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Microscopic nuclear reactions starting from the *ab initio* no-core shell model

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Nuclear Many-Body Approaches for the 21st Century

INT, Seattle, November 6, 2007

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Outline of the talk

- Our goal: *ab initio* approach to light-ions reactions
- Introduction to *ab initio* no-core shell model (NCSM)
- How do we tackle reactions? Well, that depends ...
  - The Lorentz integral transform (LIT) method
- Application of chiral effective field theory (χEFT) two- (NN) and three-nucleon (NNN) forces to the ^{4}He + $\gamma \rightarrow$ X reaction
- ^{4}He + $\gamma \rightarrow$ X reaction with χEFT NN+NNN - Conclusions
- Can we cover a wider range of nuclear reactions?
  - The resonating-group method (RGM)
- Application to *n*-^{4}He scattering
  - low-momentum V_{lowk} NN potential (bare interaction)
  - χEFT NN potential (two-body effective interaction)
- Conclusions and Outlook

Our goal: *ab initio** approach to light-ions reactions

* *non-relativistic QM, point-like nucleons, realistic NN + NNN forces*

- Why low-energy light-ion reactions?
  - underlying physics of stellar evolution
  - potential energy sources
  - rich “test-ground” for nuclear force models:
    - study NNN force effect in observables not used to fix the interaction parameters

- Why *ab initio*?
  - Provide accurate theoretical cross sections for experiments where measurements are controversial, very difficult, impossible
  - provide insight on the role of NNN interactions

- Why no-core shell model (NCSM) and low-energy reactions?
  - is a successful *ab initio* approach to nuclear structure (essential ingredient for low-energy reactions!)
  - covers nuclei beyond the *s*-shell
  - is the only method capable of employing the new chiral effective field theory (χEFT) NN + NNN potential for $A>4$

Introduction to *ab initio* NCSM

- The NCSM looks for the eigenstates of the *A*-body Hamiltonian in the form of expansions over a complete set of harmonic oscillator (HO) basis states
  - *A*-nucleon HO basis states
  - complete $N_{max}\hbar\Omega$ model space
    - excitations up to $N_{max}\hbar\Omega$ above minimum configuration energy
- Why use an HO basis?
  - Flexibility:
    - Jacobi relative coordinates
    - Cartesian single-particle coordinates
    - take advantage of second quantization shell model technique
  - Translational invariance:
    - preserved even using single-particle coordinates Slater-determinant (SD) basis (only with HO basis in a complete $N_{max}\hbar\Omega$ model space)
  - Downside:
    - Gaussian asymptotic behavior

The convergence to the exact results with increasing N_{max} is accelerated by the use of an effective interaction, which follows a unitary transformation approach

Effective interaction

	P	Q
P	H_{eff}	0
Q	0	$QXHX^{-1}Q$

	P_n	Q_n
P_n	H^n_{eff}	0
Q_n	0	$Q_n X_n H X_n^{-1} Q_n$

$2 \leq n \leq A$

- Introduce a Lee-Suzuki unitary transformation X
- $QXHX^{-1}P = 0$ *or* $PXHX^{-1}Q = 0$
- $H \rightarrow H_{eff} = PXHX^{-1}P$
- H_{eff} is an A-body operator

- Make an n-body cluster approximation ($2 \leq n \leq A$)
- solve n-body problem
- find H^n_{eff}
- in the A-body problem use

$$V_{eff} = H^n_{eff} - h_1 - h_2 \ldots - h_n$$

Two ways of reaching convergence: in a given cluster approximation by increasing the model-space size: for $P \rightarrow 1$, $H^n_{eff} \rightarrow H$; in a given model space by increasing the cluster size: for $n \rightarrow A$ and fixed P, $H^n_{eff} \rightarrow H_{eff}$

How do we tackle reactions? Well, that depends ...

- The NCSM is a bound-state technique:
  - is it possible to calculate reaction observables using expansions over localized many-body basis states?

$$R(\omega) = \sum\!\!\!\!\!\!\int_{\nu} |\langle \Psi_\nu | \hat{O} | \Psi_0 \rangle|^2 \delta(E_\nu - E_0 - \omega)$$

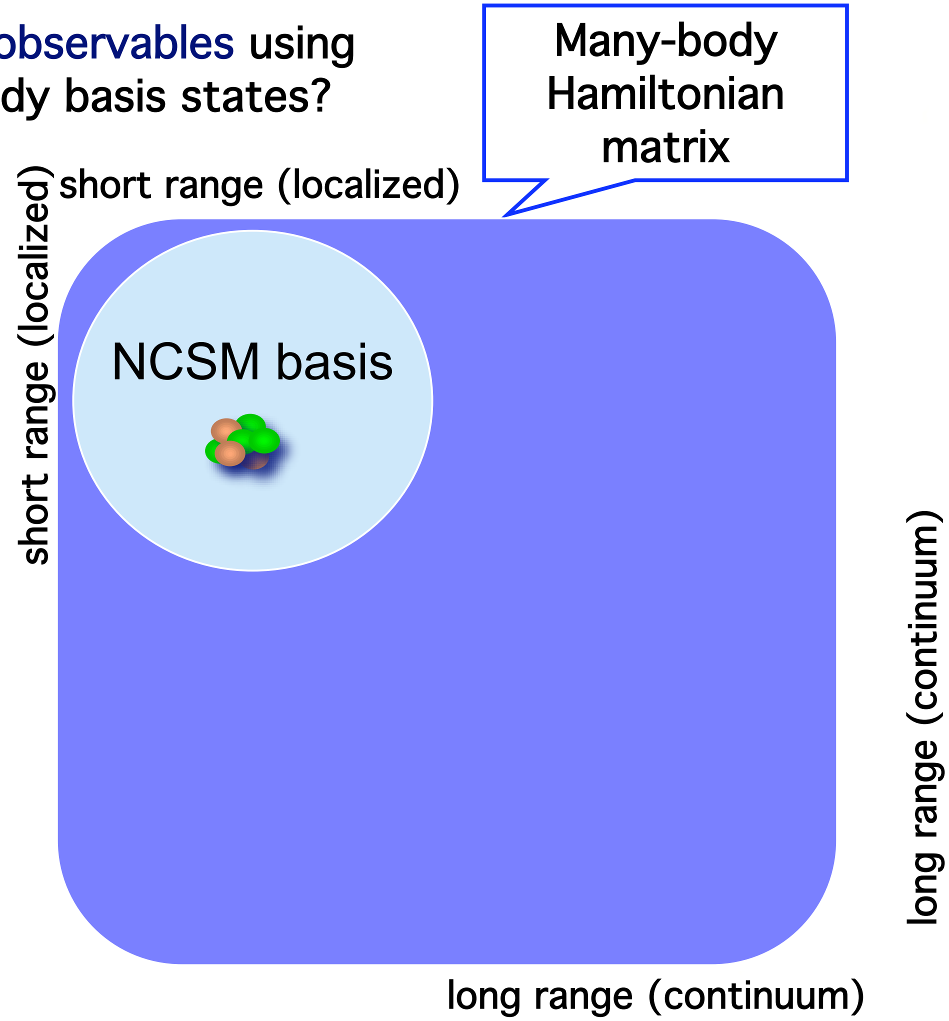
$$L(\sigma_R, \sigma_I) = \int d\omega \frac{R(\omega)}{(\omega - \sigma_R)^2 + \sigma_I^2} = \langle \tilde{\Psi} | \tilde{\Psi} \rangle$$

$$(H - E_0 - \sigma_R + i\sigma_I)|\tilde{\Psi}\rangle = \hat{O}|\Psi_0\rangle$$

$$\sigma_I \neq 0 \quad \& \quad \langle \Psi_0 | \hat{O}^\dagger \hat{O} | \Psi_0 \rangle < \infty$$

Lorentz integral transform (LIT) method

Efros *et al.*, PLB338(1994)130



The LIT method is a microscopic approach to perturbation-induced reactions (also exclusive!). The continuum problem is mapped onto a bound-state-like problem.

Application of χEFT NN and NNN forces to ^{4}He + $\gamma \rightarrow$ X

- Chiral effective filed theory (χEFT) represents our best opportunity to reach a consistent picture of the interaction among nucleons, that is based on the underlying and fundamental theory of QCD.

- χEFT provides a framework for expanding and qualifying the inter-nucleon interactions. At a given order, the interaction contains a set of low-energy constants (LECs), that need to be determined.

- It is a challenge and a necessity to apply χEFT forces to nuclei working in an *ab initio* framework.

