Nuclear structure and dynamics from *ab initio* theory

Shapes and Symmetries in Nuclei: from Experiment to Theory (SSNET’18 Conference)

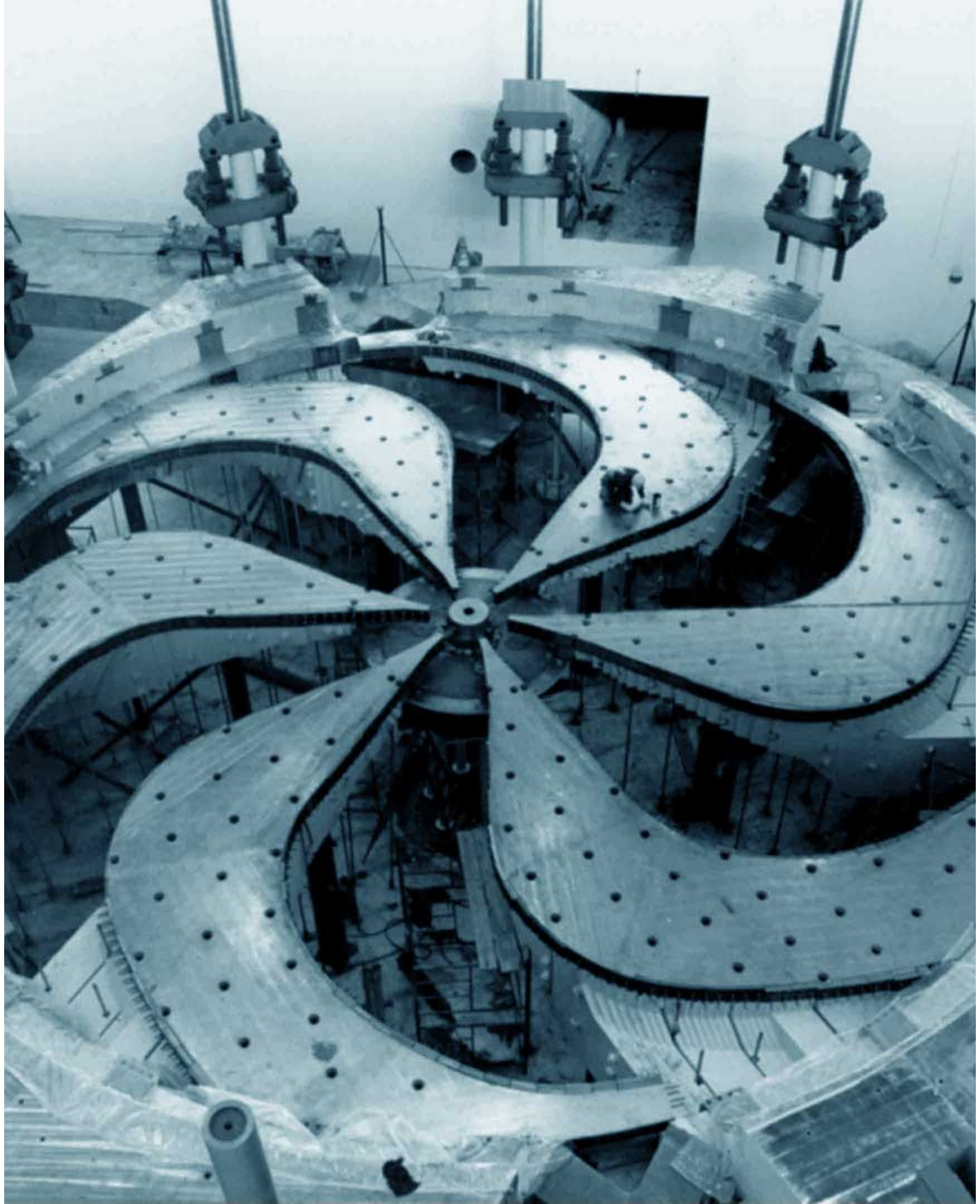
Gif-sur-Yvette, November 5th – 9th, 2018

Petr Navratil

TRIUMF

Collaborators: S. Quaglioni (LLNL), G. Hupin (Orsay), M. Vorabbi, A. Calci (TRIUMF), P. Gysbers (UBC/TRIUMF), M. Gennari (U Waterloo), J. Dohet-Eraly (ULB), F. Raimondi (Saclay), W. Horiuchi (U Hokkaido)

2018-11-13



Discovery, accelerated

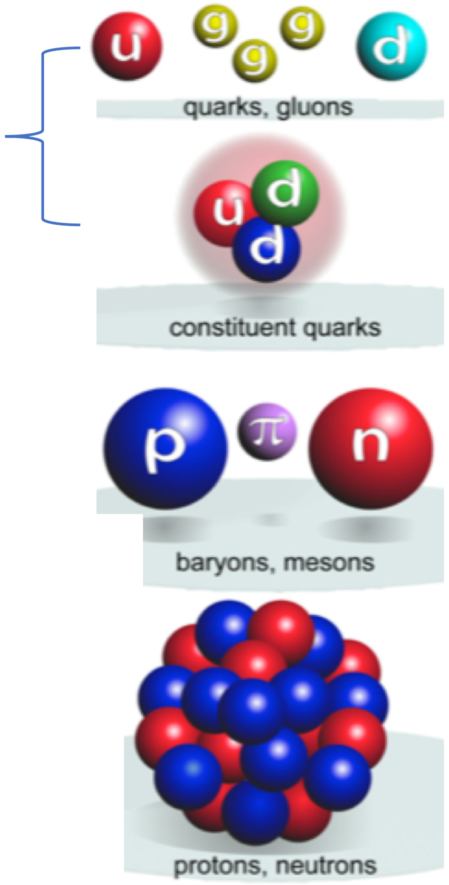
Outline

- *Ab initio* calculations in nuclear physics
- New chiral NN N^4LO + 3N
  - Beta decays of light nuclei in NCSM
  - Microscopic optical potentials from NCSM densities
  - Kinetic density from NCSM
- No-Core Shell Model with Continuum (NCSMC)
  - N-^{4}He scattering and polarized D+T fusion
  - Structure of ^{7}Be and ^{7}Li considering binary breakup thresholds

First principles or *ab initio* nuclear theory

Quantum Chromodynamics (QCD)

Genuine *Ab Initio*



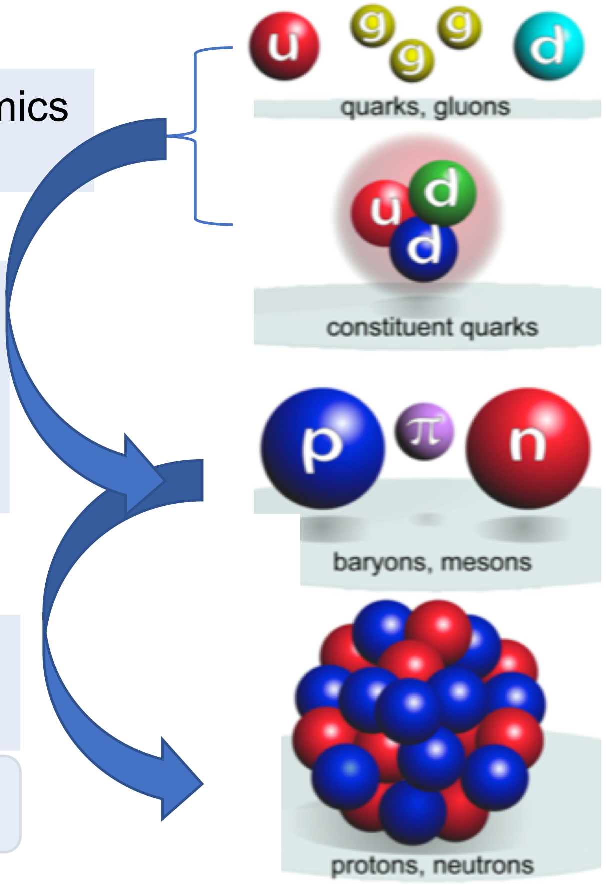
First principles or *ab initio* nuclear theory – what we do at present

Quantum Chromodynamics (QCD)

Chiral Effective Field Theory (parameters fitted to NN data)

Current *ab anitio* nuclear theory

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

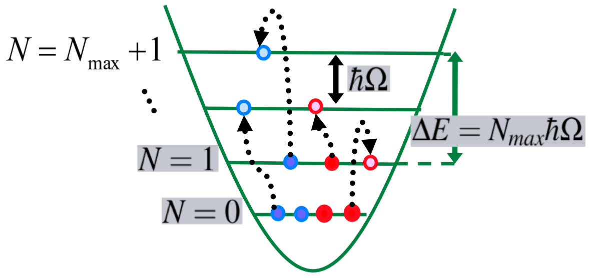


- *Ab initio*
- ✧ Degrees of freedom: Nucleons
- ✧ All nucleons are active
- ✧ Exact Pauli principle
- ✧ Realistic inter-nucleon interactions
  - ✧ Accurate description of NN (and 3N) data
- ✧ Controllable approximations

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

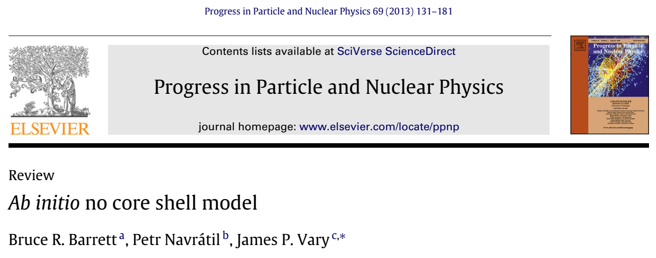
NCSM

- 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 – ^{4}He, ^{16}O, ^{40}Ca)
    - Equivalent description in relative-coordinate and Slater determinant basis
- Short- and medium range correlations
- Bound-states, narrow resonances



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

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


Progress in Particle and Nuclear Physics 69 (2013) 131–181

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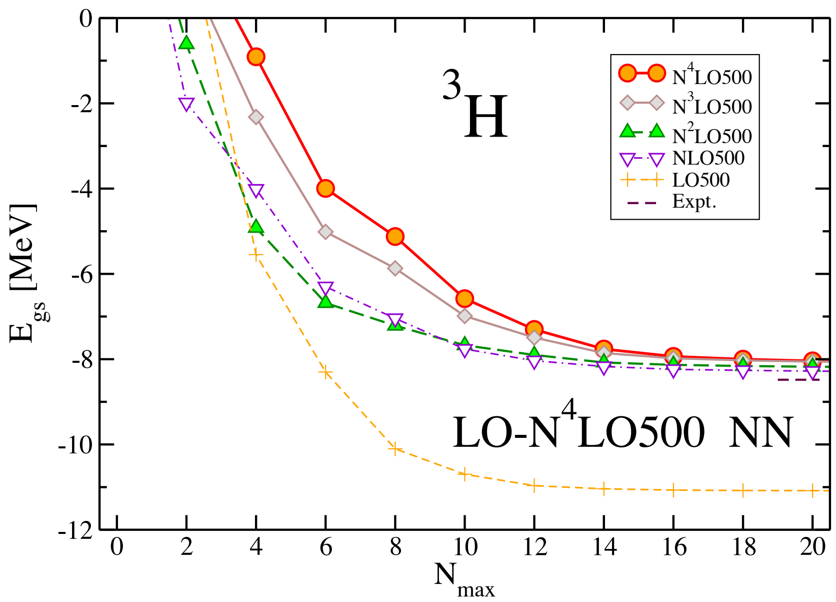
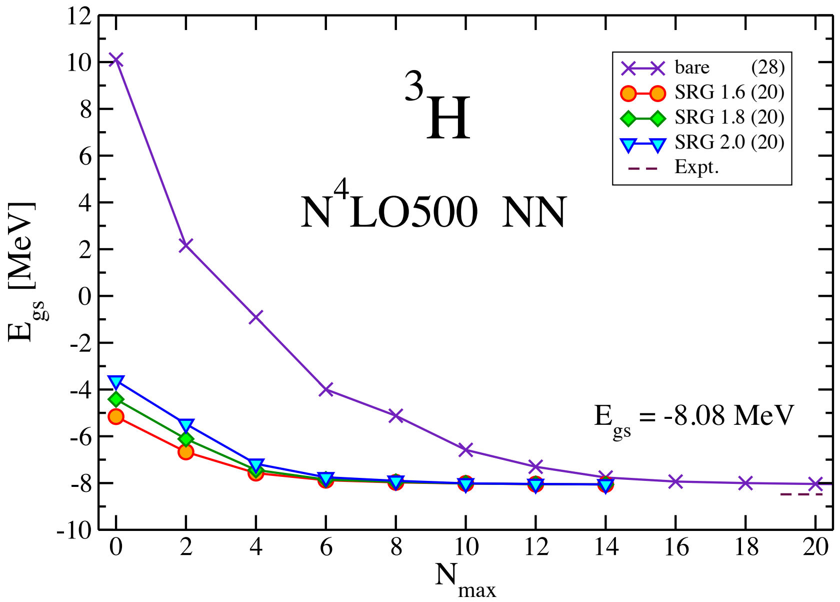
Review

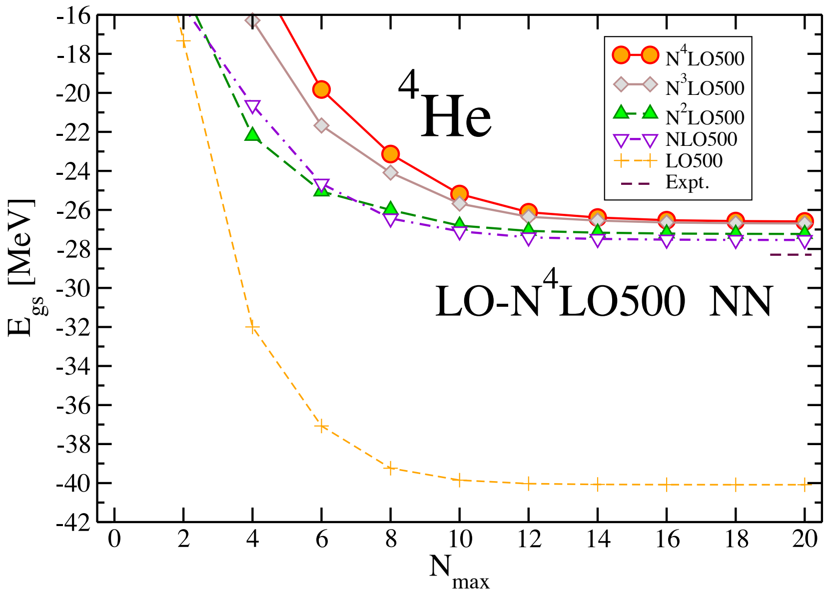
Ab initio no core shell model

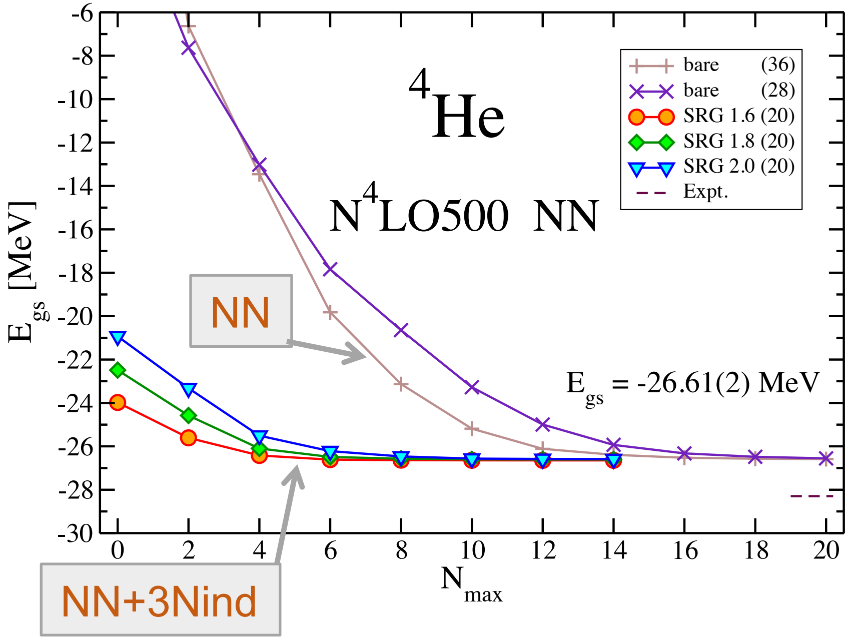
Bruce R. Barrett[a], Petr Navrátil[b], James P. Vary[c,*]

