Continuum dynamics and reactions in light nuclei

HEDS Seminar series

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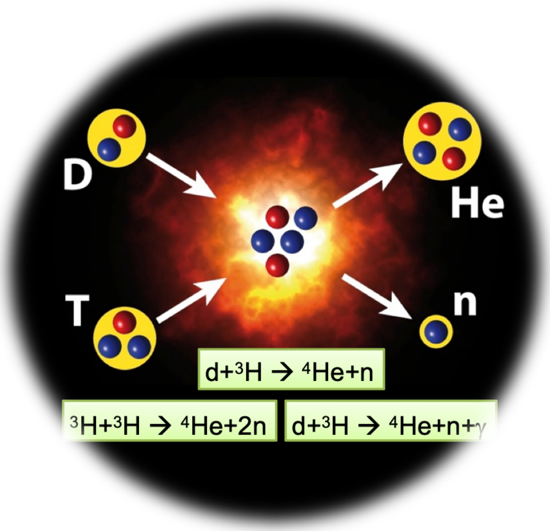
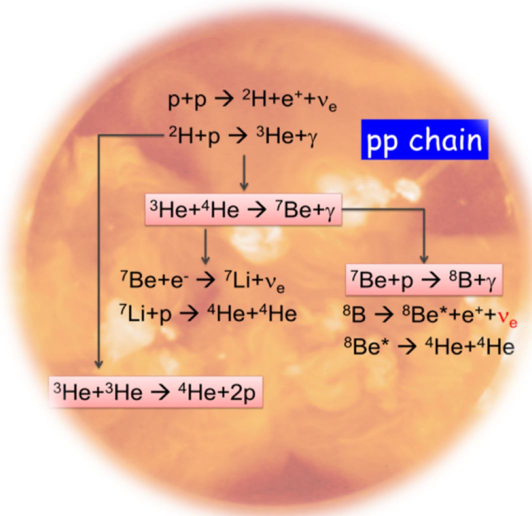
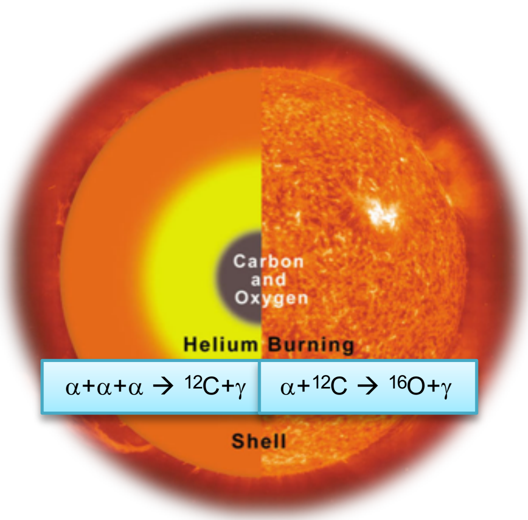
Why the interest in light-nuclei reactions?

Reactions among light nuclei in dense plasmas play an important role in applications, from fusion energy research to nuclear astrophysics







Predictive theory needed to achieve accuracy and/or provide part of nuclear data required by applications

1) The fusion process operates mainly by tunneling through the Coulomb barrier
   - Extremely low rates
2) In a accelerator expt., projectiles and targets are not fully ionized
   - Electron screening can mask "bare" nuclear cross section
3) Limitations in range of energies/angles, coincident measurements
   - Expt. determination typically incomplete

Fusion cross section

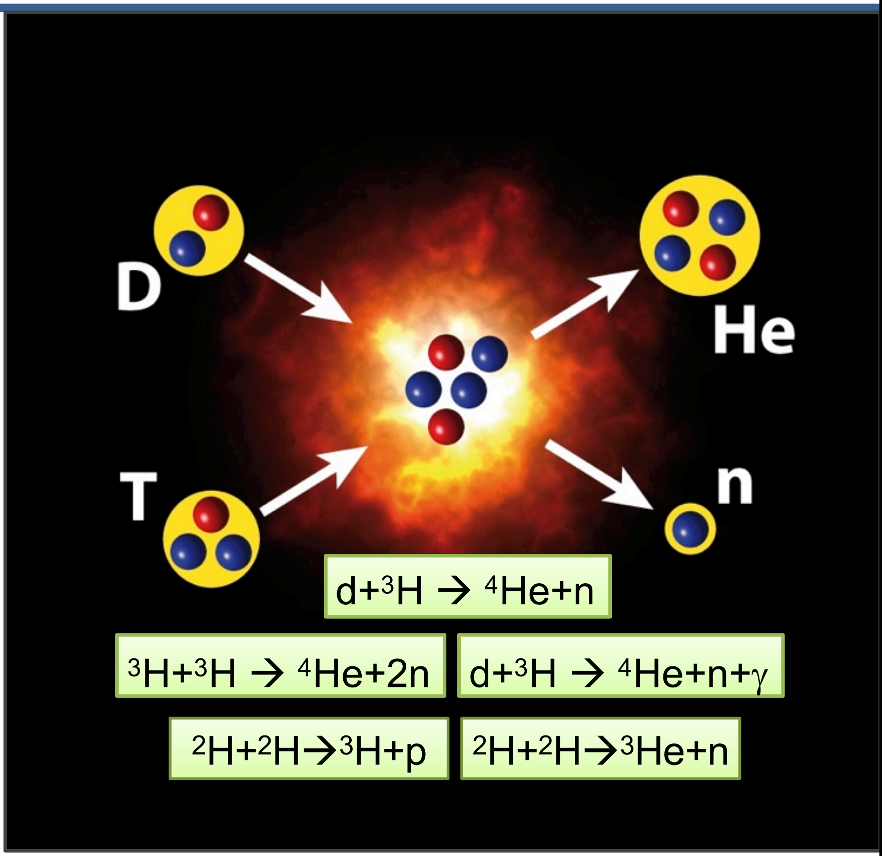
Astrophysical S-factor: nuclear contribution

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

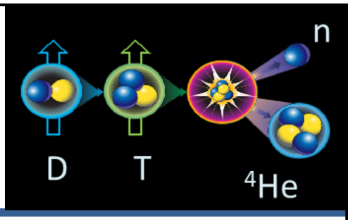
'Coulomb' contribution (tunneling)

Harnessing fusion energy

- DT most promising of the reactions that could power thermonuclear reactors of the future
- DT fusion cross section measured extensively
- Also important for diagnostic purposes: TT & DD fusion, γ branch of DT fusion
- Fusion with polarized fuel?
  - Important polarization observables not measured



Nuclear fusion with polarized fuel



- What is the effect of spin polarization in the DT fusion?
- First simple estimate by Kulsrud et al., PRL**49**, 1248 (1982)

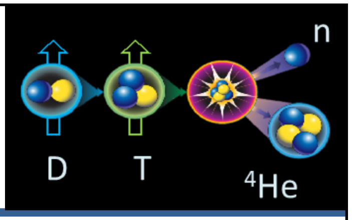
$$\sigma_{unpol} = \sum_J \frac{2J+1}{(2I_D+1)(2I_T+1)} \sigma_J \overset{\ell=0}{\approx} \frac{1}{3}\sigma_{\frac{1}{2}} + \frac{2}{3}\sigma_{\frac{3}{2}}$$

- Assumes:

1) Only $J^\pi = 3/2^+$ partial wave contributes
2) D+T pair in s-wave of relative motion

How valid are these assumptions? What is the contribution of $\ell > 0$ partial waves in the vicinity of the $3/2^+$ resonance? What is the effect on the polarized reaction rate?

Nuclear fusion with polarized fuel



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Estimated enhancement for perfect spin alignment

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

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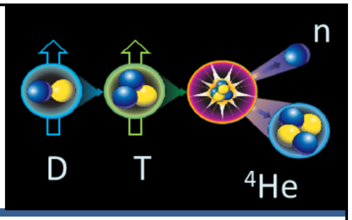
Nuclear fusion with polarized fuel



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- Assumes:
  1) Only $J^\pi = 3/2^+$ partial wave contributes
  2) D+T pair in s-wave of relative motion

Estimated angular distribution of emitted neutrons and α particles

$$\frac{d\sigma_{pol}}{d\Omega} \propto \sin^2\theta$$

How valid are these assumptions? What is the contribution of $\ell > 0$ partial waves in the vicinity of the $3/2^+$ resonance? What is the effect on the polarized reaction rate?

Nuclear fusion with polarized fuel

- What is the effect of spin polarization in the DD fusion?

$$\overset{\ell = 0}{}$$

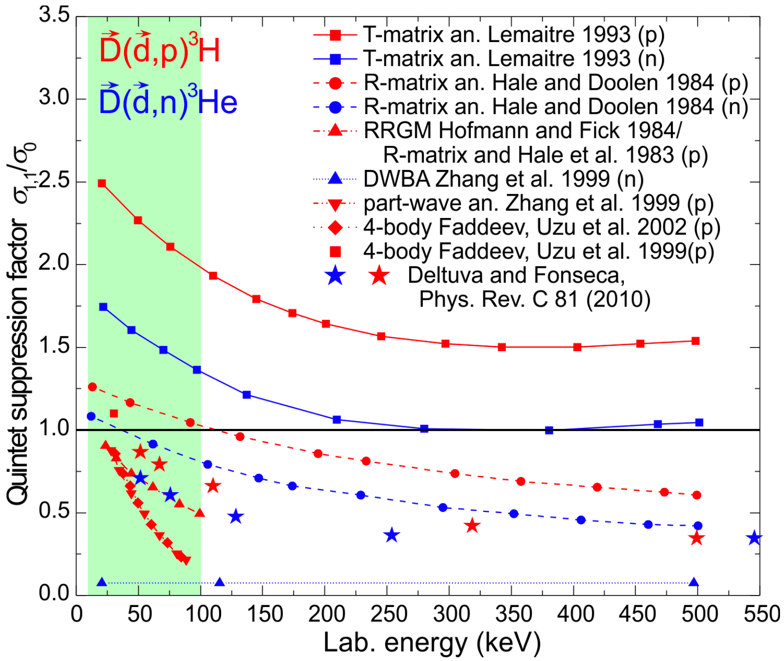
$$\sigma_{unpol} \approx \frac{1}{9}\left(2\sigma_{1,1} + 4\sigma_{1,0} + \sigma_{0,0} + 2\sigma_{1,-1}\right)$$

quintet

- But:

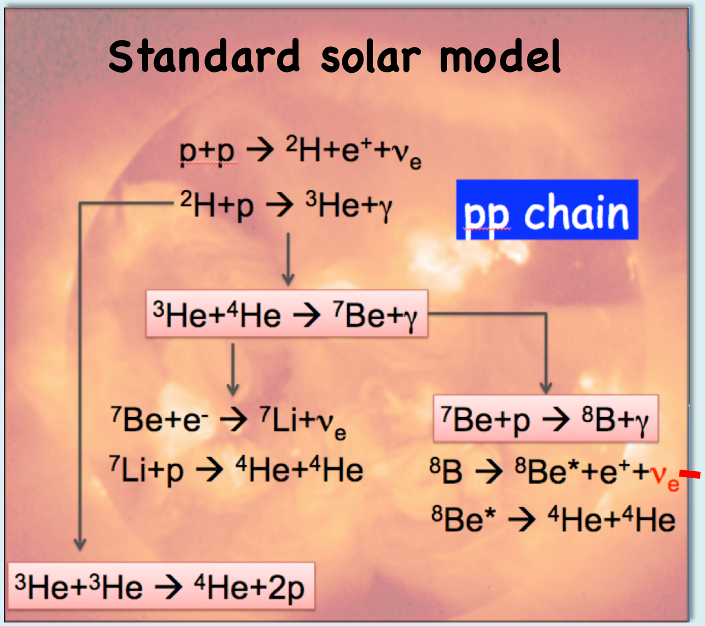
1) DD is NOT dominated by one resonance!

2) DD is NOT S-wave dominated!

