TRIUMF

Canada's national laboratory
for particle and nuclear physics
and accelerator-based science

Ab initio calculations for exotic nuclei

2018 CAP congress

Halifax – June 13, 2018

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Outline

1. Exotic structure of ^{9}He from the no-core shell model with continuum
   - Motivation
   - Basic features of the NCSMC
   - Results for ^{9}He

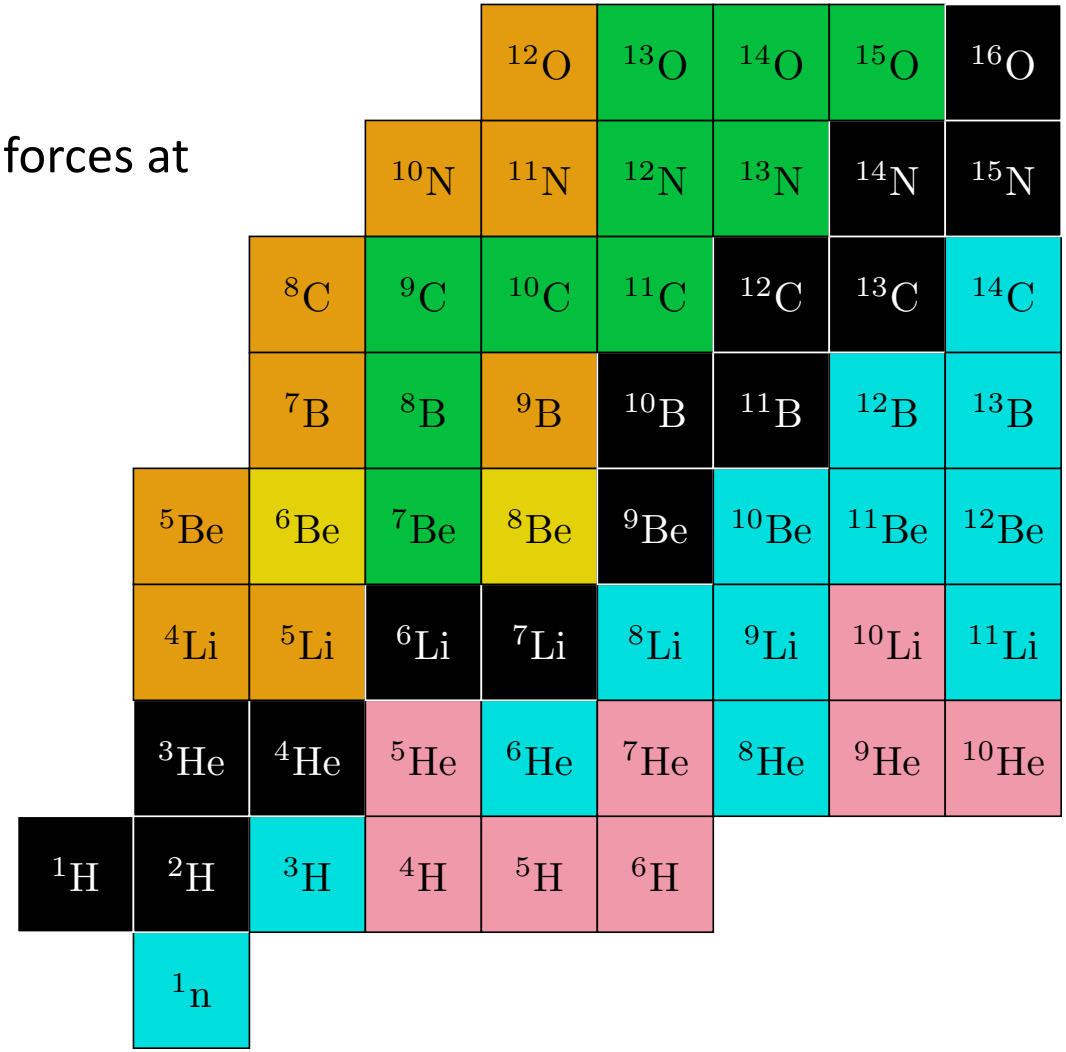
2. Microscopic optical potentials with nonlocal ab initio densities for intermediate energies
   - Results for stable nuclei
   - Results for ^{6}He and ^{8}He

1.

Exotic structure of ^{9}He

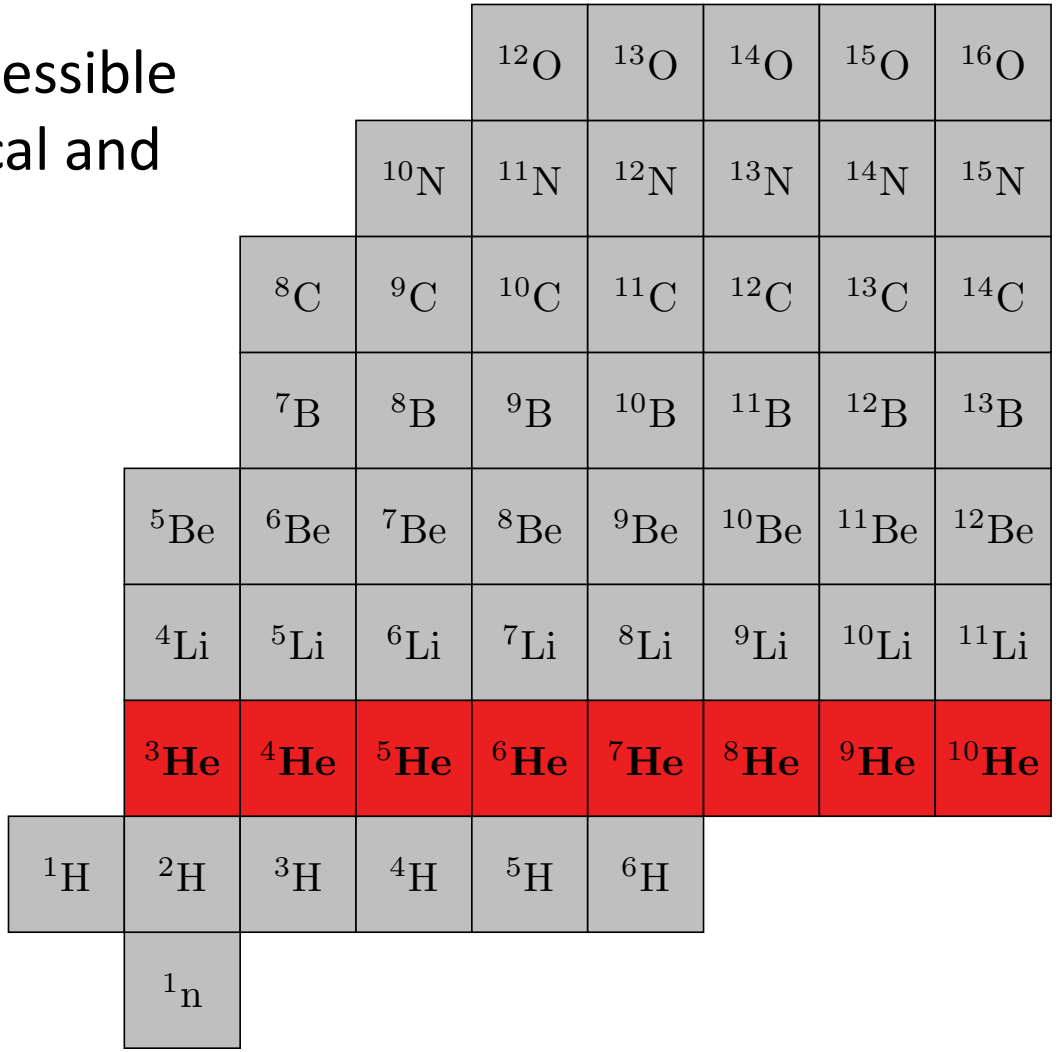
Neutron-rich nuclei

- Theory
  - Importance of many-body forces at extreme neutron excesses
  - Challenge to our current computational techniques
- Experiment
  - Difficult to produce in sufficient quantities
  - Challenging to analyze



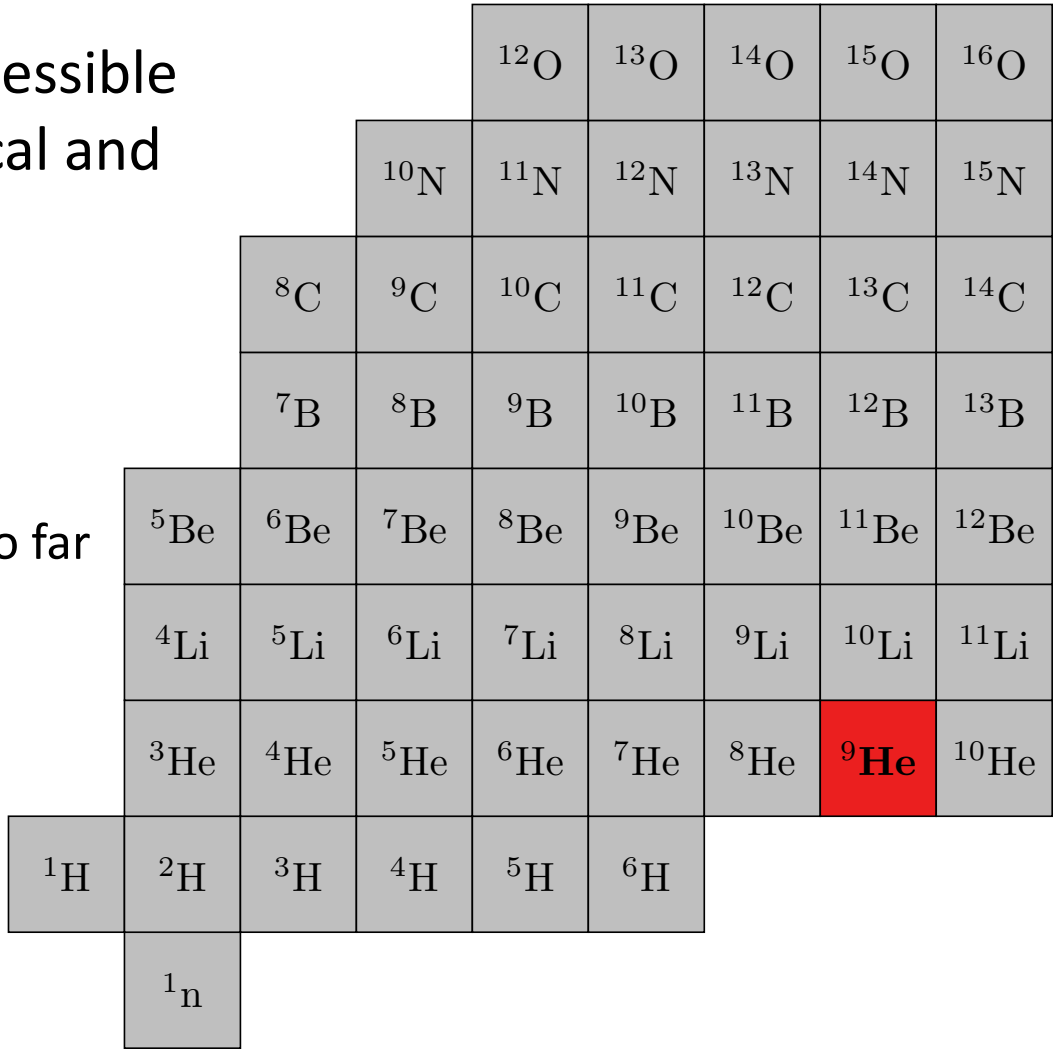
The He isotopic chain

- One of the few chains accessible to both detailed theoretical and experimental studies



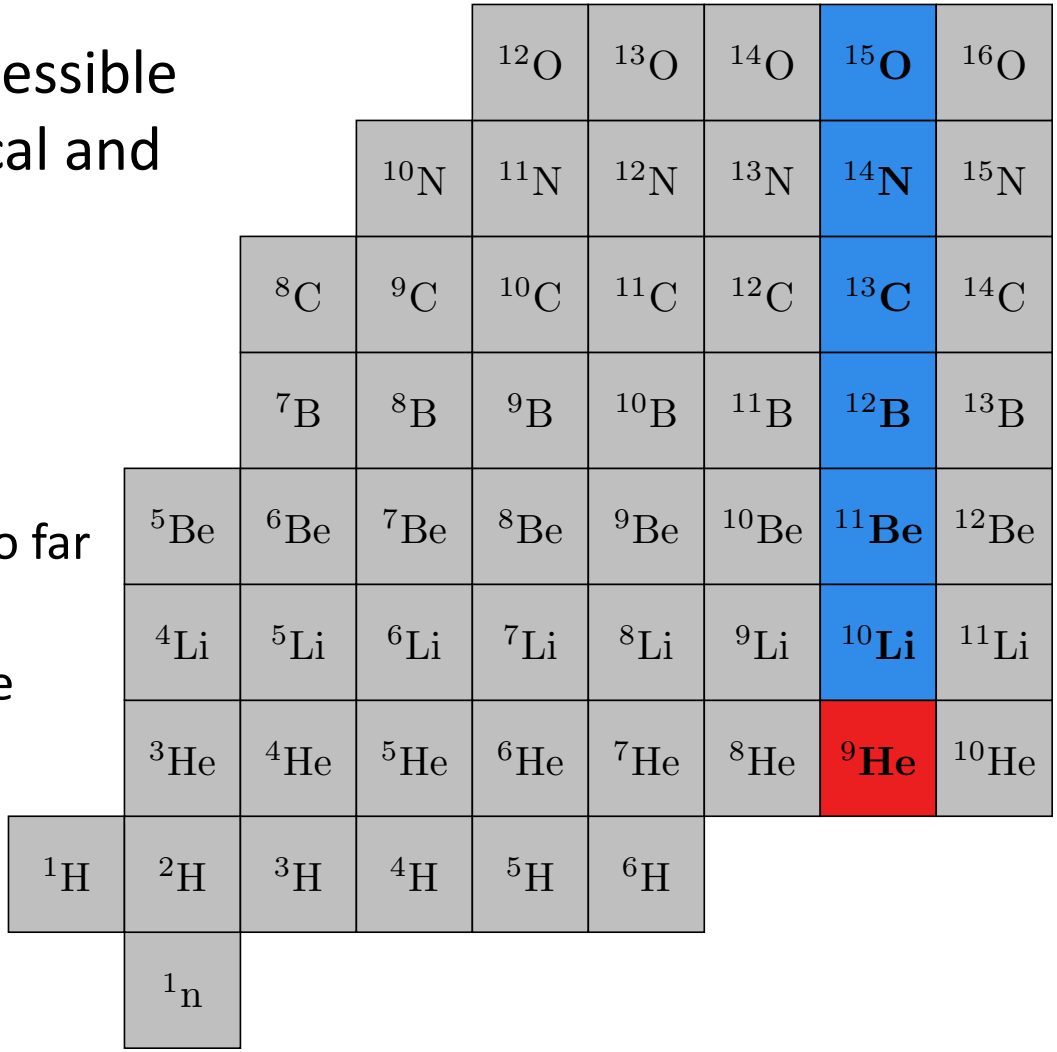
The He isotopic chain

- One of the few chains accessible to both detailed theoretical and experimental studies
- **^{9}He system**
  - Characterized by N/Z = 3.5
  - One of the most neutron extreme systems studied so far