^{3}H and ^{4}He with chiral EFT interactions up to N^{4}LO









$^3H \rightarrow {}^3He$ β decay

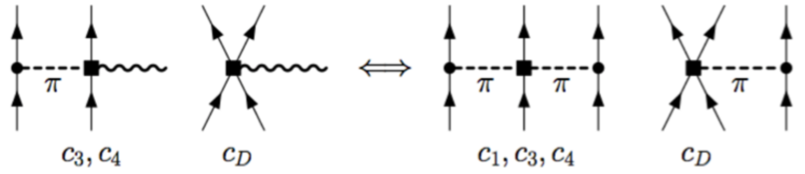
$$\hat{O} = GT^{(1)} + MEC^{(2)} \rightarrow \hat{O}_\alpha = GT^{(1)} + GT^{(2)}_\alpha + MEC^{(2)}_\alpha + \ldots$$

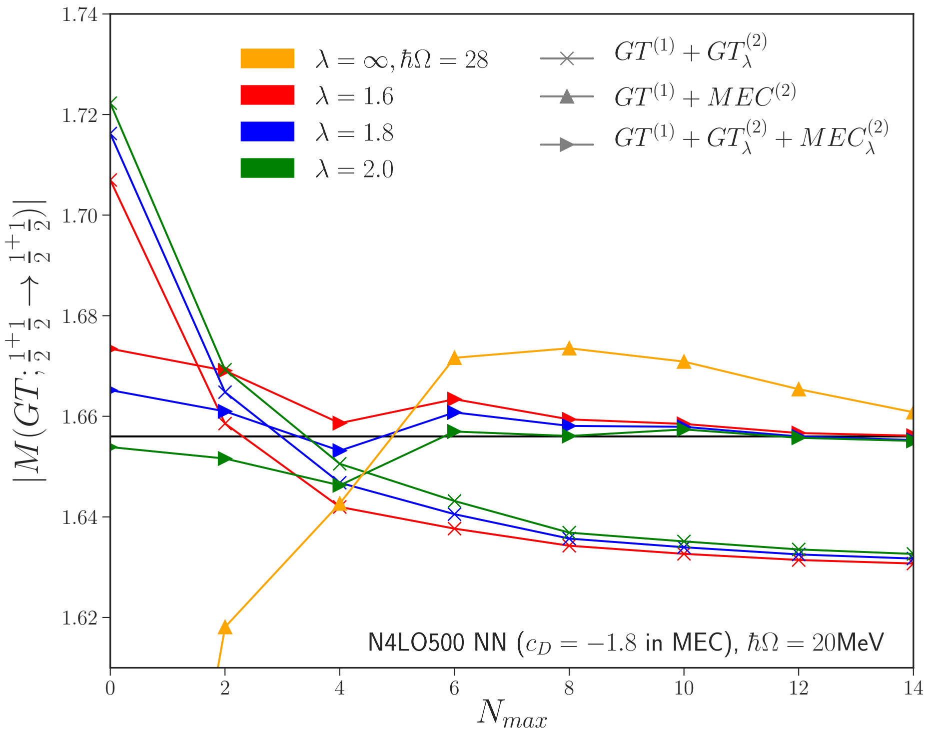
Operator:

Gamow-Teller (1-body) + chiral meson exchange current (2-body) Park (2003)

Potential: "N^{4}LO NN"

- chiral NN @ N^{4}LO, Machleidt PRC96 (2017), 500MeV cutoff
- LEC $c_D = -1.8$ determined





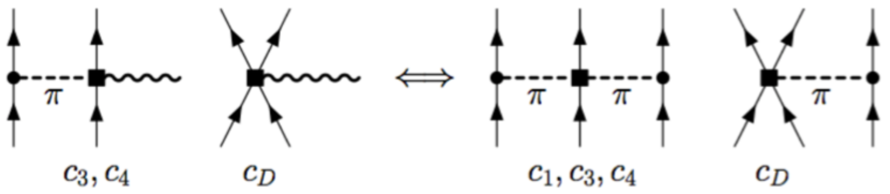
Original EM 2003 N^{3}LO NN c_D=+0.8 (3N repulsive)

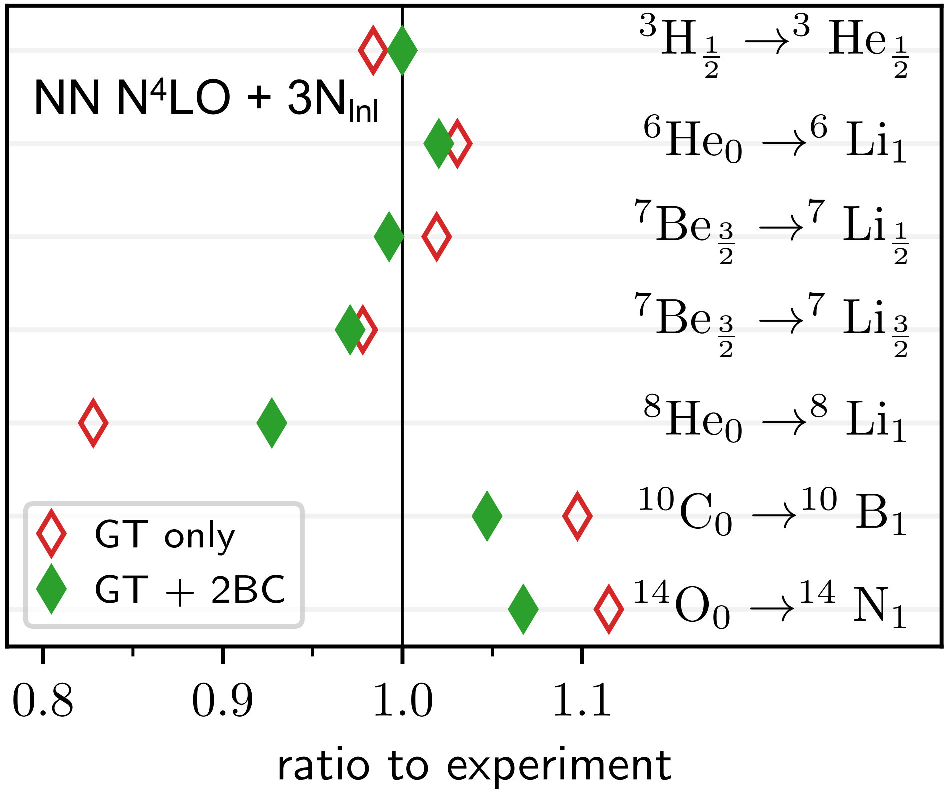
Determination of the c_D parameter relevant to chiral 3N force c_D=-1.8 (3N attractive)

Applications to β decays in p-shell nuclei and beyond

- Does inclusion of the MEC explain g_A quenching?
- In light nuclei correlations present in *ab initio* (NCSM) wave functions explain almost all of the quenching compared to the standard shell model
  - MEC inclusion overall improves agreement with experiment
- The effect of the MEC inclusion is greater in heavier nuclei
- SRG evolved matrix elements used in coupled-cluster and IM-SRG calculations (up to ^{100}Sn)

Hollow symbols – GT
Filled symbols – GT+MEC
Both Hamiltonian and operators SRG evolved
Hamiltonian and current consistent parameters





P. Gysbers *et al., "Quenching puzzle of beta decays,"* submitted.

PHYSICAL REVIEW C **97**, 034619 (2018)

Microscopic optical potentials derived from *ab initio* translationally invariant nonlocal one-body densities

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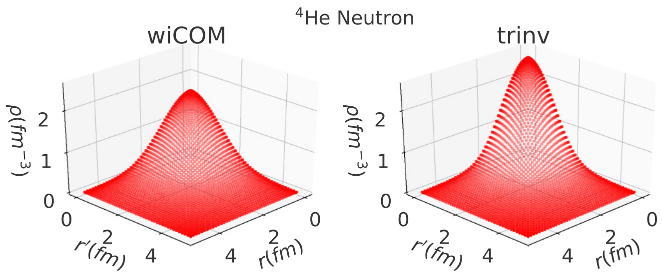
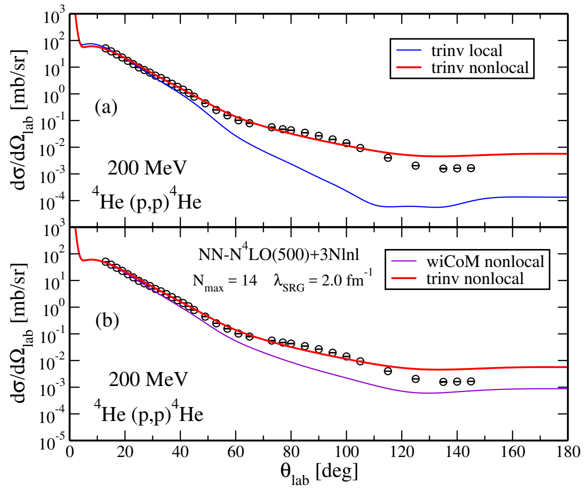
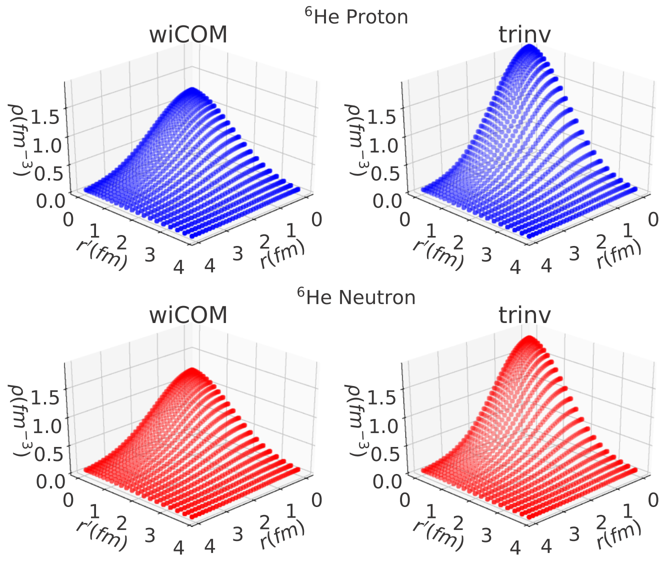
Matteo Vorabbi,† Angelo Calci, and Petr Navrátil‡
TRIUMF, 4004 Wesbrook Mall, Vancouver, British Columbia V6T 2A3, Canada

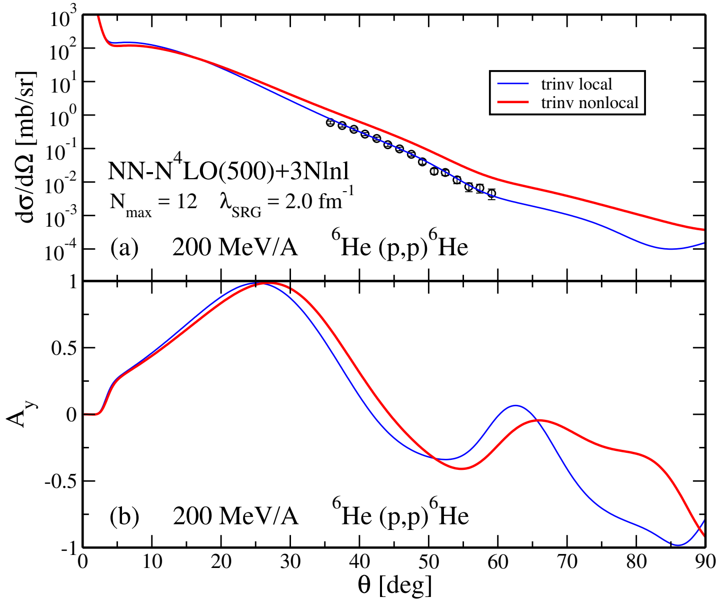
Microscopic optical potentials from NCSM densities

- Translationally-invariant non-local densities from NCSM calculations with chiral NN N^4LO + 3N N^2LO interactions
- High-energy proton-nucleus scattering with microscopic optical potentials from chiral N^4LO NN interaction and NCSM densities









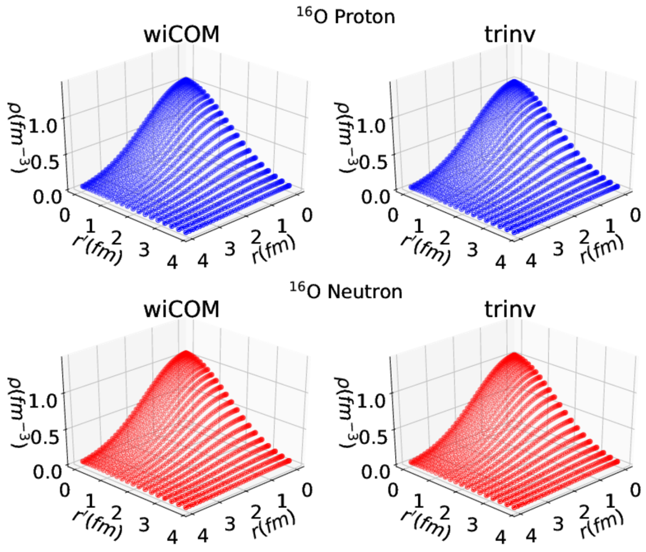
Nuclear kinetic density from NCSM wave functions

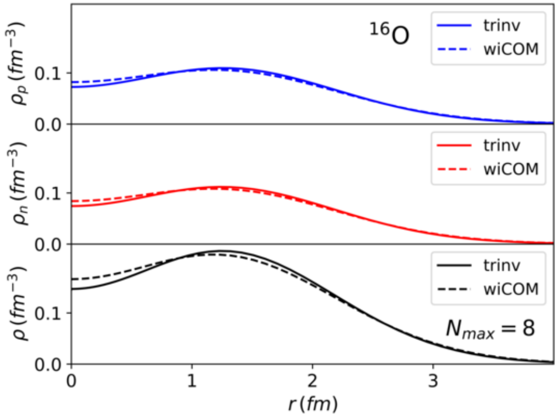
M. Gennari and P. N., arXiv:1808.10537

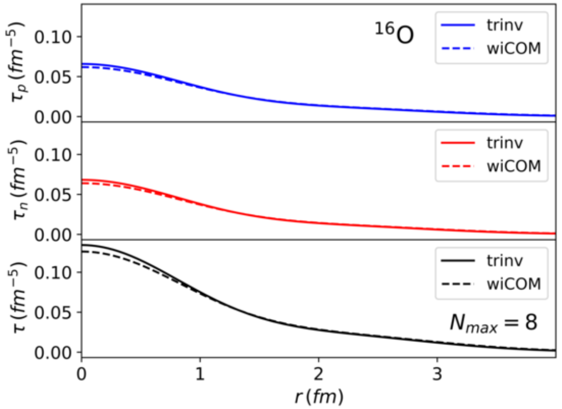
- DFT calculations include kinetic density
  - Might contain center-of-mass contamination
- Can be calculated for light nuclei in NCSM
  - Translationally invariant

$$\tau_{\mathcal{N}}(\vec{r}) = \left[\vec{\nabla}\cdot\vec{\nabla}'\rho_{\mathcal{N}}(\vec{r},\vec{r}')\right]_{\vec{r}=\vec{r}'}$$

