Nuclear & Chemical Sciences

Ab initio Calculations of Spin-Polarized Fusion

Spin-Polarized Fusion Workshop

ARPA-E Headquarters, Washington, DC, December 9-10, 2024

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G. Hupin (ICJLab), P. Navratil (TRIUMF), K. Kravvaris

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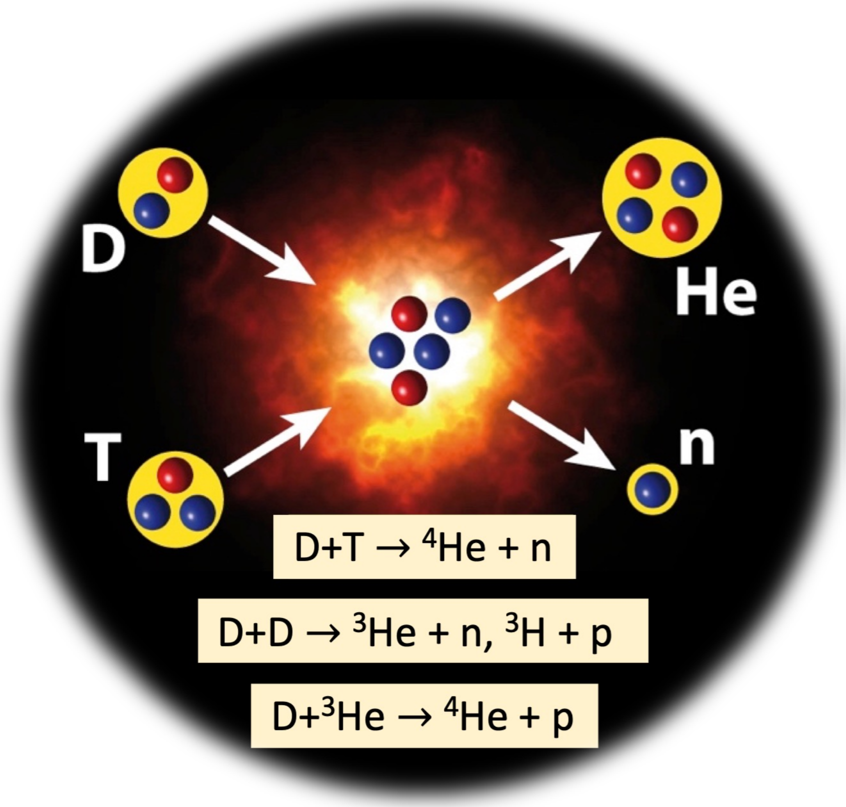
Lawrence Livermore National Laboratory

Spin-polarized fusion may offer several economical and safety advantages over unpolarized fusion ….



Increase the reaction rate

Control direction of emitted products

Reduce neutron-producing reactions

… but is challenging, not fully understood!

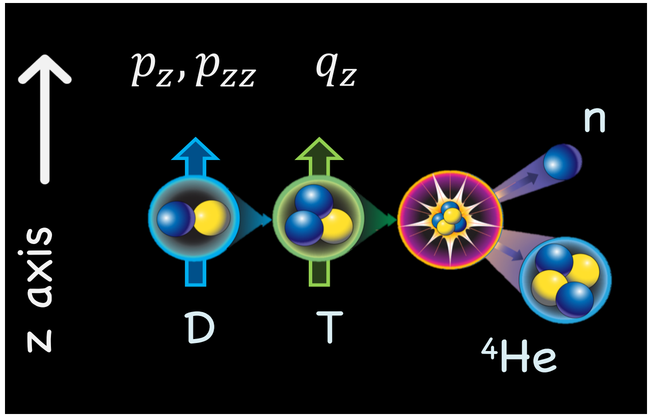
Calculations validated on "indirect" experimental data are needed to determine wanted spin-polarized fusion rates

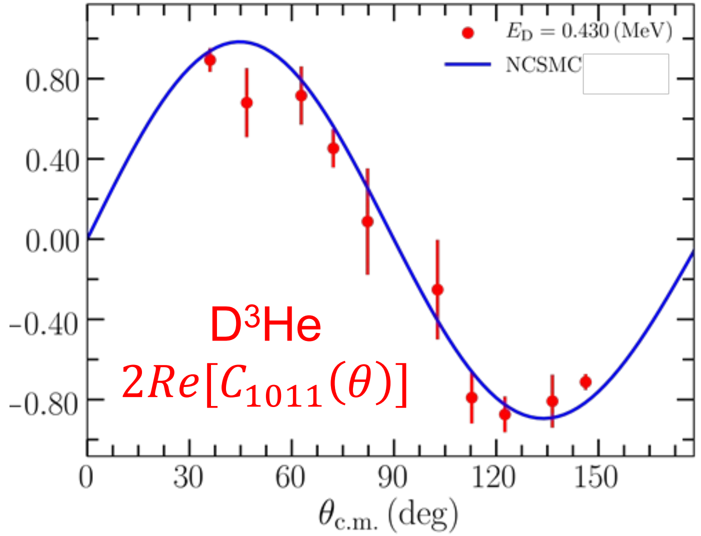
Scarce direct expt. info for polarized DT, D^3He:

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

Tensor analyzing power (only measured at $\theta = 0°$)

Spin correlation coefficient (only measured for D^3He)





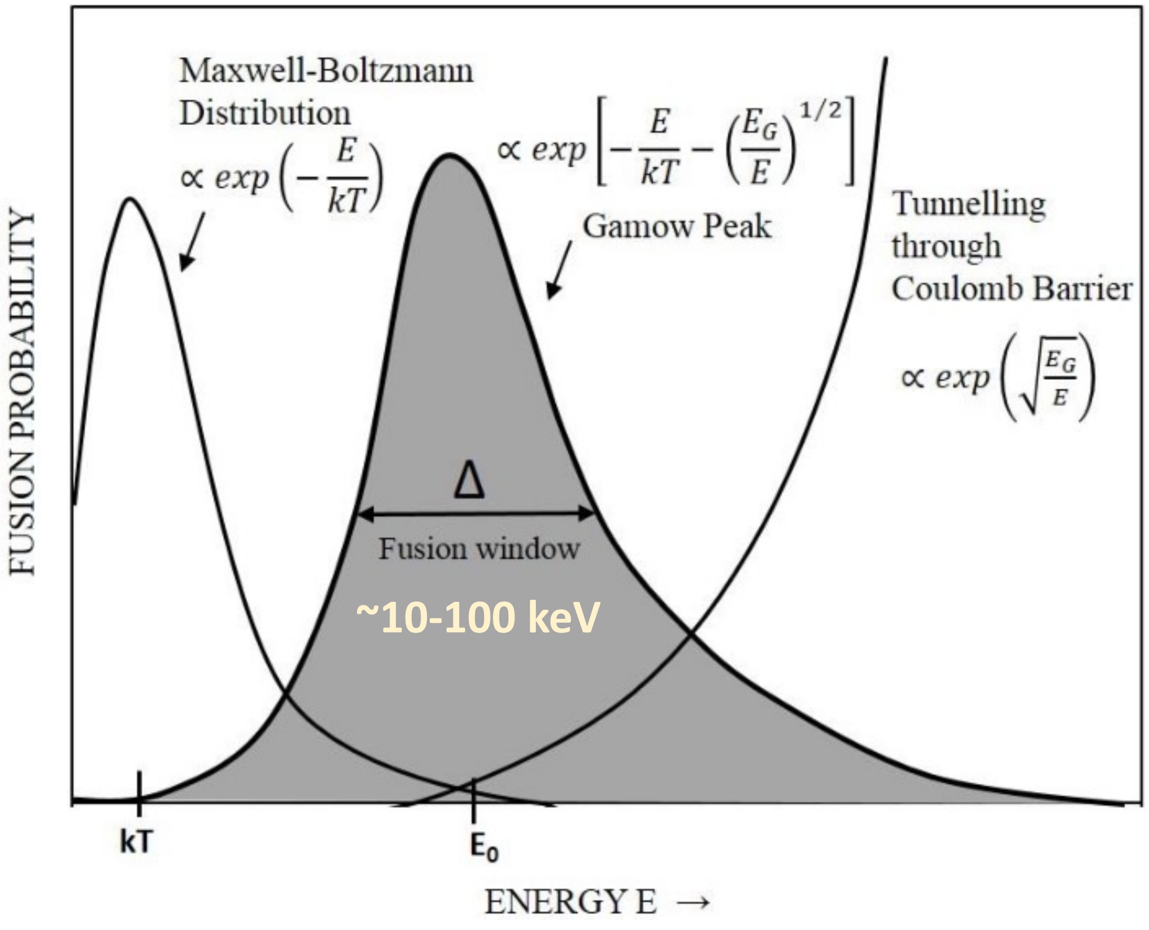
No direct expt. info for double polarized DD fusion!

