Ab initio calculations of light-ion fusion reactions

INT-12-3 Workshop Structure of Light Nuclei

October 11, 2012

Sofia Quaglioni

Lawrence Livermore National Laboratory

Collaborators:
G. Hupin (LLNL)
P. Navrátil (TRIUMF,LLNL)
C. Romero-Redondo (TRIUMF)
R. Roth (TU Darmstadt)
J. Langhammer (TU Darmstadt)

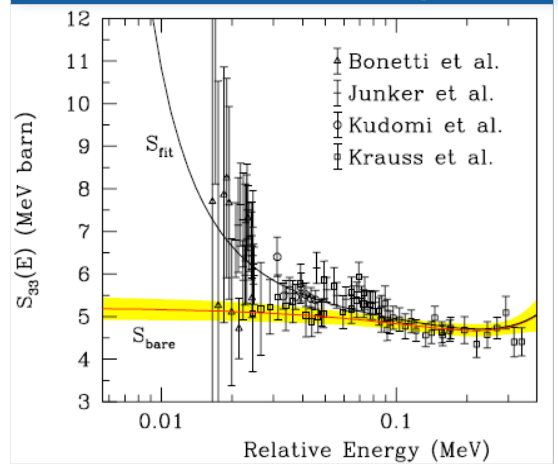
LLNL-PRES-589117
This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

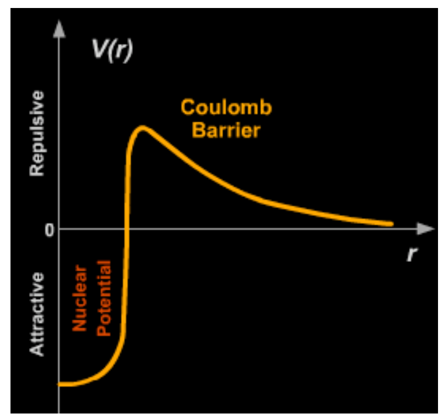
To understand the evolution of the Universe and the building blocks necessary for human life we need to understand fusion reactions

- Standard model of solar neutrinos: $^{7}Be(p,\gamma)^{8}B$, $^{3}He(\alpha,\gamma)^{7}Be$, $^{3}He(^{3}He,2p)^{4}He$, …
- Stellar nucleosyntesis: $2\alpha(\alpha,\gamma)^{12}C$, $^{12}C(\alpha,\gamma)^{16}O$, …
- But … Difficult or impossible to measure
  - Low rates due to Coulomb repulsion between projectile and target, cross section drops exponentially as $E \rightarrow 0$
  - Projectile and target not fully ionized ➔ Large electron-screening corrections
  - Astrophysical energies hard to reach in laboratory
  - Extrapolations from higher energies can be unreliable!

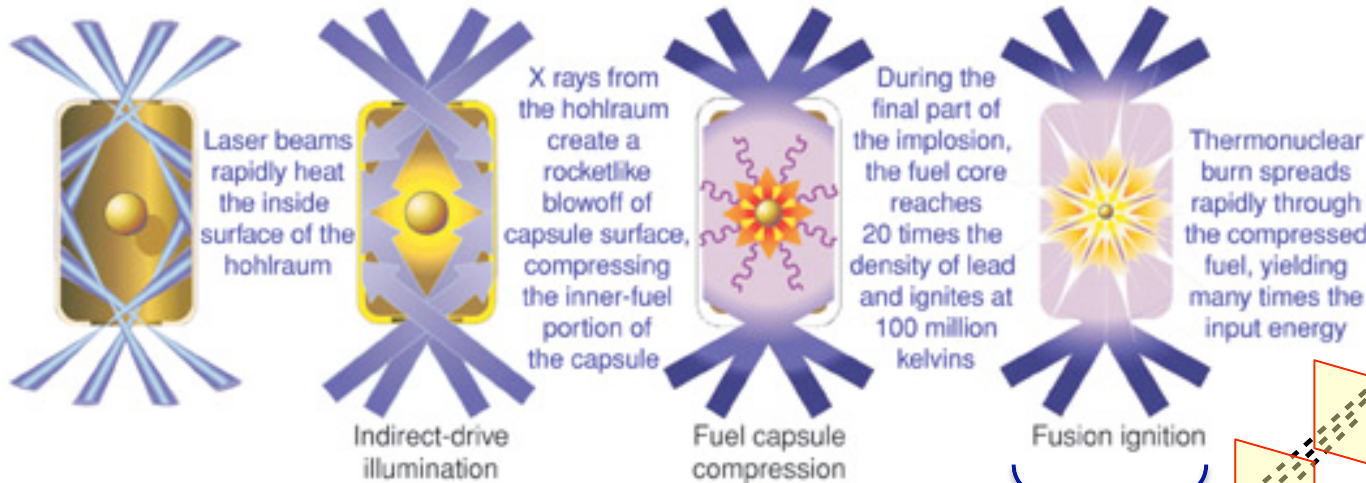
A fundamental theory is needed to enhance predictive capability of stellar modeling

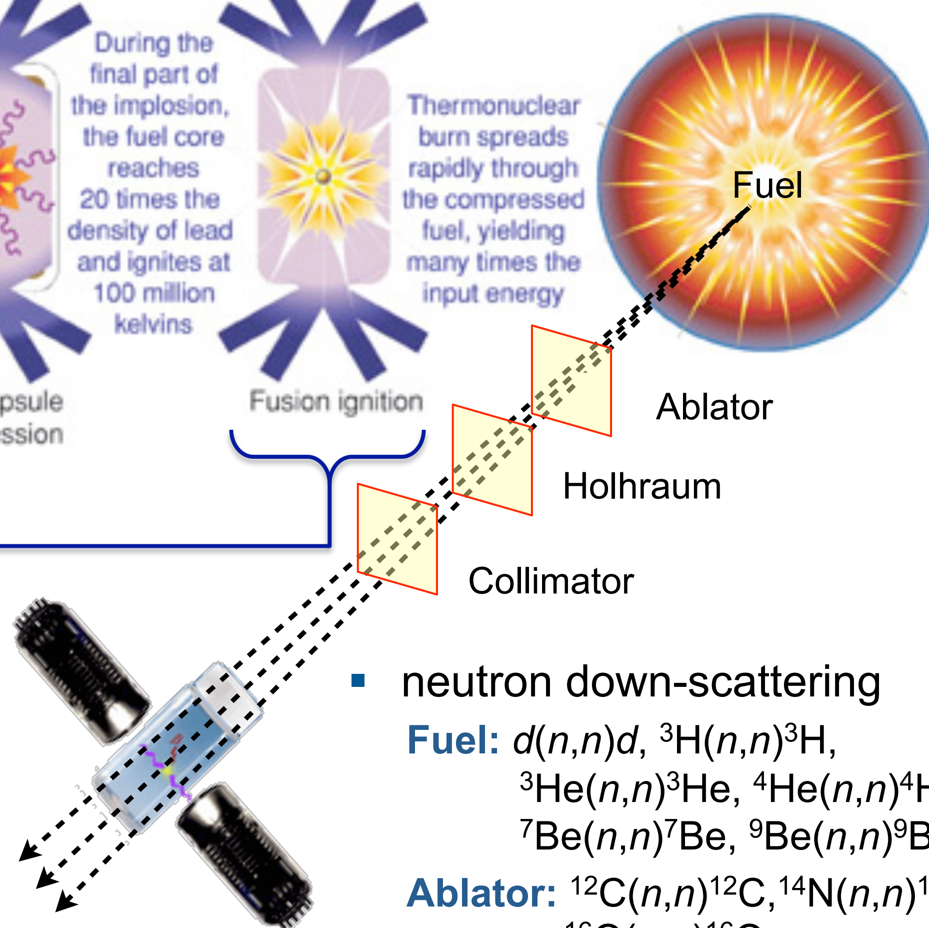
S-factor for $^{3}He(^{3}He,2p)^{4}He$





Light-ion reactions come into play in Earth-based fusion facilities (e.g., National Ignition Factility) when the fuel begins to burn





- $d + {}^3H \rightarrow {}^4He + n(14\ MeV)$
- But also:
  - $d + d \rightarrow {}^3He + n(2.45\ MeV)$
  - ${}^3H + {}^3H \rightarrow {}^4He + n + n\ (\leq 9.4\ MeV)$

Energy Production

- neutron down-scattering

Fuel: $d(n,n)d$, ${}^3H(n,n){}^3H$, ${}^3He(n,n){}^3He$, ${}^4He(n,n){}^4He$, ${}^7Be(n,n){}^7Be$, ${}^9Be(n,n){}^9Be$

Ablator: ${}^{12}C(n,n){}^{12}C$, ${}^{14}N(n,n){}^{14}N$, ${}^{16}O(n,n){}^{16}O$

Prompt Diagnostics

From nucleons to nuclei to fusion reactions

- Primary Objectives:

  Arrive at a fundamental understanding of nuclear properties from a unified theoretical standpoint rooted in the fundamental forces among nucleons

  Develop theoretical foundations for an accurate description of reactions between light ions in a thermonuclear environment

- How?
  - Solve non-relativistic Schrödinger equation for *A* (all active) nucleons interacting through two- and three-nucleon (NN+NNN) forces (= *ab initio* calculation)
  - Structural properties (bound states, narrow resonances)
    - *Ab initio* many-body approaches (A ≤ ~16); No-Core Shell Model (NCSM)
  - Dynamical properties (scattering, reactions)
    - Extend No-Core Shell-Model with the Resonating Group Method (RGM)

Can we describe nuclei and their interactions with point-like nucleons and realistic interactions?

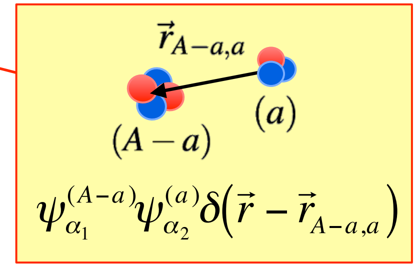
Ab initio NCSM/RGM Formalism

S. Quaglioni & P. Navrátil, Phys. Rev. Lett. 101, 092501 (2008); Phys. Rev. C 79, 044606 (2009)

- Starts from:

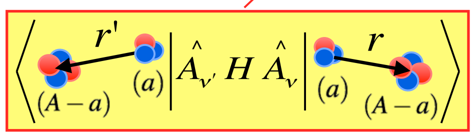
Channel basis

$$\Psi^{(A)}_{RGM} = \sum_{\nu} \int d\vec{r}\; g_\nu(\vec{r})\; \hat{A}_\nu \underbrace{\left| \Phi^{(A-a,a)}_{\nu\vec{r}} \right\rangle}_{\text{Channel basis}}$$

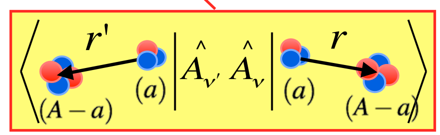


- Projects Schrödinger equation on channel basis:

$$H\Psi^{(A)}_{RGM} = E\Psi^{(A)}_{RGM} \rightarrow \sum_{\nu} \int d\vec{r}\; \left[H_{\nu'\nu}(\vec{r}',\vec{r}) - E\; N_{\nu'\nu}(\vec{r}',\vec{r}) \right] g_\nu(\vec{r}) = 0$$