- In a recent study the χEFT NN + NNN interactions have been applied to the calculation of various properties from *s*- to mid-*p*-shell nuclei using the NCSM
  - preferred choice for the two NNN LECs

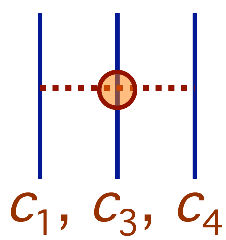
- We have applied the same χEFT NN + NNN interactions in the continuum of the four-nucleon system
  - *ab initio* calculation of the ^{4}He total photo-absorption cross section using the LIT method in the NCSM approach

$$\sigma_\gamma(\omega) = 4\pi^2 \frac{e^2}{\hbar c} \omega R(\omega) \,, \quad R(\omega) = \sum\!\!\!\!\!\!\int_\nu |\langle \Psi_\nu | \hat{D}_z | \Psi_0 \rangle|^2 \delta(E_\nu - E_0 - \omega)$$

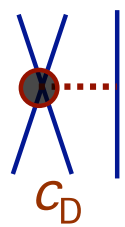
χEFT NN + NNN interactions

- A high precision fit to NN data is reached at order N^{3}LO in the chiral expansion
  - we use the N^{3}LO NN potential by Entem and Machleidt
- The strengths of the NNN interaction are determined by the NN couplings, with the exception of two LECs, c_E and c_D

N^{2}LO

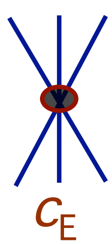


→ Two-pion exchange: c_1, c_3 and c_4 LECs appear in the chiral NN interaction
➔ determined in the A = 2 system



→ One-pion-exchange-contact: c_D is a new LEC

New!



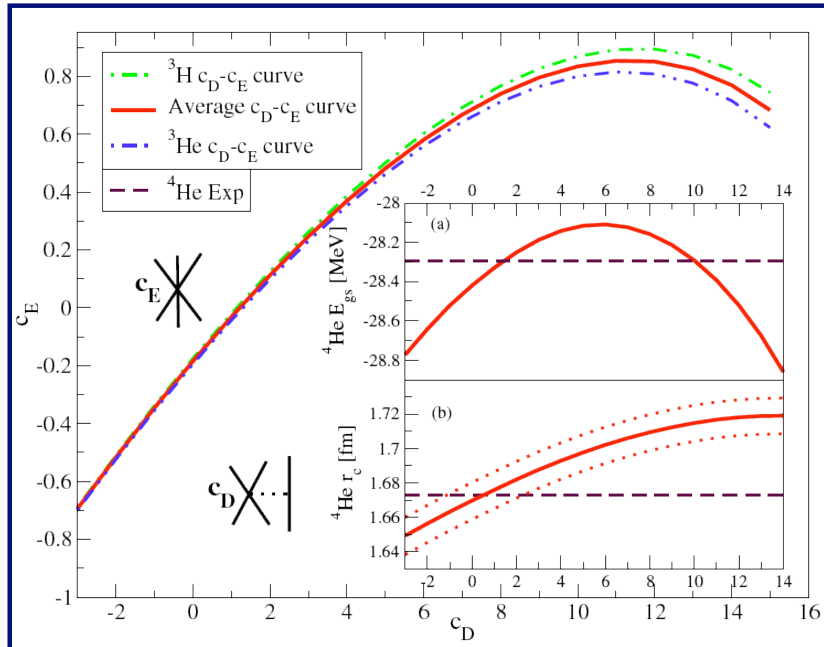
→ Contact: c_E is a new LEC

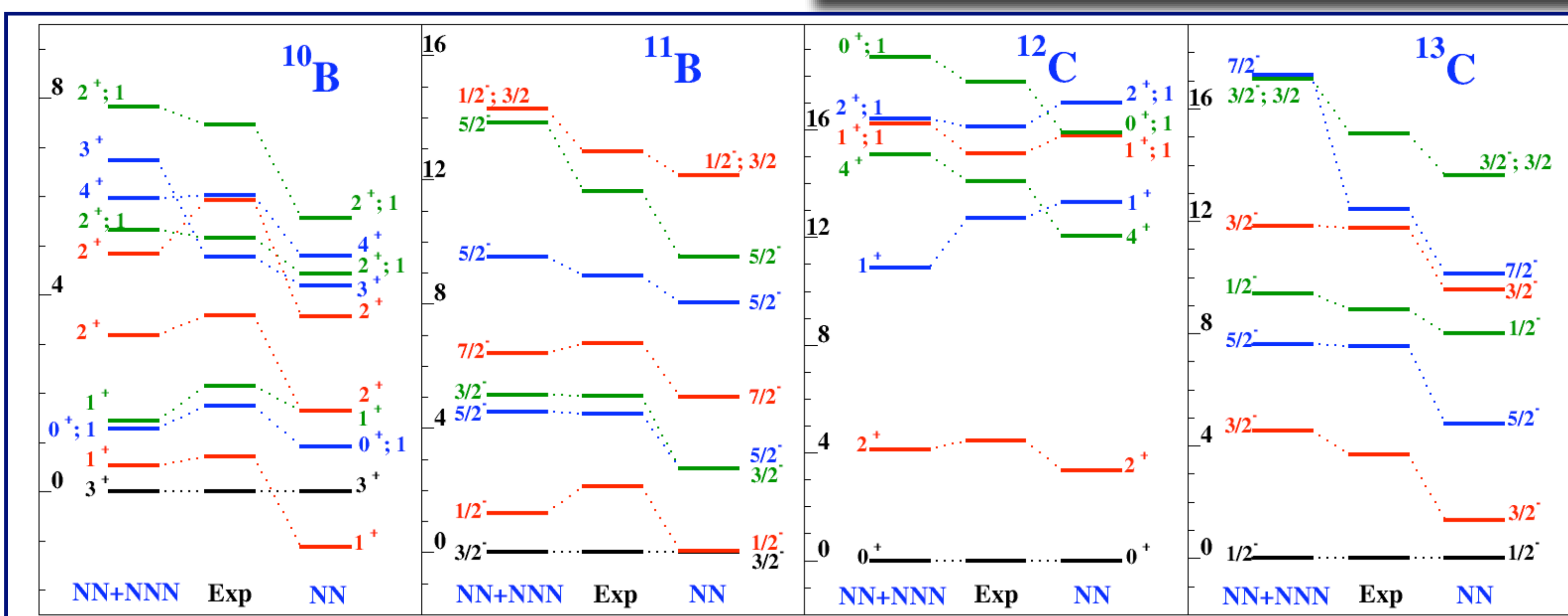
New!

Must be determined in A ≥ 3 system

Ab initio NCSM calculations with χEFT NN + NNN

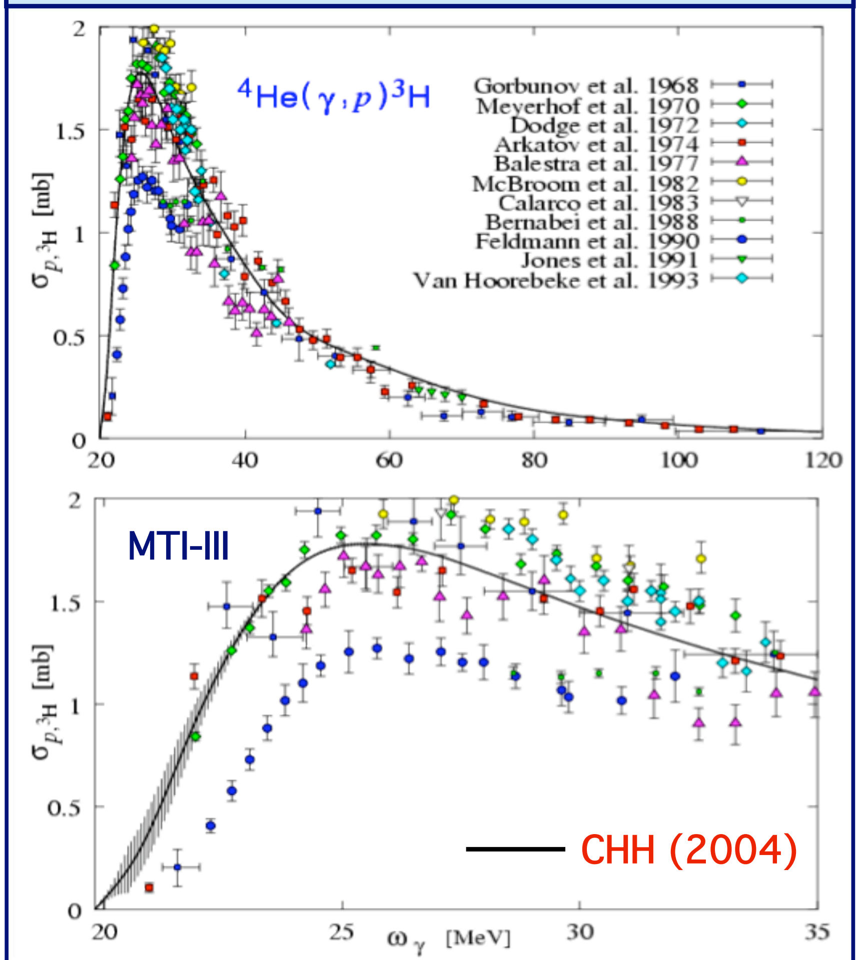
- Investigation of A = 3, ^{4}He and *p*-shell nuclei
- Globally the best results with c_D ~ -1
- NNN interaction essential to describe the structure of light nuclei
- See: P.Navratil *et al.*, Phys. Rev. Lett. 99, 042501 (2007)