We need reliable theory to accurately evaluate S-factors at fusion reactor energies

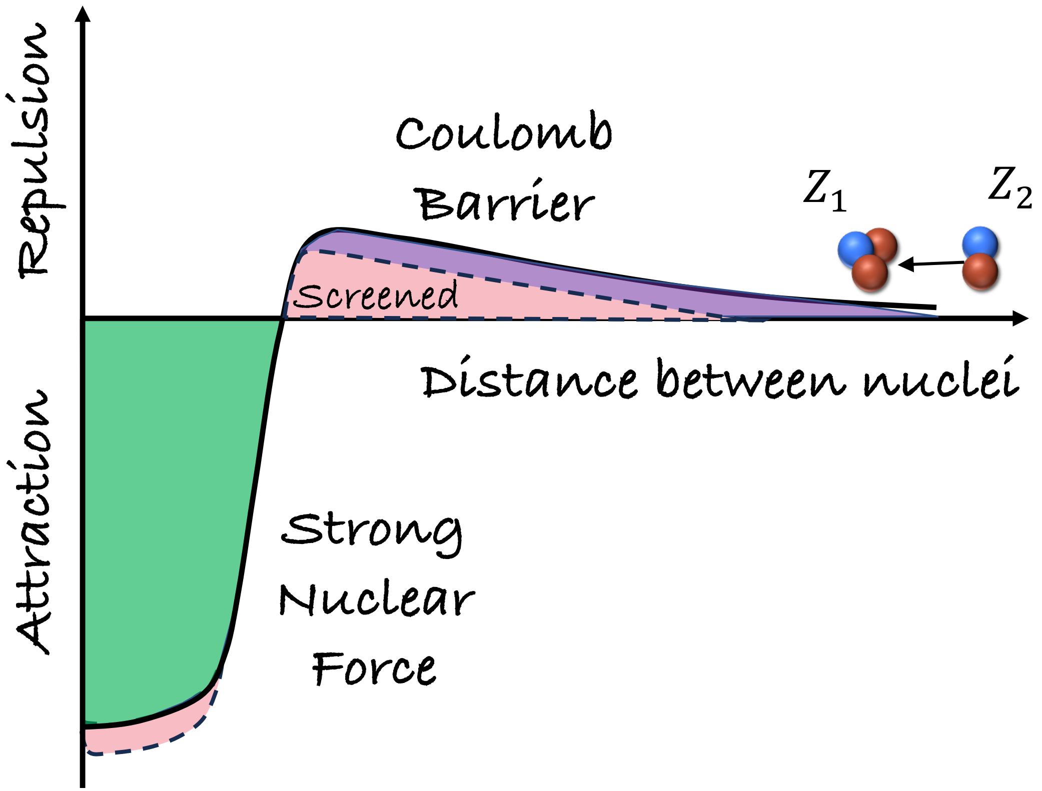
Astrophysical S-factor: nuclear contribution

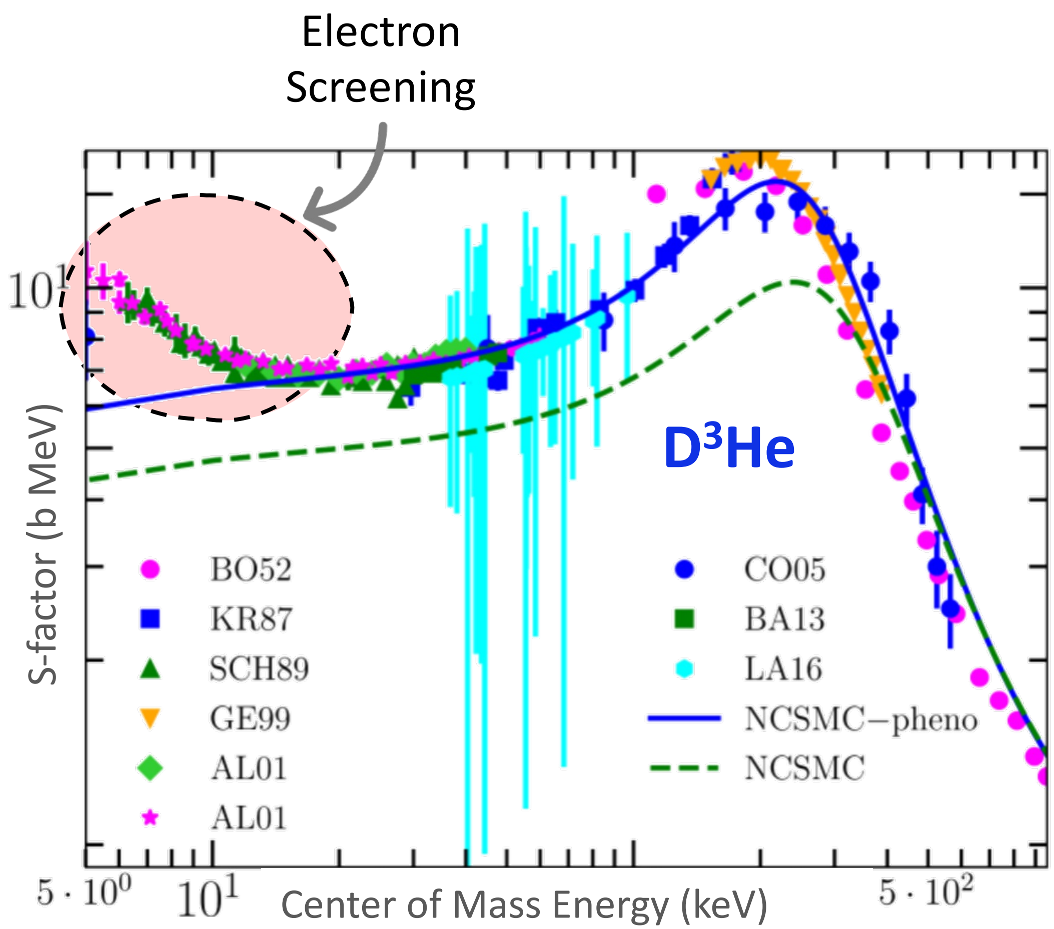
$$\sigma(E) = \frac{S(E)}{E} \exp\left(-\frac{2\pi Z_1 Z_2 e^2}{\hbar\sqrt{2E/m}}\right)$$

'Coulomb' contribution (tunneling)



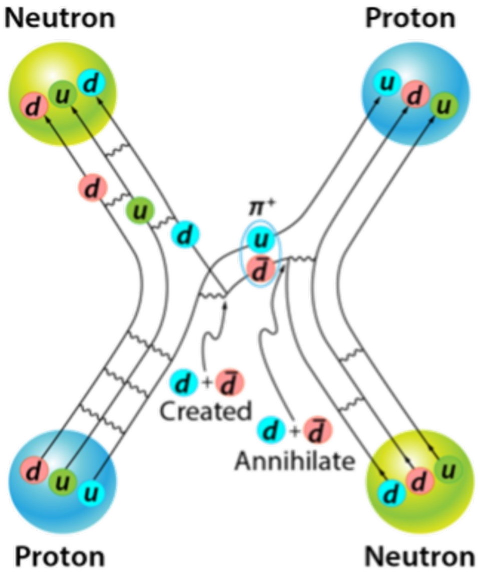
We need reliable theory to accurately evaluate S-factors at fusion reactor energies



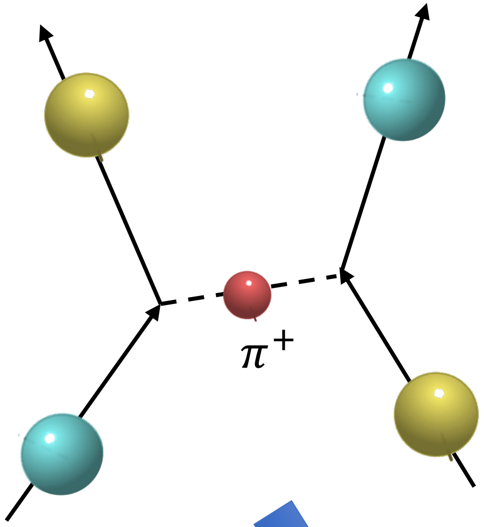


LLNL is at the forefront of developing methods to describe thermonuclear fusion from first principles

Quantum Chromodynamics

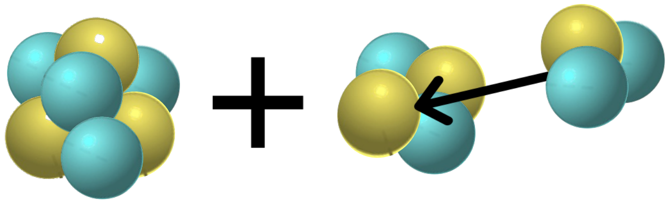


Chiral Effective Field Theory



Chiral NN+3N forces

No Core Shell Model with Continuum (NCSMC)



- All active (pointlike) nucleons, non-relativistic quantum mechanics
- Unified ab initio many-body approach to structure and reactions

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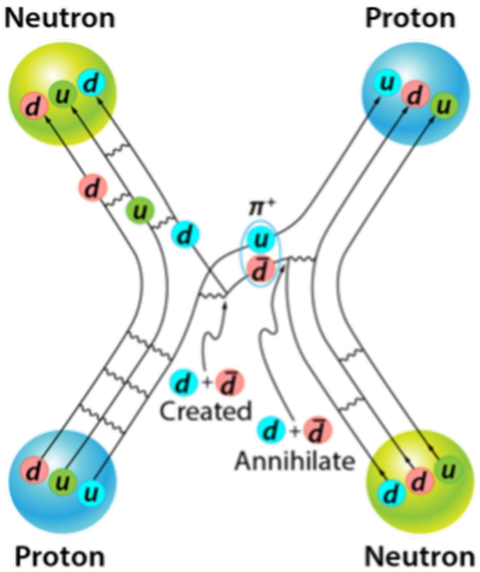
Quantum Chromodynamics