Hamiltonian kernel



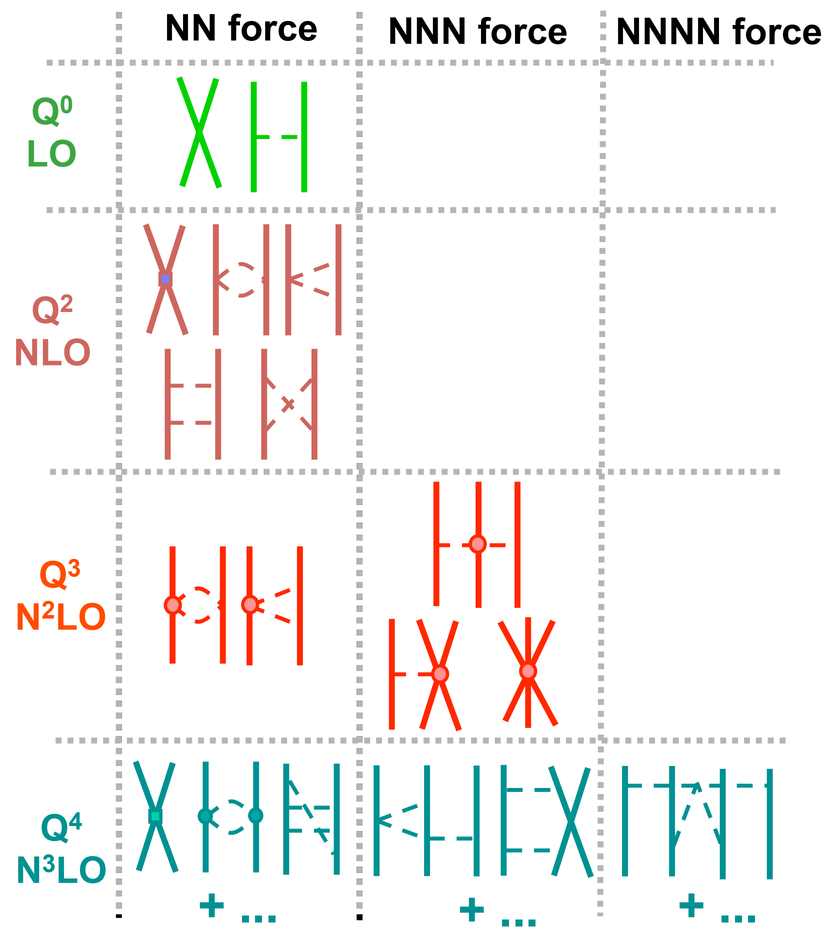
Norm (overlap) kernel

- Constructs integration kernels (≈ projectile-target potentials) starting from:
  - NN +NNN (chiral EFT) interactions
  - NCSM *ab initio* wave functions

RGM accounts for: 1) interaction (Hamiltonian kernel) and 2) Pauli principle (Norm kernel) between clusters; NCSM accounts for: internal structure of clusters

Inputs:
1) Accurate nuclear interactions (and currents)

- Nuclear forces are governed by quantum chromodynamics (QCD)
  - QCD non perturbative at low energies
- Chiral effective filed theory (χEFT)
  - retains all symmetries of QCD
  - explicit degrees of freedom: π, N
- Perturbative expansion in positive powers of $(Q/\Lambda_\chi) \ll 1$ ($\Lambda_\chi \sim 1$ Gev)
  - nuclear interactions
  - nuclear currents
- Chiral symmetry dictates operator structure
- Low-energy constants (LECs) absorb short-range physics
  - some day all from lattice QCD
  - now constrained by experiment



Worked out by Van Kolck, Keiser, Meissner, Epelbaum, Machleidt, ...

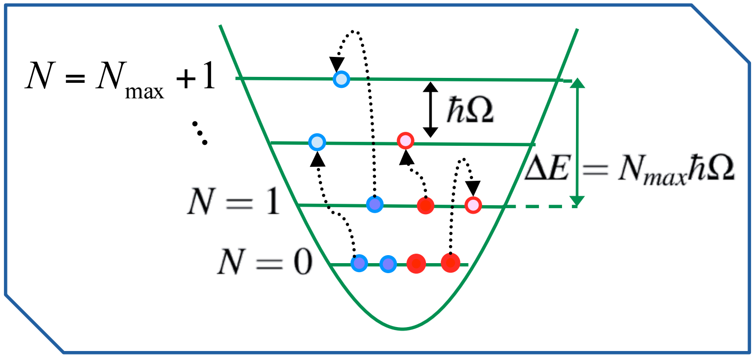
Challenge and necessity: apply χEFT forces tp nuclei

Inputs:
2) Many-body wave functions of targets and projectiles

- Solve: $$H^{(A-a)}\,\psi^{(A-a)}_{\alpha_1}(\vec{r}_1,\vec{r}_2,\cdots,\vec{r}_{A-a}) = E^{(A-a)}_{\alpha_1}\,\psi^{(A-a)}_{\alpha_1}(\vec{r}_1,\vec{r}_2,\cdots,\vec{r}_{A-a})$$
$$H^{(a)}\,\psi^{(a)}_{\alpha_2}(\vec{r}_{A-a+1},\vec{r}_{A-a+2},\cdots,\vec{r}_A) = E^{(a)}_{\alpha_2}\,\psi^{(a)}_{\alpha_2}(\vec{r}_{A-a+1},\vec{r}_{A-a+2},\cdots,\vec{r}_A)$$

- The NCSM approach:
  - Large (but finite!) expansions in *A*-body harmonic oscillator (HO) basis (Jacobi relative or Cartesian single-particle coordinates)

$$\psi^{(K)} = \sum_{N=N_{\min}}^{N_{\max}} c_N \Phi^{HO}_N(\vec{r}_1,\,\vec{r}_2,\,\ldots,\,\vec{r}_K)$$



  - Preserves translational invariance (also with Slater-Determinant basis!)
  - Can include NN+NNN interactions
  - Uses effective interaction to accelerate convergence to exact solution with $N_{\max}$

Inputs:
2) Many-body wave functions of targets and projectiles

- Solve: $H^{(A-a)}\,\psi_{\alpha_1}^{(A-a)}(\vec{r}_1,\vec{r}_2,\cdots,\vec{r}_{A-a}) = E_{\alpha_1}^{(A-a)}\,\psi_{\alpha_1}^{(A-a)}(\vec{r}_1,\vec{r}_2,\cdots,\vec{r}_{A-a})$

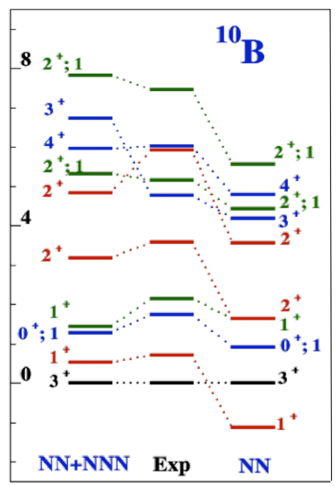
  $H^{(a)}\,\psi_{\alpha_2}^{(a)}(\vec{r}_{A-a+1},\vec{r}_{A-a+2},\cdots,\vec{r}_A) = E_{\alpha_2}^{(a)}\,\psi_{\alpha_2}^{(a)}(\vec{r}_{A-a+1},\vec{r}_{A-a+2},\cdots,\vec{r}_A)$

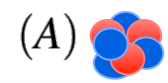
- The NCSM approach:
  - Large (but finite!) expansions in *A*-body harmonic oscillator (HO) basis (Jacobi relative or Cartesian single-particle coordinates)

$$\psi^{(K)} = \sum_{N=N_{\min}}^{N_{\max}} c_N \Phi_N^{HO}(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_K)$$

  - Preserves translational invariance (also with Slater-Determinant basis!)
  - Can include NN+NNN interactions
  - Uses effective interaction to accelerate convergence

NCSM – static properties





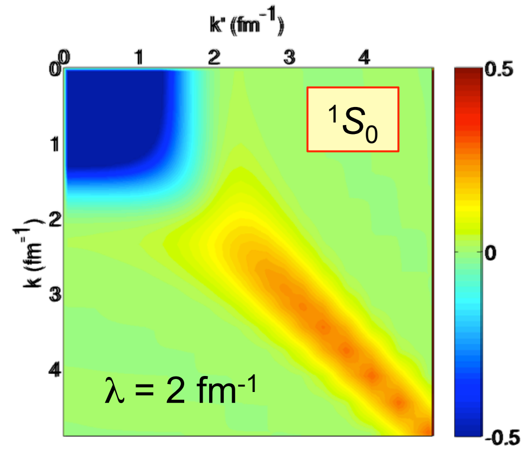
Helped revealing fundamental importance of three-nucleon (NNN) forces in structure calculations. Shown here, low-lying spectrum of ^{10}B. Without NNN force g.s. has wrong spin.

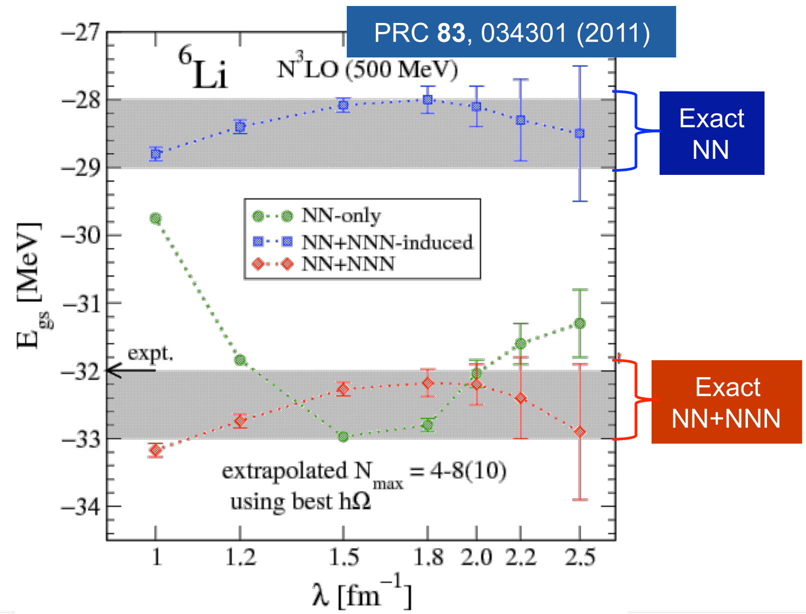
A bit of help:
3) Effective interaction

- Similarity Renormalization Group (SRG) method
  - Sequence of unitary transformations that decouple low- and high-momentum parts of the interaction

$$H_s = U_s H U_s^{+} \Rightarrow \frac{dH_s}{ds} = [[G,H_s],H_s] \qquad \left(s = 1/\lambda^4\right)$$

  - Makes the nuclear many-body problem more tractable
  - The same effective interaction used to obtain:
    1) Structure of projectiles and targets
    2) Non-local projectile-target potentials
  - Introduces three-body interactions





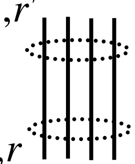
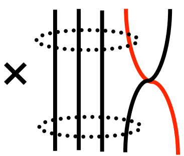
The SRG method offers a new (and improved) approach to exact descriptions of light nuclei with realistic NN, NNN interactions

Norm kernel (Pauli principle)

$$\left\langle \Phi^{(A-a',a')}_{\nu'\vec{r}\,'} \middle| \hat{A}^{(A-a',a')}\hat{A}^{(A-a,a)} \middle| \Phi^{(A-a,a)}_{\nu\vec{r}} \right\rangle$$

- Formalism is non-trivial and depends on mass numbers of projectiles: a, a'

a, a' = 1

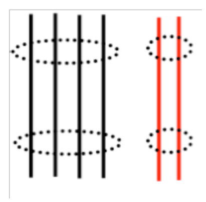
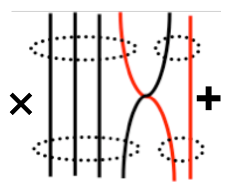
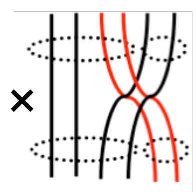
$$N_{a'=1\nu',a=1\nu}(\vec{r}\,',\vec{r}) = $$ ν',r'  ν,r **- (A-1) ×** 

$$\delta_{\nu'\nu}\frac{\delta(r'-r)}{r'r}$$

$$\sum_{n'n} R_{n'\ell'}(r')\left\langle \Phi^{(A-1,1)}_{\nu'n'} \middle| \hat{P}_{A-1,A} \middle| \Phi^{(A-1,1)}_{\nu n} \right\rangle R_{n\ell}(r)$$

localized

a, a' = 2

$$N_{a'=2\nu',a=2\nu}(\vec{r}\,',\vec{r}) = $$  **- 2(A-2) ×**  **+ (A-2)(A-3)/2 ×** 

In general, for $a \geq a'$ need many-body matrix elements of one- to up to a-body exchanges

Hamiltonian kernel (Projectile-target potentials)

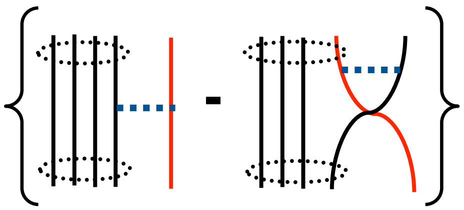
$$\left\langle \Phi^{(A-a',a')}_{\nu'\vec{r}'} \right| \hat{A}^{(A-a',a')} H \hat{A}^{(A-a,a)} \left| \Phi^{(A-a,a)}_{\nu\vec{r}} \right\rangle$$

- More complicated than norm kernel …

$a, a' = 1$

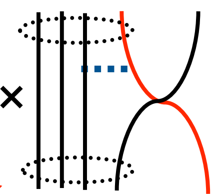
$$H_{a'=1\nu',a=1\nu}(r',r) = \left[T_{rel}(r') + V_C(r') + E^{(A-1)}_{\alpha_1}\right] N_{a'=1\nu',a=1\nu}(r',r)$$

