Three-cluster dynamics within an ab initio framework

Universality in Few-Body Systems:

Theoretical Challenges and New Directions

INT 14-1

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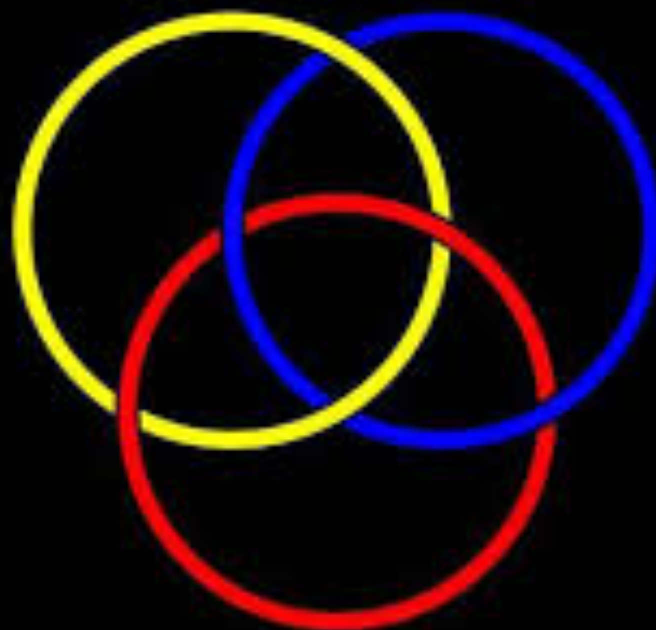
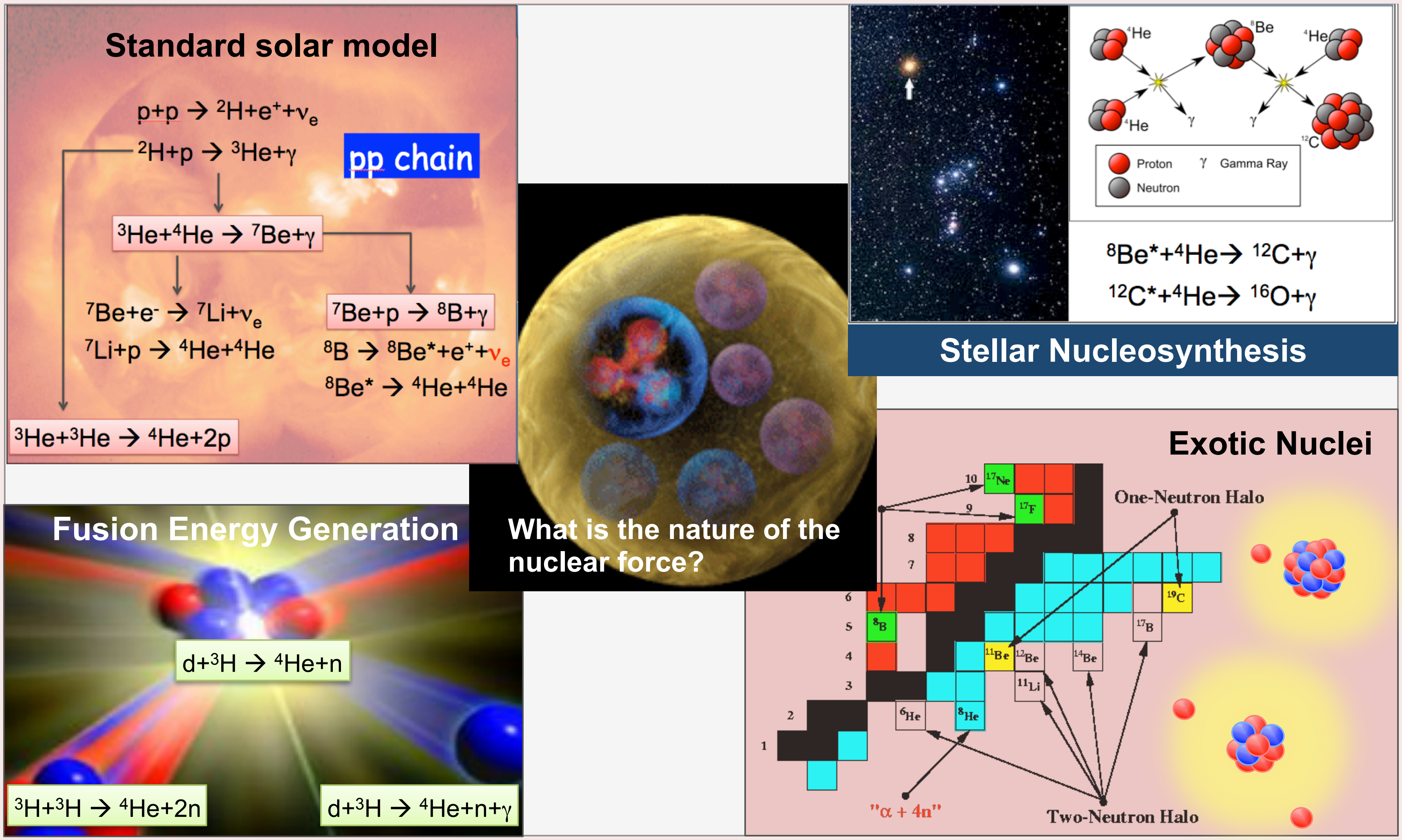


Outline

- Introduction
- Microscopic three-cluster problem
- Formalism for the (A-2)+1+1 mass partition
- Applications to ^{6}He
- Conclusions
- Outlook

Our goal is to develop a fundamental theory for the description of thermonuclear reactions and exotic nuclei

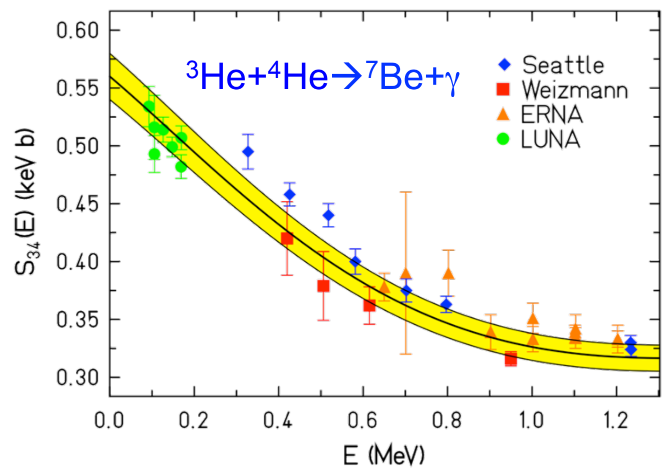


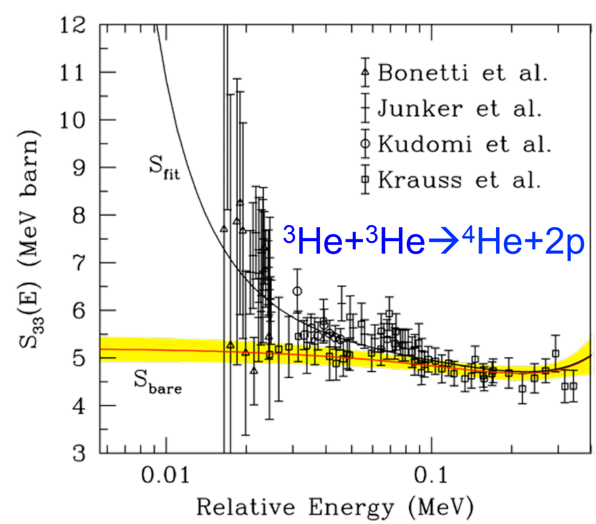
Theory needed because fusion reactions are difficult or impossible to measure at astrophysical energies

- The nuclear fusion process operates mainly by tunneling through the Coulomb barrier
  - Extremely low rates

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

- Projectiles and targets are not fully ionized
  - Electron screening can mask “bare” nuclear cross section



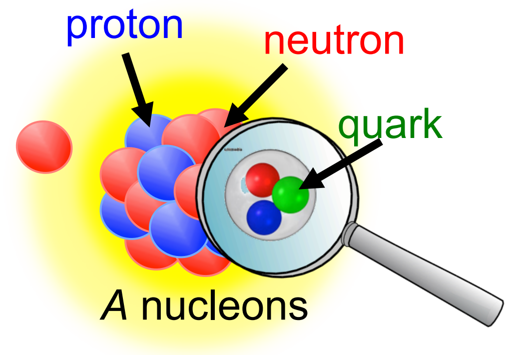


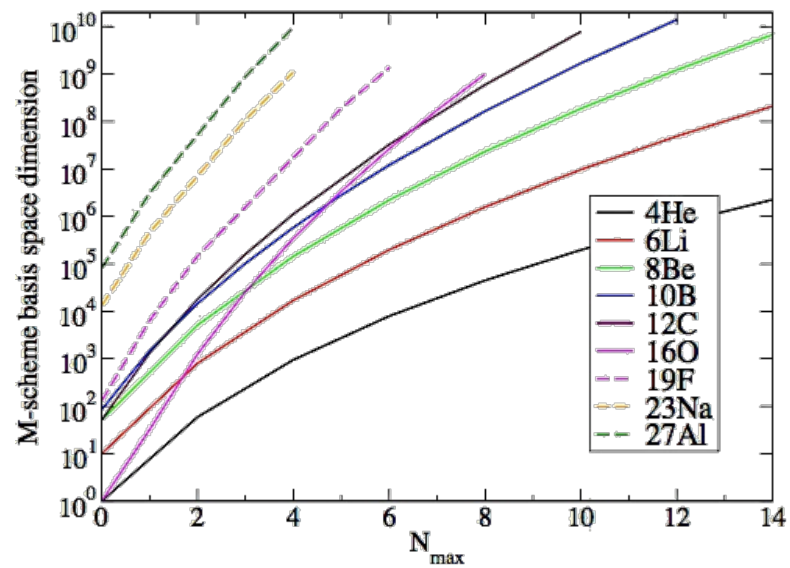
Developing such a fundamental theory is extremely complicated and a longstanding goal of nuclear theory