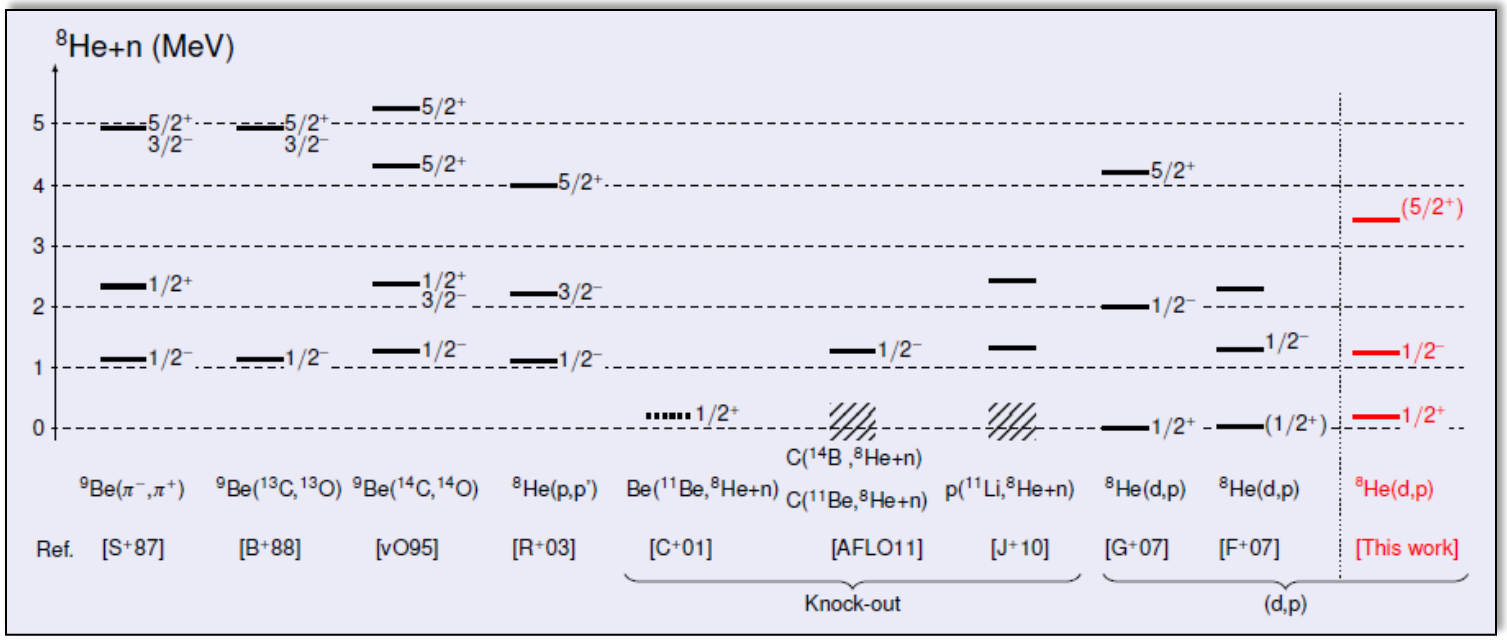


The He isotopic chain

- One of the few chains accessible to both detailed theoretical and experimental studies
- **^{9}He system**
  - Characterized by N/Z = 3.5
  - One of the most neutron extreme systems studied so far
  - Possible candidate for a positive parity ground state
    Famous example: ^{11}Be



Experimental history of ^{9}He

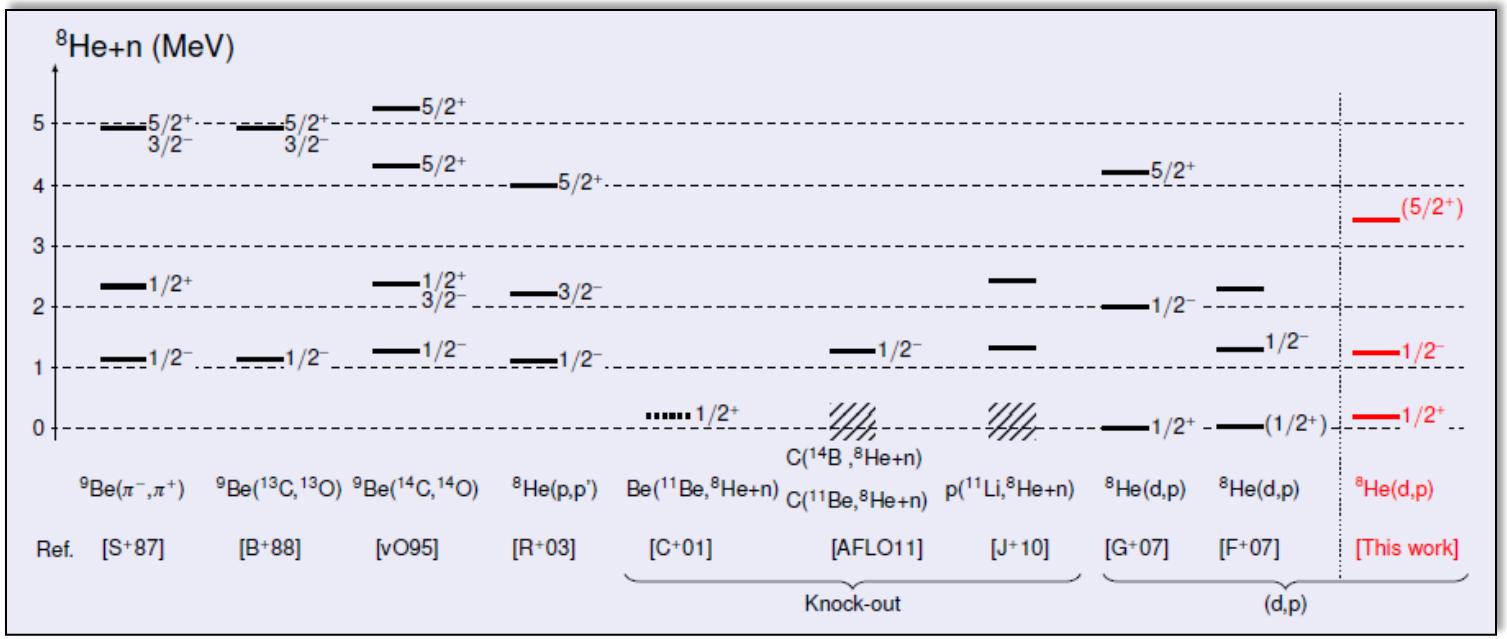


From talk by Nigel Orr at ECT* (2013)

Controversial experimental situation

- No bound state
- Most experiments see a $1/2^-$ resonance at ~ 1 MeV
- Is there a $1/2^+$ resonance? Is the ground state $1/2^+$ or $1/2^-$?
  - a_0~ -10 fm (Chen et al.)
  - a_0~ -3 fm (Al Falou, et al.)
- Any higher-lying resonances?
- Recent ^{8}He(p,p) measurement at TRIUMF by Rogachev: PLB **754** (2016) 323
  Found no T=5/2 resonances

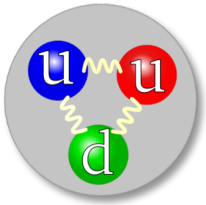
Experimental history of ^{9}He



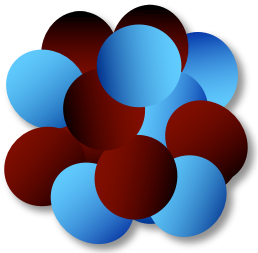
From talk by Nigel Orr at ECT* (2013)

Two long-standing problems affect the physics of the ^{9}He system

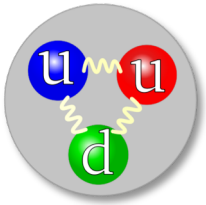
1. The existence of the $1/2^{+}$ state
2. The width of the $1/2^{-}$ state
   - Experimentally ~ 0.1 MeV
   - Theoretically ~ 1 MeV

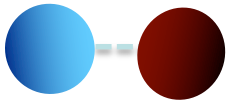


Low-energy QCD



Nuclear structure and reactions

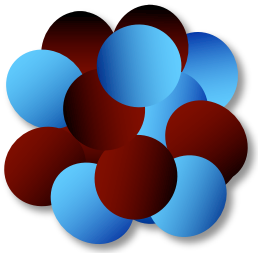




Low-energy QCD

NN+3N interactions from chiral EFT

...or accurate meson-exchange potentials



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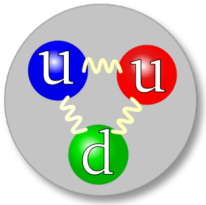

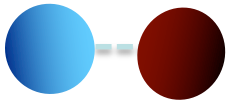

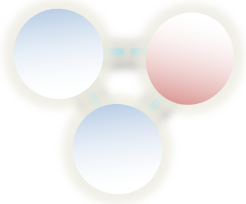

Low-energy QCD

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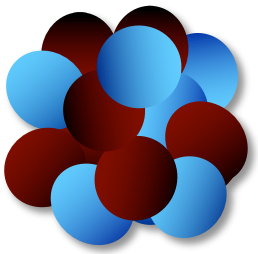
Unitary/similarity transformations

SRG
Softens NN, induces 3N

$$H|\Psi\rangle = E|\Psi\rangle$$



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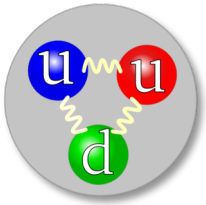

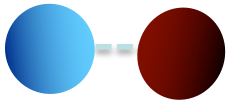

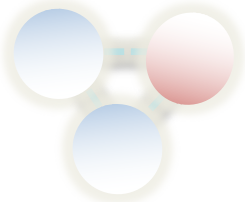

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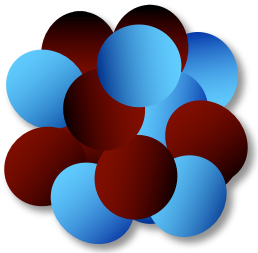


Low-energy QCD

NN+3N interactions from chiral EFT

...or accurate meson-exchange potentials

Unitary/similarity transformations

SRG
Softens NN, induces 3N

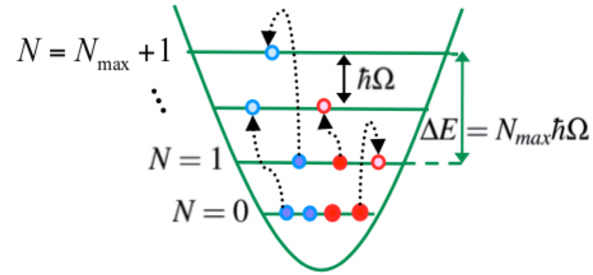
Many-Body methods

NCSM, NCSMC, CCM, IM-SRG, SCGF, GFMC, HH, Nuclear Lattice EFT...

Nuclear structure and reactions

Unified approach to bound & continuum states; to nuclear structure & reactions

- *Ab initio* no-core shell model
  - Short- and medium range correlations
  - Bound-states, narrow resonances



Harmonic oscillator basis

NCSM

$$\Psi^{(A)} = \sum_{\lambda} c_{\lambda} \left|^{(A)}\right.$$ $$, \lambda \rangle$$

Unknowns

Unified approach to bound & continuum states; to nuclear structure & reactions

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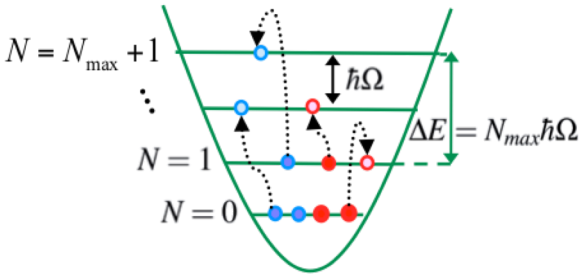
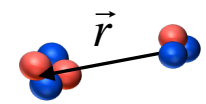


Harmonic oscillator basis

NCSM

- …with resonating group method
  - Bound & scattering states, reactions
  - Cluster dynamics, long-range correlations



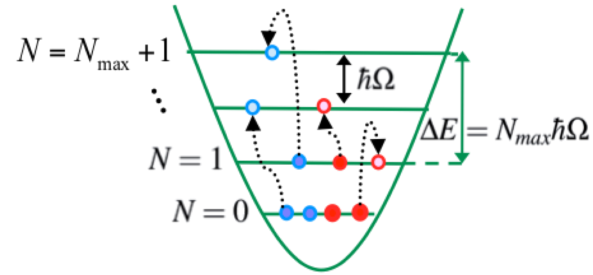
NCSM/RGM

NCSM/RGM channel states

$$\Psi^{(A)} = \sum_{\nu} \int d\vec{r}\ \gamma_{\nu}(\vec{r})\ \hat{A}_{\nu} \left| \underset{(A-a)}{\bullet} \overset{\vec{r}}{\text{———}} \underset{(a)}{\bullet}, \nu \right\rangle$$

Unknowns

- *Ab initio* no-core shell model
  - Short- and medium range correlations
  - Bound-states, narrow resonances



Harmonic oscillator basis

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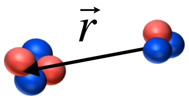


NCSM/RGM

- Most efficient: *ab initio* no-core shell model with continuum

NCSMC

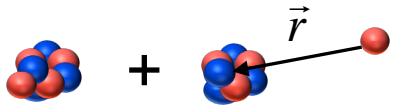
$$\Psi^{(A)} = \sum_{\lambda} c_{\lambda} \left| {}^{(A)} \; , \lambda \right\rangle + \sum_{\nu} \int d\vec{r} \; \gamma_{\nu}(\vec{r}\,) \; \hat{A}_{\nu} \left| \underset{(A-a)}{} \; \vec{r} \; \underset{(a)}{} \; , \nu \right\rangle$$

NCSM eigenstates (over the first term); NCSM/RGM channel states (over the second term)

Unknowns (c_{λ} and γ_{ν})