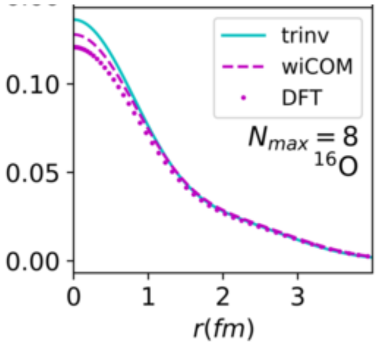
$$\tau_{DFT}(\vec{r}) = \left(1-\frac{1}{A}\right)\tau_{wiCOM}(\vec{r})$$





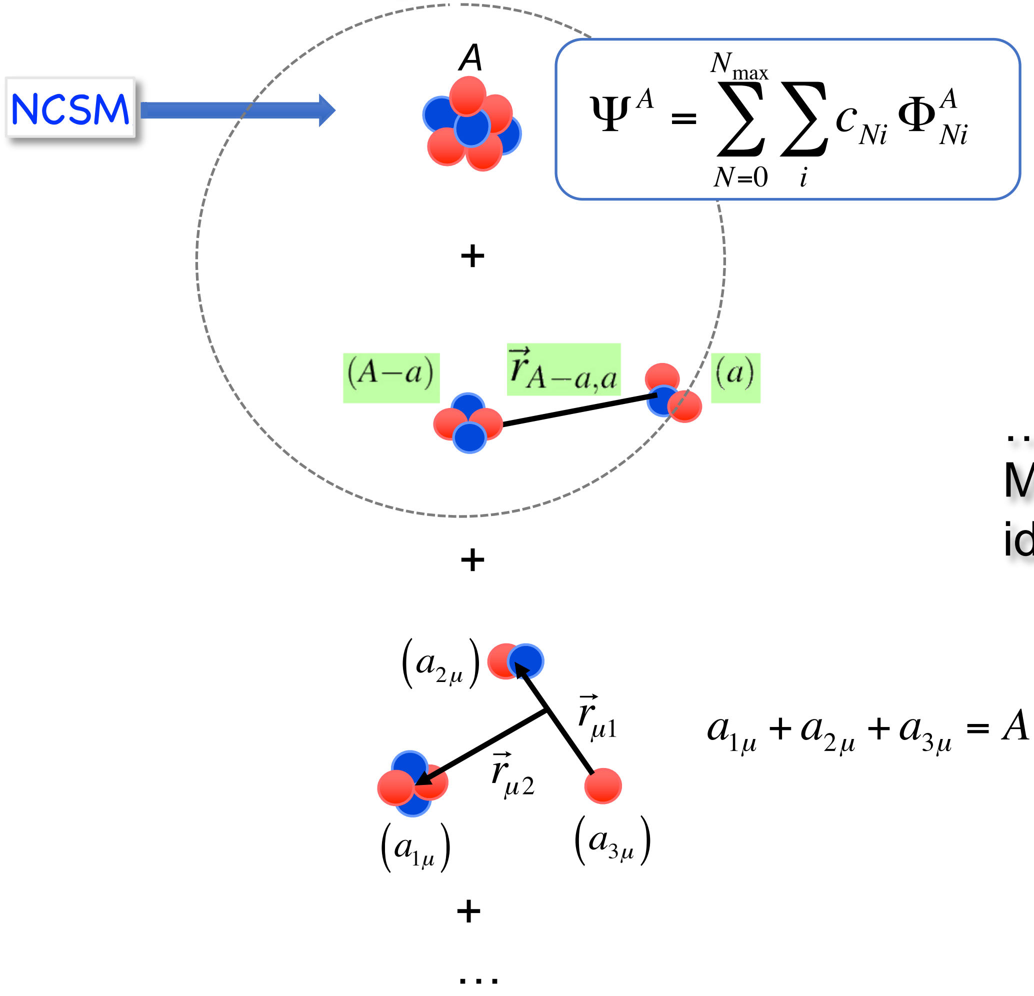


Nucleus	$N_{\max}$	$\langle T_{int}\rangle$	$\langle T_{wiCOM}\rangle$	$\langle T_{DFT}\rangle$
^{4}He	14	51.91	66.91	50.18
^{6}He	12	78.26	93.26	77.72
^{8}He	10	116.30	131.30	114.89
^{12}C	8 IT	219.84	234.84	215.27
^{16}O	8 IT	301.69	316.69	296.90



Extending no-core shell model beyond bound states

Include more many nucleon correlations…

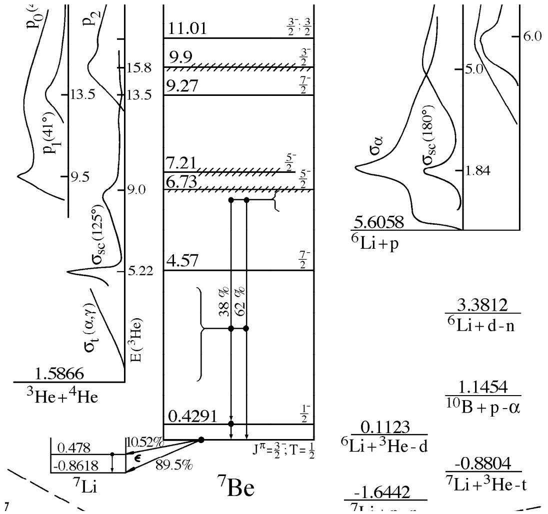


$$\Psi^A = \sum_{N=0}^{N_{max}} \sum_i c_{Ni} \Phi^A_{Ni}$$

$$\vec{r}_{A-a,a}$$

$$(a_{1\mu}) \quad (a_{2\mu}) \quad (a_{3\mu}) \quad \vec{r}_{\mu 1} \quad \vec{r}_{\mu 2}$$

$$a_{1\mu} + a_{2\mu} + a_{3\mu} = A$$



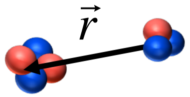
…using the Resonating Group Method (RGM) ideas

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

- NCSM with Resonating Group Method (NCSM/RGM)
  - cluster expansion, clusters described by NCSM
  - proper asymptotic behavior
  - long-range correlations



NCSM/RGM

- Most efficient: *ab initio* no-core shell model with continuum (NCSMC)

NCSMC

$$\Psi^{(A)} = \sum_{\lambda} c_{\lambda} \left|^{(A)}, \lambda \right\rangle + \sum_{\nu} \int d\vec{r}\; \gamma_{\nu}(\vec{r})\; \hat{A}_{\nu} \left|_{(A-a)} \overset{\vec{r}}{\longleftrightarrow} (a), \nu \right\rangle$$

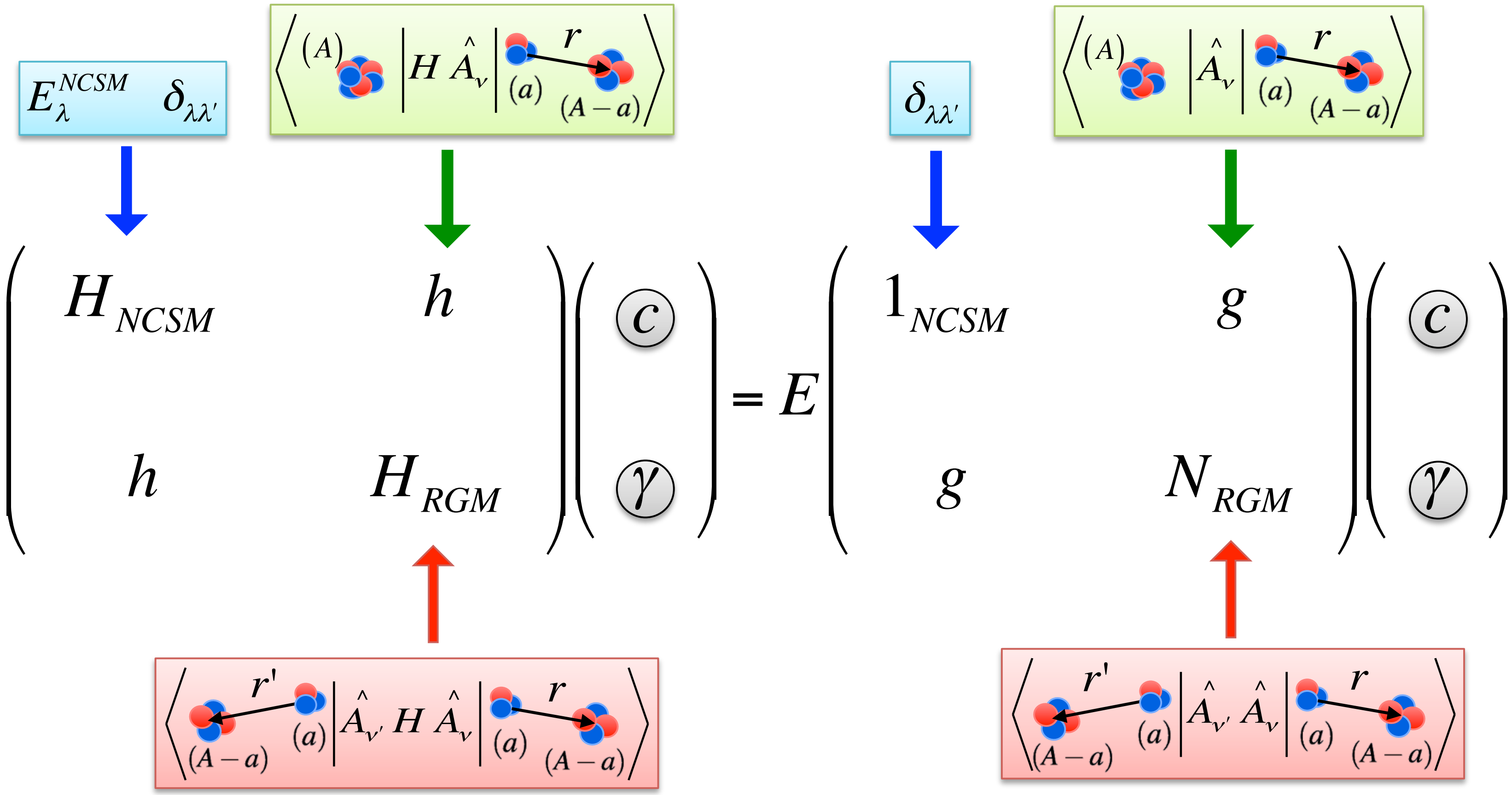
Unknowns

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

Coupled NCSMC equations

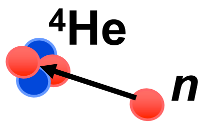
$$H\,\Psi^{(A)} = E\,\Psi^{(A)}$$

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

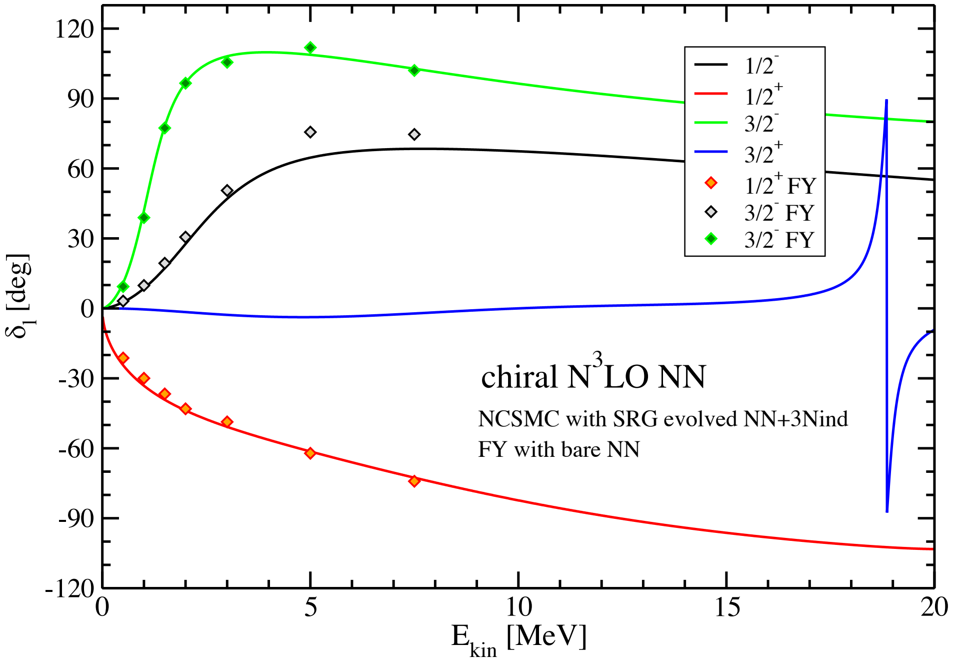


Solved by Microscopic R-matrix theory on a Lagrange mesh – efficient for coupled channels

n-^{4}He scattering within NCSMC



n-^{4}He scattering phase-shifts for chiral NN



FY: Faddeev-Yakubovsky method - Rimantas Lazauskas

IOP Publishing | Royal Swedish Academy of Sciences — Physica Scripta

Phys. Scr. **00** (2016) 000000 (37pp)

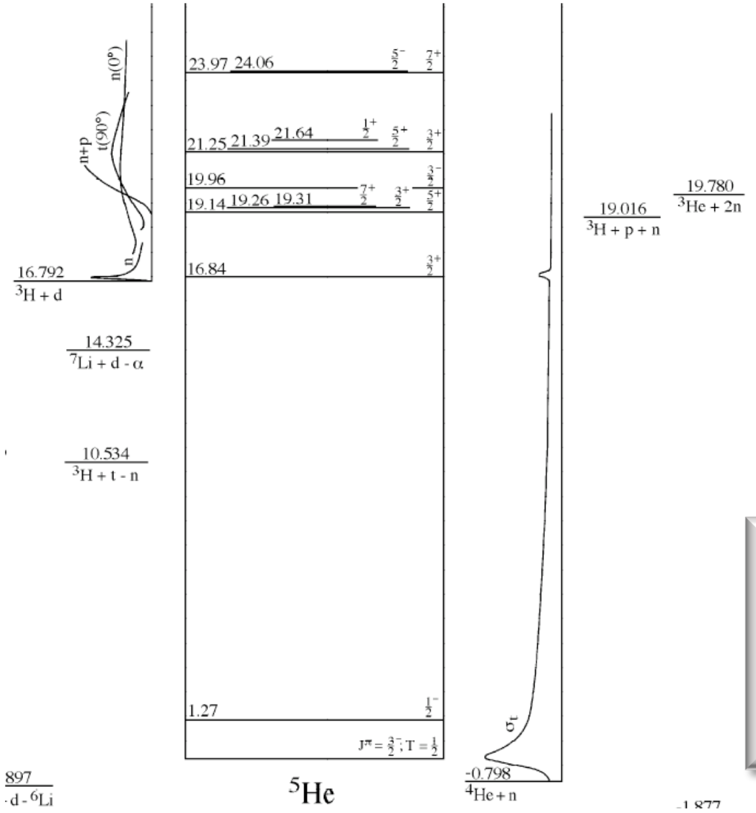
Invited Comment

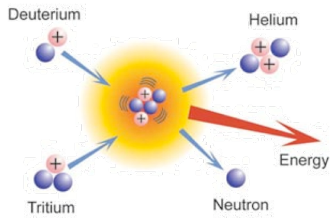
Unified *ab initio* approaches to nuclear structure and reactions

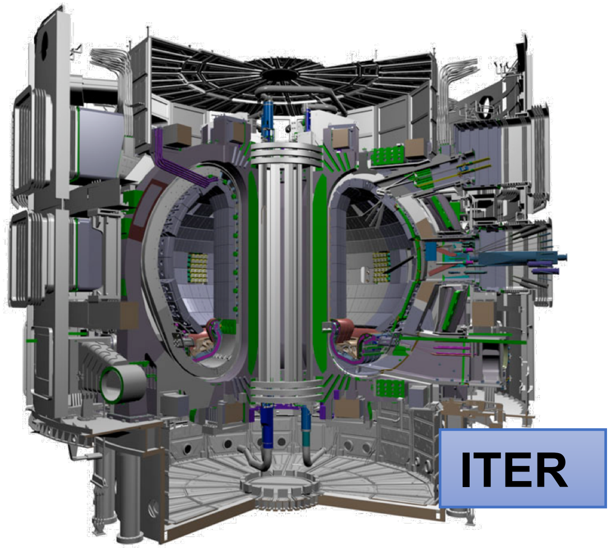
Petr Navrátil[1], Sofia Quaglioni[2], Guillaume Hupin[3,4], Carolina Romero-Redondo[2] and Angelo Calci[1]