Ab initio many-body calculations:

- A (all active) point-like nucleons
- Nuclear two- and three-body (NN+NNN) forces guided by Quantum Chromodynamics (QCD)
- Unitary transformation to soften bare Hamiltonian: e.g., Similarity Renormalization Group (SRG)

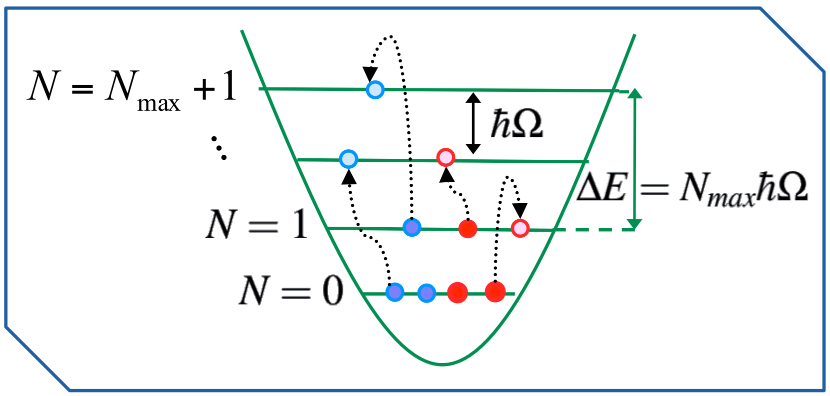
Efficient theoretical framework and High Performance Computing (HPC)



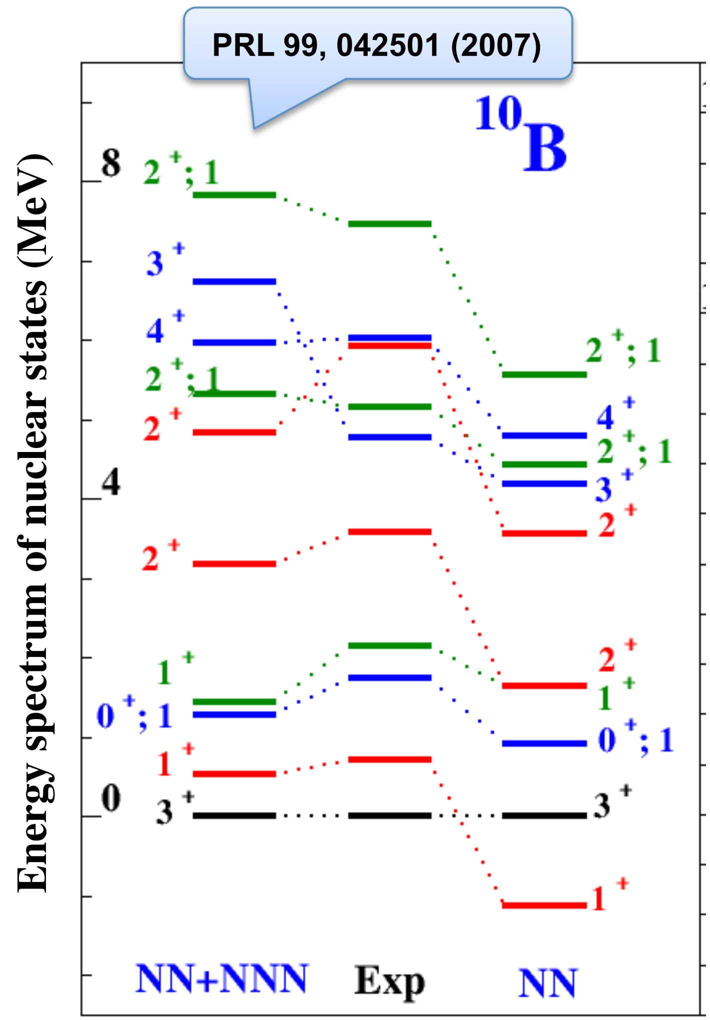


Our starting point is a method to describe static properties of light nuclei from first principles

- *Ab initio* no-core shell model (NCSM) approach

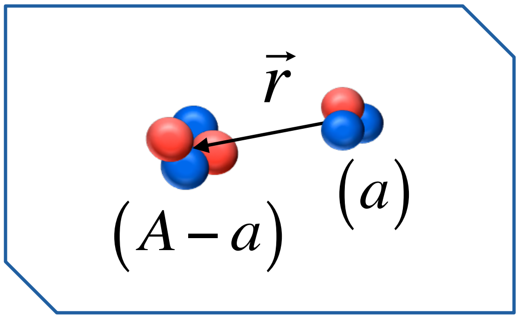


Helped to point out the fundamental importance of three-nucleon (NNN) forces in structure calculations.



We extended this approach by adding the dynamics between nuclei with the resonating-group method (RGM)

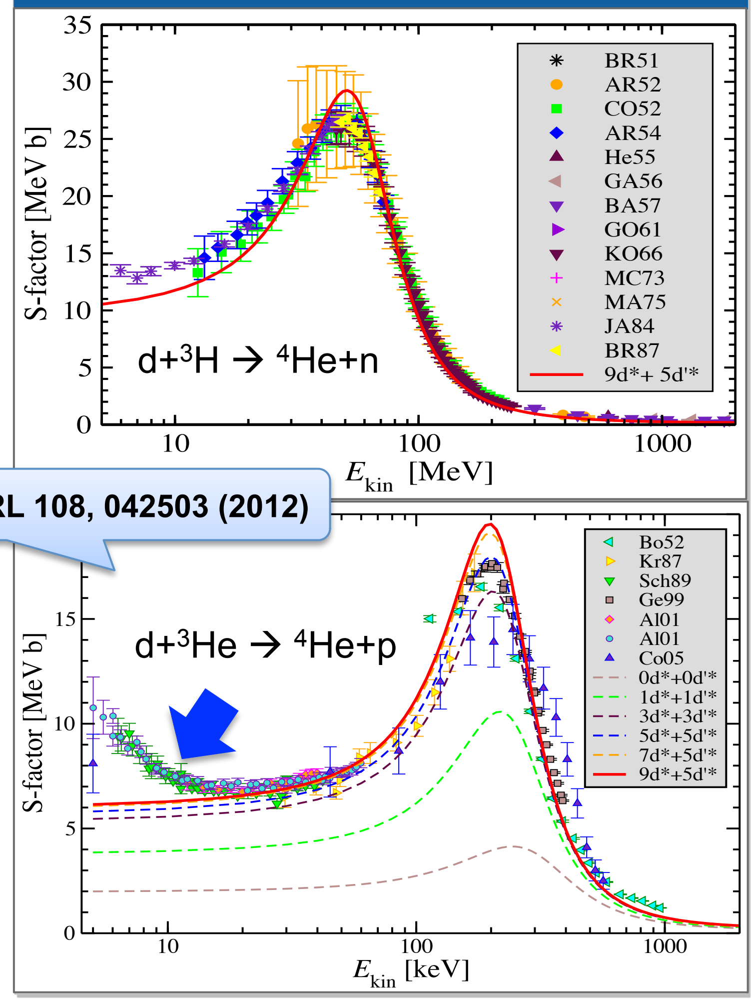
- NCSM/RGM approach



- *Ab initio* NCSM wave functions of the nuclei
- NN interactions

Pioneered ab initio calculations of light-nuclei fusion reactions

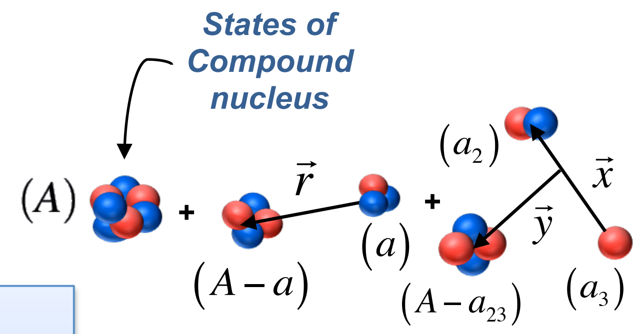
Astrophysical S-factors



PRL 108, 042503 (2012)

We are now working to complete this picture

- Extended NCSM/RGM to include:
  1) NNN force in reactions
  2) States of the compound nucleus
  3) Three-cluster states in the continuum