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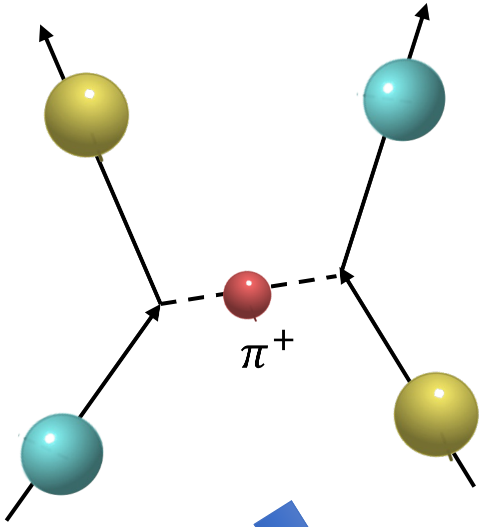

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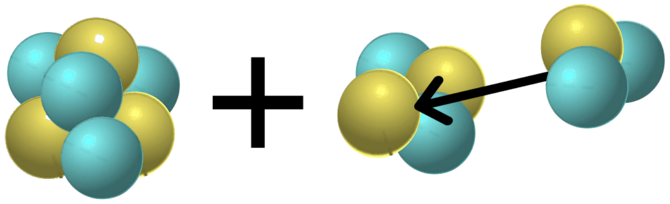


Possibility to fine-tune some energy levels

NCSMC-pheno

LLNL is at the forefront of developing methods to describe thermonuclear fusion from first principles

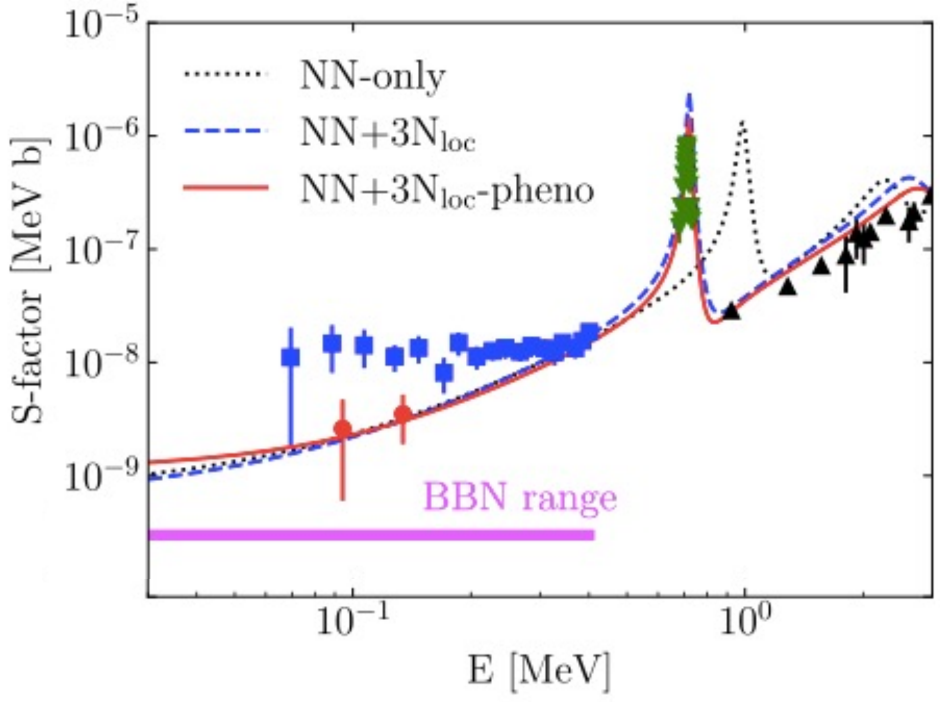
Sole input: interactions among the protons and neutrons

Use a large portion of a HPC machine, require multiple runs, and can scale with machine size

Accurate predictions for fusion reactions in mass $A = 5$ to 8; Can push up to mass $A \approx 12$

LLNL is at the forefront of developing methods to describe thermonuclear fusion from first principles

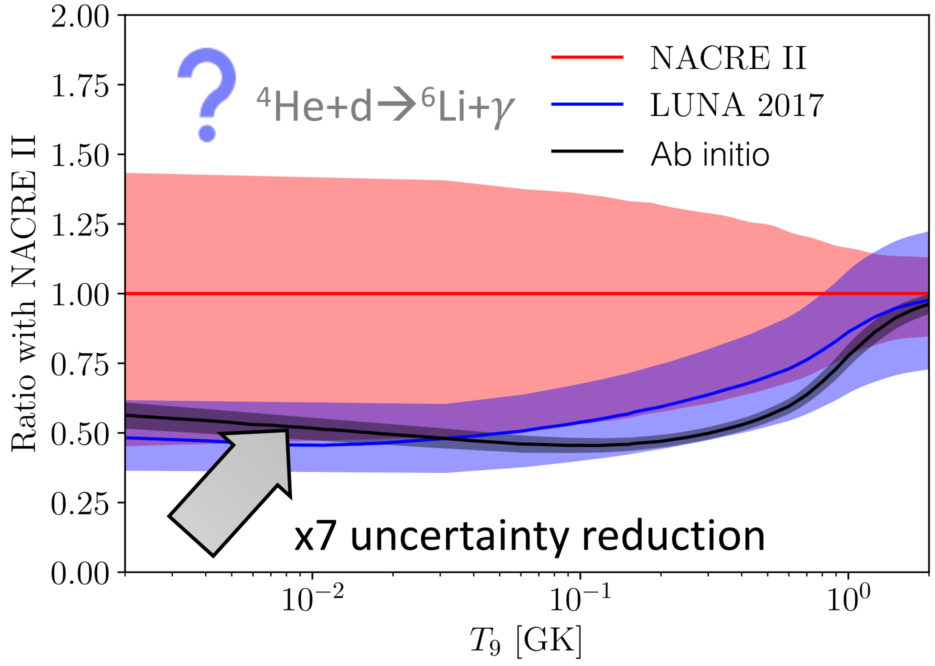
$^{4}He(d,\gamma)^{6}He$ S-factor (Big Bang)



Hebborn C et al. (2022), Phy. Rev. Lett. 129, 042503

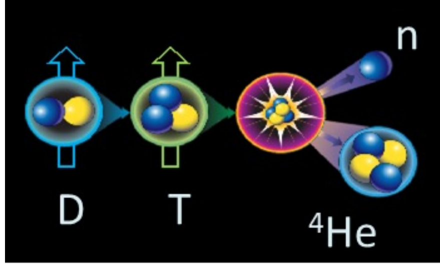
LLNL is at the forefront of developing methods to describe thermonuclear fusion from first principles

Cosmological Lithium Puzzle



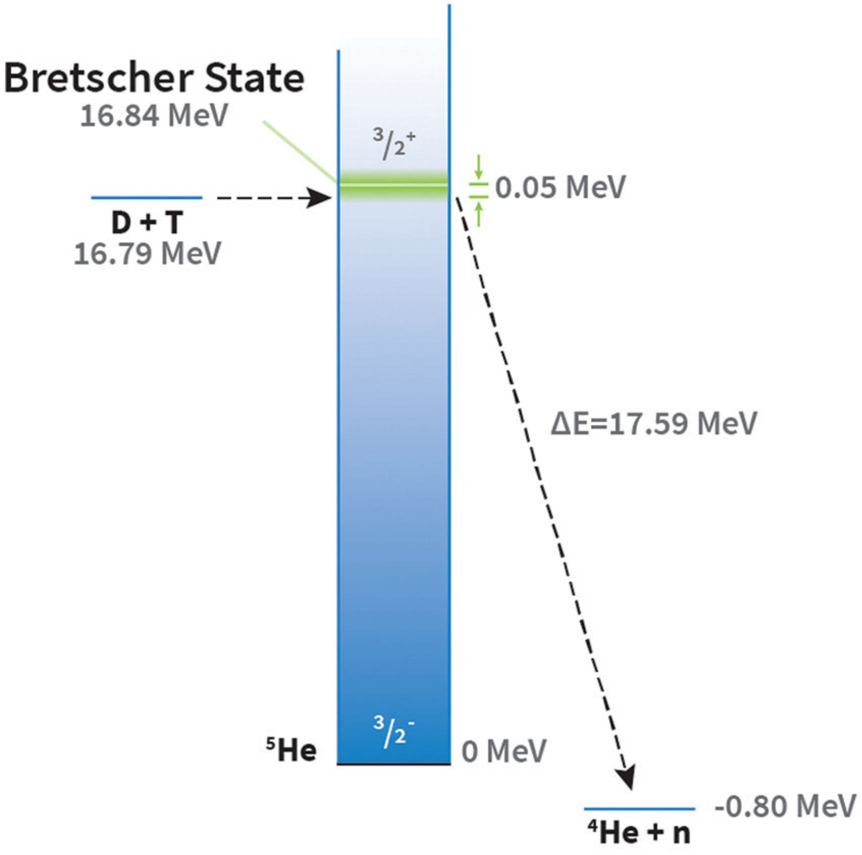
Hebborn C et al. (2022), Phy. Rev. Lett. 129, 042503

How does spin polarization affect the DT fusion?



- First simple estimate by Kulsrud et al., PRL**49**, 1248 (1982)

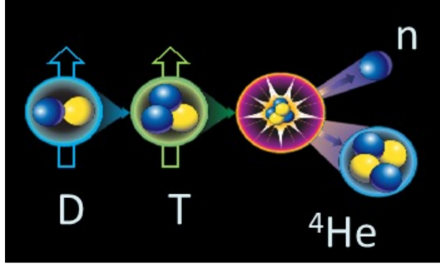
$$\sigma_{unpol} = \sum_J \frac{2J+1}{(2I_D+1)(2I_T+1)} \sigma_J \overset{\ell=0}{\approx} \frac{1}{3}\sigma_{\frac{1}{2}} + \frac{2}{3}\sigma_{\frac{3}{2}}$$



- Assume:
  1) D+T pair in s-wave of relative motion

Figure from Paris, MW & Chadwick, MB (2024), *Fusion Science and Technology*, *80*(sup1), S110

How does spin polarization affect the DT fusion?