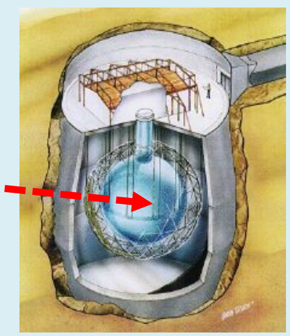


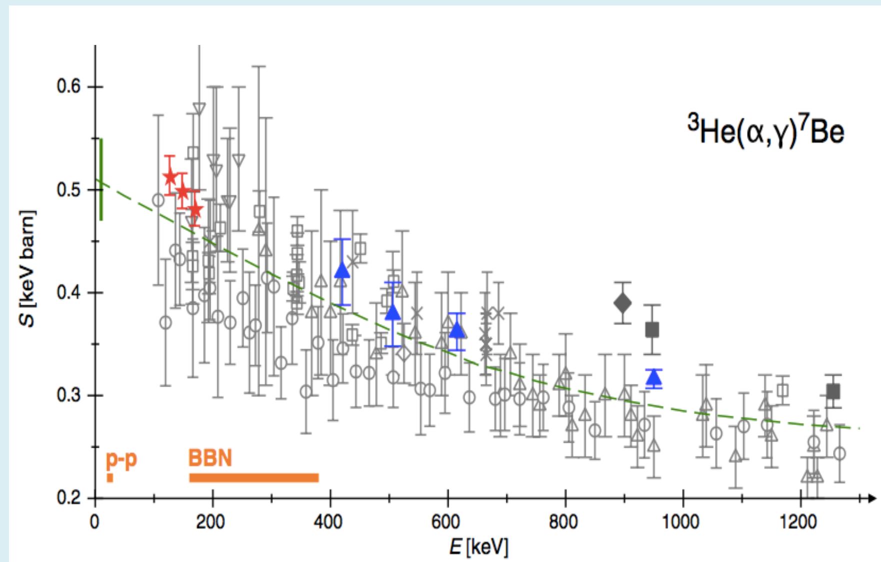
Predictions for parallell spins (quintet suppression factor = $\sigma_{1,1}/\sigma_{unpol}$) span from a factor 10 suppression for D+D→^{3}He+n to a factor 2.5 enhancement of D+D→^{3}H+p

Our Sun: one of the best tools for studying neutrinos



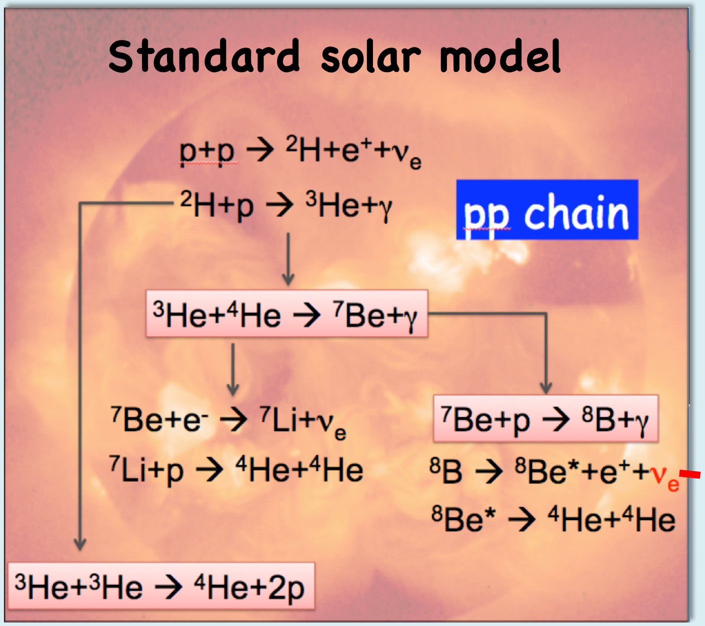
Neutrino oscillations
2015 Noble Prize in Physics





Several other examples of insufficiently known reactions among light nuclei that play an important role in understanding the origin, evolution, and inner workings of our universe

Our Sun: one of the best tools for studying neutrinos



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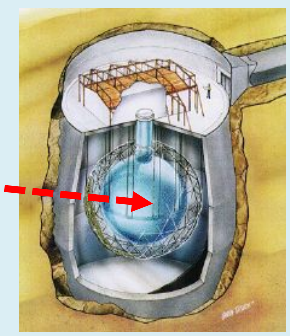
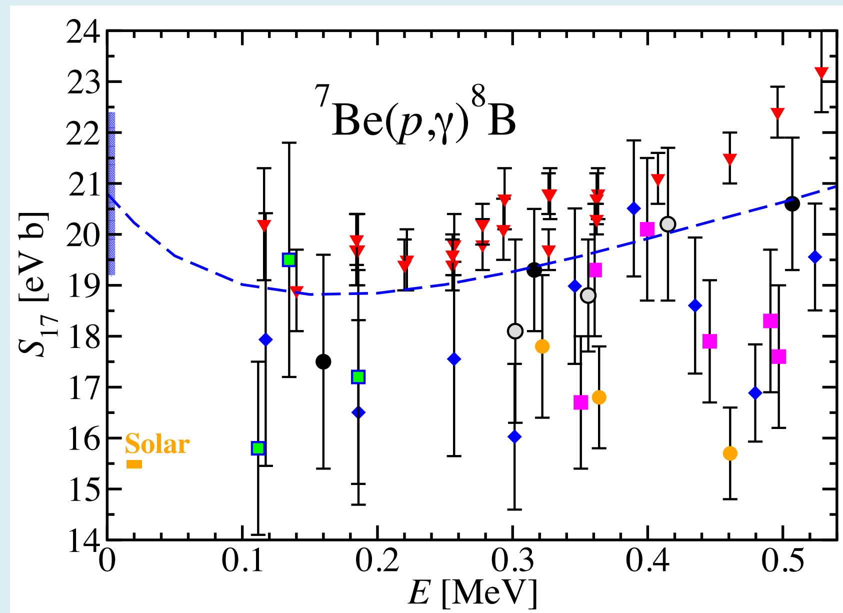
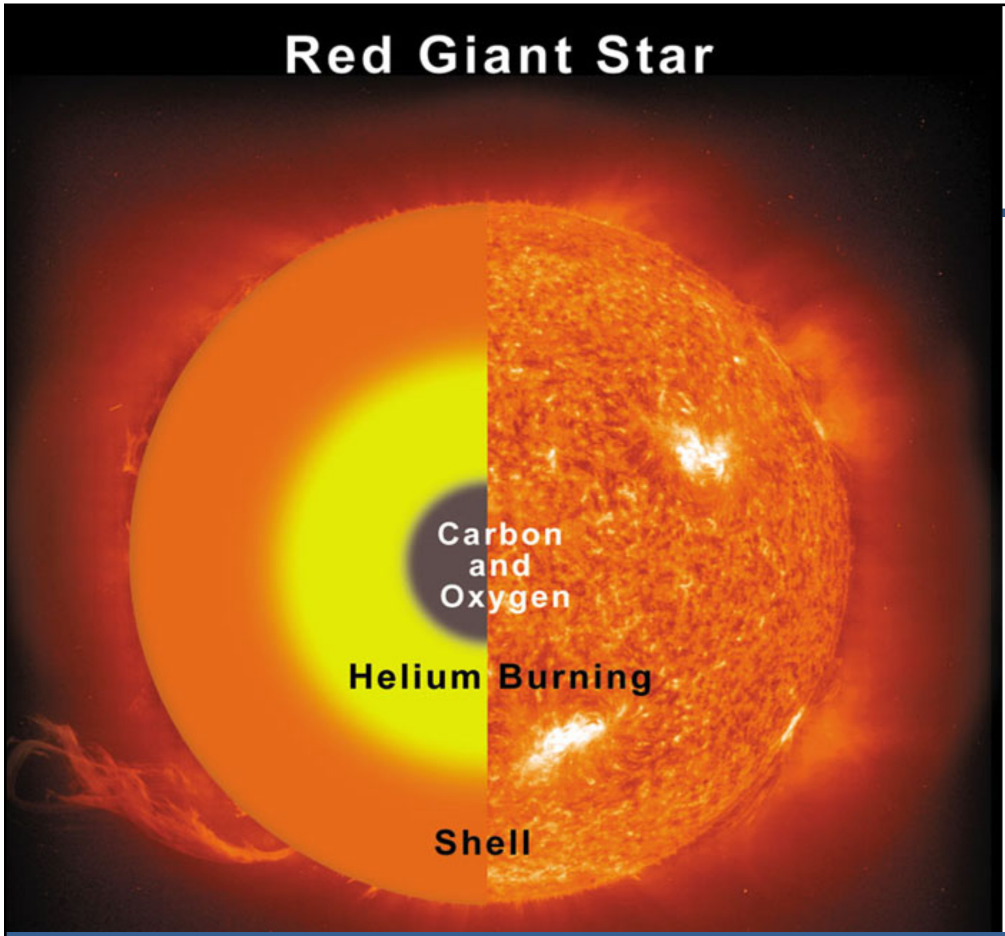
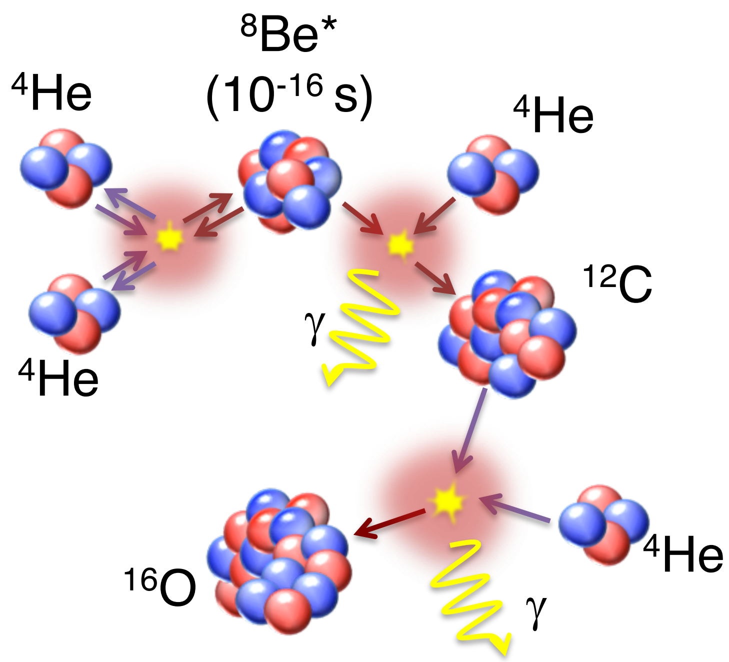




Several other examples of insufficiently known reactions among light nuclei that play an important role in understanding the origin, evolution, and inner workings of our universe



Helium burning

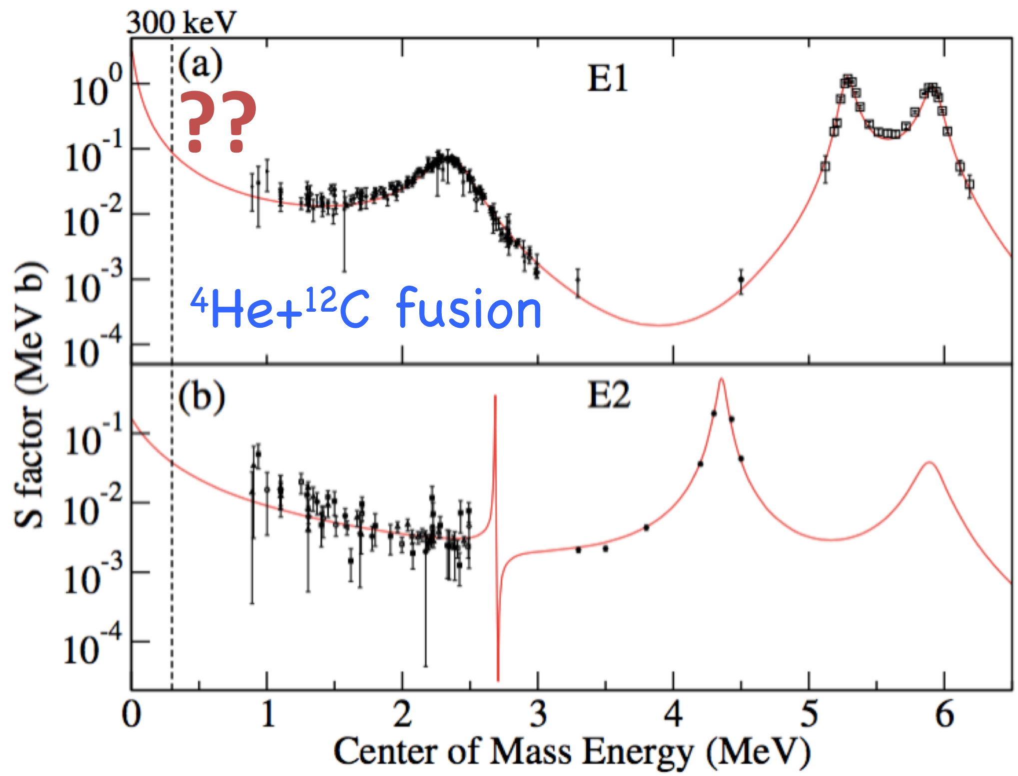


"Not only important for the development of the chemical building blocks of life but also for the entire scheme and sequence of nucleosynthesis events as we imagine them now." (2015 LRP)

