^{7}Li in the no-core shell model with continuum framework with coupling of mass partitions

Jakub Herko

Collaborators: Petr Navratil, Konstantinos Kravvaris, Sofia Quaglioni, Guillaume Hupin, Mark A. Caprio

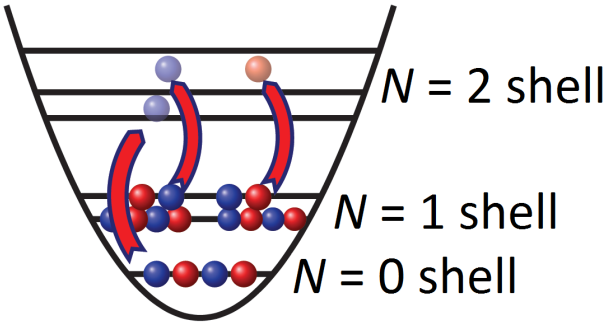
Outline

- No-core shell model (NCSM)
- No-core shell model with continuum (NCSMC)
- First NCSMC calculations
  with 3 coupled mass partitions: ^{4}He + ^{3}H, ^{6}Li + n, ^{6}He + p

  - Energies of bound states of ^{7}Li
  - Resonances in ^{7}Li - experimentally observed and predicted
  - Reactions ^{6}Li$(n,n)^6$Li, ^{6}Li$(n,p)^6$He,
    ^{6}He$(p,p)^6$He, ^{6}He$(p,n)^6$Li, ^{6}He$(p,t)^4$He

No-core shell model (NCSM)

- System of nucleons described by intrinsic Hamiltonian $H = T_{\text{int}} + \sum_{i<j} V_{ij}$
- Schrödinger equation $H|\Psi\rangle = E|\Psi\rangle$ solved as eigenvalue problem for Hamiltonian matrix
- Basis of Slater determinants constructed from harmonic oscillator single-particle states with frequency Ω
- Each basis state carries $N = N_0 + N_{\text{ex}}$ oscillator quanta
  N_0 ... number of oscillator quanta in lowest Pauli-allowed configuration



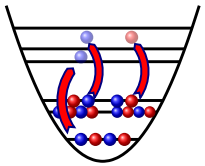
- Basis truncated by keeping only states with $N_{\text{ex}} \leq N_{\text{max}}$

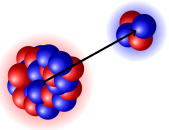
Figure courtesy of K. Kravvaris

No-core shell model with continuum (NCSMC)

- Describes both bound and scattering states
- Combines NCSM and NCSM/RGM methods
- NCSM/RGM organizes nucleons into clusters, each described within NCSM
- First, NCSM calculations for the whole system and the clusters are done
- Wave function expanded in terms of NCSM eigenstates and NCSM/RGM binary-cluster states:

$$\Psi = \sum_{\lambda} c_{\lambda} \left| \right\rangle + \sum_{\nu} \int dr u_{\nu}(r) \left| \right\rangle$$





r ... parameter coordinate playing role of distance between clusters
$u_{\nu}(r)$ ... continuous amplitudes representing intercluster relative motion

- Distribution of nucleons between clusters is called “mass partition”
- Expansion coefficients c_{λ} and amplitudes $u_{\nu}(r)$ calculated by solving NCSMC equations on Lagrange mesh

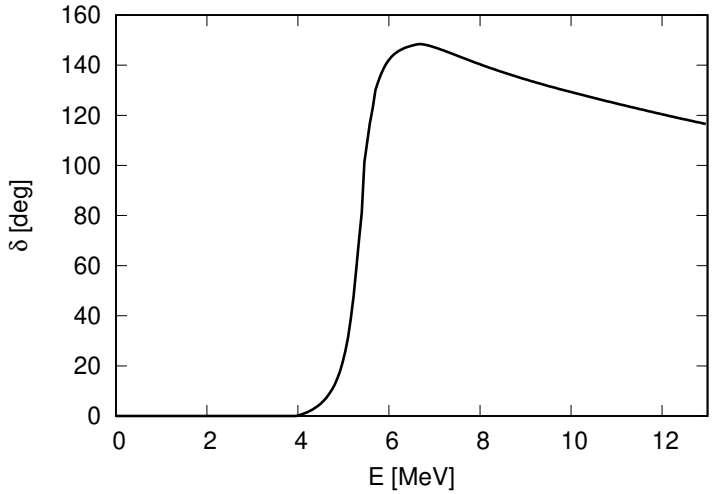
Figure courtesy of K. Kravvaris

No-core shell model with continuum (NCSMC)

- NCSMC equations can be solved for bound or scattering states by choosing asymptotic form of $u_\nu(r)$
- For scattering states:

$$u_\nu(r \to \infty) \propto \delta_{\nu i} I_\nu(r) - S_{\nu i} O_\nu(r)$$

  i ... initial channel
  $I_\nu(r)$, $O_\nu(r)$ ... ingoing and outgoing Coulomb wave functions
  $S_{\nu i}$ ... scattering matrix $\to$ cross sections
- Scattering matrix is unitary $\Rightarrow$ eigenvalues $e^{2i\delta}$
  δ ... eigenphase shifts $\to$ resonances:



Calculations for ^{7}Li within NCSMC coupling mass partitions ^{4}He + ^{3}H, ^{6}Li + n, and ^{6}He + p

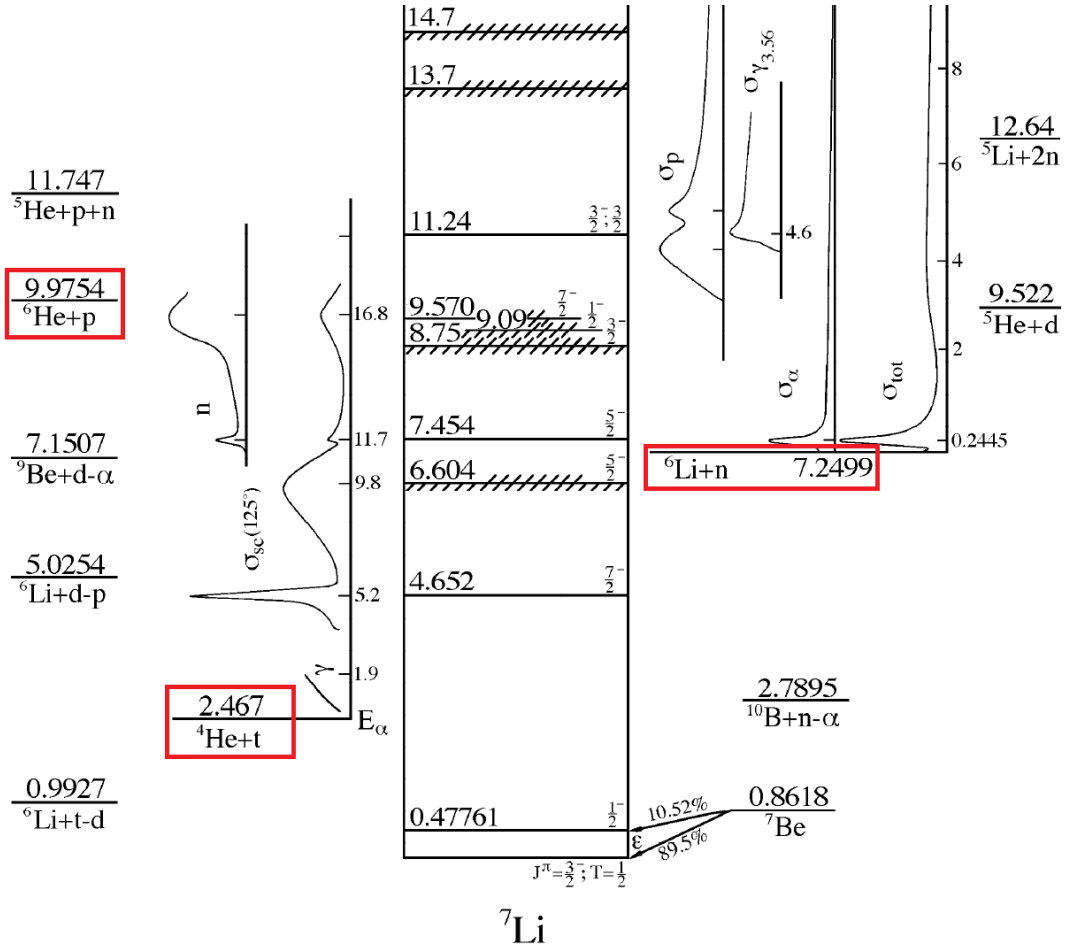


Figure from `https://nucldata.tunl.duke.edu`

Calculations for ^{7}Li within NCSMC coupling mass partitions ^{4}He + ^{3}H, ^{6}Li + n, and ^{6}He + p