Deuterium-Tritium fusion

- The d+^{3}H$\rightarrow n$+^{4}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}He(d,p)^{4}He, important for Big Bang nucleosynthesis



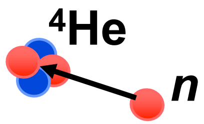




Resonance at E_{cm} =48 keV (E_d=105 keV) in the J=3/2$^+$ channel
Cross section at the peak: 4.88 b

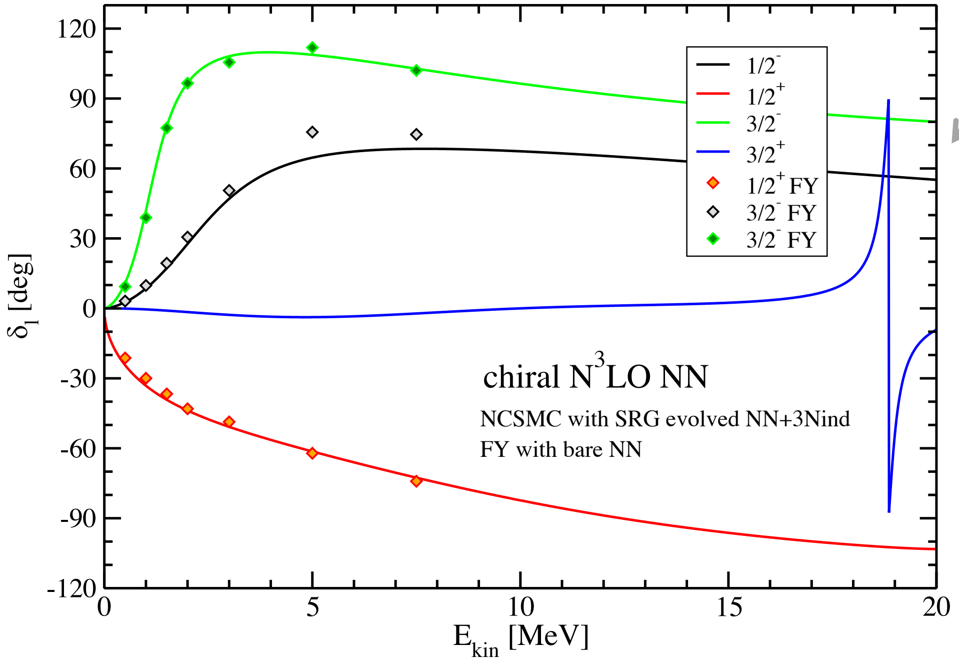
17.64 MeV energy released:
14.1 MeV neutron and 3.5 MeV alpha

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



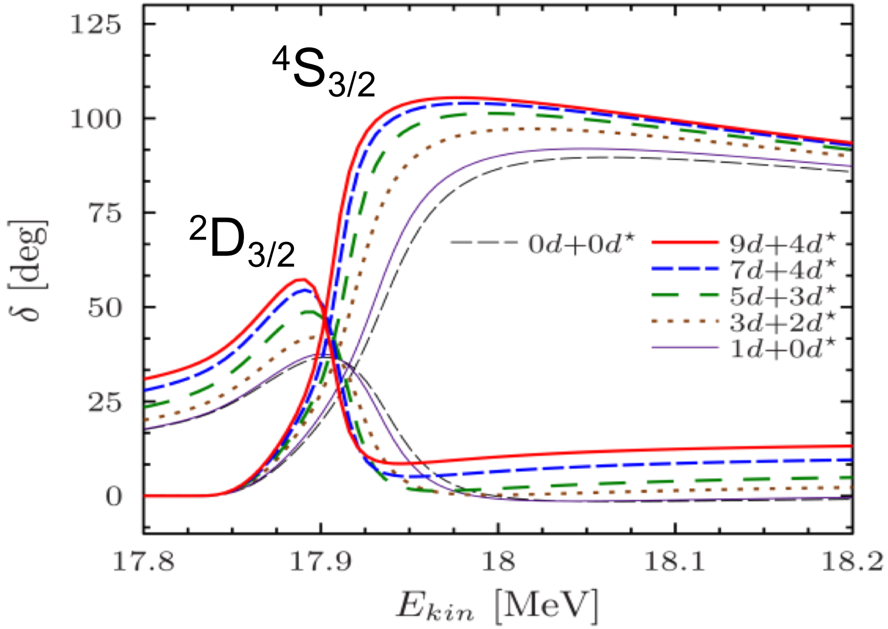
n-^{4}He scattering phase-shifts for chiral NN

^{4}He+n



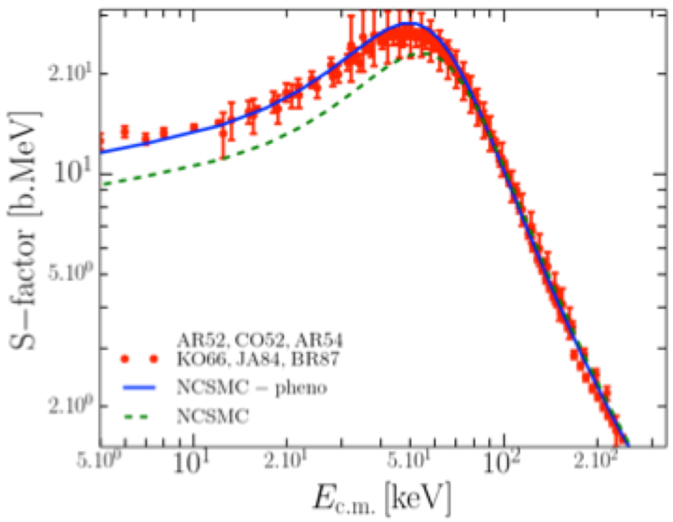
FY: Faddeev-Yakubovsky method - Rimantas Lazauskas

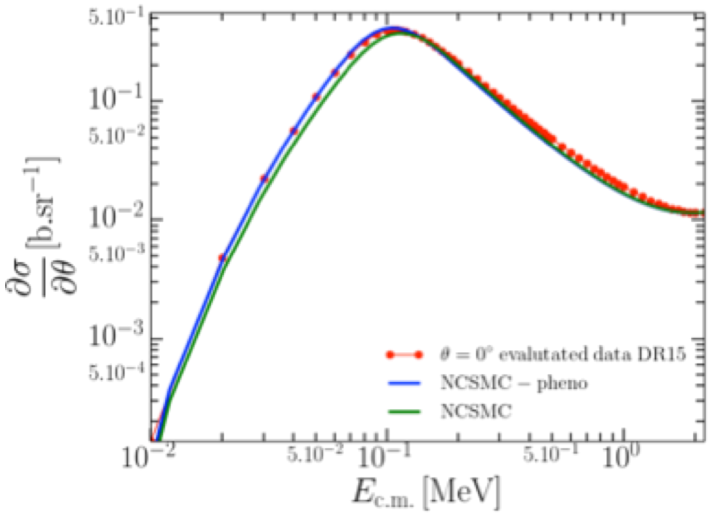
^{4}He+n -> ^{3}H+d



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

$^{3}H(d,n)^{4}He$ with chiral NN+3N500 interaction





$$S(E) = E\sigma(E)\exp[2\pi\eta(E)]$$

$$\eta(E) = Z_{A-a}Z_{a}e^{2} / \hbar v_{A-a,a}$$

NCSMC phenomenology

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

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

$$E_{\lambda}^{NCSM}\;\delta_{\lambda\lambda'} \qquad \left\langle (A) \right| H \hat{A}_{\nu} \left| (a)\;\; r\;\; (A-a) \right\rangle \qquad \delta_{\lambda\lambda'} \qquad \left\langle (A) \right| \hat{A}_{\nu} \left| (a)\;\; r\;\; (A-a) \right\rangle$$

$$\begin{pmatrix} H_{NCSM} & h \\ h & H_{RGM} \end{pmatrix} \begin{pmatrix} c \\ \gamma \end{pmatrix} = E \begin{pmatrix} 1_{NCSM} & g \\ g & N_{RGM} \end{pmatrix} \begin{pmatrix} c \\ \gamma \end{pmatrix}$$

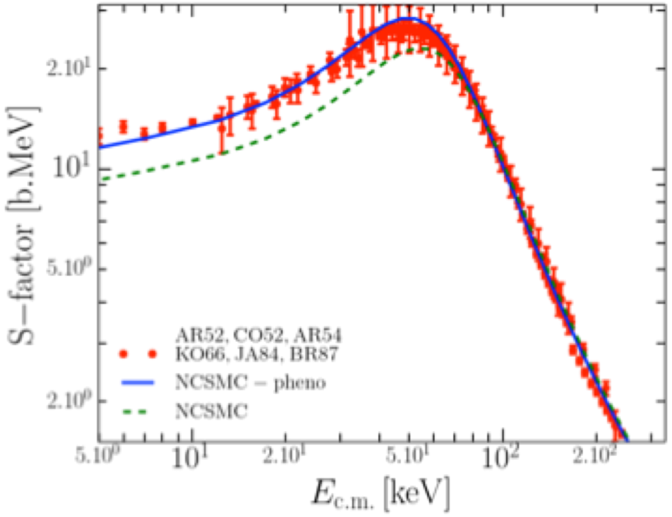
$$\left\langle (A-a)\;\; r'\;\; (a) \right| \hat{A}_{\nu'} H \hat{A}_{\nu} \left| (a)\;\; r\;\; (A-a) \right\rangle \qquad \left\langle (A-a)\;\; r'\;\; (a) \right| \hat{A}_{\nu'} \hat{A}_{\nu} \left| (a)\;\; r\;\; (A-a) \right\rangle$$

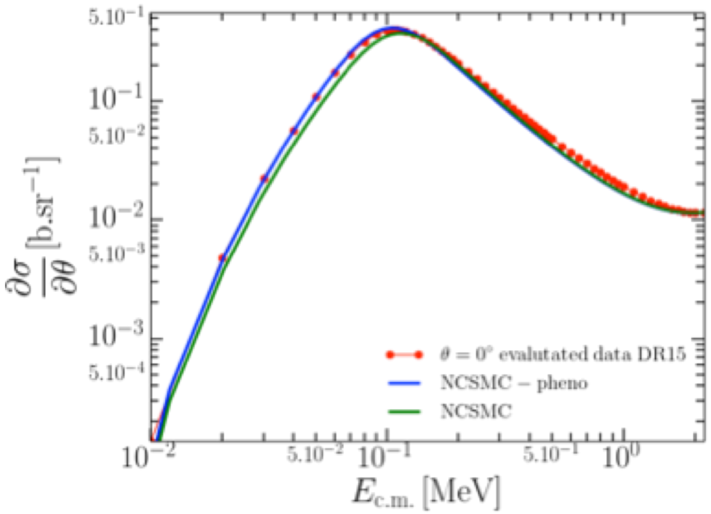
E_{λ}^{NCSM} energies treated as adjustable parameters

***Ab initio* predictions for *polarized* DT thermonuclear fusion**
Nature Communications (accepted); arXiv:1803.11378
Guillaume Hupin[1,2,3], Sofia Quaglioni[3] and Petr Navrátil[4]

$^{3}H(d,n)^{4}He$ with chiral NN+3N500 interaction

Polarized fusion



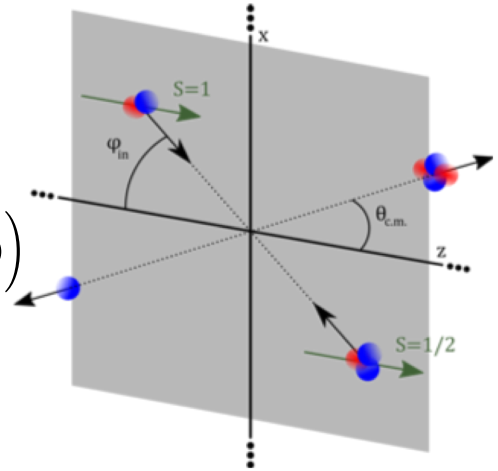


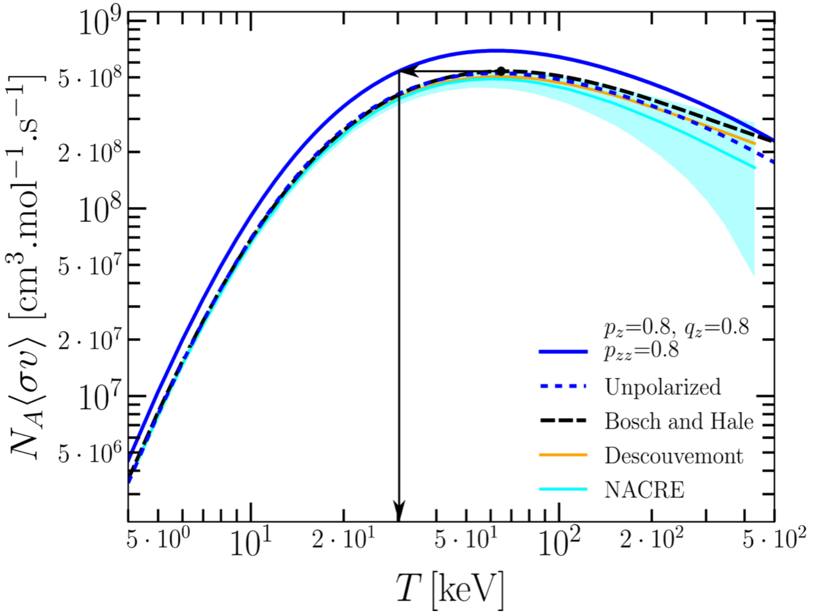
$$S(E) = E\sigma(E)\exp[2\pi\eta(E)]$$

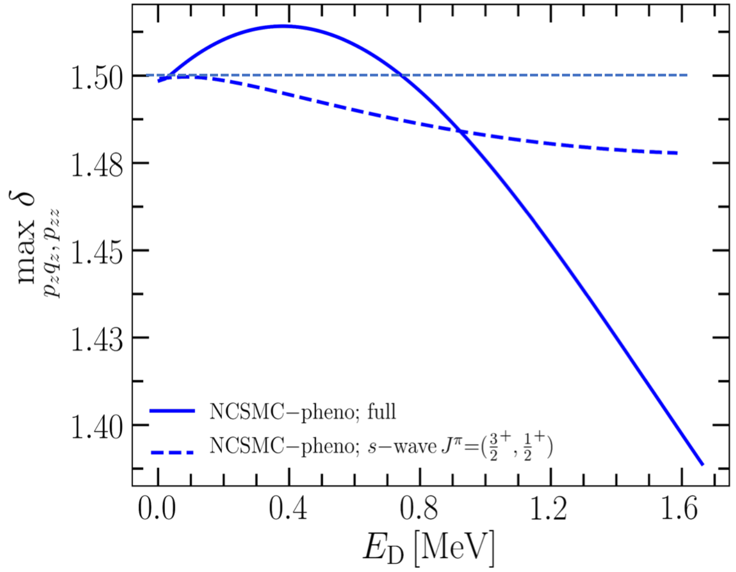
$$\eta(E) = Z_{A-a}Z_a e^2 / \hbar v_{A-a,a}$$