We need reliable theory to estimate the S-factor at stellar energies

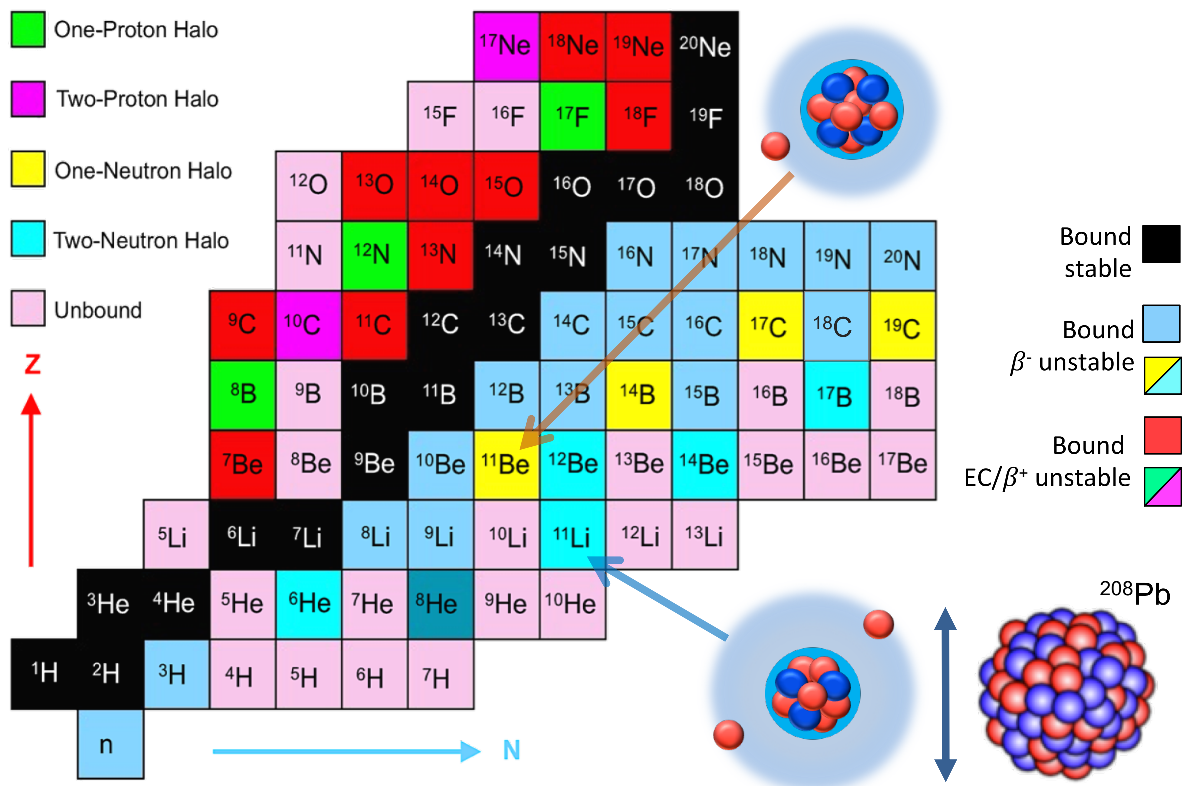
- Direct measurements at 300 keV (helium burning conditions) so far impossible
- Major hurdle in precisely determining carbon-to-oxygen ratio produced in stars, introduces large uncertainties in stellar-evolution models and in the predictions of stellar nucleosynthesis

In-depth review: R.J. deBoer et al., Rev. Mod. Phys. **89**, 035007

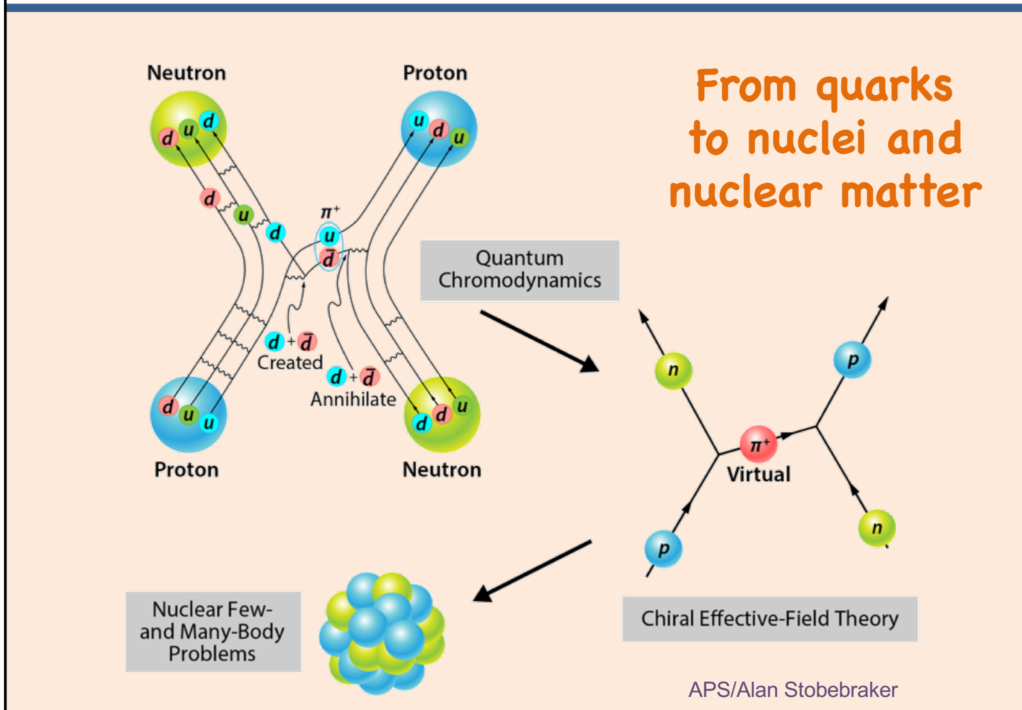


A fundamental understanding of continuum dynamics is needed to arrive at a predictive theory of nuclei

- Nuclear structure at the limits of stability (neutron and proton driplines)
- Halo nuclei: weakly-bound states of clusters of nucleons with unusually large radii
- Unbound nuclei existing only as metastable states called resonances
- And more …



Currently best path to predictive theory: Effective field theories of QCD combined with ab initio many-body methods



- *Ab initio* many-body calculations
  - A (all active) point-like nucleons
  - Nucleon-nucleon and three-nucleon (NN+3N) interactions derived within chiral effective field theory (EFT)
  - Non relativistic Quantum Mechanics

The ab initio nuclear many-body problem is extremely complicated and among the most computationally intensive fields of science. Requires efficient theoretical frameworks and high-performance computing.

How to describe the phenomena of low-energy nuclear reactions based on colliding nuclei made of interacting nucleons?

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Ab initio no-core shell model with continuum (NCSMC)

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

Unknowns

Ab initio no-core shell model with continuum (NCSMC)

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Localized A-nucleon solutions (eigenstates) computed with the NCSM

$$\left| {}^{(A)}, \lambda \right\rangle = \sum_{k}^{N} b_k^{(\lambda)} \phi_k(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_A)$$

$$(H^{(A)} - E_{\lambda}) \left| {}^{(A)}, \lambda \right\rangle = 0$$

Ab initio no-core shell model with continuum (NCSMC)

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

$$\left| {}_{(A-a)} \overset{\vec{r}}{\longleftarrow} {}_{(a)} , \nu \right\rangle = \left| {}^{(A-a)} , \nu_1 \right\rangle \left| {}^{(a)} , \nu_2 \right\rangle \delta(\vec{r} - \vec{r}_{A-a,a})$$

Continuous microscopic cluster states made of projectile-target pairs in relative motion

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Describe efficiently the wave function when all A nucleons are close together

Describe efficiently the wave function when the reactants/ reaction products are far apart

Ab initio no-core shell model with continuum (NCSMC)

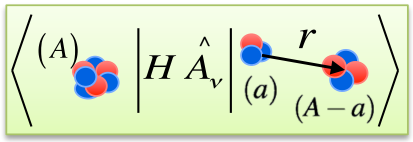
$$\Psi^{(A)} = \sum_{\lambda} c_{\lambda} \left| {}^{(A)}, \lambda \right\rangle + \sum_{\nu} \int d\vec{r}\; u_{\nu}(\vec{r})\; \hat{A}_{\nu} \left| {}_{(A-a)} \xleftarrow{\vec{r}} {}^{(a)}, \nu \right\rangle$$

Works well for describing clustering in nuclei (halo nuclei)

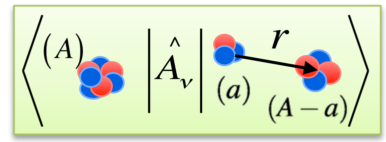
Works well for describing both bound and scattering state

Discrete and continuous variational amplitudes are determined by solving the coupled NCSMC equations

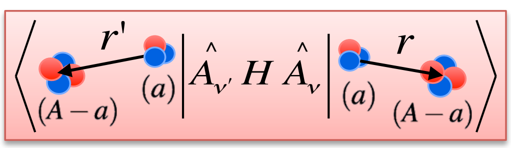
$E_\lambda^{NCSM}\,\delta_{\lambda\lambda'}$

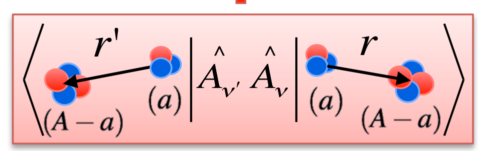


$\delta_{\lambda\lambda'}$



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





The NCSMC equations can be solved using R-matrix theory

Expansion on a basis (square-integrable)

$$u_c(r) = \sum_n A_{cn} f_n(r)$$

Bound state asymptotic behavior

$$u_c(r) = C_c W(k_c r)$$

$$\boxed{k_c = \sqrt{\frac{2\mu_c E_c}{\hbar^2}}}$$

$$C_c W(k_c r) \propto \exp\left(-\sqrt{\frac{2\mu_c E_c}{\hbar^2}}\, r\right)$$

The NCSMC equations can be solved using R-matrix theory

Expansion on a basis (square-integrable)

$$u_c(r) = \sum_n A_{cn} f_n(r)$$

Bound state asymptotic behavior

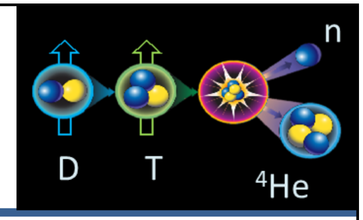
$$u_c(r) = C_c W(k_c r)$$

Scattering state asymptotic behavior

$$u_c(r) = \frac{i}{2} v_c^{-\frac{1}{2}} \left[\delta_{ci} I_c(k_c r) - S_{ci} O_c(k_c r) \right]$$

Predictions for polarized DT and D^{3}He fusion

G. Hupin, S.Q., P. Navratil, Nature Communications **10**, 351 (2019)



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Estimated enhancement for perfect spin alignment

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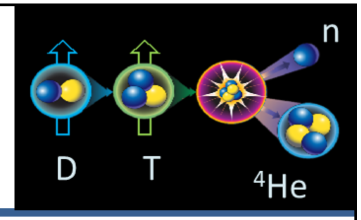
$$\boxed{\sigma_{pol} \approx 1.5\,\sigma_{unpol}}$$

How valid are these assumptions? What is the contribution of $\ell > 0$ partial waves in the vicinity of the $3/2^+$ resonance? What is the effect on the polarized reaction rate?