- Motivation: nuclear astrophysics, primordial nucleosynthesis, ^{3}H for fusion energy generation via ^{6}Li$(n,t)^{4}$He
- Previous work [1,2] took into account these mass partitions in separate calculations
- We include mass partitions ^{4}He + ^{3}H, ^{6}Li + n, and ^{6}He + p in single calculation
- Coupling of mass partitions allows for calculation of charge-exchange and nucleon-transfer reactions

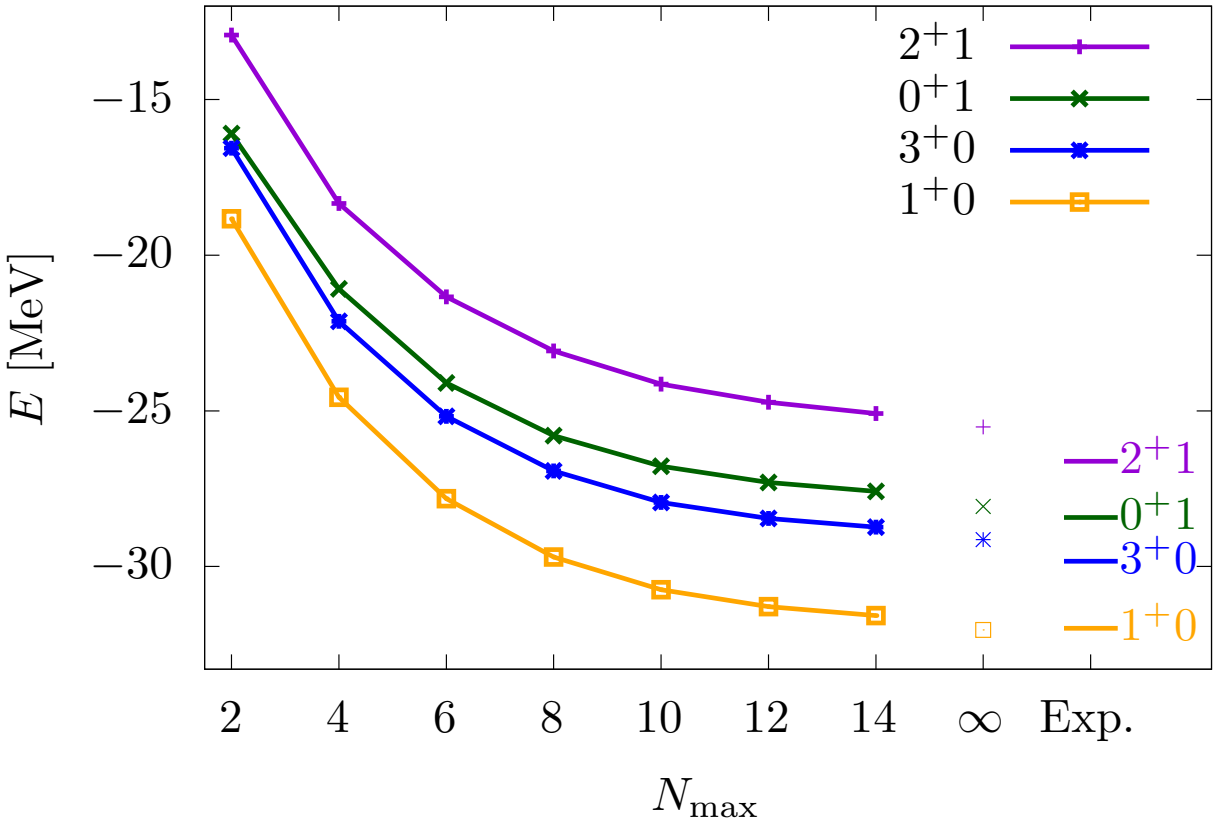
[1] Dohet-Eraly *et al.* Phys. Lett. B **757**, 430 (2016)
[2] Vorabbi *et al.* Phys. Rev. C **100**, 024304 (2019)

Calculations for ^{7}Li within NCSMC coupling mass partitions ^{4}He + ^{3}H, ^{6}Li + n, and ^{6}He + p

- SRG-evolved chiral N^{3}LO nucleon-nucleon interaction as in [1,2] used
- NCSM eigenstates taken into account:
  - 1 state of ^{4}He (0^+0) and 1 state of ^{3}H ($1/2^+1/2$)
  - 4 states of ^{6}Li: 1^+0, 3^+0, 0^+1, 2^+1
  - 2 states of ^{6}He: 0^+1, 2^+1
  - Lowest 12 negative-parity and lowest 6 positive-parity states of ^{7}Li
- $\hbar\Omega = 20$ MeV, $N_{\max} = 11$
- Calculated quantities: bound-state energies, energies and widths of resonances, cross sections of ^{6}Li$(n,n)^{6}$Li, ^{6}Li$(n,p)^{6}$He, ^{6}He$(p,p)^{6}$He, ^{6}He$(p,n)^{6}$Li, ^{6}He$(p,t)^{4}$He

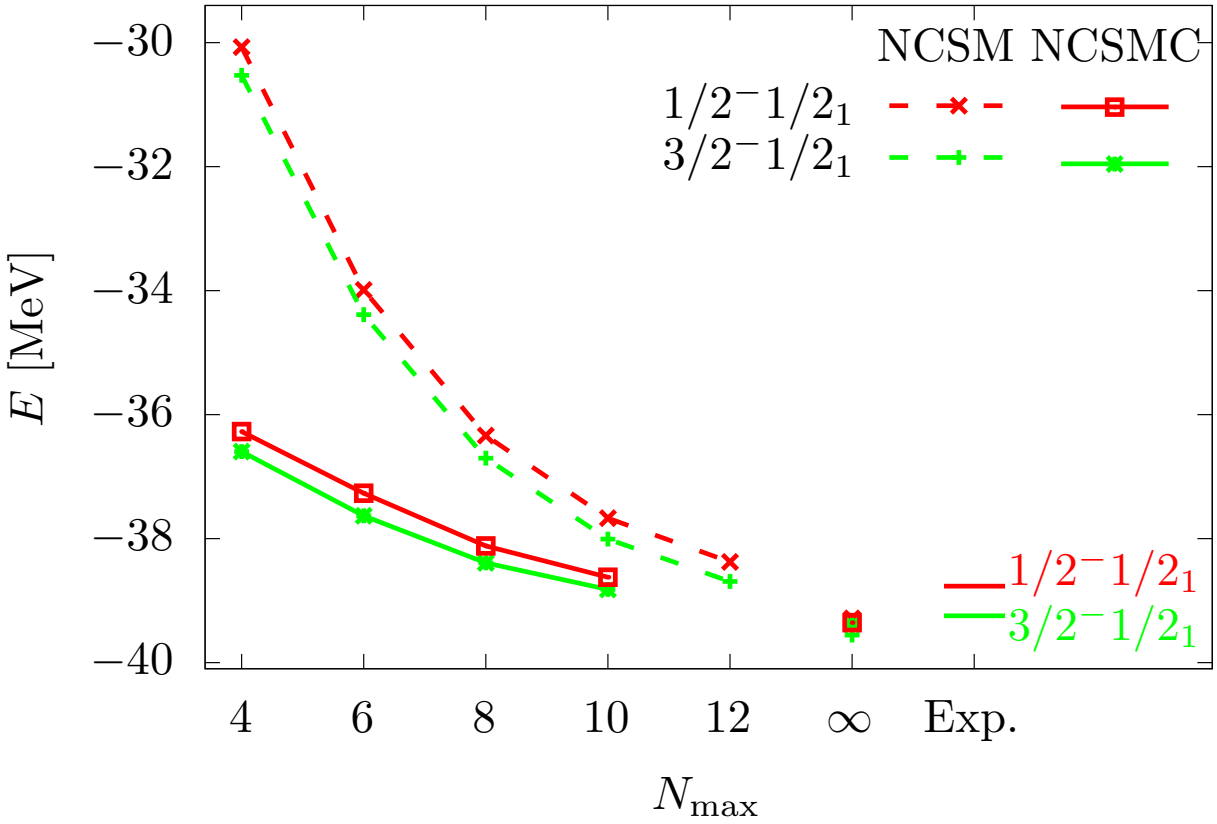
[1] Dohet-Eraly *et al.* Phys. Lett. B **757**, 430 (2016)
[2] Vorabbi *et al.* Phys. Rev. C **100**, 024304 (2019)