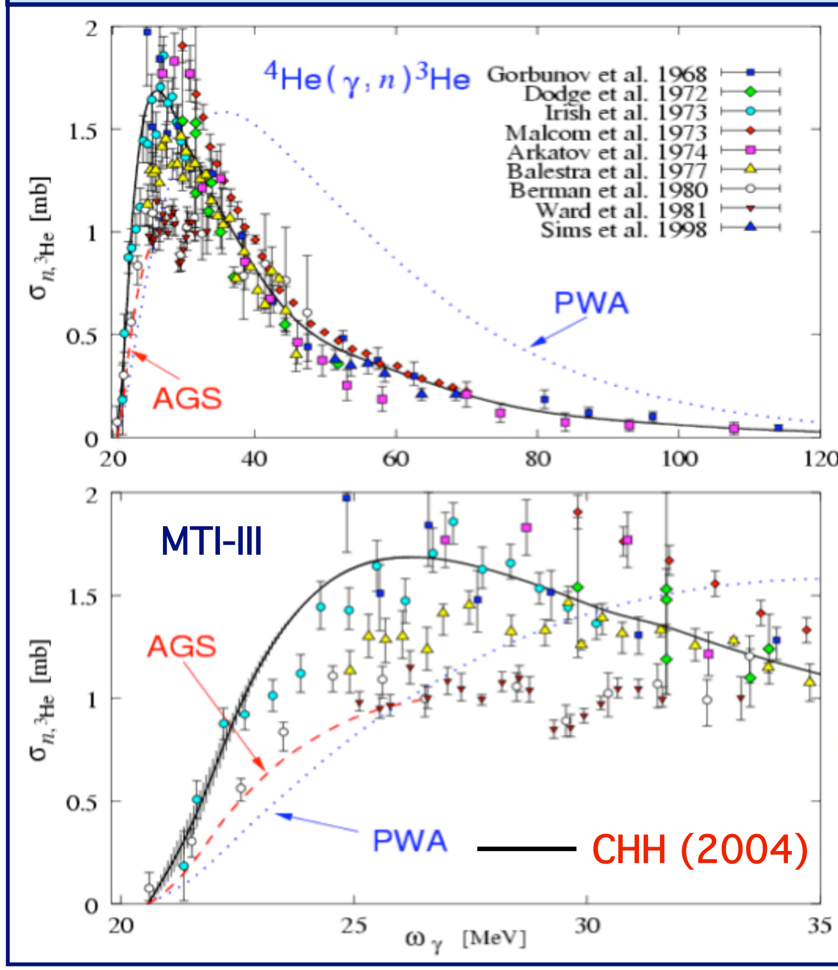


^{4}He photo-disintegration: a history of discrepancies

The ^{4}He(γ,p)^{3}H disintegration channel



The ^{4}He(γ,n)^{3}He disintegration channel

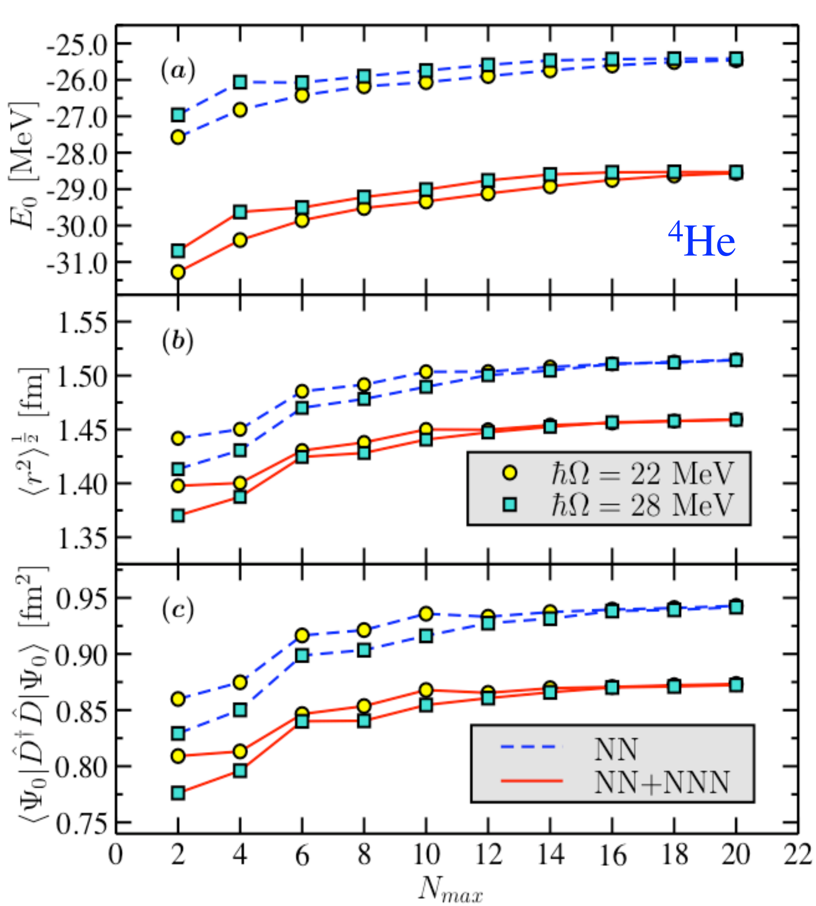


Large discrepancies between different experimental data. Early calculations with semi-realistic NN interactions show better agreement with high-peaked experiment.
Can the χEFT NN + NNN interaction explain the low-lying data?

Ab initio NCSM calculation of the ^{4}He ground state

- χEFT NN + NNN interaction: convergence reached with three-body effective interaction

^{4}He ground-state convergence



- χEFT NN and NN + NNN:
  - similar patterns
  - accurate convergence

	E_0 [MeV]	$\langle r_p^2 \rangle^{1/2}$ [fm]	$\langle \Psi_0 \vert \hat{D}^\dagger \hat{D} \vert \Psi_0 \rangle$ [fm^2]
NN	−25.39(1)	1.515(2)	0.943(1)
NN + NNN	−28.60(3)	1.458(2)	0.868(1)
Expt.	−28.296	1.455(7)*	–
NN (HH)	−25.38	1.516	–
NN (FY)	−25.37	–	–