- NCSMC calculations with several interactions
  - N^2LO_{sat} NN + 3N
  - NN N^3LO + 3N N^2LO
  - **SRG-N^4LO500 NN**

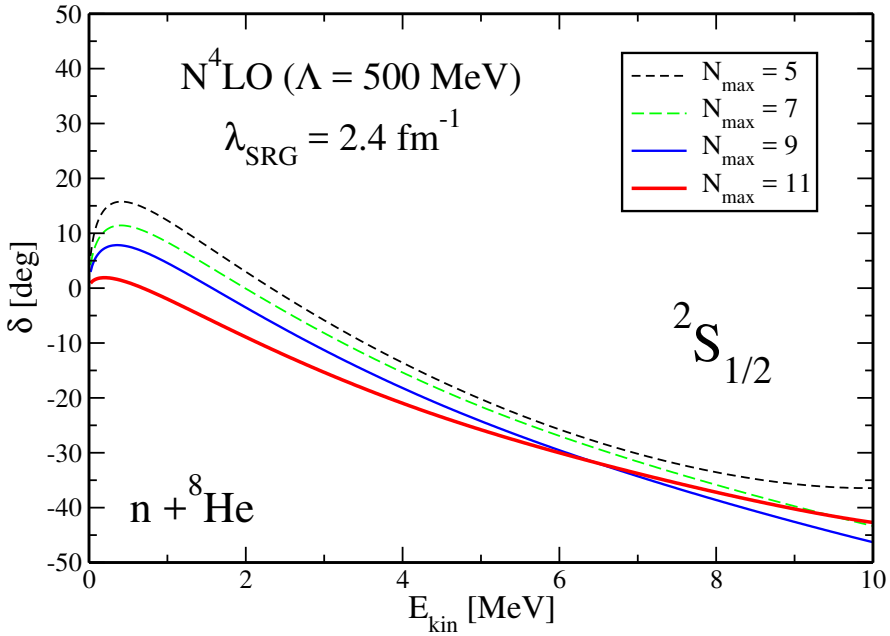
- Calculations with SRG-N^4LO500 NN
  - $^{9}He \sim (^{9}He)_{NCSM} + (n\text{-}^{8}He)_{NCSM/RGM}$
    - ^{8}He: 0^+ and 2^+ NCSM eigenstates
    - ^{9}He: 4 negative-parity NCSM eigenstates
      6 positive-parity NCSM eigenstates



  - Importance of large N_{max} basis:
    - SRG-N^4LO500 NN with λ=2.4 fm^{-1}
      up to N_{max} = 11 with ^{9}He NCSM (m-scheme basis of 350 million)

Phase shift convergence with SRG-N^{4}LO500 NN λ=2.4 fm^{-1}

Vorabbi, Calci, Navratil, Kruse, Quaglioni, Hupin, PRC **97**, 034314 (2018)



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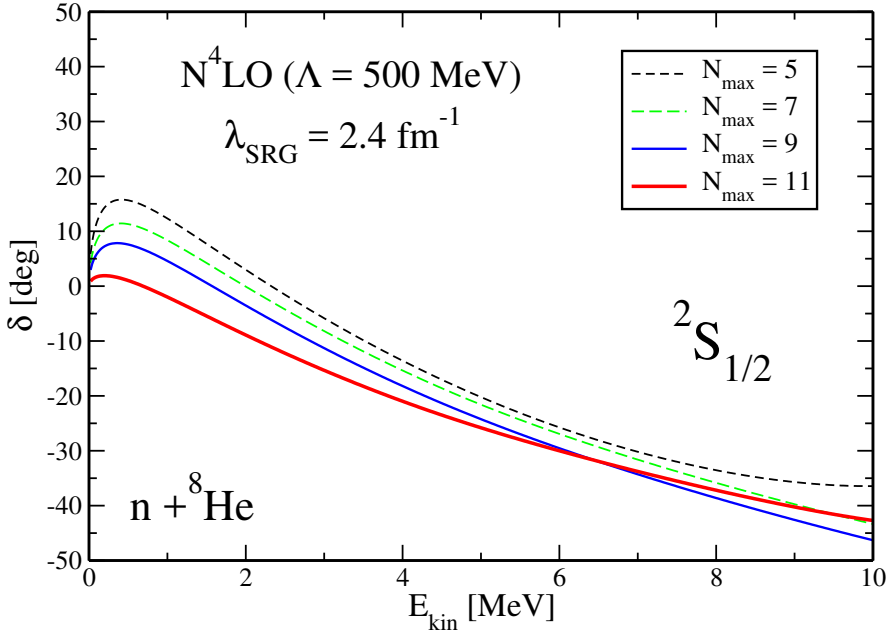

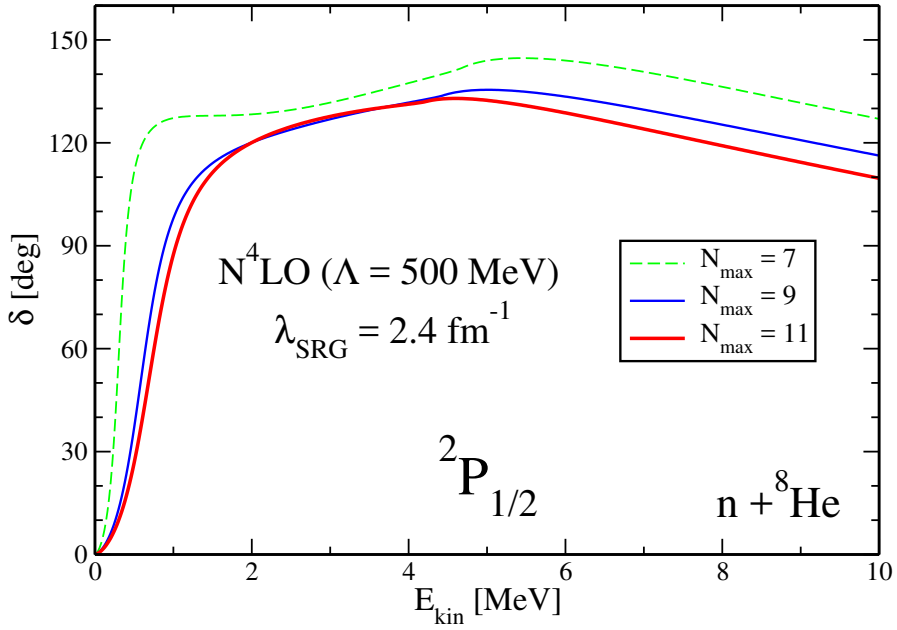

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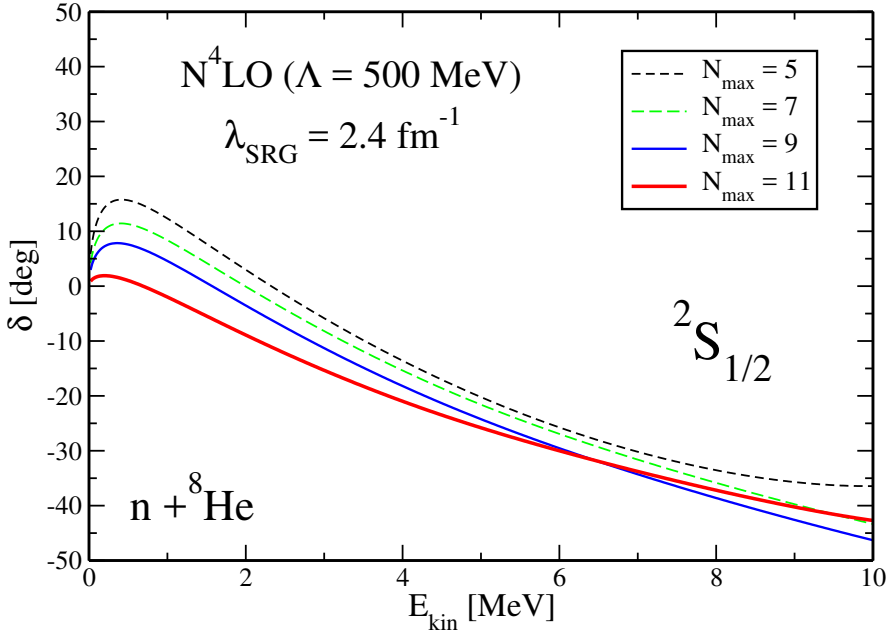
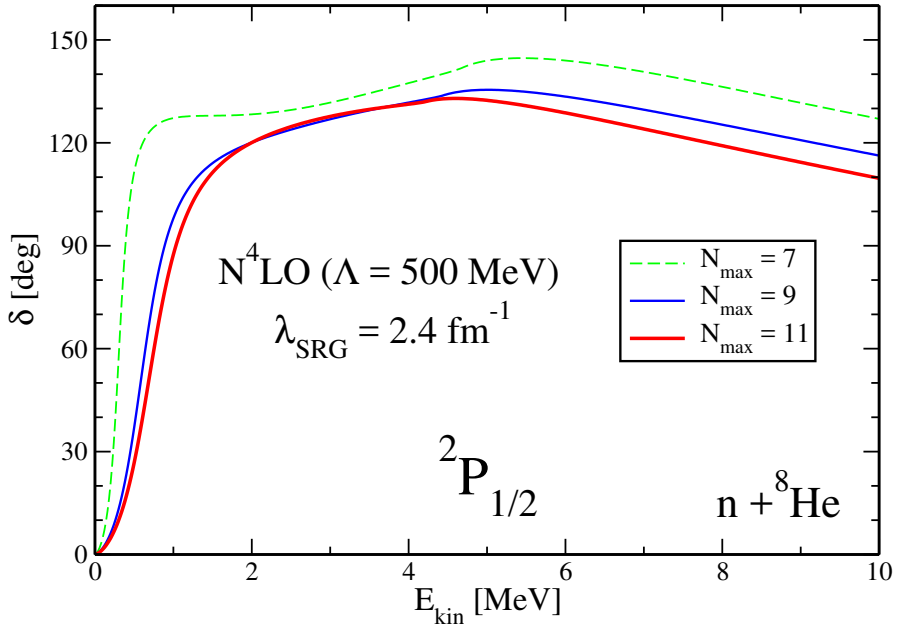
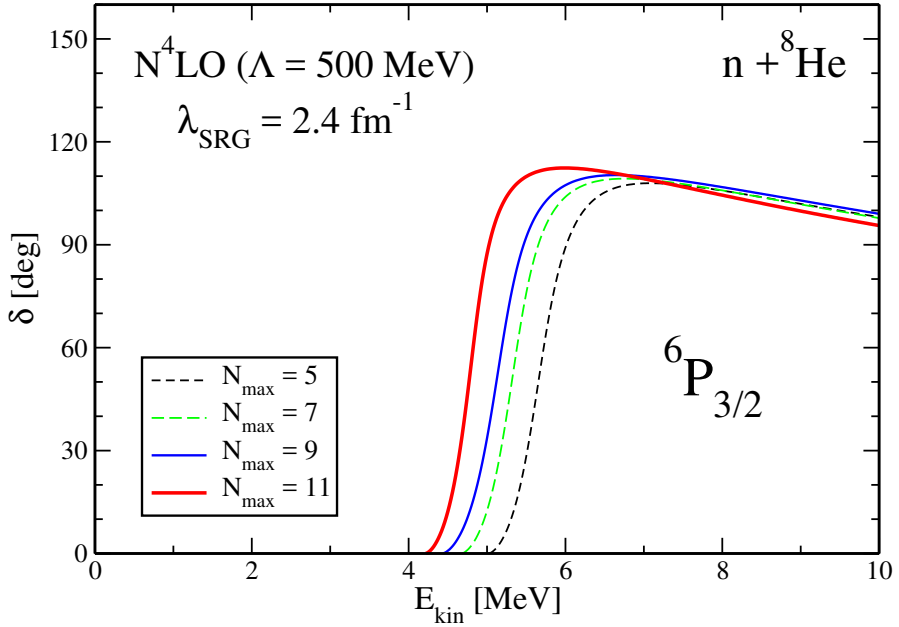






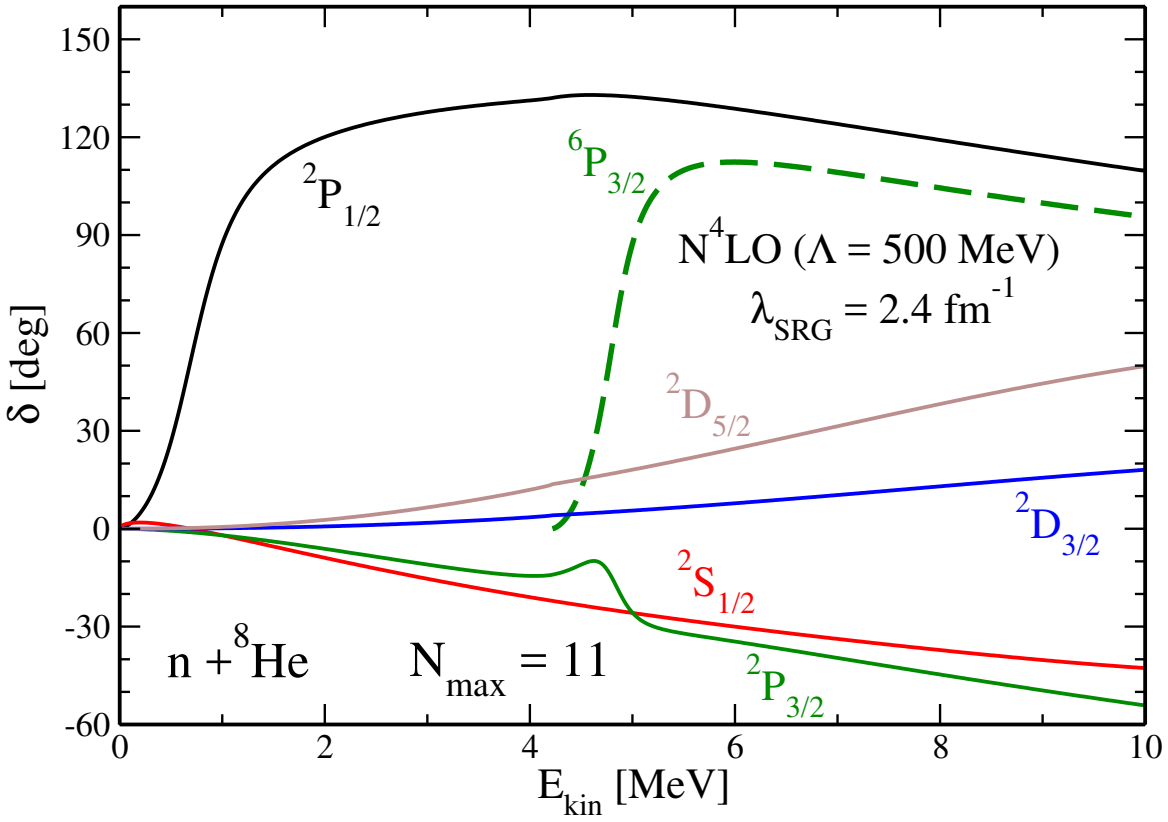
Phase shifts with SRG-N^{4}LO500 NN λ=2.4 fm^{-1}