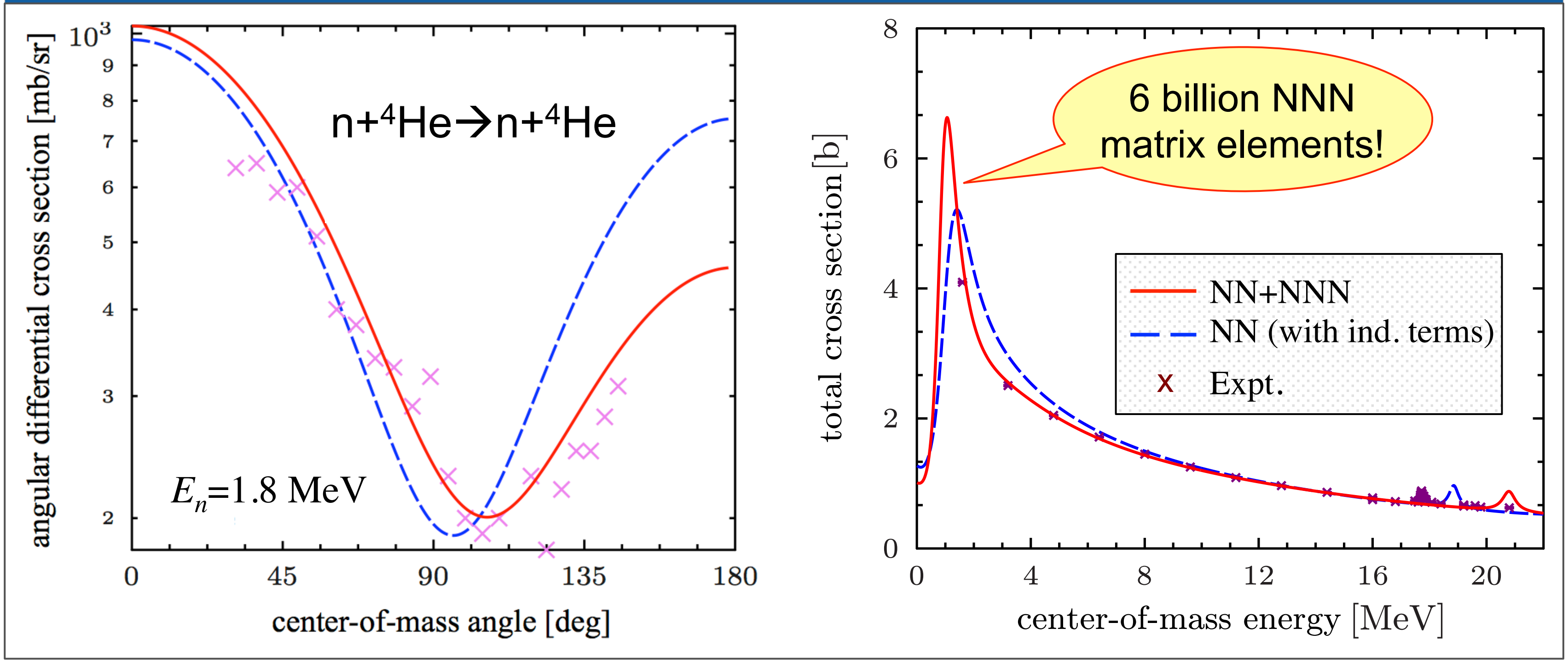


This talk

1) Importance of the NNN force in reactions

G. Hupin, J. Langhammer, P. Navratil, S. Quaglioni, A. Calci and R. Roth, Phys. Rv. C 88, 054622 (2013)

Elastic scattering of neutrons on ^{4}He

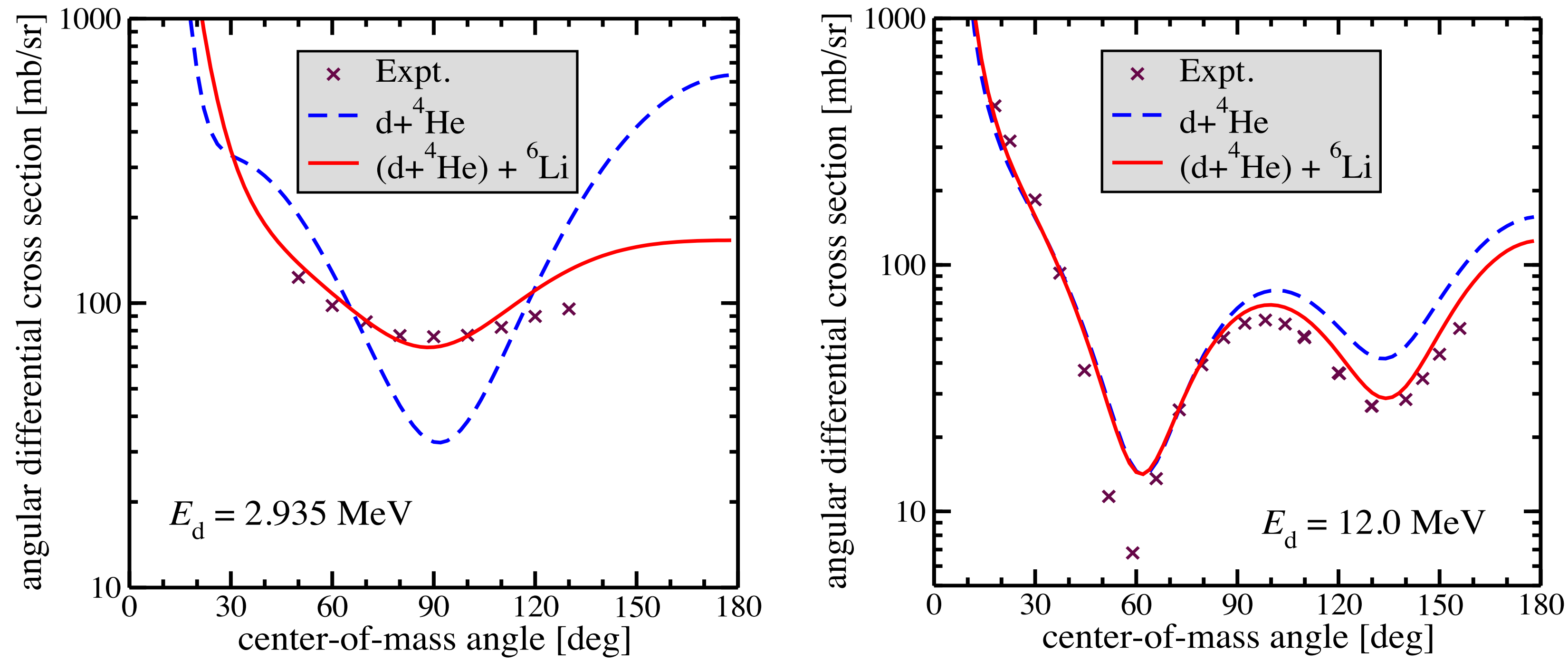


This work sets the stage for a truly accurate prediction of the d+^{3}H→^{4}He+n fusion from QCD-based NN+NNN forces

2) Importance of states of the compound system

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

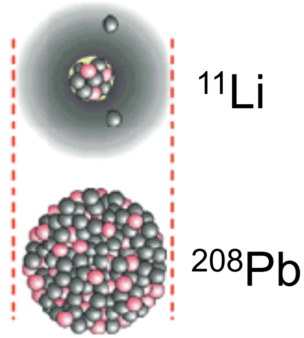
d+^{4}He→d+^{4}He with & without inclusion of ^{6}Li states

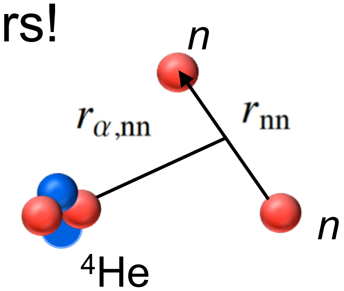


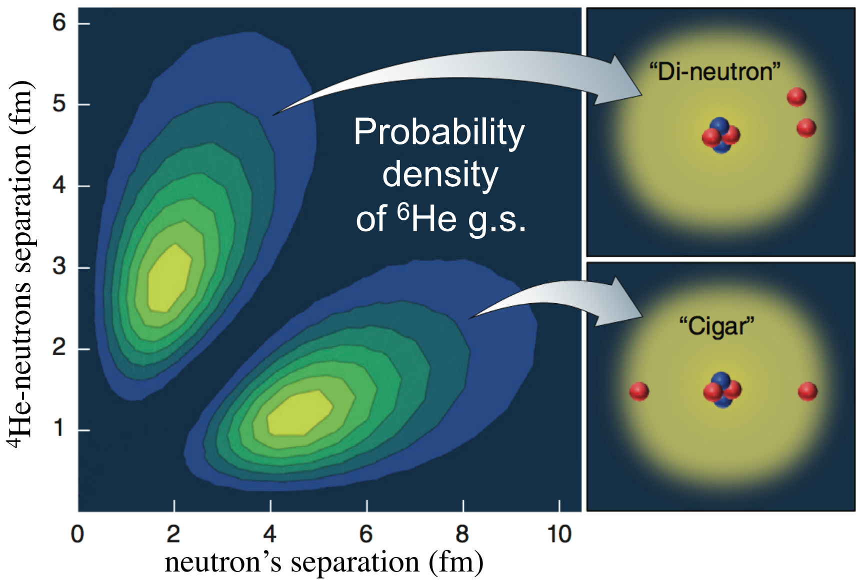
Six-body correlations important also for binding energy (~1 MeV)

3) We want to describe also systems for which the lowest threshold for particle decay is of the 3-body nature

- Exotic nuclei, (Borromean halos, dripline nuclei)
  - ^{6}He (= ^{4}He + n + n)
  - ^{6}Be (= α + p + p)
  - ^{11}Li (= ^{9}Li + n + n)
  - ^{14}Be (= ^{12}Be + n + n)
  - …
- Constituents do not bind in pairs!