- NNN effects:
  - more binding
  - reduced size
  - reduced dipole strength

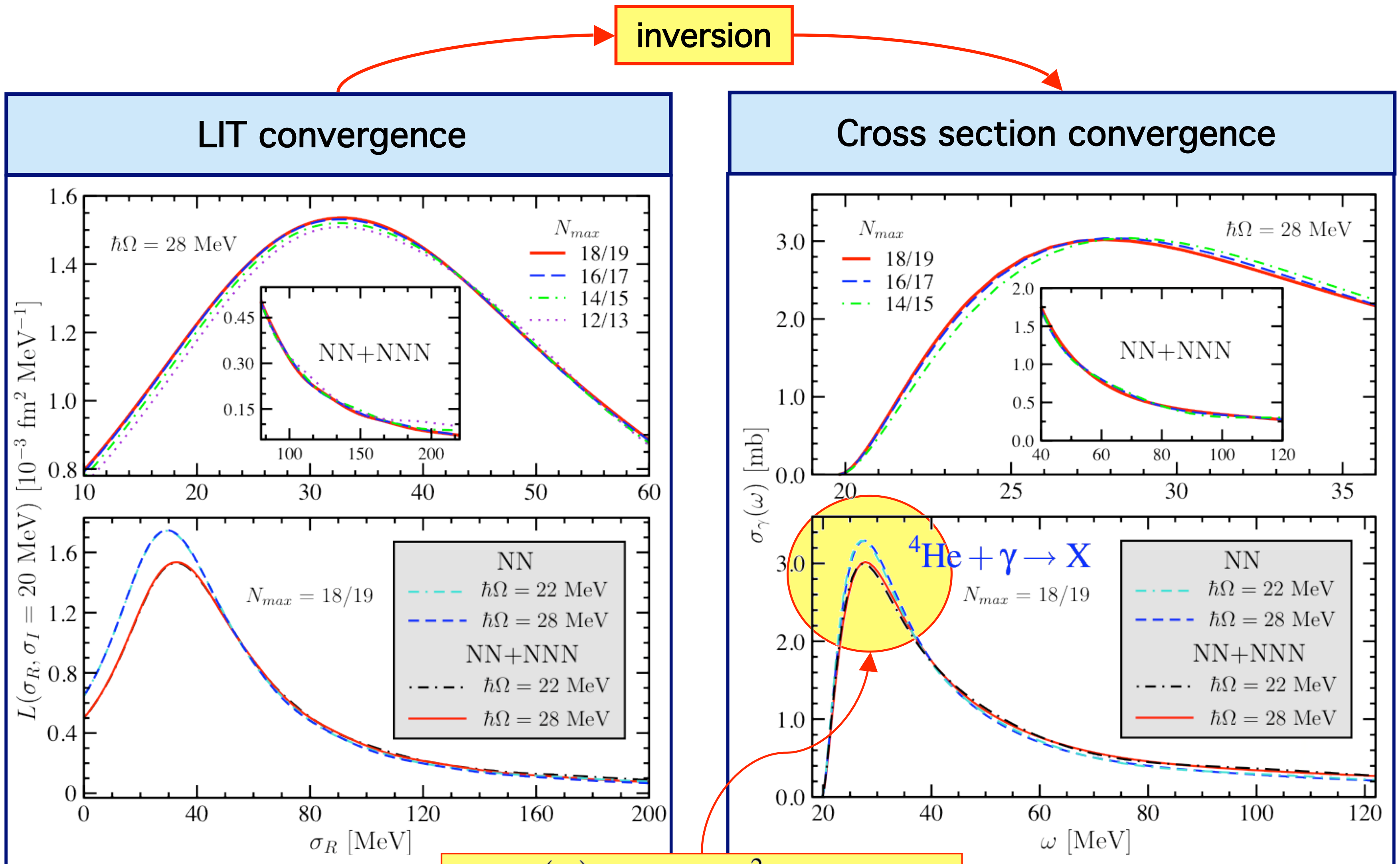
$$\langle \Psi_0 | \hat{D}^\dagger \hat{D} | \Psi_0 \rangle \simeq \frac{ZN}{3(A-1)} \langle r_p^2 \rangle$$

pure symmetric spatial w. f.
(9% off)

*deduced from: $\langle r_c^2 \rangle^{1/2} = 1.673(1)$ fm, $\langle R_p^2 \rangle^{1/2} = 0.895(18)$ fm, and $\langle R_n^2 \rangle = -0.120(5)$ fm^2

NCSM/LIT *ab initio* calculation of ^{4}He + $\gamma \rightarrow$ X

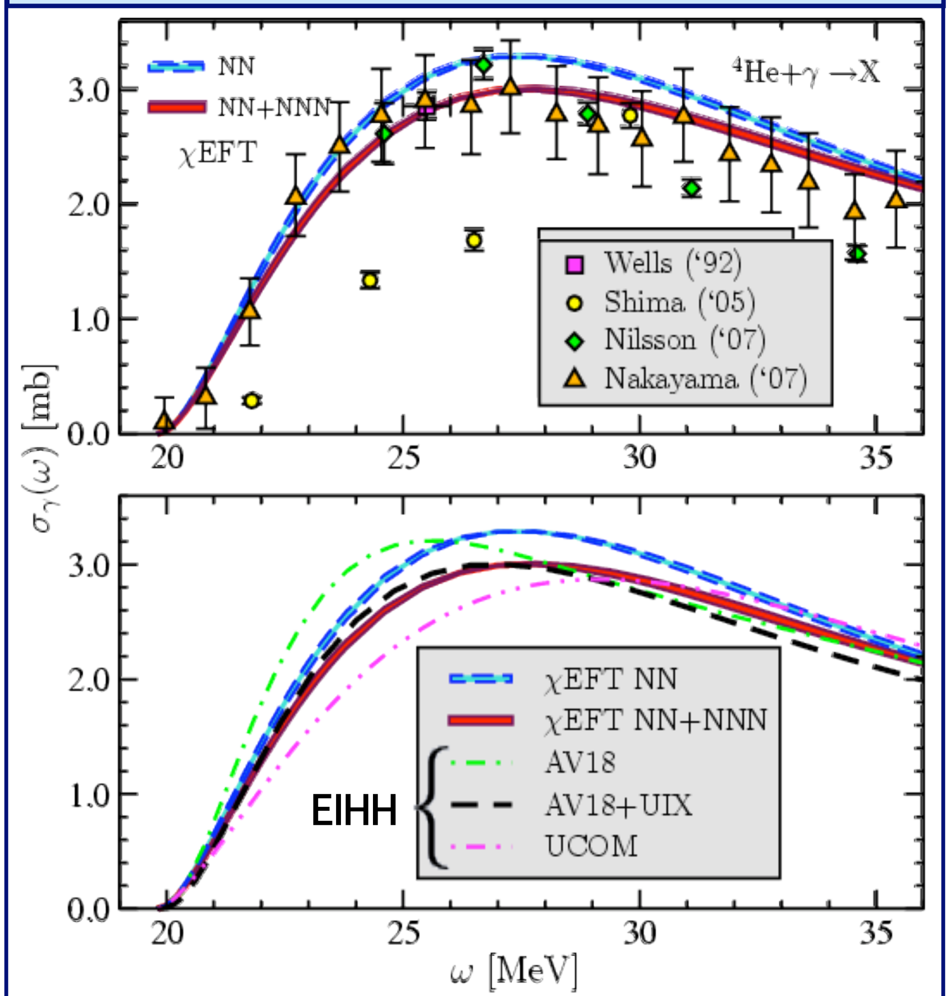
- χEFT NN + NNN interaction: convergence reached with three-body effective interaction



$$\int_{E_{th}}^{\infty} \frac{\sigma_\gamma(\omega)}{\omega} d\omega = 4\pi^2 \frac{e^2}{\hbar c} \langle \Psi_0 | \hat{D}^\dagger \hat{D} | \Psi_0 \rangle$$

$^4He + \gamma \rightarrow X$ reaction with χEFT NN+NNN - Conclusions

^{4}He photo-absorption cross section



- Still large discrepancies between different experimenal data
  - up to 100% disagreement on the peak-height
- The NNN force induces a suppression of the peak
  - not enough to explain data by Shima *et al.*
  - Overall better agreement with recent data by Nakayama *et al.*
- In the peak region χEFT NN+NNN and AV18 + UIX curves are relatively close:
  - weak sensitivity to the details of NNN force
  - expect larger effects in *p*-shell nuclei
- See: S.Q. and P. Navratil, Phys. Lett. B 652 (2007) 370

Sizable effect of NNN force. However, differences in the realistic calculations far below the experimental uncertainties: urgency for further experimental activity to clarify the situation.

Can we cover a wider range of nuclear reactions?