Energy spectrum

No bound state

Two resonances in the $2P_{1/2}$ and $^6P_{3/2}$ channels

No resonance in the $^2S_{1/2}$ state



Vorabbi, Calci, Navratil, Kruse, Quaglioni, Hupin, PRC **97**, 034314 (2018)

Eigenphase shifts with SRG-N^{4}LO500 NN λ=2.4 fm^{-1}

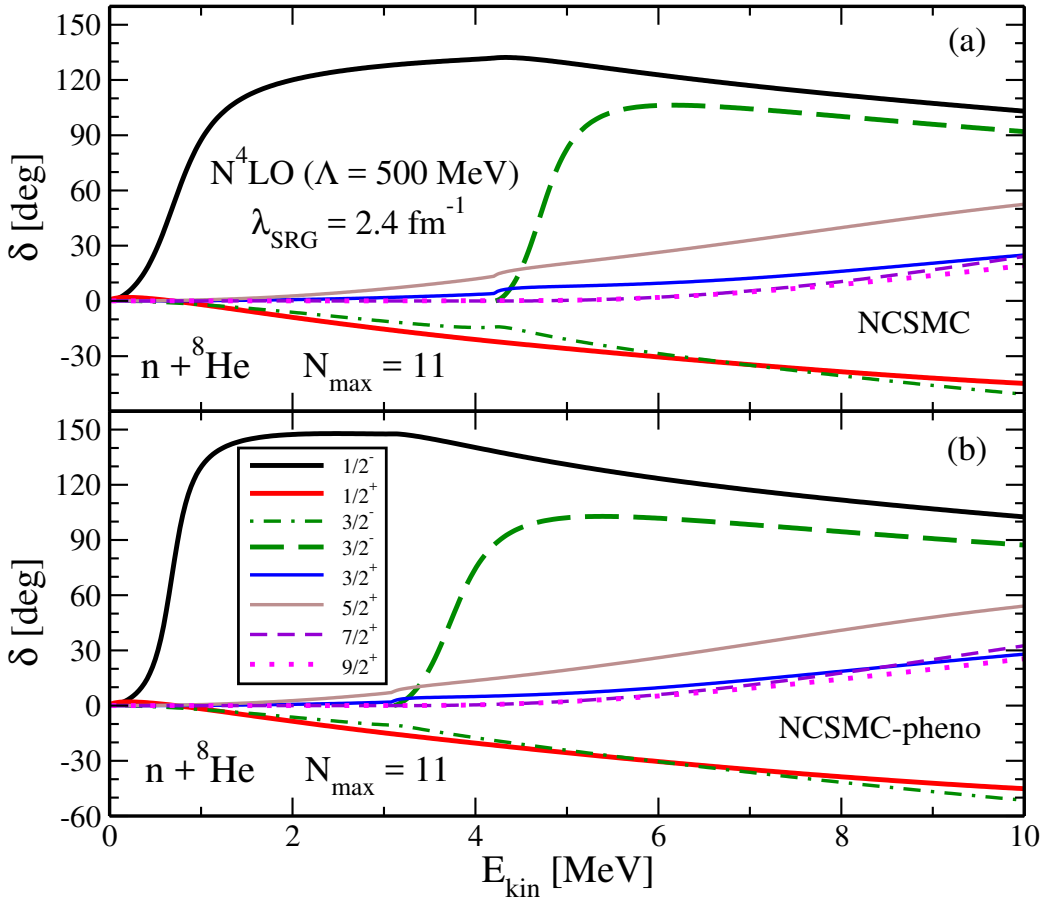
Vorabbi, Calci, Navratil, Kruse, Quaglioni, Hupin, PRC **97**, 034314 (2018)

Summary

Robust results for **1/2$^-$** (~ 1MeV) and **3/2$^-$** (~4 MeV) **P-wave** resonances (3/2$^-$ resonance in n-^{8}He(2$^+$) channel)

1/2$^+$ S-wave with vanishing scattering length: a_s= 0 ~ -1 fm

No evidence for other higher lying resonances



J^π	NCSMC		NCSMC-pheno	
$1/2^-$	$E_R = 0.69$	$\Gamma = 0.83$	$E_R = 0.68$	$\Gamma = 0.37$
$3/2^-$	$E_R = 4.70$	$\Gamma = 0.74$	$E_R = 3.72$	$\Gamma = 0.95$

2.

Microscopic optical potentials for intermediate energies

The first-order optical potential

- The elastic nucleon-nucleus scattering amplitude

$$T_{\rm el}(\boldsymbol{k}', \boldsymbol{k}; E) = U(\boldsymbol{k}', \boldsymbol{k}; E) + \int d^3p \frac{U(\boldsymbol{k}', \boldsymbol{p}; E)\, T_{\rm el}(\boldsymbol{p}, \boldsymbol{k}; E)}{E - E(p) + i\epsilon}$$

- The first-order optical potential
  - Obtained from the multiple scattering theory
  - Impulse approximation

$$U(\boldsymbol{q}, \boldsymbol{K}; E) = \sum_{\alpha=n,p} \int d^3\boldsymbol{P}\, \eta(\boldsymbol{P}, \boldsymbol{q}, \boldsymbol{K}) t_{p\alpha} \left[\boldsymbol{q}, \frac{1}{2}\left(\frac{A+1}{A}\boldsymbol{K} - \boldsymbol{P}\right); E\right] \times \rho_\alpha \left(\boldsymbol{P} - \frac{A-1}{2A}\boldsymbol{q}, \boldsymbol{P} + \frac{A-1}{2A}\boldsymbol{q}\right)$$

- Extension of: Navratil, PRC **70**, 014317 (2004)

- Non-local nuclear density operator

$$\rho_{\mathrm{op}} = \sum_{i=1}^{A} \delta(\boldsymbol{r} - \boldsymbol{r}_i)\delta(\boldsymbol{r}' - \boldsymbol{r}'_i)$$

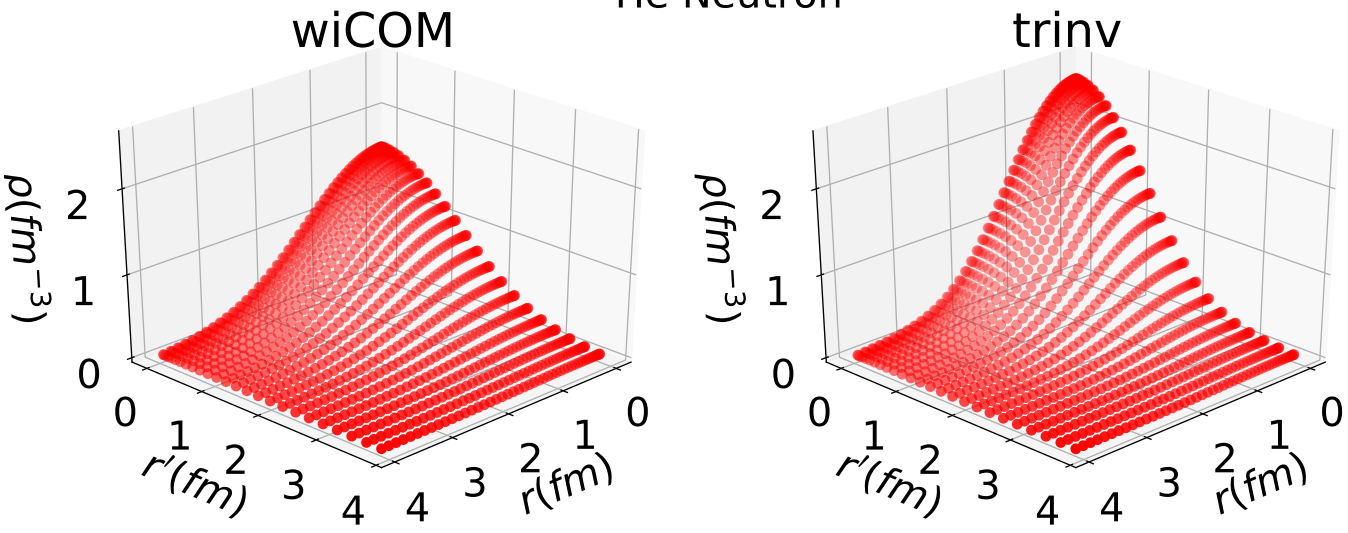
- The matrix elements between a general initial and final state are obtained from the NCSM in the Cartesian coordinate single-particle Slater determinant basis

- Removal of the COM component is required
  - Enabled by the factorization of the Slater determinant and Jacobi eigenstates

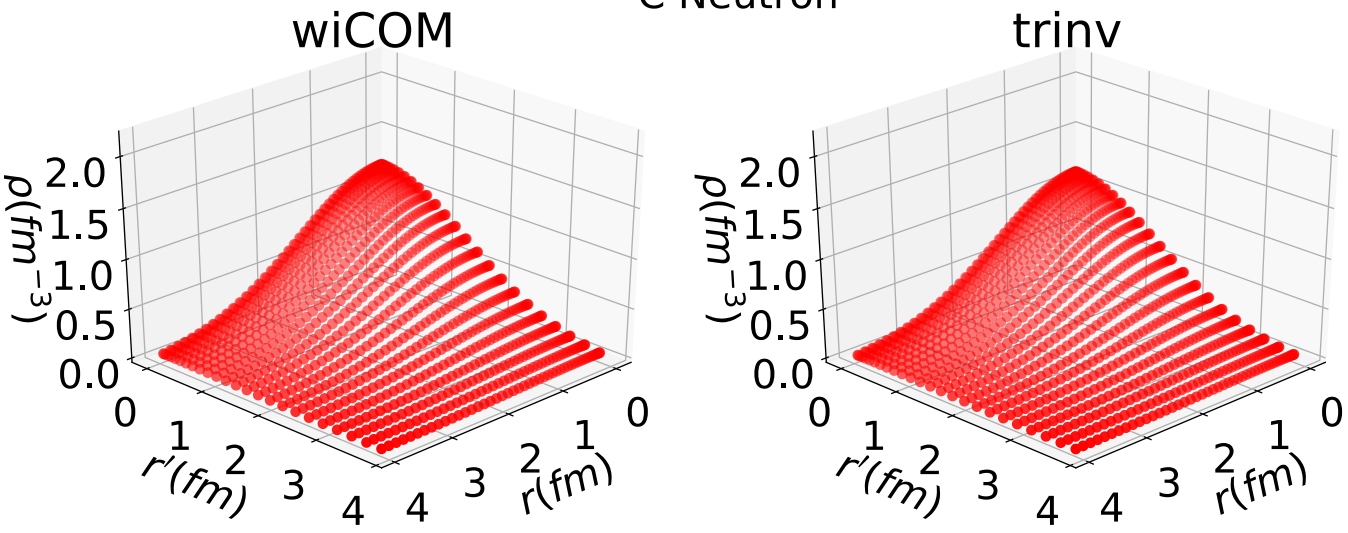
Non-local densities

Gennari, Vorabbi, Calci, Navratil, PRC **97**, 034619 (2018)

^{4}He Neutron

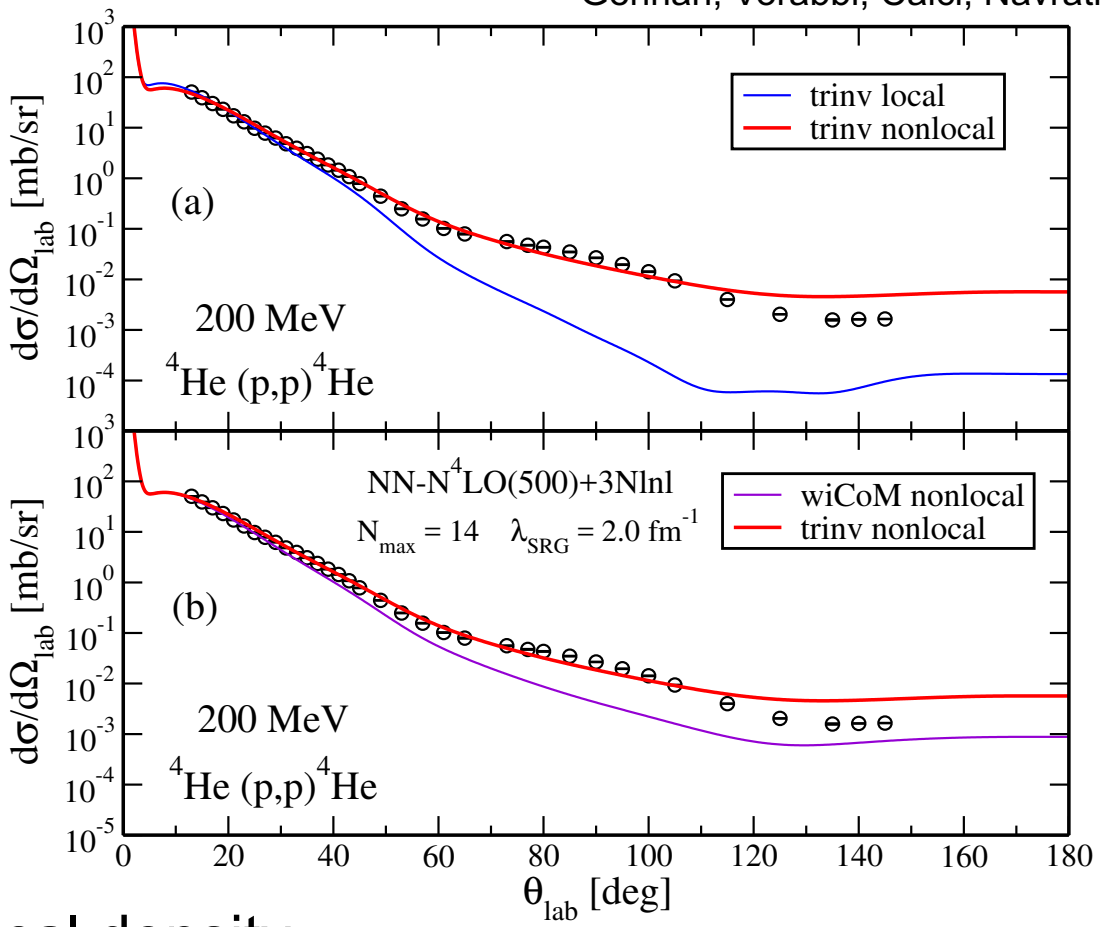


^{12}C Neutron



Scattering observables – Stable nuclei

Gennari, Vorabbi, Calci, Navratil, PRC **97**, 034619 (2018)