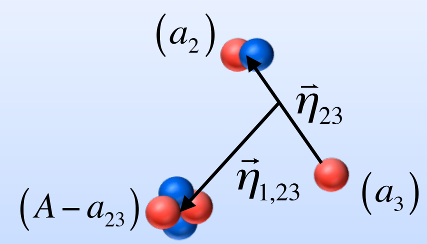
S. Quaglioni, C. Romero-Redondo, P. Navrátil, Phys. Rev. C 88, 034320 (2013)

Microscopic three-cluster problem

- Starts from:

3-body channels

$$\Psi^{(A)} = \sum_{\nu} \iint d\vec{x}\, d\vec{y}\; G_{\nu}(\vec{x},\vec{y})\; \hat{A}_{\nu} \left| \Phi_{\nu\vec{x}\vec{y}} \right\rangle$$



$$\psi_{\alpha_1}^{(A-a_{23})}\psi_{\alpha_2}^{(a_2)}\psi_{\alpha_3}^{(a_3)}\delta(\vec{x}-\vec{\eta}_{23})\delta(\vec{y}-\vec{\eta}_{1,23})$$

- Projects $(H-E)\Psi^{(A)}=0$ onto the channel basis:

$$\sum_{\nu} \iint d\vec{x}\, d\vec{y}\; \left[H_{\nu'\nu}(\vec{x}',\vec{y}',\vec{x},\vec{y}) - E\;\; N_{\nu'\nu}(\vec{x}',\vec{y}',\vec{x},\vec{y}) \right]\; G_{\nu}(\vec{x},\vec{y}) = 0$$

$$\left\langle \Phi_{\nu'\vec{x}'\vec{y}'} \right| \hat{A}_{\nu'} H \hat{A}_{\nu} \left| \Phi_{\nu\vec{x}\vec{y}} \right\rangle$$

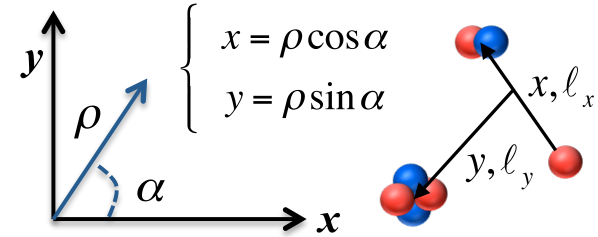
Hamiltonian kernel

$$\left\langle \Phi_{\nu'\vec{x}'\vec{y}'} \right| \hat{A}_{\nu'} \hat{A}_{\nu} \left| \Phi_{\nu\vec{x}\vec{y}} \right\rangle$$

Norm or Overlap kernel

This can be turned into a set of coupled-channels Schrödinger equations for the hyperradial motion

- Hyperspherical Harmonic (HH) functions form a natural basis:



$$\left|\Phi_{\nu\vec{x}\vec{y}}\right\rangle = \sum_K \phi_K^{*\ell_x,\ell_y}(\alpha)\left|\Phi_{\nu K\rho}\right\rangle$$

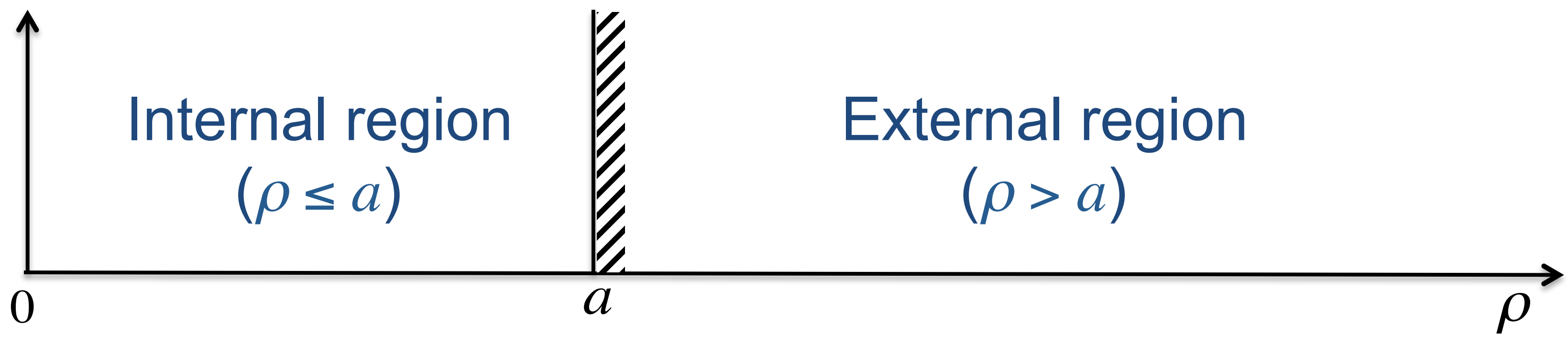
$$\propto \Upsilon_L^{K\ell_x\ell_y}(\alpha_\eta,\hat{\eta}_{1,23},\hat{\eta}_{23})\frac{\delta(\rho-\rho_\eta)}{\rho^{5/2}\rho_\eta^{5/2}}$$

- Then, with orthogonalization and projection over $\phi_{K'}^{\ell'_x,\ell'_y}(\alpha')$:

$$\sum_{\nu K}\int d\rho\ \rho^5\left[N^{-1/2}H\ N^{-1/2}\right]_{\nu'\nu}(\rho',\rho)\ \frac{u_{K\nu}(\rho)}{\rho^{5/2}} = E\,\frac{u_{K'\nu'}(\rho')}{\rho'^{5/2}}$$

$$\left[N^{1/2}G\right]_\nu(x,y) = \rho^{-5/2}\sum_K u_{\nu K}(\rho)\ \ \phi_K^{\ell_x\ell_y}(\alpha)$$

These equations can be solved using R-matrix theory



Expansion on a basis

$$u_{K\nu}(\rho) = \sum_n c_n^{K\nu} f_n(\rho)$$

Bound state asymptotic behavior

$$u_{K\nu}(\rho) = C_{K\nu} \sqrt{k\rho}\ K_{K+2}(k\rho)$$

Scattering state asymptotic behavior

$$u_{K\nu}(\rho) = A_{K\nu}\left[\mathrm{H}_K^-(k\rho)\ \delta_{\nu\nu'}\delta_{KK'} - S_{\nu K,\nu' K'}\mathrm{H}_K^+(k\rho)\right]$$

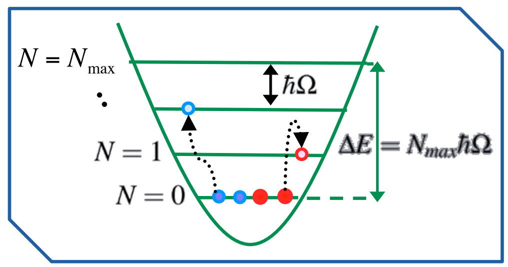
^{4}He+n+n within the NCSM/RGM

S. Quaglioni, C. Romero-Redondo, P. Navratil, Phys. Rev. C 88, 034320 (2013)

- Accurate soft NN interaction: SRG-evolved chiral N^{3}LO potential with Λ=1.5 fm^{-1}
  - Fits NN data with high accuracy
  - But: misses both chiral initial and SRG-induced NNN force
  - **Fortuitously**: two effects mostly compensate each other for very light systems

- ^{4}He ab initio wave function obtained within the NCSM

$$H^{(A-2)}\psi^{(A-2)}_{\beta_1}(\vec{r}_1,\vec{r}_2,\cdots,\vec{r}_{A-2}) = E^{(A-2)}_{\beta_1}\psi^{(A-2)}_{\beta_1}(\vec{r}_1,\vec{r}_2,\cdots,\vec{r}_{A-2})$$

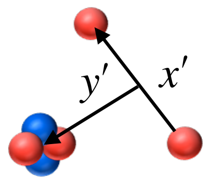


  - Large expansions in *A*-body harmonic oscillator (HO) basis
  - Preserves: 1) Pauli principle, and 2) translational invariance
  - Can include NNN interactions
  - ^{4}He binding energy close to experiment: 28.22 MeV (expt.: 28.3 MeV)

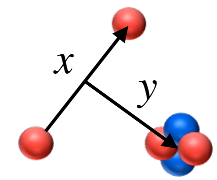
- Fully antisymmetric channel states: $$\hat{A}_\nu = \sqrt{\frac{(A-2)!2!}{A!}}\left[1-\sum_{i=1}^{A-2}\sum_{k=A-1}^{A}\hat{P}_{i,k}+\sum_{i<j=1}^{A-2}\hat{P}_{i,A-1}\hat{P}_{j,A}\right]\frac{1-\hat{P}_{A-1,A}}{\sqrt{2}}$$

The formalism is general for (A-2)+1+1 mass partitions

Norm or overlap kernel (Pauli principle)



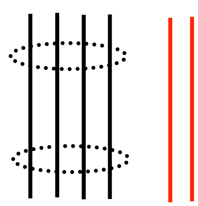
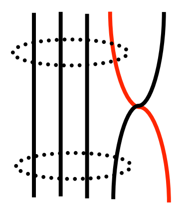
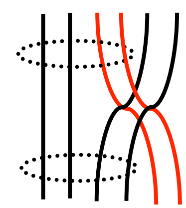
$$\left\langle \cdots \right| \left(1-\sum_{i=1}^{A-2}\sum_{k=A-1}^{A}\hat{P}_{i,k}+\sum_{i<j=1}^{A-2}\hat{P}_{i,A-1}\hat{P}_{j,A}\right)\left(1-\hat{P}_{A-1,A}\right)\left| \cdots \right\rangle$$



$$N_{\nu'\nu}(x',y',x,y)=\frac{1}{2}\left[1-(-1)^{\ell'_x+S'_{23}+T'_{23}}\right]\left[1-(-1)^{\ell_x+S_{23}+T_{23}}\right]\times\left\{\delta_{\nu'\nu}\frac{\delta(x'-x)}{x'x}\frac{\delta(y'-y)}{y'y}\right.$$

$$-2(A-2)\sum_{n'_x n'_y}\sum_{n_x n_y}R_{n'_x\ell'_x}(x')R_{n'_y\ell'_y}(y')\left\langle\Phi_{\nu'_3 n'_x n'_y}\middle|P_{A-2,A}\middle|\Phi_{\nu_3 n_x n_y}\right\rangle R_{n_x\ell_x}(x)R_{n_y\ell_y}(y)$$

$$\left.+\frac{(A-2)(A-3)}{2}\sum_{n'_x n'_y}\sum_{n_x n_y}R_{n'_x\ell'_x}(x')R_{n'_y\ell'_y}(y')\left\langle\Phi_{\nu'_3 n'_x n'_y}\middle|P_{A-3,A-1}P_{A-2,A}\middle|\Phi_{\nu_3 n_x n_y}\right\rangle R_{n_x\ell_x}(x)R_{n_y\ell_y}(y)\right\}$$