- The NCSM is a bound state technique: we need to include
  - clustering and resonant and non resonant continuum

Ansatz:

$$\Psi^{(A)} = \sum_\nu \hat{\mathcal{A}} \left[\psi_{1\nu}^{(A-a)} \psi_{2\nu}^{(a)} \varphi_\nu(\vec{r}_{A-a,a}) \right] = \sum_\nu \int d\vec{r}\, \varphi_\nu(\vec{r})\, \hat{\mathcal{A}}\, \Phi_{\nu\vec{r}}^{(A-a,a)}$$

$$\Phi_{\nu\vec{r}}^{(A-a,a)} = \psi_{1\nu}^{(A-a)} \psi_{2\nu}^{(a)} \delta(\vec{r} - \vec{r}_{A-a,a})$$

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

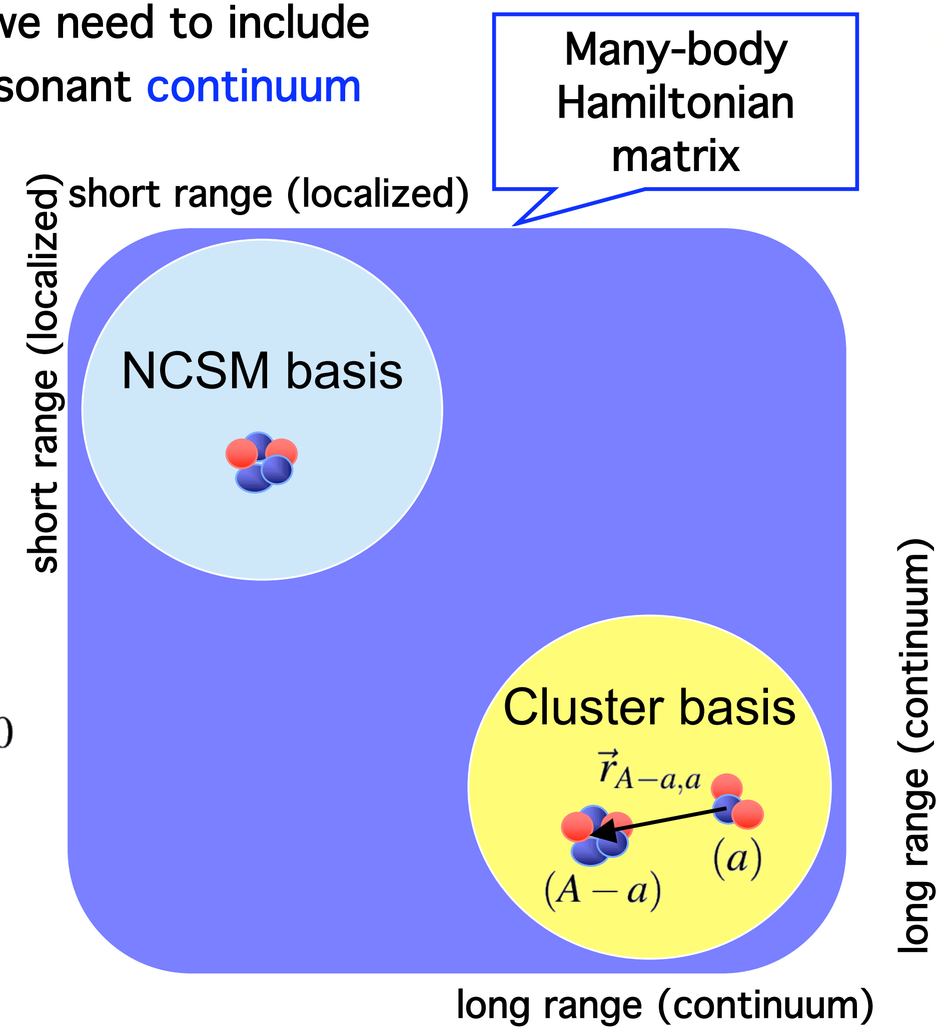
$$\sum_\nu \int d\vec{r} \left[\mathcal{H}_{\mu\nu}^{(A-a,a)}(\vec{r}^{\,\prime},\vec{r}) - E\mathcal{N}_{\mu\nu}^{(A-a,a)}(\vec{r}^{\,\prime},\vec{r}) \right] \varphi_\nu(\vec{r}) = 0$$

$$\langle \Phi_{\mu\vec{r}^{\,\prime}}^{(A-a,a)} | \hat{\mathcal{A}} H \hat{\mathcal{A}} | \Phi_{\nu\vec{r}}^{(A-a,a)} \rangle$$

Hamiltonian kernel

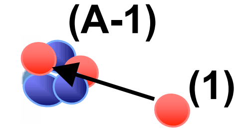
$$\langle \Phi_{\mu\vec{r}^{\,\prime}}^{(A-a,a)} | \hat{\mathcal{A}}^2 | \Phi_{\nu\vec{r}}^{(A-a,a)} \rangle$$

Norm kernel

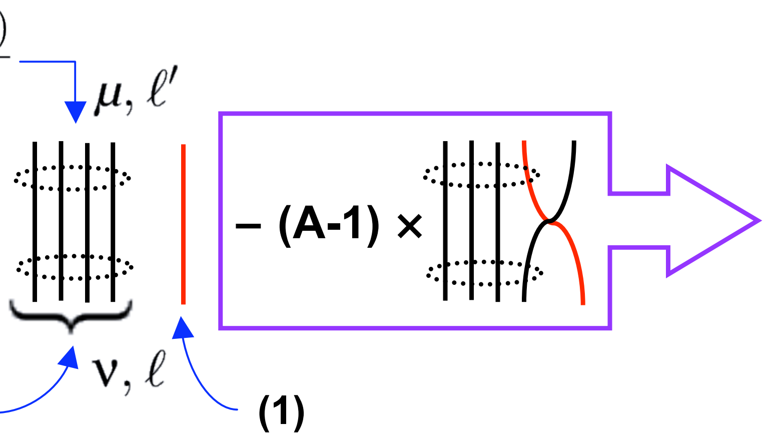


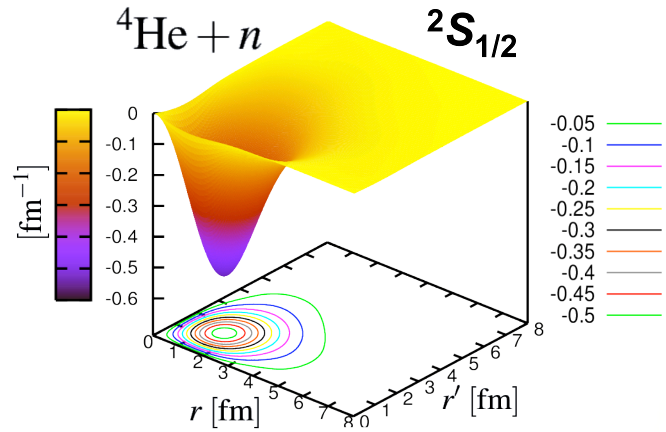
Resonating group method (RGM): many-body problem mapped onto various channels of nucleon clusters and their relative motion. We will use NCSM microscopic wave functions for the clusters, and effective interactions derived from realistic forces.

The RGM kernels in the single-nucleon projectile basis



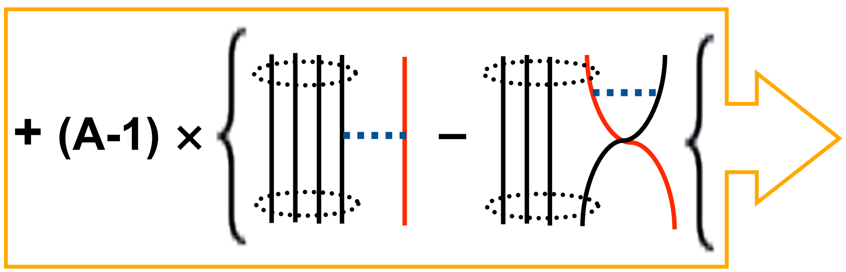
$$\mathcal{N}^{(A-1,1)}_{\mu\ell',\nu\ell}(r',r) = \delta_{\mu\nu}\,\delta_{\ell'\ell}\frac{\delta(r'-r)}{r'r} - (A\text{-}1)\times \ldots$$

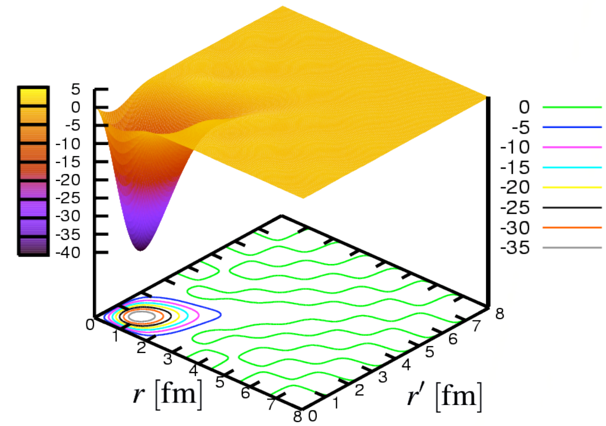




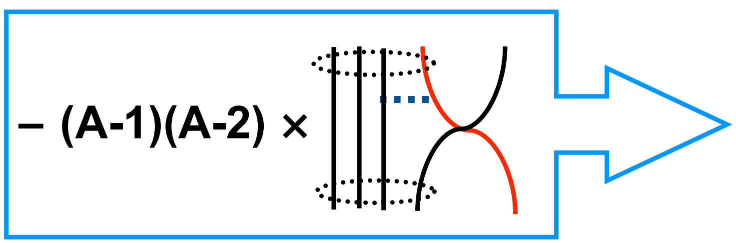
$$\mathcal{H}^{(A-1,1)}_{\mu\ell',\nu\ell}(r',r) = (E_{A-1} + \mathcal{T}_{rel})\,\mathcal{N}^{(A-1,1)}_{\mu\ell',\nu\ell}(r',r)$$