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

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







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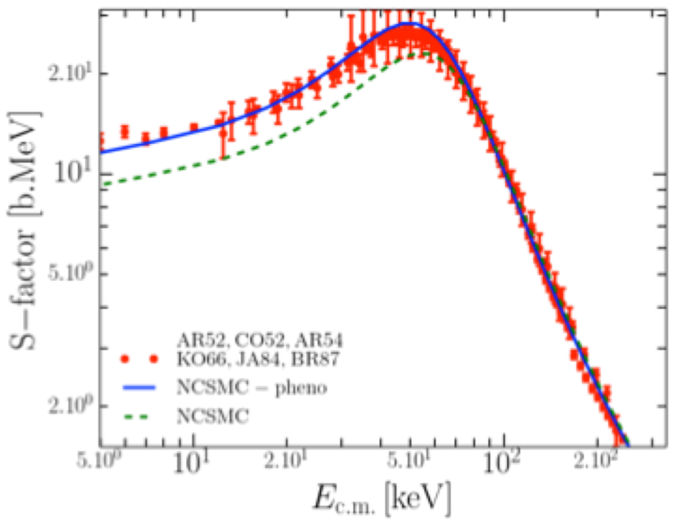
Polarized fusion

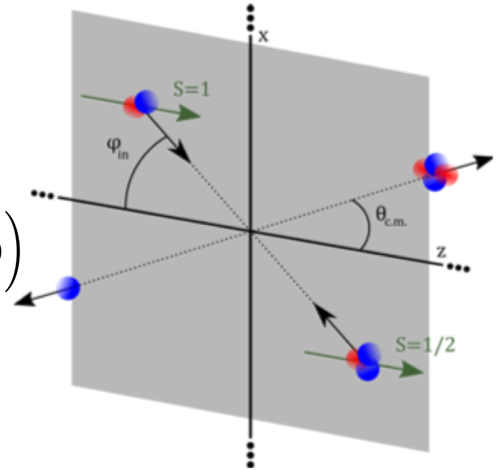


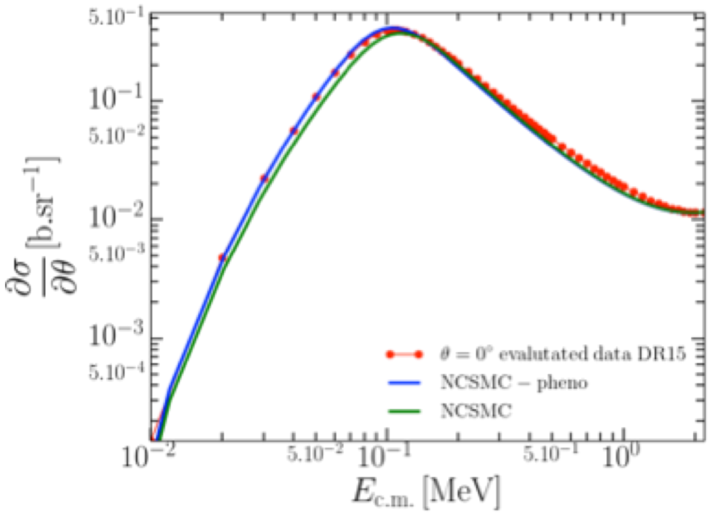
$$S(E) = E\sigma(E)\exp[2\pi\eta(E)]$$

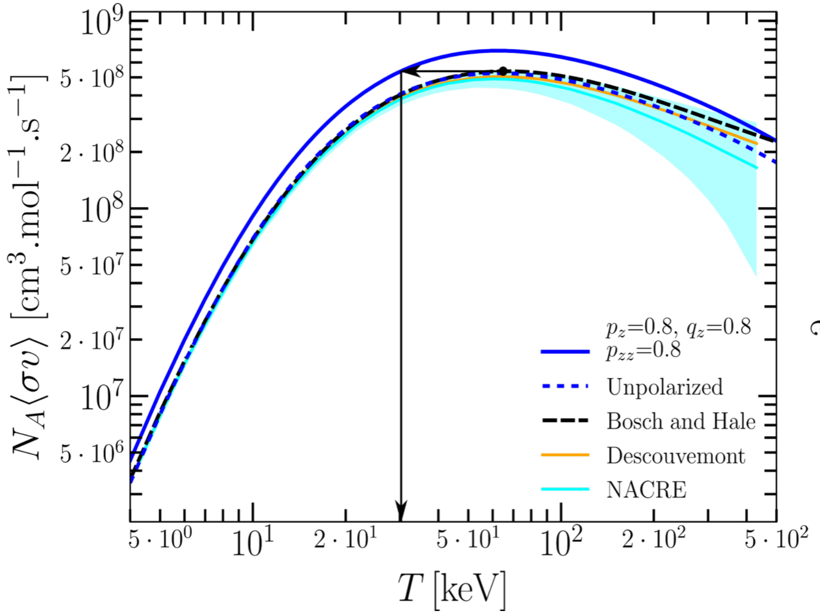
$$\eta(E) = Z_{A-a}Z_a e^2 / \hbar v_{A-a,a}$$

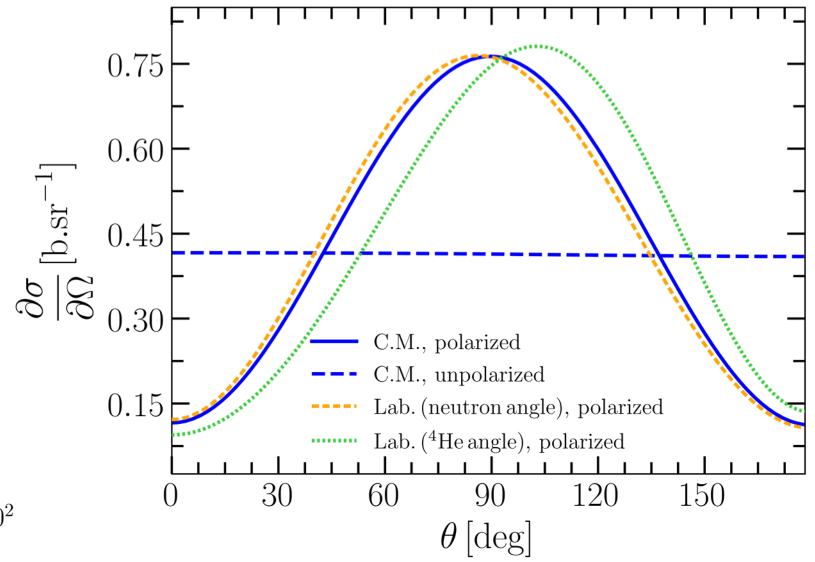
$$\frac{\partial\sigma_{pol}}{\partial\Omega_{c.m.}}(\theta_{\rm c.m.}) = \frac{\partial\sigma_{unpol}}{\partial\Omega_{c.m.}}(\theta_{\rm c.m.})\left(1+\frac{1}{2}p_{zz}A_{zz}^{(b)}(\theta_{\rm c.m.})+\frac{3}{2}p_z q_z C_{z,z}(\theta_{\rm c.m.})\right)$$

