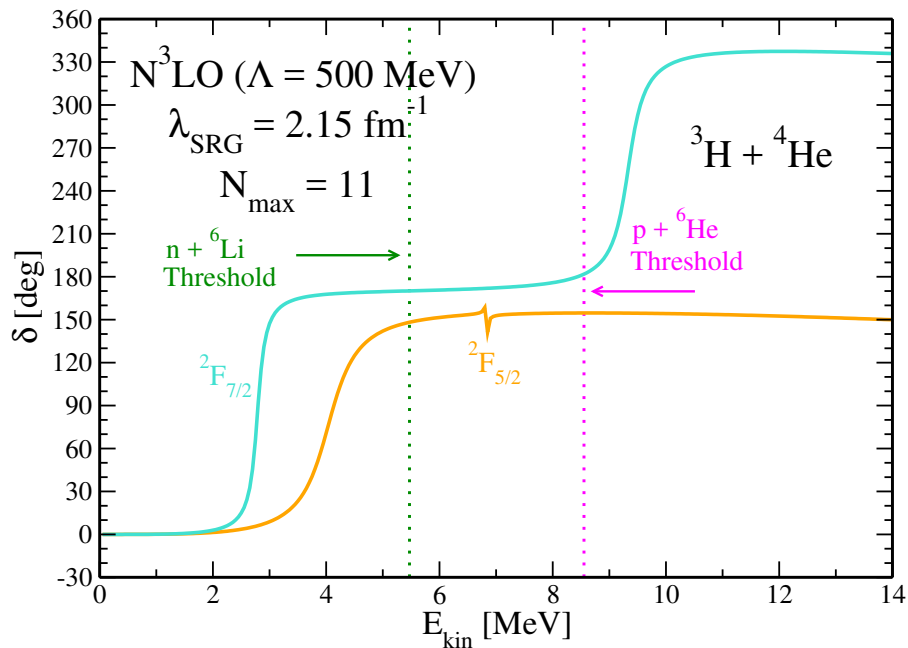
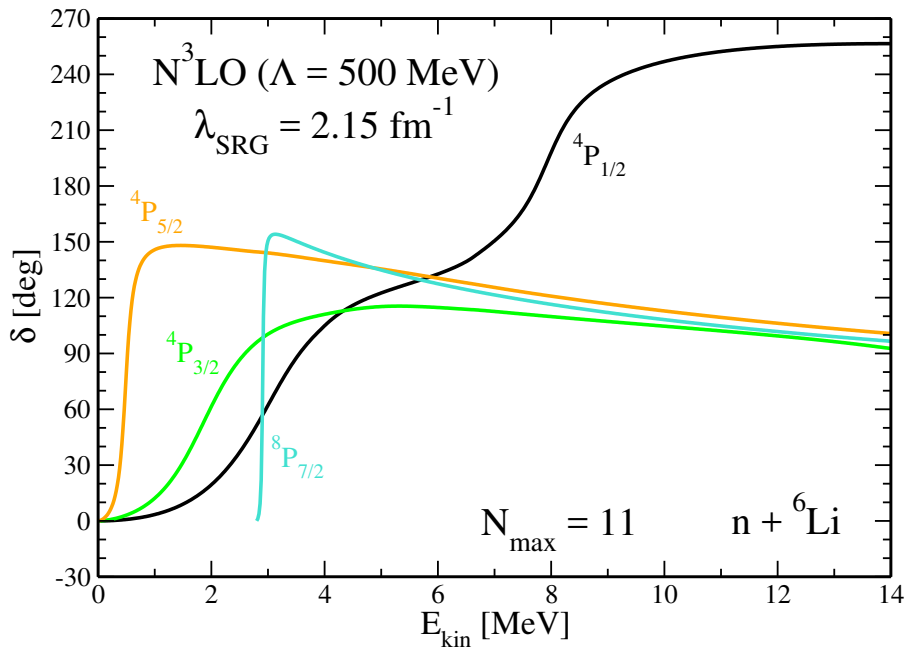
${}^3\text{H} + {}^4\text{He}$	$J^\pi = 3/2^-$	$J^\pi = 1/2^-$
E_{bound}	-2.432	-2.153
E [MeV]	-38.65	-38.37

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

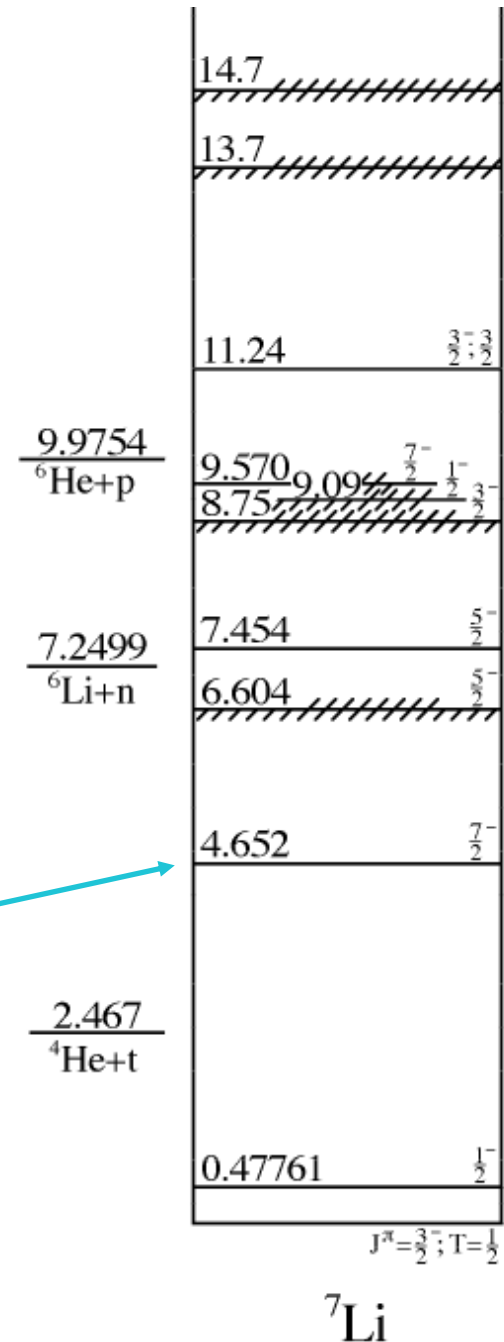
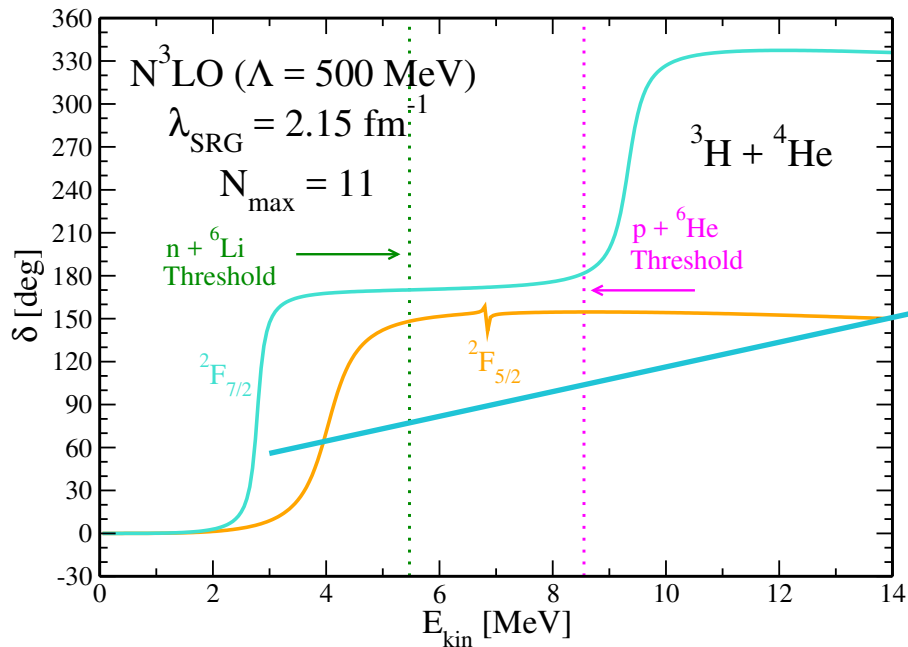
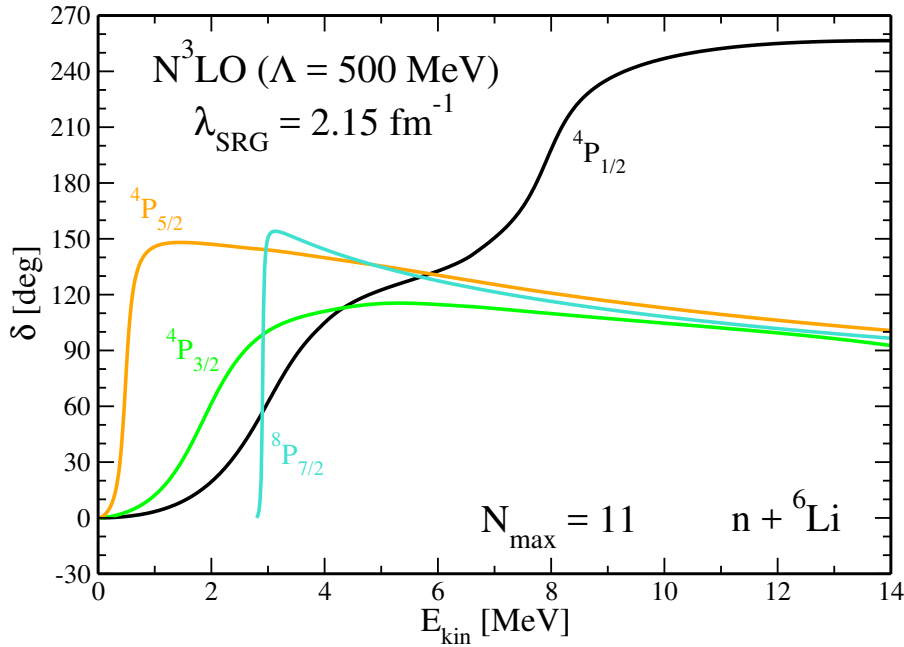
$p + {}^6\text{He}$	$J^\pi = 3/2^-$	$J^\pi = 1/2^-$
E_{bound}	-10.40	-10.06
E [MeV]	-38.06	-37.73