Energies of NCSM states of ^{6}Li



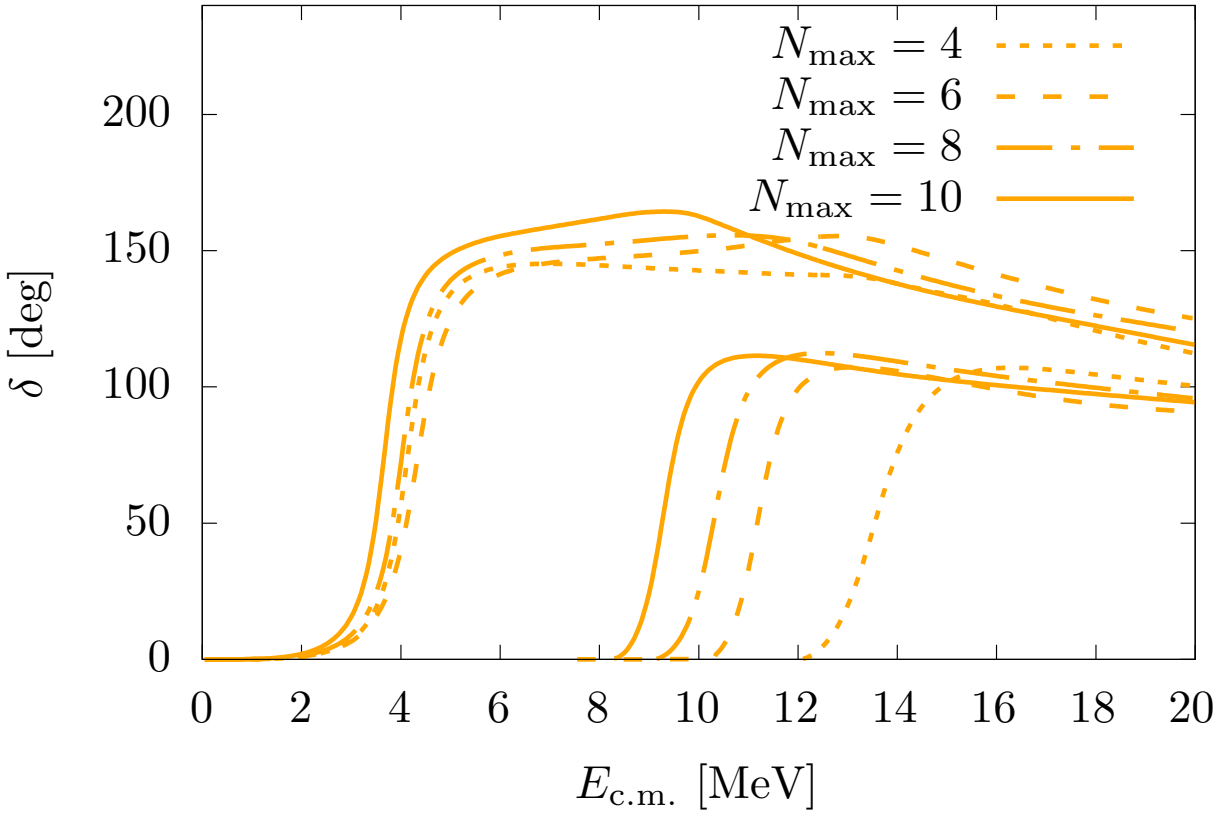
- Similar for ^{6}He
- Better for ^{4}He and ^{3}H

Energies of bound states of ^{7}Li



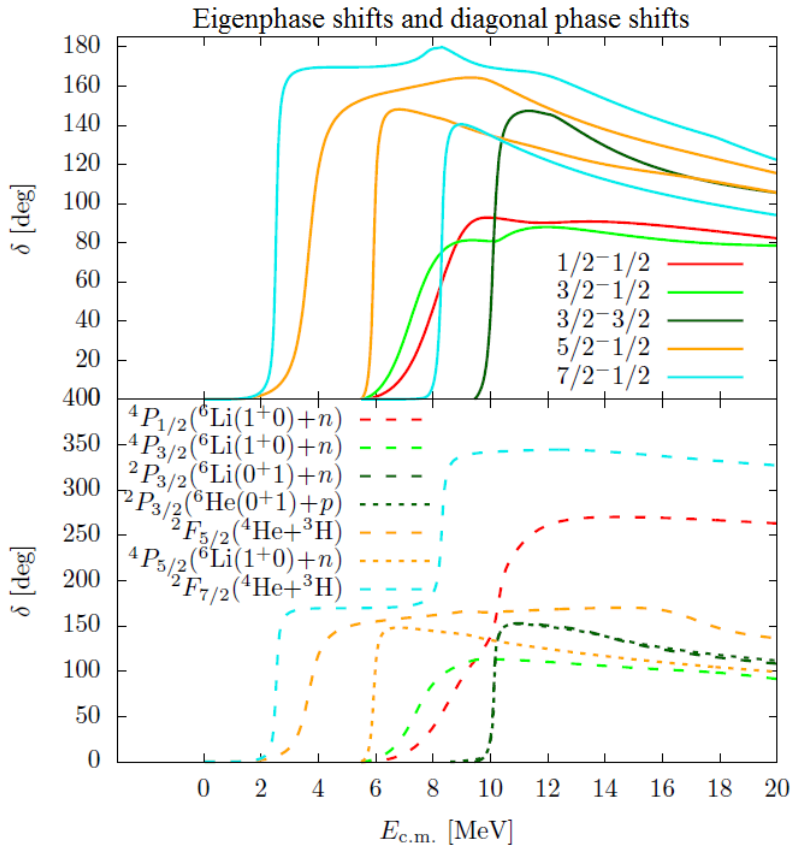
- NCSMC states more bound
- Extrapolated NCSM and NCSMC energies are the same

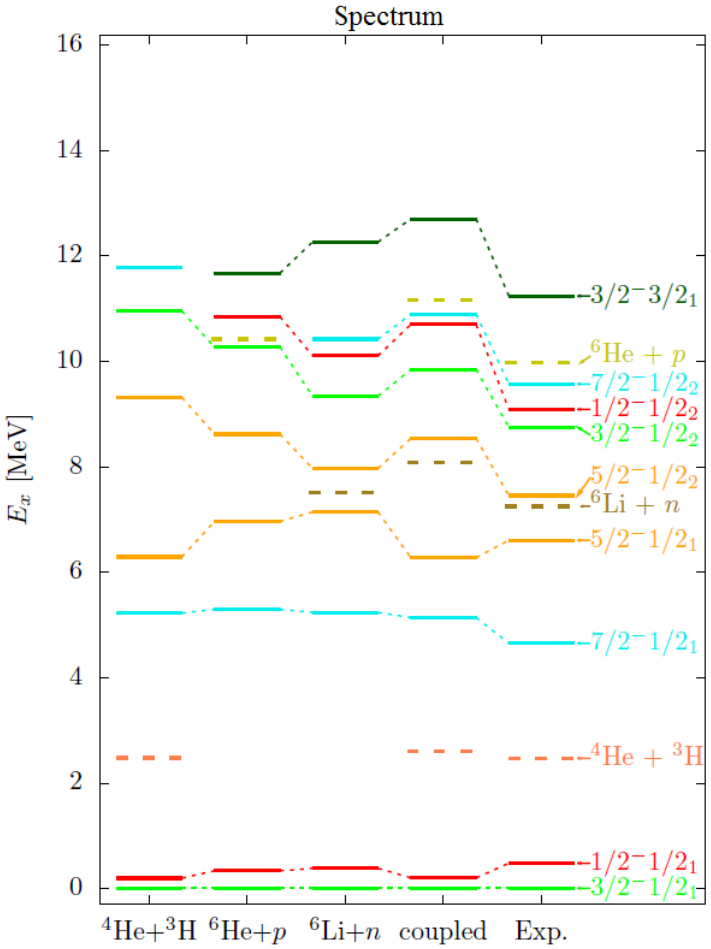
$5/2^-1/2$ eigenphase shifts



- Reasonable convergence for $5/2^-1/2_1$ resonance, similar for $7/2^-1/2_1$
- Less satisfactory convergence for other eigenphase shifts

