TRIUMF

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

Ab initio calculations for exotic nuclei

Recent advances and challenges in the description of nuclear reactions at the limit of stability

Trento - 2018/03/08

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Papers: arXiv:1712.05824, arXiv:1712.02879

Outline

1. Exotic structure of ^{9}He from the no-core shell model with continuum
   - ^{6}He and ^{8}He NCSM calculations
   - ^{9}He NCSMC calculations

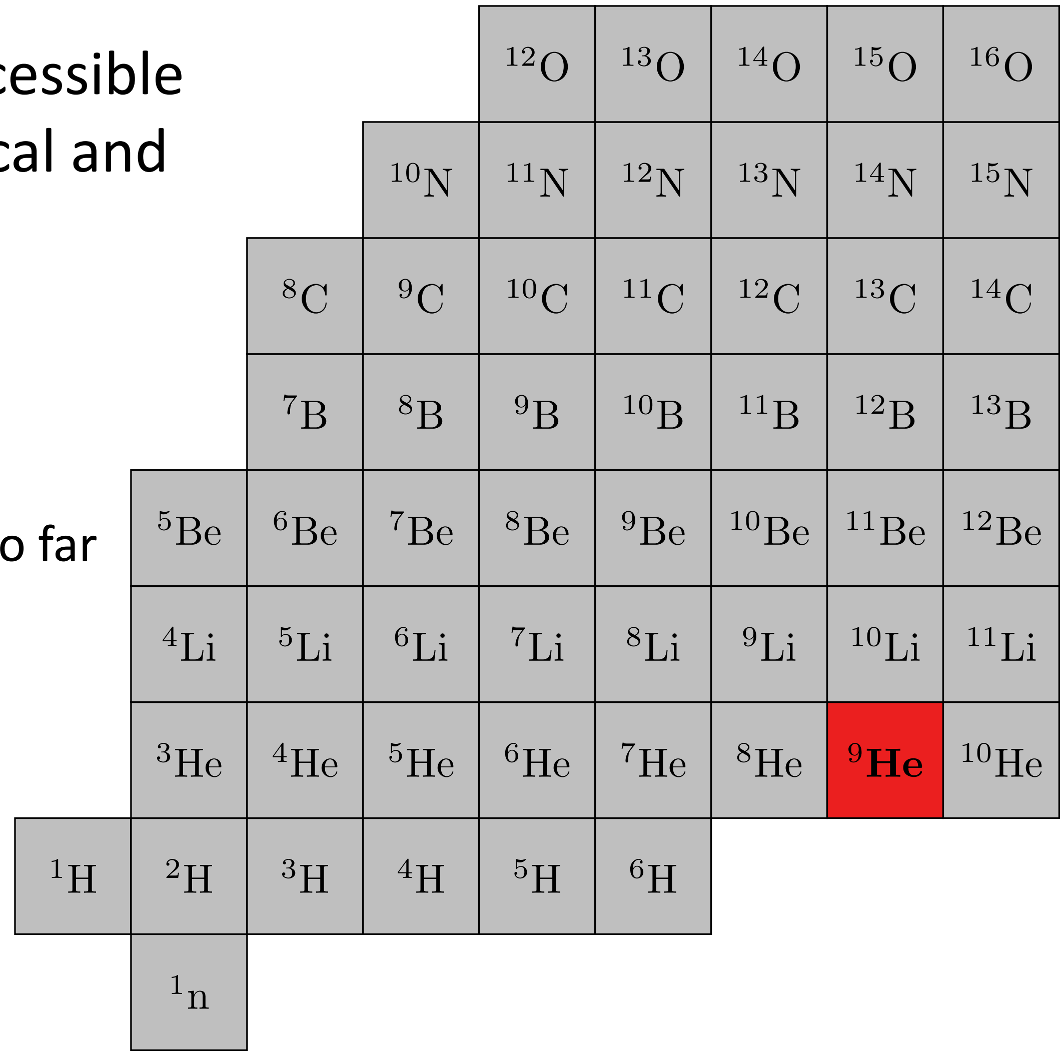
2. Microscopic optical potentials with nonlocal ab initio densities for intermediate energies
   - Results for stable nuclei
   - Results for ^{6}He and ^{8}He

1.