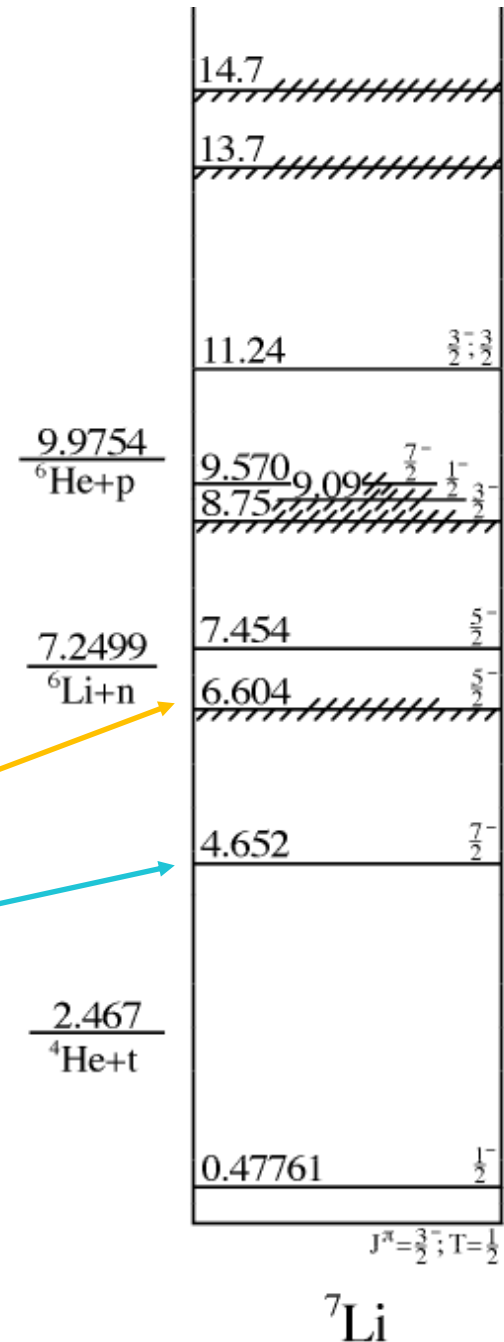
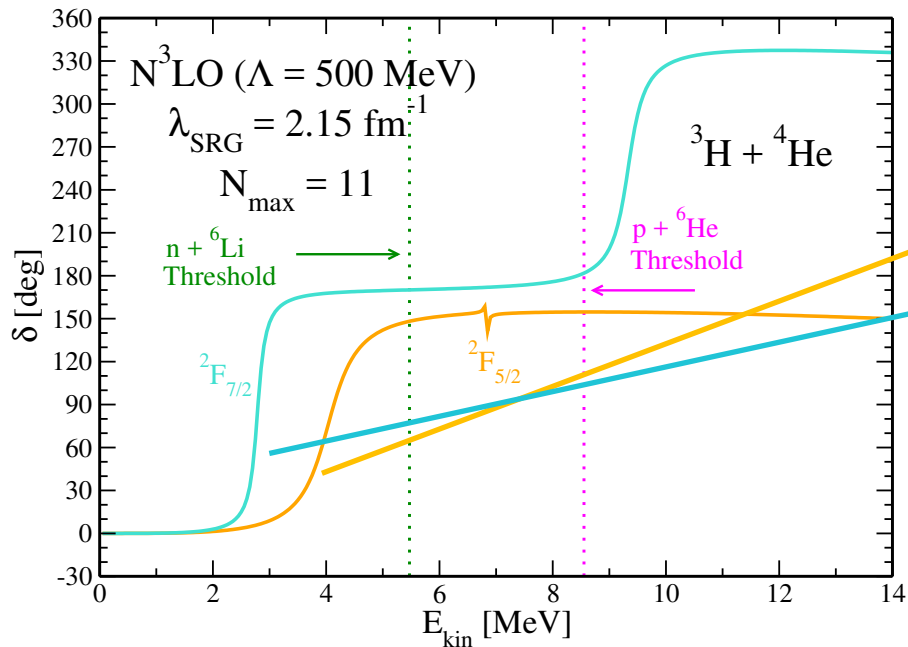
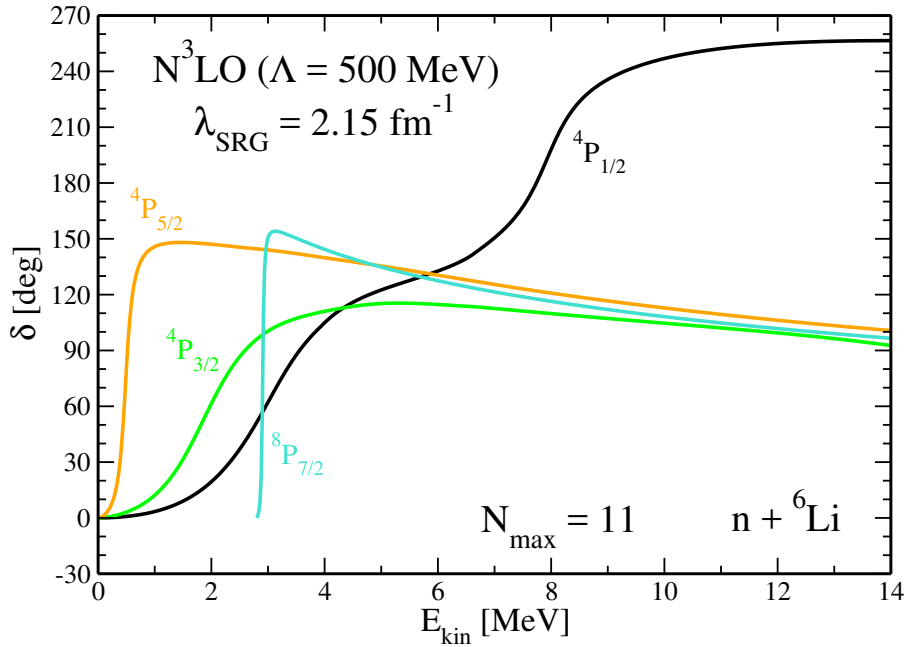
${}^7\text{Li}$ – Reproducing the energy spectrum



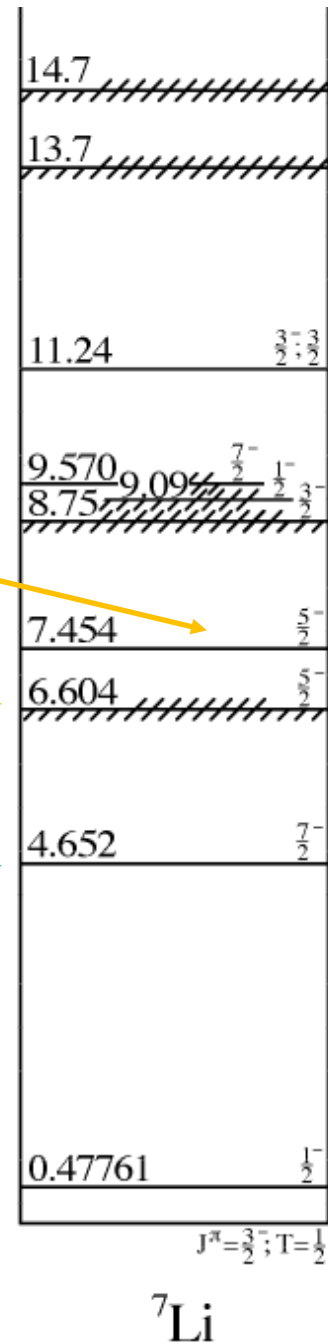
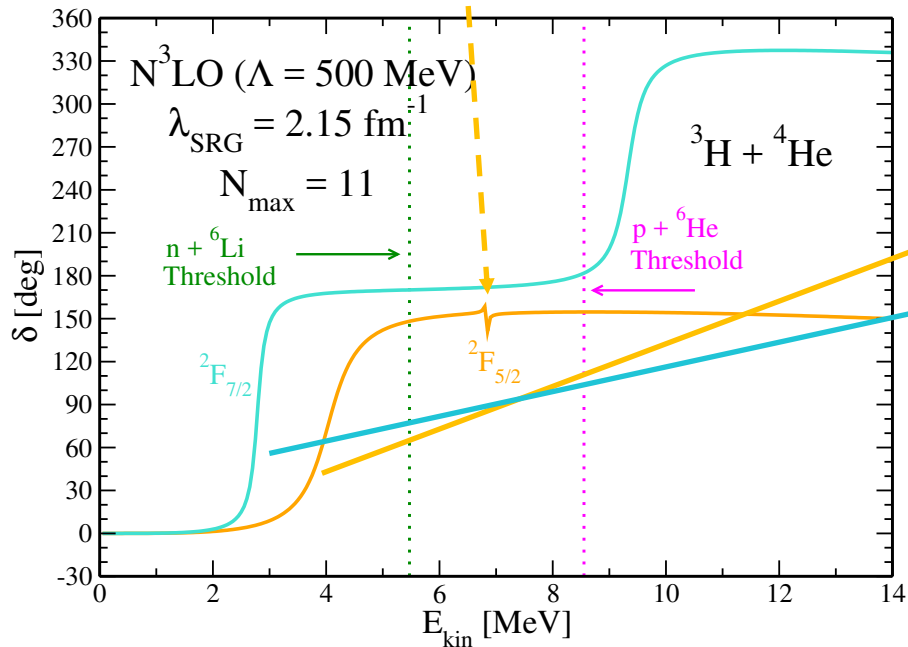
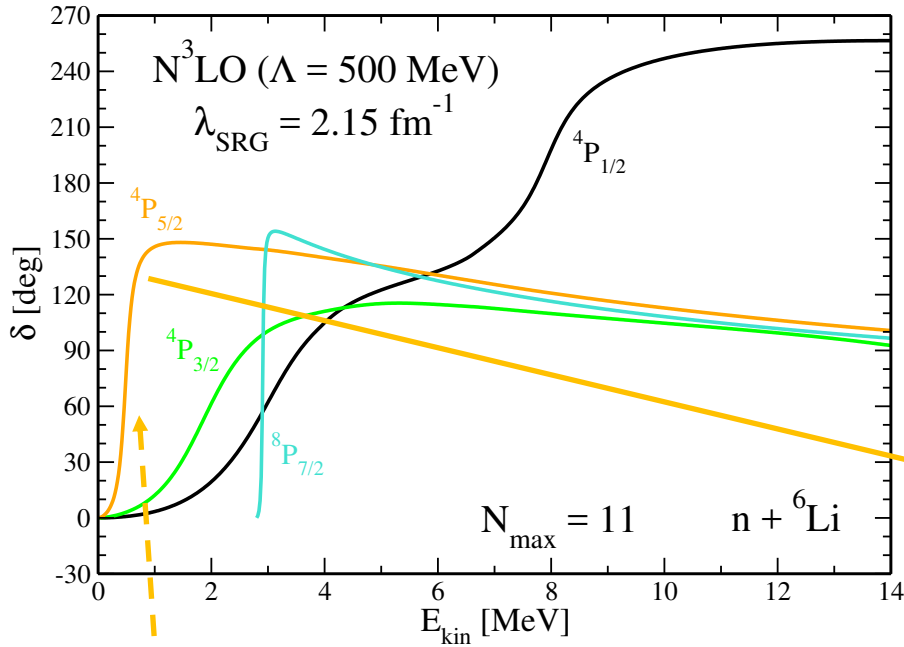
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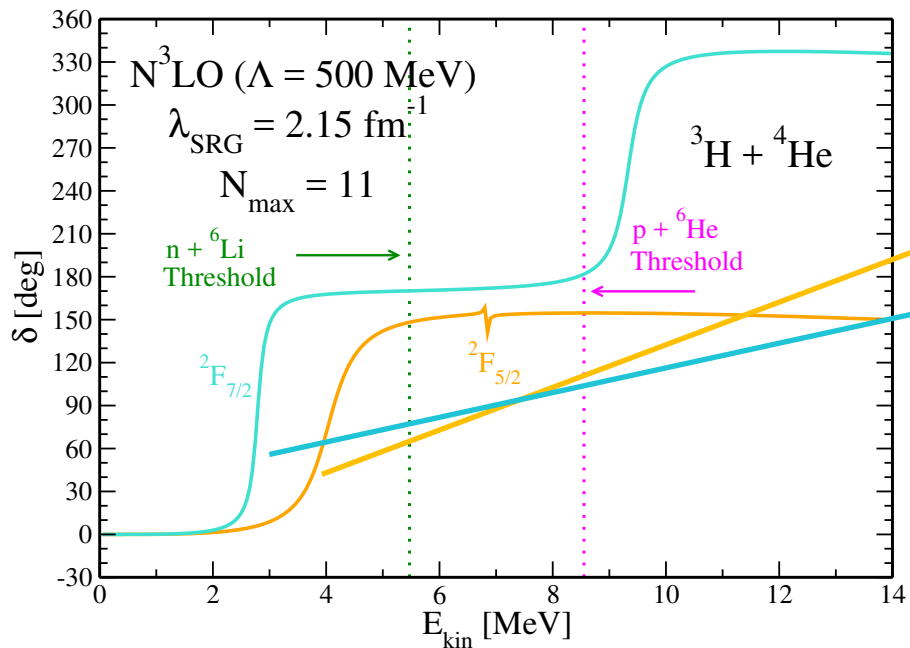
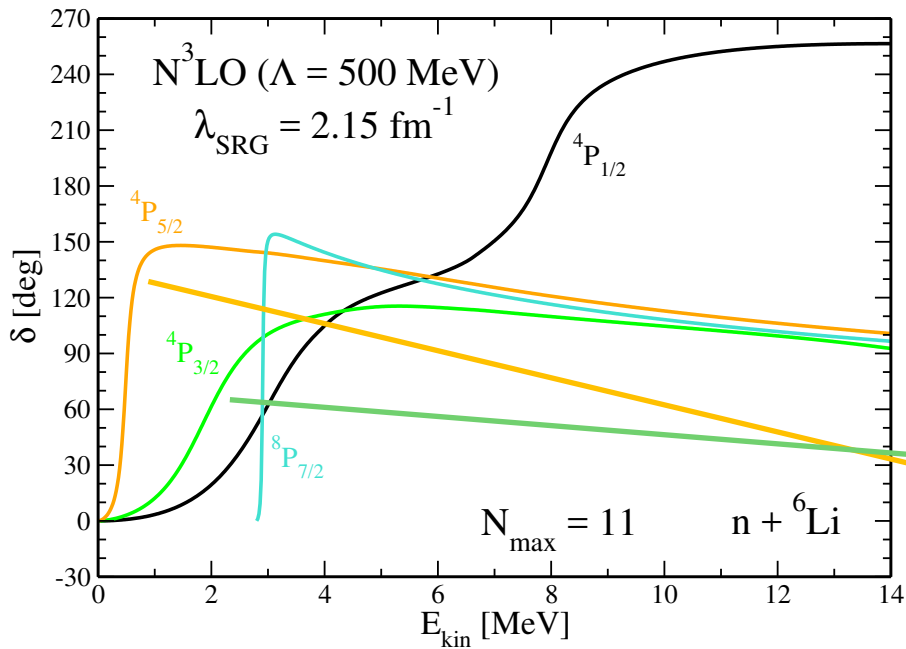
${}^7\text{Li}$ – Reproducing the energy spectrum