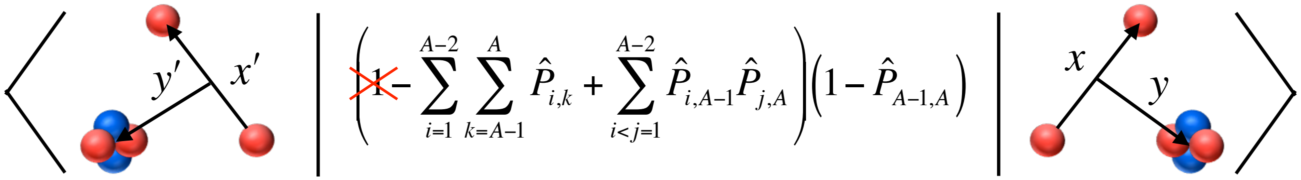
 **- 2(A-2) ×**  **+ (A-2)(A-3)/2 ×** 

$${}_{SD}\left\langle\psi_{\mu_1}^{(A-2)}\middle|a^+a\middle|\psi_{\nu_1}^{(A-2)}\right\rangle_{SD}$$

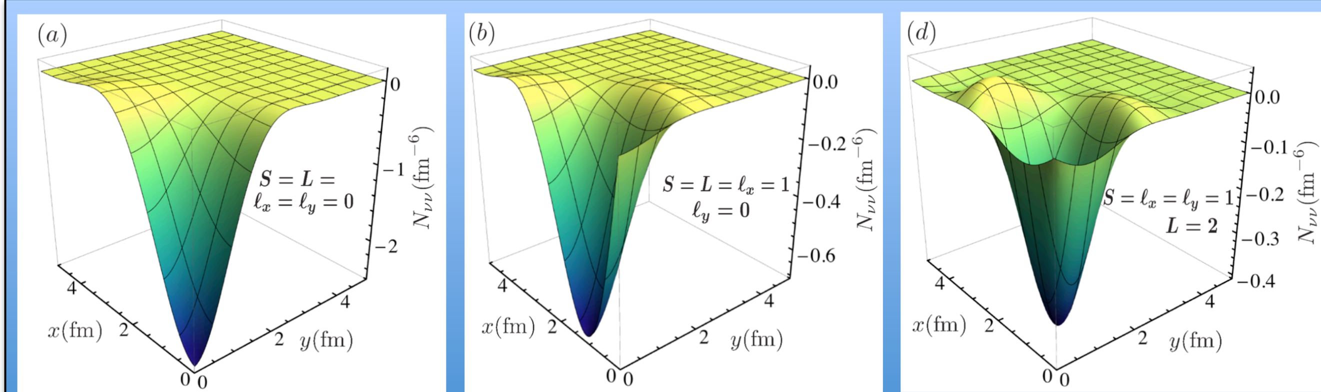
$${}_{SD}\left\langle\psi_{\mu_1}^{(A-2)}\middle|a^+a^+\,a\,a\middle|\psi_{\nu_1}^{(A-2)}\right\rangle_{SD}$$

The formalism is general for (A-2)+1+1 mass partitions

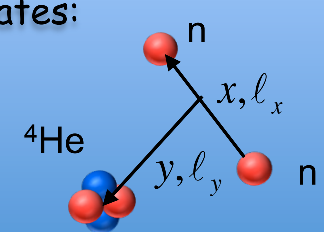
Norm or overlap kernel (Pauli principle)

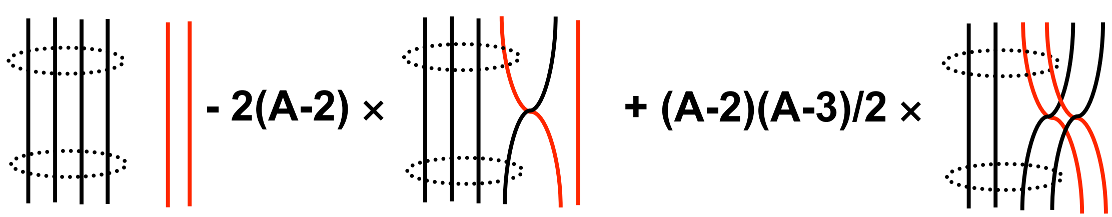


$$\left\langle \ \right| \left(\cancel{1} - \sum_{i=1}^{A-2} \sum_{k=A-1}^{A} \hat{P}_{i,k} + \sum_{i<j=1}^{A-2} \hat{P}_{i,A-1}\hat{P}_{j,A} \right)\left(1-\hat{P}_{A-1,A}\right) \left| \ \right\rangle$$



Matrix element $\left\langle \hat{A}_\nu^2 - 1 \right\rangle$ over three-cluster states:



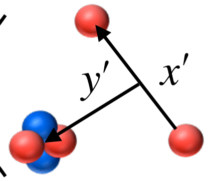


$${}_{\mathrm{SD}}\left\langle \psi_{\mu_1}^{(A-2)} \middle| a^+ a \middle| \psi_{\nu_1}^{(A-2)} \right\rangle_{\mathrm{SD}}$$

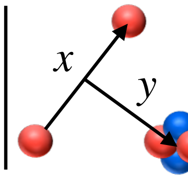
$${}_{\mathrm{SD}}\left\langle \psi_{\mu_1}^{(A-2)} \middle| a^+ a^+ a\, a \middle| \psi_{\nu_1}^{(A-2)} \right\rangle_{\mathrm{SD}}$$

The formalism is general for (A-2)+1+1 mass partitions

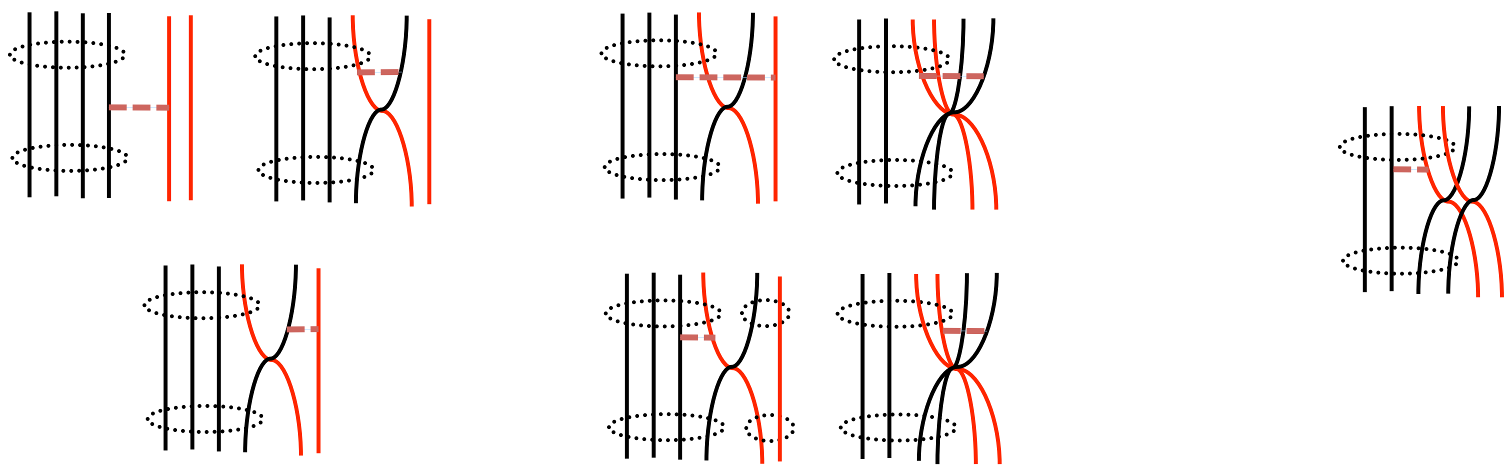
Hamiltonian kernel (nucleon-nucleon-target potentials)



$$\left\langle \cdots \right| \left(\sum_{l=1}^{A-2} \sum_{m=A-1}^{A} V_{lm} + V_{A-1A} \right) \left(1 - \sum_{i=1}^{A-2} \sum_{k=A-1}^{A} \hat{P}_{i,k} + \sum_{i<j=1}^{A-2} \hat{P}_{i,A-1} \hat{P}_{j,A} \right) \left(1 - \hat{P}_{A-1,A} \right) \left| \cdots \right\rangle$$



$$= V(x') N_{\nu'\nu}(x',y',x,y) +$$

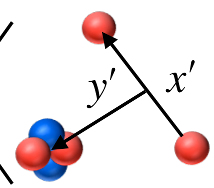


$$_{SD}\left\langle \psi_{\mu_1}^{(A-2)} \middle| a^+ a \middle| \psi_{\nu_1}^{(A-2)} \right\rangle_{SD}$$

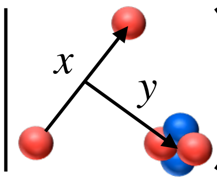
$$_{SD}\left\langle \psi_{\mu_1}^{(A-2)} \middle| a^+ a^+ a\, a \middle| \psi_{\nu_1}^{(A-2)} \right\rangle_{SD}$$

$$_{SD}\left\langle \psi_{\mu_1}^{(A-2)} \middle| a^+ a^+ a^+ a\, a\, a \middle| \psi_{\nu_1}^{(A-2)} \right\rangle_{SD}$$