Exotic structure of ^{9}He

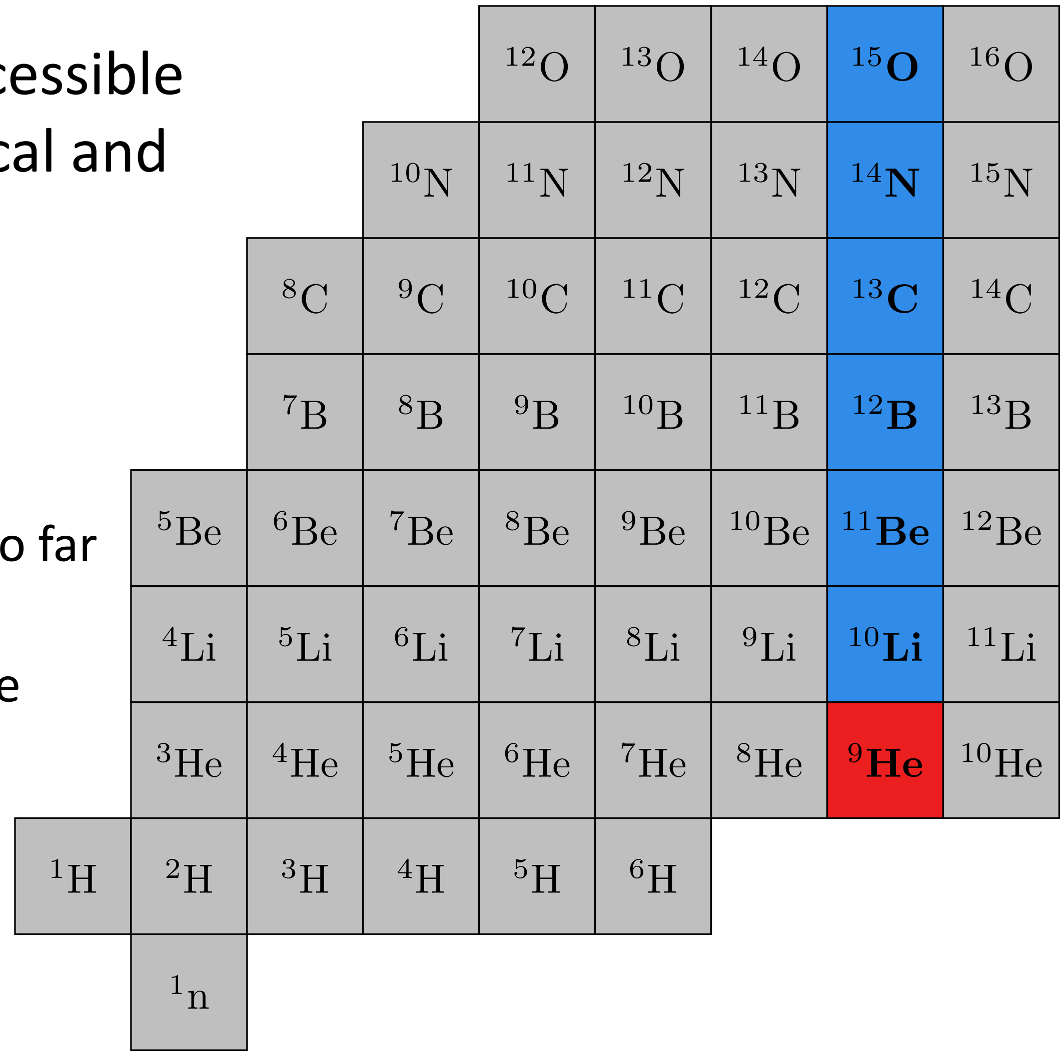
The He isotopic chain

- 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

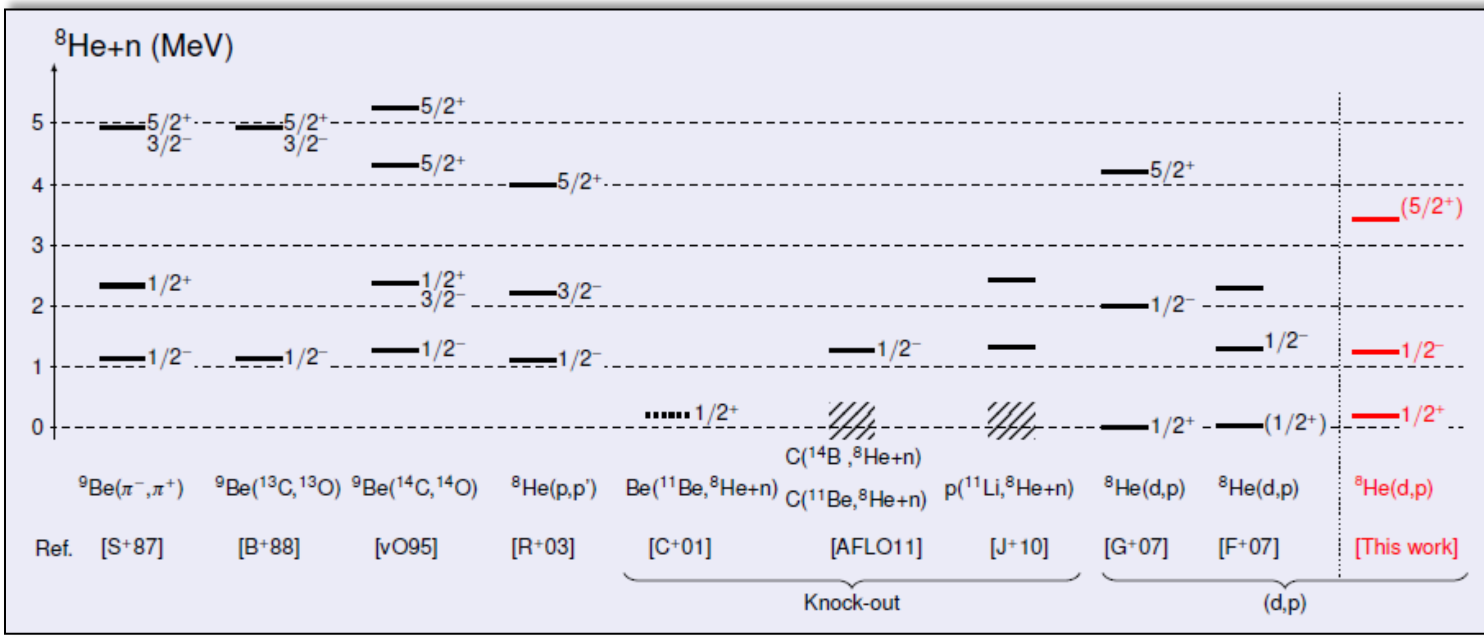


The He isotopic chain

- 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

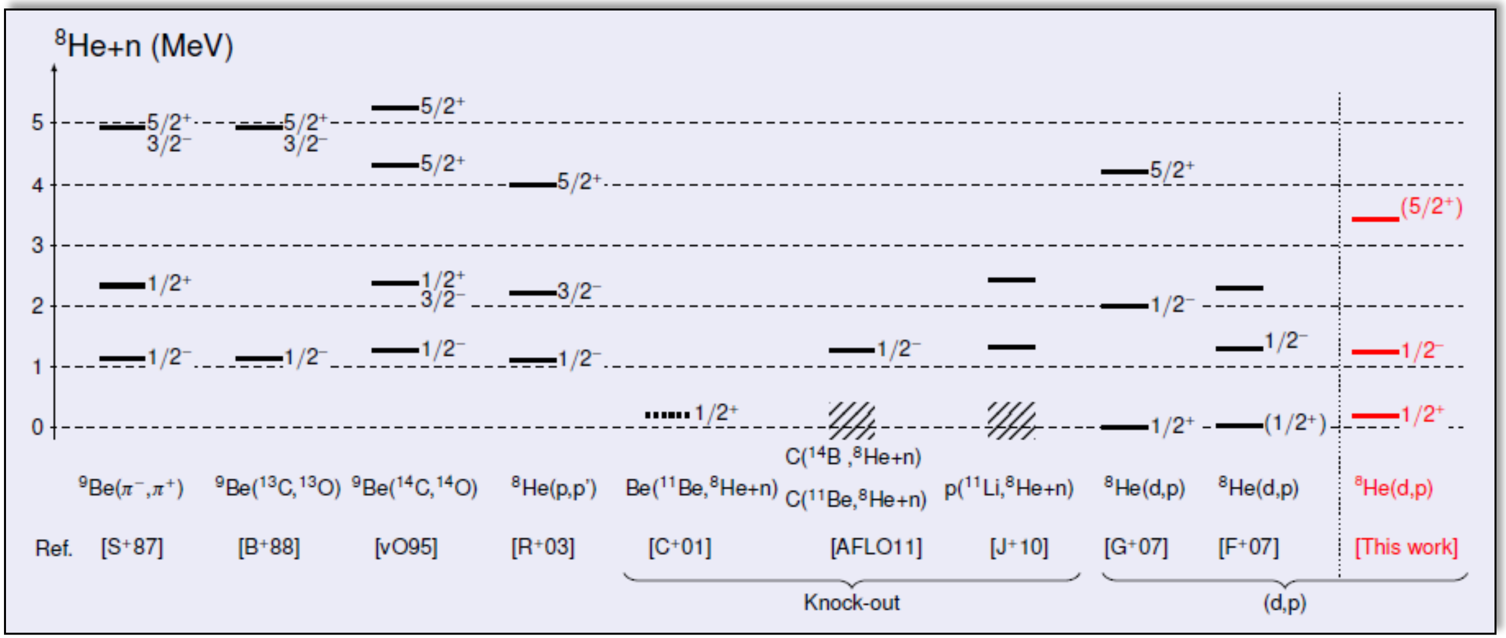


From talk by Nigel Orr at ECT* (2013)