FF from local density

$$\rho_\alpha(q) = 4\pi \int_0^\infty dr r^2 j_0(qr)\rho_\alpha(r)$$

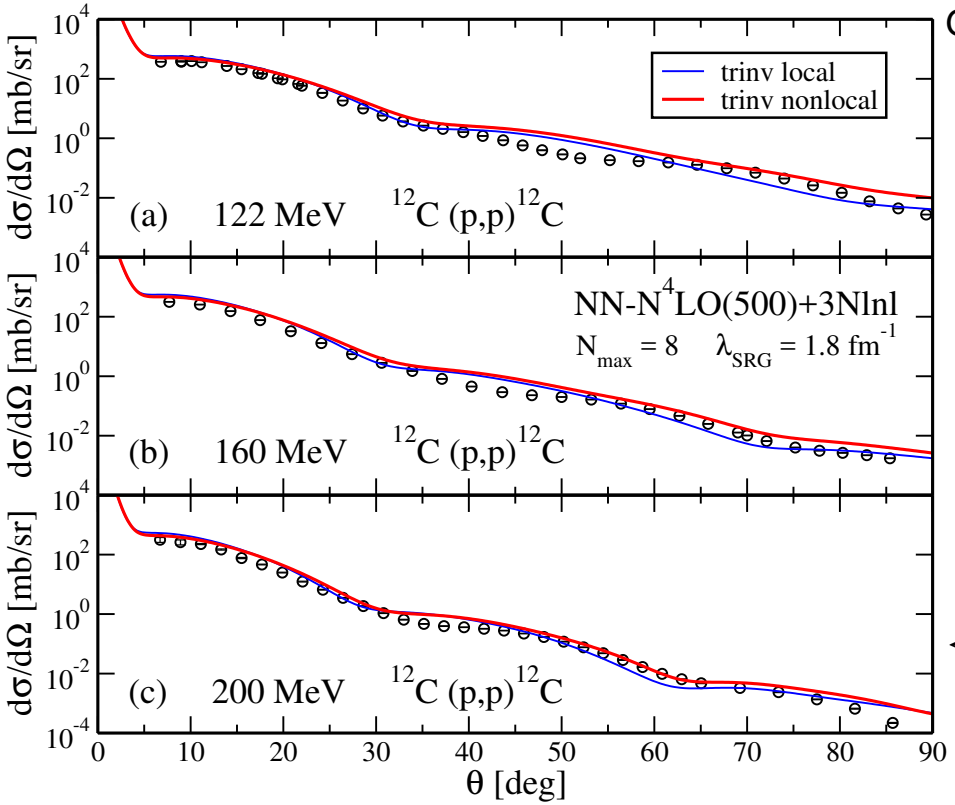
Navratil, PRC **70**, 014317 (2004)

Factorized optical potential

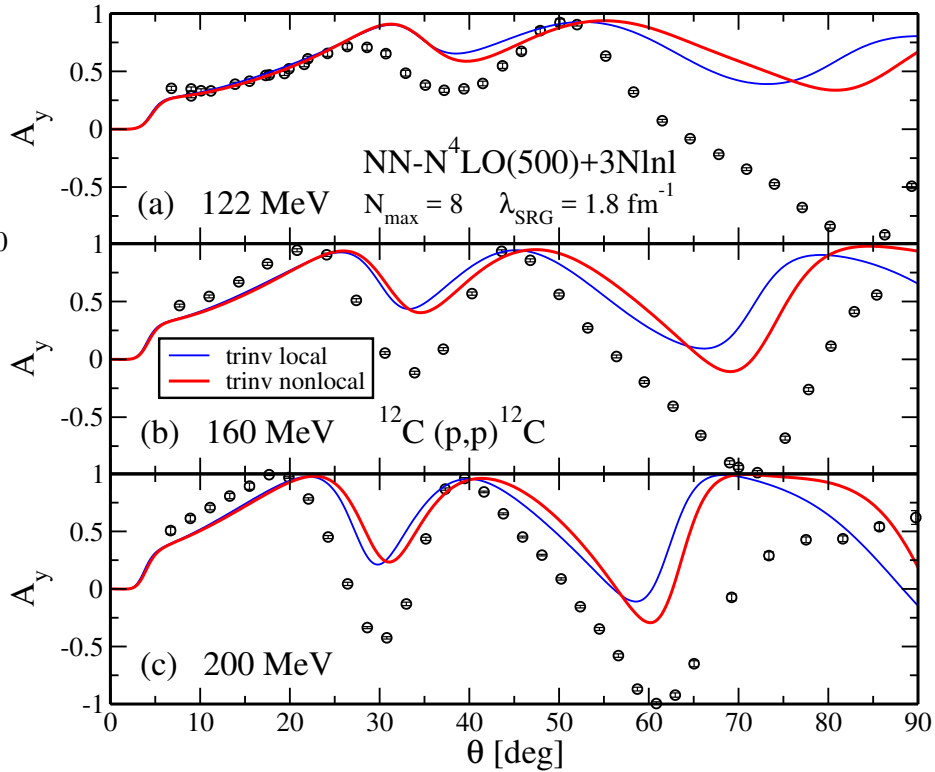
$$U(\boldsymbol{q}, \boldsymbol{K}; E) \sim \sum_{\alpha=n,p} t_{p\alpha}\left[\boldsymbol{q}, \frac{A+1}{2A}\boldsymbol{K}; E\right]\rho_\alpha(q)$$

Scattering observables – Stable nuclei

Gennari, Vorabbi, Calci, Navratil, PRC **97**, 034619 (2018)



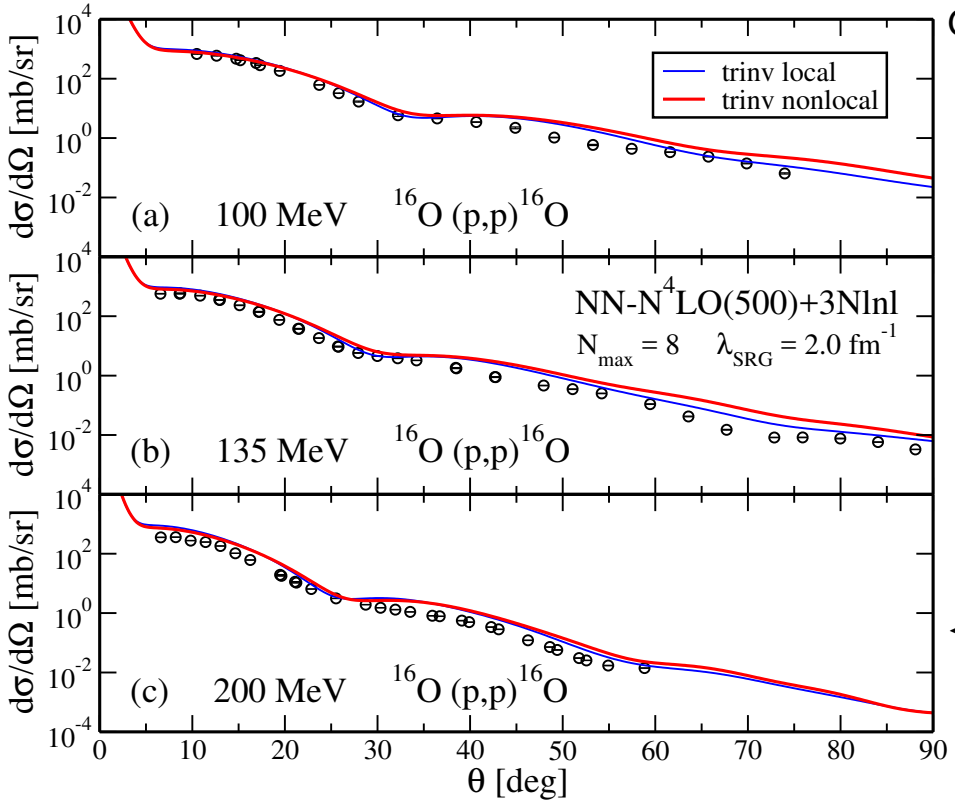
Good description of differential cross sections

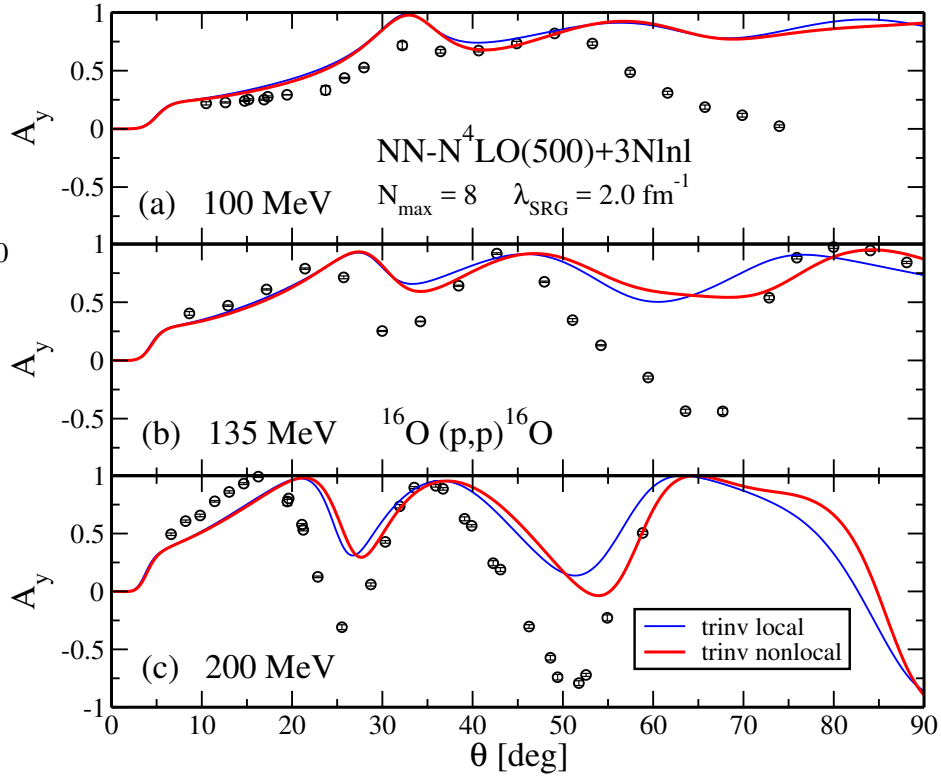


Reproduction of the general trend of the A_y

Scattering observables – Stable nuclei

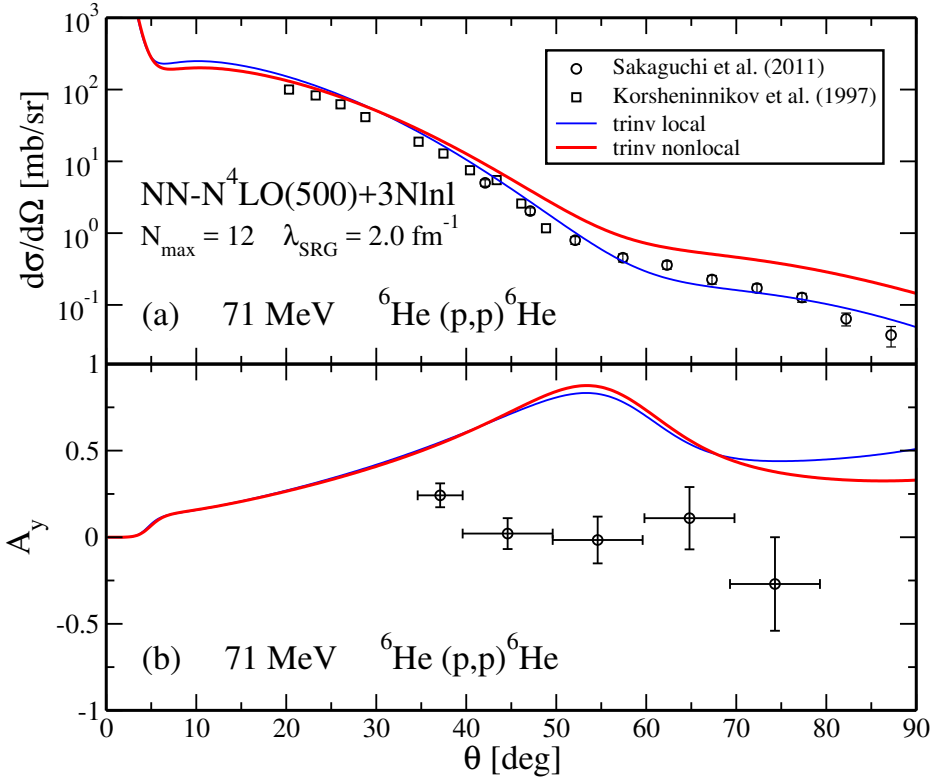
Gennari, Vorabbi, Calci, Navratil, PRC **97**, 034619 (2018)



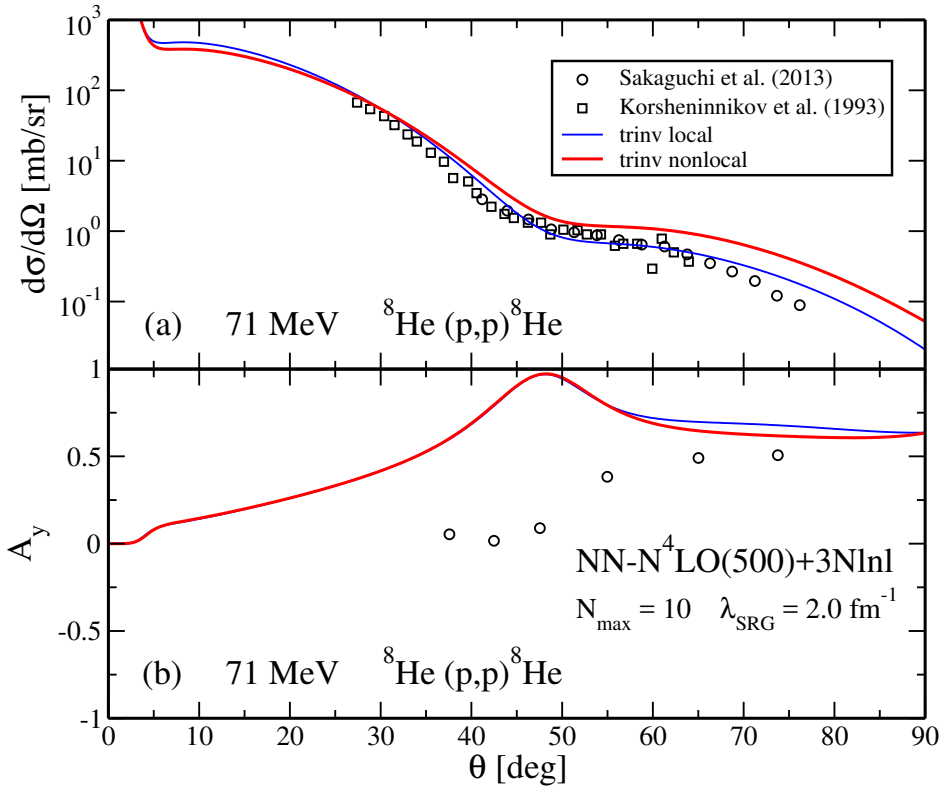


Scattering observables – Halo nuclei

Gennari, Vorabbi, Calci, Navratil, PRC **97**, 034619 (2018)