Part of the interaction kernel is localized only in x, x’



$$\left\langle \quad \middle| V_{A-1A}\left(1-\hat{P}_{A-1,A}\right) \middle| \quad \right\rangle$$



$$\propto \sum_{n'_x n_x} R_{n'_x \ell'_x}(x') R_{n_x L_x}(x) \left\langle n'_x \ell'_x s_{23} J_{23} T_{23} \middle| V \middle| n_x L_x s_{23} J_{23} T_{23} \right\rangle$$

$$\times \left(1-(-1)^{\ell_x + s_{23} + T_{23}}\right) \delta_{\tilde{\gamma}'\gamma} \frac{\delta(y'-y)}{y'y}$$

$$\approx \sum_{n_y} R_{n_y \ell_y}(y') R_{n_y \ell_y}(y)$$

Extended-size HO expansion

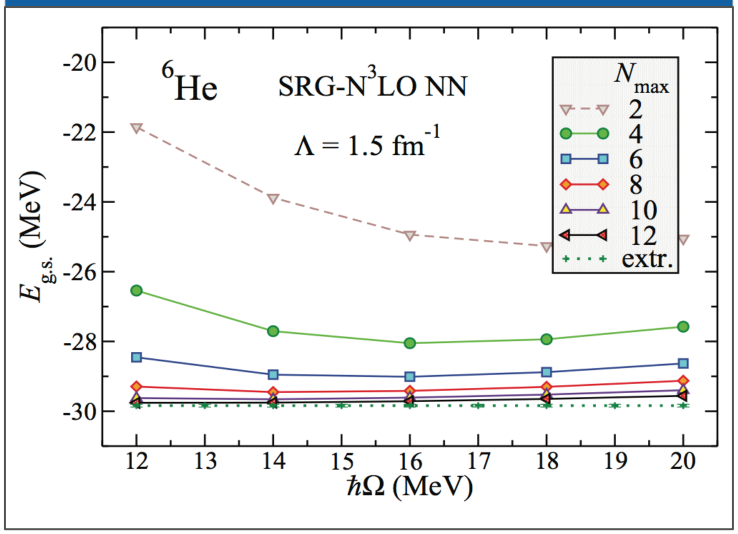
$N_{\mathrm{ext}} >> N_{\mathrm{max}}$

Results for ^{6}He ground state

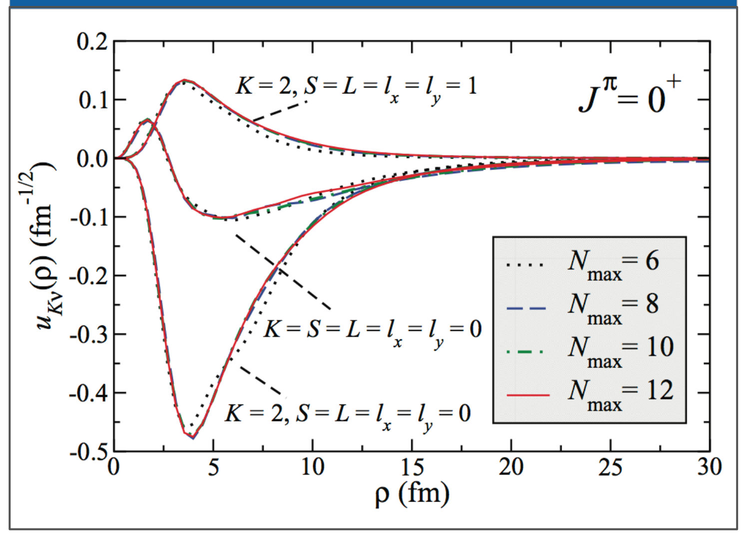
6-body diagonalization vs ^{4}He(g.s)+n+n calculation

$$\chi_\nu(x,y) = \frac{1}{\rho^{5/2}} \sum_K u_{\nu K}(\rho)\, \phi_K^{\ell_x \ell_y}(\alpha)$$

NCSM 6-body diagonalization



NCSM/RGM ^{4}He(g.s.)+n+n

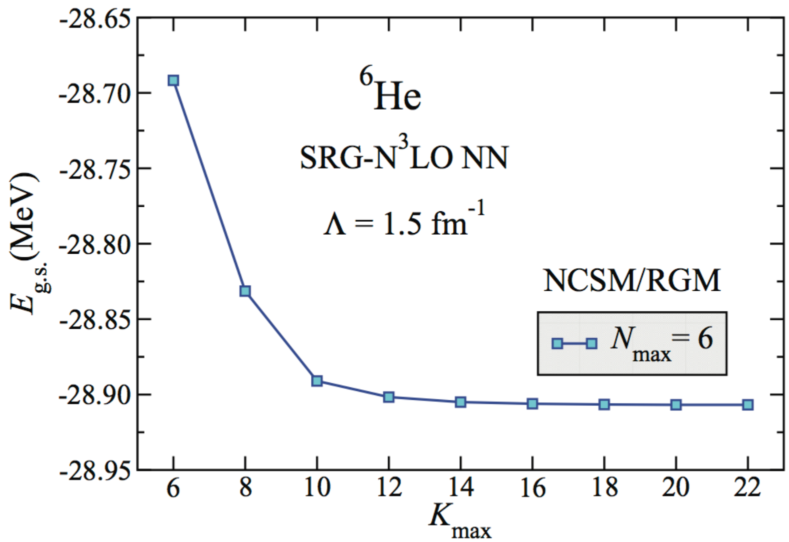


$N_{tot} = N_0 + N_{max}$	^{4}He NCSM	^{6}He NCSM/RGM	^{6}He NCSM
6	– 27.984	– 28.907	– 27.705
8	– 28.173	– 28.616	– 28.952
10	– 28.215	– 28.696	– 29.452
12	– 28.224	– 28.697	– 29.658
Extrapolation	– 28.230(5)	– 28.70(3)	– 29.84(4)
Experimental	– 28.296	– 29.268	

- Differences between NCSM 6-body and NCSM/RGM ^{4}He(g.s.)+n+n results due to core polarization
- Contrary to NCSM, NCSM/RGM wave function has appropriate asymptotic behavior

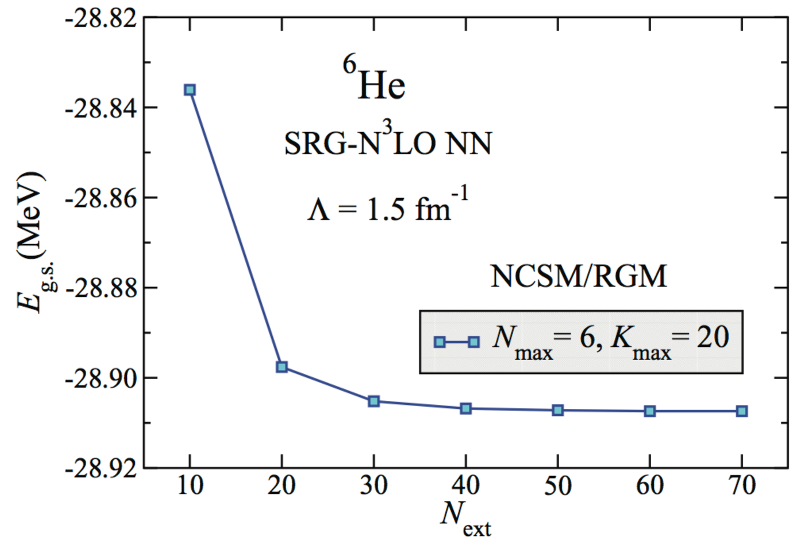
Other convergence tests

- HH expansion



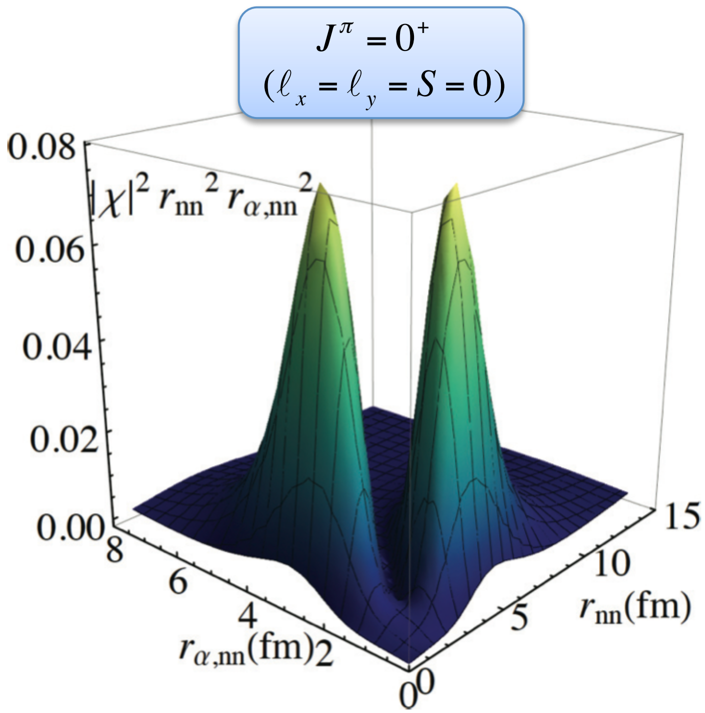
$$\chi_\nu(x,y) = \frac{1}{\rho^{5/2}} \sum_K^{K_{max}} u_{\nu K}(\rho)\, \phi_K^{\ell_x \ell_y}(\alpha)$$