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

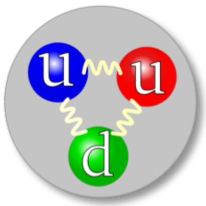


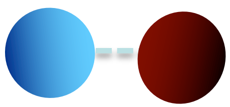
From talk by Nigel Orr at ECT* (2013)

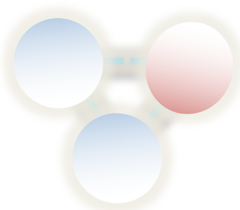
Two long-standing problems affect the physics of the ^{9}He system

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

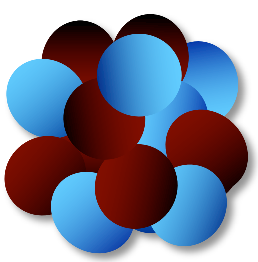
From QCD to nuclei







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



Low-energy QCD

↓

NN+3N interactions from chiral EFT

↓

SRG
Softens NN, induces 3N

↓

NCSMC
(Binary-cluster formulation)

↓

Nuclear structure and reactions

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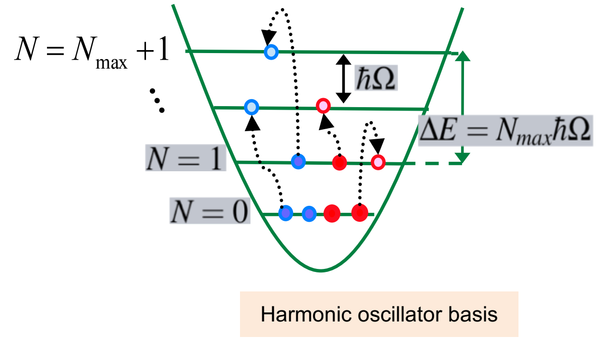
Unified approach to bound & continuum states; to nuclear structure & reactions

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



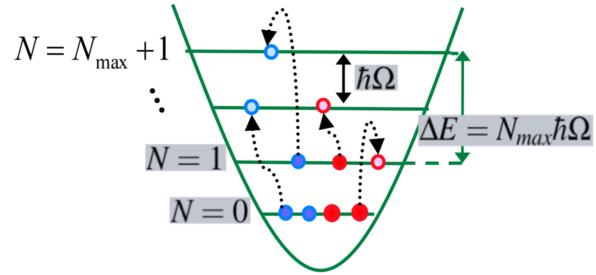
NCSM

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

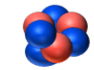
Unknowns

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

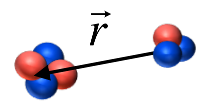


Harmonic oscillator basis



NCSM

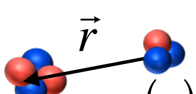
- …with resonating group method
  - Bound & scattering states, reactions
  - Cluster dynamics, long-range correlations



NCSM/RGM

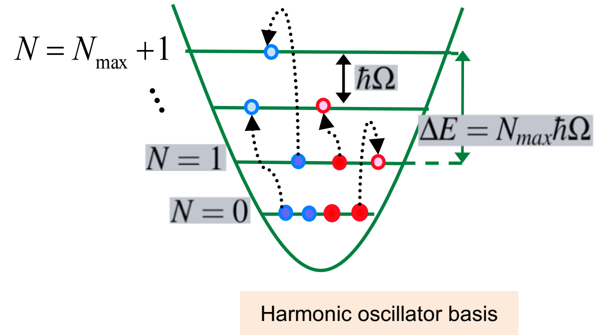
NCSM/RGM channel states

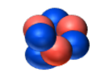
$$\Psi^{(A)} = \sum_{\nu} \int d\vec{r}\; \gamma_{\nu}(\vec{r}\,)\; \hat{A}_{\nu} \left| \;_{(A-a)} \quad \vec{r} \quad (a)\;, \nu \right\rangle$$



Unknowns

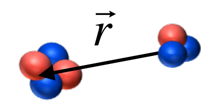
- *Ab initio* no-core shell model
  - Short- and medium range correlations
  - Bound-states, narrow resonances





NCSM

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



NCSM/RGM

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

NCSMC

NCSM eigenstates

NCSM/RGM channel states

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

Unknowns

Coupled NCSMC equations

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

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

$$E_{\lambda}^{NCSM}\,\delta_{\lambda\lambda'} \qquad \left\langle (A) \left| H\,\hat{A}_{\nu} \right| (a) \overset{r}{\longleftrightarrow} (A-a) \right\rangle \qquad \delta_{\lambda\lambda'} \qquad \left\langle (A) \left| \hat{A}_{\nu} \right| (a) \overset{r}{\longleftrightarrow} (A-a) \right\rangle$$

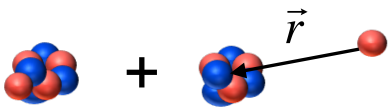
$$\begin{pmatrix} H_{NCSM} & h \\ h & H_{RGM} \end{pmatrix} \begin{pmatrix} c \\ \gamma \end{pmatrix} = E \begin{pmatrix} 1_{NCSM} & g \\ g & N_{RGM} \end{pmatrix} \begin{pmatrix} c \\ \gamma \end{pmatrix}$$