No-core shell model (NCSM) with continuum calculation of the DT fusion at a glance



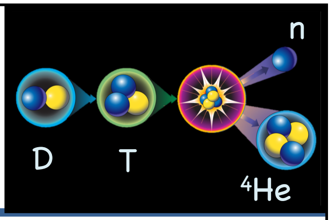
$$|\Psi\rangle = \sum_{\lambda} c_{\lambda} \left| {}^{5}\mathrm{He}, \lambda \right\rangle + \int d\vec{r}\, u_{\nu_{DT}}(\vec{r}) \hat{A}_{DT} \left| \mathrm{T} \overset{\vec{r}}{—} D, \nu_{DT} \right\rangle + \int d\vec{r}\, u_{\nu_{n\alpha}}(\vec{r}) \hat{A}_{n\alpha} \left| \alpha \overset{\vec{r}}{\longleftarrow} n, \nu_{n\alpha} \right\rangle$$

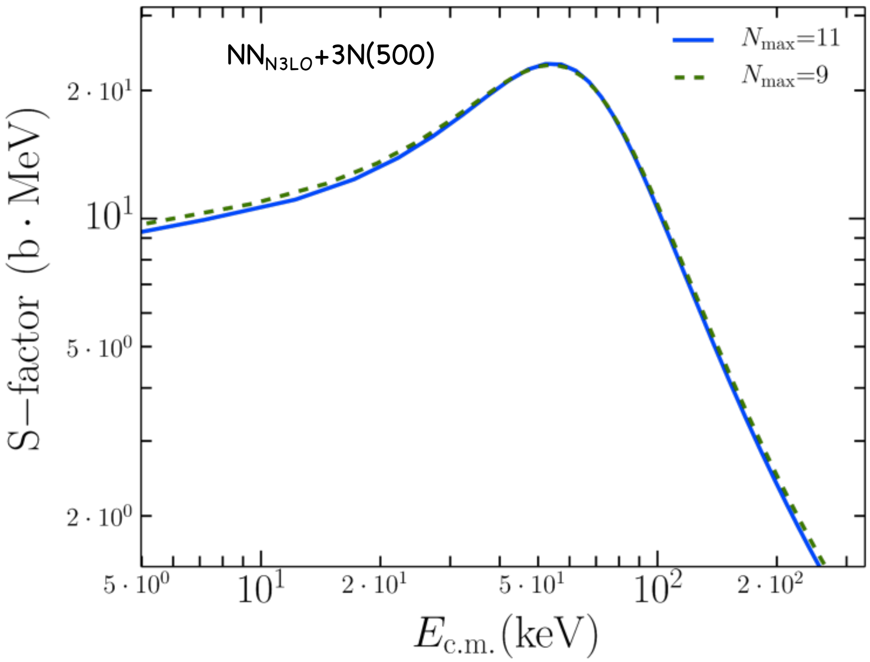
- 2x7 static ^{5}He eigenstates computed with the NCSM (N_{max}=11)
- Continuous D-T(g.s.) cluster states (entrance channel)
  - Including positive-energy eigenstates of D to account for distortion
- Continuous n-^{4}He(g.s.) cluster states (exit channel)
- N^{3}LO NN + N^{2}LO 3N (local) with 500 MeV cutoff, a.k.a NN+3N(500)

A formidable challenge for ab initio reaction theory: Integrated and comprehensive description of the interweaving of nuclear shell structure and reaction dynamics

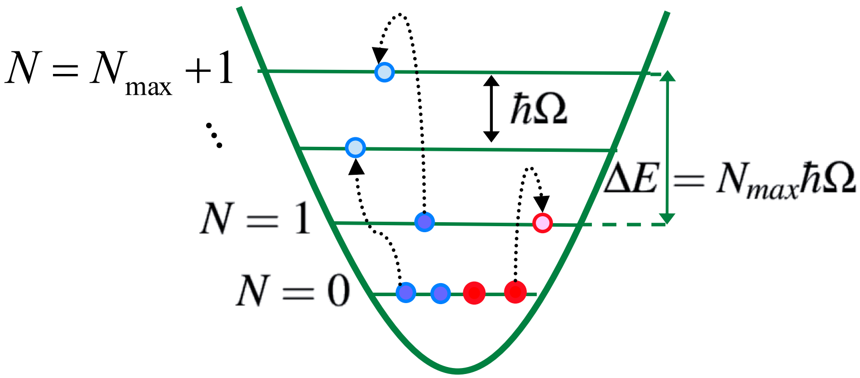
The unpolarized astrophysical S-factor

Dependence on the size of the HO model space





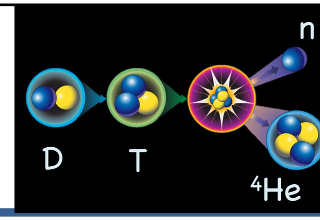
- We use an expansion in harmonic oscillator (HO) basis states to represent T, D, ^{5}He (in the example), and D-T relative motion in the internal region

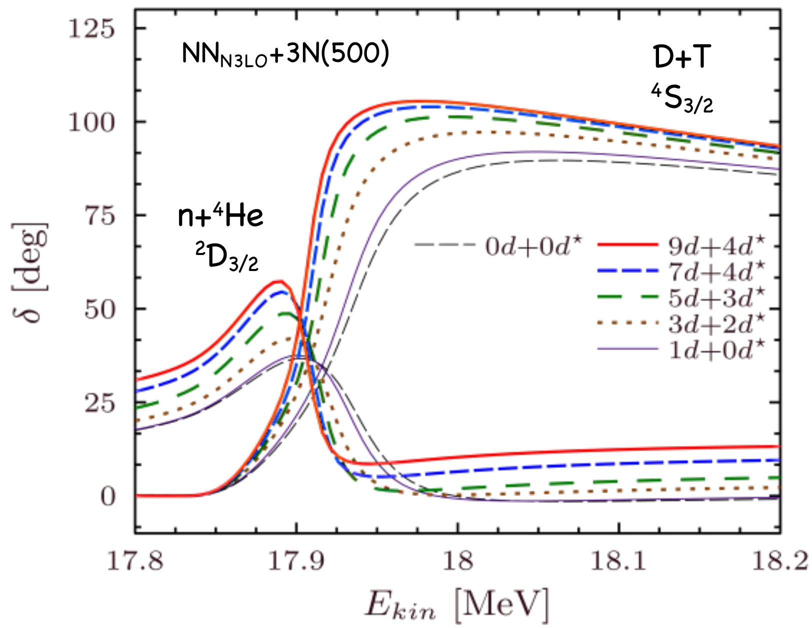


A formidable challenge for ab initio reaction theory: Integrated and comprehensive description of the interweaving of nuclear shell structure and reaction dynamics

Phase shifts in 3/2+ channel of ^{5}He

Influence of D positive-energy states





- Positive-energy eigenstates of D used to describe the projectile deformation
- Number of available states depends on N_{max}

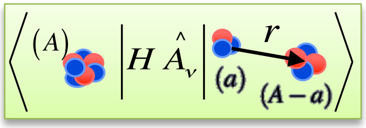
The resonance centroid and width

^{5}He(3/2+)	NCSMC	R-Matrix
E_R (keV)	55	47
Γ_R (keV)	110	74

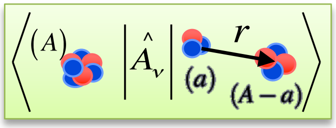
A formidable challenge for ab initio reaction theory: Integrated and comprehensive description of the interweaving of nuclear shell structure and reaction dynamics

Discrete and continuous variational amplitudes are determined by solving the coupled NCSMC equations

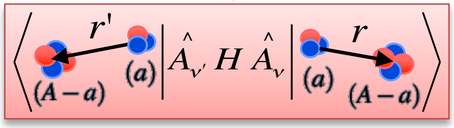
$E_\lambda \delta_{\lambda\lambda'}$

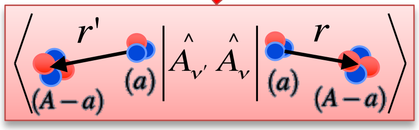


$\delta_{\lambda\lambda'}$



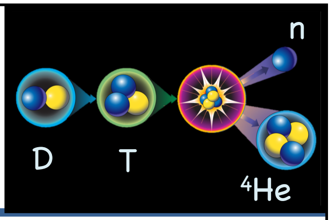
$$\begin{pmatrix} H_{NCSM} & h \\ h & H_{cont} \end{pmatrix} \begin{pmatrix} c \\ u \end{pmatrix} = E \begin{pmatrix} 1_{NCSM} & g \\ g & N_{cont} \end{pmatrix} \begin{pmatrix} c \\ u \end{pmatrix}$$



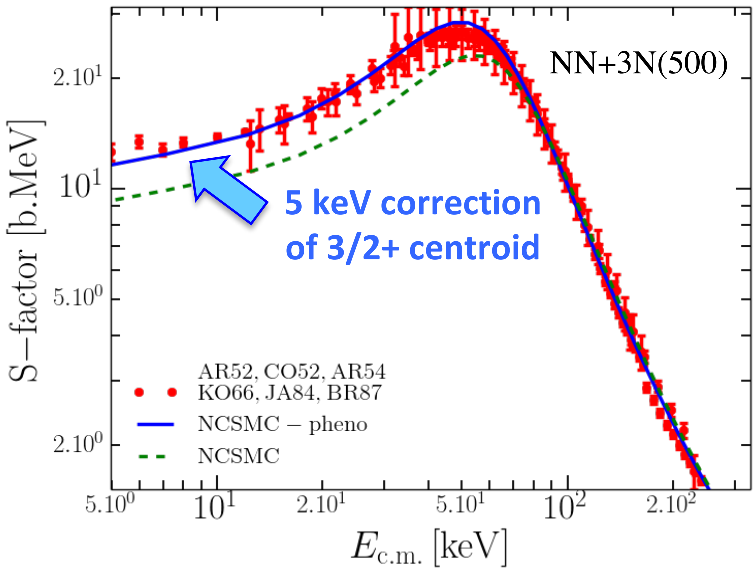


5 keV correction of the 3/2+ resonance centroid.
All other characteristics of the S-matrix still predicted from ab initio theory.

Phenomenological adjustment
NCSMC-pheno



Astrophysical S-factor



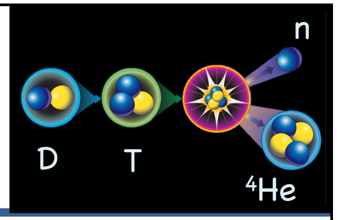
The resonance centroid and width

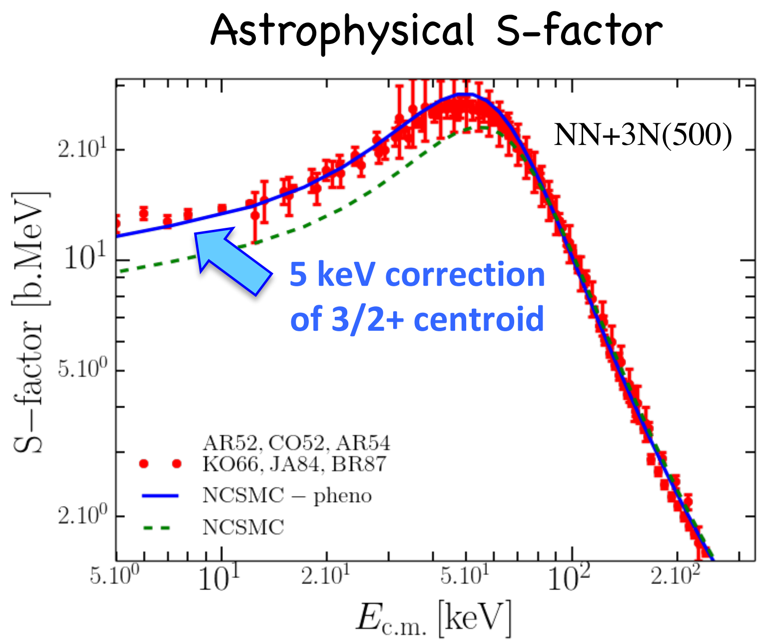
^{5}He(3/2+)	NCSMC-pheno	R-Matrix
E_R (keV)	50	47
Γ_R (keV)	98	74

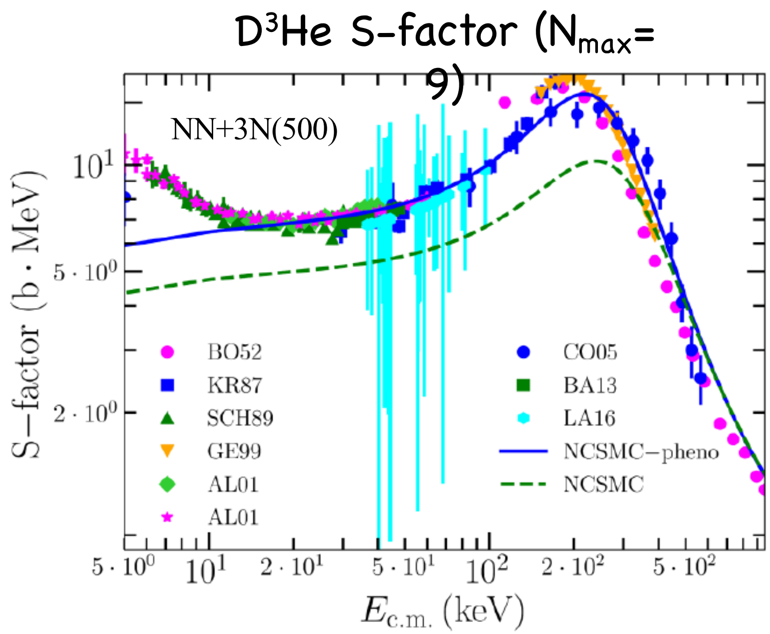
$3/2^+$ input energy eigenvalue adjusted to reproduce experimental S-factor data for energy below the resonance. Computed 3/2+ resonance width somewhat larger than R-matrix fit.