+(A-1) ×



$$\sum_{n'n} R_{n'\ell'}(r') \left\langle \Phi^{(A-1,1)}_{\nu'n'} \right| V_{A-1,A}(1-\hat{P}_{A-1,A}) \left| \Phi^{(A-1,1)}_{\nu n} \right\rangle R_{n\ell}(r)$$

- (A-1)(A-2) ×



$$\sum_{n'n} R_{n'\ell'}(r') \left\langle \Phi^{(A-1,1)}_{\nu'n'} \right| V_{A-2,A}\hat{P}_{A-1,A} \left| \Phi^{(A-1,1)}_{\nu n} \right\rangle R_{n\ell}(r)$$

+ terms containing NNN potential

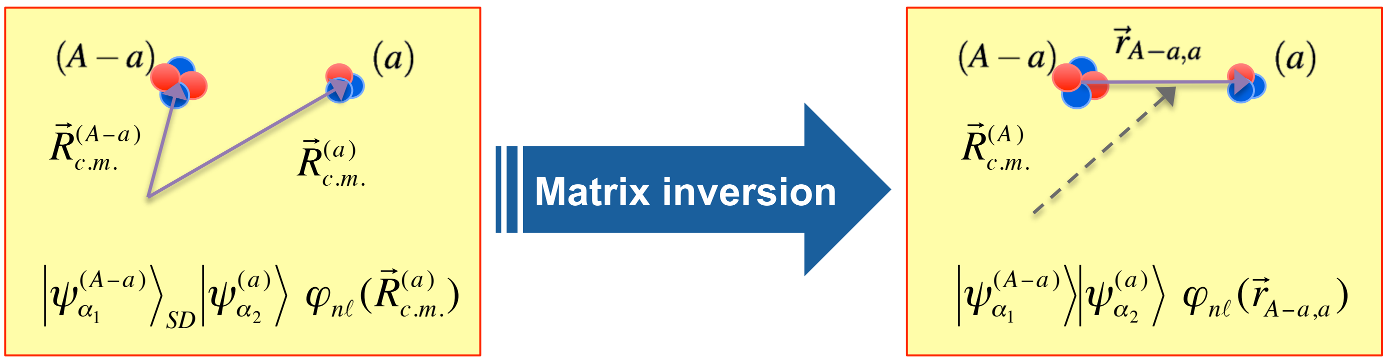
The matrix elements of the potential are all localized and can be expanded in HO radial wfs

Matrix elements of translationally invariant operators

- Translational invariance is preserved (exactly!) also with SD cluster basis

$$ {}_{SD}\left\langle \Phi^{(A-a',a')}_{f_{SD}} \middle| \hat{O}_{t.i.} \middle| \Phi^{(A-a,a)}_{i_{SD}} \right\rangle_{SD} = \sum_{i_R f_R} M_{i_{SD} f_{SD}, i_R f_R} \left\langle \Phi^{(A-a',a')}_{f_R} \middle| \hat{O}_{t.i.} \middle| \Phi^{(A-a,a)}_{i_R} \right\rangle $$

Calculate these **Interested in these**



- Advantage: can use powerful second quantization techniques

$$ {}_{SD}\left\langle \Phi^{(A-a',a')}_{\nu' n'} \middle| \hat{O}_{t.i.} \middle| \Phi^{(A-a,a)}_{\nu n} \right\rangle_{SD} \propto {}_{SD}\left\langle \psi^{(A-a')}_{\alpha_1'} \middle| a^+ a \middle| \psi^{(A-a)}_{\alpha_1} \right\rangle_{SD}, \; {}_{SD}\left\langle \psi^{(A-a')}_{\alpha_1'} \middle| a^+ a^+ a a \middle| \psi^{(A-a)}_{\alpha_1} \right\rangle_{SD}, \; \cdots $$

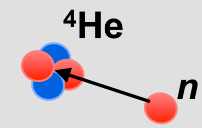
Solving the RGM equations

- The many-body problem has been reduced to a two-body problem!
  - Macroscopic degrees of freedom: nucleon clusters
  - Unknowns: relative wave function between pairs of clusters
- Non-local integral-differential coupled-channel equations:

$$\left[T_{rel}(r)+V_C(r)+E_{\alpha_1}^{(A-a)}+E_{\alpha_2}^{(a)}\right]u_\nu(r)+\sum_{\nu'}\int dr'r'\; W_{\nu\nu'}(r,r')u_{\nu'}(r')=0$$

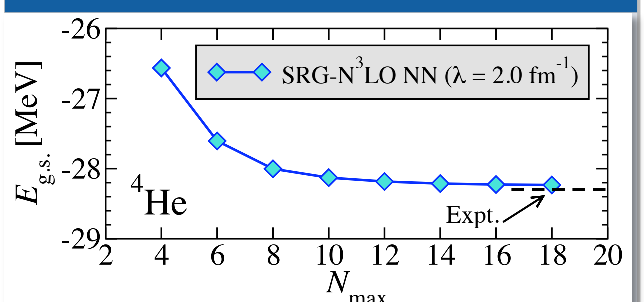
- Solve with microscopic R-matrix theory
  - Bound state boundary conditions → eigenenergy + eigenfunction
  - Scattering state boundary conditions → Scattering matrix
    - Phase shifts
    - Cross sections
    - …

Convergence with respect to HO basis size (N_{max})

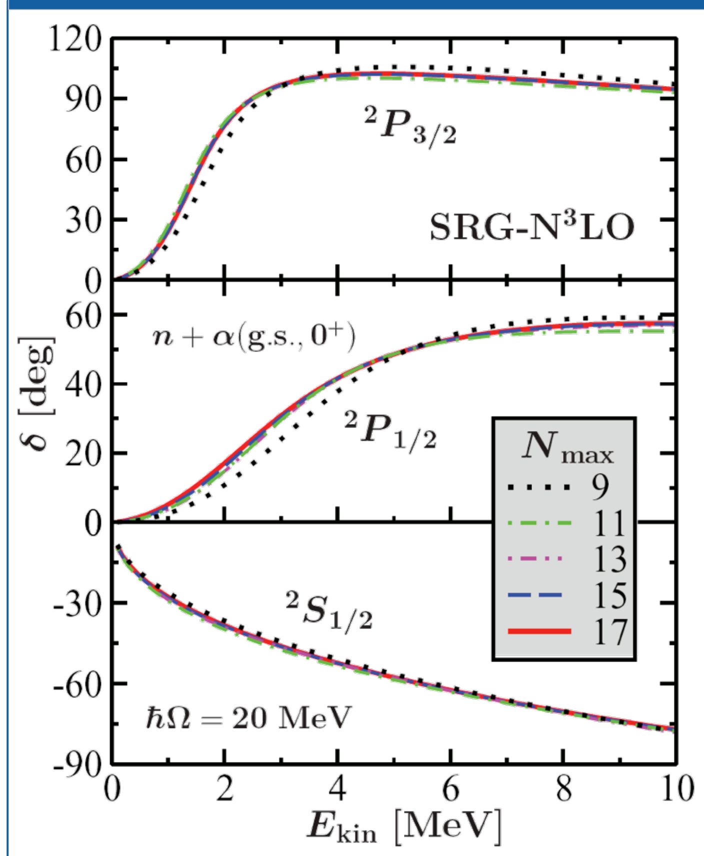


- Influenced by:
  1) Convergence of target and projectile wave functions
  2) Convergence of localized parts of the integration kernels
- Here:
  - *n* + 4He(g.s.,0^+) phase shifts
  - SRG-N³LO NN potential (λ = 2 fm^{-1})

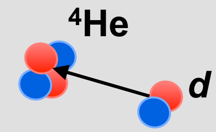
⁴He ground-state energy



⁴He(*n*,*n*)⁴He phase shifts



Convergence with respect to RGM model space (number/type of binary clusters)

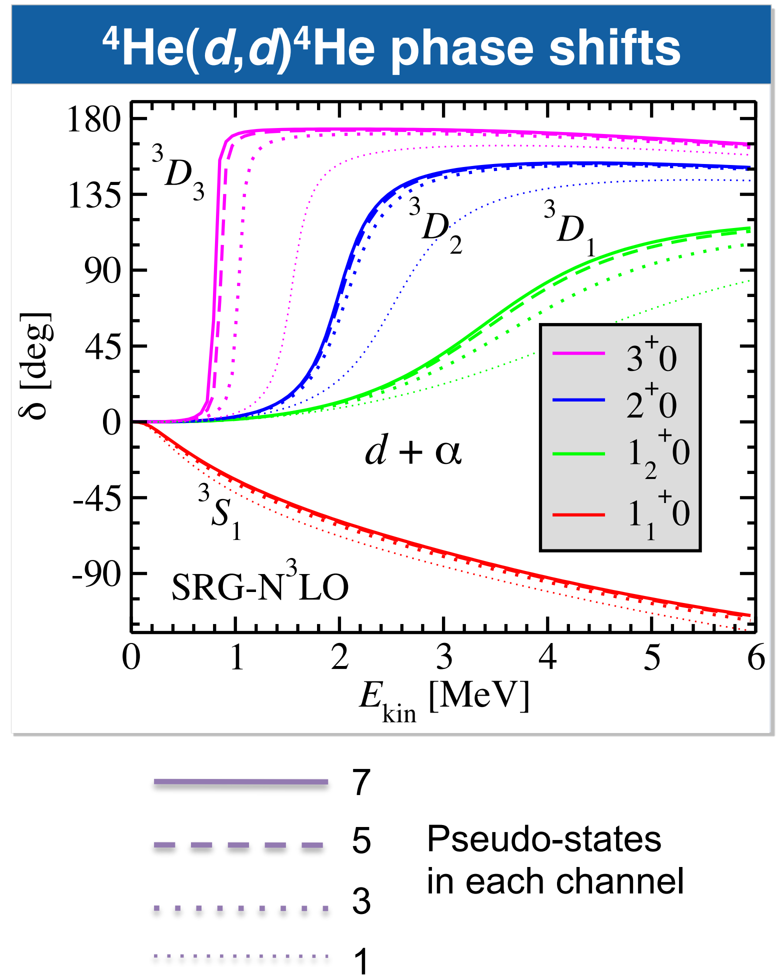


- NCSM/RGM describes binary reactions (below three-body breakup threshold)
- If projectile (or target) can be easily deformed or broken apart
  - Need to account for virtual breakup
  - Approximate treatment:

    Include multiple excited (pseudo-) states of the clusters
  - Exact treatment:

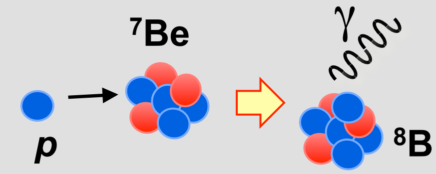
    1) Inclusion of three-body clusters

    2) Solution of three-body scattering
- Here:
  - d(g.s.,$^3S_1$-$^3D_1$, $^3D_2$, $^3D_3$-$^3G_3$) + ^{4}He(g.s.)
  - SRG-N^{3}LO NN potential (λ = 1.5 fm^{-1})