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

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

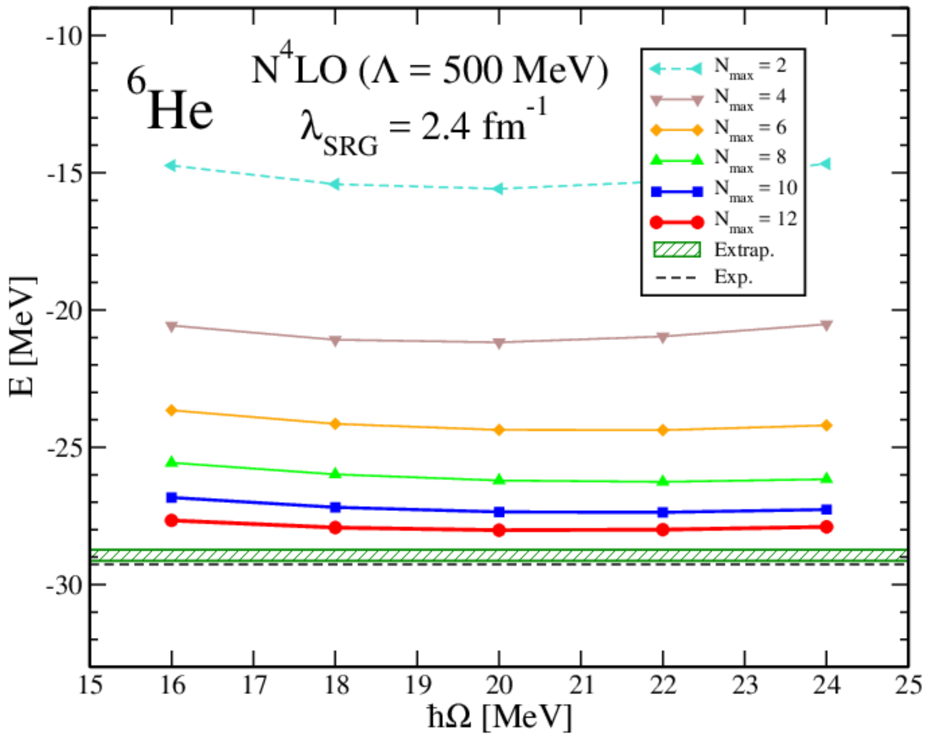
- NCSMC calculations with several interactions
  - N^2LO_{sat} NN + 3N
  - NN N^3LO + 3N N^2LO
  - **SRG-N^4LO500 NN**

- 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

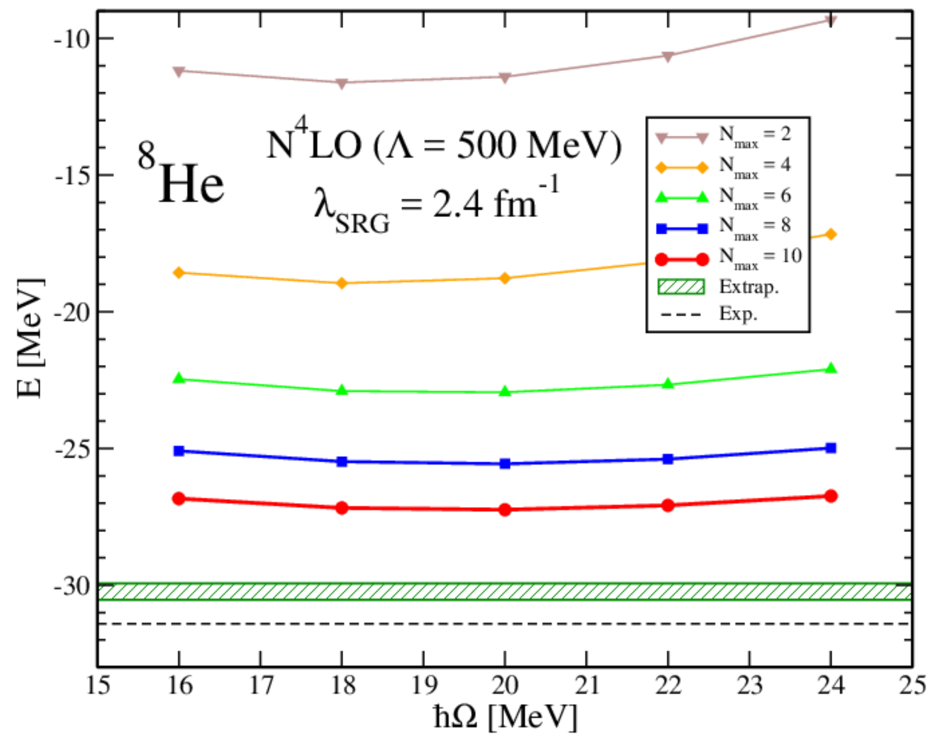


  - Importance of large N_{max} basis:
    - SRG-N^4LO500 NN with λ=2.4 fm^{-1}
      up to N_{max} = 11 with ^{9}He NCSM (m-scheme basis of 350 million)