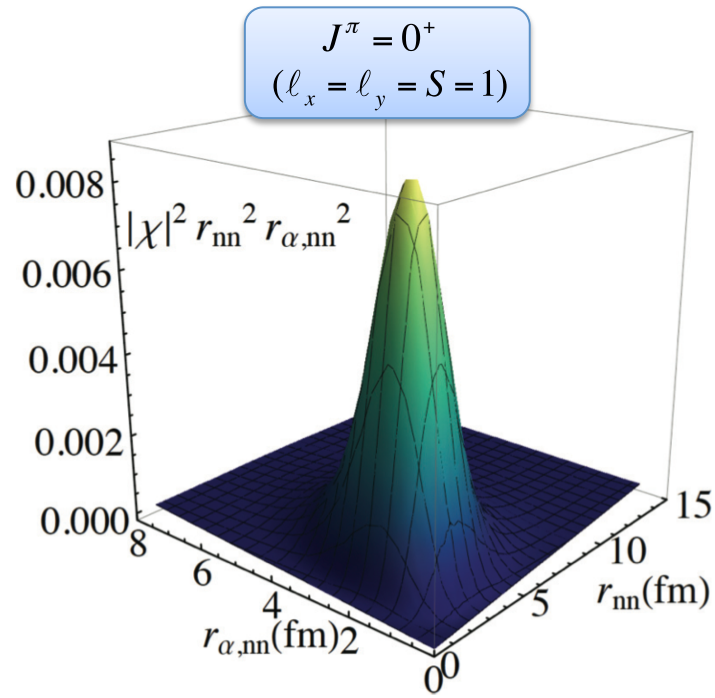
- Extended-size HO expansion



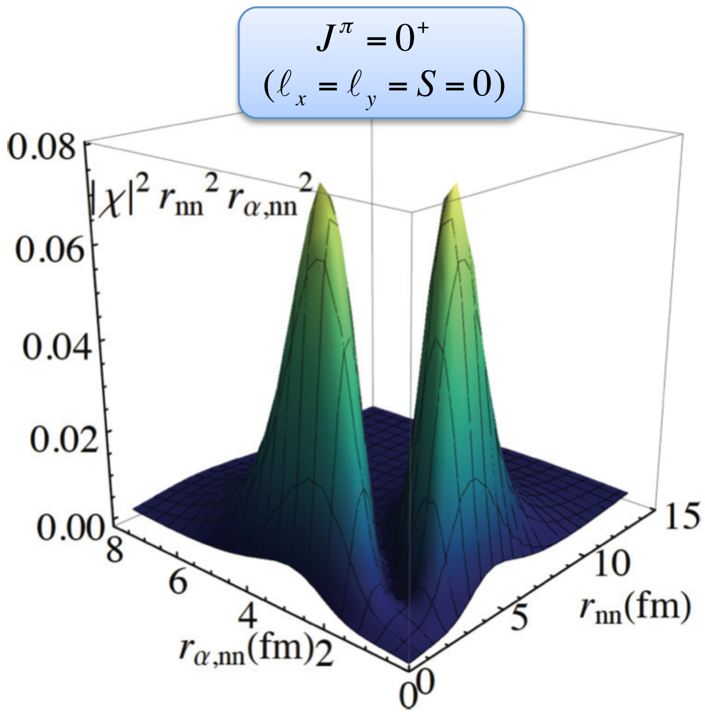
$$\left\langle V_{A-1A}\left(1-\hat{P}_{A-1,A}\right)\right\rangle \propto \sum_{n_y} R_{n_y \ell_y}(y') R_{n_y \ell_y}(y)$$

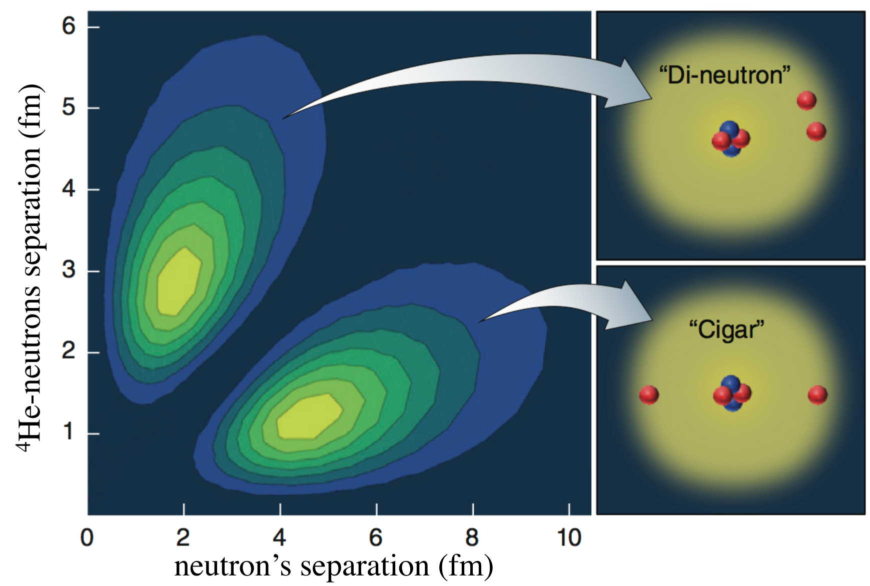
Probability density of ^{6}He ground state