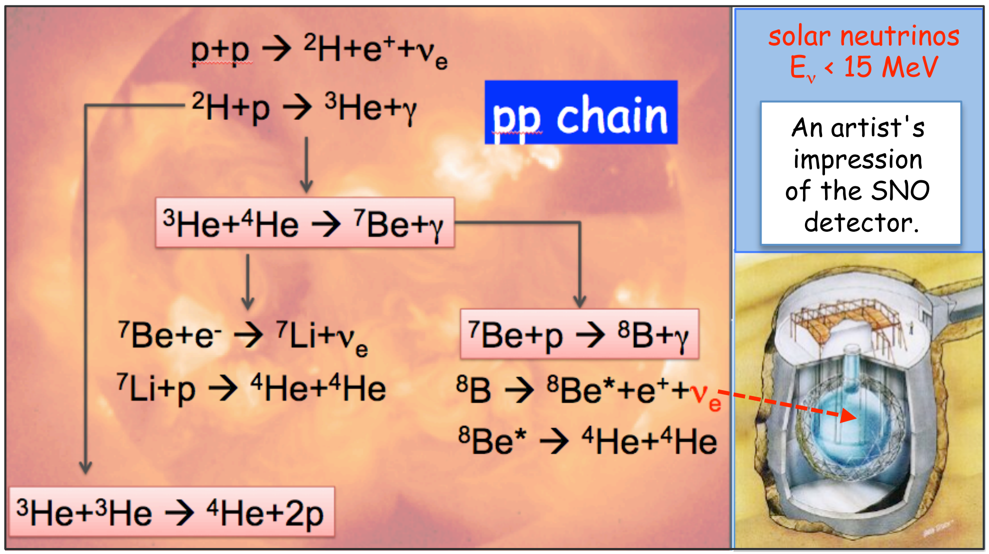
The ^{7}Be(p,γ)^{8}B radiative capture

P. Navrátil, R. Roth, and S.Q., Phys. Lett. B704, 379 (2011)



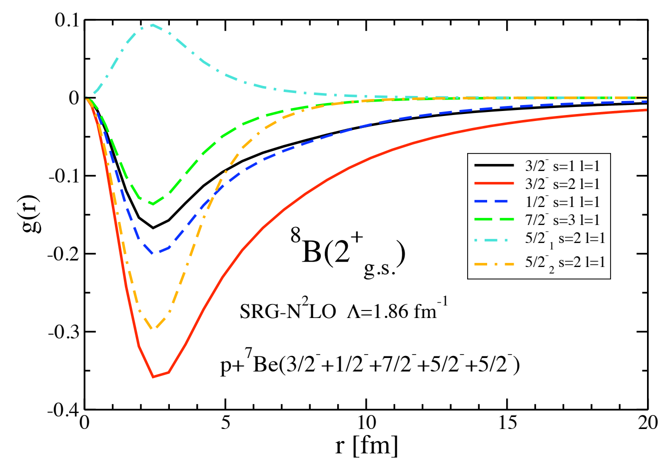
Solar neutrino problem:

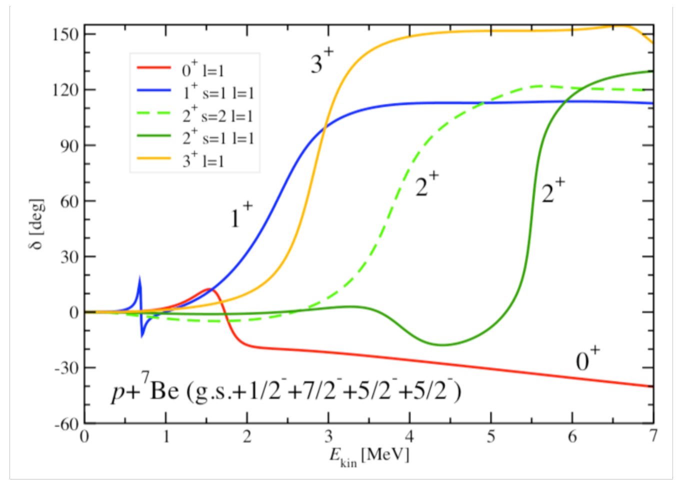
The ^{7}Be(p,γ)^{8}B is the final step in the nucleosynthetic chain leading to ^{8}B and one of the main inputs of the Standard Solar Model



- ~10% error in latest $S_{17}(0)$: dominated by uncertainty in theoretical models

^{8}B g.s. and p+^{7}Be phase shifts



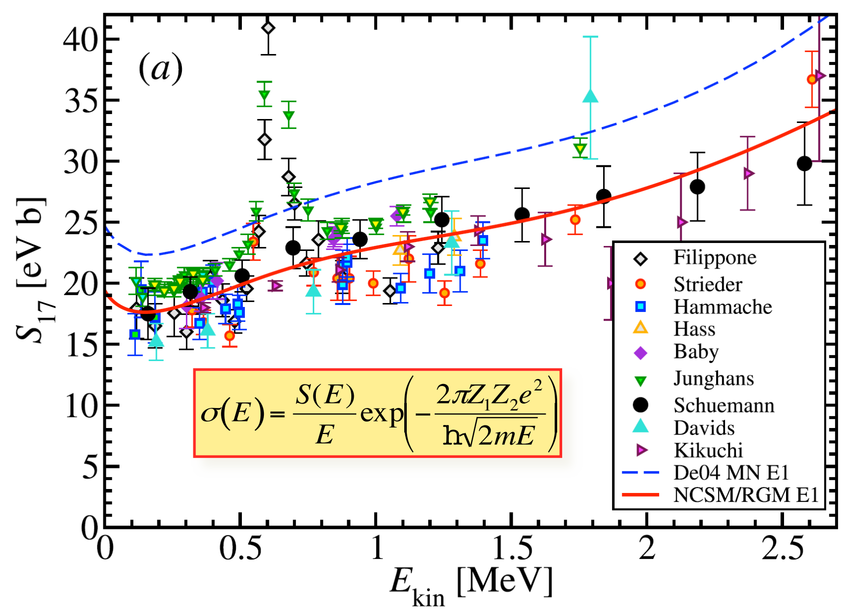


Ab initio many-body calculation of the $^7Be(p,\gamma)^8B$ radiative capture

P. Navrátil, R. Roth, and S. Quaglioni, Phys. Lett. B704, 379 (2011)

- NCSM/RGM results with largest realistic model space (N_{max} = 10):
  - $p+^7Be$(g.s., $1/2^-$, $7/2^-$, $5/2_1^-$, $5/2_2^-$)
  - Siegert's E1 transition operator
- Parameter Λ of SRG NN interaction chosen to reproduce separation energy: 136 keV (Expt. 137 keV)
- $S_{17}(0)$ = 19.4(7) eV b on the lower side of, but consistent with latest evaluation
- Study of dependence on the HO basis size N_{max} and influence of higher-energy excited states of ^7Be used to estimate 0.7 eV b uncertainty on $S_{17}(0)$

$^7Be(p,\gamma)^8B$ astrophysical S-factor



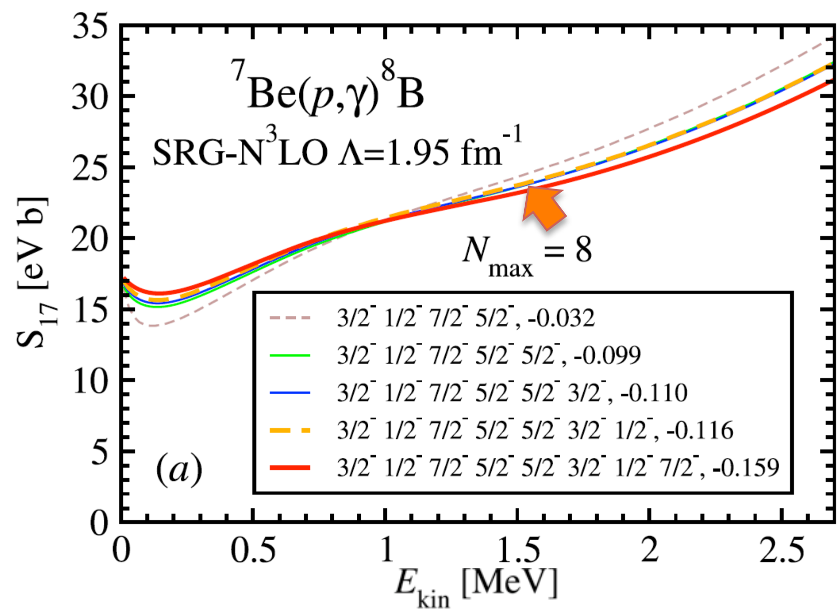
Ab initio theory predicts simultaneously both normalization and shape of S_{17}. Inclusion of $5/2_2^-$ state improves S-factor energy dependence above 1.5 MeV.

Ab initio many-body calculation of the $^{7}Be(p,\gamma)^{8}B$ radiative capture

P. Navrátil, R. Roth, and S. Quaglioni, Phys. Lett. B704, 379 (2011)

- NCSM/RGM results with largest realistic model space (N_{max} = 10):
  - $p+^{7}$Be(g.s., $1/2^-$, $7/2^-$, $5/2_1^-$, $5/2_2^-$)
  - Siegert's E1 transition operator
- Parameter Λ of SRG NN interaction chosen to reproduce separation energy: 136 keV (Expt. 137 keV)
- $S_{17}(0)$ = 19.4(7) eV b on the lower side of, but consistent with latest evaluation
- Study of dependence on the HO basis size N_{max} and influence of higher-energy excited states of ^{7}Be used to estimate 0.7 eV b uncertainty on $S_{17}(0)$

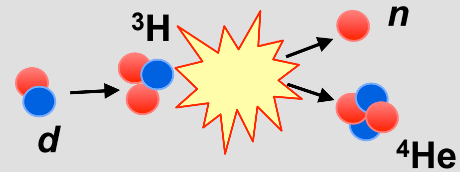
$^{7}Be(p,\gamma)^{8}B$ astrophysical S-factor



Ab initio theory predicts simultaneously both normalization and shape of S_{17}. Inclusion of $5/2_2^-$ state improves S-factor energy dependence above 1.5 MeV.

The $^3H(d,n)^4He$ and $^3He(d,p)^4He$ fusion

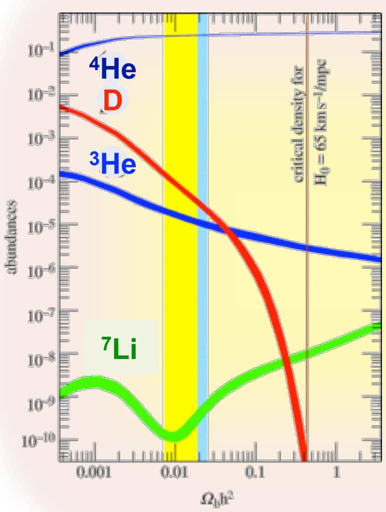
P. Navrátil, S. Quaglioni, PRL 108, 042503 (2012)

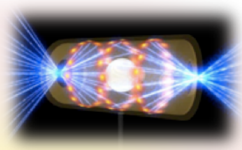


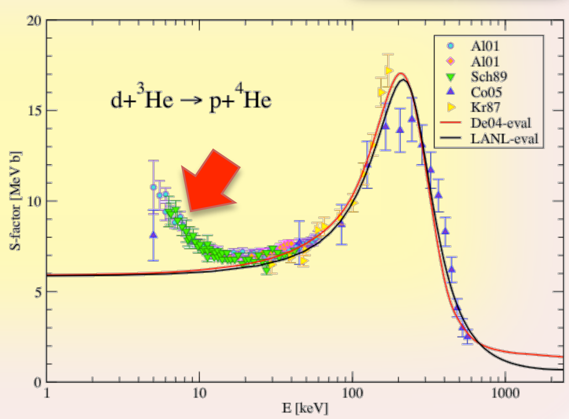
Nuclear astrophysics: Predictions of Big Bang nucleosystesis for light-nucleus abundances

Fusion research and Plasma physics: *d*+T is the easiest fusion to achieve on Earth; $^3H(d,\gamma)^5He$ branch useful for diagnostic, not known well enough

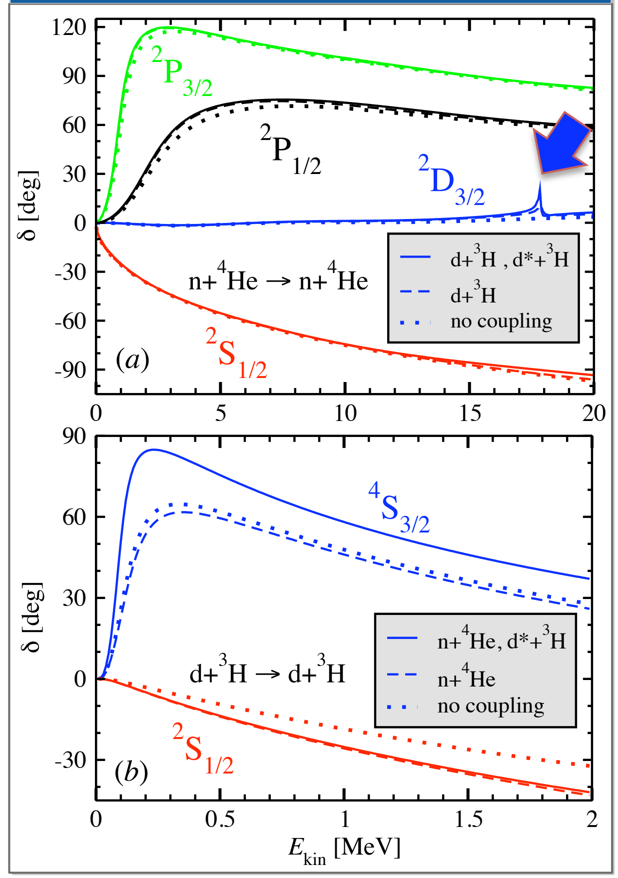
Atomic physics: Considerable electron-screening effects in *d*+^{3}He not completely understood