Phenomenological adjustment

NCSMC-pheno



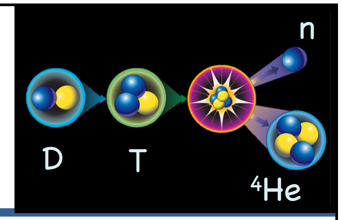




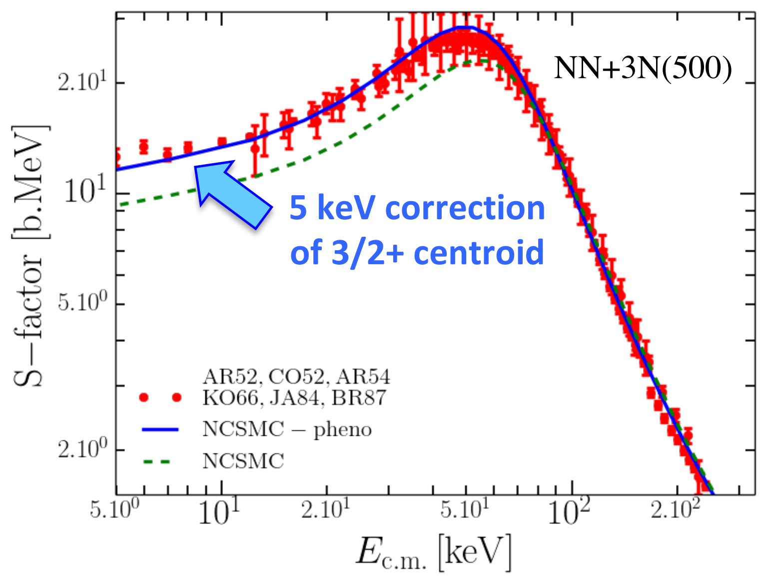
The experimental peak at the DT (D^{3}He) center-of-mass energy of 49.7 keV (427 keV) corresponds to the enhancement from the 3/2$^+$ resonance of ^{5}He (^{5}Li)

Phenomenological adjustment

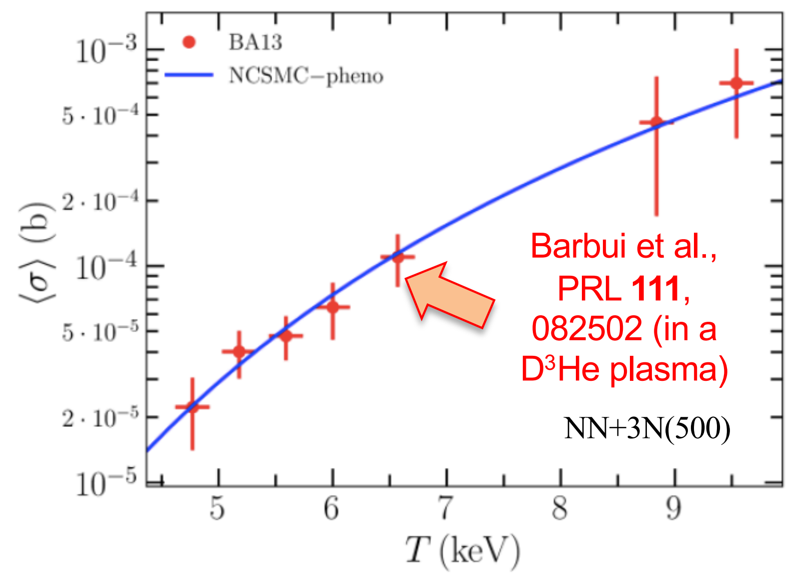
NCSMC-pheno



Astrophysical S-factor

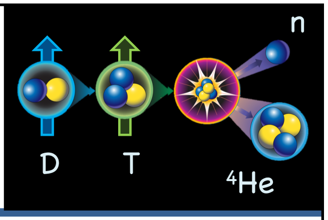


D^{3}He heated cross section (N_{max}= 9)



The experimental peak at the DT (D^{3}He) center-of-mass energy of 49.7 keV (427 keV) corresponds to the enhancement from the 3/2$^+$ resonance of ^{5}He (^{5}Li)

What is the effect of spin-polarization?



- Special case of reactants aligned along the z-axis:

$$\frac{d\sigma_{pol}}{d\Omega} = \frac{d\sigma_{unpol}}{d\Omega}(\theta)\left(1 + \frac{1}{2}p_{zz}A_{zz}^{(b)}(\theta) + \frac{3}{2}p_z q_z C_{z,z}(\theta)\right)$$

D, T vector polarization

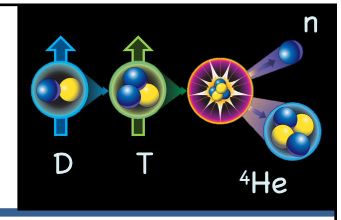
D tensor polarization

Tensor analyzing power

Spin correlation coefficient

At the energies relavant for the DT fusion $A_{zz}^{(b)}$ measured only at $\theta = 0°$: −0.929 ± 0.014.
No DT experimental data on $C_{z,z}$. Spin correlation coefficients measured for D^{3}He.

What is the effect of spin-polarization?



- Special case of reactants aligned along the z-axis:

$$\frac{d\sigma_{pol}}{d\Omega} = \frac{d\sigma_{unpol}}{d\Omega}(\theta)\left(1 + \frac{1}{2}p_{zz}A_{zz}^{(b)}(\theta) + \frac{3}{2}p_z q_z C_{z,z}(\theta)\right)$$

Estimated enhancement of up to 1.5

- Assuming:
  1) Only $J^{\pi} = 3/2^{+}$ partial wave contributes
  2) D+T pair in s-wave of relative motion

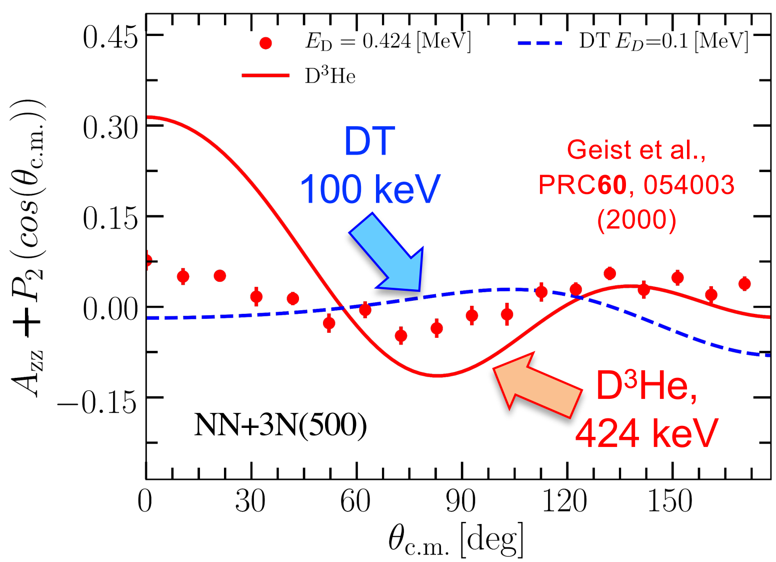
$$\sigma_{pol} \approx \sigma_{unpol}\left(1 + \frac{1}{2}p_z q_z\right)$$

Paetz gen.Schieck, Lecture Notes in Physics **842** (Springer,Heidelberg,2012)

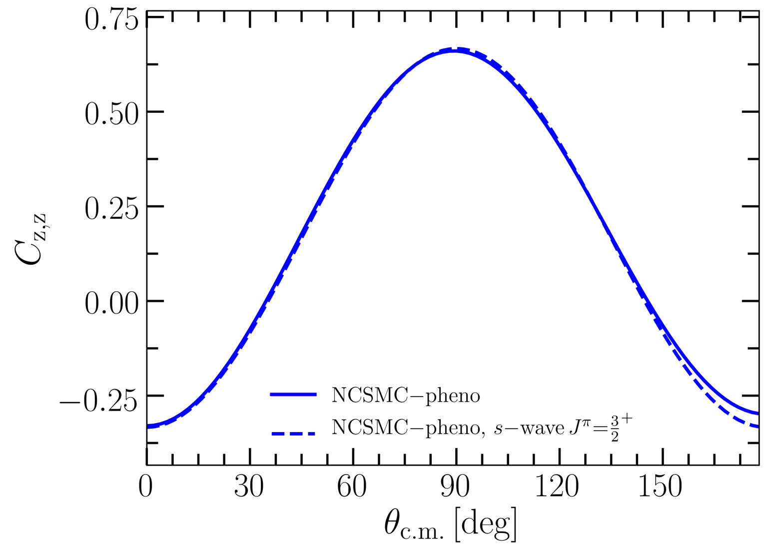
How valid are these assumptions? What is the contribution of $\ell > 0$ partial waves in the vicinity of the $3/2^{+}$ resonance? What is the effect on the polarized reaction rate?

Tensor analyzing power and spin correlation coefficients: ℓ>0 contributions near 3/2+ resonance

Tensor Analyzing Power - ℓ=0 contribution



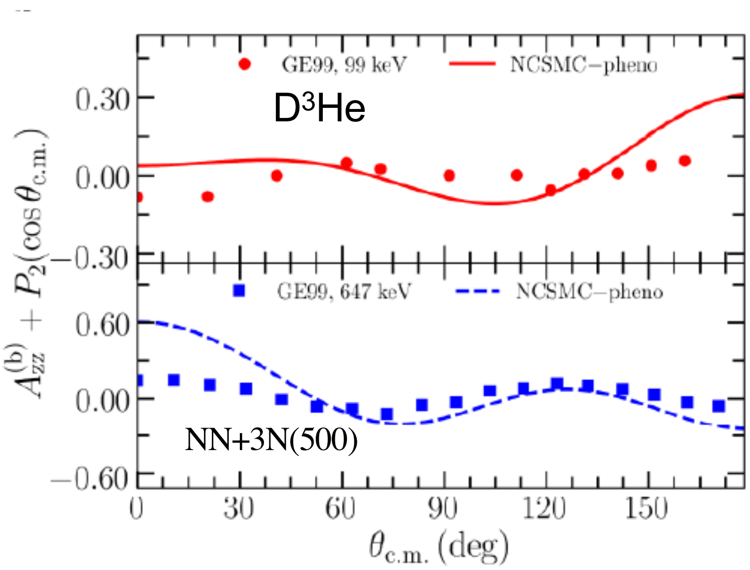
DT Spin Correlation Coefficient



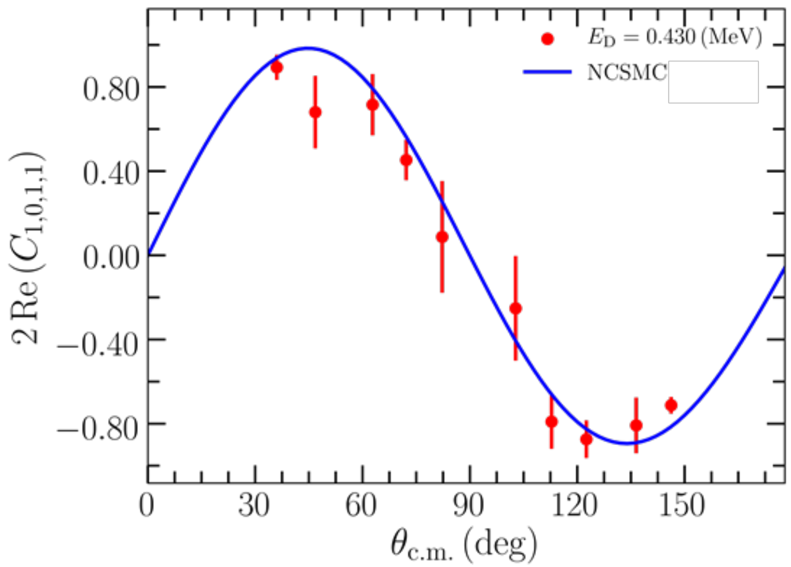
$A_{zz}^{(b)}$ measured only at 0° (−0.929±0.014); NCSMC-pheno:−0.975. Prediction for $C_{z,z}$!