Experimentally observed states in ^{7}Li

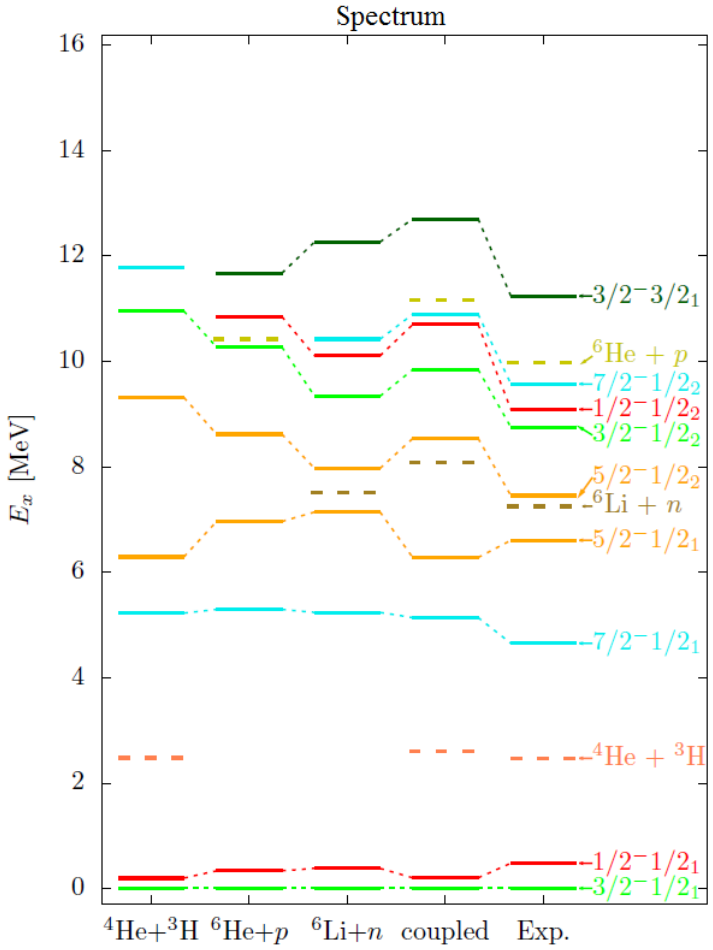




- Experimentally observed states reproduced in correct order
- Results depend on mass partition, effect of coupling

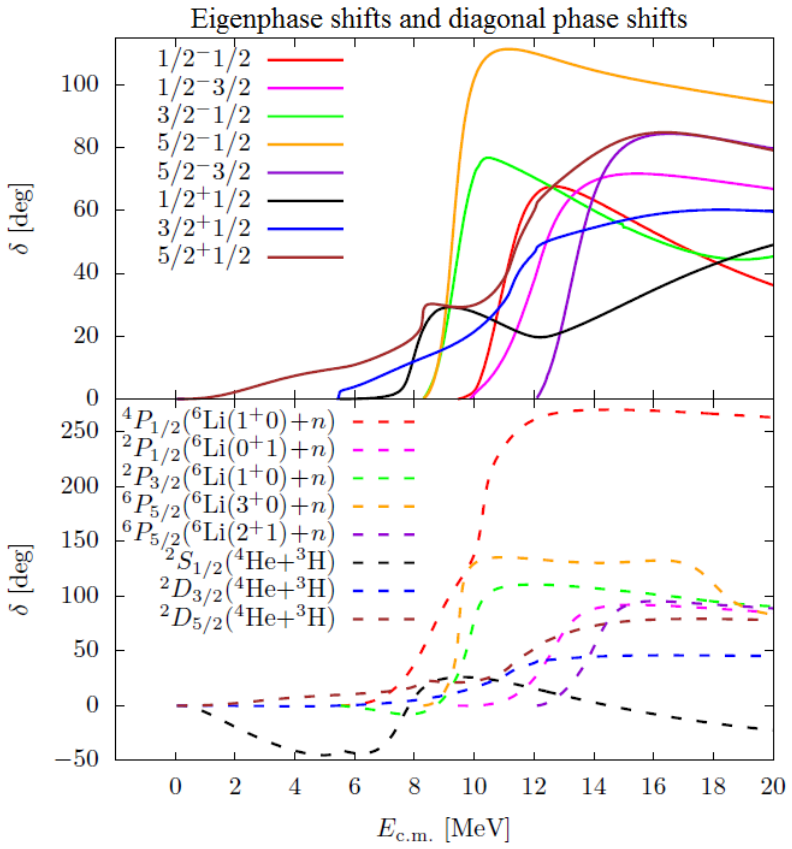
Experimentally observed states in ^{7}Li

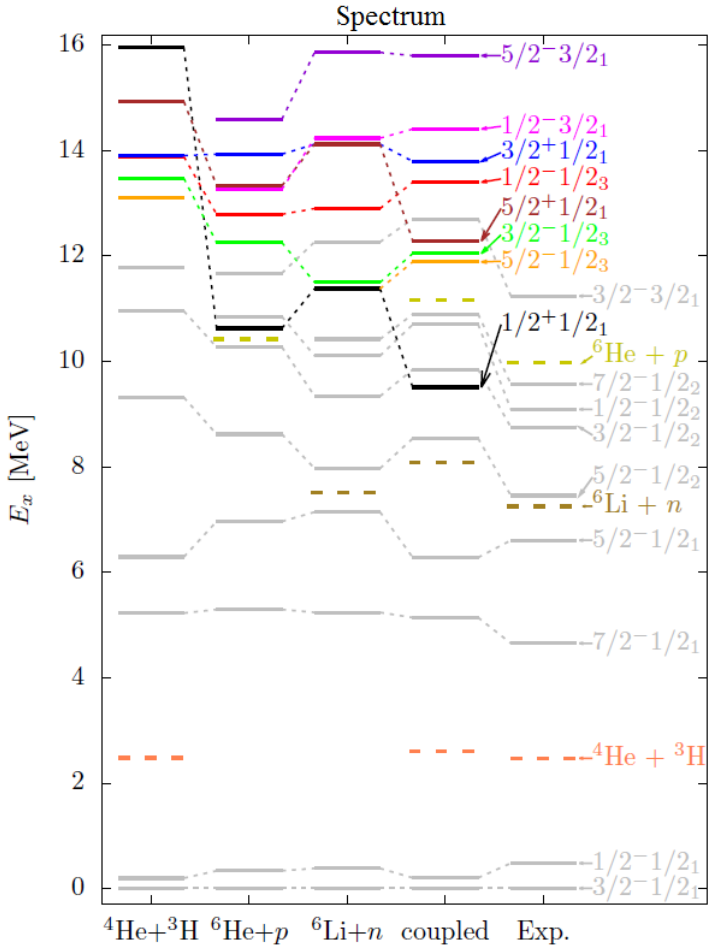
	^{4}He+^{3}H	^{6}He+p	^{6}Li+n	coupled		Exp.	
$J^{\pi}T_i$	Γ	Γ	Γ	E_r	Γ	E_r	Γ
$7/2^{-}1/2_1$	0.2			2.5	0.2	2.19	0.07
$5/2^{-}1/2_1$	0.8			3.7	0.7	4.14	0.92
$5/2^{-}1/2_2$	0.006		0.2	5.9	0.2	4.99	0.08
$3/2^{-}1/2_2$	0.3		1.7	7.2	2.1	6.28	4.71
$1/2^{-}1/2_2$	not found		2.6	8.1	2.4	6.62	2.75
$7/2^{-}1/2_2$	0.4		0.04	8.3	0.2	7.10	0.44
$3/2^{-}3/2_1$		0.4	0.4	10.1	0.3	8.77	0.26