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



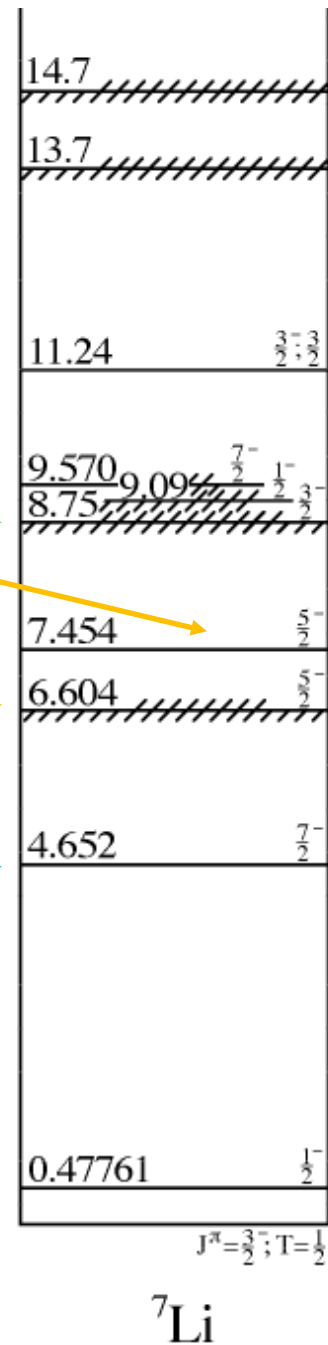
${}^7\text{Li}$ – Reproducing the energy spectrum



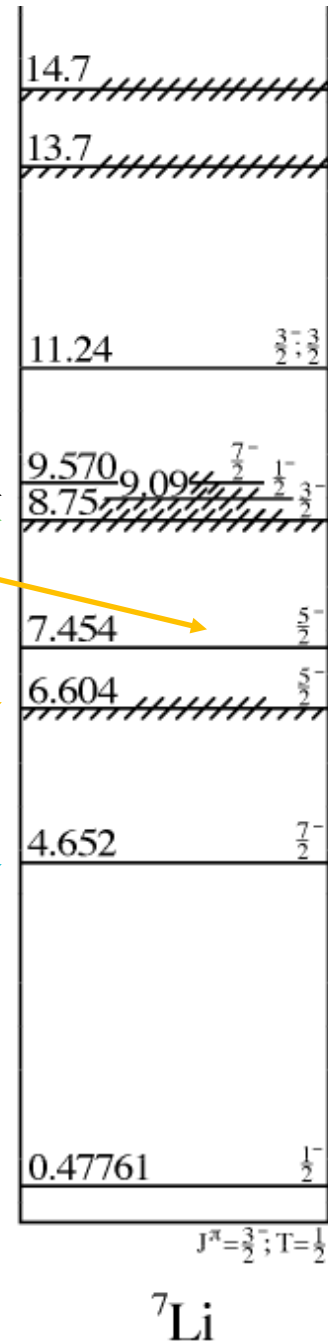
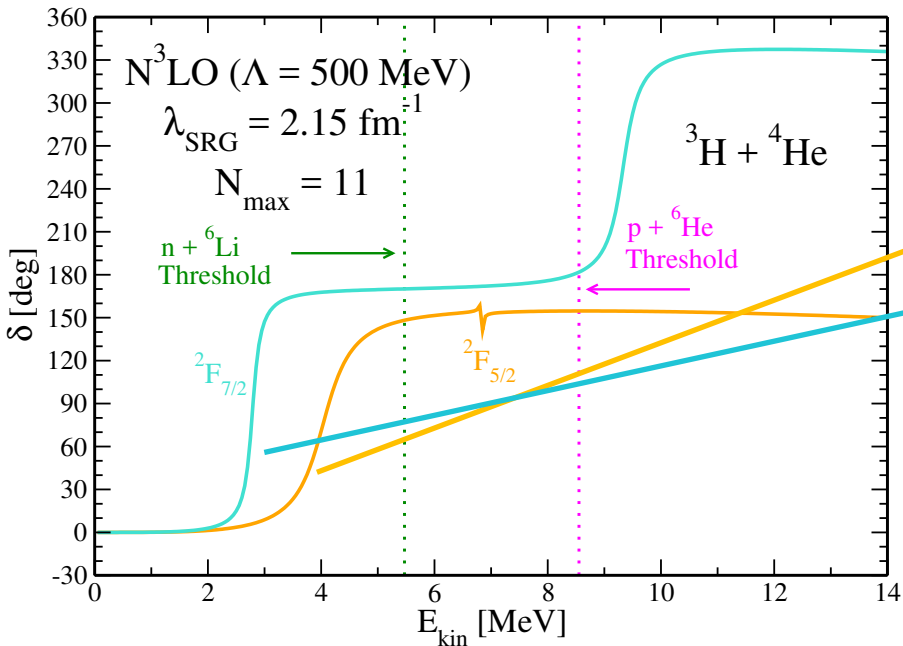
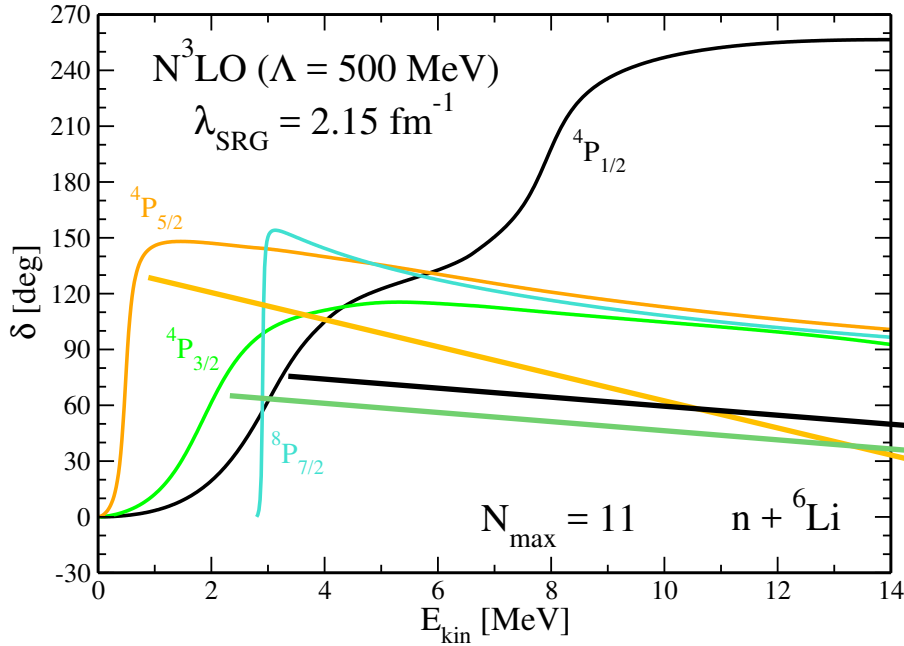
$$\frac{9.9754}{{}^6\text{He}+p}$$

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

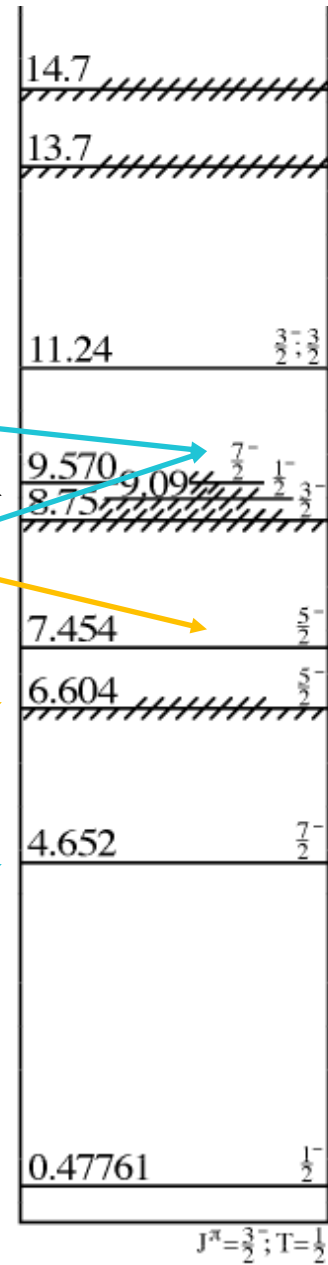
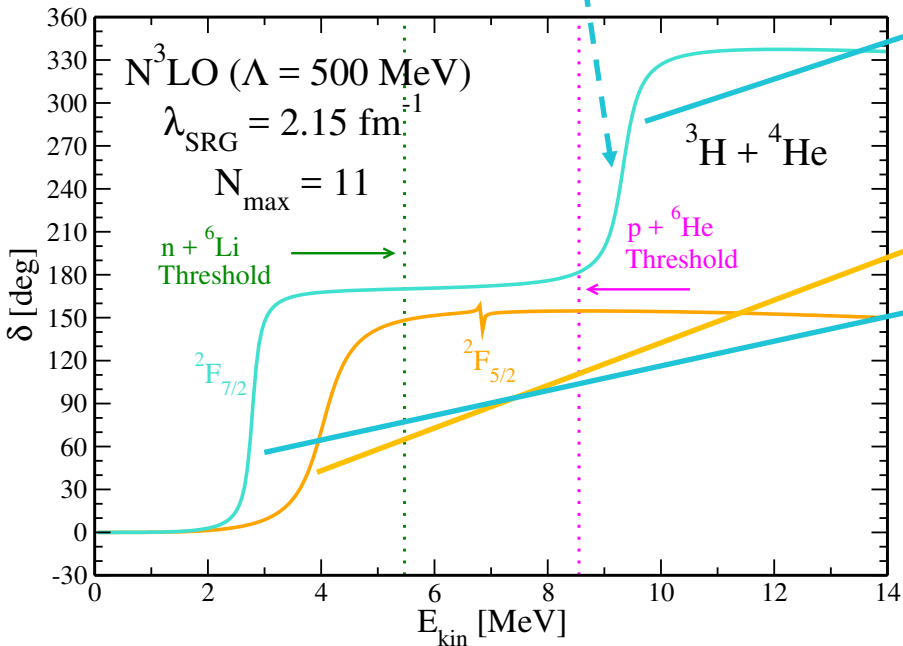
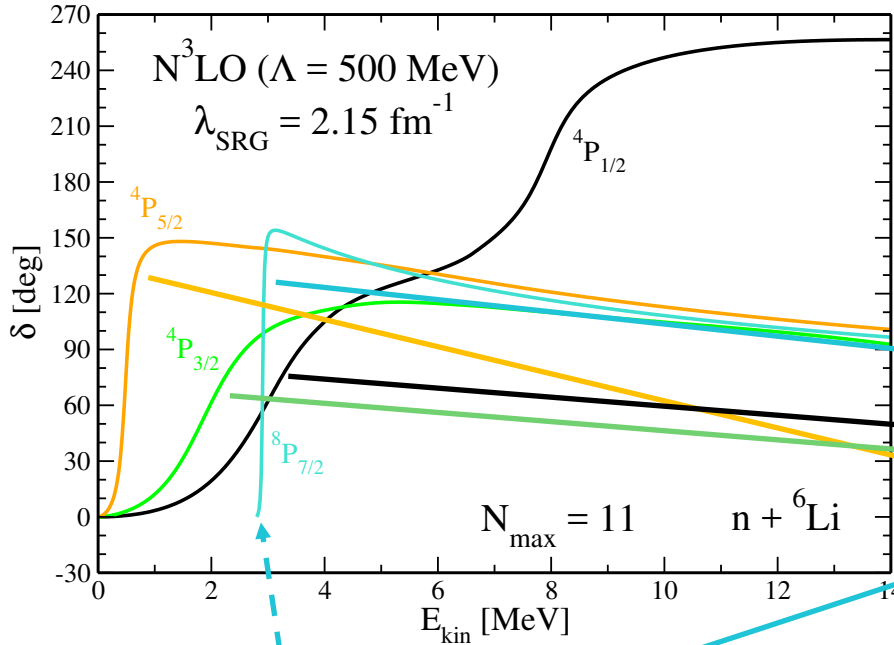
$$\frac{2.467}{{}^4\text{He}+t}$$