Tensor analyzing power and spin correlation coefficients: ℓ>0 contributions near 3/2+ resonance

D3He Tensor Analyzing Power - ℓ=0 contribution

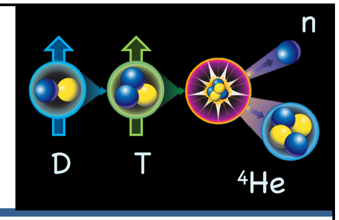


D3He Spin Correlation Coefficient

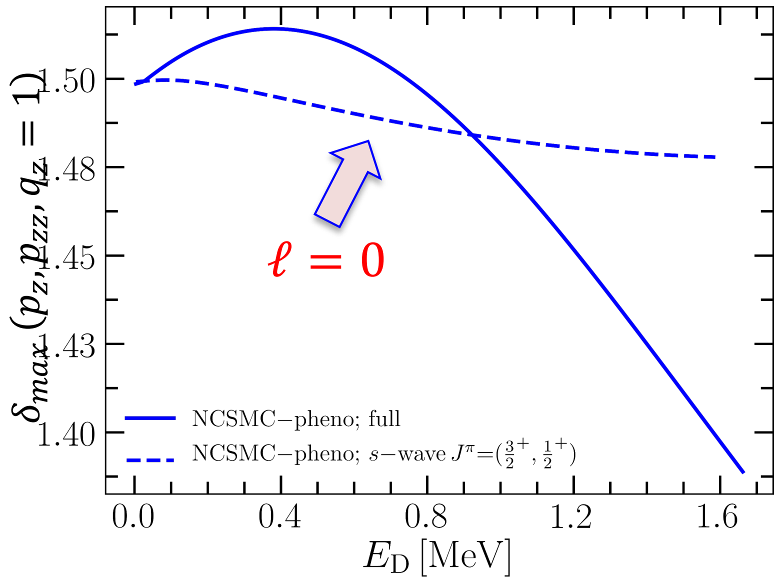


Comparison with experimental data for D3He demonstrates predictive power of calculation

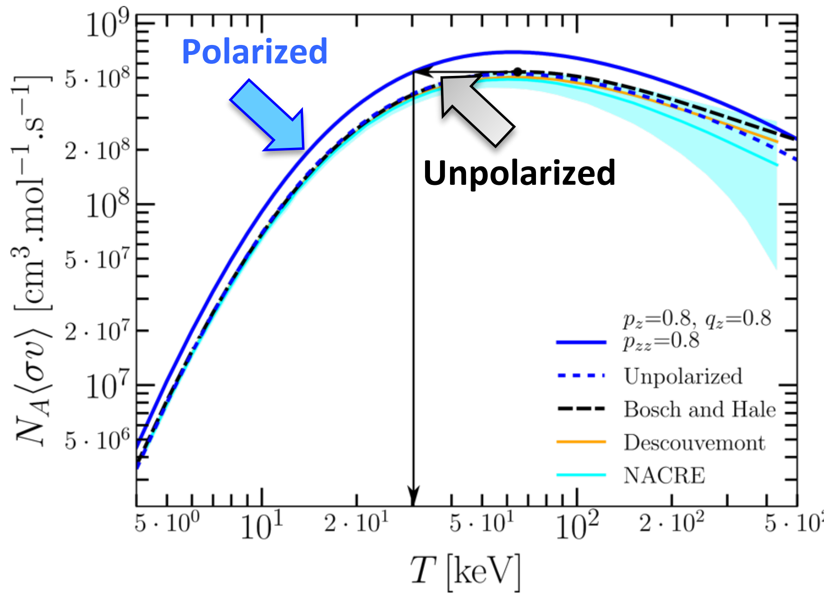
What is the enhancement factor?
And the polarized reaction rate?



Enhancement factor: $\delta = \sigma_{pol}/\sigma_{unpol}$



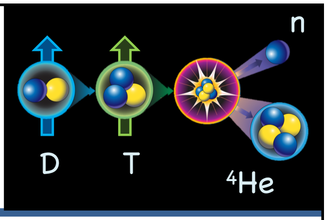
DT Reaction rate

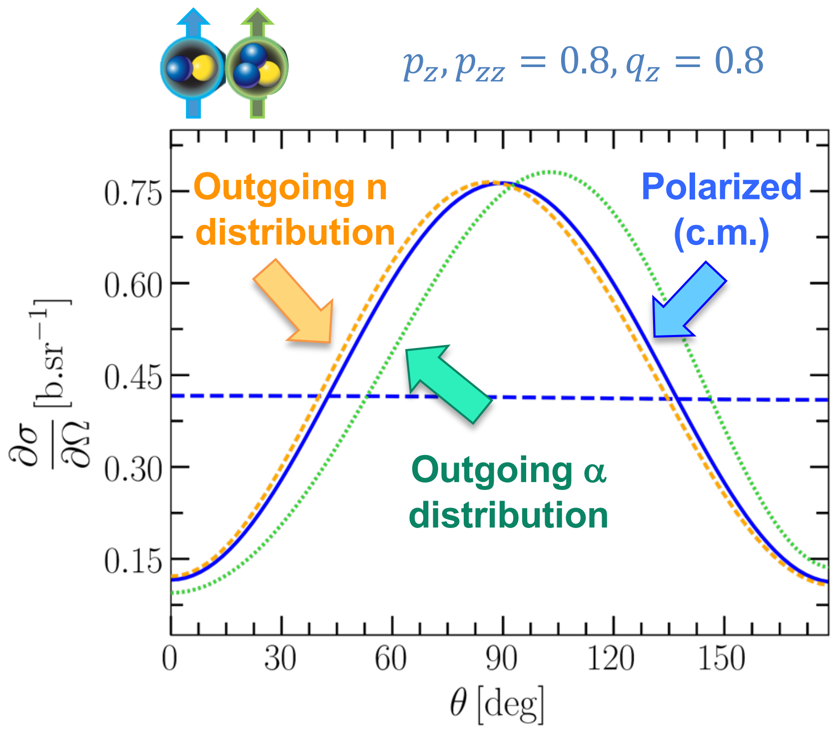


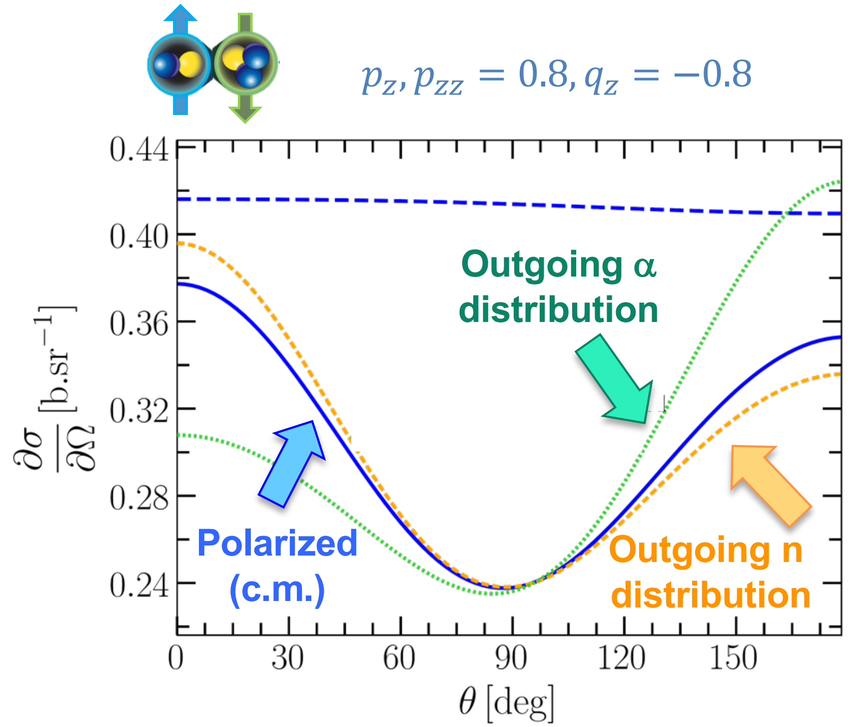
For realistic polarization of the reactants ($p_z, q_z = 0.8$) the reaction rate can be enhanced by about 32%, or same reaction rate can be achieved at ~45% lower temperature

Polarized differential cross section

Reactants aligned along the z-axis







Polarized DT fuel allows to control the direction of the emitted neutron and α particle

What about the polarized DD fusion?

- Special case of reactants aligned along the z-axis:

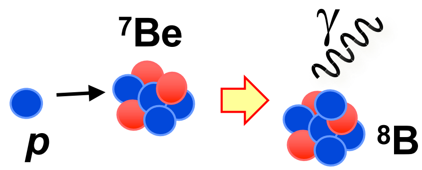
$$\frac{d\sigma_{pol}}{d\Omega} = \frac{d\sigma_{unpol}}{d\Omega}(\theta)\left\{1 + \frac{3}{2}\left(p_{zz}A_{zz}^{(b)}(\theta) + q_{zz}A_{zz}^{(t)}(\theta)\right) + \frac{9}{4}p_z q_z C_{z,z}(\theta) + \frac{1}{4}p_{zz}q_{zz}C_{zz,zz}(\theta)\right\}$$

Paetz gen.Schieck, Lecture Notes in Physics **842** (Springer,Heidelberg,2012)

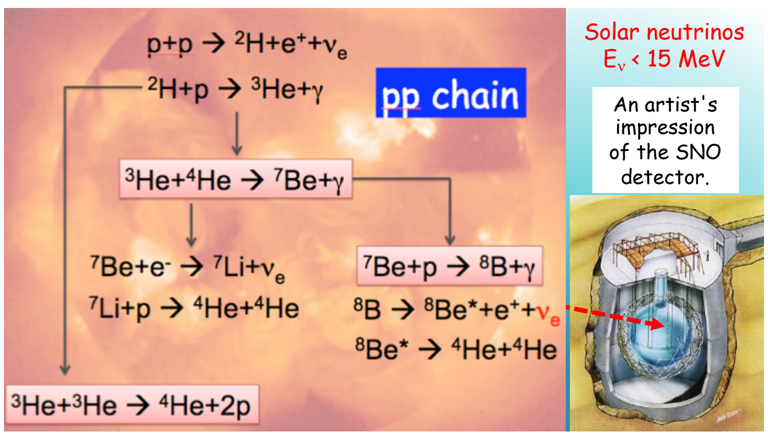
- More complicated
  - Both projectile and target have tensor components of the polarization
  - New terms arise even in the simplest case

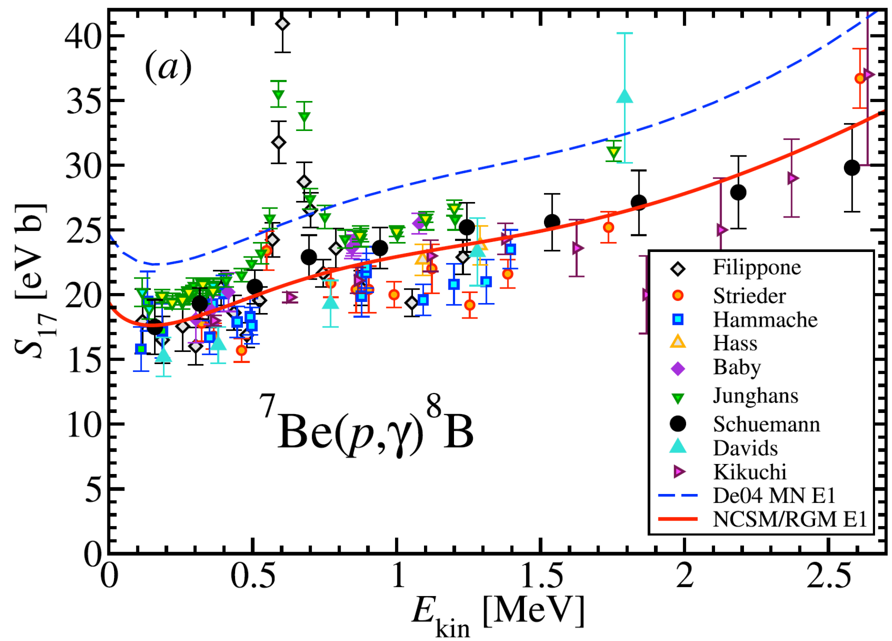
Requires some extra formalism/codes… currently in our bucket list

Now gradually building up capability to describe solar pp-chain reactions



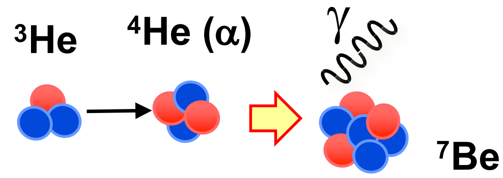
- The ^{7}Be(p, γ)^{8}B and ^{3}He(α,γ)^{7}Be fusion rates are essential to evaluate the flux of pp-chain ^{7}Be versus ^{8}B solar neutrinos
- Complete NCSMC calculation with 3N forces (not included here) now in progress