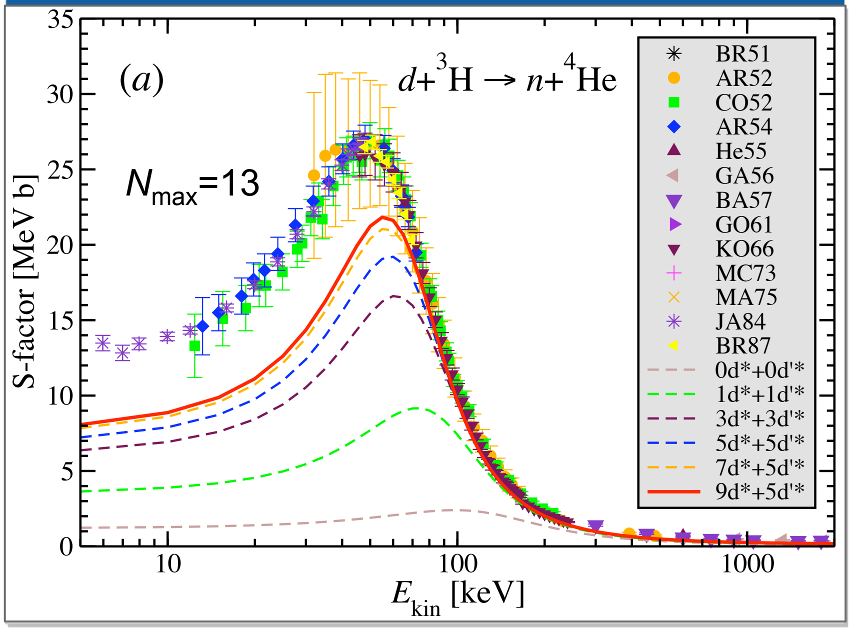
$^4He(n,n)^4He$ & $^3He(d,p)^4He$ elastic phase shifts



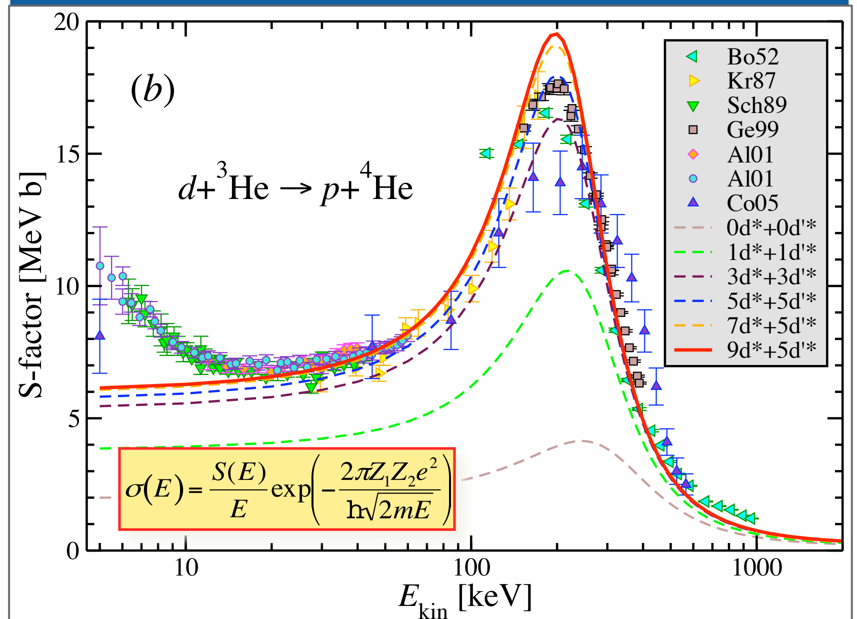
Ab initio many-body calculations of the $^3H(d,n)^4He$ and $^3He(d,p)^4He$ fusion

P. Navrátil, S. Quaglioni,
PRL 108, 042503 (2012)

$^3H(d,n)^4He$ astrophysical S-factor



$^3He(d,p)^4He$ astrophysical S-factor



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

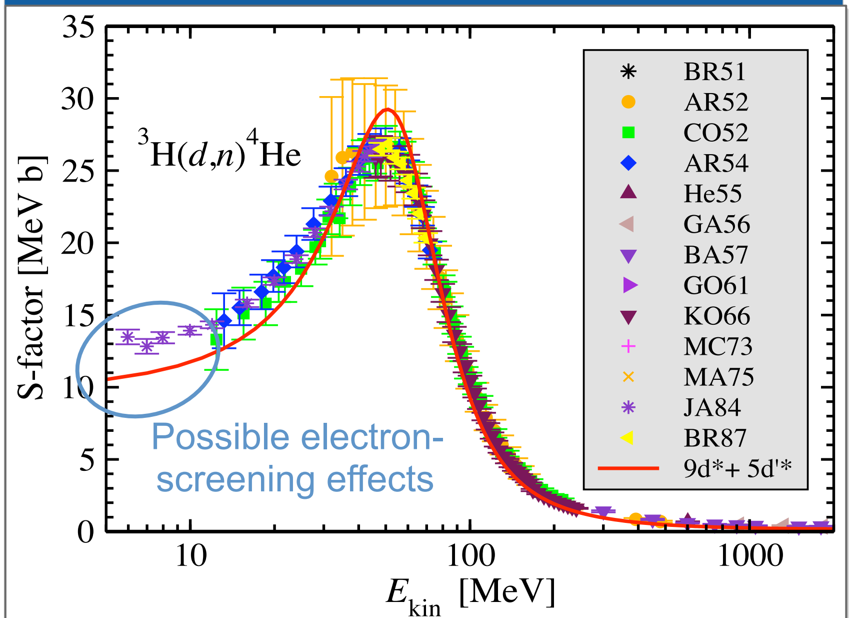
Calculated S-factors improve with the inclusion of the virtual breakup of the deuterium, obtained by means of excited $^3S_1$-$^3D_1$ (d^*) and $^3D_2$ (d'^*) pseudo-states.

NCSM/RGM results for the $^3He(d,p)^4He$ astrophysical S-factor compared to beam-target measurements. Data curve up and deviate from theoretical results at low energy due to laboratory electron-screening.

Ab initio many-body calculations of the ^{3}H(*d*,*n*)^{4}He and ^{3}He(*d*,*p*)^{4}He fusion

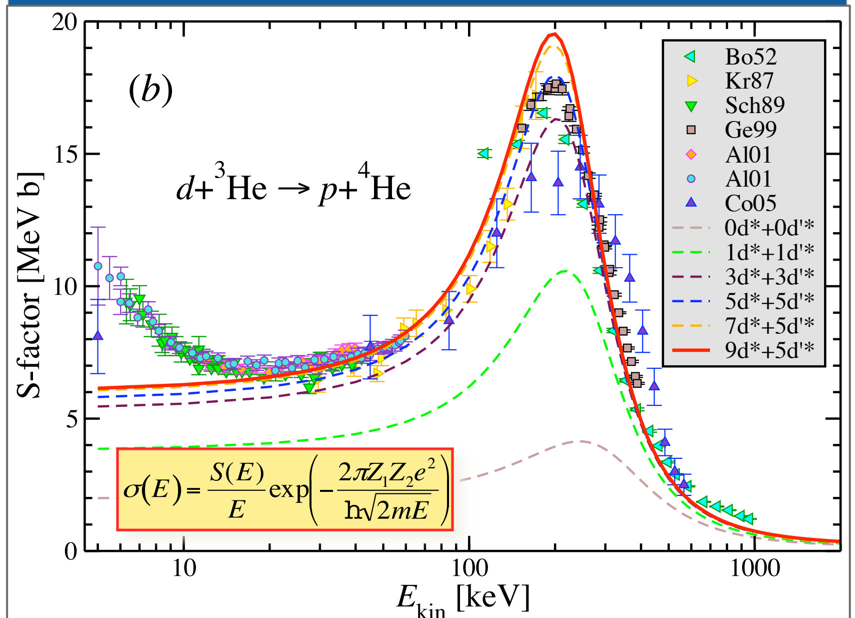
P. Navrátil, S. Quaglioni, PRL 108, 042503 (2012)

^{3}H(*d*,*n*)^{4}He astrophysical S-factor



Changing the evolution parameter λ of the SRG NN interaction from 1.5 to 1.45 fm^{-1} improves agreement with data (expt. Q value reproduced within 0.3%)

^{3}He(*d*,*p*)^{4}He astrophysical S-factor



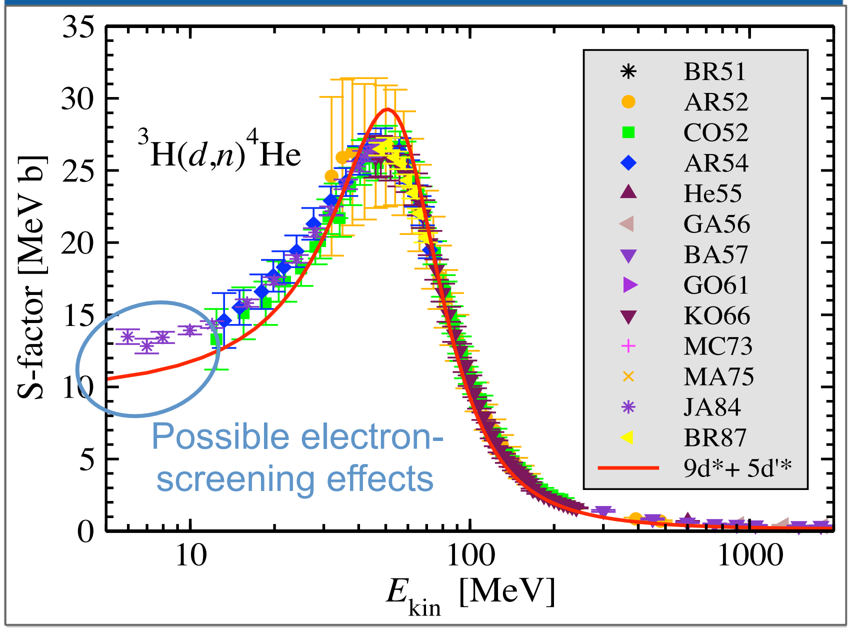
$$\sigma(E) = \frac{S(E)}{E}\exp\left(-\frac{2\pi Z_1 Z_2 e^2}{\hbar\sqrt{2mE}}\right)$$

NCSM/RGM results for the ^{3}He(*d*,*p*)^{4}He astrophysical S-factor compared to beam-target measurements. Data curve up and deviate from theoretical results at low energy due to laboratory electron-screening.

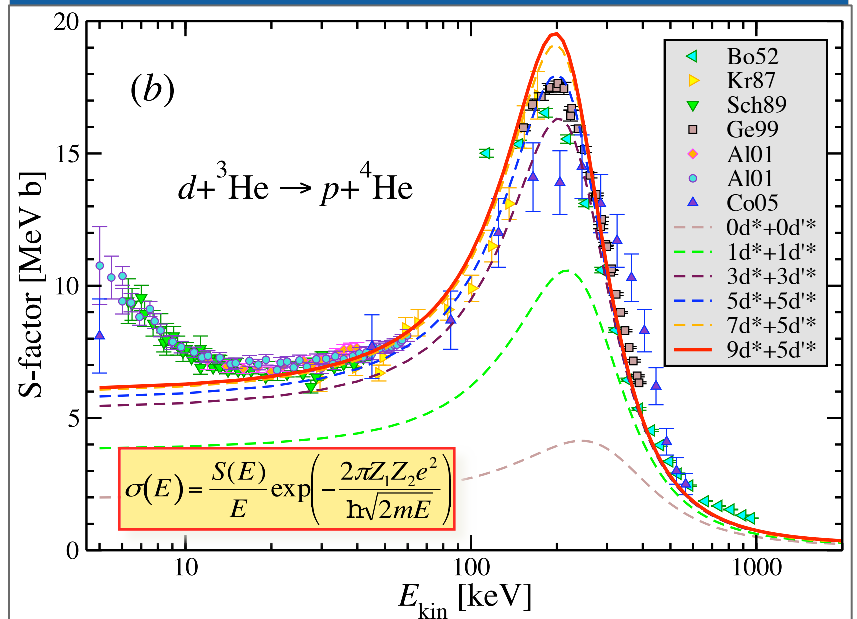
Ab initio many-body calculations of the ^{3}H(*d*,*n*)^{4}He and ^{3}He(*d*,*p*)^{4}He fusion