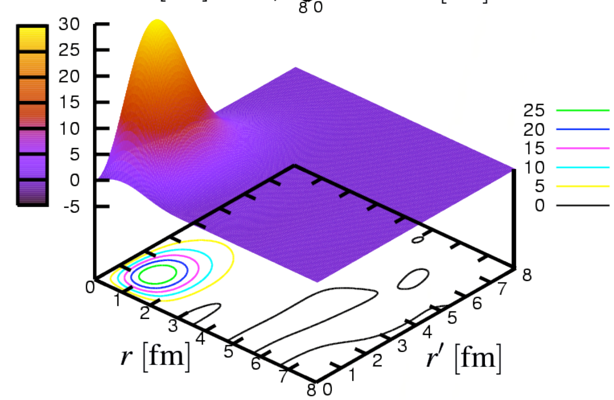
"direct potential"





"exchange potential"





Application to n-^{4}He scattering

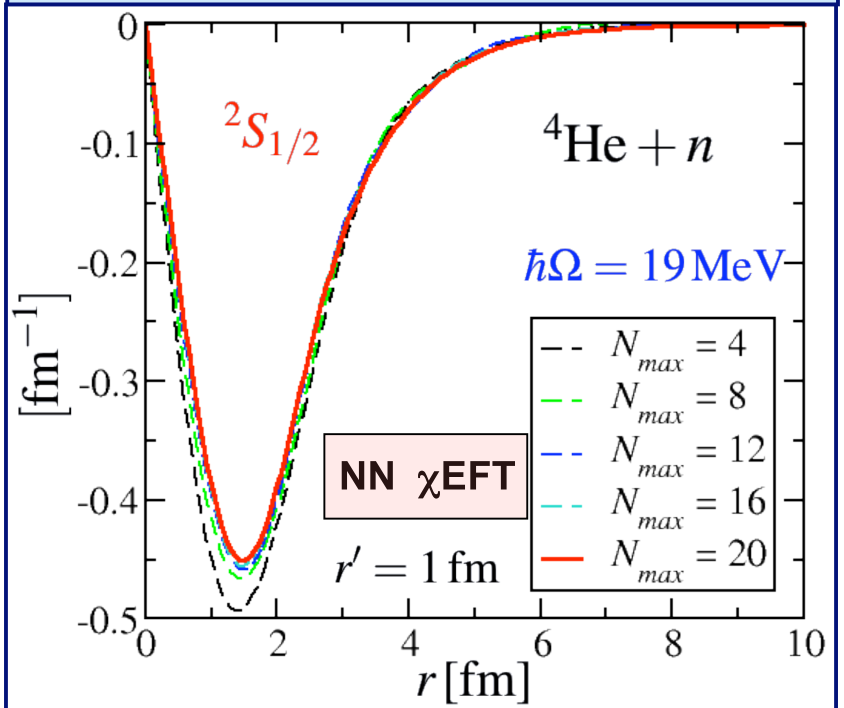
- The n-^{4}He system represents a convenient "training-ground" for low-energy nuclear scattering calculations
  - the A = 5 system does not have a bound state
  - there are two resonances in the *p*-waves
    - a sharp, low-energy resonance in the $3/2^-$ channel
    - a broader, higher-energy resonance in $1/2^-$ channel
  - the A = 5 system presents large effects of the Pauli Exclusion Principle
  - the ^{4}He is a tightly-bound nucleus
    - single channel scattering is valid up to E~20 MeV

- We have performed *ab initio* NCSM/RGM calculation with
  - low-momentum V_{lowk} NN potential (bare interaction)
  - χEFT NN potential (two-body effective interaction)

Describing correctly the low-energy neutron scattering on ^{4}He represents the first step towards a coherent picture of light-ion reactions

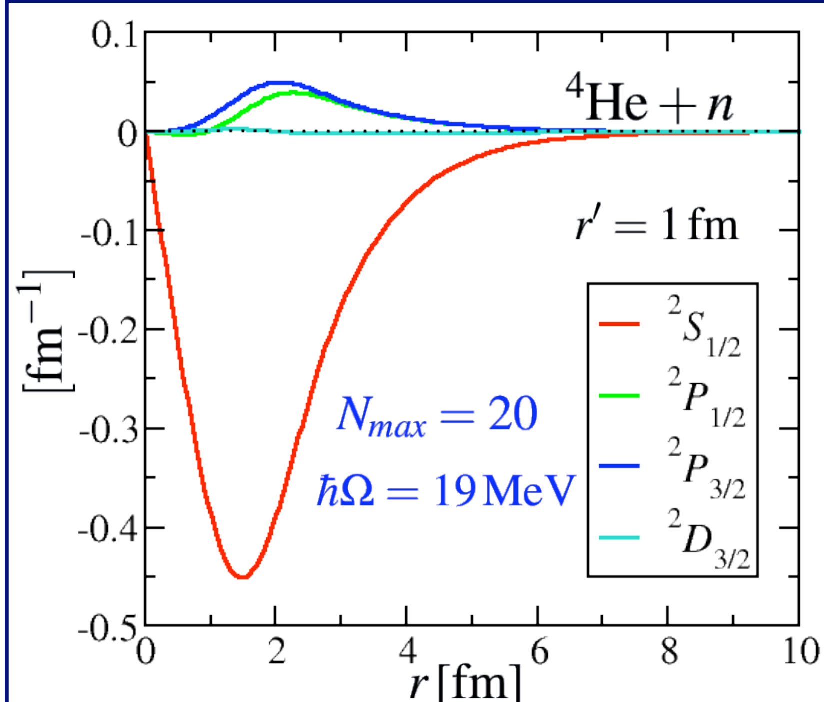
The ^{4}He+n system and the Pauli Exclusion Principle

– (A-1) × : convergence pattern



Good convergence with respect to the model space of the ^{4}He

– (A-1) × for different channels

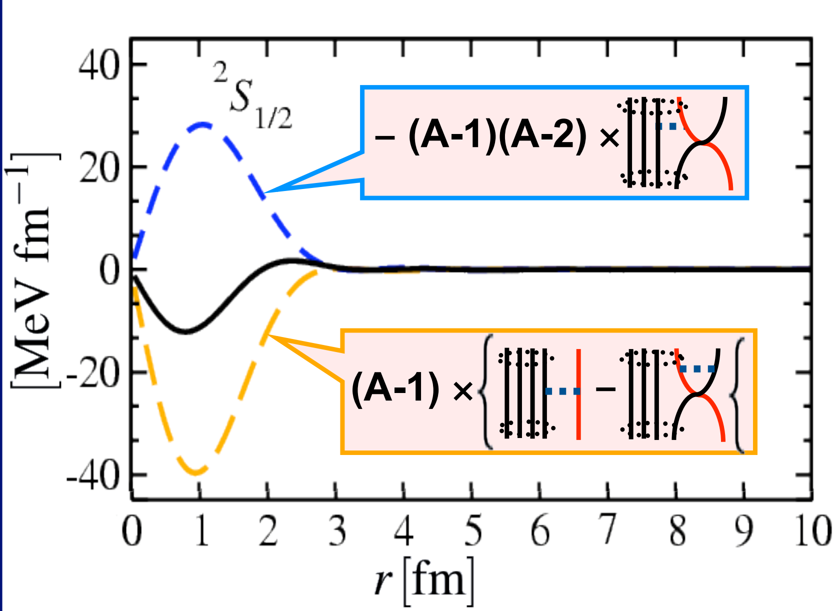


The $^2S_{1/2}$ channel shows large effects of the Pauli exclusion principle

All kernels have been verified using two independent derivations and codes based on the Jacobi and single-particle SD basis, respectively. The latter formalism will allow the application of the NCSM/RGM approach to *p*-shell nuclei