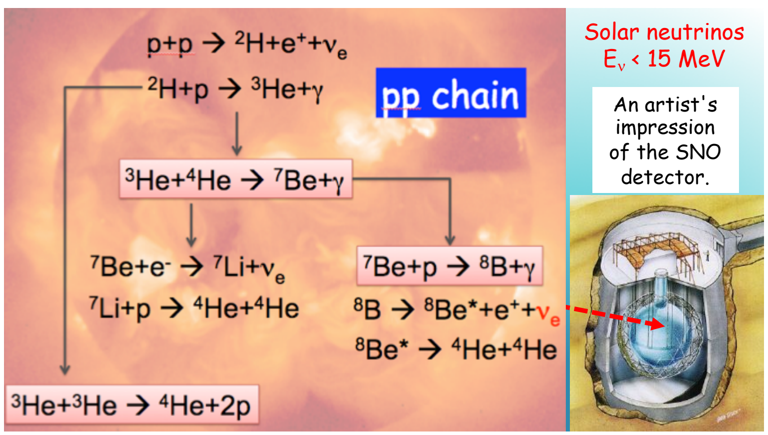


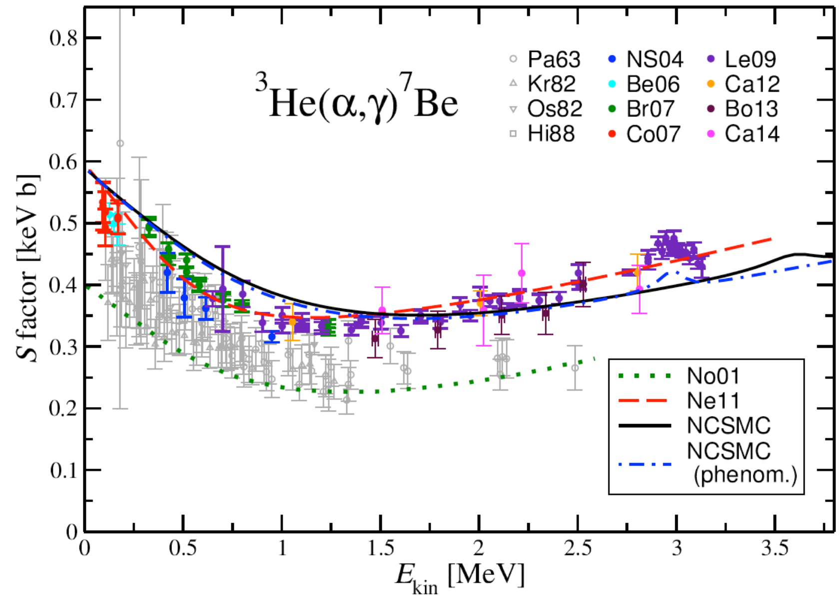
P. Navrátil, R. Roth, S.Q., Phys. Lett. B 704, 379

Now gradually building up capability to describe solar pp-chain reactions



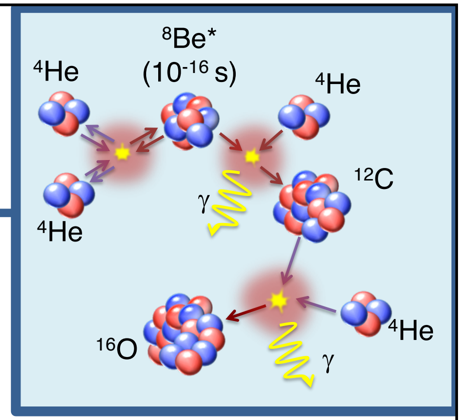
- The ^{3}He(α,γ)^{7}Be and ^{7}Be(p, γ)^{8}B fusion rates are essential to evaluate the flux of pp-chain ^{7}Be versus ^{8}B solar neutrinos
- Quantitative comparison still requires inclusion of 3N forces

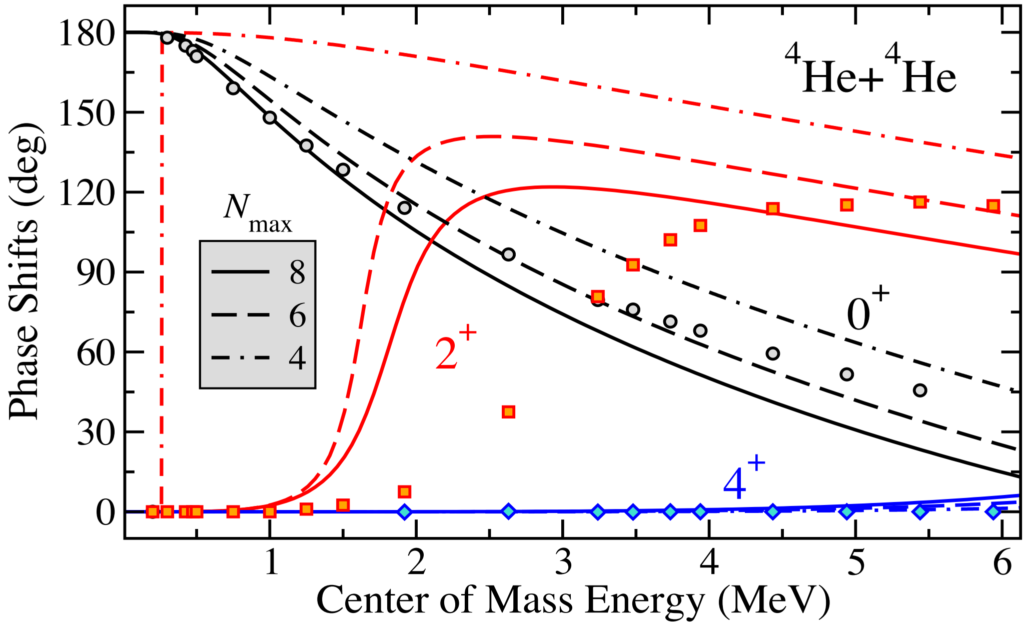




J. Dohet-Eraly et al., Phys. Lett. B 757, 430

α-induced reactions had been out of reach of NCSMC. Now possible!



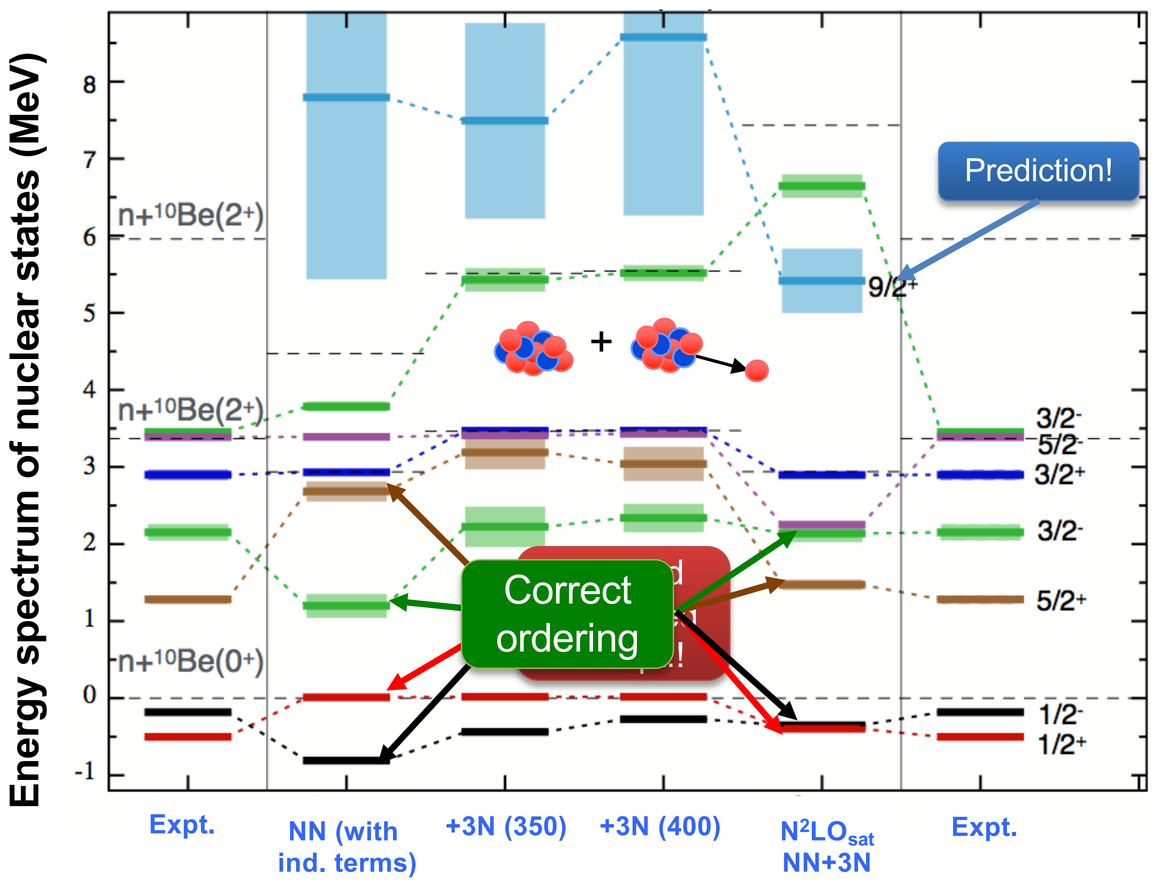


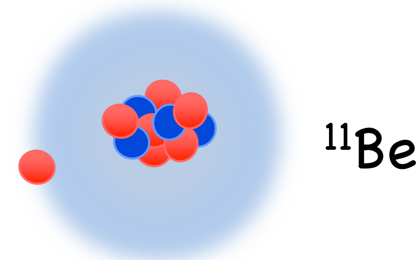
Preliminary Results!

- Previous formalism laborious, not easily extensible to heavier projectiles
  - Second quantization techniques used for targets, but not projectiles!
  - Required new derivations/codes for each different projectile.

Breakthrough enabled by new methods and codes to construct the channel basis and evaluate the matrix elements in second quantization. Work towards complete study is in progress.

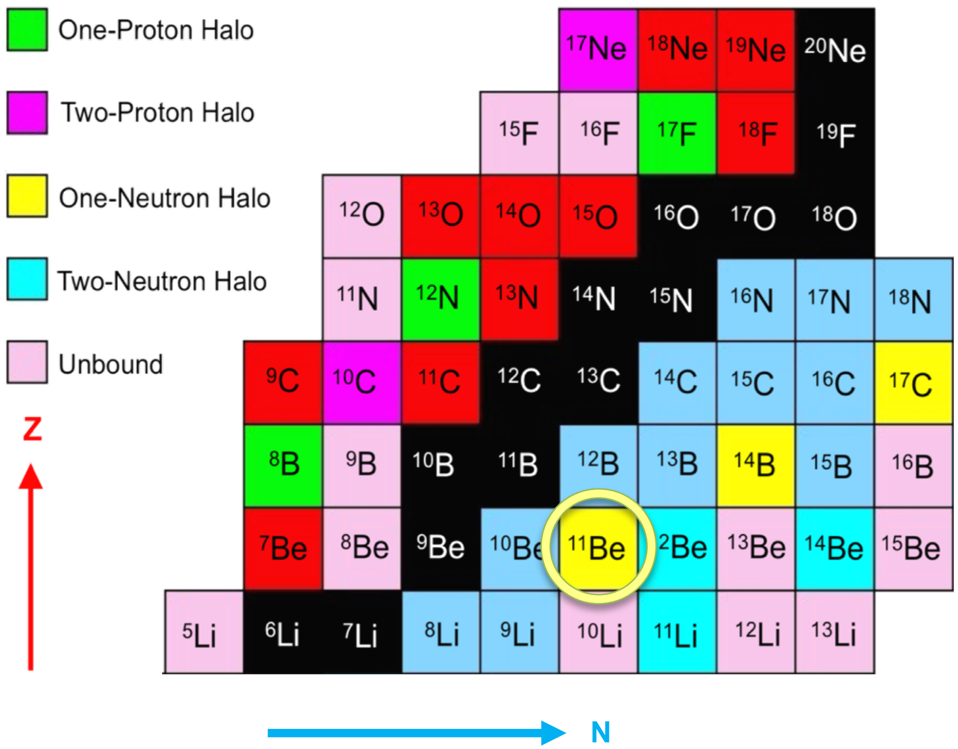
Can ab initio theory explain the phenomenon of parity inversion in ^{11}Be?