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

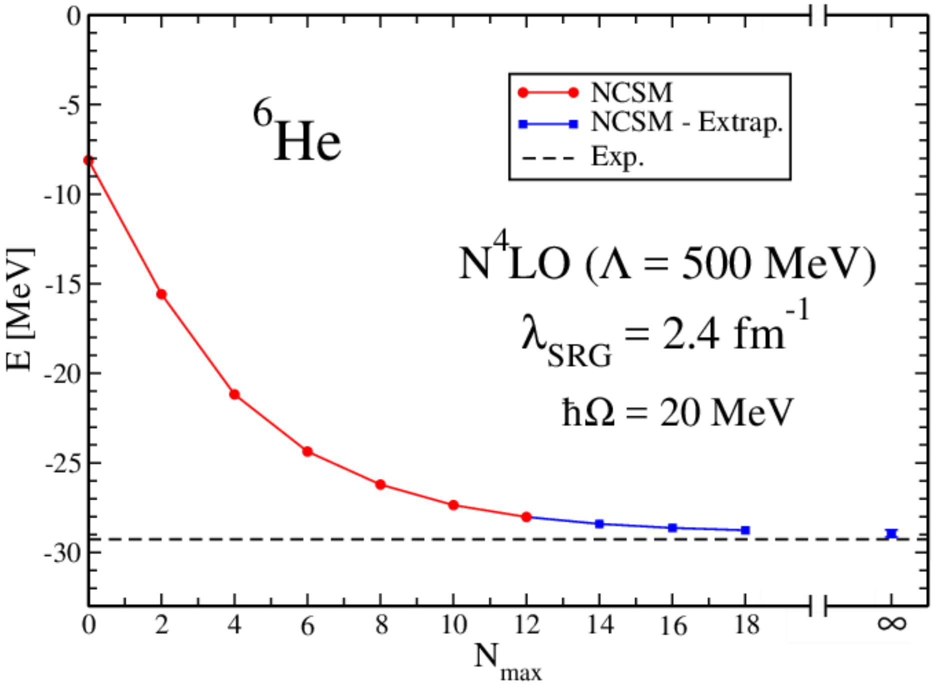


Ground-state energies as function of ħΩ for different values of N_{max}



Minimum at ħΩ = 20 MeV

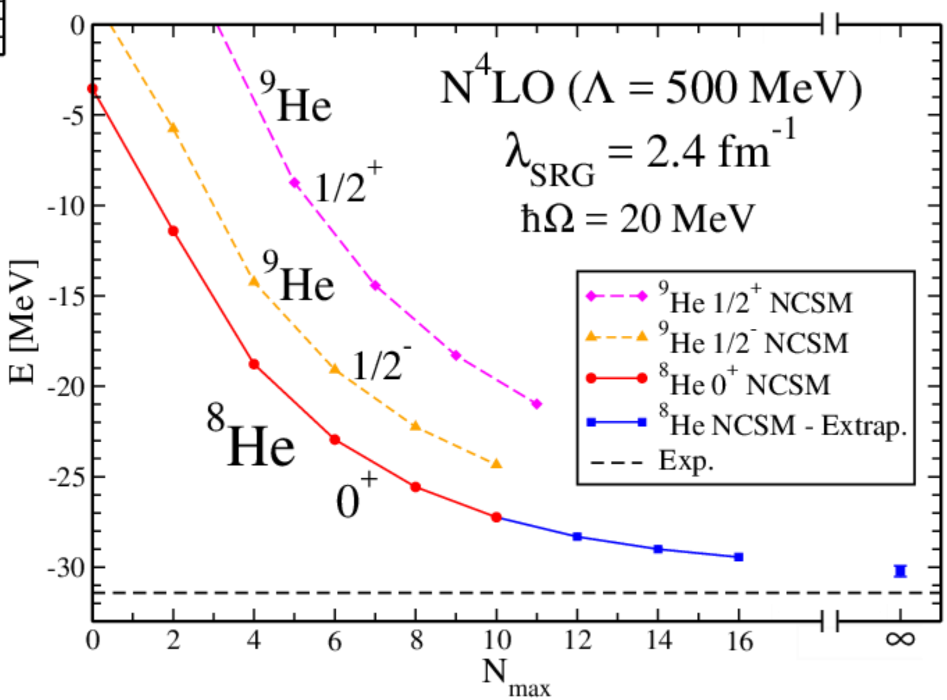
NCSM ground-state energies



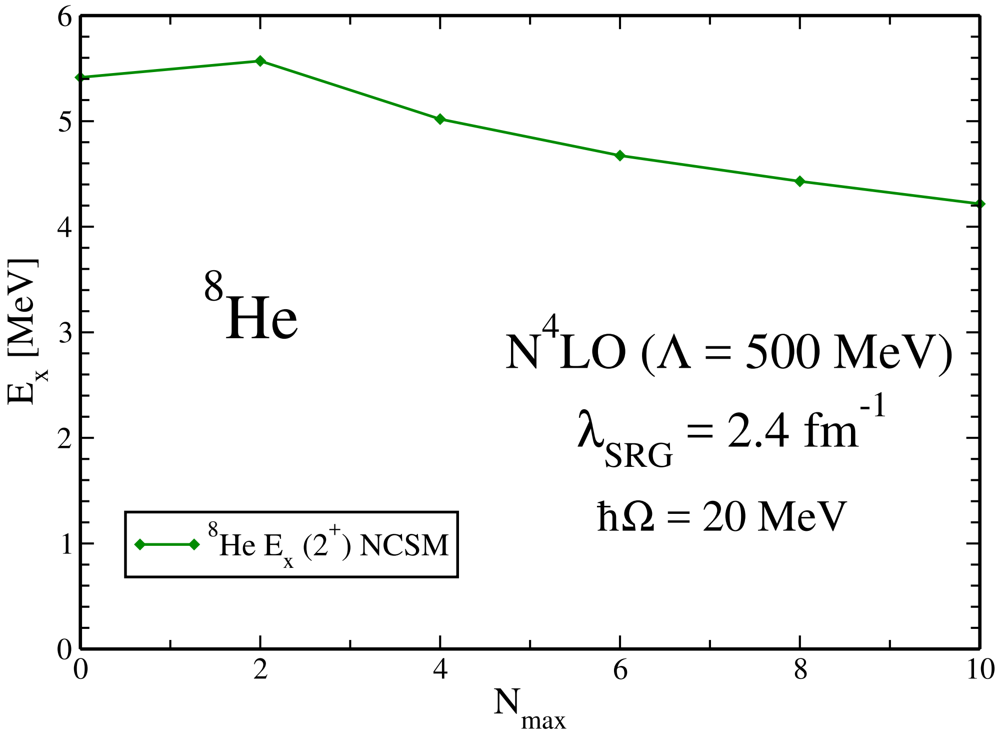
G.s. energy [MeV]	^{4}He	^{6}He	^{8}He
NCSM	-28.36	-28.9(2)	-30.1(3)
Expt	-28.30	-29.27	-31.41