Reasonable description of the differential cross section



Outlook

- Investigation of the ^{9}He structure with the inclusion of the three-nucleon interaction
  - Introducing a controlled approximation for the 3N terms
- Calculation of the p+^{8}He scattering process
  - New TRIUMF experiment for ^{8}He(p,p) reaction
- Improvement of optical potential
  - Inclusion of the three-nucleon interaction
  - Inclusion of medium effects
- Calculation of the (e,e'p) quasi-elastic reactions with microscopic nonlocal optical potentials

Backup Slides

Coupled NCSMC equations

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

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

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

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

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

$\delta_{\lambda\lambda'}$

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

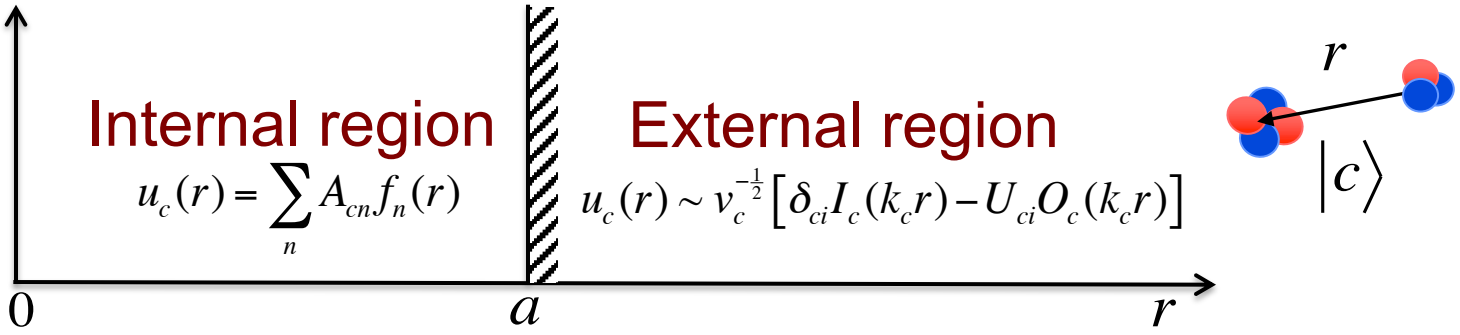
$\left\langle r', (A-a), (a) \left| \hat{A}_{\nu'}\, H\, \hat{A}_{\nu} \right| r, (a), (A-a) \right\rangle$

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

Scattering matrix (and observables) from matching solutions to known asymptotic with microscopic *R*-matrix on Lagrange mesh

Microscopic *R*-matrix theory on Lagrange mesh

Separation into "internal" and "external" regions at the channel radius a



- This is achieved through the Bloch operator: $L_c = \frac{\hbar^2}{2\mu_c}\delta(r-a)\left(\frac{d}{dr} - \frac{B_c}{r}\right)$
- System of Bloch-Schrödinger equations:

$$\left[\hat{T}_{rel}(r) + L_c + \overline{V}_{Coul}(r) - (E - E_c)\right] u_c(r) + \sum_{c'} \int dr' r' W_{cc'}(r,r') u_{c'}(r') = L_c u_c(r)$$

- Internal region: expansion on Lagrange square-integrable basis $u_c(r) = \sum_n A_{cn} f_n(r)$
- External region: asymptotic form for large r

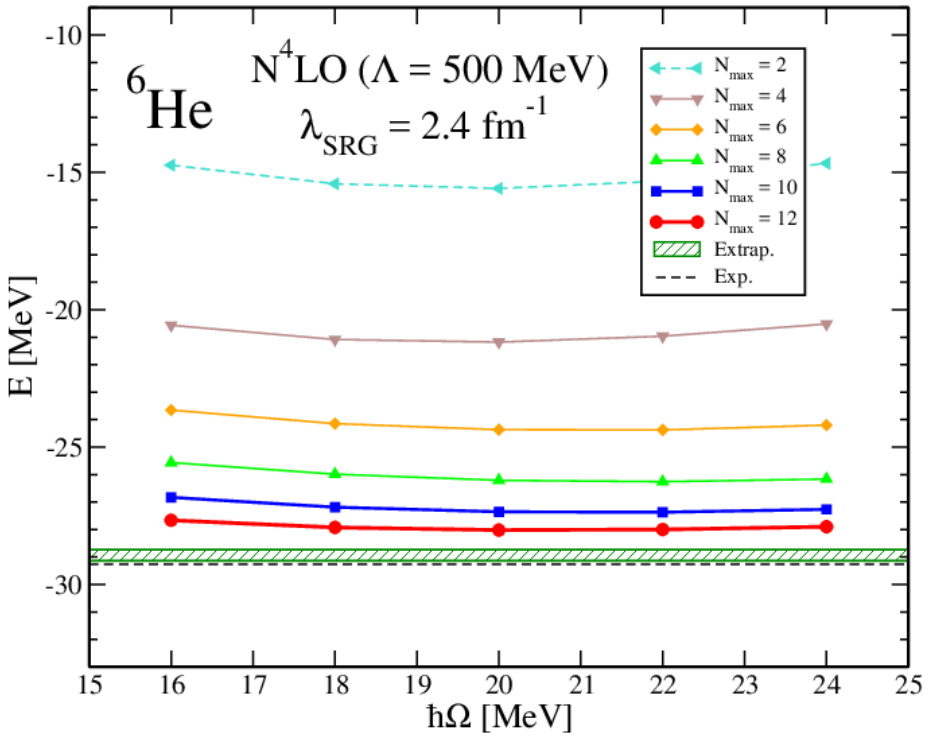
$u_c(r) \sim C_c W(k_c r)$ or $u_c(r) \sim v_c^{-\frac{1}{2}} \left[\delta_{ci} I_c(k_c r) - U_{ci} O_c(k_c r)\right]$

Scattering matrix

Bound state

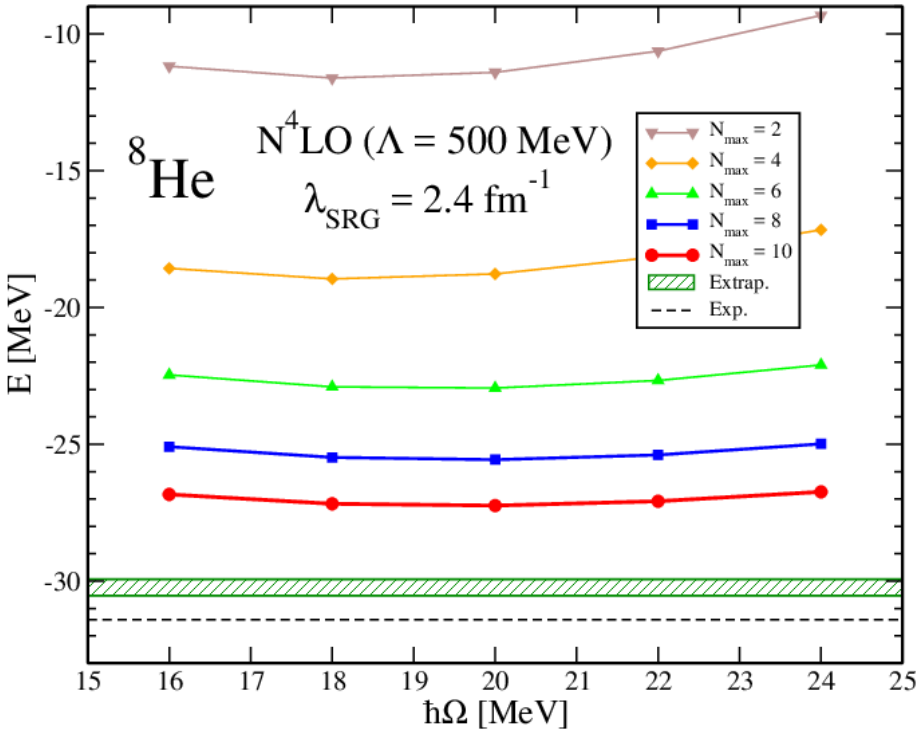
Scattering state

^{6}He and ^{8}He NCSM ground-state energies



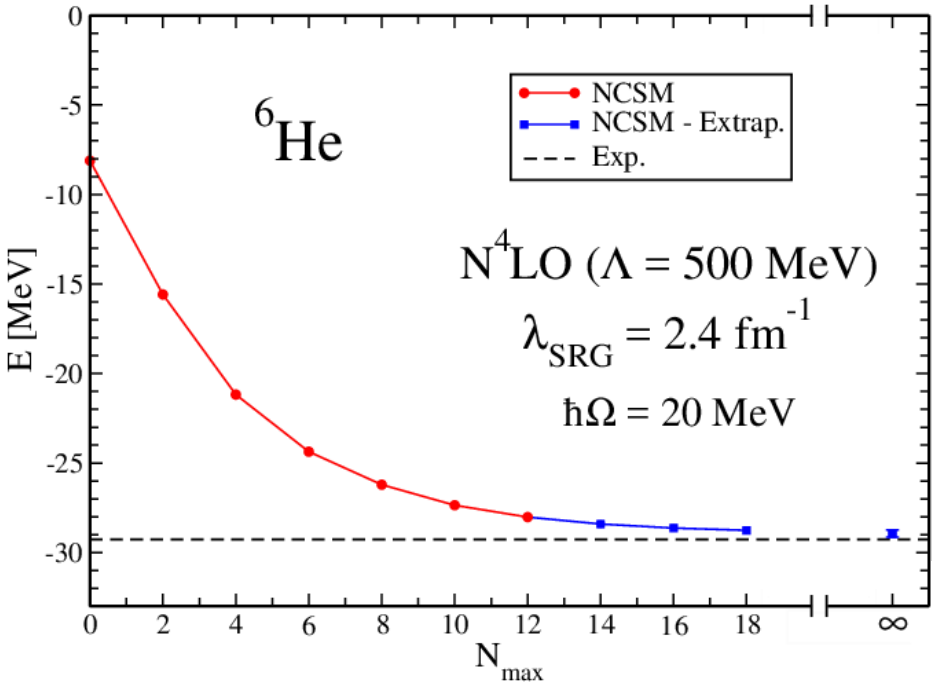
Vorabbi, Calci, Navratil, Kruse, Quaglioni, Hupin, PRC **97**, 034314 (2018)

Ground-state energies as function of ħΩ for different values of N_{max}



Minimum at ħΩ = 20 MeV

NCSM ground-state energies

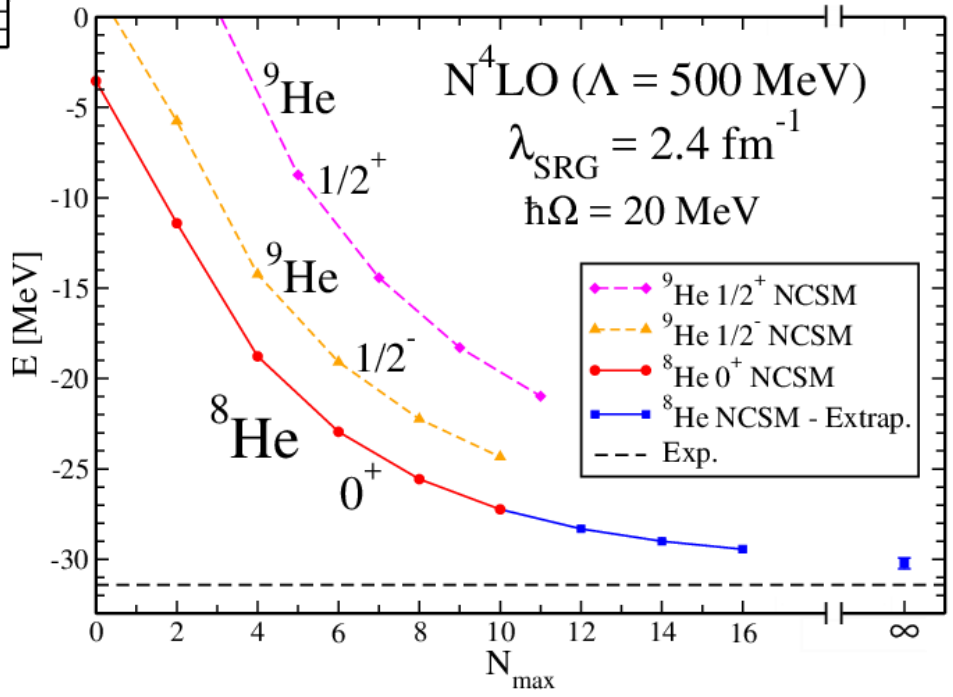


Vorabbi, Calci, Navratil, Kruse, Quaglioni, Hupin, PRC **97**, 034314 (2018)