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

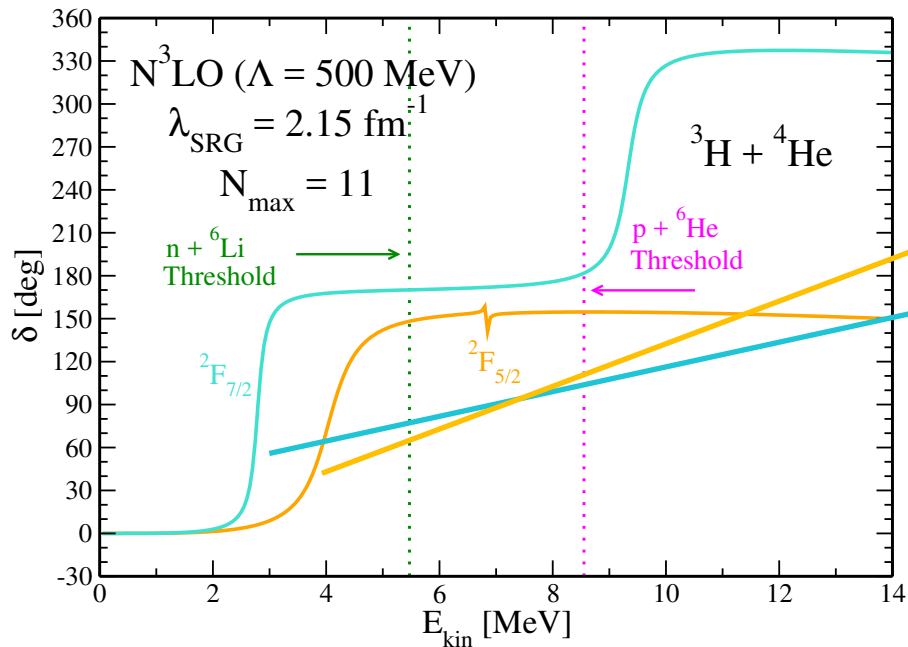
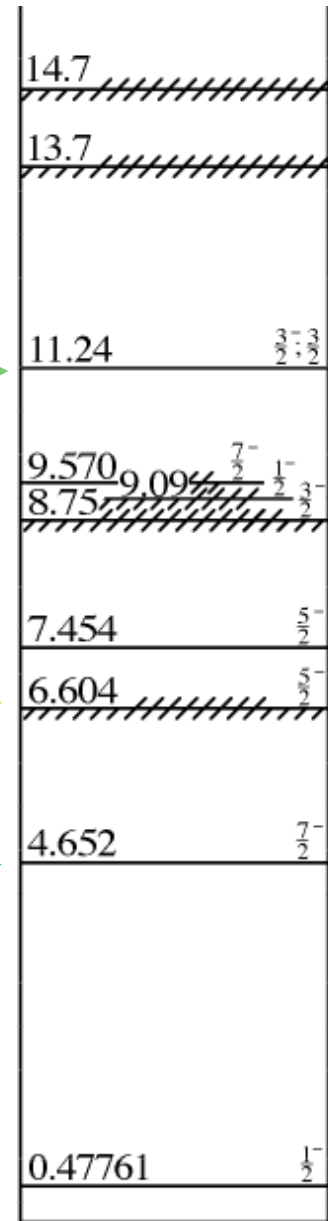
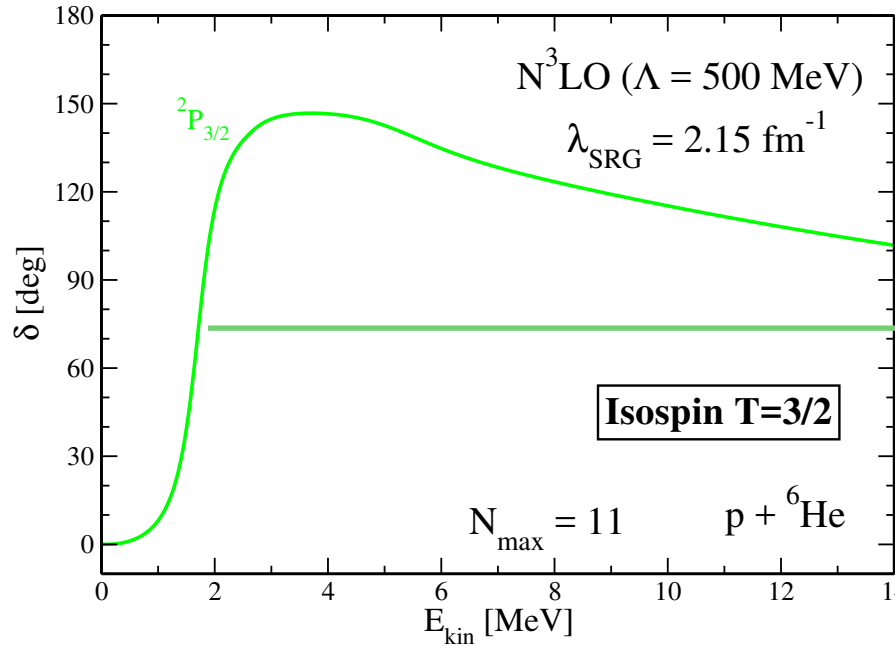


${}^7\text{Li}$ – Reproducing the energy spectrum



${}^7\text{Li}$

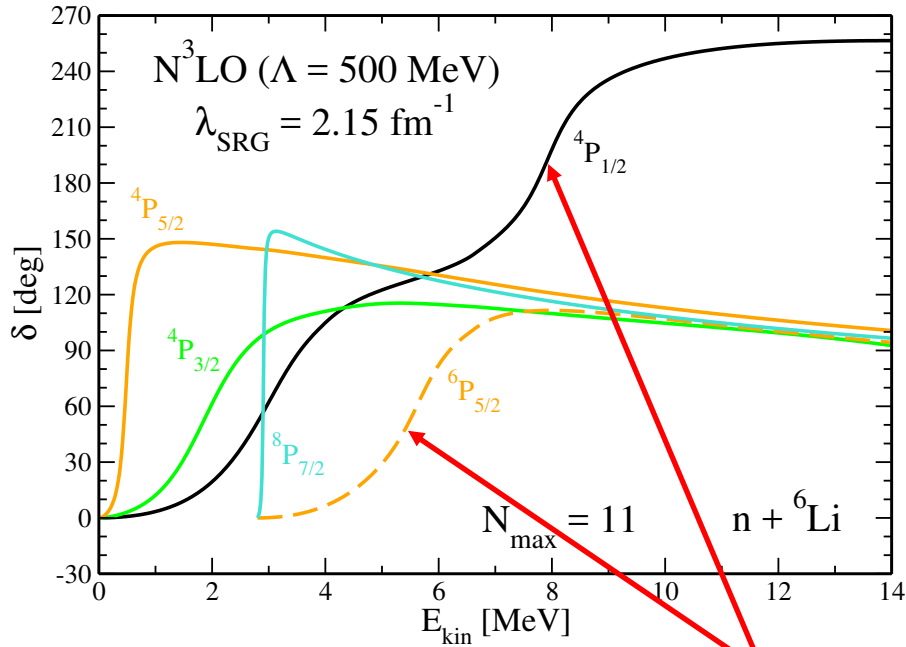
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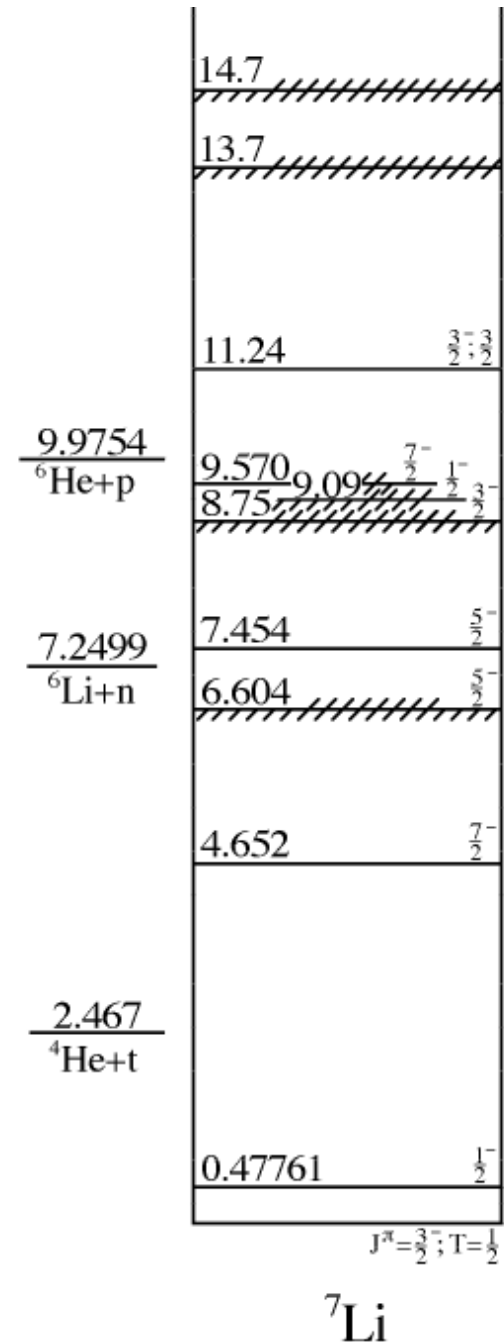
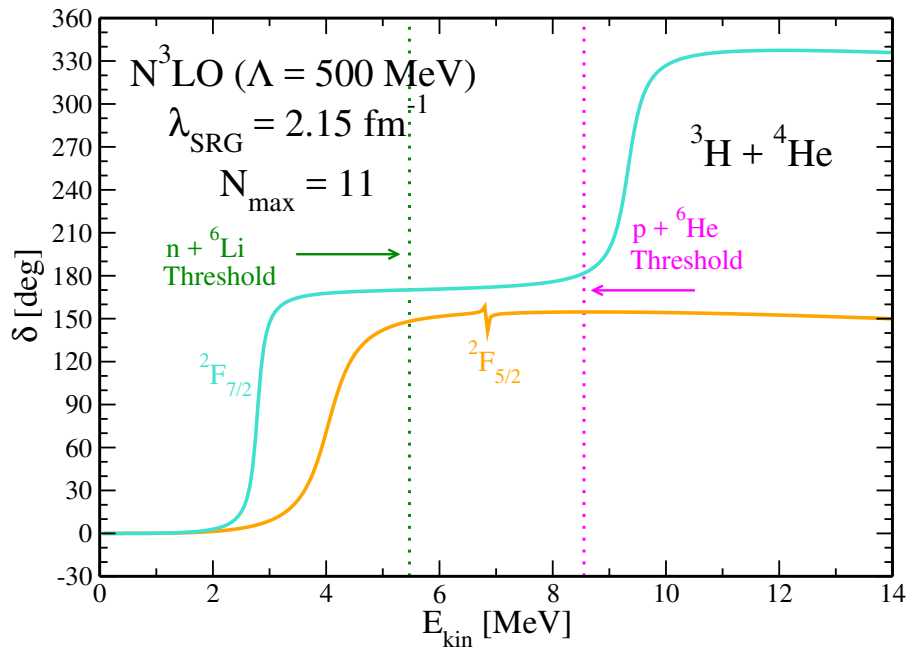
${}^7\text{Li}$