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









Structure of ^{7}Be and ^{7}Li considering binary breakup thresholds

NCSMC with SRG evolved chiral NN

^{7}Be system

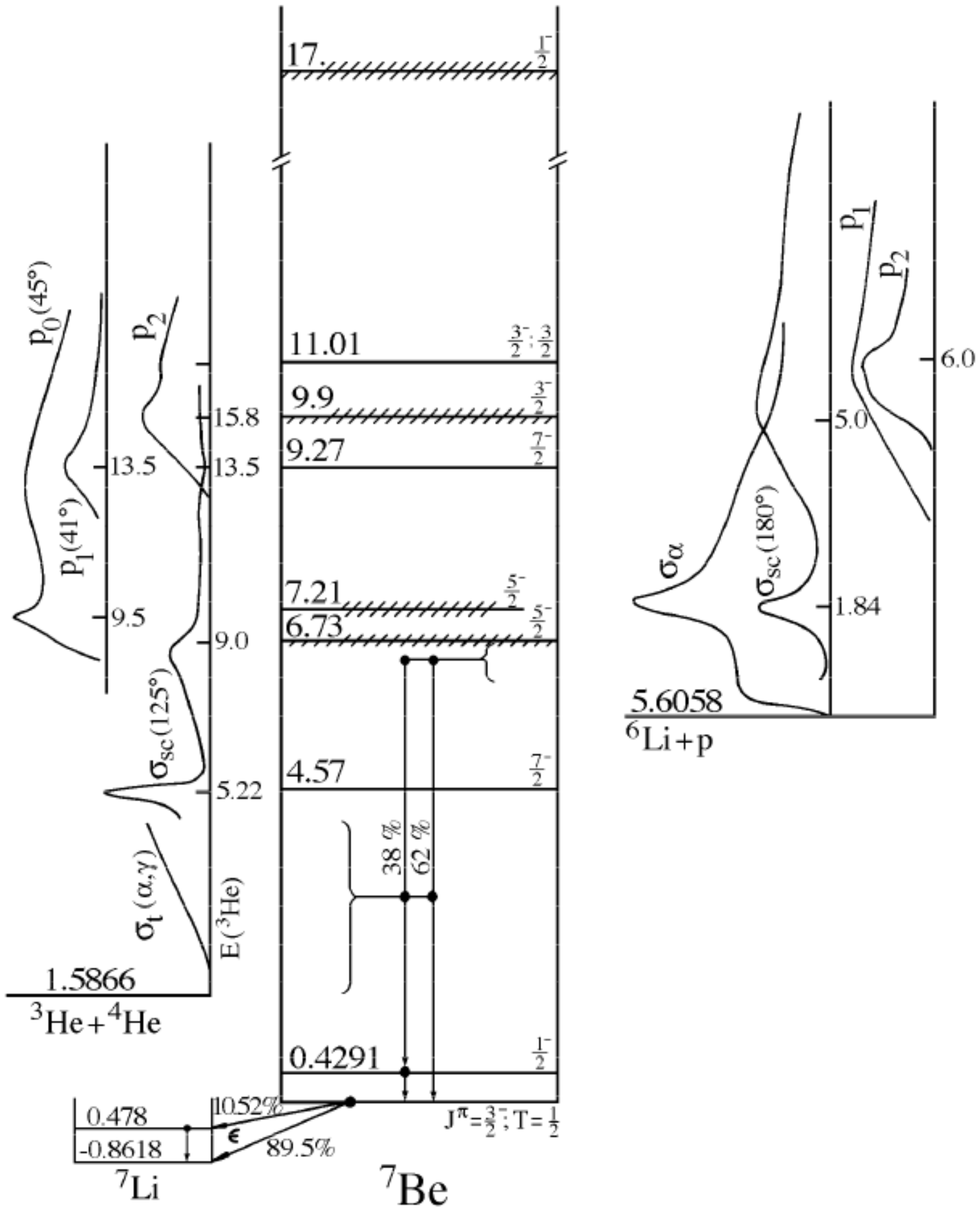
Analyzed mass partitions

- ^{3}He + ^{4}He
- p + ^{6}Li

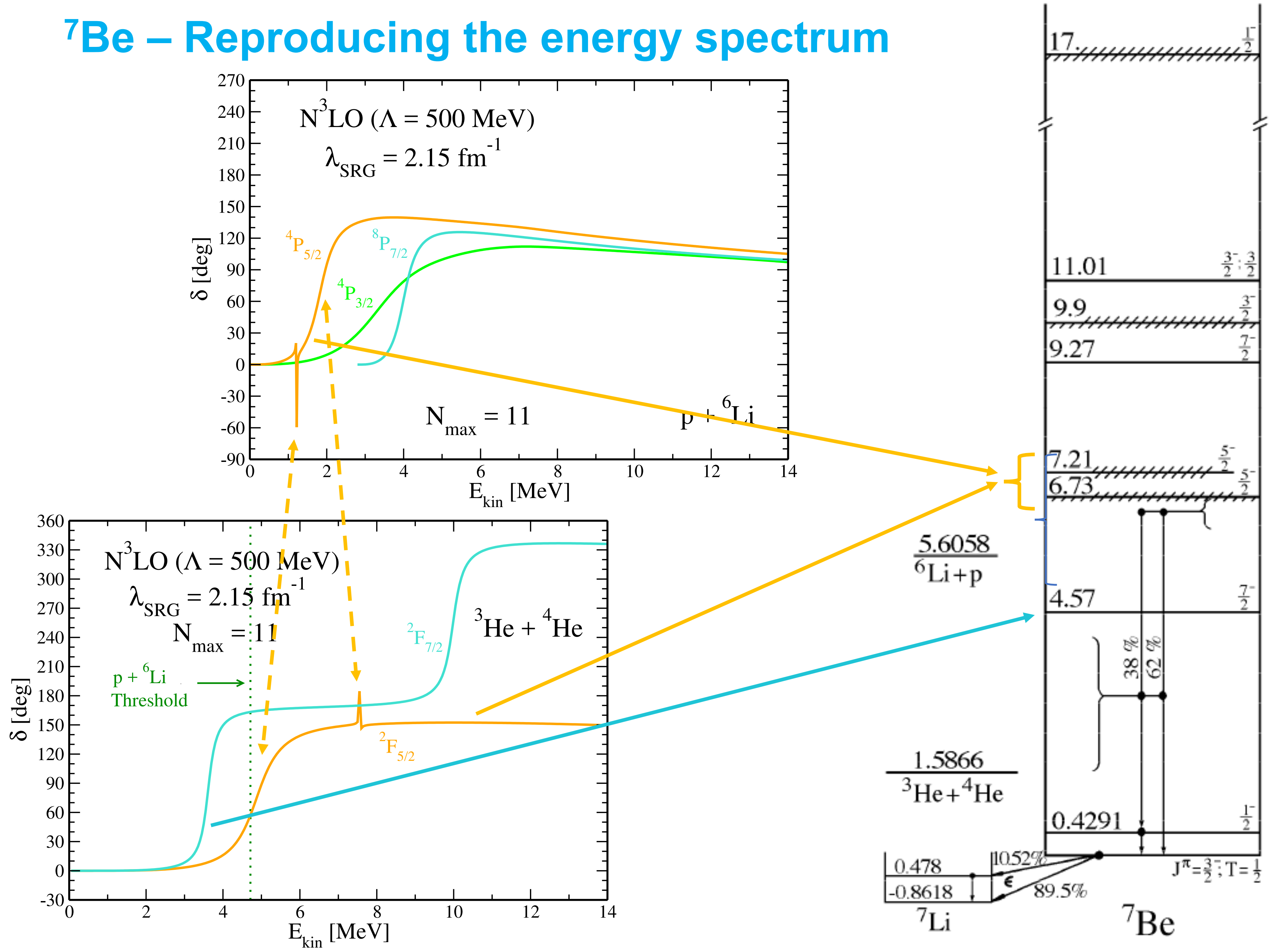
Exp.	$J^\pi = 3/2^-$
E [MeV]	-37.60

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

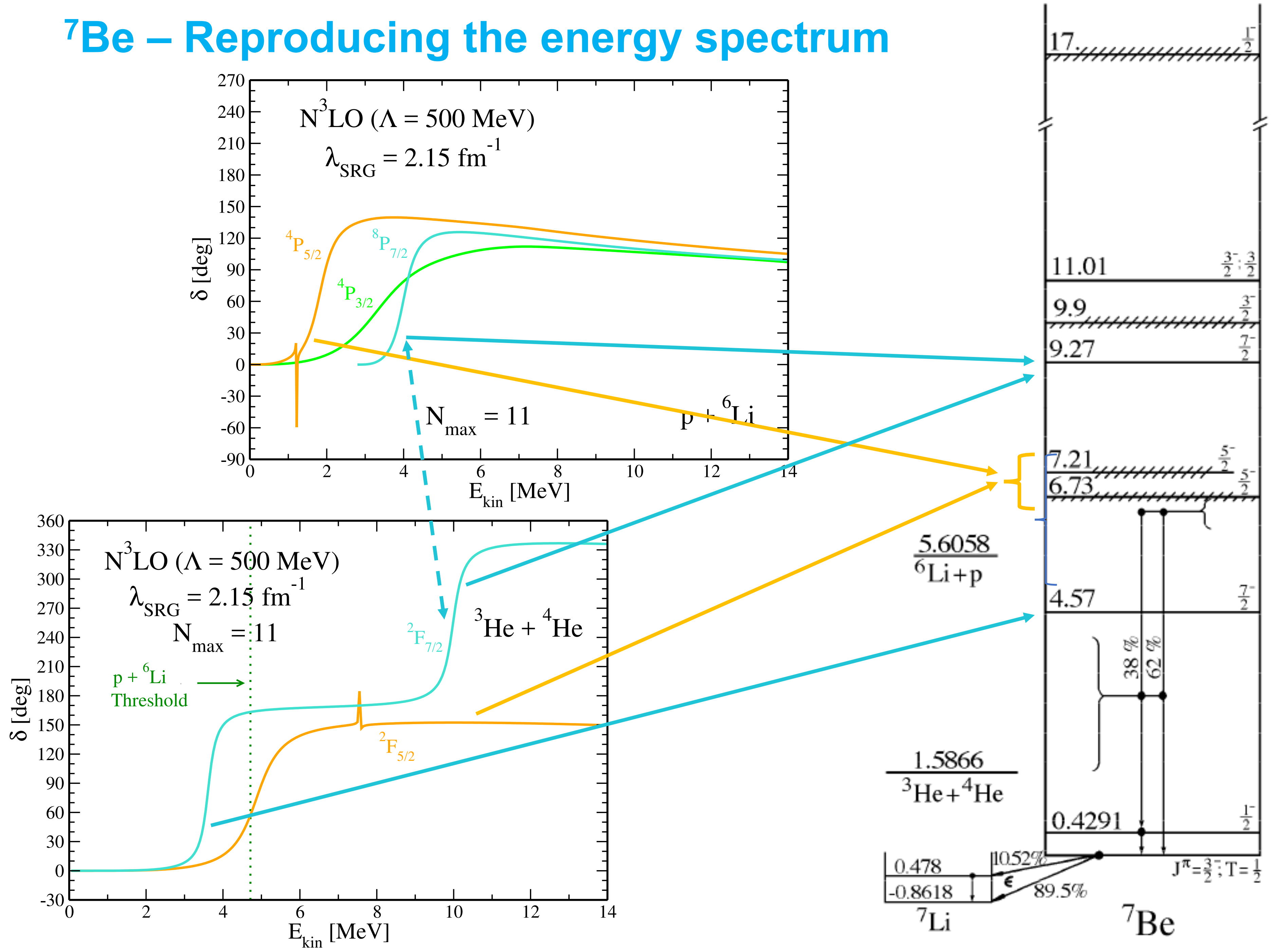
p + ^{6}Li	$J^\pi = 3/2^-$	$J^\pi = 1/2^-$
E_{bound}	-5.729	-5.389
E [MeV]	-36.47	-36.13



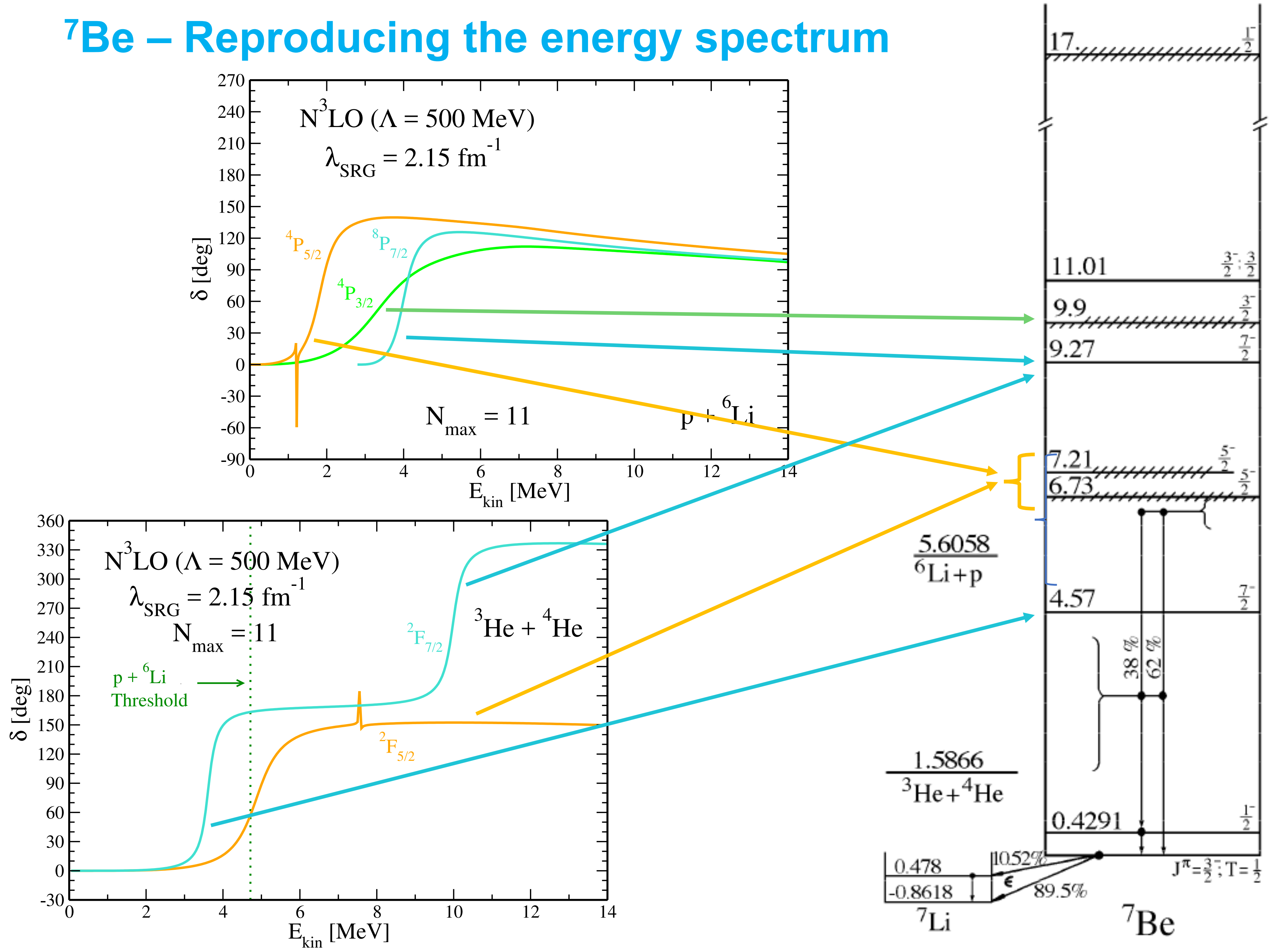
^{7}Be – Reproducing the energy spectrum



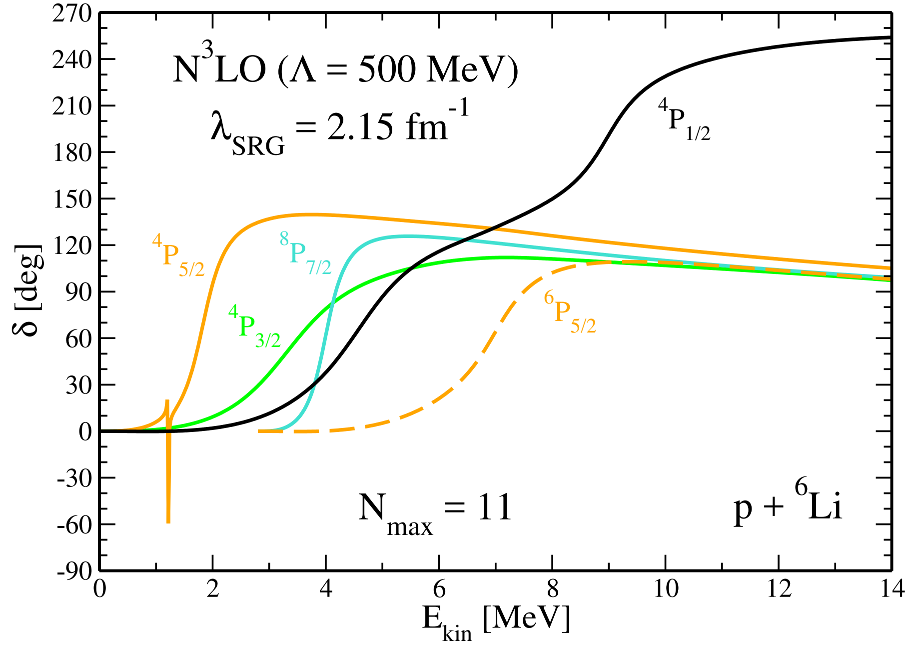
^{7}Be – Reproducing the energy spectrum

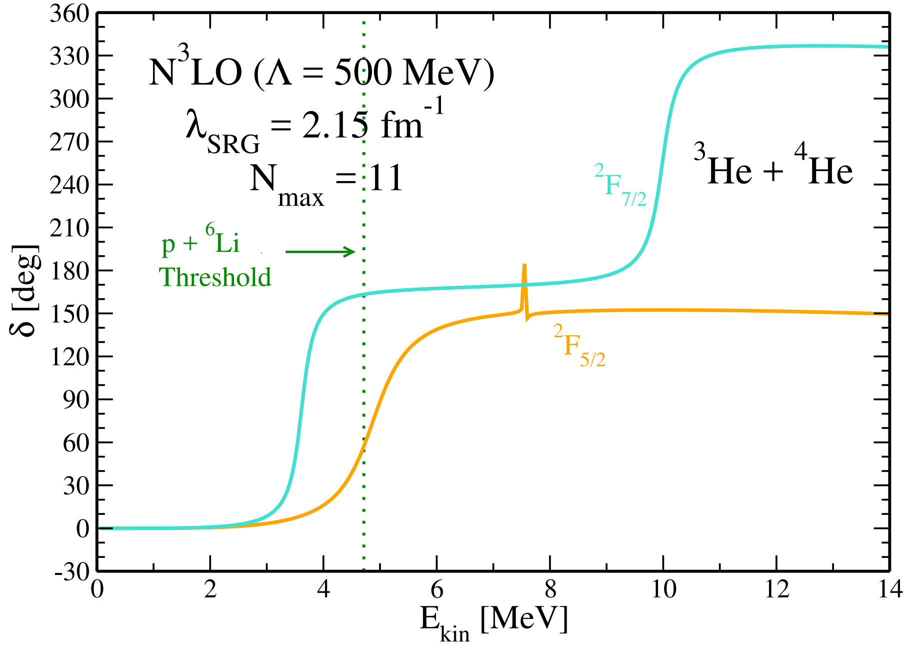


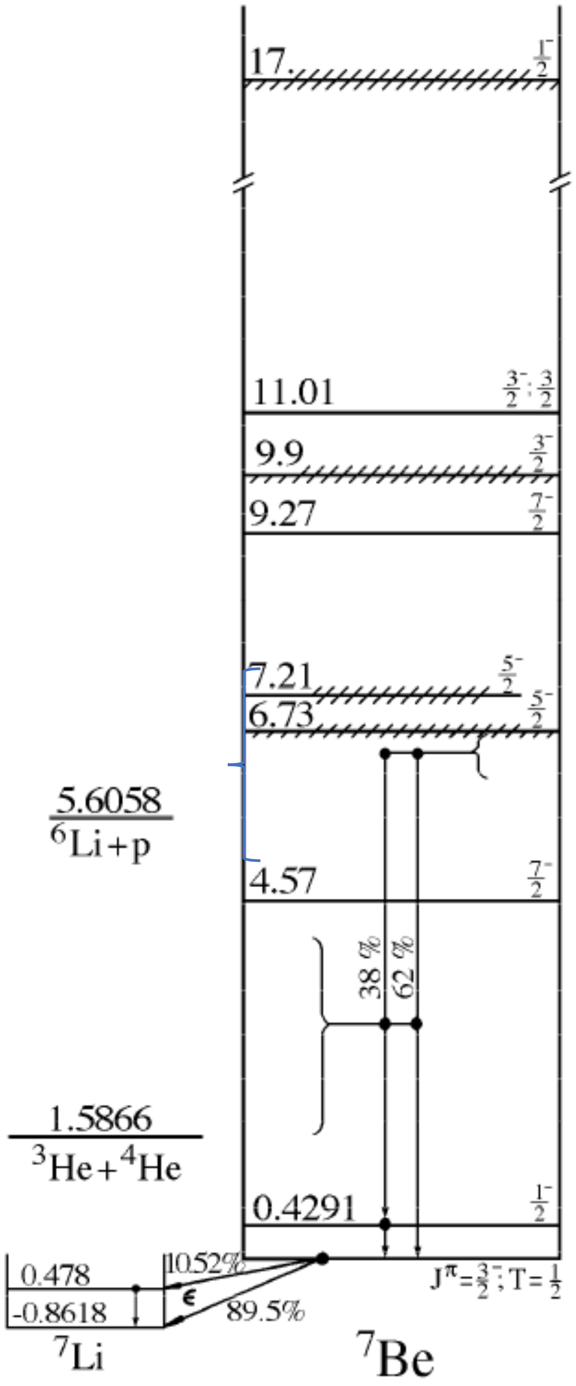
⁷Be – Reproducing the energy spectrum



^{7}Be – New negative-parity states







^{7}Li system

Analyzed mass partitions

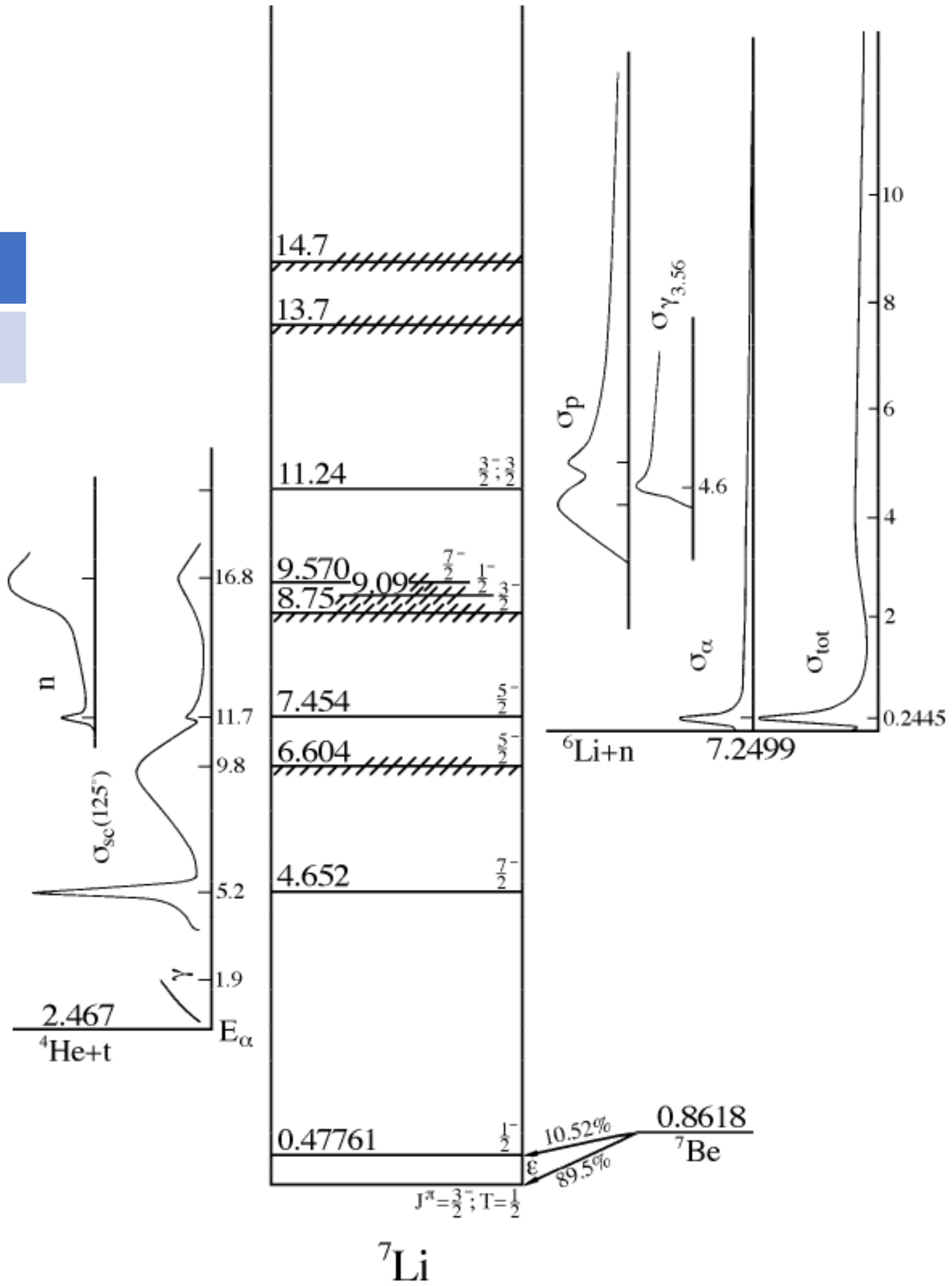
- ^{3}H + ^{4}He
- n + ^{6}Li
- p + ^{6}He