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

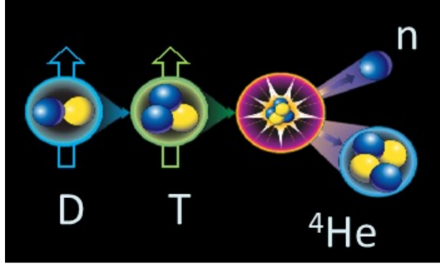
Estimated enhancement for perfect spin alignment

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

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

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?

How does spin polarization affect the DT fusion?



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

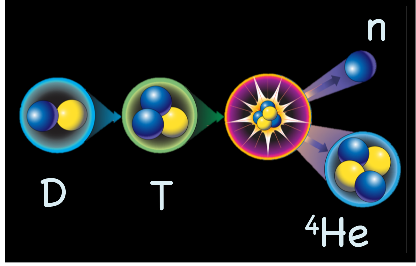
Estimated angular distribution of emitted neutrons and α particles

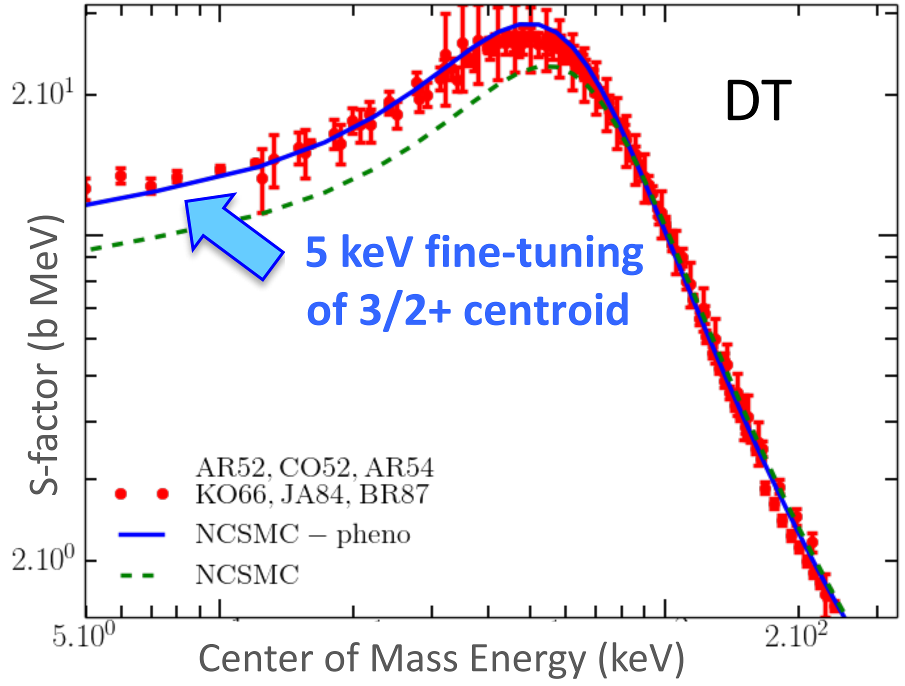
- Assume:
  1) D+T pair in s-wave of relative motion
  2) Only $J^\pi = 3/2^+$ partial wave contributes

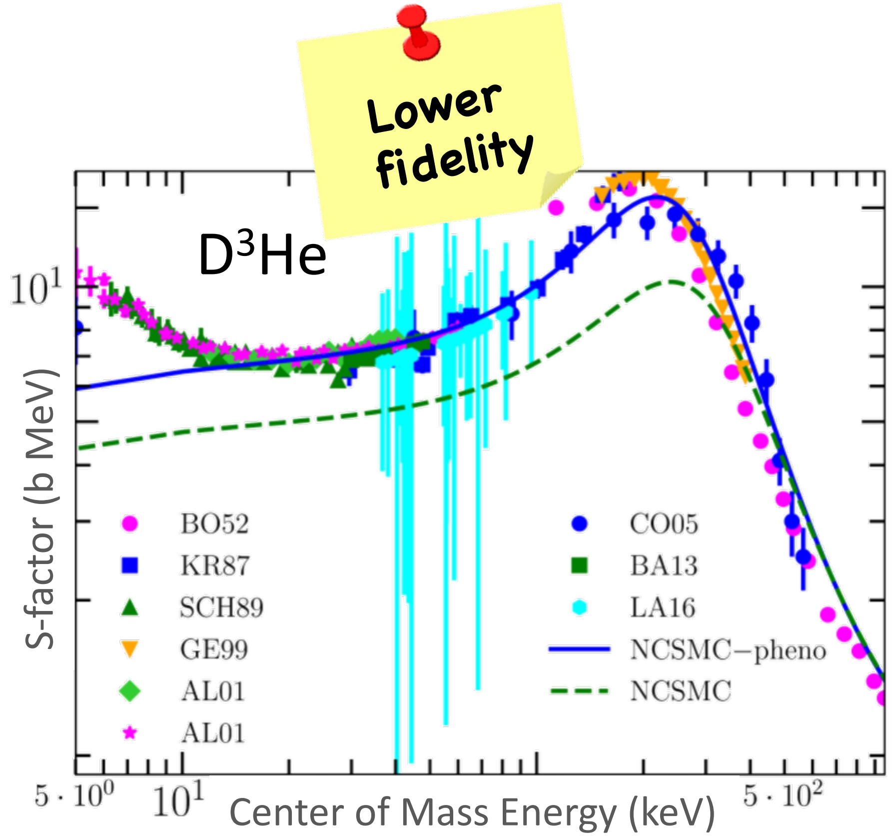
$$\frac{d\sigma_{pol}}{d\Omega} \propto \sin^2\theta$$

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?

Ab initio calculations accurately predict unpolarized S-factors and other observables for DT and D^3He



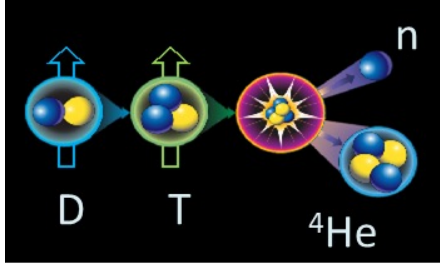




Hupin, G etal. (2019) Nature Communication 10, 351

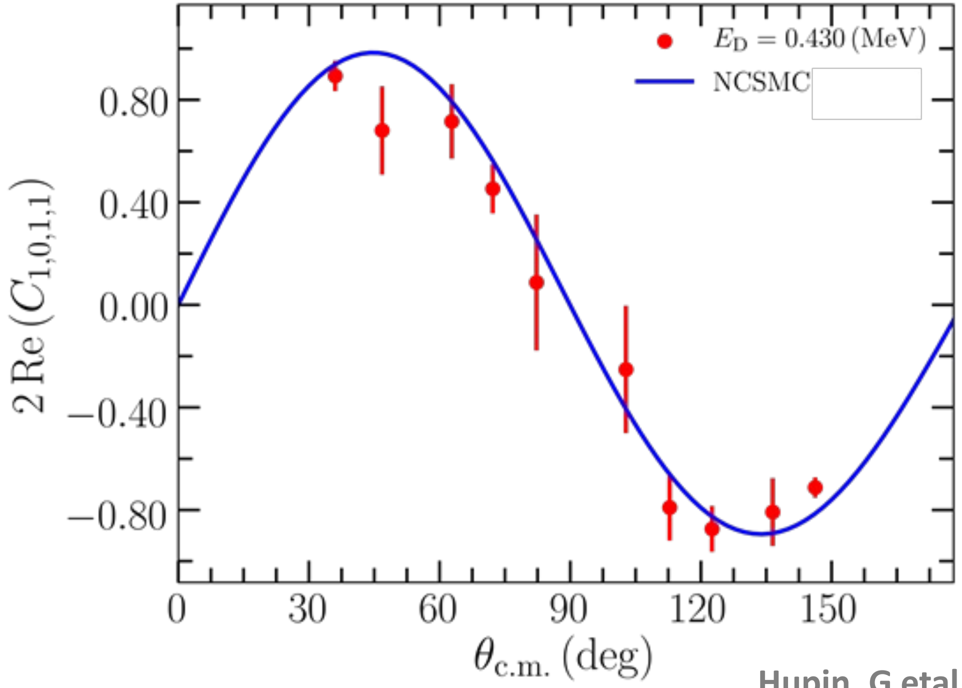
The experimental peak at the DT (D^3He) center-of-mass energy of 49.7 keV (427 keV) corresponds to the enhancement from the $3/2^+$ resonance of ^5He (^5Li)

Further validation on polarized D^3He observables demonstrates predictive power for DT calculation