- Experimentally observed states reproduced in correct order, widths consistent with experiment
- Results depend on mass partition, effect of coupling

Predicted resonances in ^{7}Li

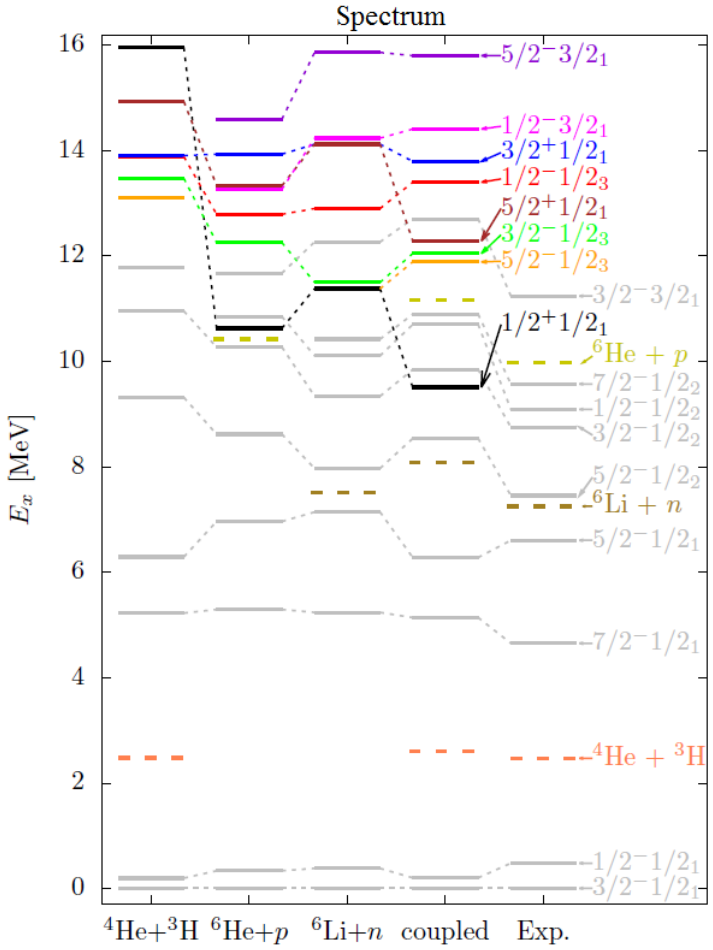




- Eight resonances predicted, including $T = 3/2$ resonances
- Results depend on mass partitions, effect of coupling

Predicted resonances in ^{7}Li

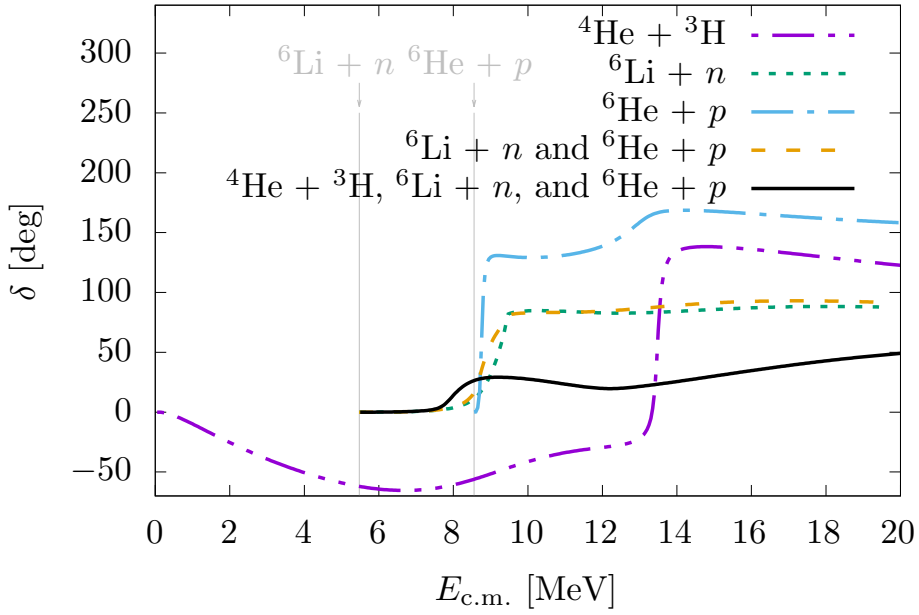
	^{4}He+^{3}H	^{6}He+p	^{6}Li+n	coupled	
$J^\pi T_i$	Γ	Γ	Γ	E_r	Γ
$1/2^+1/2_1$	0.2	0.1	1.2	6.9	4.9
$5/2^-1/2_3$	0.2	not found	1.0	9.3	0.9
$3/2^-1/2_3$	0.3	0.5	1.7	9.4	2.2
$5/2^+1/2_1$	5.1	0.5	1.2	9.7	6.3
$1/2^-1/2_3$	0.3	0.1	1.5	10.8	2.1
$3/2^+1/2_1$	0.1	1.1	0.1	11.2	5.0
$1/2^-3/2_1$		2.4	2.8	11.8	3.5
$5/2^-3/2_1$		2.1	2.7	13.2	2.2



- Eight resonances predicted, including $T = 3/2$ resonances
- Results depend on mass partitions, effect of coupling

$1/2^+$ eigenphase shift and diagonal phase shifts

- Previous NCSMC calculations neglecting coupling of mass partitions [2] predict S-wave $1/2^+$ resonance in ^{6}He + p just above proton separation threshold
- No such resonance was experimentally observed [3]

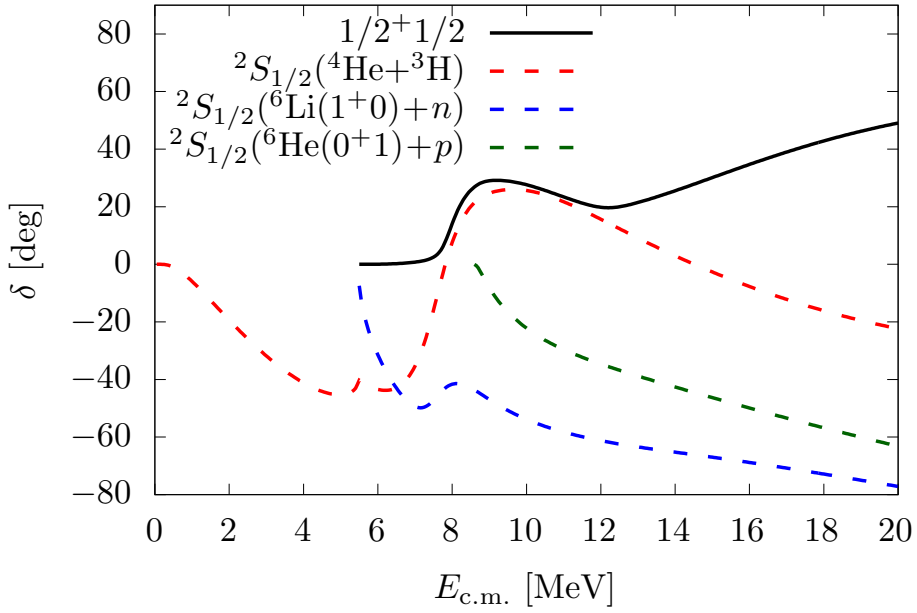


- In present calculation the $1/2^+$ resonance is below ^{6}He + p threshold and dominated by $^2S_{1/2}$(^{4}He + ^{3}H) channel

[2] Vorabbi *et al.* Phys. Rev. C **100**, 024304 (2019)
[3] Dronchi *et al.* Phys. Rev. C **107**, L061303 (2023)