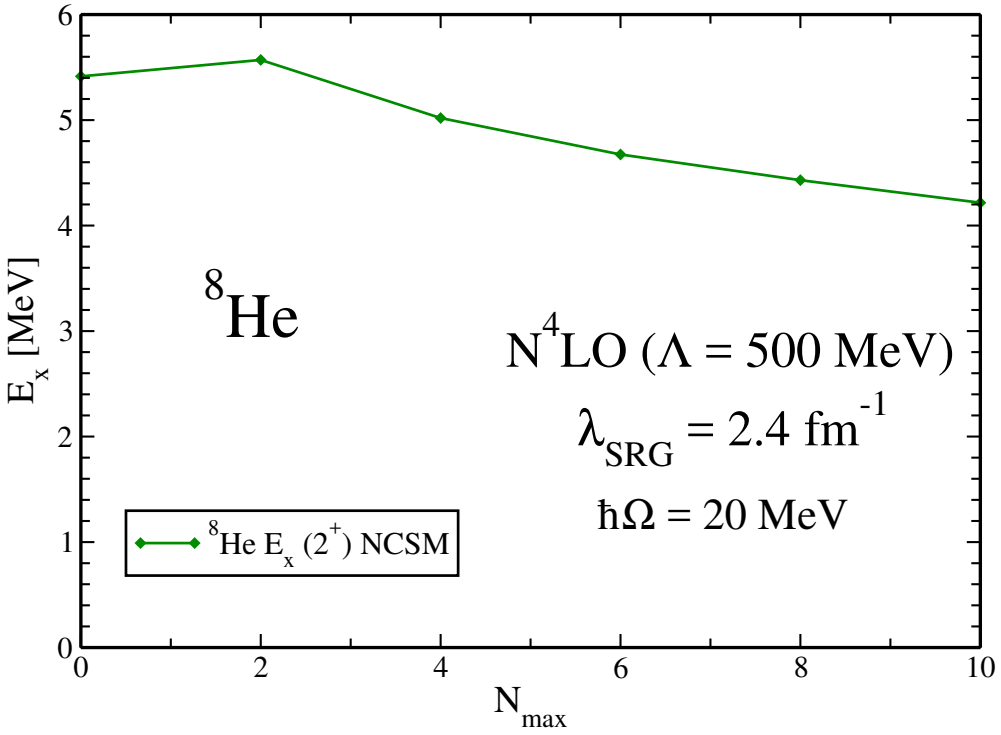
G.s. energy [MeV]	^{4}He	^{6}He	^{8}He
NCSM	-28.36	-28.9(2)	-30.1(3)
Expt	-28.30	-29.27	-31.41

Energy extrapolation

$$E(N_{\max}) = E_\infty + ae^{-bN_{\max}}$$



^{8}He NCSM excitation energies



^{8}He 2^+ state

Experimentally unbound

Important for subsequent NCSMC calculations

^{8}He first-excited state	
N_{max}	E_x (2^+) [MeV]
6	4.67
10	4.22

- Translationally invariant non-local densities

$$
\begin{aligned}
&\langle A\lambda_j J_j M_j \,|\rho_{op}^{trinv}(\vec{r}-\vec{R},\vec{r}\,'-\vec{R})|\, A\lambda_i J_i M_i\rangle \\
&= \left(\frac{A}{A-1}\right)^{\frac{3}{2}} \sum \frac{1}{\hat{J}_f}(J_i M_i K k|J_f M_f) \\
&\quad \times \left(M^K\right)^{-1}_{nln'l',n_1l_1n_2l_2} \left(Y_l^*(\widehat{\vec{r}-\vec{R}})\, Y_{l'}^*(\widehat{\vec{r}\,'-\vec{R}})\right)^{(K)}_k \\
&\quad \times R_{n,l}\left(\sqrt{\frac{A}{A-1}}|\vec{r}-\vec{R}|\right) R_{n',l'}\left(\sqrt{\frac{A}{A-1}}|\vec{r}\,'-\vec{R}|\right) \\
&\quad \times (-1)^{l_1+l_2+K+j_2-\frac{1}{2}}\, \hat{j}_1\hat{j}_2 \left\{ \begin{array}{ccc} j_1 & j_2 & K \\ l_2 & l_1 & \frac{1}{2} \end{array} \right\} \\
&\quad \times {}_{SD}\langle A\lambda_f J_f||\, (a^\dagger_{n_1,l_1,j_1}\, \tilde{a}_{n_2,l_2,j_2})^{(K)}\, ||A\lambda_i J_i\rangle_{SD}
\end{aligned}
$$

- Translationally invariant non-local densities

$$\langle A\lambda_j J_j M_j \,|\rho_{op}^{trinv}(\vec{r}-\vec{R},\vec{r}\,'-\vec{R})|\, A\lambda_i J_i M_i\rangle$$
$$= \left(\frac{A}{A-1}\right)^{\frac{3}{2}} \sum \frac{1}{\hat{J}_f}(J_i M_i K k|J_f M_f)$$
$$\times \left(M^K\right)^{-1}_{nln'l',n_1l_1n_2l_2} \left(Y_l^*(\widehat{\vec{r}-\vec{R}})\, Y_{l'}^*(\widehat{\vec{r}\,'-\vec{R}})\right)^{(K)}_k$$
$$\times R_{n,l}\left(\sqrt{\frac{A}{A-1}}|\vec{r}-\vec{R}|\right) R_{n',l'}\left(\sqrt{\frac{A}{A-1}}|\vec{r}\,'-\vec{R}|\right)$$
$$\times (-1)^{l_1+l_2+K+j_2-\frac{1}{2}}\, \hat{j}_1\hat{j}_2 \left\{ \begin{array}{ccc} j_1 & j_2 & K \\ l_2 & l_1 & \frac{1}{2} \end{array} \right\}$$
$$\times {}_{SD}\langle A\lambda_f J_f||\, (a^\dagger_{n_1,l_1,j_1}\, \tilde{a}_{n_2,l_2,j_2})^{(K)}\, ||A\lambda_i J_i\rangle_{SD}$$

- Ground-state density for even-even nuclei

$$\rho(\boldsymbol{r},\boldsymbol{r}') = \sum_l \rho_l(r,r')(-1)^l \frac{\sqrt{2l+1}}{4\pi} P_l(\cos\omega)$$

- Translationally invariant non-local densities

$$\langle A\lambda_j J_j M_j \,|\rho_{op}^{trinv}(\vec{r}-\vec{R},\vec{r}\,'-\vec{R})|\, A\lambda_i J_i M_i\rangle$$

$$= \left(\frac{A}{A-1}\right)^{\frac{3}{2}} \sum \frac{1}{\hat{J}_f}(J_i M_i K k|J_f M_f)$$

$$\times \left(M^K\right)^{-1}_{nln'l',n_1l_1n_2l_2} \left(Y_l^*(\widehat{\vec{r}-\vec{R}})\, Y_{l'}^*(\widehat{\vec{r}\,'-\vec{R}})\right)^{(K)}_k$$

$$\times R_{n,l}\left(\sqrt{\frac{A}{A-1}}|\vec{r}-\vec{R}|\right) R_{n',l'}\left(\sqrt{\frac{A}{A-1}}|\vec{r}\,'-\vec{R}|\right)$$

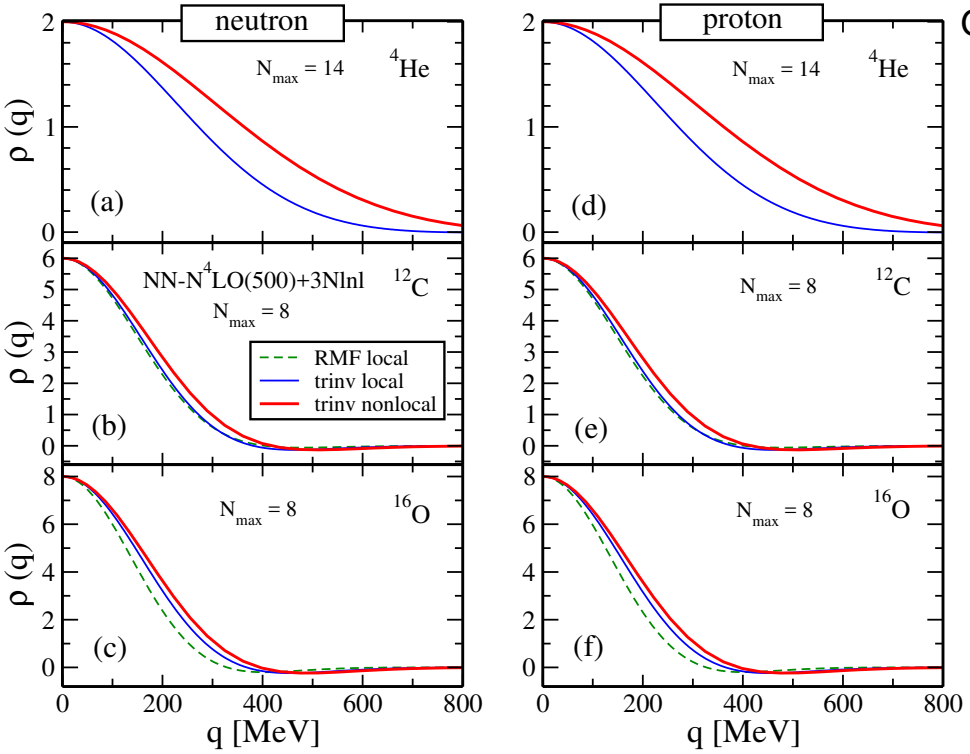
$$\times (-1)^{l_1+l_2+K+j_2-\frac{1}{2}}\, \hat{j}_1\hat{j}_2 \begin{Bmatrix} j_1 & j_2 & K \\ l_2 & l_1 & \frac{1}{2} \end{Bmatrix}$$

$$\times {}_{SD}\langle A\lambda_f J_f||\, (a^\dagger_{n_1,l_1,j_1}\, \tilde{a}_{n_2,l_2,j_2})^{(K)}\, ||A\lambda_i J_i\rangle_{SD}$$

Angular part

- Ground-state density for even-even nuclei

$$\rho(\boldsymbol{r},\boldsymbol{r}') = \sum_l \rho_l(r,r')(-1)^l \frac{\sqrt{2l+1}}{4\pi} P_l(\cos\omega)$$



Gennari, Vorabbi, Calci, Navratil, PRC **97**, 034619 (2018)

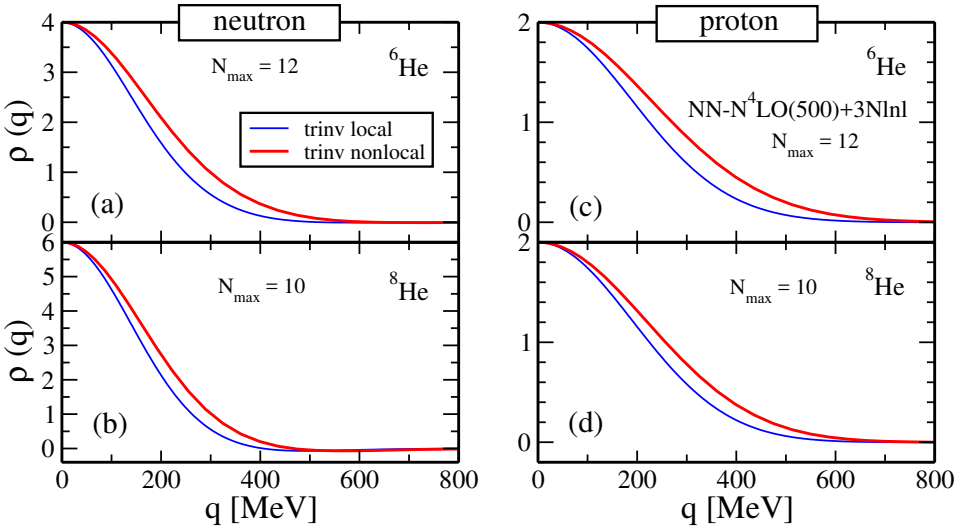
FF from local density

$$\rho_\alpha(q) = 4\pi \int_0^\infty dr r^2 j_0(qr) \rho_\alpha(r)$$

PRC **70**, 014317 (2004)

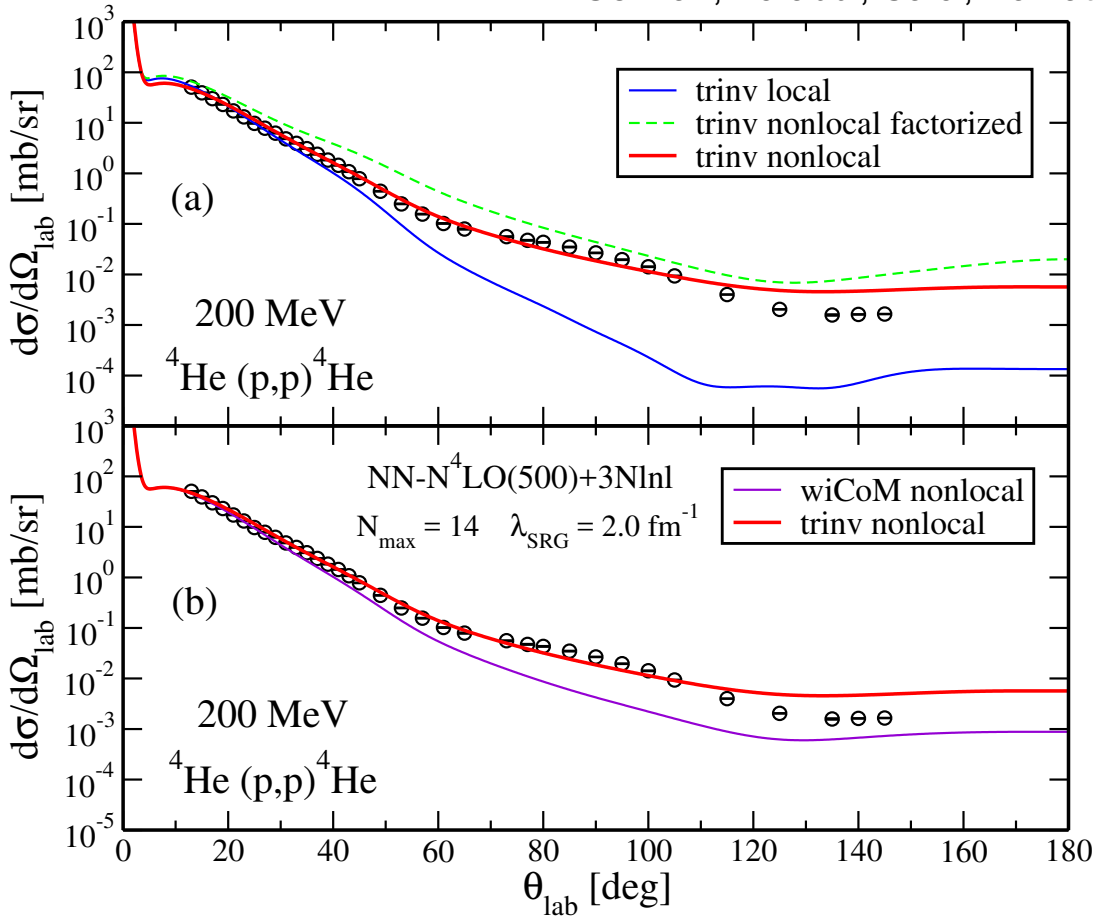
FF from non-local density

$$\rho_\alpha(q) = \int d^3\boldsymbol{P}\, \rho_\alpha\left(\boldsymbol{P} - \frac{A-1}{2A}\boldsymbol{q}, \boldsymbol{P} + \frac{A-1}{2A}\boldsymbol{q}\right)$$