Energy extrapolation

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



^{8}He NCSM excitation energies



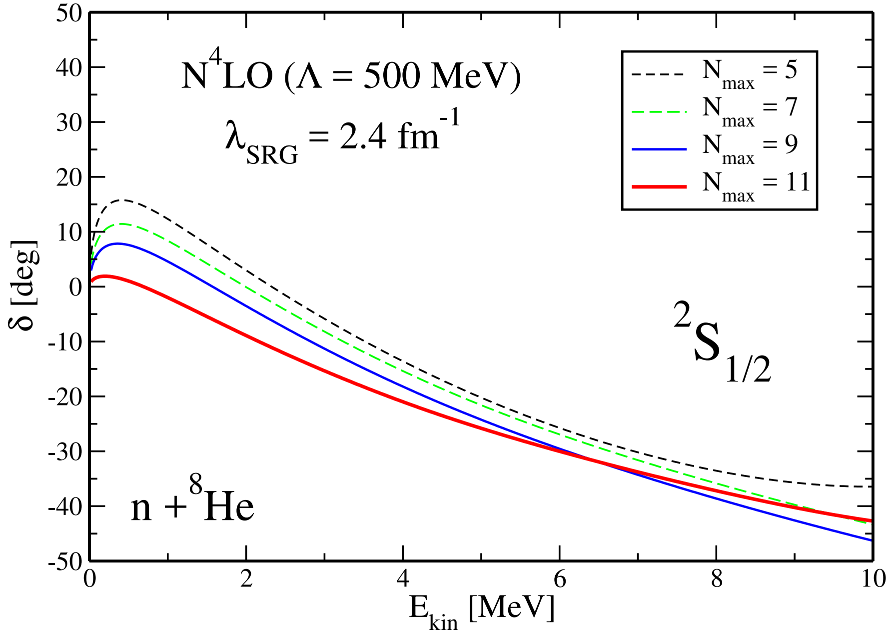
^{8}He 2^+ state

Experimentally unbound

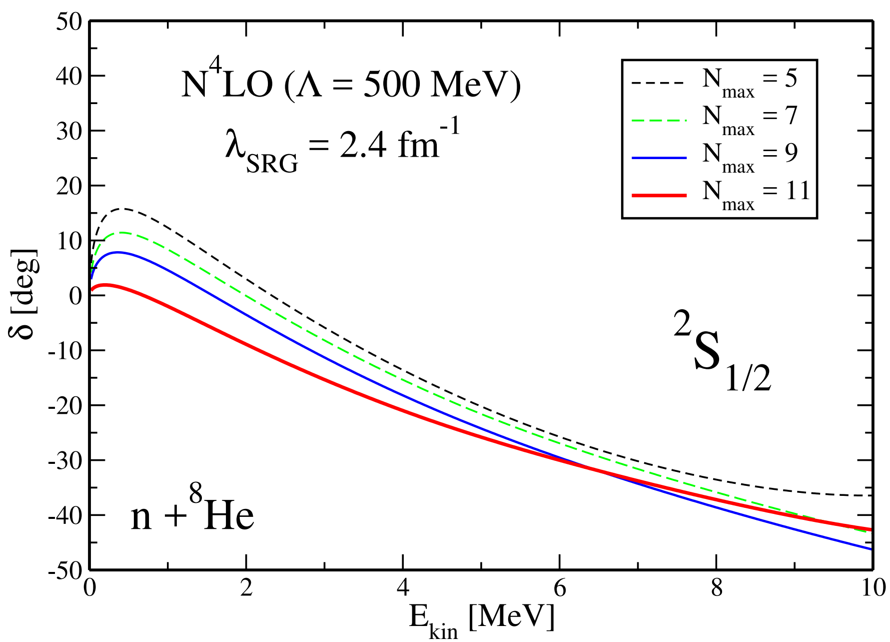
^{8}He first-excited state	
N_{max}	E_x (2^+) [MeV]
6	4.67
10	4.22

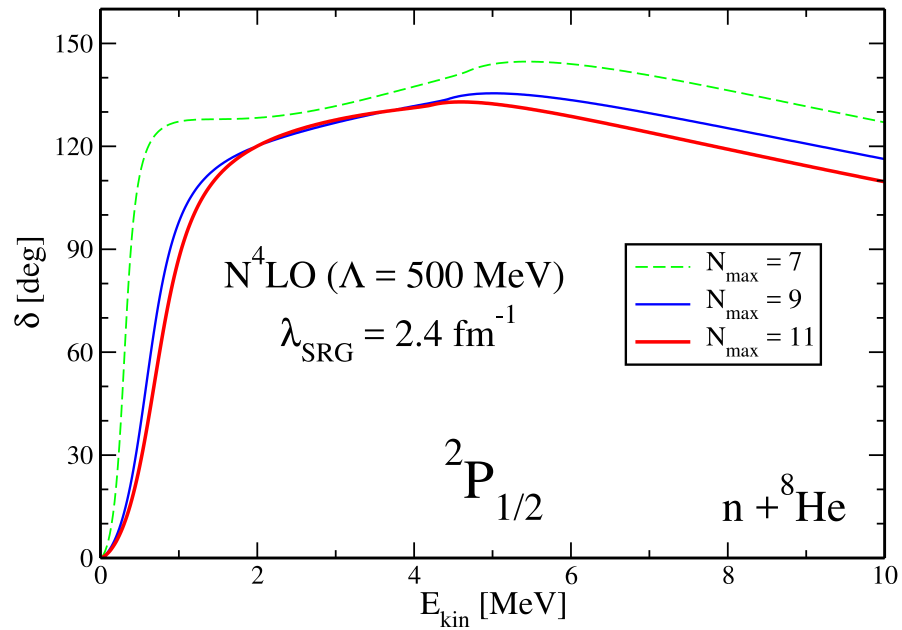
Important for subsequent NCSMC calculations

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

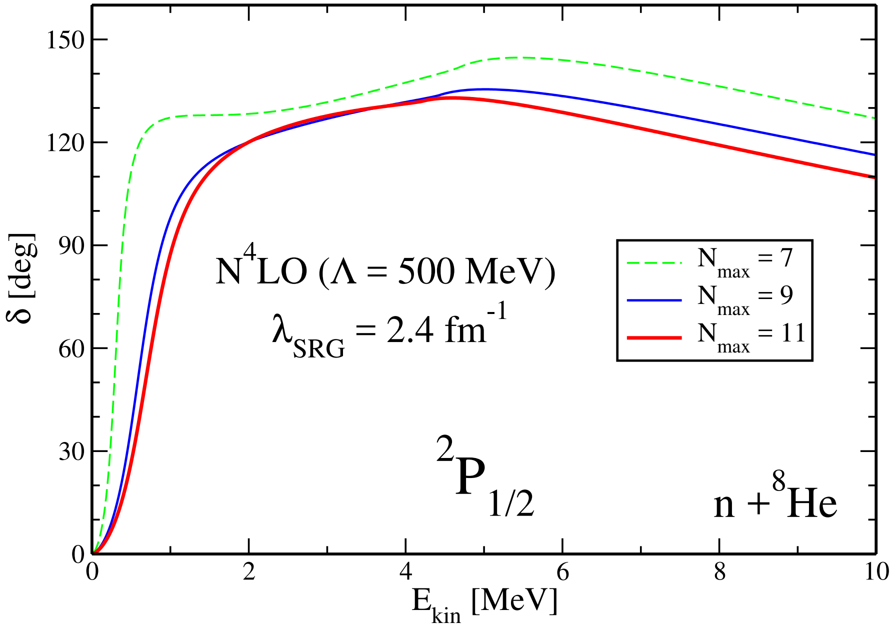


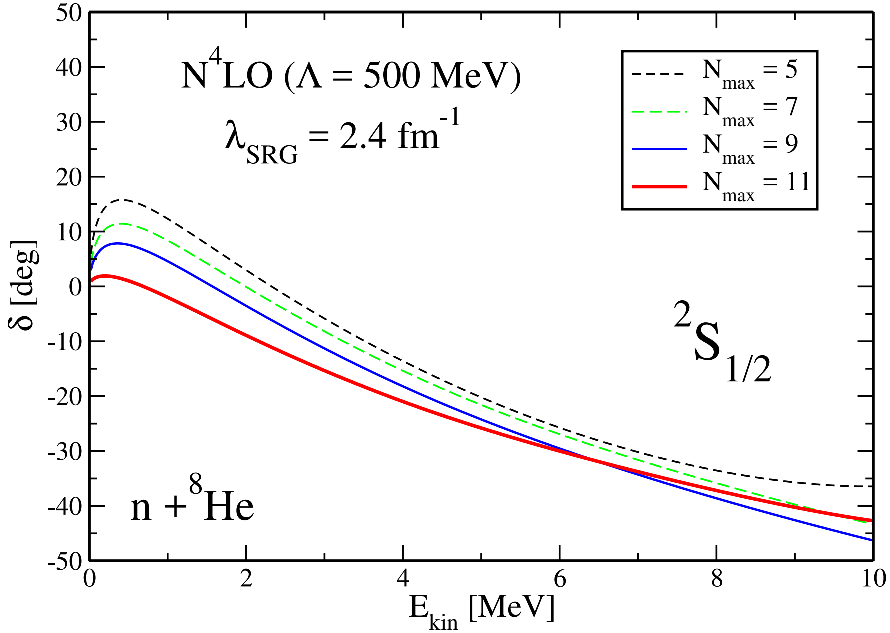
Phase shift convergence with SRG-N^{4}LO500 NN λ=2.4 fm^{-1}