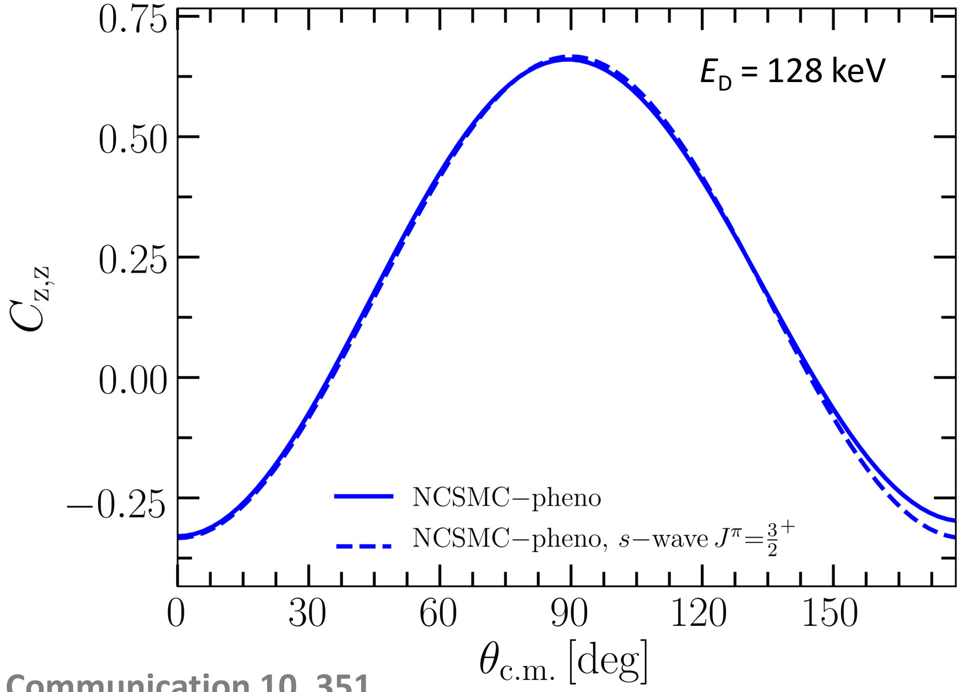


$$\frac{d\sigma_{pol}}{d\Omega} = \frac{d\sigma_{unpol}}{d\Omega}(\theta)\left(1 + \frac{1}{2}p_{zz}A_{zz}^{(b)}(\theta) + \frac{3}{2}p_z q_z C_{z,z}(\theta)\right)$$

D^3He Spin Correlation Coefficient



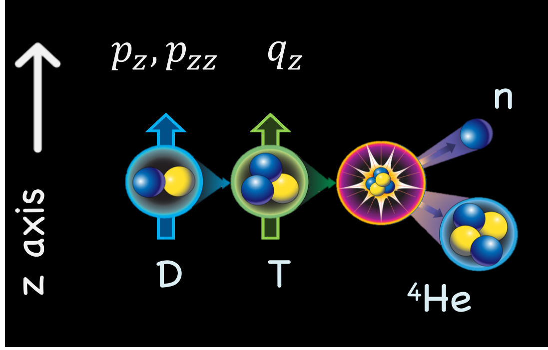
DT Spin Correlation Coefficient



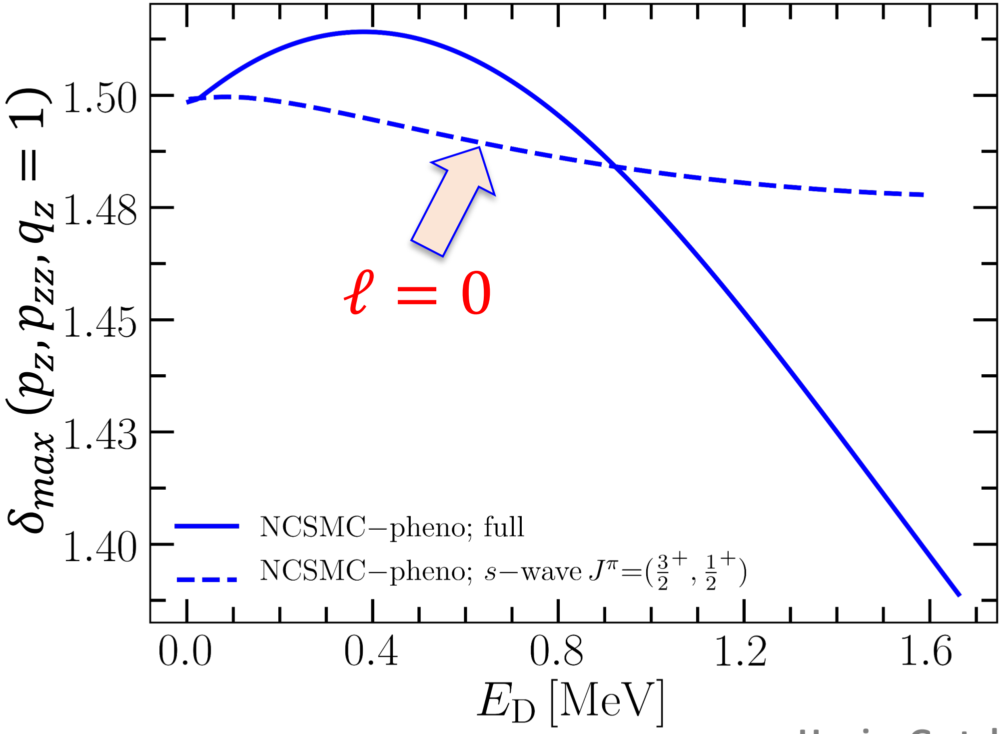
Hupin, G etal. (2019) Nature Communication 10, 351

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

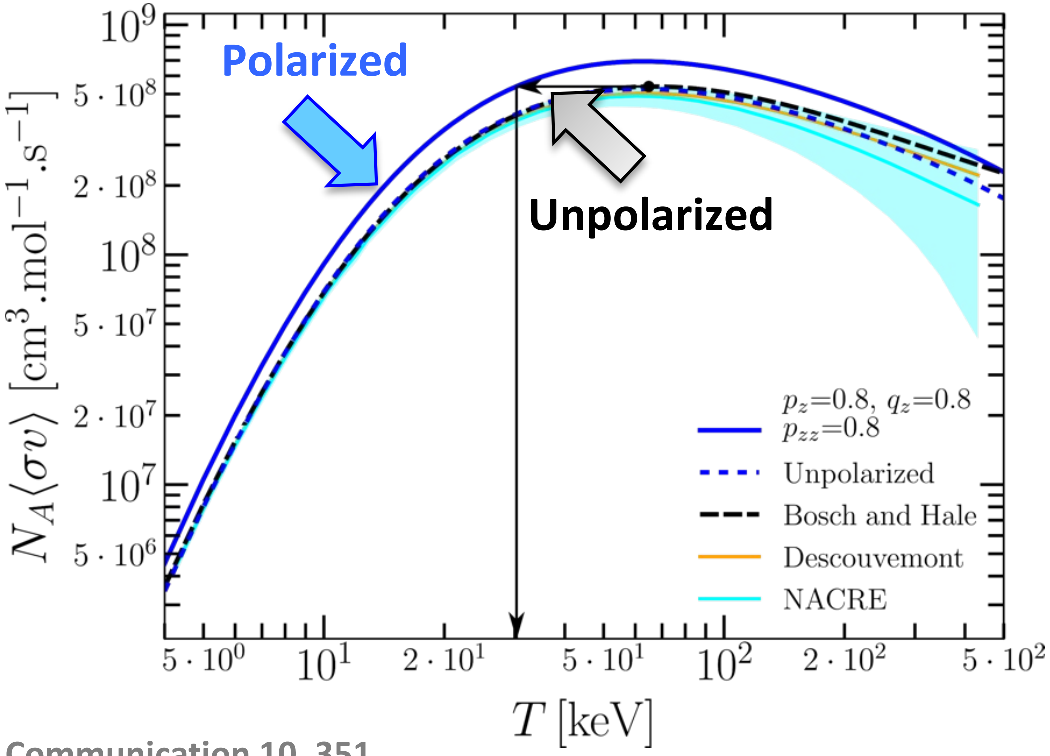
What is the enhancement factor?
And the polarized reaction rate?