$1/2^+$ eigenphase shift and diagonal phase shifts

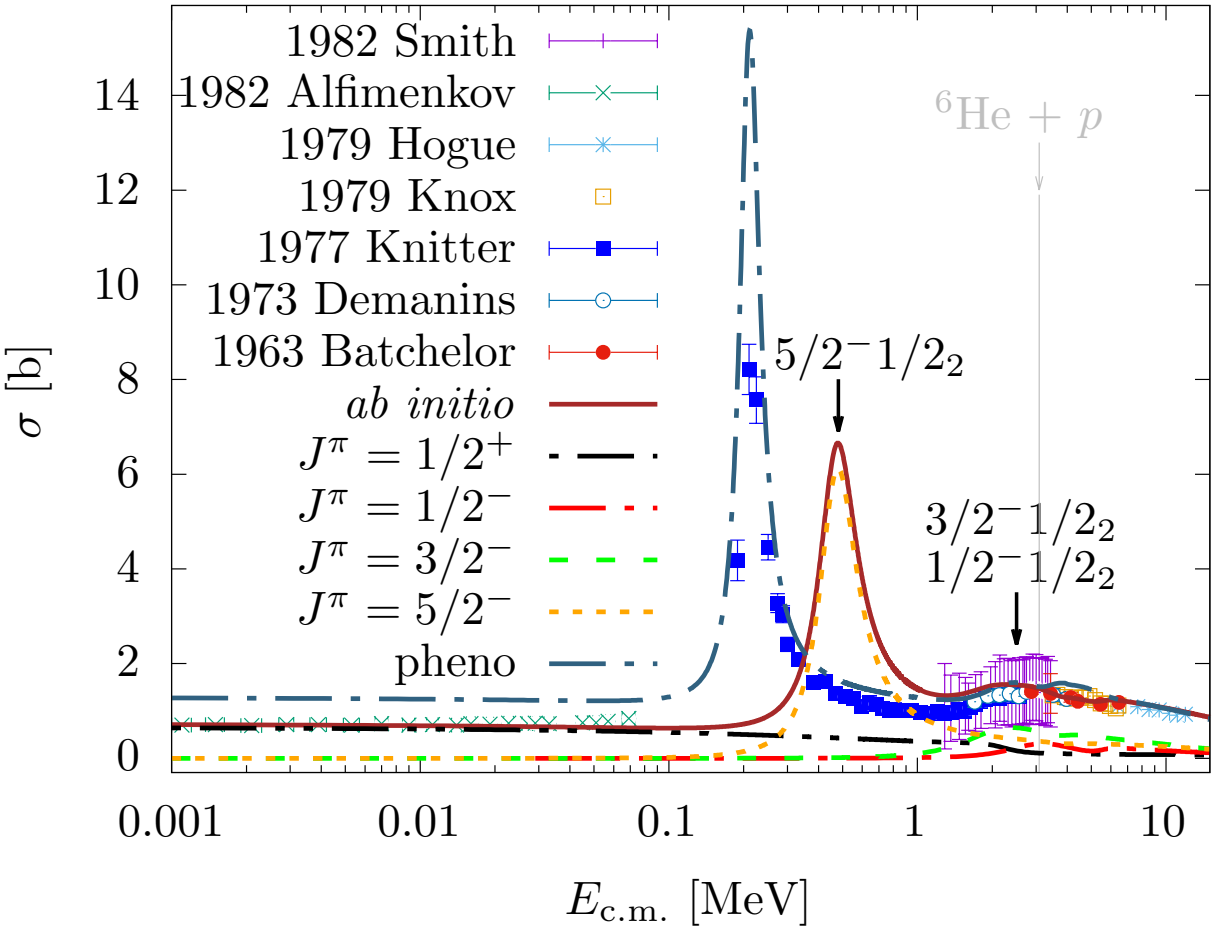
- Previous NCSMC calculations neglecting coupling of mass partitions [2] predict S-wave $1/2^+$ resonance in ^{6}He + p just above proton separation threshold
- No such resonance was experimentally observed [3]



- In present calculation the $1/2^+$ resonance is below ^{6}He + p threshold and dominated by $^2S_{1/2}(^4$He + ^{3}H) channel

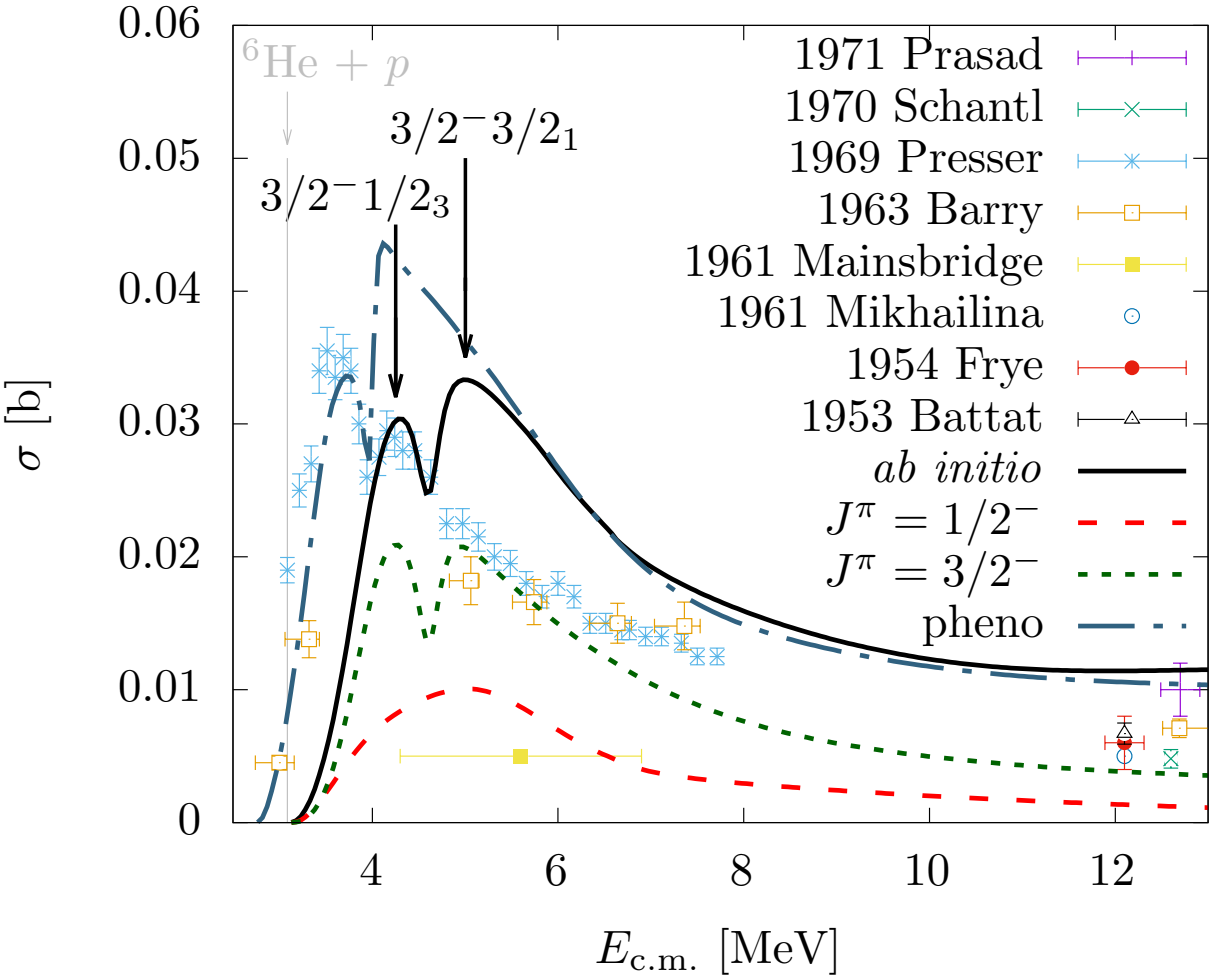
[2] Vorabbi *et al.* Phys. Rev. C **100**, 024304 (2019)
[3] Dronchi *et al.* Phys. Rev. C **107**, L061303 (2023)