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

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

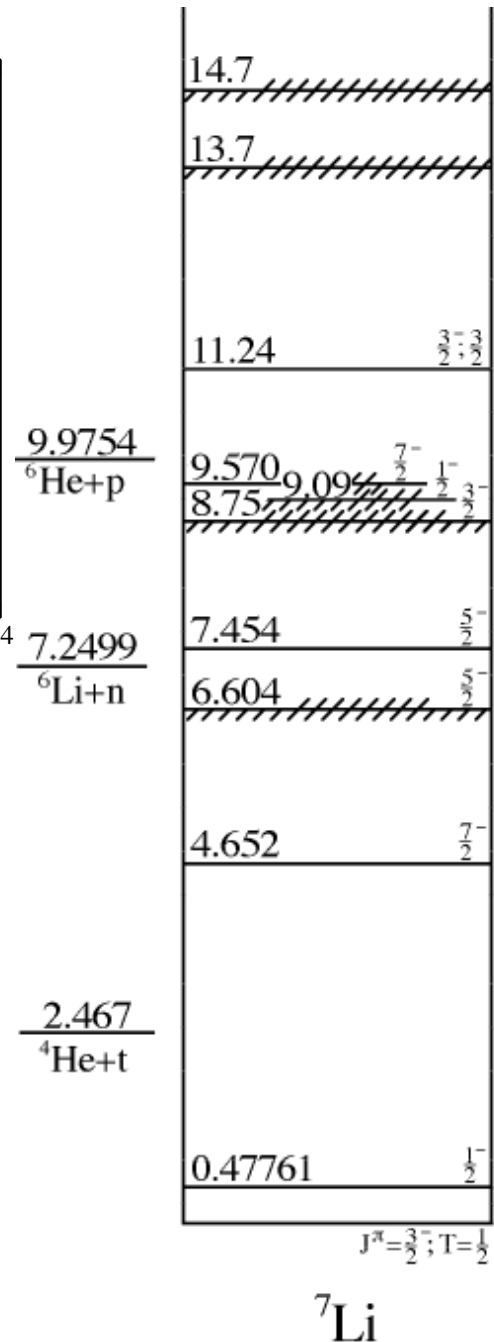
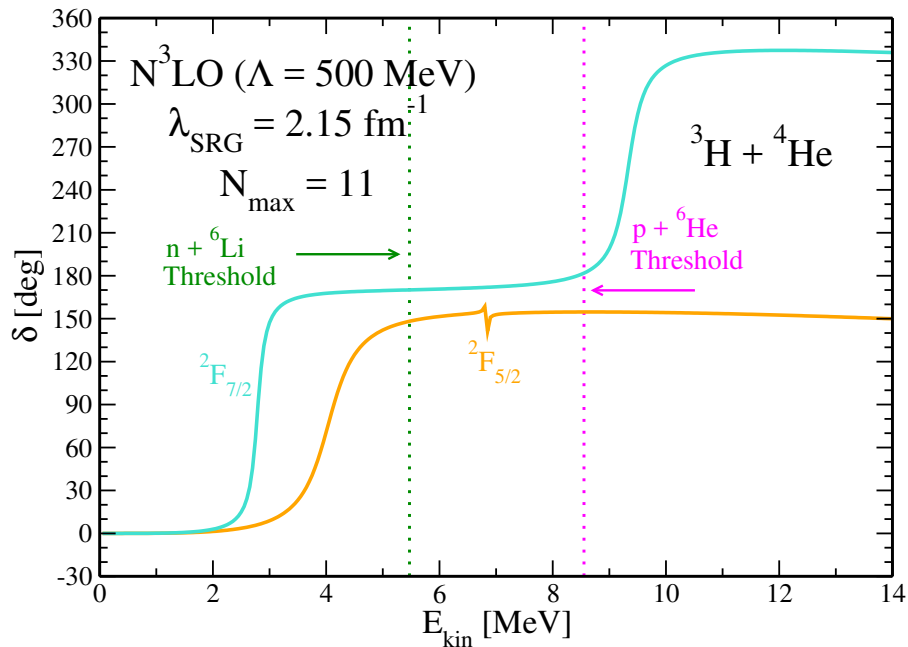
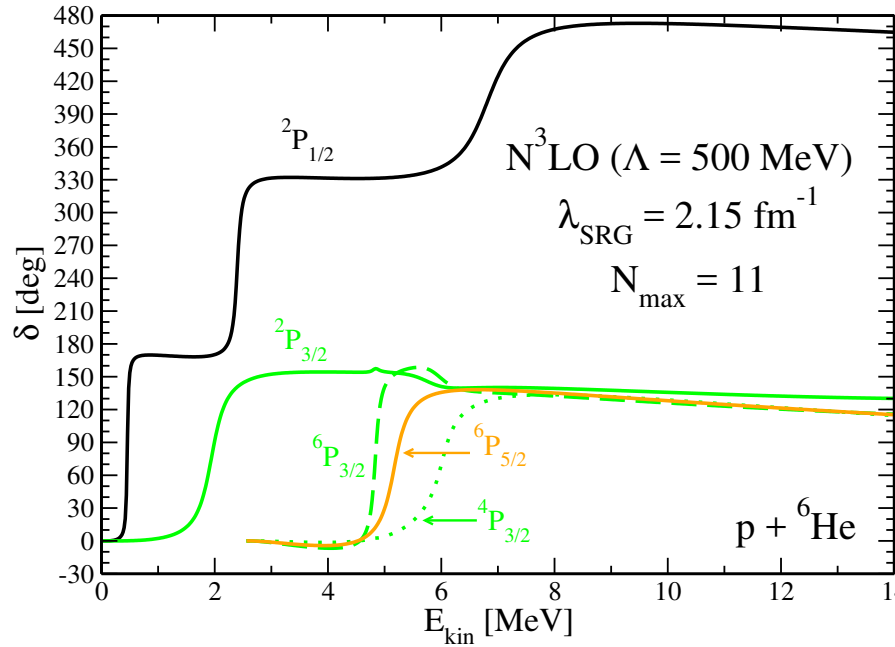


NEW



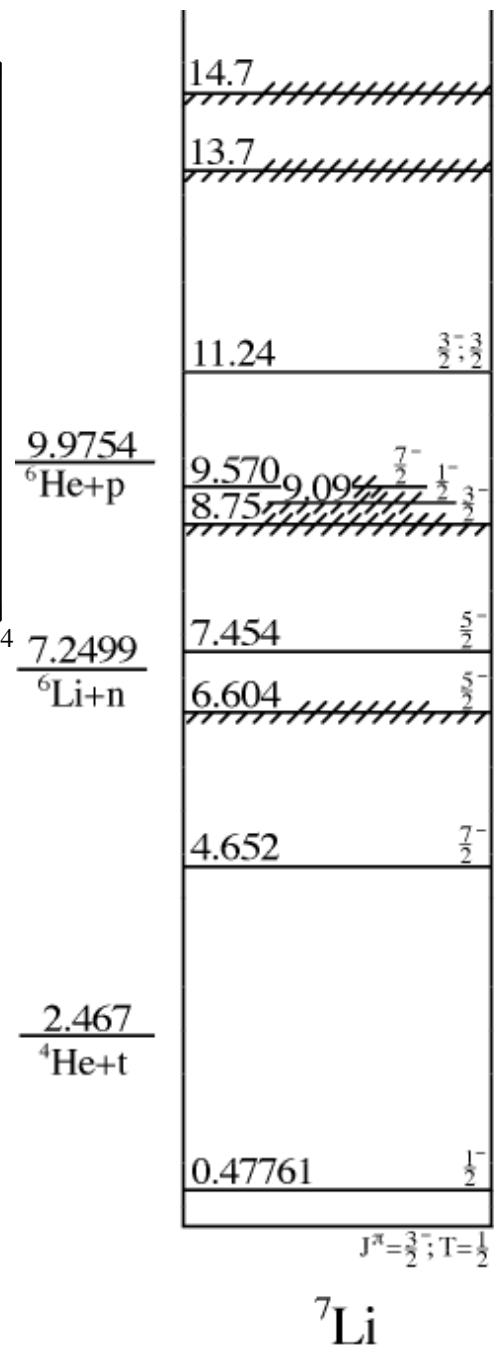
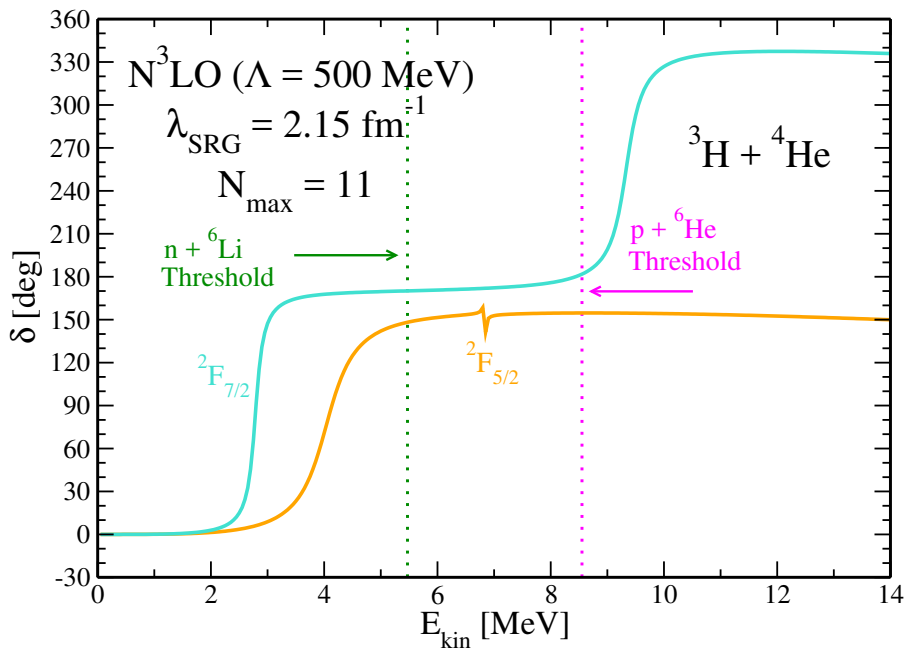
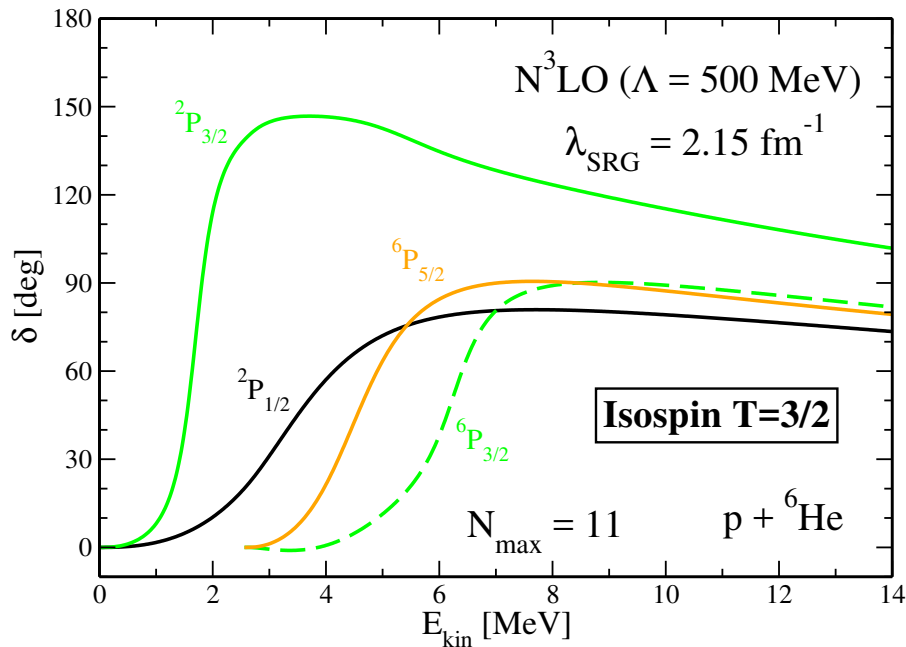
${}^7\text{Li}$ – New negative-parity states