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



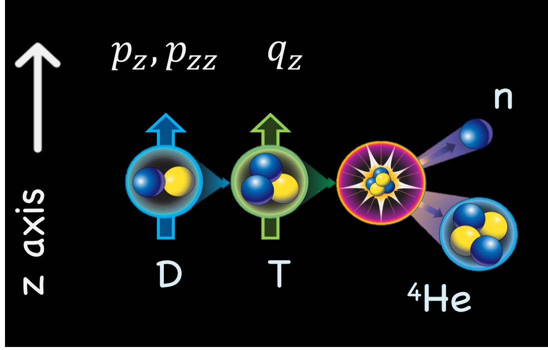
DT reaction rate

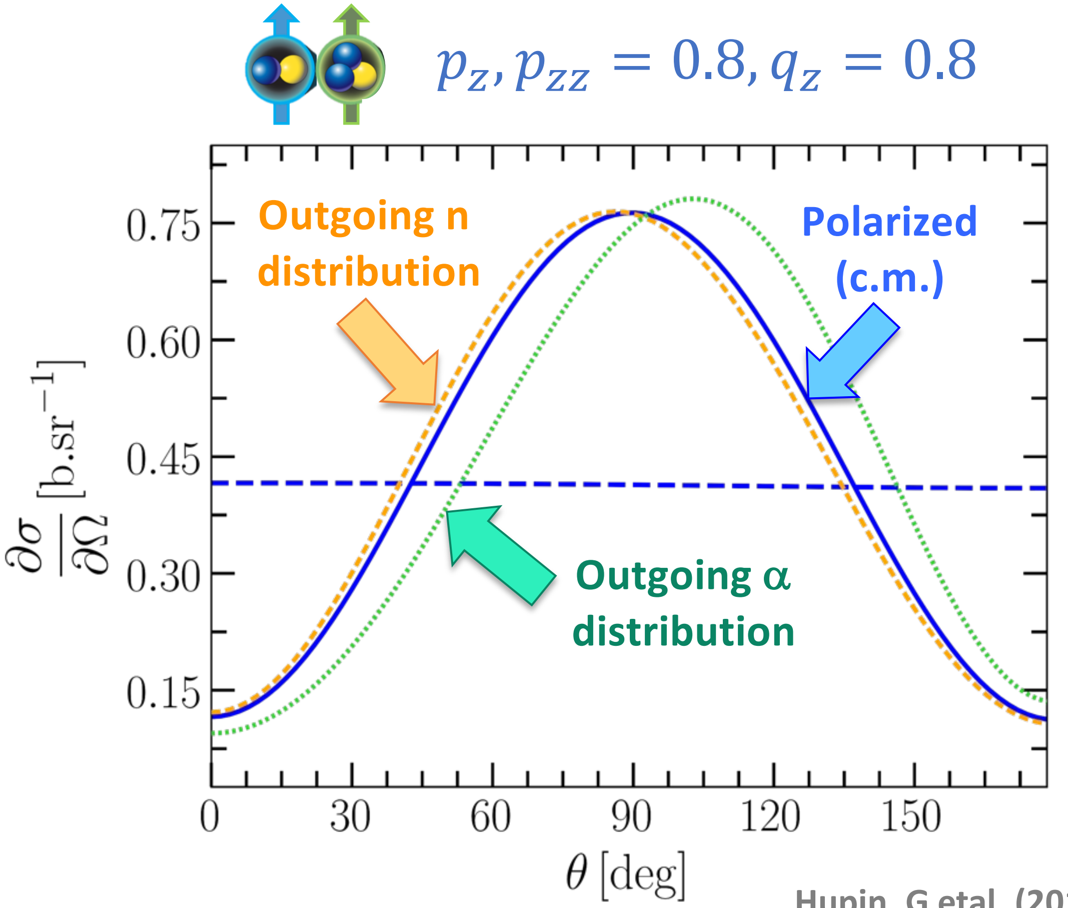


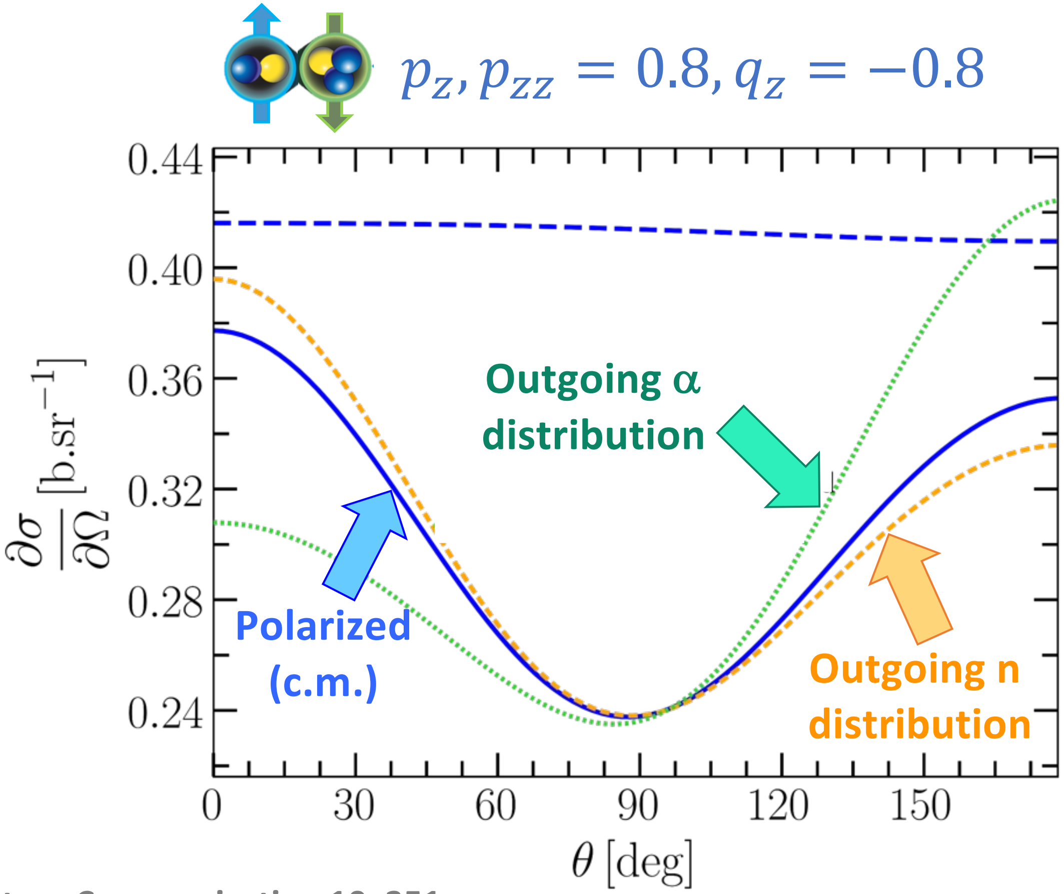
Hupin, G etal. (2019) Nature Communication 10, 351

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

What is the change in the products' angular distributions?



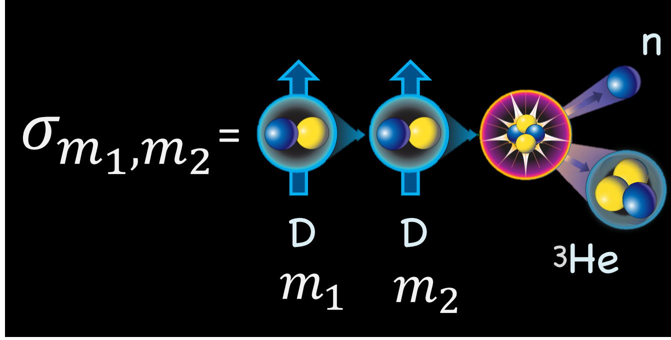




Hupin, G etal. (2019) Nature Communication 10, 351

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

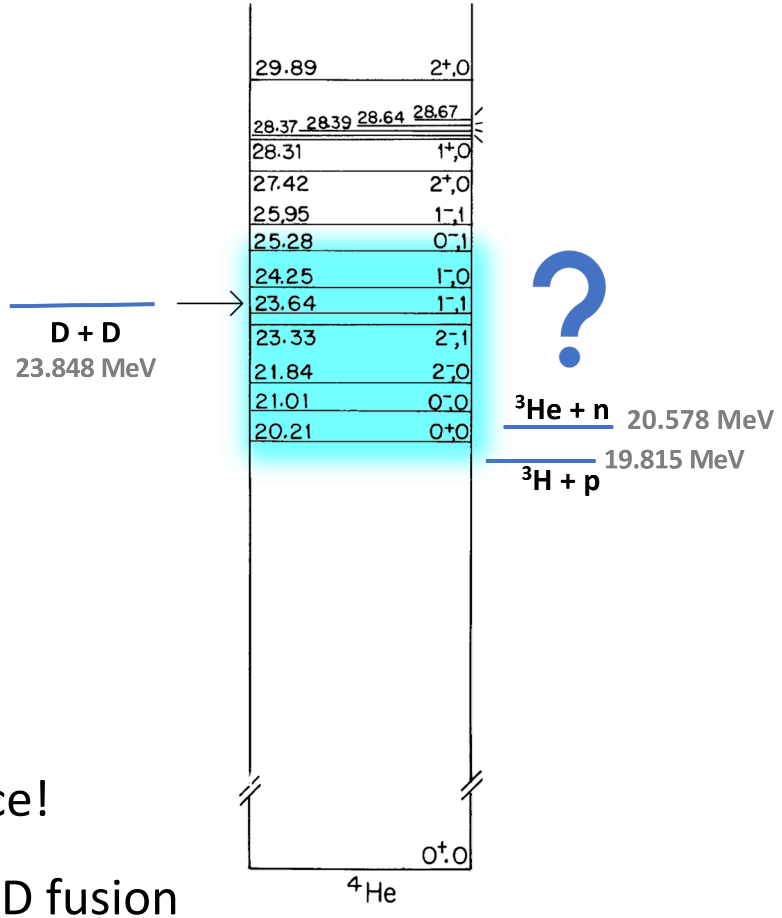
What about the spin-polarized DD fusion?



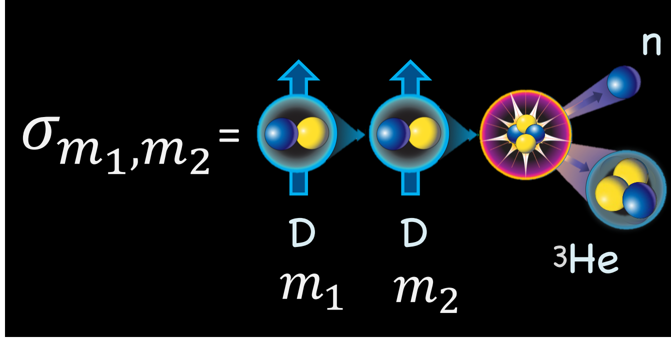
- H. Paetz gen. Schieck, Eur. Phys. J. A 44, 321 (2010):

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

Quintet $(S = 2)$ Triplet $(S = 1)$ Singlet $(S = 0)$



- Much more complicated:
  1) The fusion does not proceed through a single narrow resonance!
  2) Several relative partial waves ($\ell = 0, 1, 2$) can contribute to DD fusion



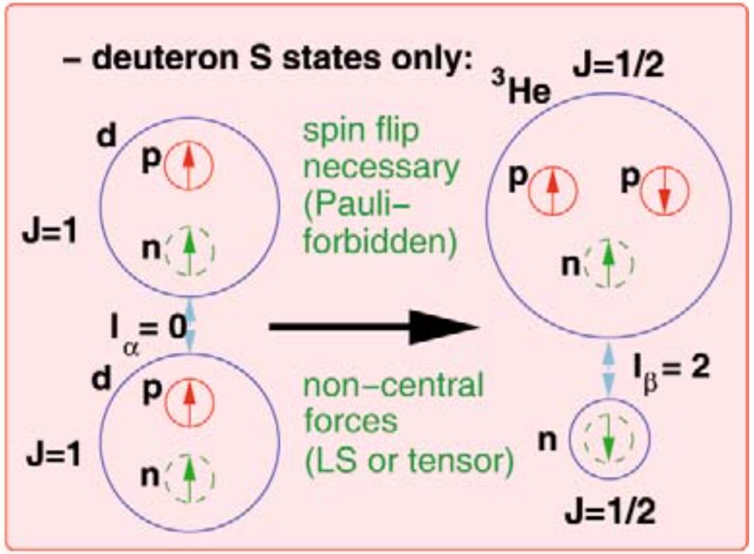
What about the spin-polarized DD fusion?