Probability density of ^6He ground state

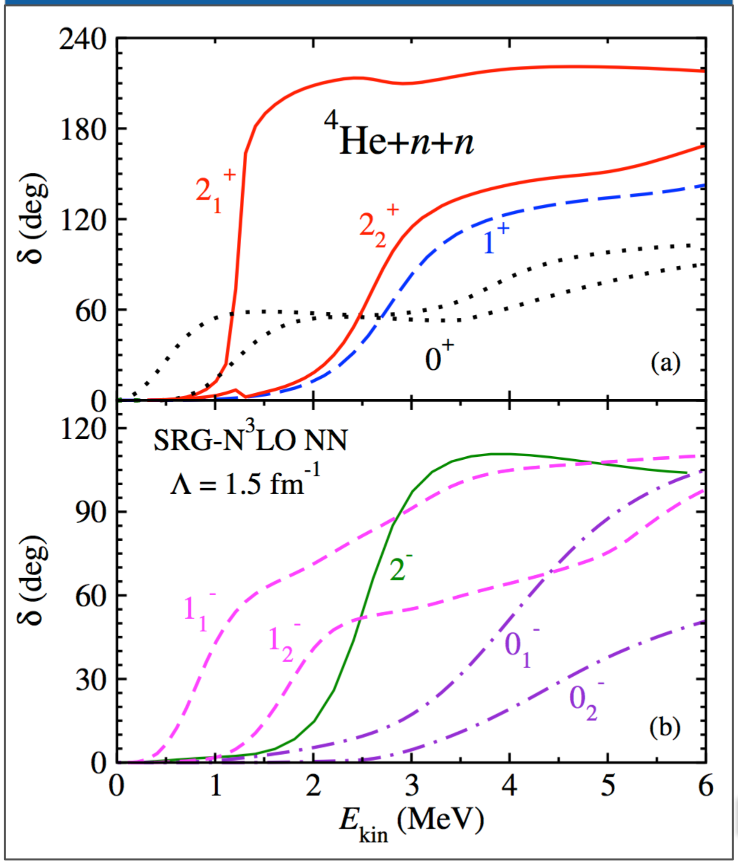




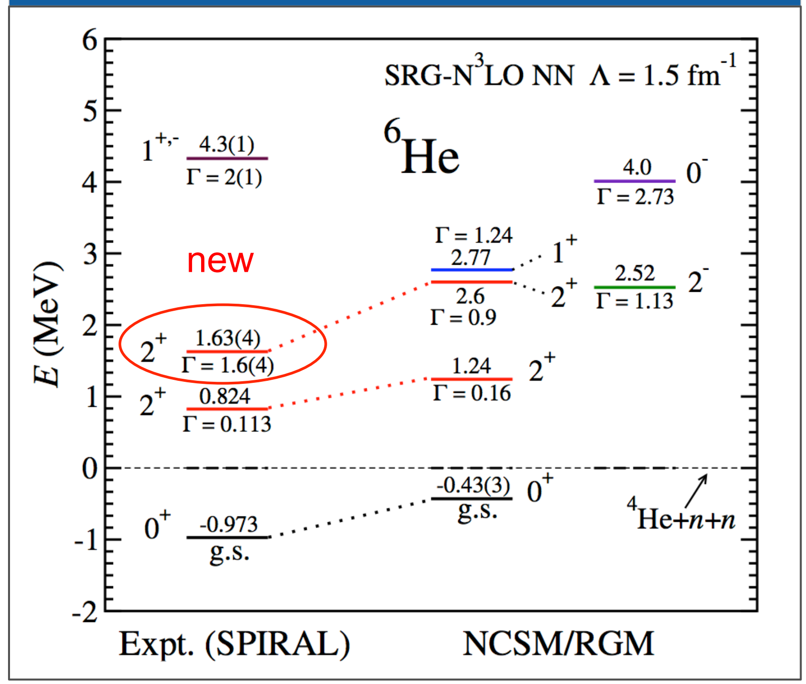
Results for ^{4}He(g.s.)+n+n continuum

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

Scattering phase shifts

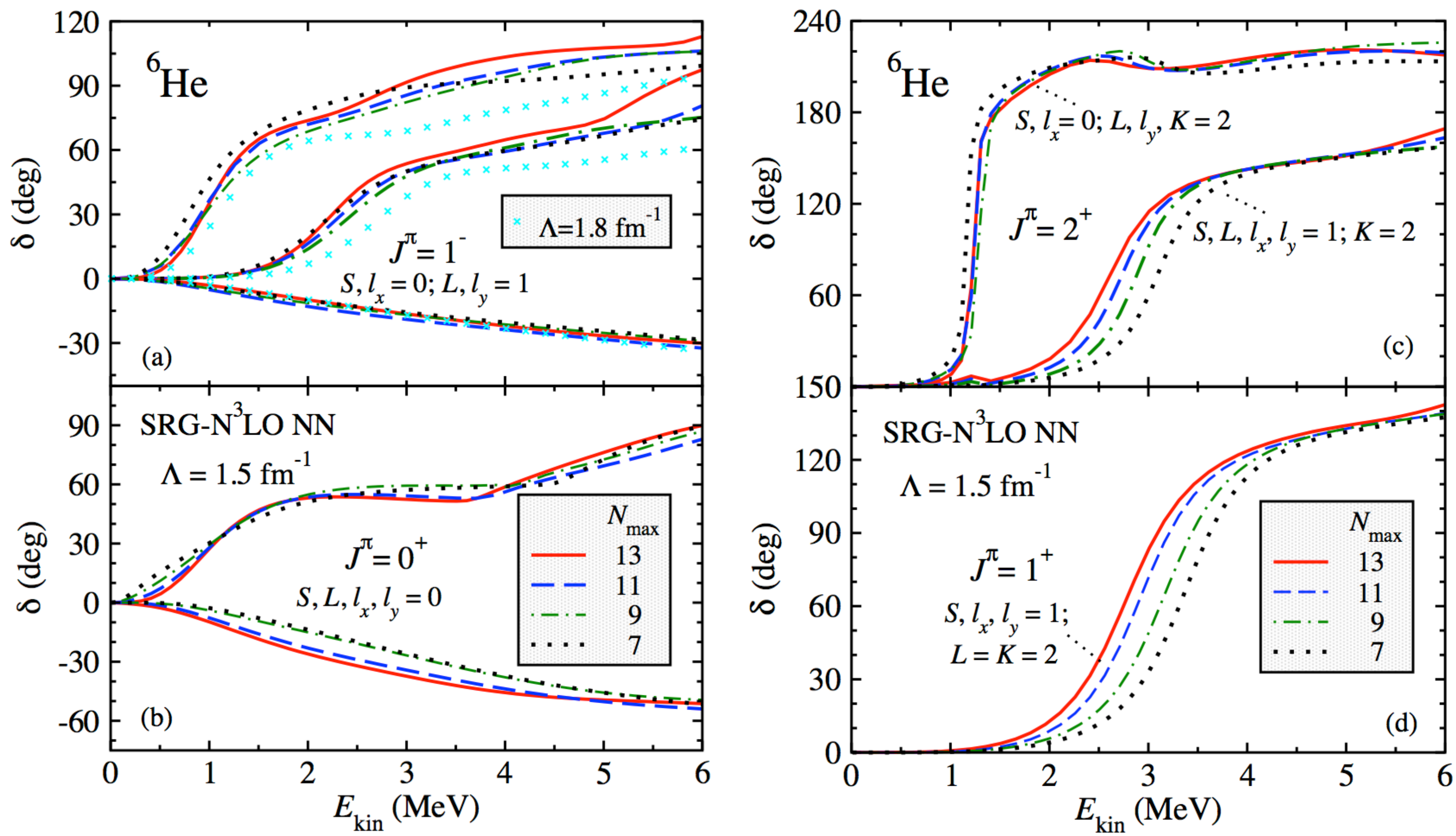


Energy spectrum of states

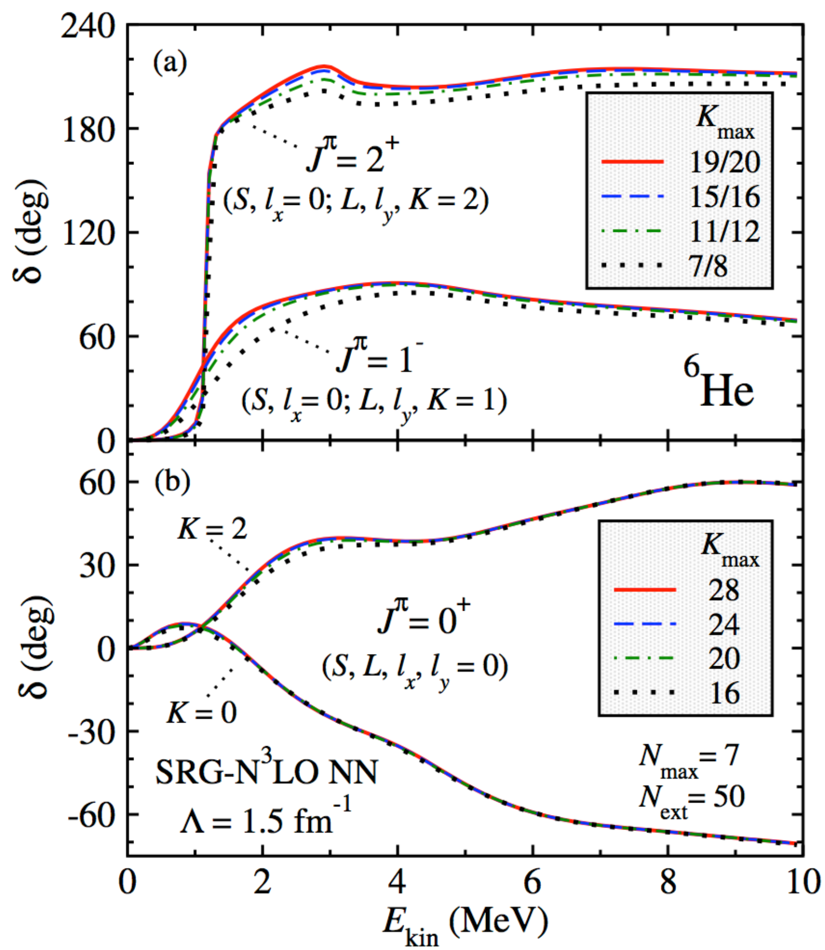


$$\Gamma = \frac{2}{\left.\dfrac{d\delta(E)}{dE}\right|_{E=E_R}}$$

Convergence with respect to HO model space size



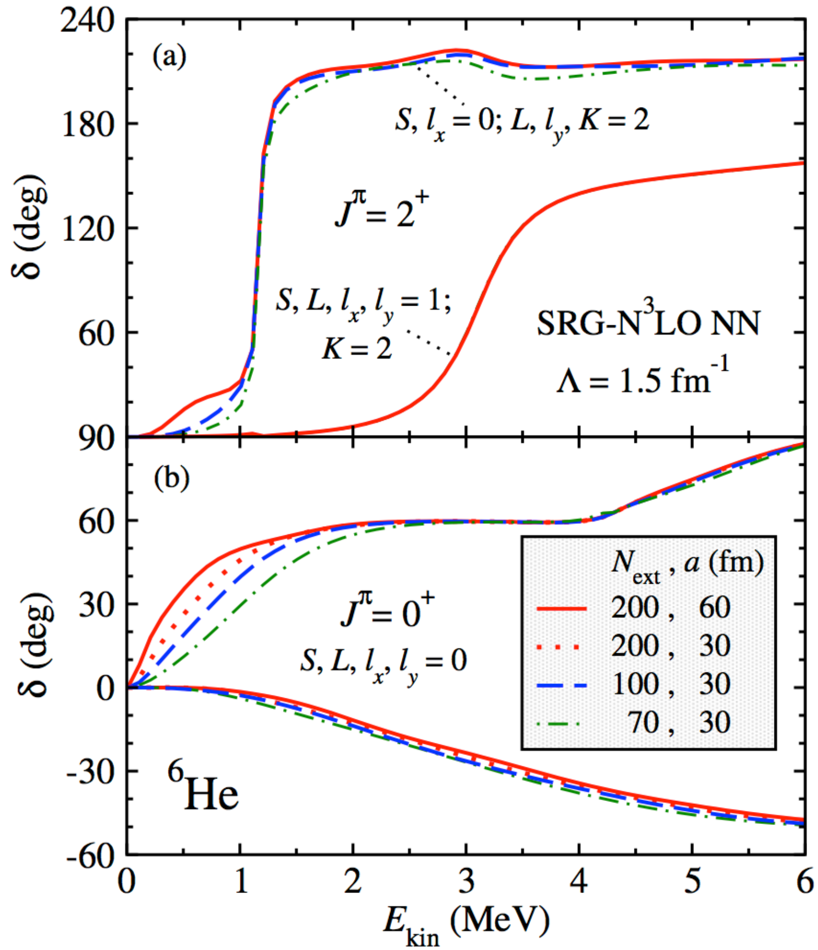
Other convergence tests



- HH expansion

$$\chi_\nu(x,y) = \frac{1}{\rho^{5/2}} \sum_{K}^{K_{max}} u_{\nu K}(\rho)\, \phi_K^{\ell_x \ell_y}(\alpha)$$

Other convergence tests



- Extended-size HO expansion

$$\left\langle V_{A-1A}\left(1-\hat{P}_{A-1,A}\right)\right\rangle \propto \sum_{n_y}^{N_{ext}} R_{n_y\ell_y}(y')R_{n_y\ell_y}(y)$$

- Sizable effects only when neutrons are in $^1S_0$ partial wave (strong attraction)

Conclusions

- We are building an efficient ab initio theory including the continuum
  - NCSM eigenstates → short- to medium-range A-body structure
  - NCSM/RGM cluster states → scattering physics of the system
- We map the many-body problem into a few-cluster problem
  - The Pauli exclusion principle is treated exactly
  - Inter-cluster interactions arise from underlying nuclear Hamiltonian
- First ab initio description of three-cluster dynamics
  - ^{4}He+n+n bound and continuum states
  - Good qualitative description of the low-lying spectrum of ^{6}He

Outlook

- For a complete picture we need to:
  - Run calculations with NNN forces (codes are ready)
  - Introduce core excitations by coupling to NCSM A-body eigenstates
- Future applications of three-cluster formalism
  - Calculations of radii, electric dipole transitions
  - Other systems: ^{5}H (^{3}H+n+n), ^{11}Li (=^{9}Li+n+n), ^{12}Be(=^{10}Be+n+n)
- Ultimate goal: binary & ternary light-nucleus fusion reactions
  - Transfer reactions: ^{3}H(^{3}H,2n)^{4}He