7 new $T=1/2$
resonances

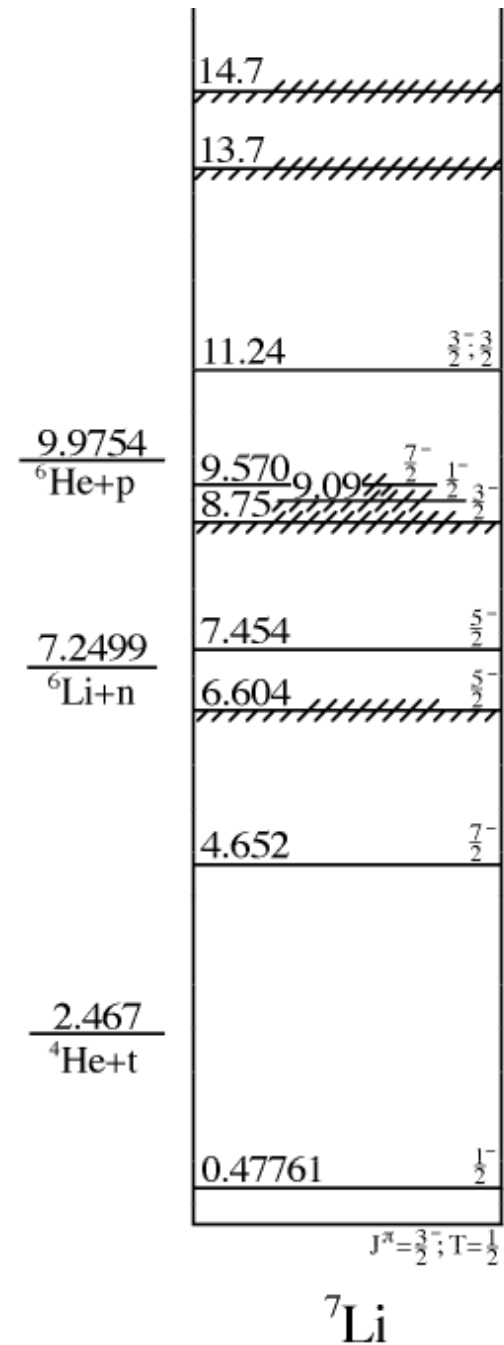
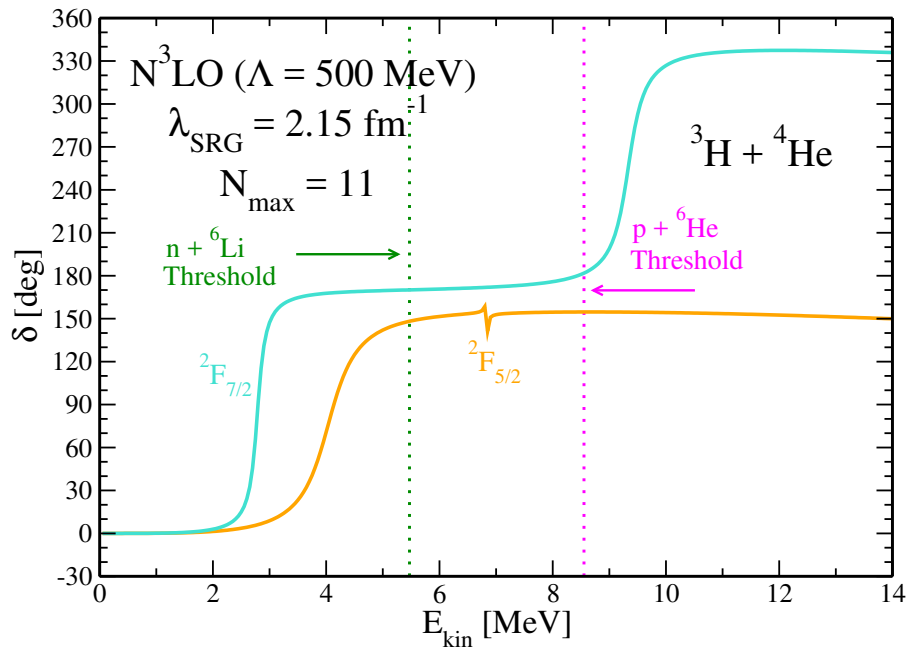
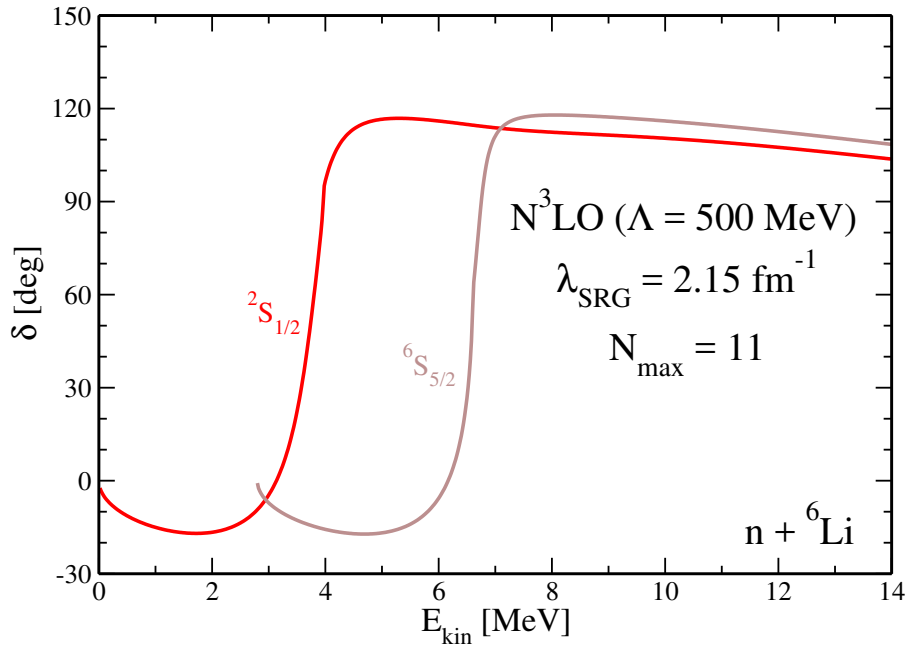


${}^7\text{Li}$ – New negative-parity states

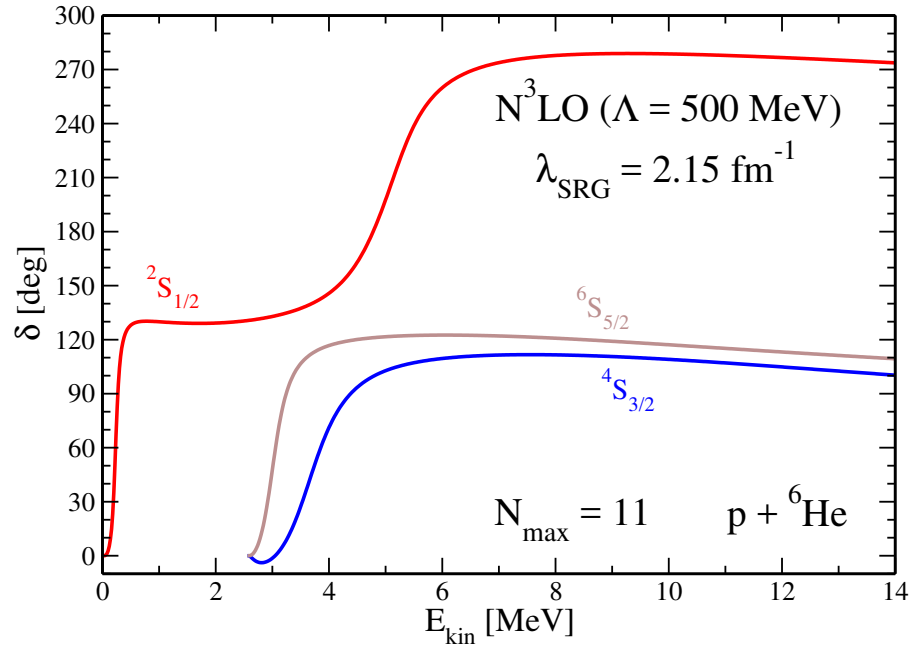
3 new $T=3/2$ resonances



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

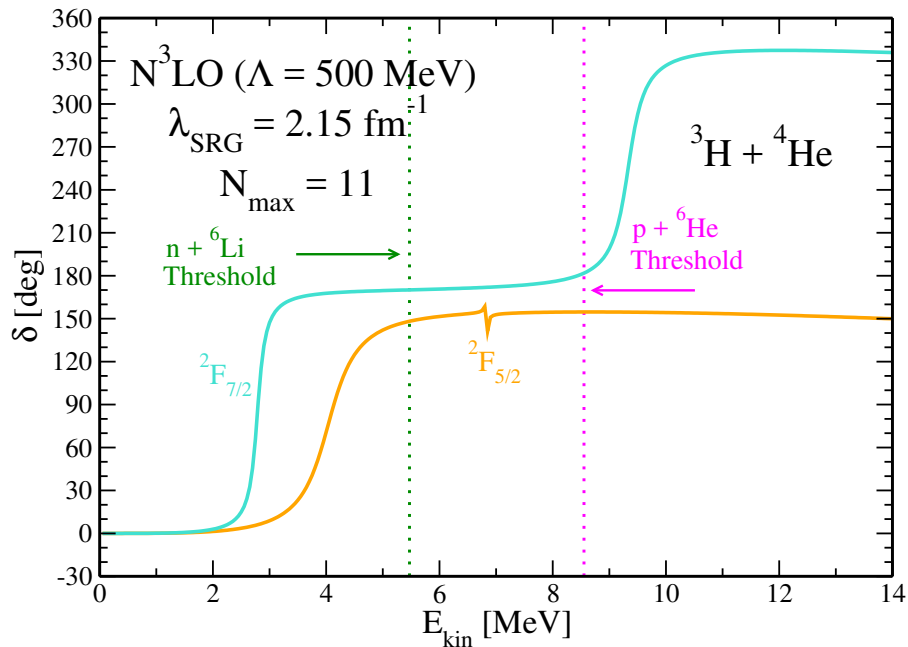
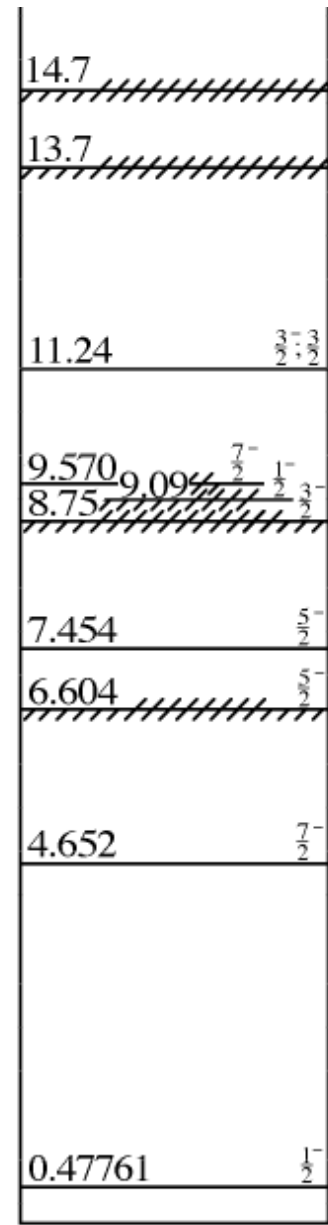