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

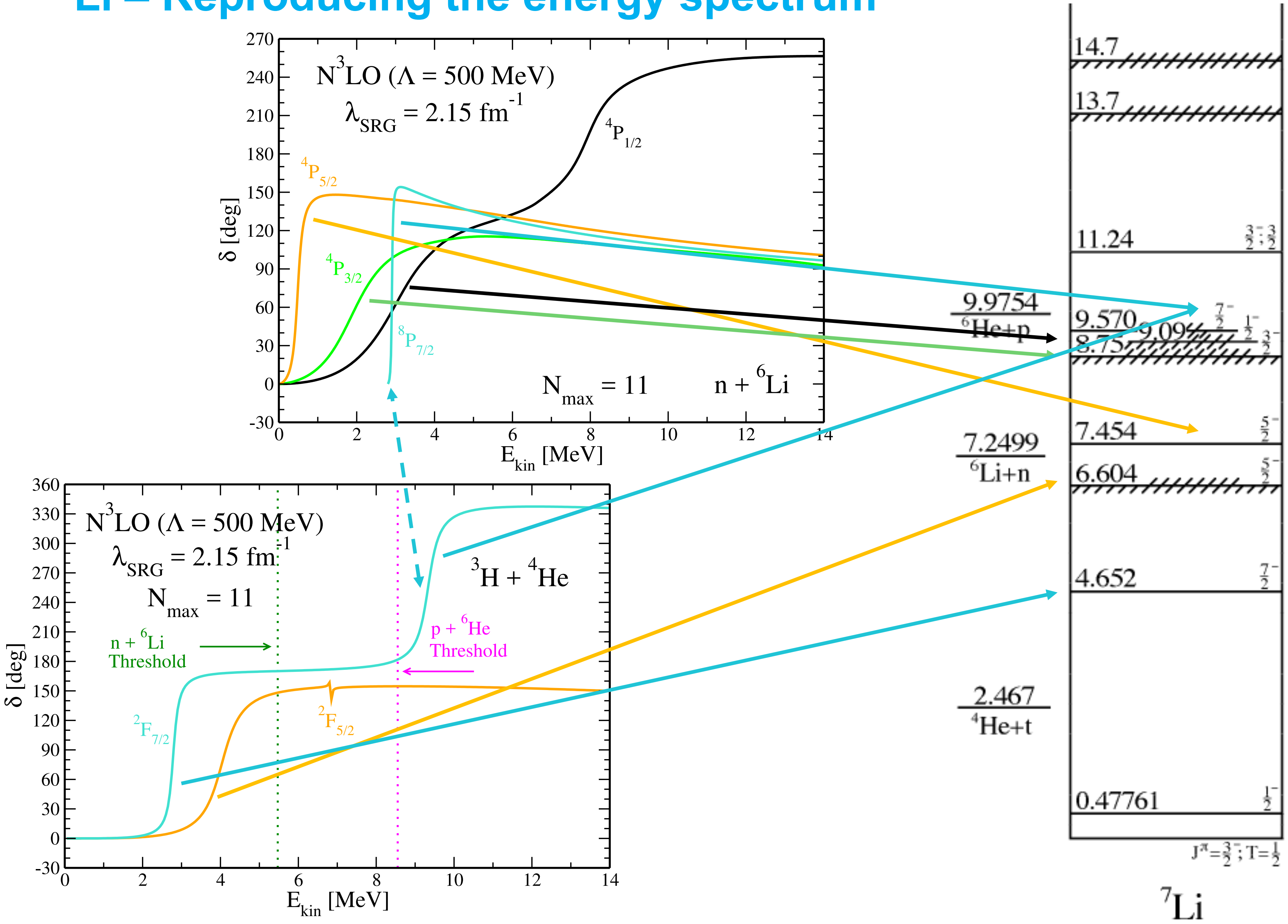
^{3}H + ^{4}He	$J^\pi = 3/2^-$	$J^\pi = 1/2^-$
E_{bound}	-2.432	-2.153
E [MeV]	-38.65	-38.37

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

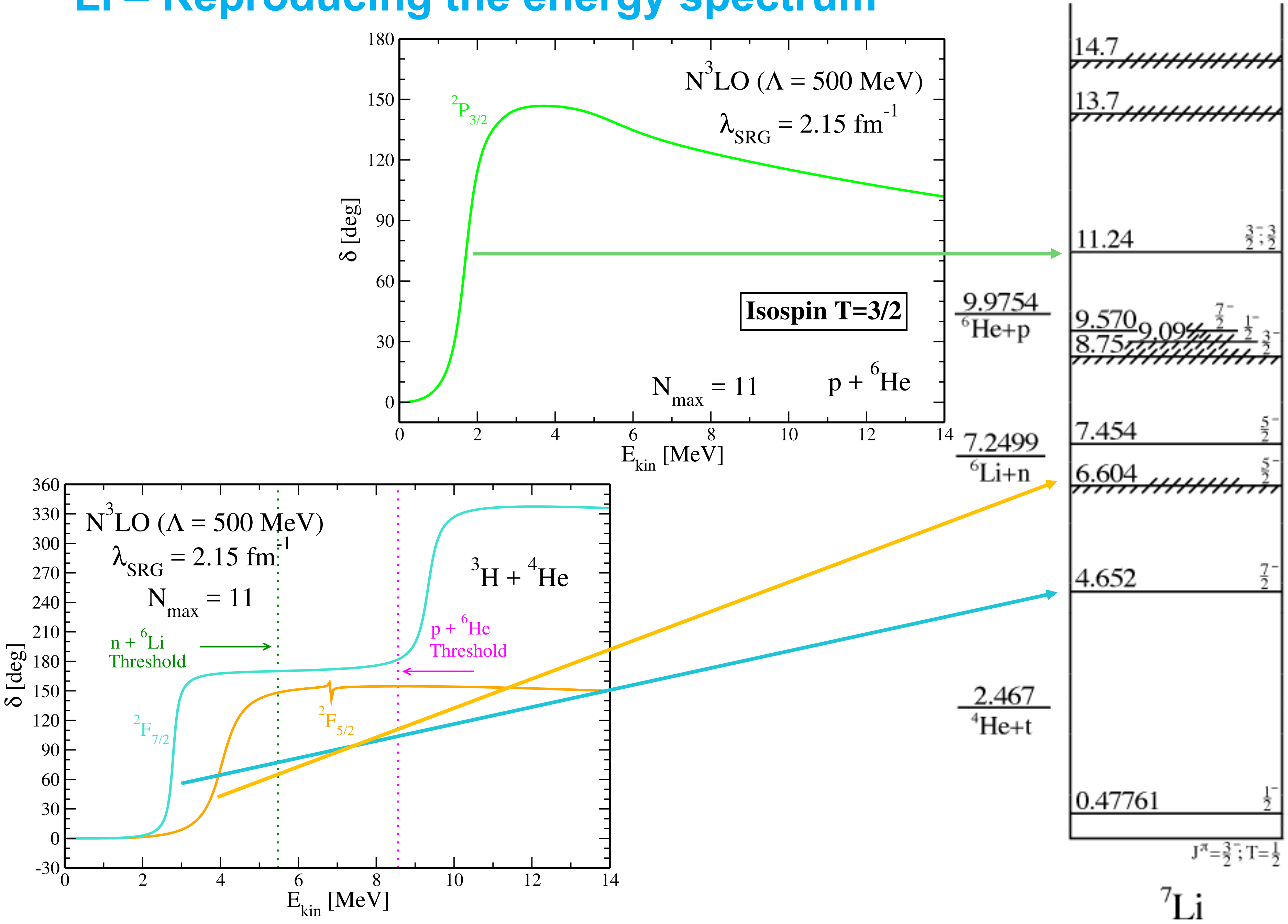
p + ^{6}He	$J^\pi = 3/2^-$	$J^\pi = 1/2^-$
E_{bound}	-10.40	-10.06
E [MeV]	-38.06	-37.73



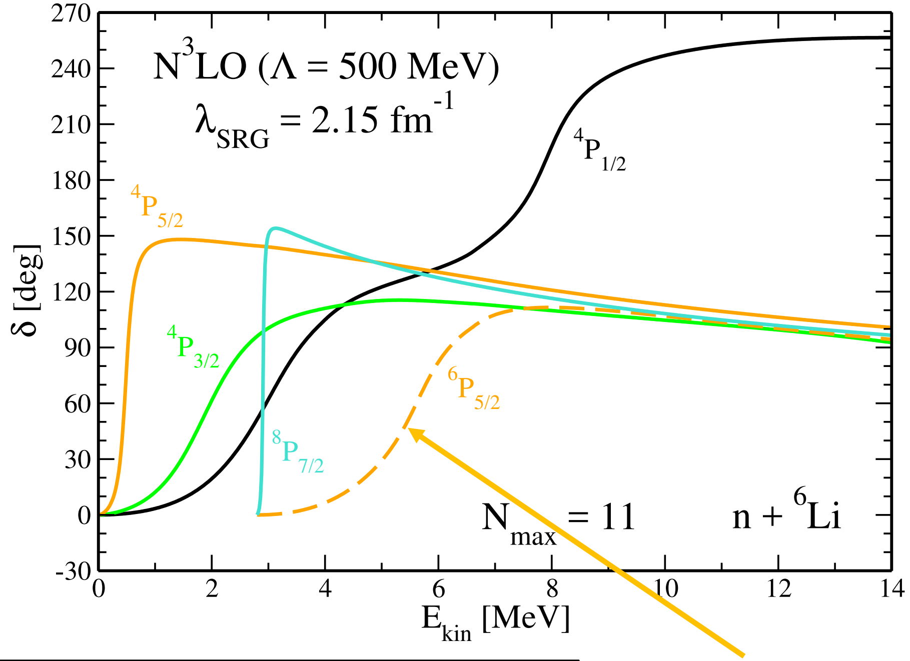
^{7}Li – Reproducing the energy spectrum

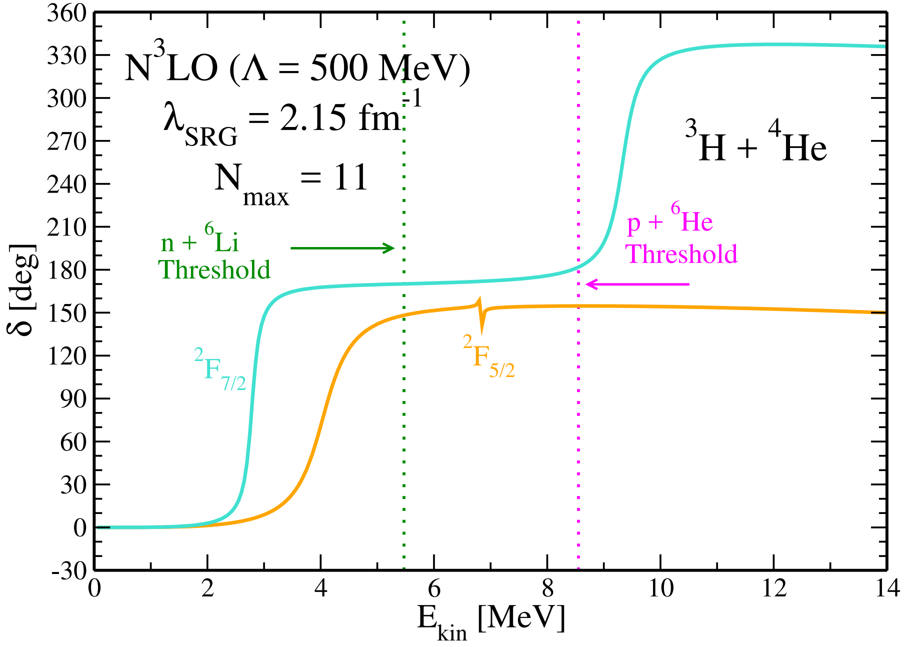


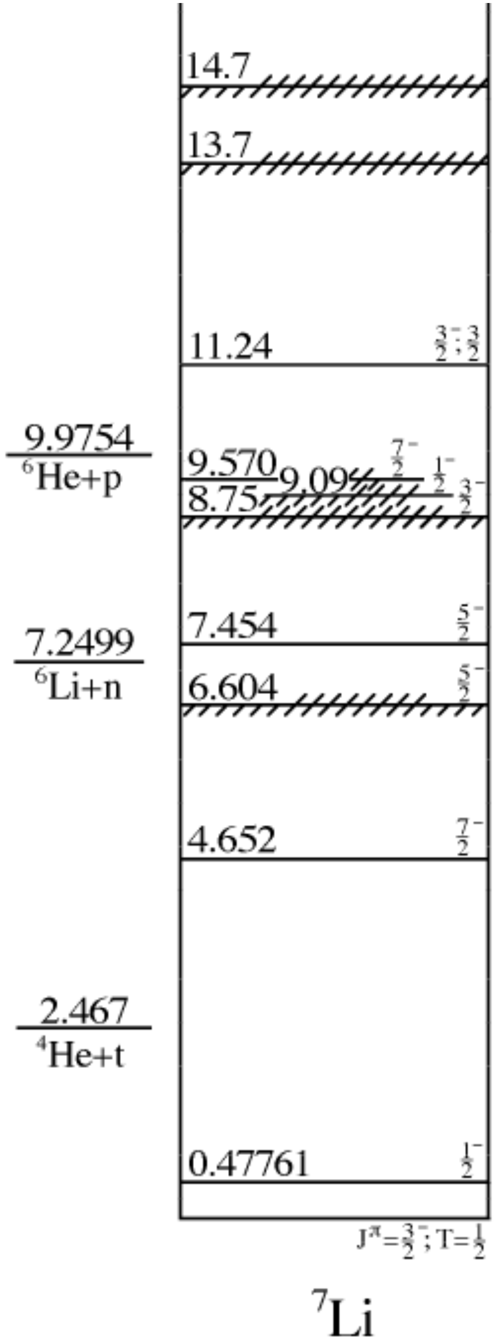
^{7}Li – Reproducing the energy spectrum