P. Navrátil, S. Quaglioni,
PRL 108, 042503 (2012)

^{3}H(*d*,*n*)^{4}He astrophysical S-factor



^{3}He(*d*,*p*)^{4}He astrophysical S-factor



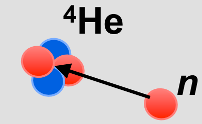
Fundamental description still requires:

1) **NNN force (SRG-induced + "real")**
2) **3-body cluster states & solution of 3-body scattering problem**

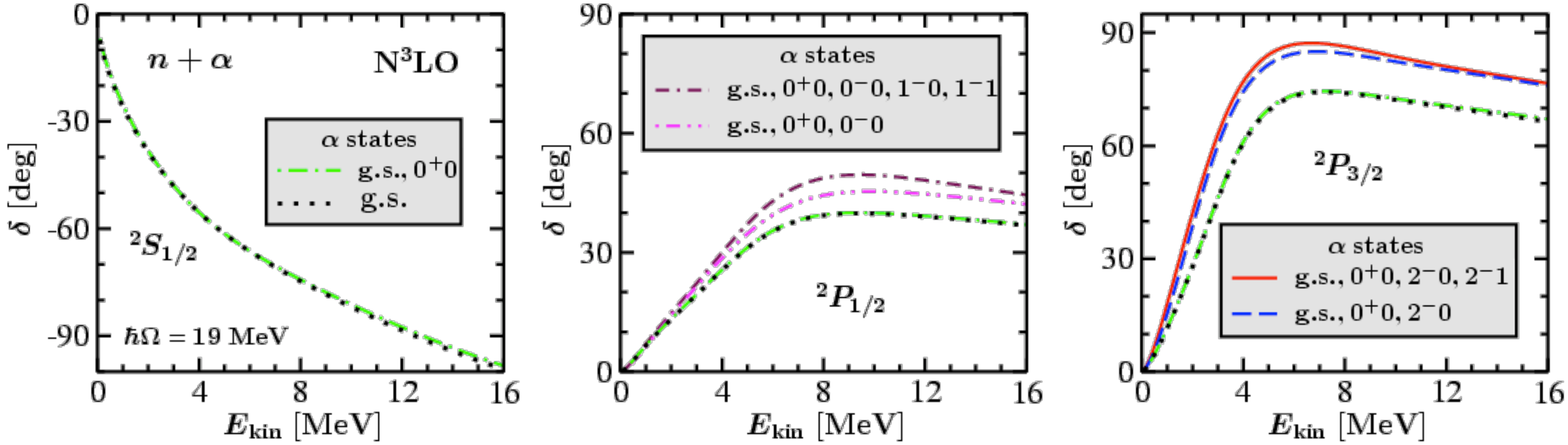
NCSM/RGM results for the ^{3}He(*d*,*p*)^{4}He astrophysical S-factor compared to beam-target measurements. Data curve up and deviate from theoretical results at low energy due to laboratory electron-screening.

Back to where we started: n+^{4}He scattering

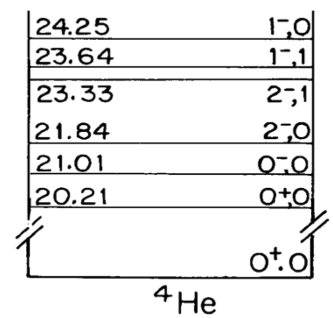
Convergence with respect to RGM model space



- NCSM/RGM calculation with n+^{4}He(ex), N_{max} = 15, $\hbar\Omega$ = 19 MeV
- χEFT N^{3}LO NN potential: convergence reached with two-body effective interaction



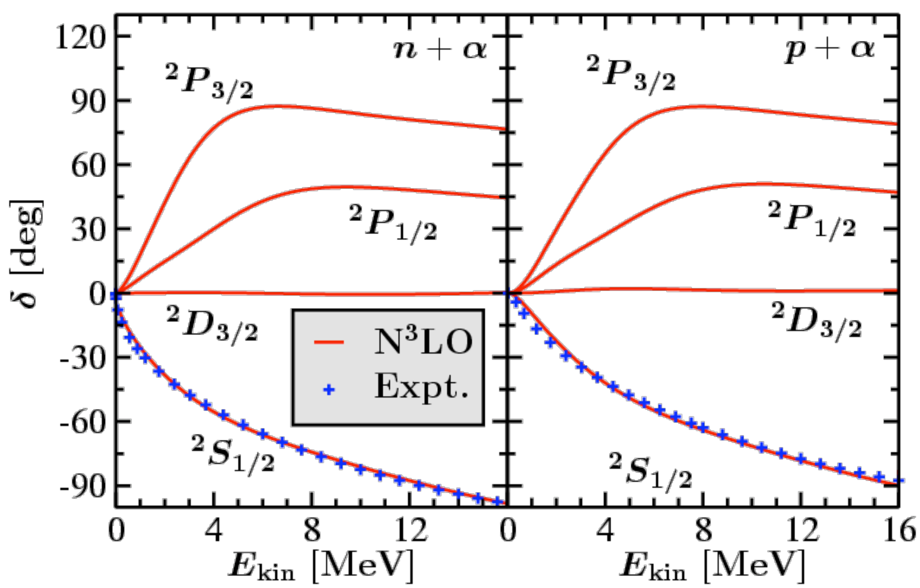
- very mild effects of 0^+0 on $^2S_{1/2}$
- the negative-parity states have larger effects on $^2P_{1/2}$ and $^2P_{3/2}$
    - 0^-0, 1^-0 and 1^-1 affect $^2P_{1/2}$
    - 2^-0 and 2^-1 affect $^2P_{3/2}$

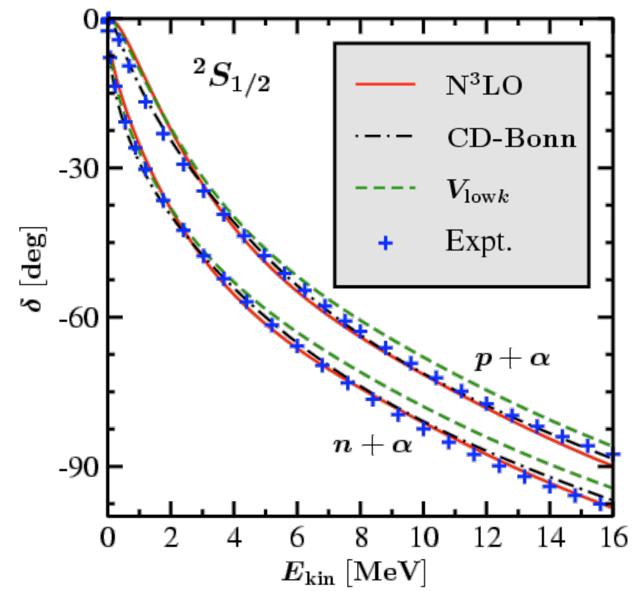


The resonances are sensitive to the inclusion of the first six excited states of ^{4}He

Nucleon-α phase-shifts with χEFT N^{3}LO NN interaction

- NCSM/RGM calculation with N+^{4}He(g.s., 0^+0, 0^-0, 1^-0, 1^-1, 2^-0, 2^-1)
- χEFT N^{3}LO NN potential: convergence with 2-body effective interaction

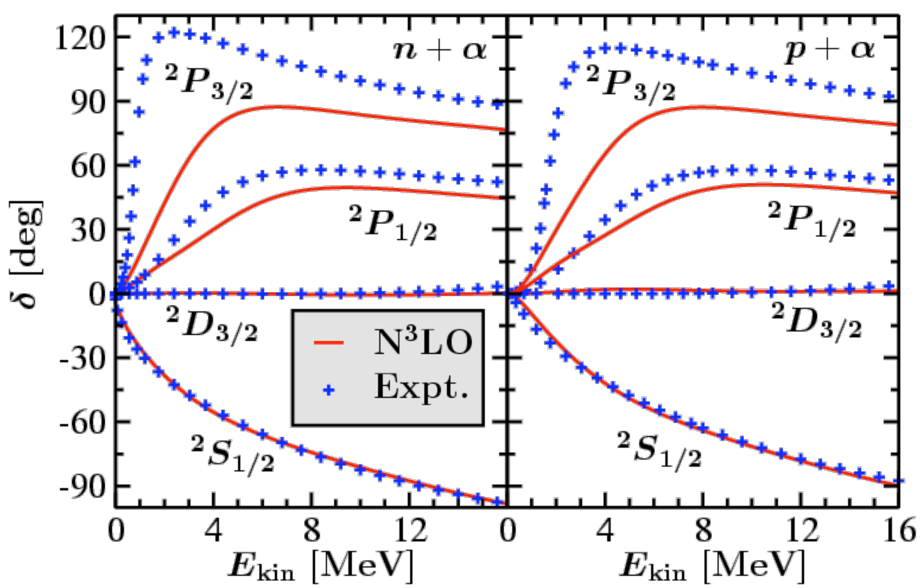


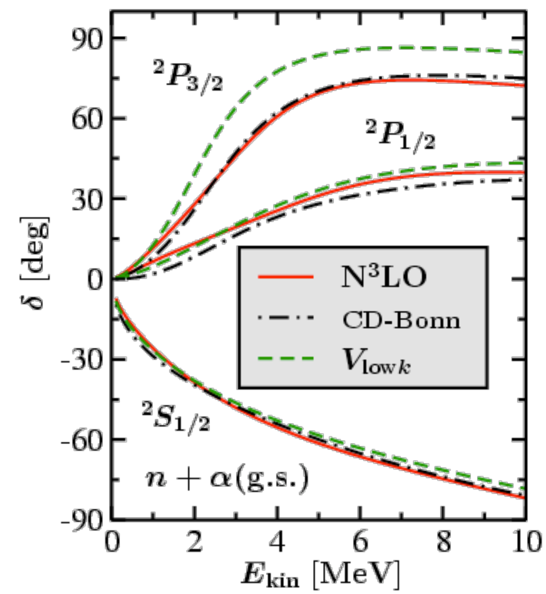


- $^2S_{1/2}$ in agreement with Expt. (dominated by N-α repulsion - Pauli principle)

Nucleon-α phase-shifts with χEFT N^{3}LO NN interaction

- NCSM/RGM calculation with N+^{4}He(g.s., 0^+0, 0^-0, 1^-0, 1^-1, 2^-0, 2^-1)
- χEFT N^{3}LO NN potential: convergence with 2-body effective interaction





- $^2S_{1/2}$ in agreement with Expt. (dominated by N-α repulsion - Pauli principle)
- Insufficient spin-orbit splitting between $^2P_{1/2}$ and $^2P_{3/2}$ (sensitive to interaction)

Including the NNN force into the NCSM/RGM approach

Nucleon-nucleus formalism

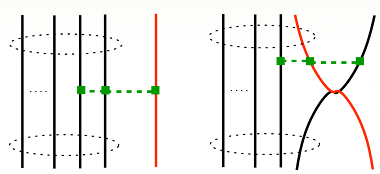
$$\left\langle \Phi^{J^\pi T}_{\nu' r'} \right| \hat{A}_{\nu'} V^{NNN} \hat{A}_{\nu} \left| \Phi^{J^\pi T}_{\nu r} \right\rangle = \left\langle (A-1) \;\; r' \;\; (a'=1) \right| V^{NNN}\left(1-\sum_{i=1}^{A-1}\hat{P}_{iA}\right) \left| (a=1) \;\; r \;\; (A-1) \right\rangle$$

$$\mathcal{V}^{NNN}_{\nu'\nu}(r,r') = \sum R_{n'l'}(r') R_{nl}(r) \left[\frac{(A-1)(A-2)}{2} \langle \Phi^{J^\pi T}_{\nu' n'} | V_{A-2A-1A}(1-2P_{A-1A}) | \Phi^{J^\pi T}_{\nu n} \rangle \right.$$

$$\left. -- \frac{(A-1)(A-2)(A-3)}{2} \langle \Phi^{J^\pi T}_{\nu' n'} | P_{A-1A} V_{A-3A-2A-1} | \Phi^{J^\pi T}_{\nu n} \rangle \right] .$$

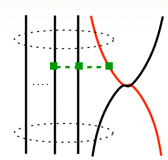
Direct potential: in the model space (interaction is localized!)

Exchange potential: in the model space (interaction is localized!)