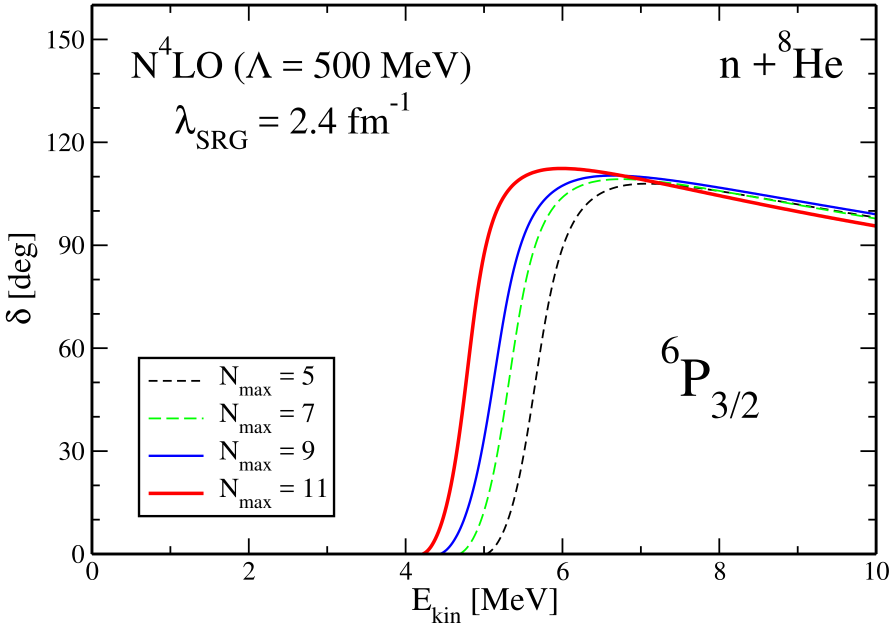




Phase shift convergence with SRG-N^{4}LO500 NN λ=2.4 fm^{-1}







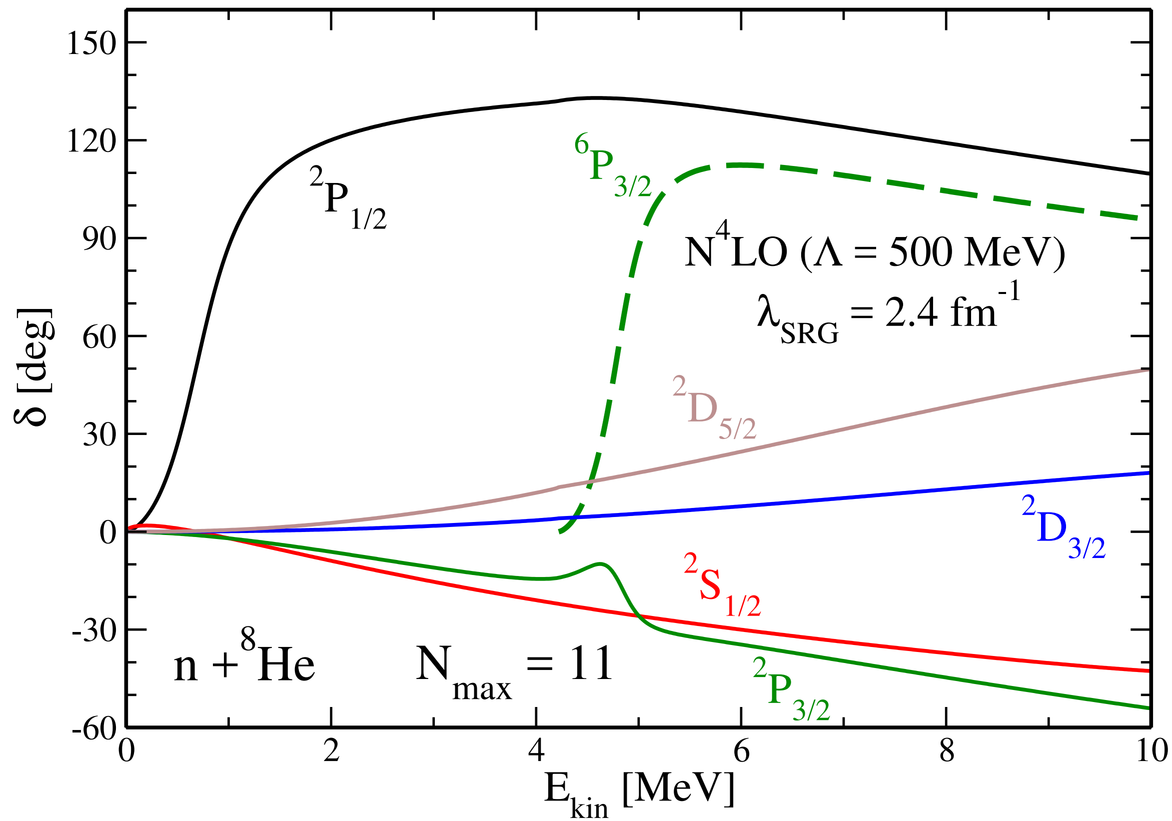
Phase shifts with SRG-N^{4}LO500 NN λ=2.4 fm^{-1}