^{7}Li – New negative-parity states

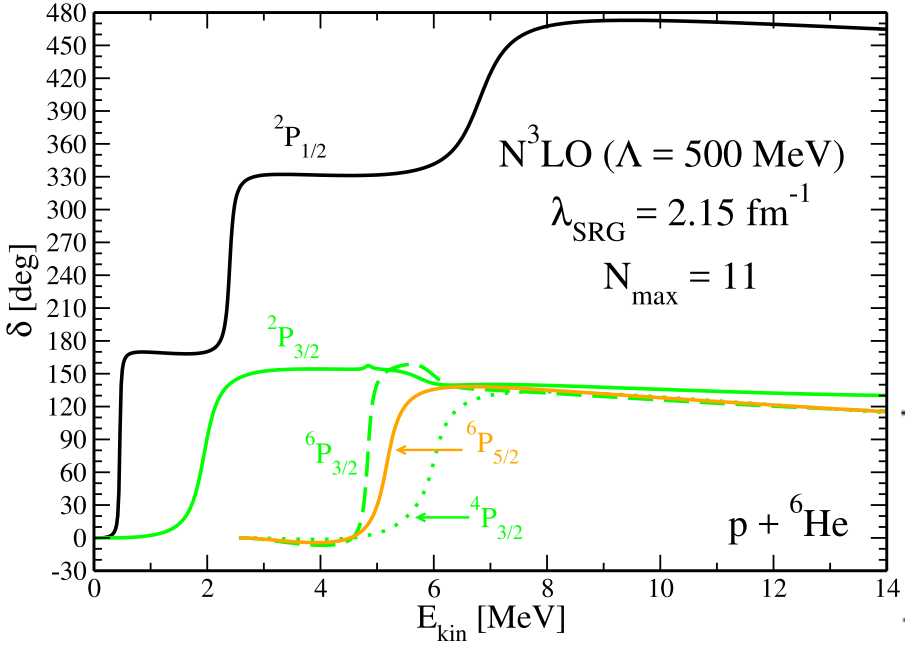


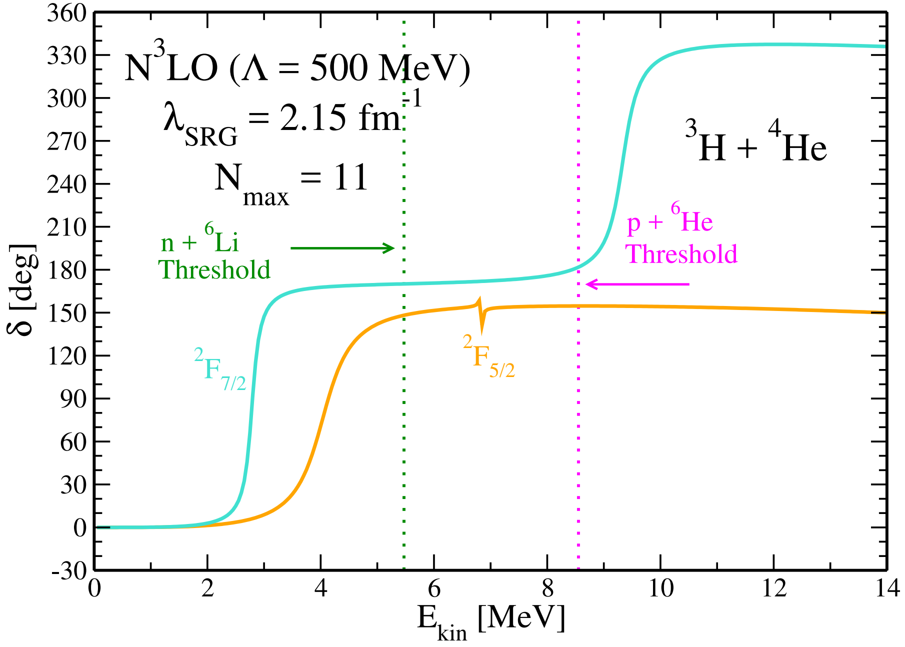


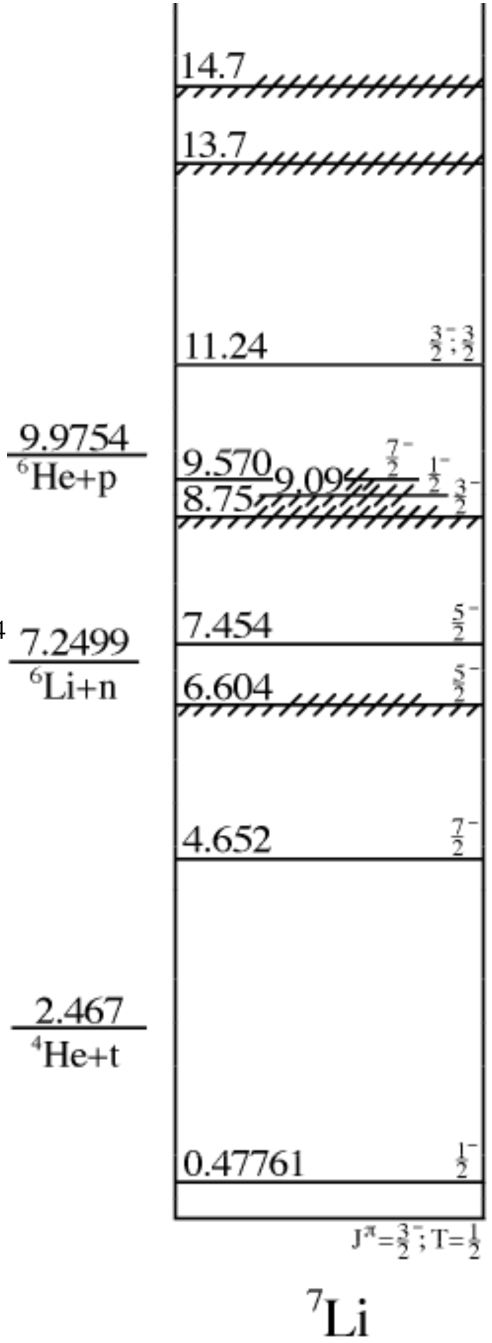


^{7}Li – New negative-parity states

5 new T=1/2 resonances

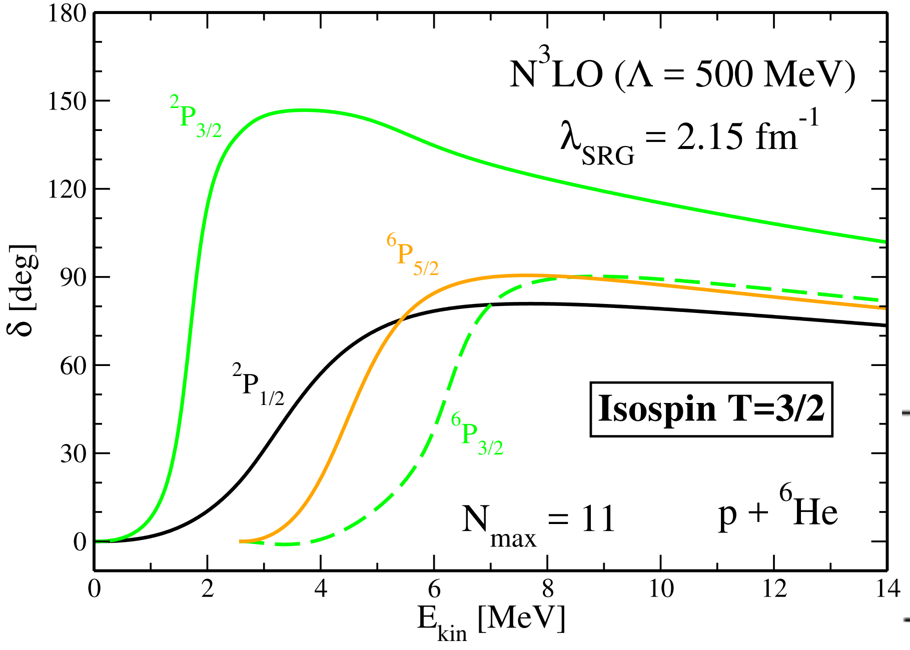


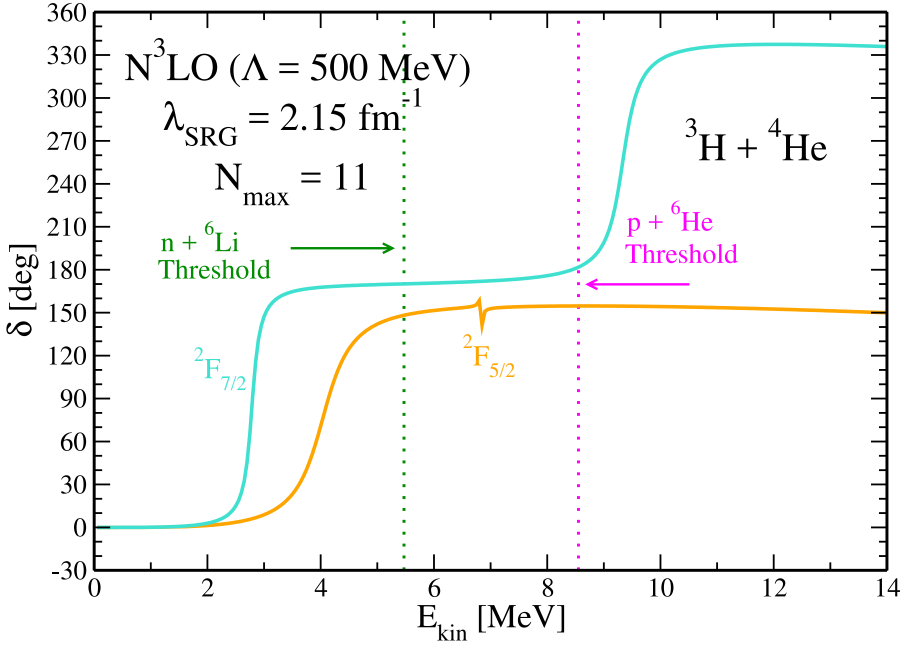


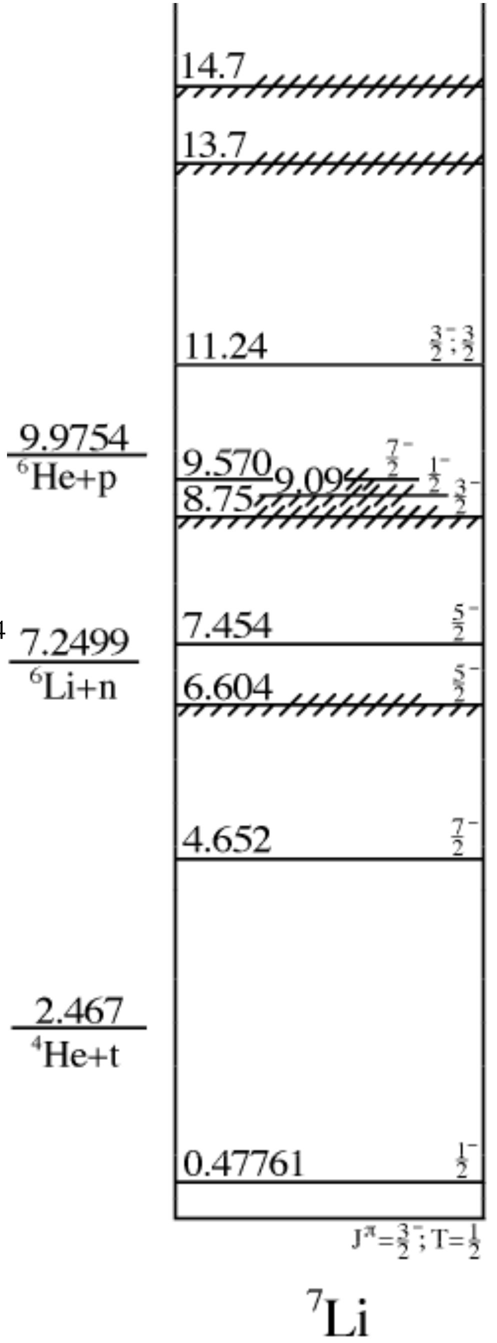


^{7}Li – New negative-parity states

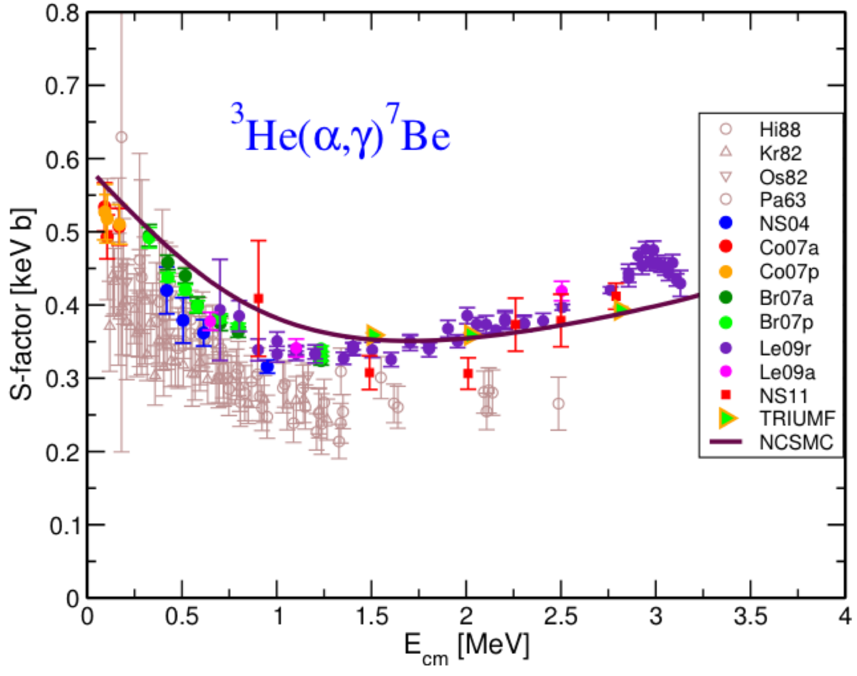
3 new T=3/2 resonances







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



Cross section and S-factor

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

Sommerfeld parameter

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

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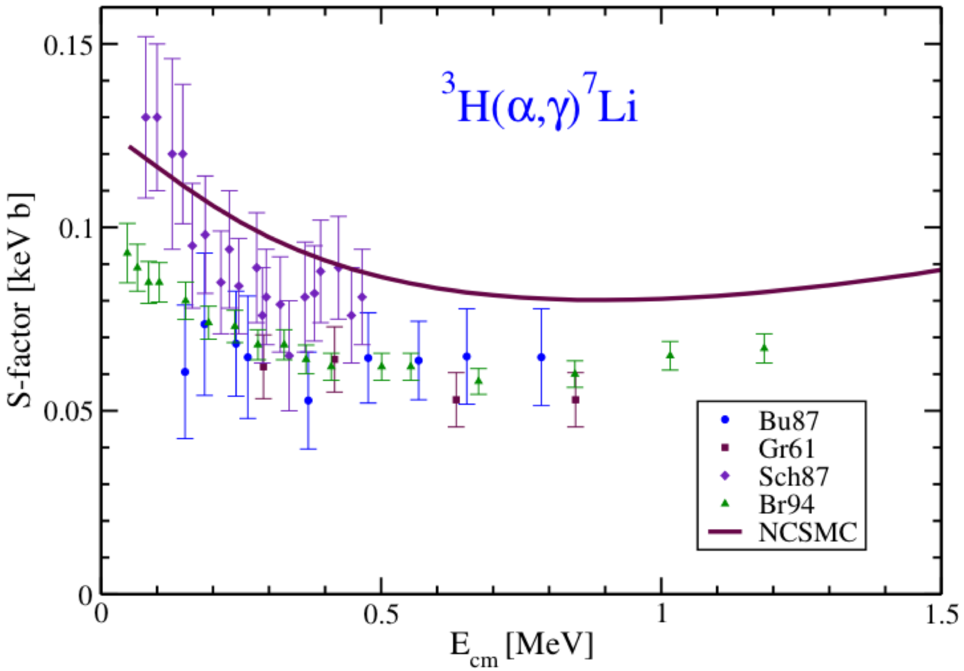
^{3}He$(\alpha,\gamma)^7$Be and ^{3}H$(\alpha,\gamma)^7$Li astrophysical S factors from the no-core shell model with continuum

CrossMark

Jérémy Dohet-Eraly [a,*], Petr Navrátil [a], Sofia Quaglioni [b], Wataru Horiuchi [c], Guillaume Hupin [b,d,1], Francesco Raimondi [a,2]



Conclusions

- *Ab initio* calculations of nuclear structure and reactions with predictive power becoming feasible beyond the lightest nuclei
- *Ab initio* structure calculations can even reach (selected) medium & medium-heavy mass nuclei
- These calculations make connections between the low-energy QCD, many-body systems, and nuclear astrophysics

TRIUMF

Thank you!

Merci!

Discovery,
accelerated