Scattering observables – Stable nuclei

Gennari, Vorabbi, Calci, Navratil, PRC **97**, 034619 (2018)



FF from nonlocal density

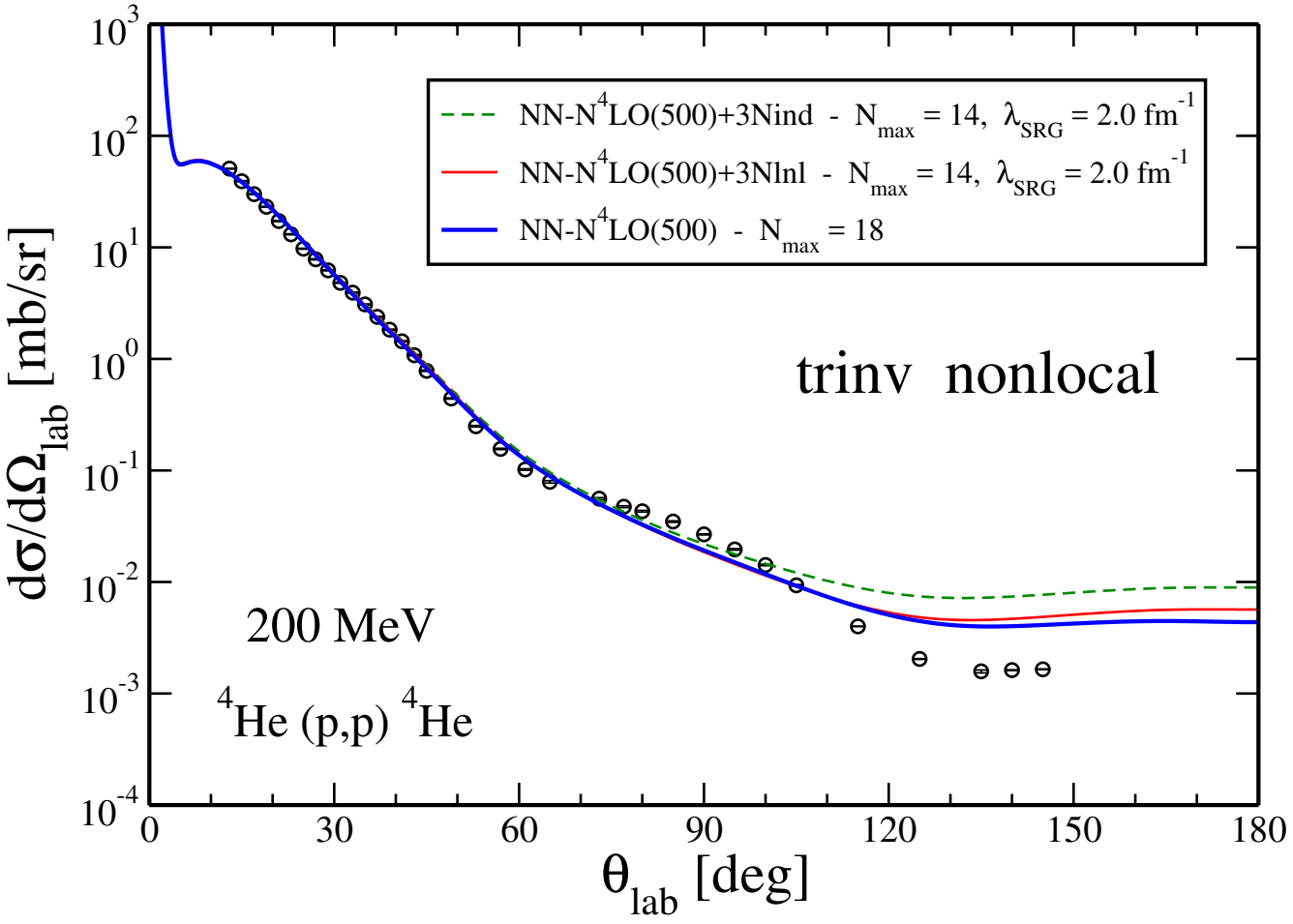
$$\rho_\alpha(q) = \int d\boldsymbol{P}\, \rho_\alpha\left(\boldsymbol{P} - \frac{A-1}{2A}\boldsymbol{q}, \boldsymbol{P} + \frac{A-1}{2A}\boldsymbol{q}\right)$$

Factorized optical potential

$$U(\boldsymbol{q}, \boldsymbol{K}; E) \sim \sum_{\alpha=n,p} t_{p\alpha}\left[\boldsymbol{q}, \frac{A+1}{2A}\boldsymbol{K}; E\right] \rho_\alpha(q)$$

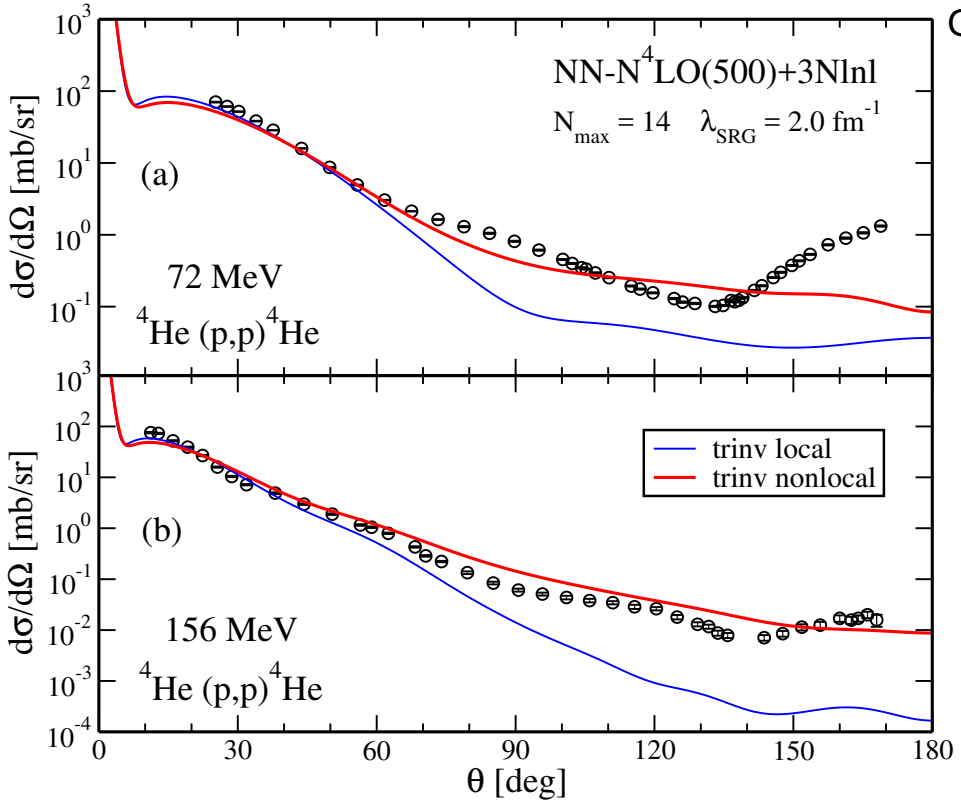
Scattering observables – Consistency

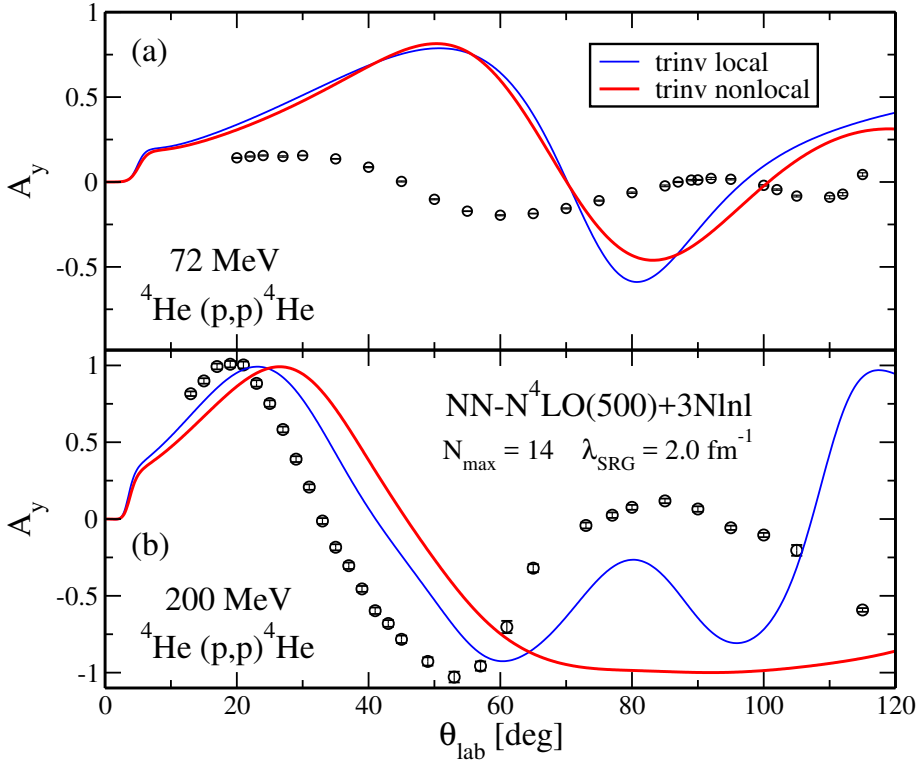
Gennari, Vorabbi, Calci, Navratil, PRC **97**, 034619 (2018)



Scattering observables – Stable nuclei

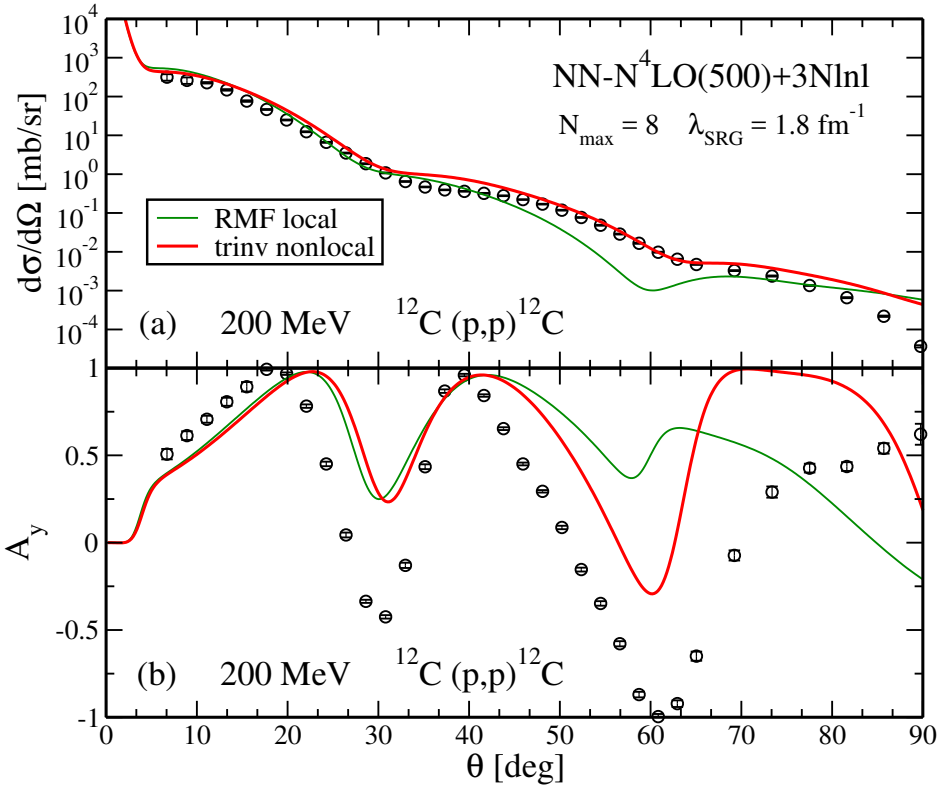
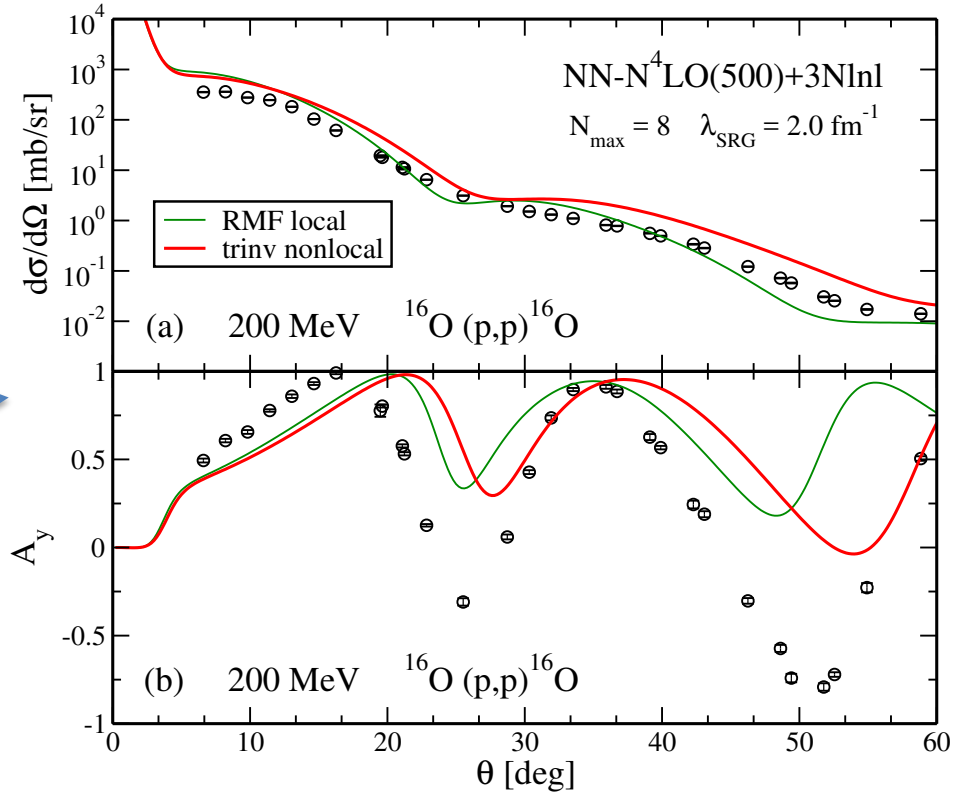
Gennari, Vorabbi, Calci, Navratil, PRC **97**, 034619 (2018)





Comparison with RMF

Gennari, Vorabbi, Calci, Navratil, PRC **97**, 034619 (2018)



Shift with respect the RMF results