- First inidications by Kulsrud et al., PRL**49**, 1248 (1982)

$\ell = 0$ Suppressed Enhanced

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

Quintet ($S = 2$) Triplet ($S = 1$) Singlet ($S = 0$)



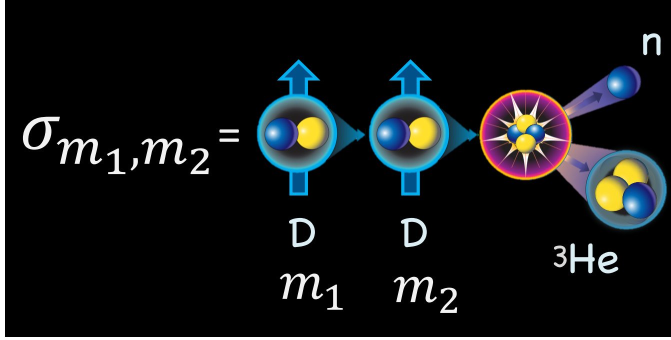
- Assume:

1) Below 100 keV, D+D pair mainly in S-wave (ℓ = 0) relative motion, i.e. $\sigma_{1,0} \approx 0$ (ℓ = 1)

2) D is a pure S ($\ell_D = 0$) state, therefore $\sigma_{1,1}$ would require spin flip ⇒ it is suppressed

Figure adapted from H. Paetz gen. Schieck, Eur. Phys. J. A 44, 321 (2010)

What about the spin-polarized DD fusion?



- First indications by Kulsrud et al., PRL**49**, 1248 (1982)

$\ell = 0$ — Suppressed ($\sigma_{1,1}$) — Enhanced ($\sigma_{0,0} + 2\sigma_{1,-1}$)

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

Quintet ($S = 2$) Triplet ($S = 1$) Singlet ($S = 0$)

- Singlet states beneficial for DD reactor concept
- Quintet state beneficial for aneutronic D^{3}He reactor concept

- Conjectures:

1) Enhancement of order 2 by polarizing beam and target D either transverse to the magnetic field or in opposite direction relative to the field

2) Suppression by a significant factor by polarizing both ions parallel to the field

But, estimates from fits on indirect expt. data show no or very little neutron suppression in the Quintet state, appreciable differences

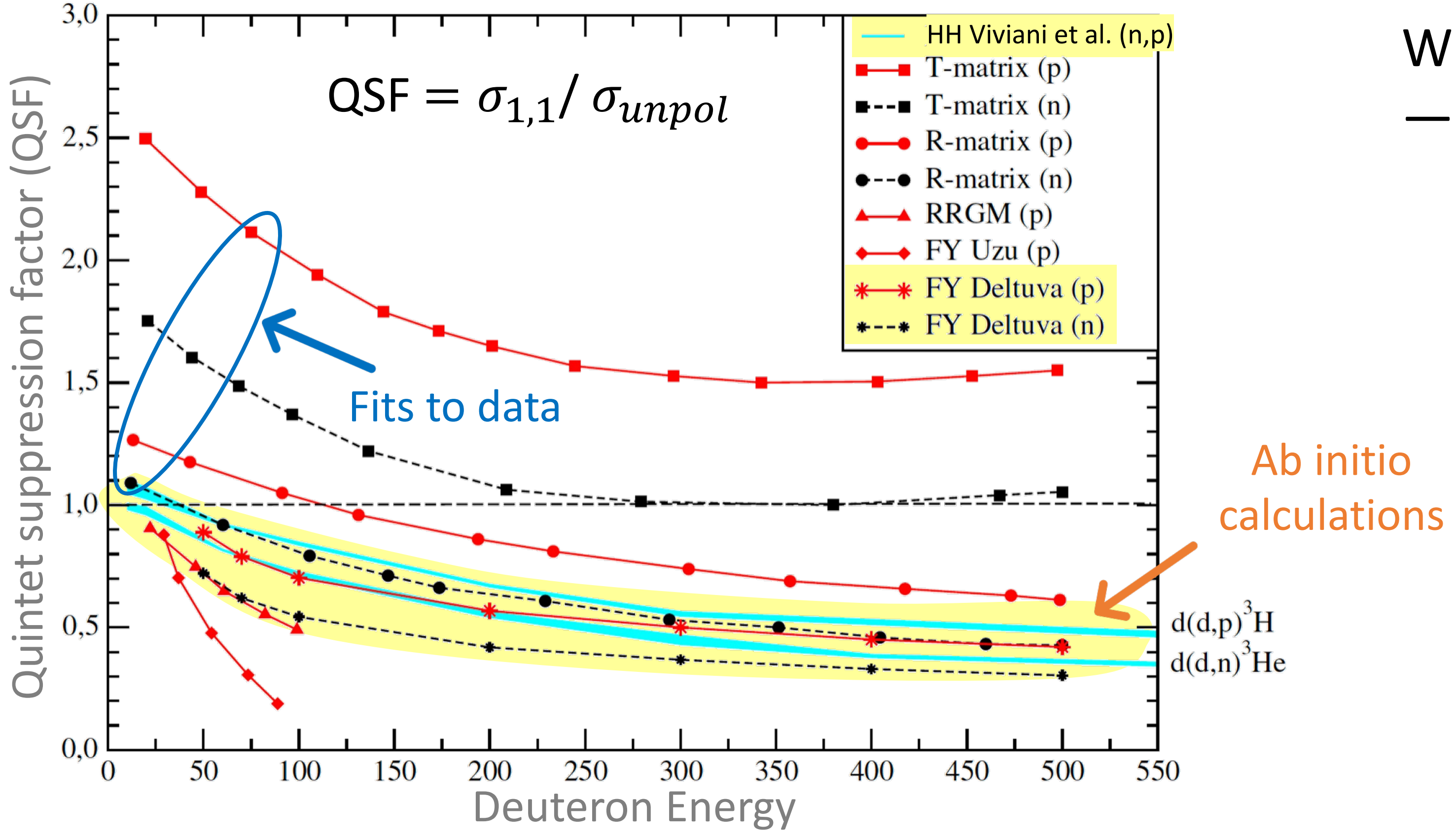


Figure adapted from Viviani, M et al, (2023) PRL 130, 122501

What did Kulsrud miss?
— D has also a small *D* ($\ell_D = 2$) state!

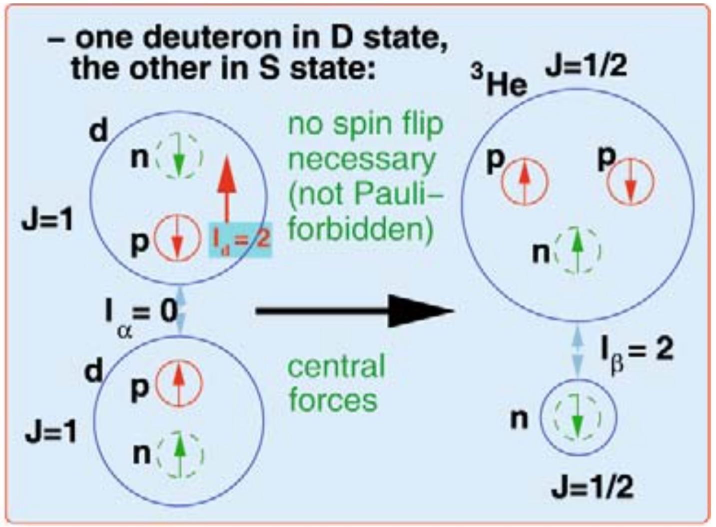


Figure adapted from H. Paetz gen. Schieck, Eur. Phys. J. A 44, 321 (2010)

Ab initio calculations suggest no, or only very mild suppression in quintet state below 100 keV. Contributions: singlet and quintet states ($\ell = 0$) are dominant; triplet state ($\ell = 1$) also sizable!

Spin-polarized DT fusion is now well understood, thanks in part to ab initio NCSMC calculations

Measurements of DT spin-correlation coefficient would be desirable!

What would be the gains of muon catalyzed, polarized DT fusion?