(a) (b)

$$\propto {}_{SD}\left\langle \psi^{(A-1)}_{\alpha_1'} \right| a_i^+ a_j^+ a_l a_k \left| \psi^{(A-1)}_{\alpha_1} \right\rangle_{SD}$$



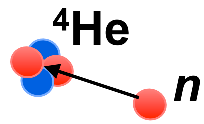
(c)

$$\propto {}_{SD}\left\langle \psi^{(A-1)}_{\alpha_1'} \right| a_h^+ a_i^+ a_j^+ a_m a_l a_k \left| \psi^{(A-1)}_{\alpha_1} \right\rangle_{SD}$$

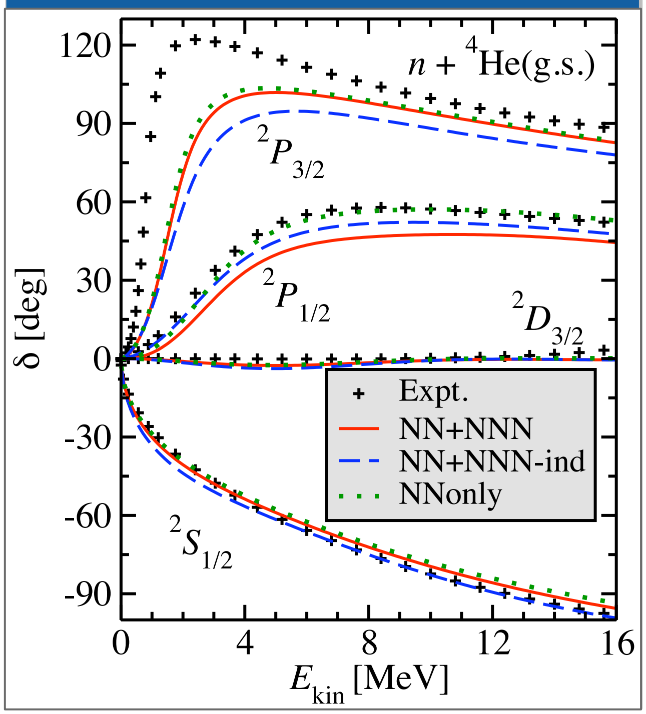
^{4}He(n,n)^{4}He with SRG-evolved N^{3}LO NN + N^{2}LO NNN

G. Hupin, J. Langhammer, S. Quaglioni, P. Navratil, R. Roth, work in progress

- n+^{4}He(g.s.), N_{max}=13, $\hbar\Omega$ = 20 MeV
- SRG-(N^{3}LO NN +N^{2}LO NNN) potential with λ = 2 fm^{-1}

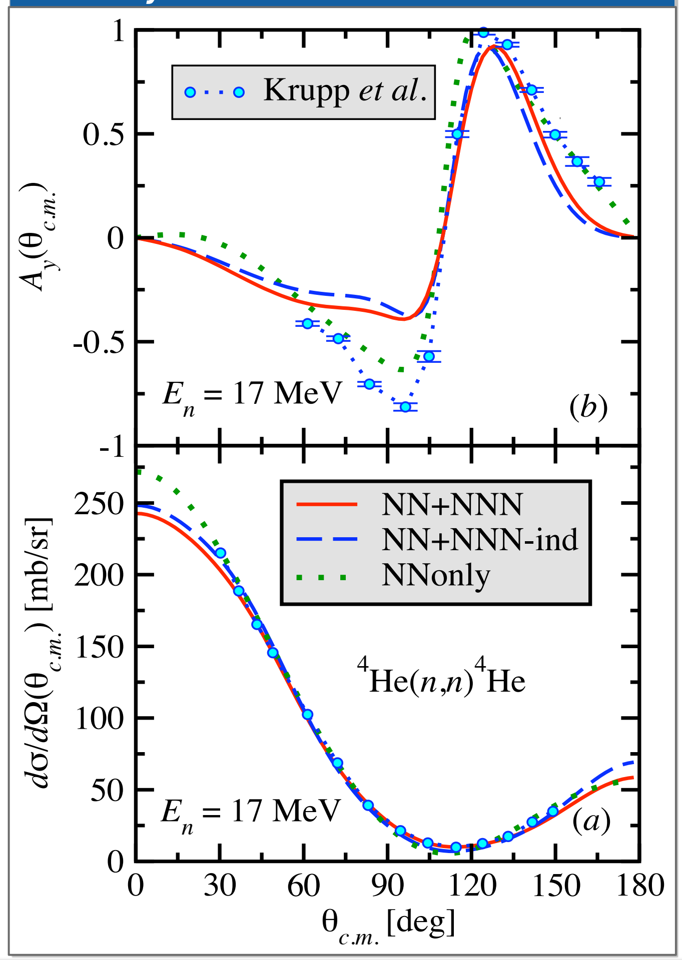


Phase shifts



Still missing: excited states of ^{4}He

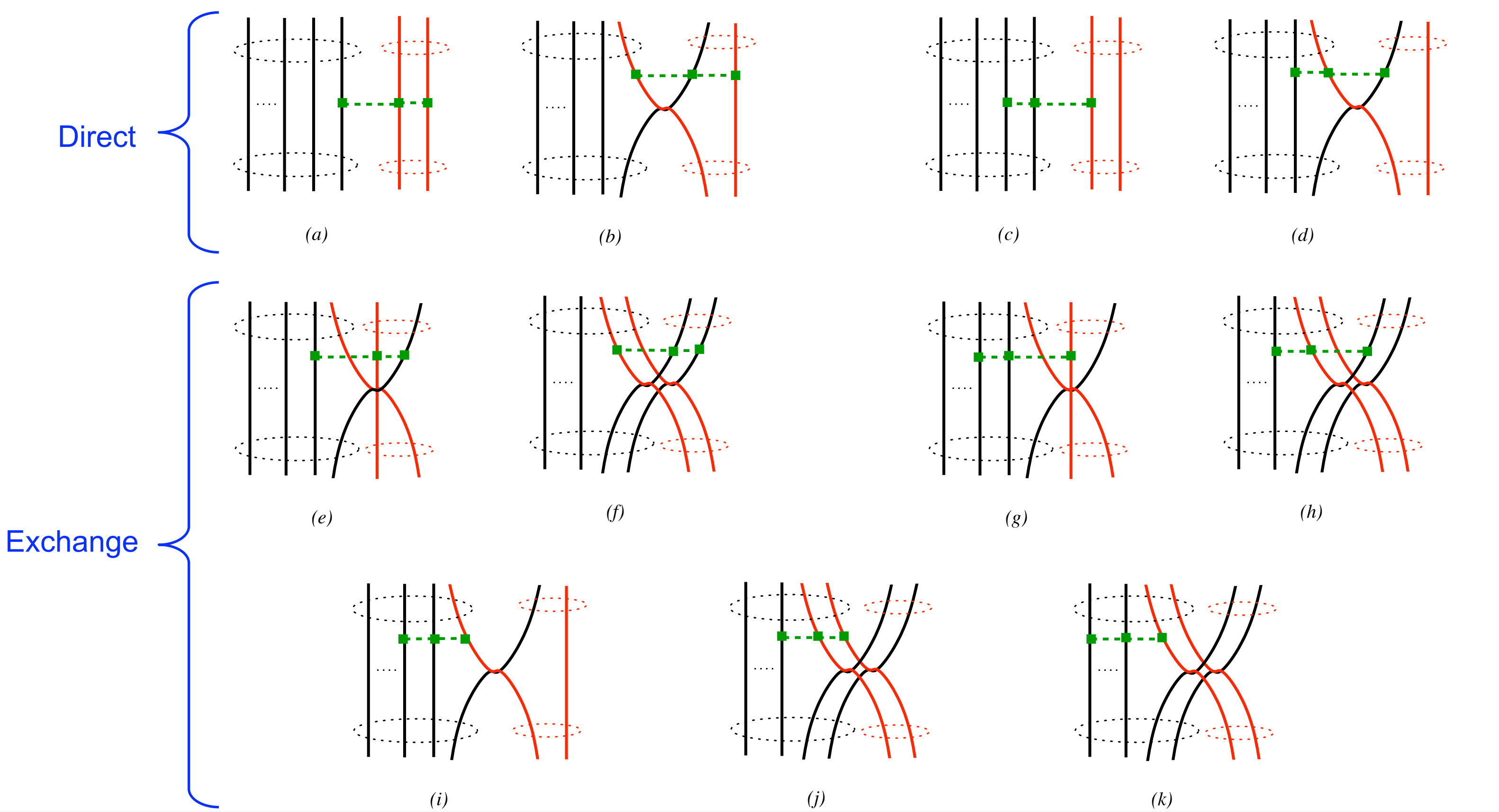
A_y and cross section



Including the NNN force into the NCSM/RGM approach

Deuteron-nucleus formalism

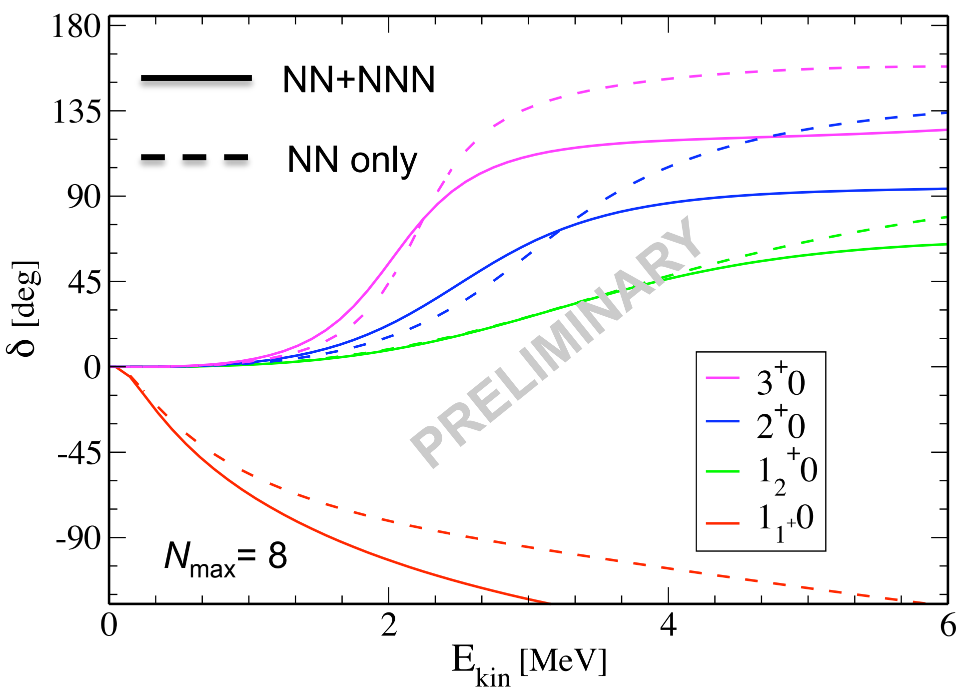
$$\left\langle \Phi^{J^\pi T}_{\nu' r'} \right| \hat{A}_{\nu'} V^{NNN} \hat{A}_{\nu} \left| \Phi^{J^\pi T}_{\nu r} \right\rangle = \left\langle \begin{matrix}(A-2)\\ r' \\ (a'=2)\end{matrix} \right| V^{NNN} \left(1 - \sum_{i=1}^{A-2} \sum_{k=A-1}^{A} \hat{P}_{i,k} + \sum_{i<j=1}^{A-2} \hat{P}_{i,A-1} \hat{P}_{j,A} \right) \left| \begin{matrix}(A-2)\\ r \\ (a=2)\end{matrix} \right\rangle$$



^{4}He(d,d)^{4}He with SRG-evolved chiral NN+NNN force

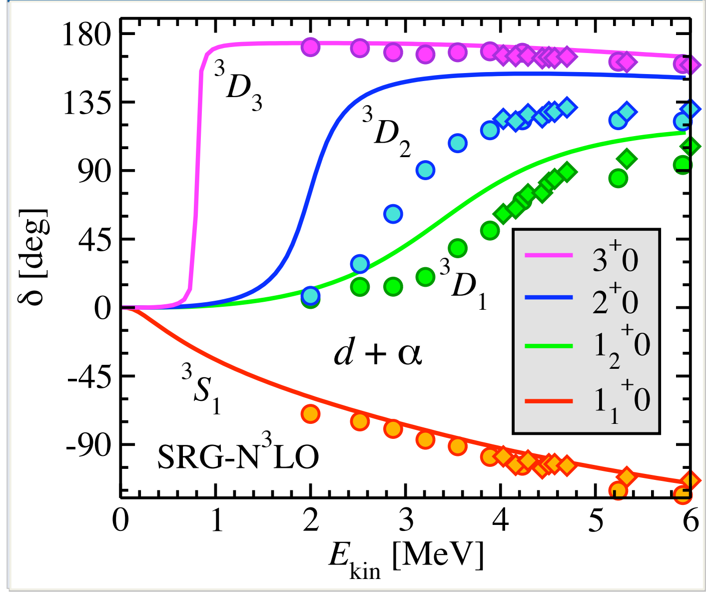
G. Hupin, S. Quaglioni, P. Navratil, work in progress

Phase shifts with λ = 2 fm^{-1}



Here:
d(g.s.) + ^{4}He(g.s.) scattering phase shifts for
SRG-(chiral NN+NNN) potential with (λ=2 fm^{-1}).