Cross section of ^{6}Li + *n* elastic scattering



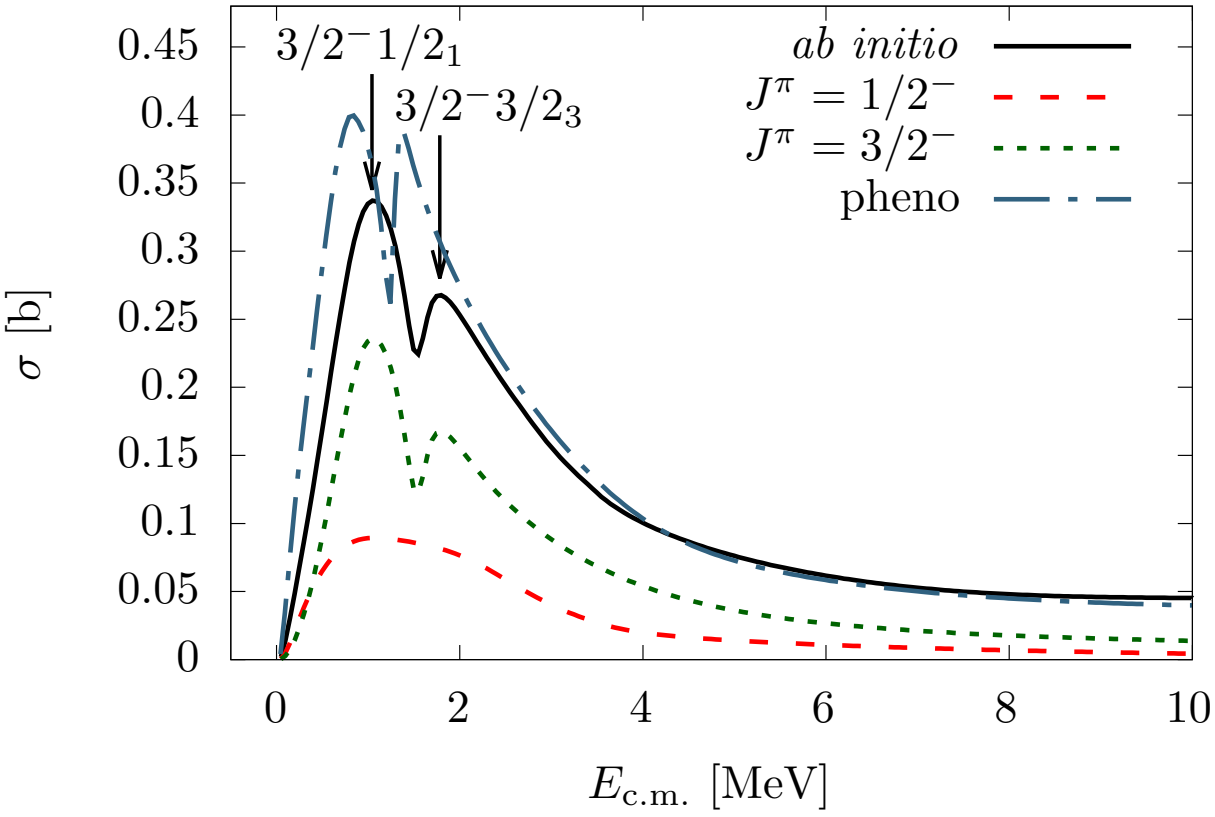
- Energy of $5/2^-1/2_2$ resonance with respect to ^{6}Li + n threshold overestimated

Cross section of ^{6}Li(n,p)^{6}He reaction

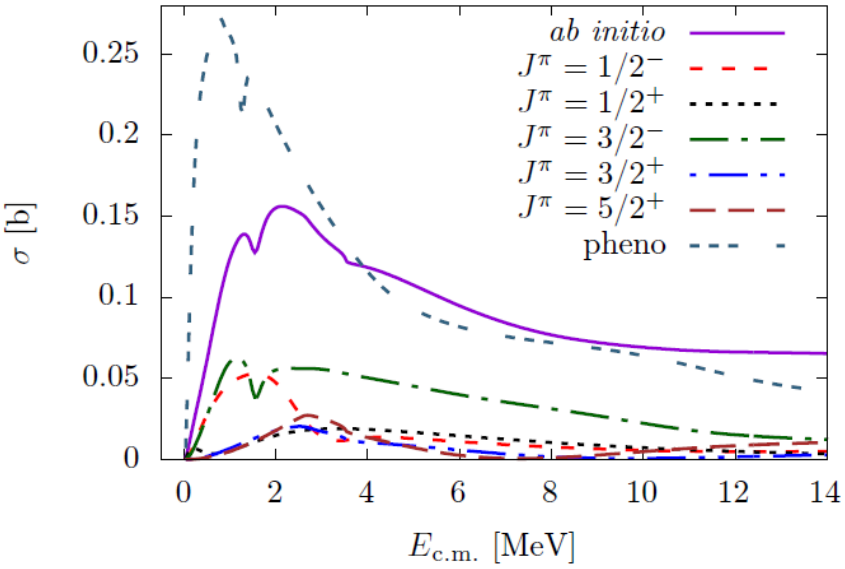


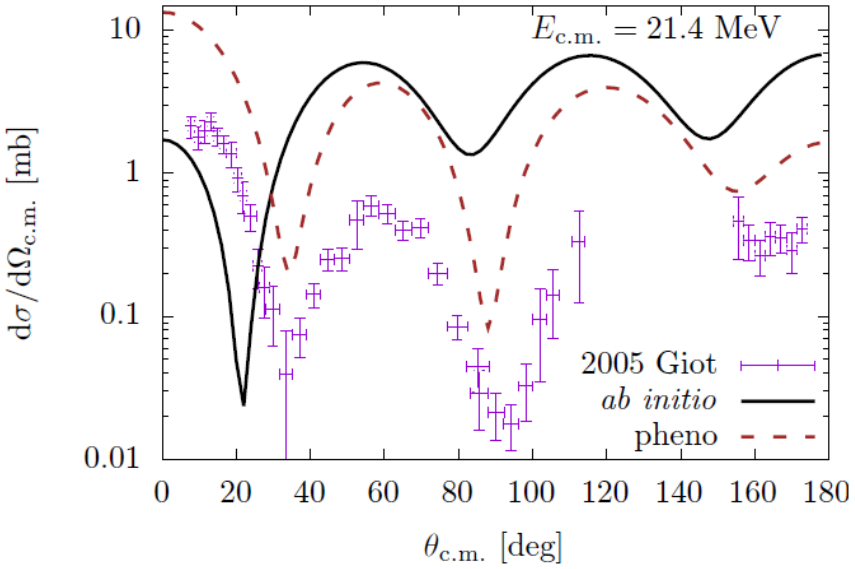
- Overall shape reproduced

Cross section of ^{6}He(p,n)^{6}Li reaction



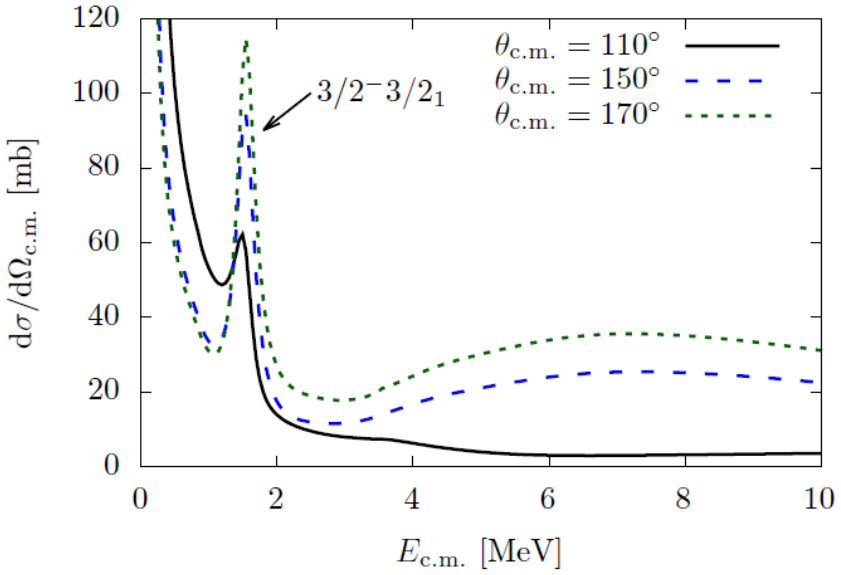
Cross sections of ^{6}He(*p*,*t*)^{4}He reaction