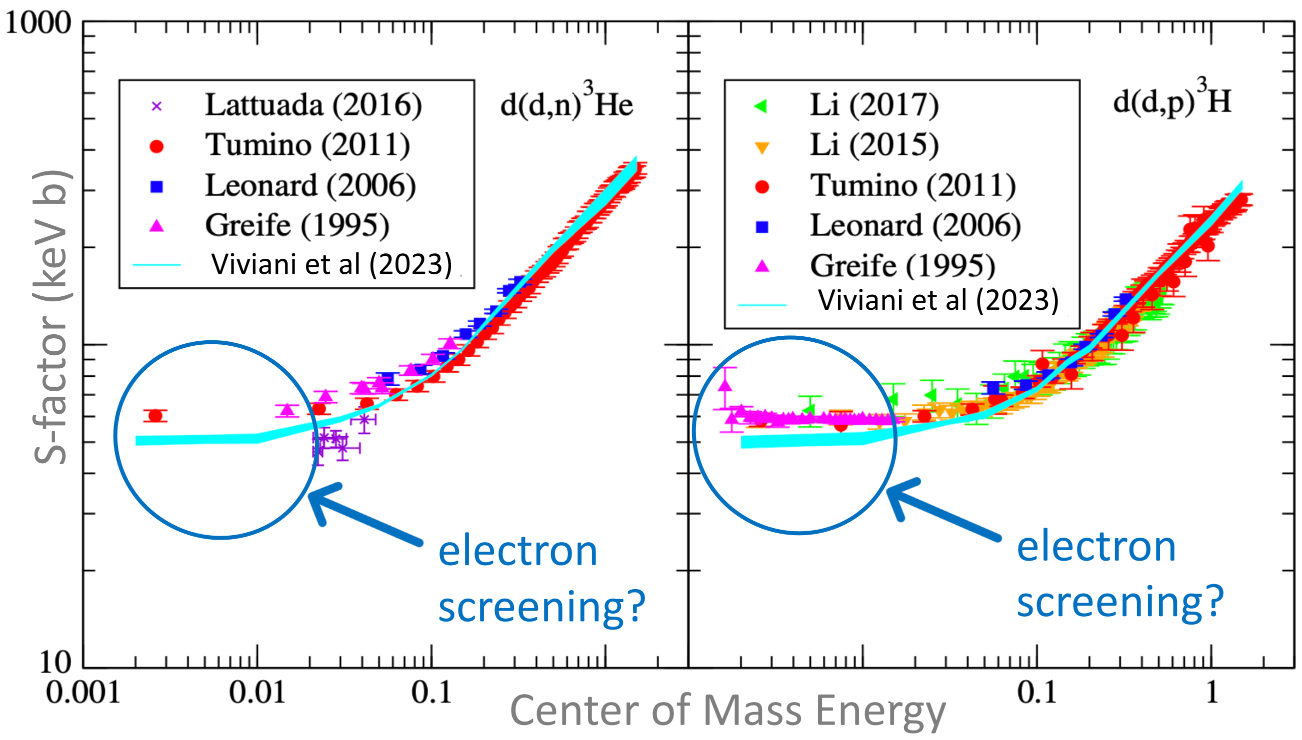
Need experimental and theoretical effort (See talk from A. Knaian)

How does the enhancement factor vary with energy in polarized D^3He fusion?

Higher fidelity ab initio NCSMC predictions for polarized D^3He could answer this question and are possible

Ab initio calculations started to place double polarized DD fusion on firmer ground, but more work is needed!

Figure adapted from Viviani, M et al, (2023) PRL 130, 122501



All evidence so far points to no or only very mild suppression in the Quintet state

Ab initio calculations from Viviani et al. most reliable, but ~15% off data below ~100 keV

Systematic theoretical uncertainties only partially assessed

There are no (reported) predictions for the enhancement factor in the *Singlet* state

Ab initio NCSMC predictions possible with some extra formalism/code development

Fully uncertainty quantified ab initio calculations of DD fusion **and** direct spin-correlated DD cross section measurements are still lacking, but highly desirable!

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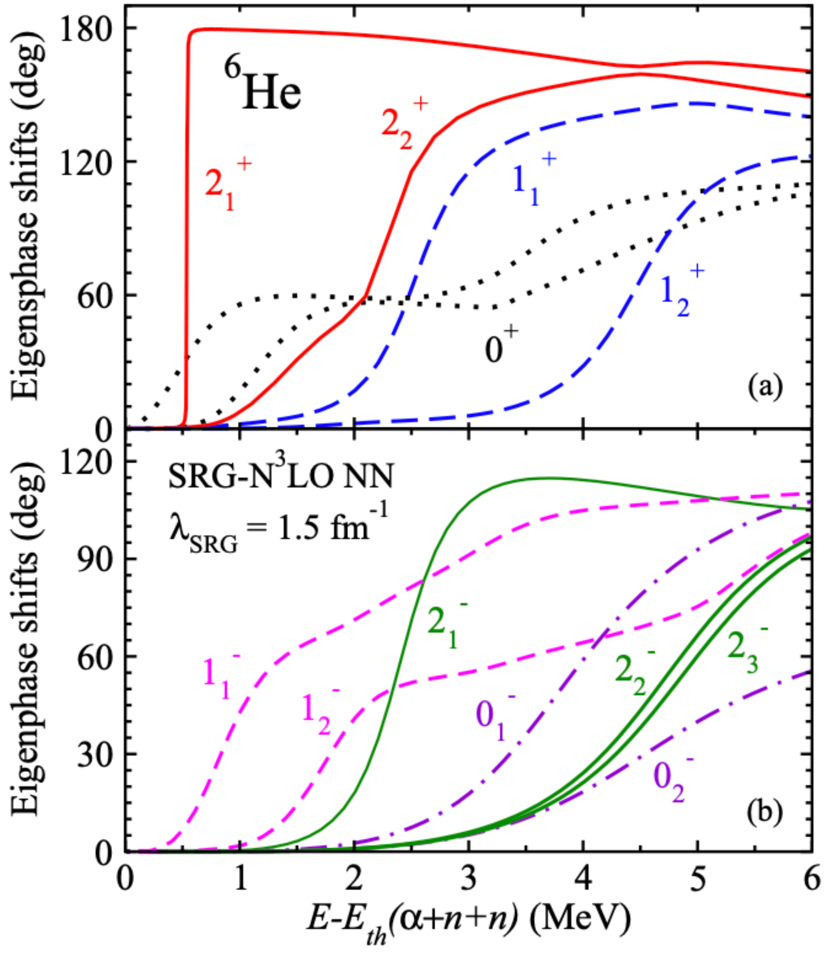
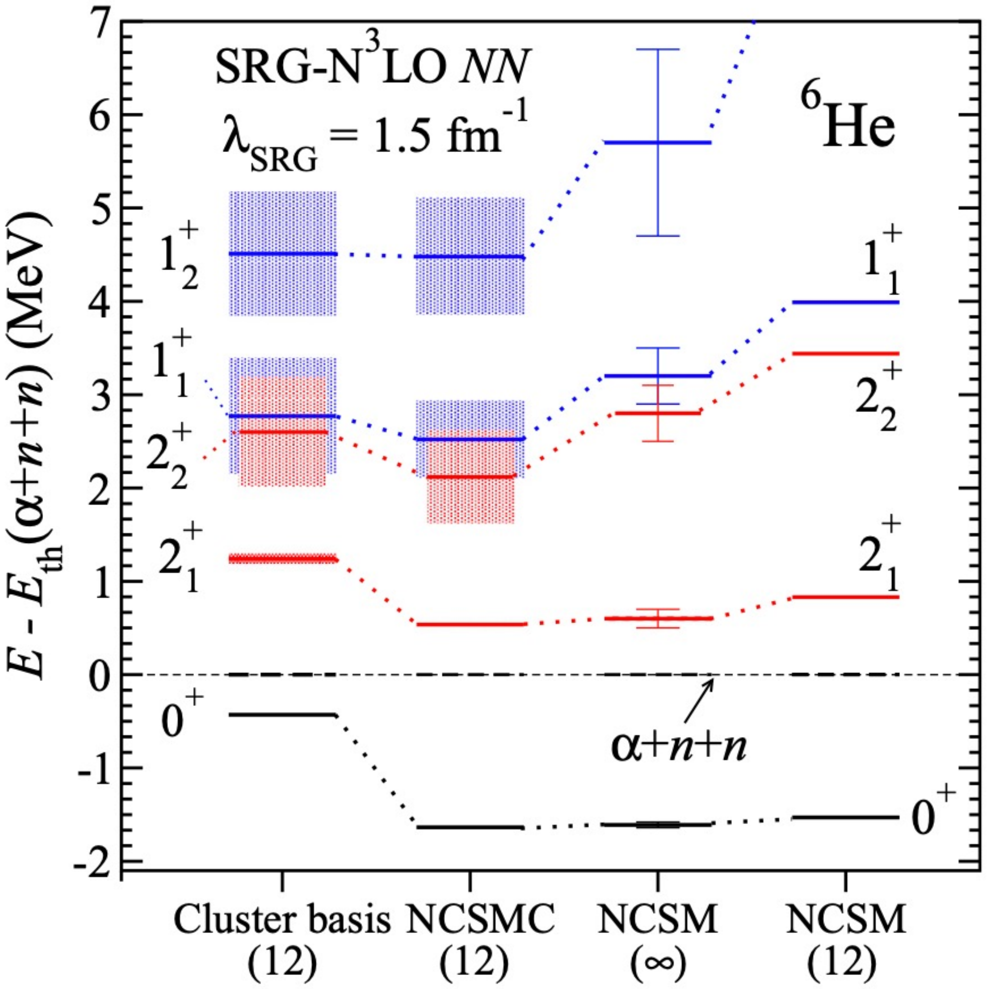
Are there 1^+ states in the ^{6}Be spectrum?
There are some predictions for the charge symmetric ^{6}He





Quaglioni, S et al (2018) Phys. Rev. C 97, 034332