Phase shifts with λ = 1.5 fm^{-1}



Here: N_{max}= 12
d(g.s., $^3S_1$-$^3D_1$, $^3D_2$, $^3D_3$-$^3G_3$) + ^{4}He(g.s.)
SRG-N^{3}LO NN potential (λ=1.5 fm^{-1})

Preliminary results in a small model space and with only d and 4He g.s., look promising

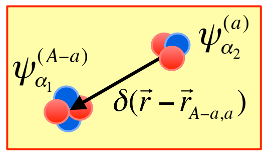
Extended *ab initio* NCSM/RGM Formalism

Three-body cluster dynamics

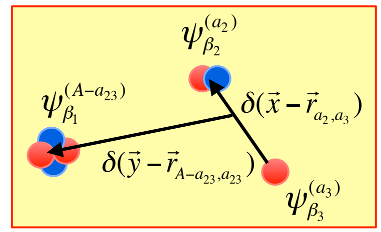
- Starts from:

$$\Psi^{(A)}_{RGM} = \sum_{\nu_2} \int g_{\nu_2}(\vec{r}\,)\hat{A}_{\nu_2} \left|\phi_{\nu_2 \vec{r}}\right\rangle d\vec{r} + \sum_{\nu_3} \iint G_{\nu_3}(\vec{x},\vec{y})\ \hat{A}_{\nu_3} \left|\Phi_{\nu_3 \vec{x}\vec{y}}\right\rangle d\vec{x}d\vec{y}$$

2-body channels



plus

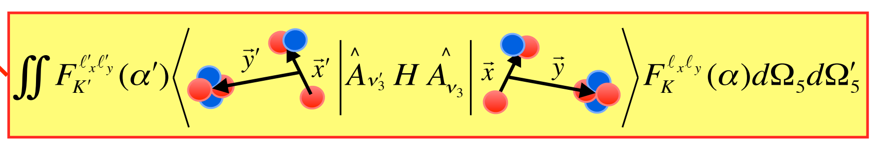


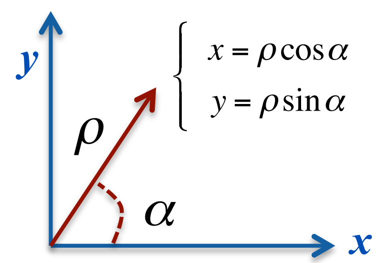
3-body channels

- 3-body dynamics within Hyperspherical Harmonics: **x,y** → **ρ, Ω_5={α, Ω_x, Ω_y}**

$$\sum_{\nu K} \int d\rho\ \rho^5 \left[H^{K',K}_{\nu',\nu}(\rho',\rho) - E\ N^{K',K}_{\nu',\nu}(\rho',\rho)\right]\ \rho^{-5/2} \chi_{\nu K}(\rho) = 0$$

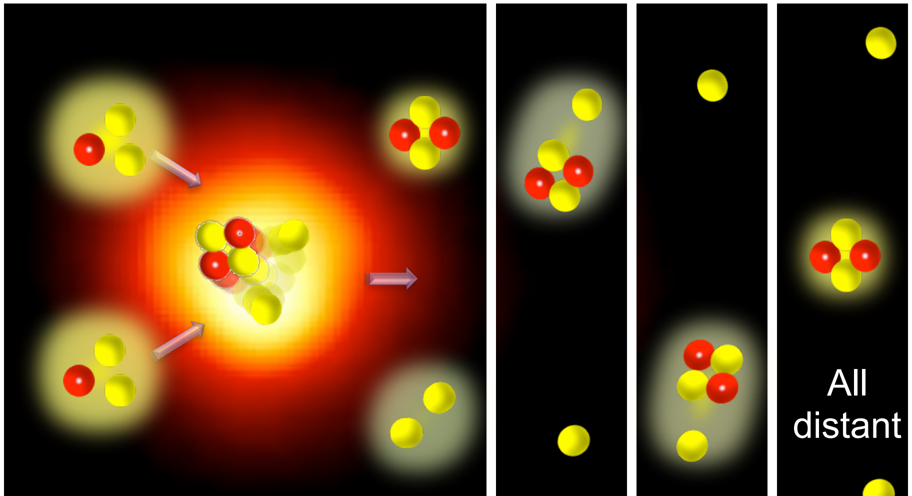
Hamiltonian kernel **Norm (overlap) kernel**





Towards ^{3}H(^{3}H,2n)^{4}He and ^{3}He(^{3}He,2p)^{4}He

Three-body breakup reactions



An artist's impression of the ^{3}H+^{3}H fusion reaction.

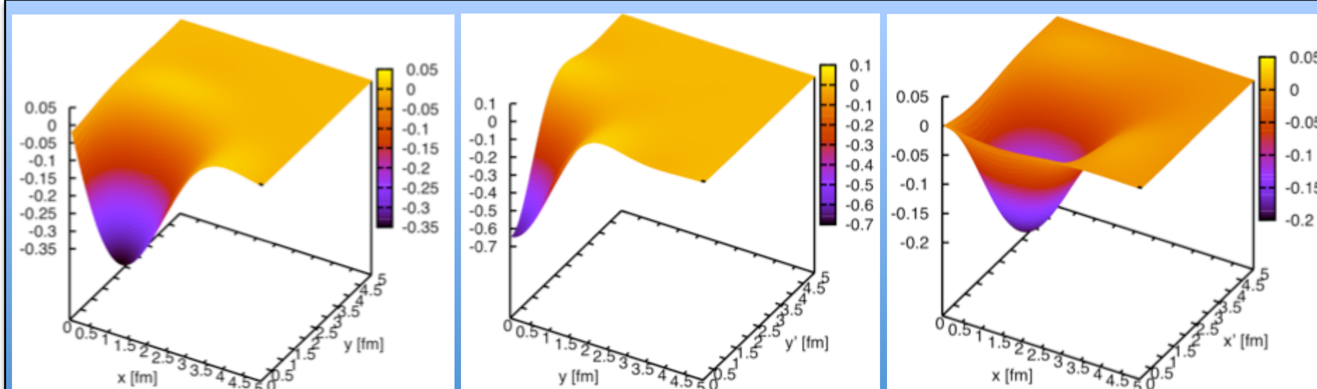
The ^{3}H+^{3}H fusion is often studied with the help of a sequential decay model:

^{3}H+^{3}H→ 2n+^{4}He, Q=11.3 MeV

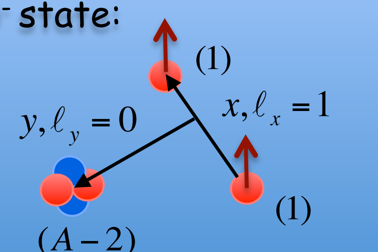
^{3}H+^{3}H→ n+^{5}He(g.s.), Q=10.4 MeV

^{3}H+^{3}H→ n+^{5}He(e.s.), Q=9.2 MeV

All (two-body breakup mechanisms included) are a manifestation of the three-body continuum



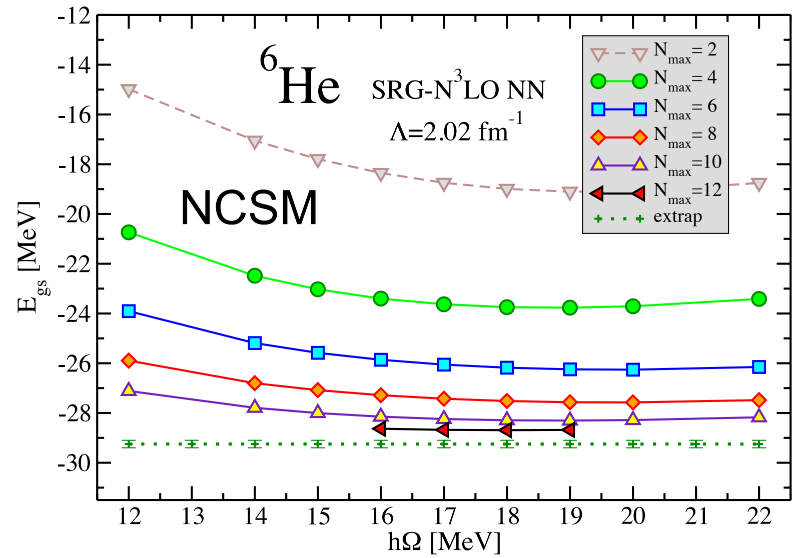
Matrix element $\langle \hat{A}^2 - 1 \rangle$ over three-cluster 0^- state:



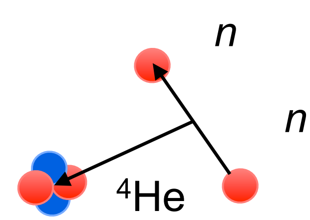
First results for ^{6}He ground state

S. Quaglioni, C. Romero-Redondo, P. Navratil, work in progress

- Preliminary NCSM/RGM results
  - n+n+^{4}He(g.s.), N_{max} = 12, $\hbar\Omega$ = 16 MeV
  - SRG-N^{3}LO NN with λ = 1.5 fm^{-1}
- Comparison with NCSM:
  - ~1 MeV difference in binding energy due to excitations of ^{4}He core, at present included only in NCSM
  - Contrary to NCSM, NCSM/RGM ^{4}He+n+n w.f. has appropriate asymptotic behavior
    - Essential to describe ^{6}He excited states in the continuum (*e.g.*, 1$^-$ soft dipole resonance)

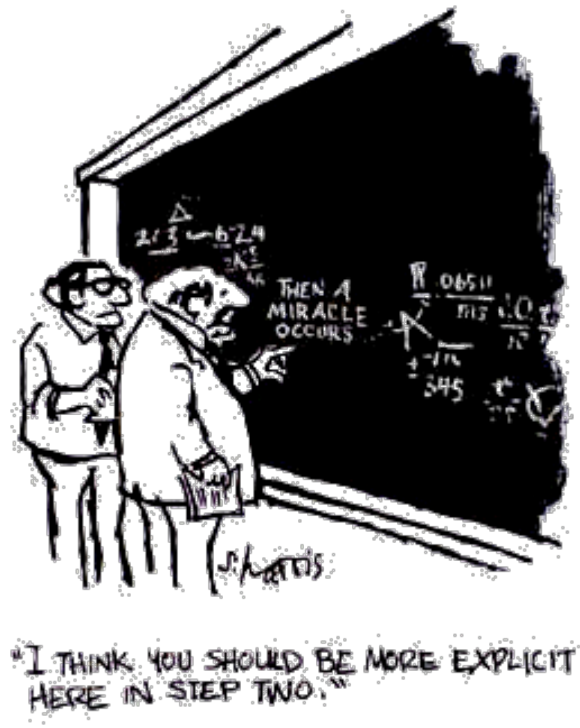


HO model space	$E_{g.s.}$ (^{4}He) (NCSM)	$E_{g.s.}$ (^{6}He) (NCSM)	$E_{g.s.}$ (^{6}He) (NCSM/RGM) PRELIMINARY
N_{max} = 12	-28.22 MeV	-29.75 MeV	-28.72 MeV



Conclusions and Outlook

- With the NCSM/RGM approach we are extending the *ab initio* effort to describe low-energy reactions and weakly-bound systems
- Ability to describe:
  - Nucleon-nucleus collisions
  - Deuterium-nucleus collisions
  - (d,N) transfer reactions
  - ^{3}H- and ^{3}He-nucleus collisions
- Recent results with SRG-N^{3}LO NN pot.:
  - ^{3}H(n,n)^{3}H, ^{4}He(d,d)^{4}He, ^{3}H(d,n)^{4}He, ^{3}He(d,p)^{4}He, ^{7}Be(p,γ)^{8}B



- Work in progress
  - Inclusion of NNN force in N-nucleus and d-nucleus formalism
  - Three-cluster NCSM/RGM and treatment of three-body continuum:
    - First results for ^{6}He ground state within ^{4}He+n+n cluster basis
  - Initial results for ^{3}He-^{4}He scattering
  - …