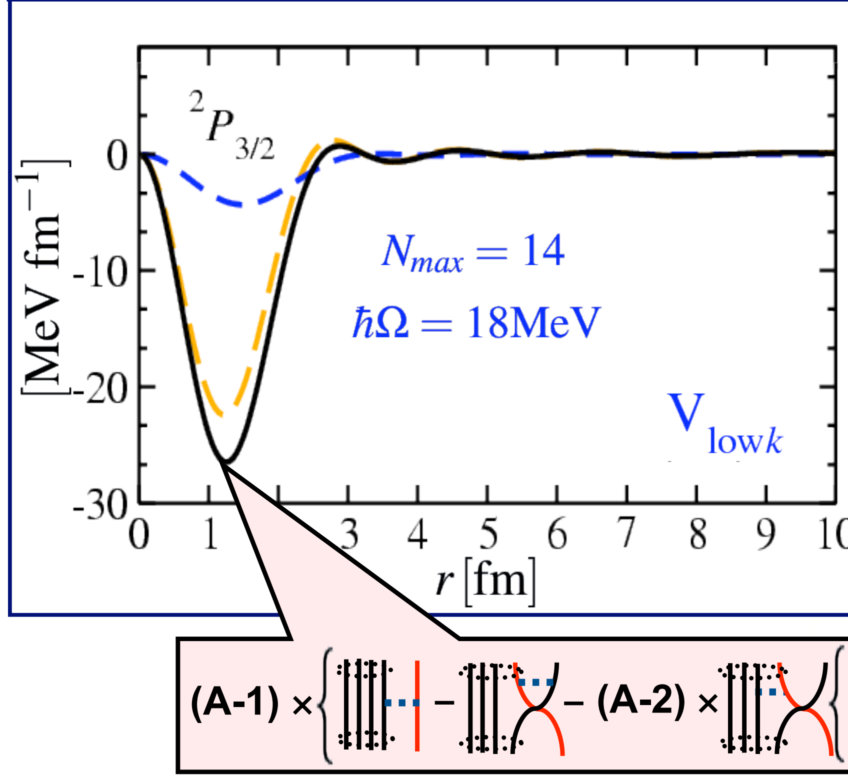
The ^{4}He+n system and the Pauli Exclusion Principle

Interaction kernels: $^2S_{1/2}$ channel



The $^2S_{1/2}$ channel shows large effects of the Pauli exclusion principle

interaction kernels: $^2P_{3/2}$ channel



All kernels have been verified using two independent derivations and codes based on the Jacobi and single-particle SD basis, respectively. The latter formalism will allow the application of the NCSM/RGM approach to p-shell nuclei

Solving the RGM equations

- Non-local integro-differential coupled-channel equations:

$$-\frac{\hbar^2}{2\mu_c}\frac{d}{dr^2}$$

$$[T_c + V_c(r) - E]u_c(r) + \sum_{c'} \int W_{cc'}(r,r')u_{c'}(r')dr' = 0$$

$$\varepsilon_c + \frac{\hbar^2}{2\mu_c}\frac{\ell_c(\ell_c+1)}{r^2} + \frac{Z_{c1}Z_{c2}e^2}{r} \qquad (\varepsilon_c - E)\mathcal{N}^E_{cc'}(r,r') + \mathcal{T}^E_{cc'}(r,r') + V^D_{cc'}(r,r') + V^E_{cc'}(r,r')$$

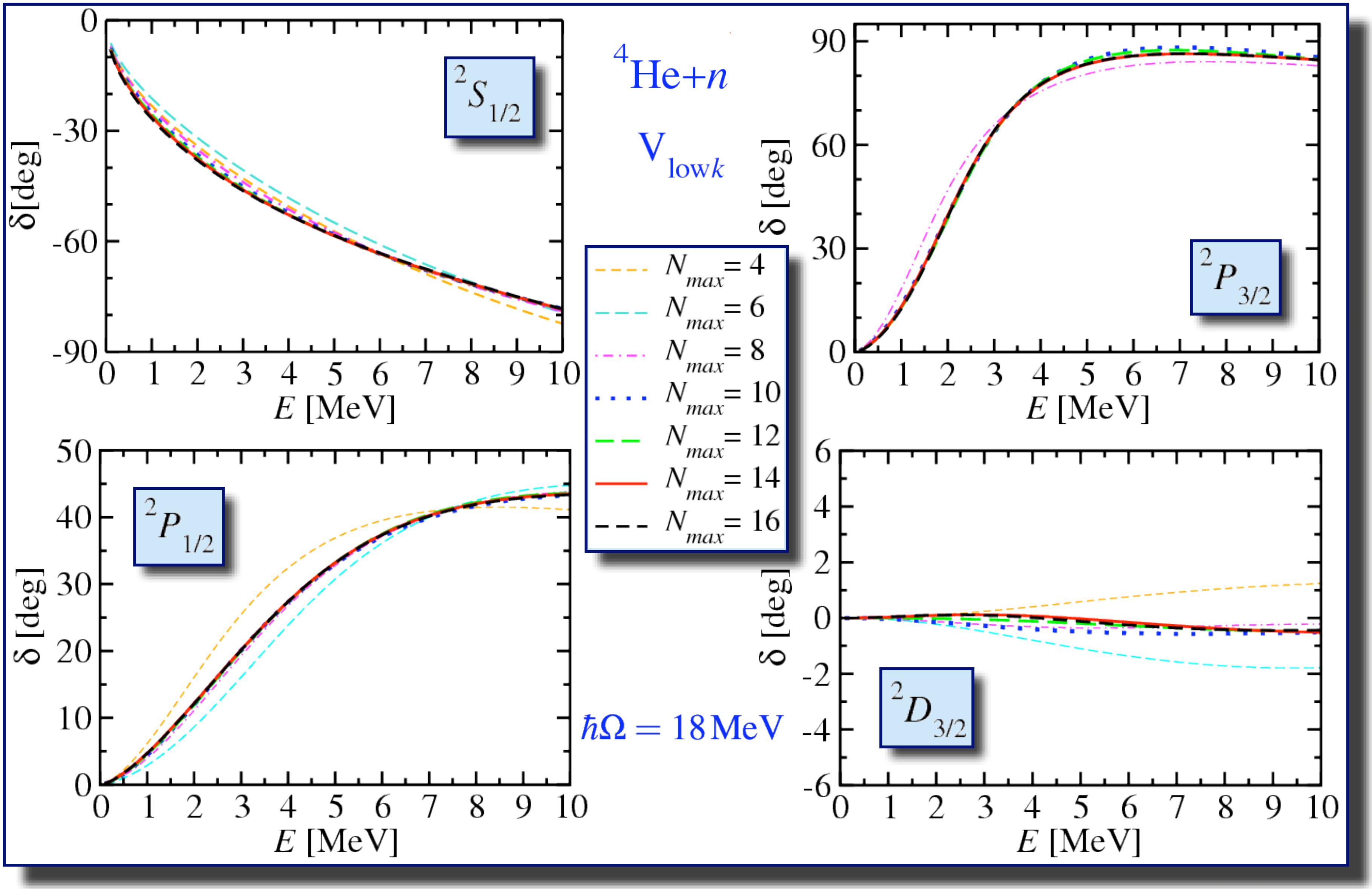
- Solution by Numerov's method
  - finite-difference approximations + Simpson integration
  - need ~200 quadrature points for a matching radius a = 10 fm
  - ➡ find simultaneously radial wave function and K-matrix ➔ S-matrix

- Solution by R-matrix method on a Lagrange mesh
  - exact analytical expression for kinetic operator
  - only values of local and non-local potential at mesh points needed
  - need ~20 quadrature points for a matching radius a = 10 fm
  - ➡ calculate R-matrix ➔ S-matrix

Both methods implemented and tested. They yield to identical results for n+^{4}He phase shifts calculated within the NCM/RGM approach.