${}^7\text{Li}$ – New positive-parity states



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

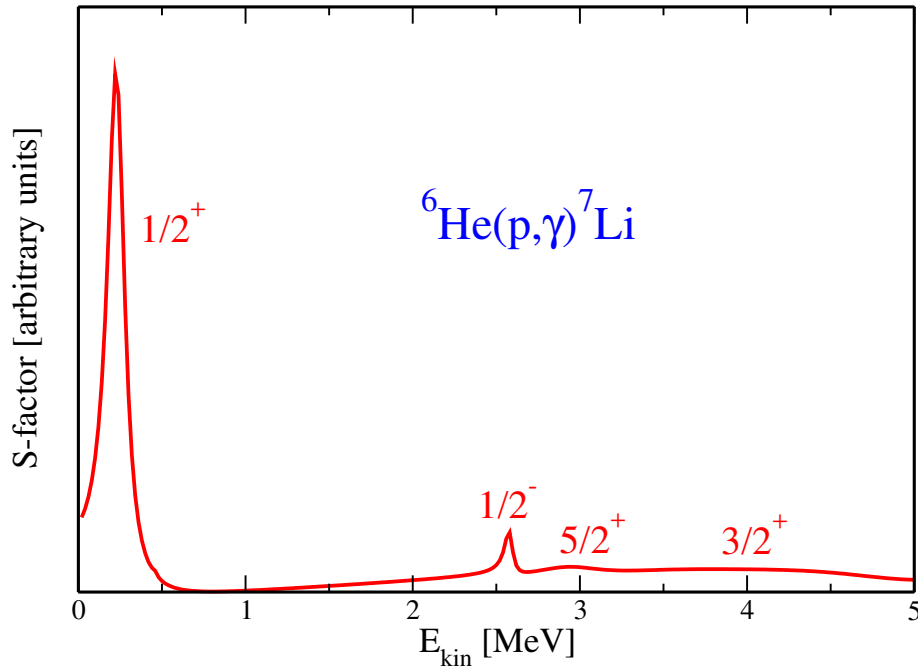
$\frac{7.2499}{{}^6\text{Li}+n}$



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

${}^7\text{Li}$

S-factors

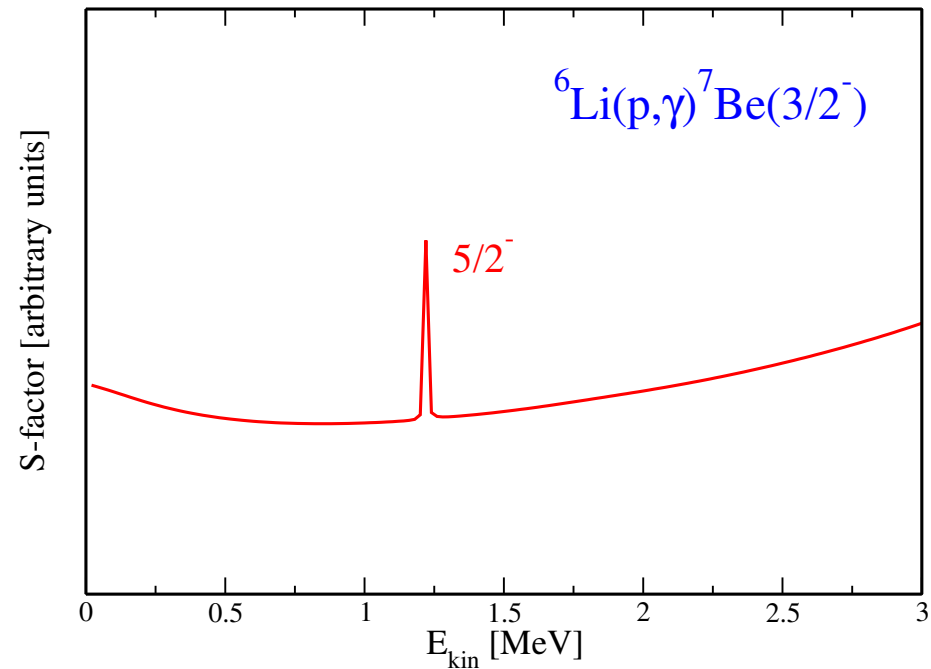


Cross section and S-factor

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

Sommerfeld parameter

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



2.

**Microscopic optical potentials for
intermediate energies**

Motivation

1. Facility for Antiprotons and Ion Research (FAIR) is currently under construction and experiments on antiproton scattering off nuclear targets will probably experience a renaissance
2. A new $\bar{N}N$ chiral interaction has been recently derived up to N³LO in the chiral expansion scheme
 - ➔ Dai, Haidenbauer, Meißner, JHEP **2017**, 78 (2017)

Purpose: Construction of a microscopic Optical Potential (OP) for antiproton elastic scattering off nuclei

- ➔ No fitting to $N(\bar{N})$ - nucleus elastic scattering data
- ➔ More predictive power where experimental data do not exist

Method: Extension of the Watson multiple scattering theory to antiproton-nucleus scattering

Statement of the problem

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

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

All two particle 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 projectile-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

$$P + Q = 1$$

$$[G_0, P] = 0$$

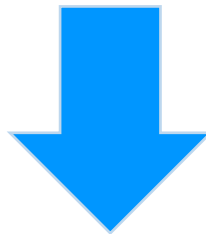
In the case of elastic scattering,
 P projects onto the elastic channel

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

Statement of the problem

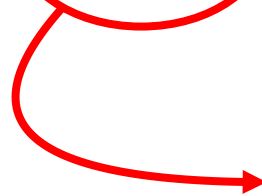
Lippmann-Schwinger (LS) equation for the projectile-nucleus transition amplitude

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



Transition amplitude T for elastic scattering

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

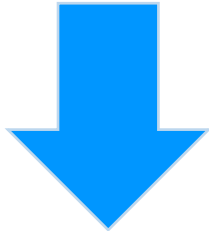


we need to calculate PUP

Statement of the problem

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

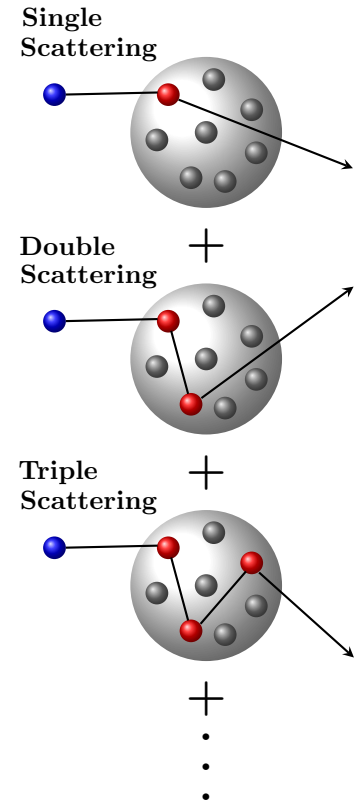
$$T_{\text{el}} = PUP + PUPG_0(E)T_{\text{el}}$$



Spectator expansion for U

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

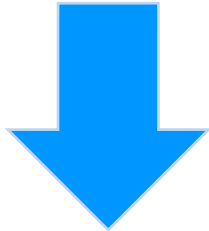
$$U = \sum_{i=1}^A \tau_i + \sum_{i,j \neq i}^A \tau_{ij} + \sum_{i,j \neq i, k \neq i,j}^A \tau_{ijk} + \dots$$



Single scattering approximation

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

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

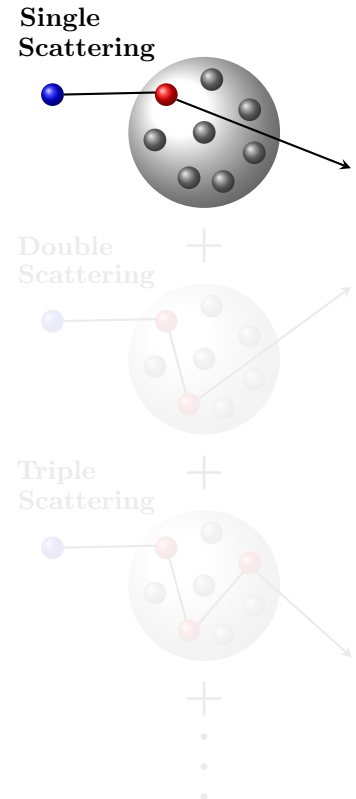


Spectator expansion for U

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

Single scattering approximation

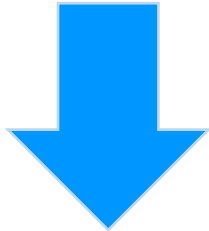
$$U = \sum_{i=1}^A \tau_i + \sum_{i,j \neq i}^A \tau_{ij} + \sum_{i,j \neq i, k \neq i,j}^A \tau_{ijk} + \dots$$



Impulse approximation

Lippmann-Schwinger (LS) equation for the projectile-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

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

$$\times \rho_N \left(\mathbf{P} - \frac{A-1}{2A} \mathbf{q}, \mathbf{P} + \frac{A-1}{2A} \mathbf{q} \right)$$

$$\mathbf{q} = \mathbf{k}' - \mathbf{k}$$

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

Basic ingredients

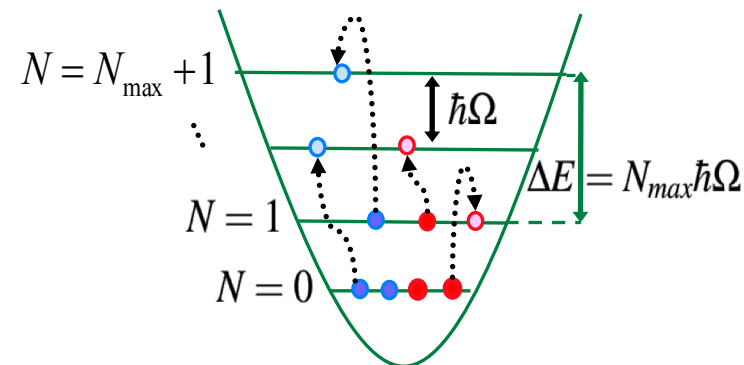
- (Anti)nucleon-nucleon scattering matrix $t_{\alpha N}$
- Non-local nuclear densities

Projectiles

$$\alpha = (p, n, \bar{p})$$

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

The matrix elements between a general initial and final state are obtained from the NCSM
 PRC **97**, 034619 (2018)

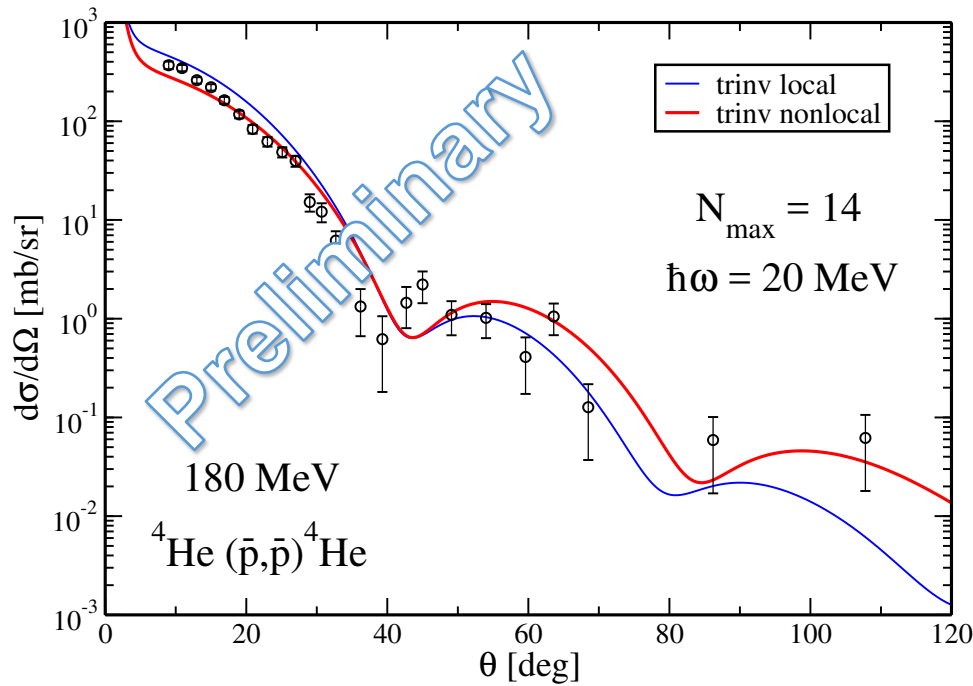


Chiral interaction

- Target density
 - NN - N⁴LO500 Entem, Machleidt, Nosyk, PRC **96** 024004 (2017)
 - + 3N - N²LO Navratil, Few-Body Syst. **41** 117 (2007)