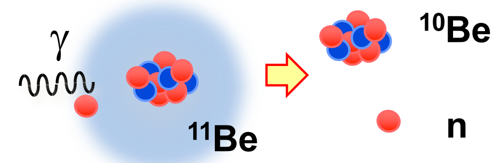


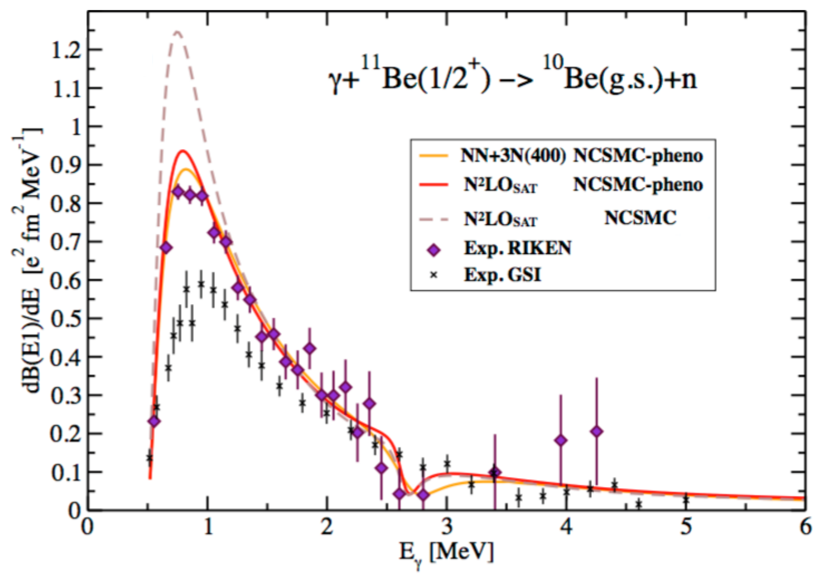
A. Calci, P. Navratil, R. Roth, **J. Dohet-Eraly**, S.Q., and G. Hupin, Phys. Rev. Lett. 117, 242501

Scattering and reactions in dripline nuclei



A. Calci et al.,
Phys. Rev. Lett.
117, 242501





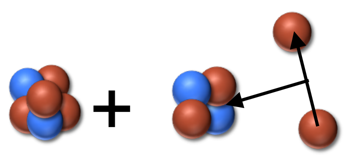
C. Romero

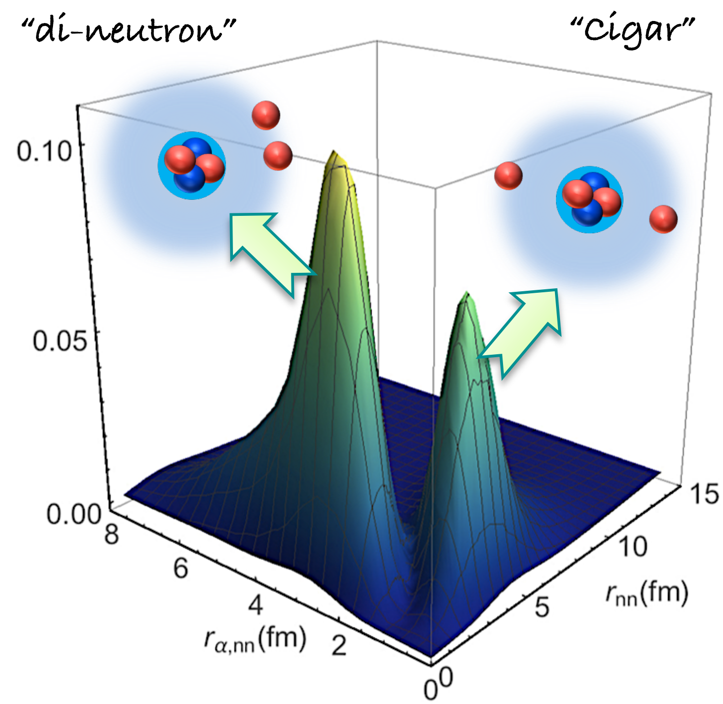
Ab initio description of three-cluster dynamics

S.Q., C. Romeoro-Redondo, P. Navrátil, and G. Hupin, Phys. Rev. C 97, 034332 (2018)

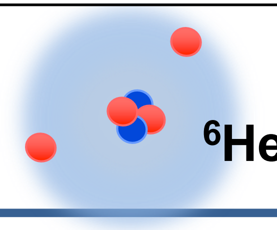
- Reactions with ternary channels
- Borromean halos (dripline nuclei):
  - **^{6}He (= ^{4}He+n+n)**
  - ^{11}Li (= ^{9}Li+n+n)
  - ^{14}Be (= ^{12}Be+n+n)
  - …

- No-core shell model with continuum:





Ab initio calculations simultaneously address many-body correlations and 3-cluster dynamics



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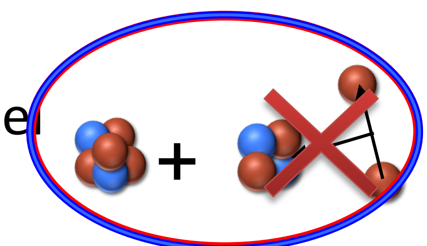
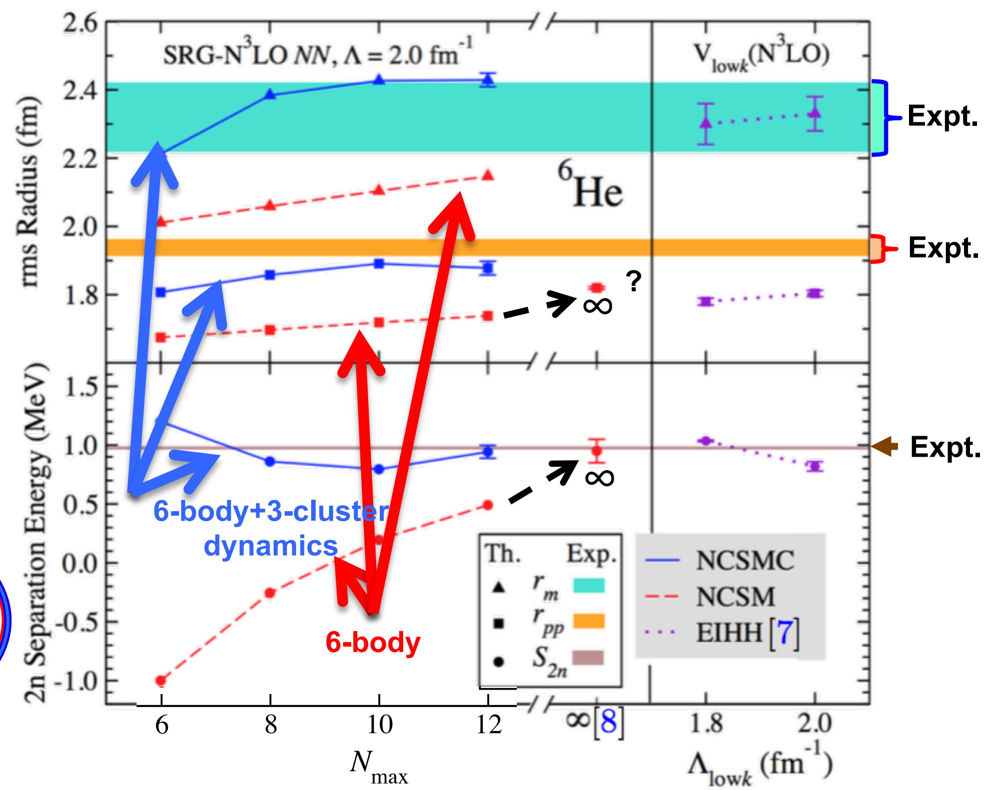
- No-core shell model with continuum





C. Romero-Redondo, S. Quaglioni, P.Navratil, and G. Hupin, Phys. Rev. Lett. 117, 222501 (2016)

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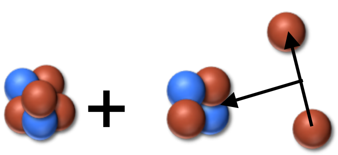

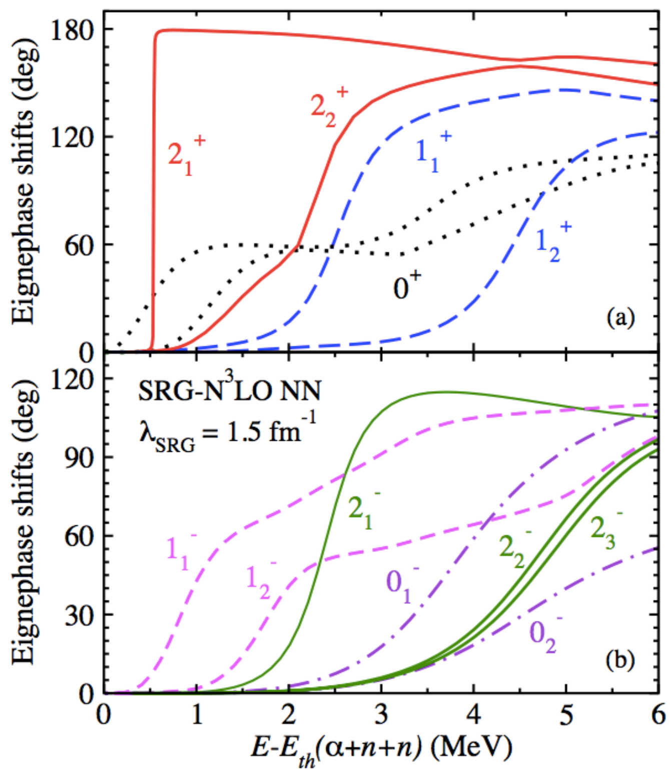

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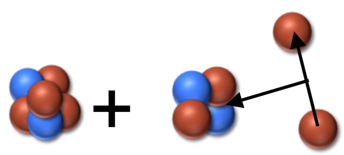

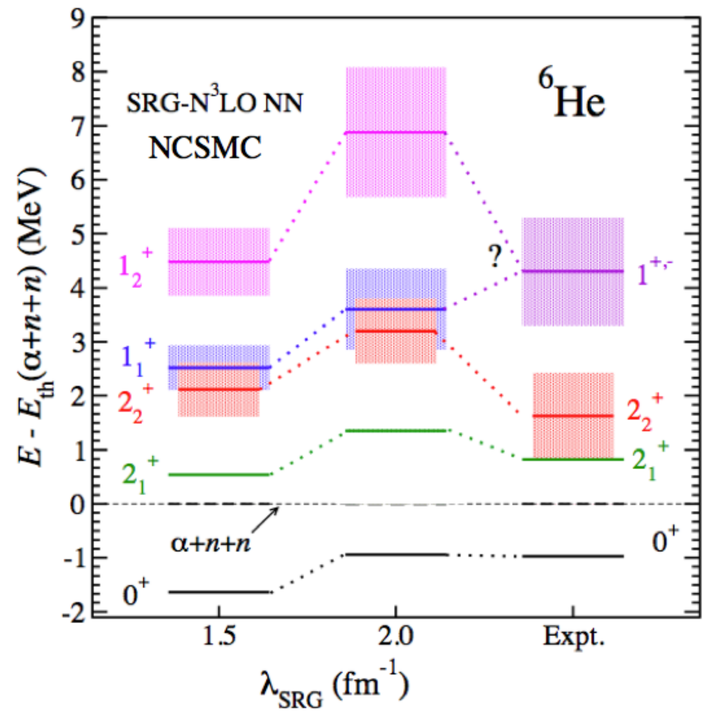

For now, qualitative agreement with available experimental data. Need inclusion of 3N forces (underway) and more experimental data for the excitation spectrum!

Collaborators

- K. Kravvaris (LLNL)
- C. Romero Redondo
- G. Hupin (IN2P3/CNRS)
- P. Navratil, M. Vorabbi, P. Gysbers (TRIUMF)
- A. Calci
- J. Dohet-Eraly (ULB)
- R. Roth (TUD)

Conclusions and Prospects

- Predictive theory of nuclear reactions needed to achieve accuracy and/or provide part of nuclear data required by applications
- Demonstrated role of anisotropies, placed on firmer footing understanding of the rate of DT thermonuclear fusion in a polarized plasma
- Open questions about the polarized DD fusion: more work is needed to address them
- Ongoing and upcoming efforts:
  - Complete calculations of solar fusion cross sections (with, now missing, effect of 3N forces)
  - New more efficient implementation of NCSMC, for reactions induced by α and p-shell projectiles
  - UQ with machine learning methodology
  - Joint effort to measure and predict ab initio beta-delayed particle emission – FY19 LDRD ER, Gallant
  - Calculations of charge-exchange reactions, ^{7}Be(n,p)^{7}Li (Lithium problem) – FY20 LDRD LW, Kravvaris