NCSM/RGM *ab initio* calculation of *n*-^{4}He phase-shifts

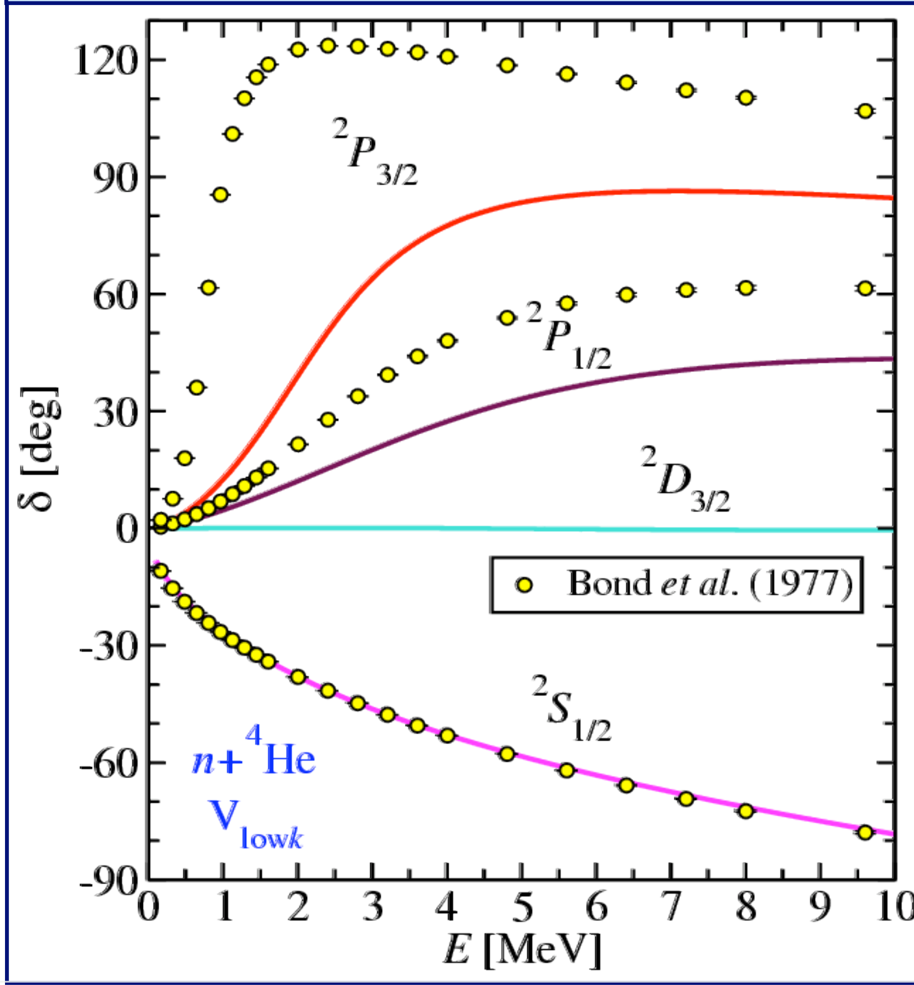
- Low-momentum V_{lowk} NN potential: convergence reached with bare interaction



n-^{4}He phase-shifts with V_{lowk} NN interaction

- NCSM/RGM calculation:
  - low-momentum V_{lowk} NN potential
  - bare interaction
  - N_{max}=16 @ $\hbar\Omega$ = 18 MeV
- $^2S_{1/2}$ phase-shift in agreement with experiment
  - known to be insensitive to NNN interaction
- $^2P_{1/2}$ and $^2P_{3/2}$ phase-shifts underestimate data
  - incorrect resonant pole positions
  - insufficient spin-orbit splitting
- The resonance are sensitive to NNN interaction

n-^{4}He phase-shifts

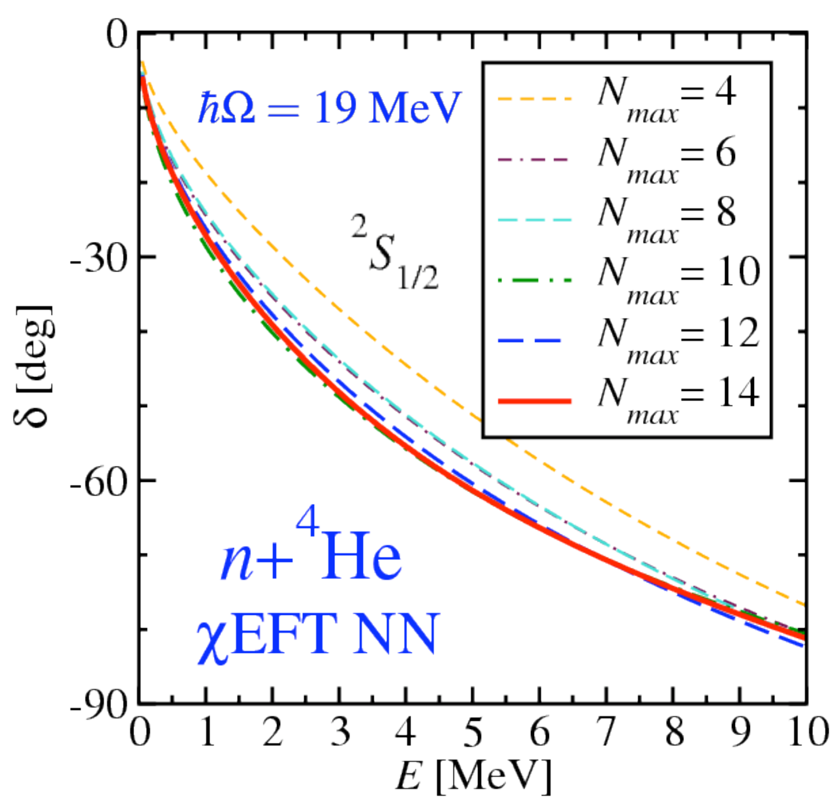


The first n+^{4}He phase shifts calculation within the NCSM/RGM approach. Fully *ab initio*, very promising results. The resonances are sensitive to NNN interaction.

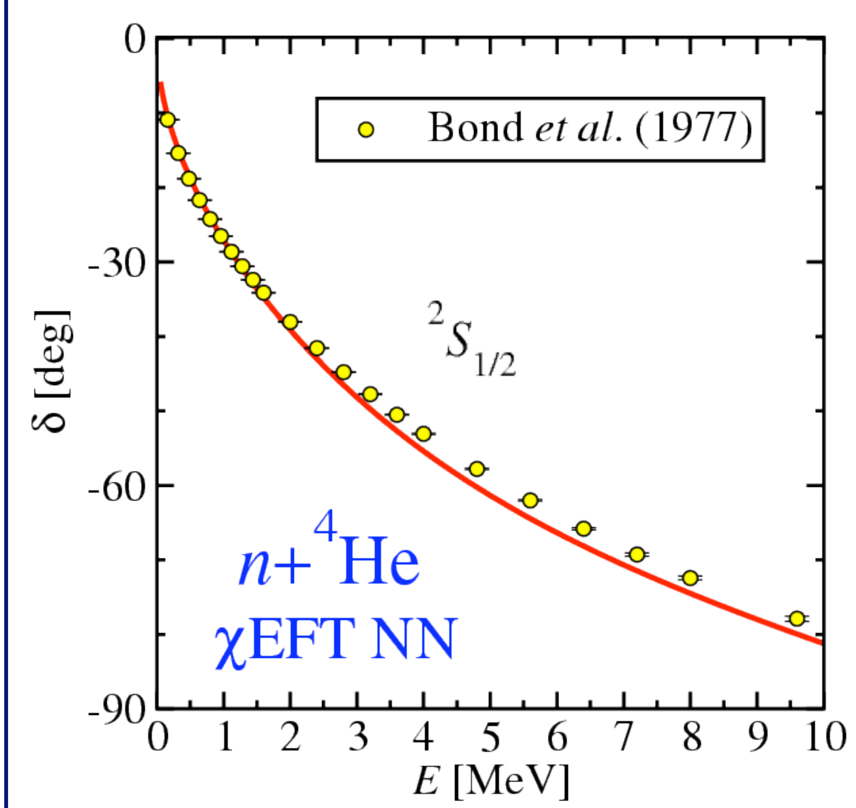
NCSM/RGM *ab initio* calculation of n-^{4}He phase-shifts

- χEFT N^{3}LO NN potential: convergence reached with two-body effective interaction

Convergence patterns with χEFT NN



Comparison with experiment



The first n+^{4}He phase shifts calculation within the NCSM/RGM approach. Fully *ab initio*, very promising results.

Conclusions and Outlook

- We are extending the *ab initio* NCSM to treat low-energy light-ion reactions
- Our recent achievements:
  - *n*-^{4}He scattering phase-shifts with realistic NN potentials
- Merging the NCSM and the RGM approaches represents our best opportunity to build a more complete theory to describe
  - structure
  - resonant and non resonant continuum
- Coming next:
  - inclusion of NNN potential terms
  - two-, three-, four-nucleon projectiles
- Ultimate goal:
  - *ab initio* NCSM with continuum (NCSMC)