- Scattering matrix
 - $\bar{N}N - N^3LO$ Dai, Haidenbauer, Meißner, JHEP **2017**, 78 (2017)
 - Local regulator for the long range part: $R = 0.9$ fm
 - Non-local regulator for the contact terms: $\Lambda = 2 R^{-1}$
 - The $\bar{N}N$ interaction is connected to the NN one through the G-parity in an unambiguous way

Scattering observables



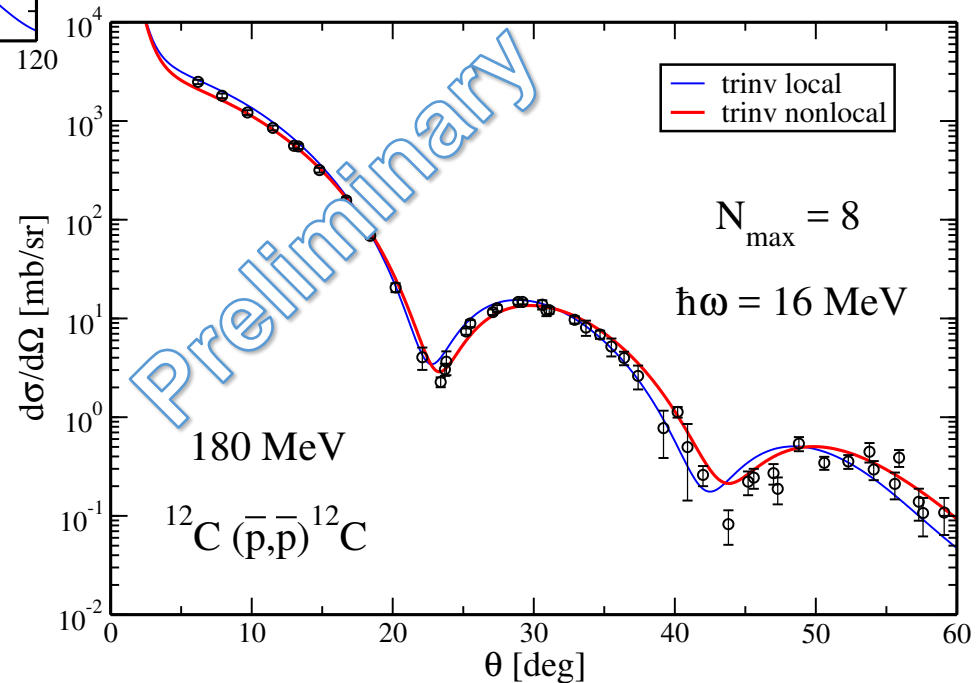
Experimental data are from the LEAR collaboration at CERN

Factorized optical potential

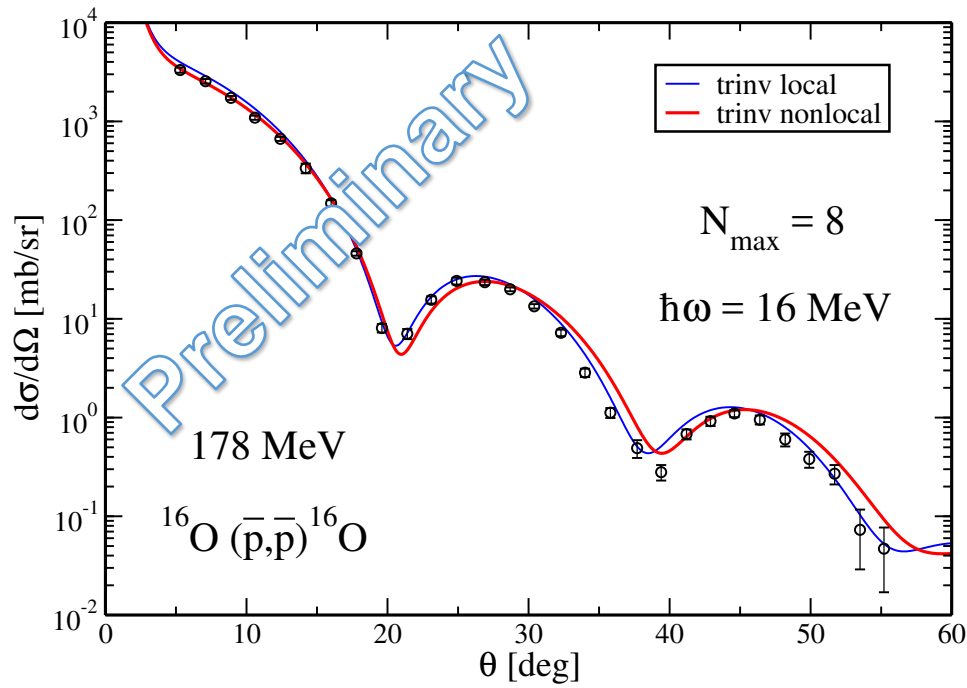
$$U(\mathbf{q}, \mathbf{K}; E) \sim \sum_{\alpha=n,p} t_{p\alpha} \left[\mathbf{q}, \frac{A+1}{2A} \mathbf{K}; E \right] \rho_{\alpha}(q)$$

FF from local density

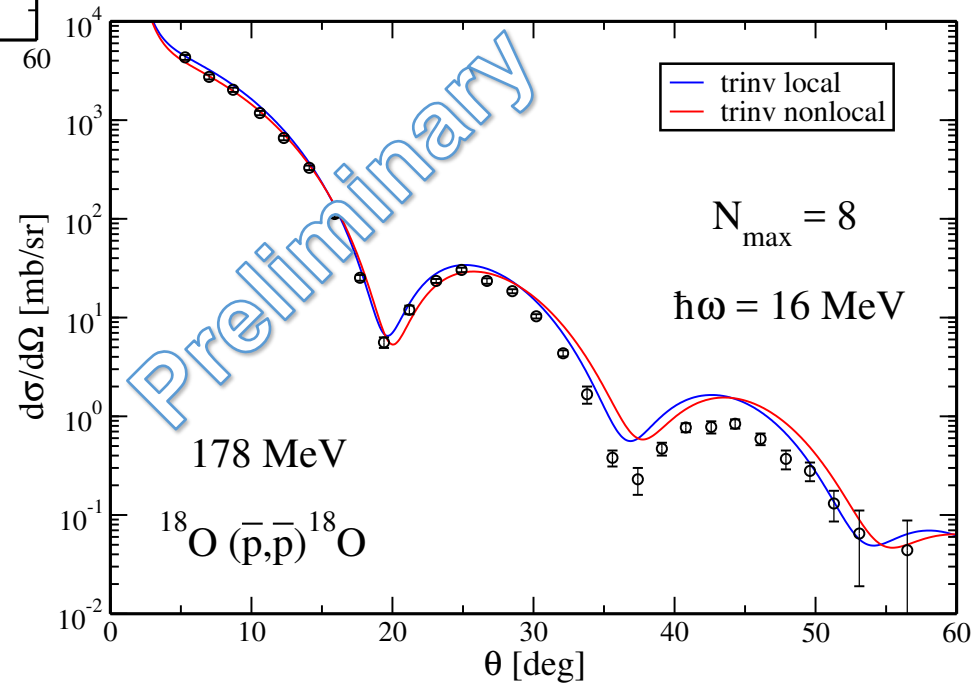
$$\rho_{\alpha}(q) = 4\pi \int_0^{\infty} dr r^2 j_0(qr) \rho_{\alpha}(r)$$



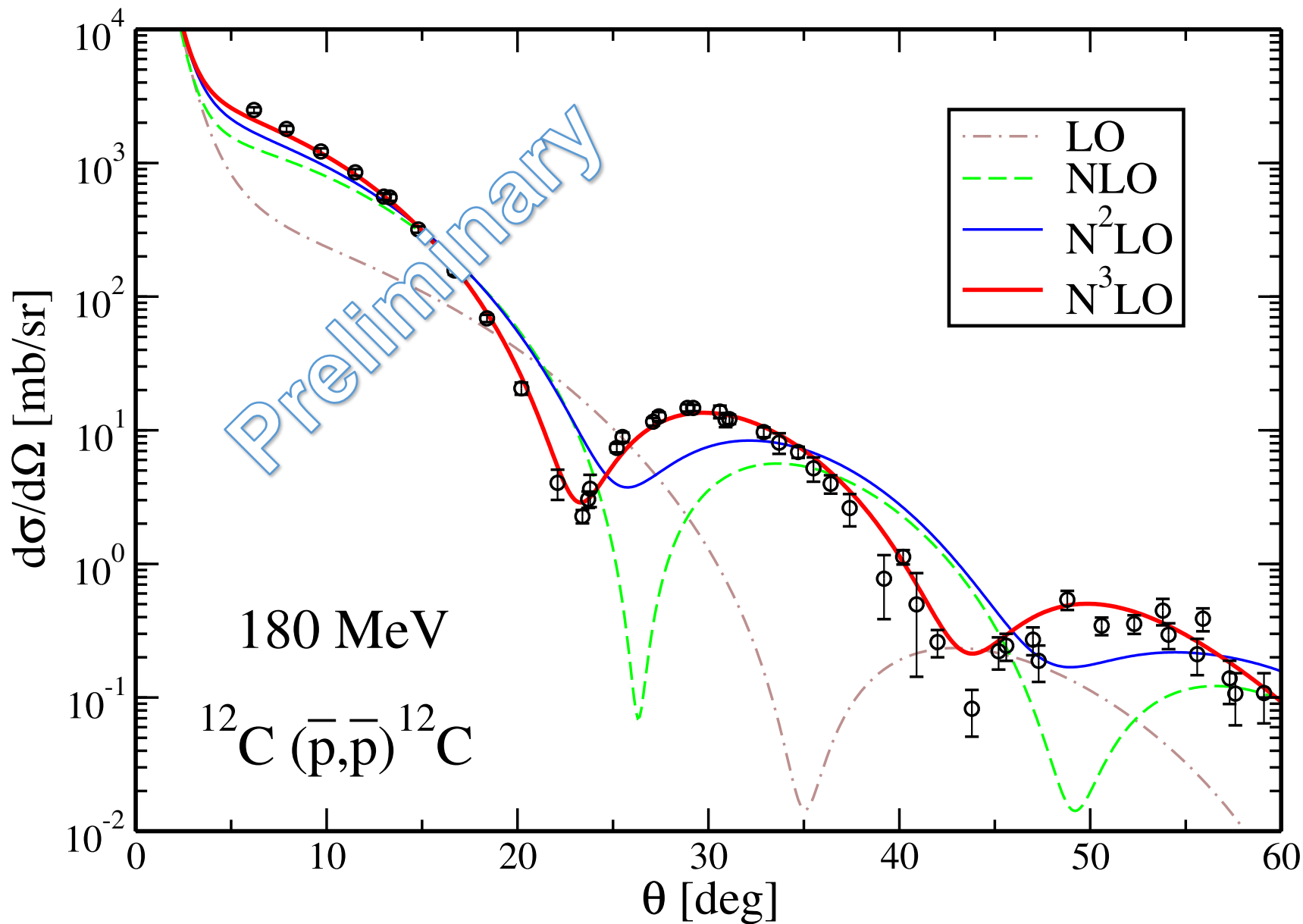
Scattering observables



Experimental data are from the
LEAR collaboration at CERN



Scattering observables



Summary & Outlook

- Reproduction of the experimental spectrum of ${}^7\text{Be}$ and ${}^7\text{Li}$
- Predictions for possible new resonant states ($\pi=+,-$)
 - ➔ Coupling between different mass partitions
 - ➔ Inclusion of the 3N force
- Good description of the data with the microscopic OP
 - ➔ Inclusion of the 3N force in NA scattering
 - ➔ Inclusion of medium effects
- Importance of $\bar{\text{N}}\text{NN}$ force