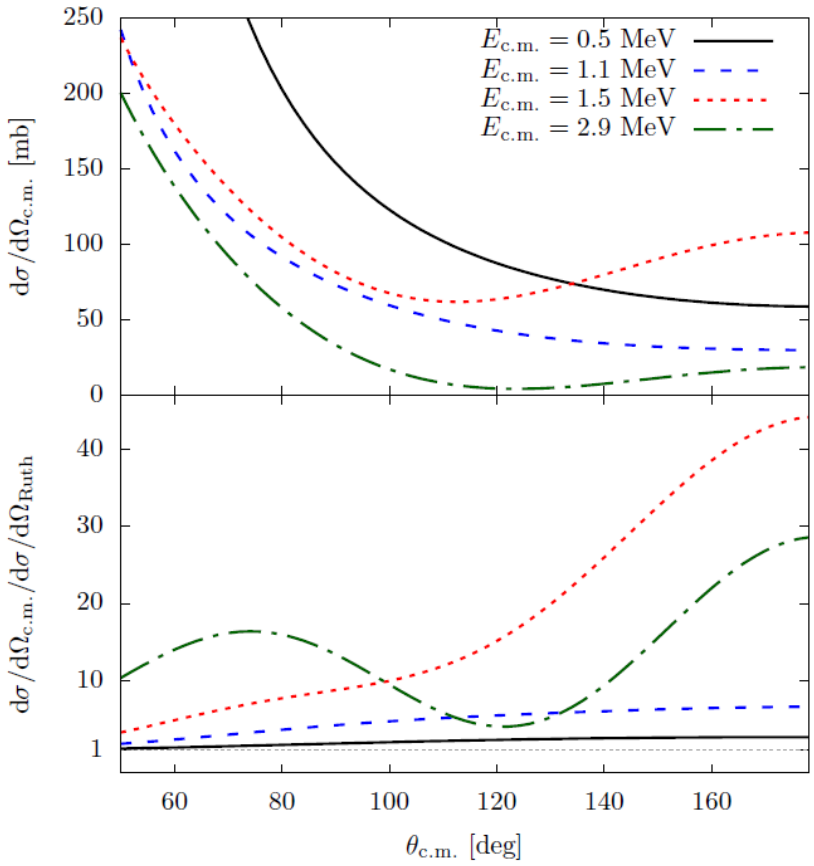




- $E_{\mathrm{c.m.}} = 21.4$ MeV beyond applicability of current setup due to omitted channels $\rightarrow$ overestimated values

Differential cross sections of ^{6}He + *p* elastic scattering





Conclusion

- First NCSMC calculations coupling 3 mass partitions, namely ^{4}He + ^{3}H, ^{6}Li + n, and ^{6}He + p, done
- Experimentally observed states in ^{7}Li reproduced
- Energies and widths of resonances affected by coupling of mass partitions
- 1/2$^+$ resonance predicted, but below ^{6}He + p threshold in ^{4}He + ^{3}H
  - discrepancy between previous NCSMC prediction and experiment explained
- Cross sections of ^{6}Li$(n,n)^6$Li and ^{6}Li$(n,p)^6$He calculated
  - overall shapes reproduced
- Cross sections of ^{6}He$(p,p)^6$He, ^{6}He$(p,n)^6$Li, and ^{6}He$(p,t)^4$He calculated for comparison with future experiments
- Future work: Include three-nucleon iteraction

Collaborators

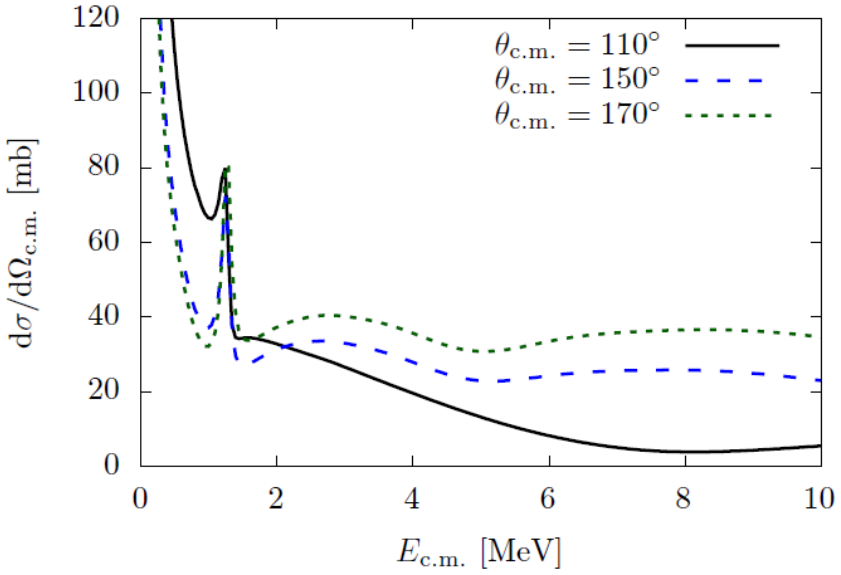
Konstantinos Kravvaris, Sofia Quaglioni
Lawrence Livermore National Laboratory

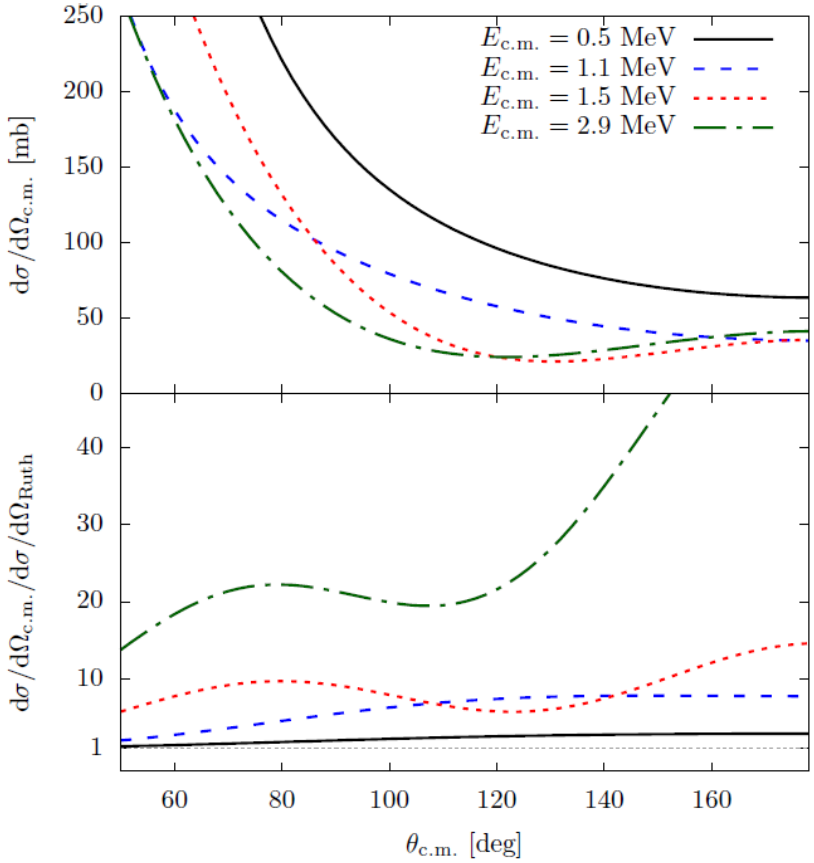
Petr Navrátil
TRIUMF

Guillaume Hupin
Université Paris-Saclay, CNRS/IN2P3, IJCLab

Mark A. Caprio
University of Notre Dame

^{6}He + *p* elastic scattering with pheno shifts





NCSM energy of ground state of ^{6}Li