Energy spectrum

No bound state

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

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



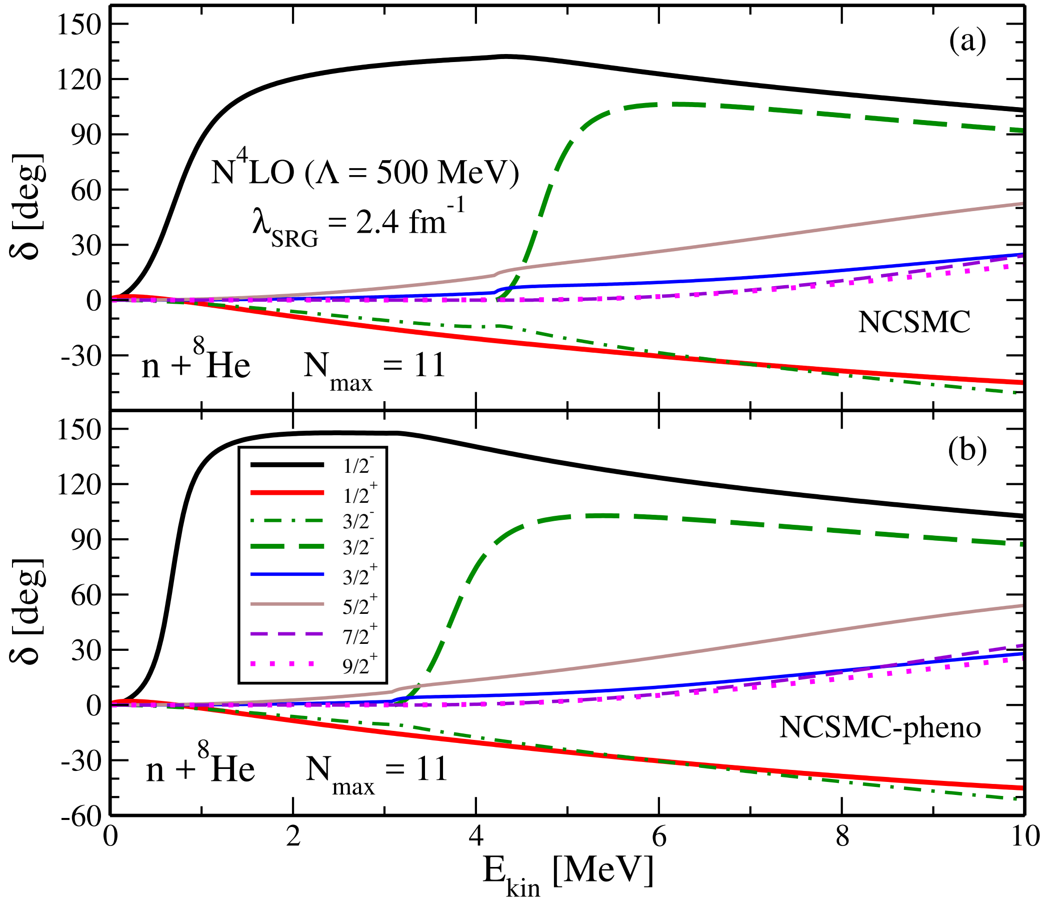
Eigenphase shifts with SRG-N^4LO500 NN λ=2.4 fm^{-1}

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

- Lippmann-Schwinger equation for nucleon-nucleus (NA) scattering

$$T = V + VG_0(E)T$$

- Separation of the LS equation

$$T = U + UG_0(E)PT$$

$$U = V + VG_0(E)QU$$

- Transition operator for the elastic scattering

$$T_{\mathrm{el}} \equiv PTP = PUP + PUPG_0(E)T_{\mathrm{el}}$$

- Spectator expansion [Chinn, Elster, Thaler, Weppner, PRC **52,** 1992 (1995)]

$$U = \sum_{i=1}^{A} \tau_i + \sum_{i,j\neq i}^{A} \tau_{ij} + \sum_{i,j\neq i,k\neq i,j}^{A} \tau_{ijk} + \cdots$$

Free propagator

$$G_0(E) = (E - H_0 + i\epsilon)^{-1}$$

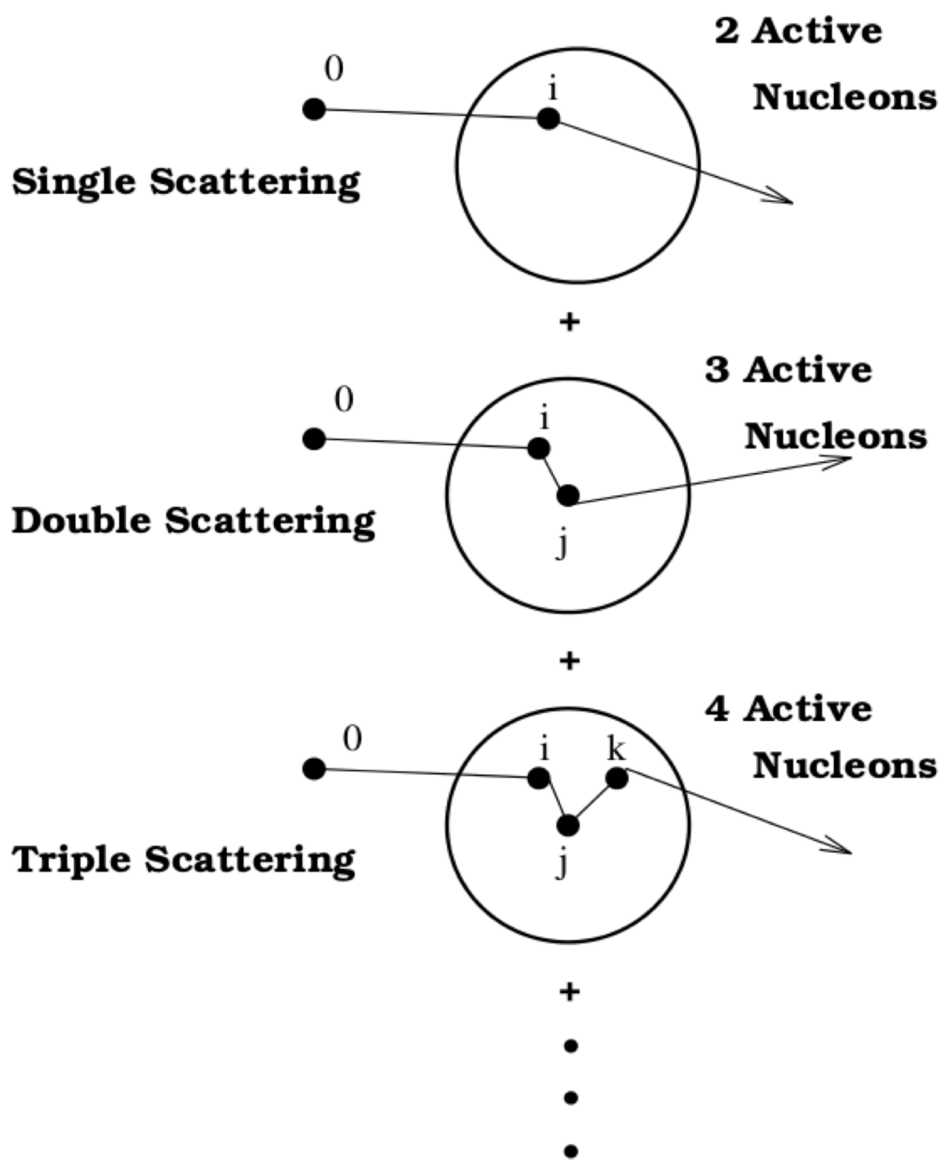
Free Hamiltonian

$$H_0 = h_0 + H_A$$

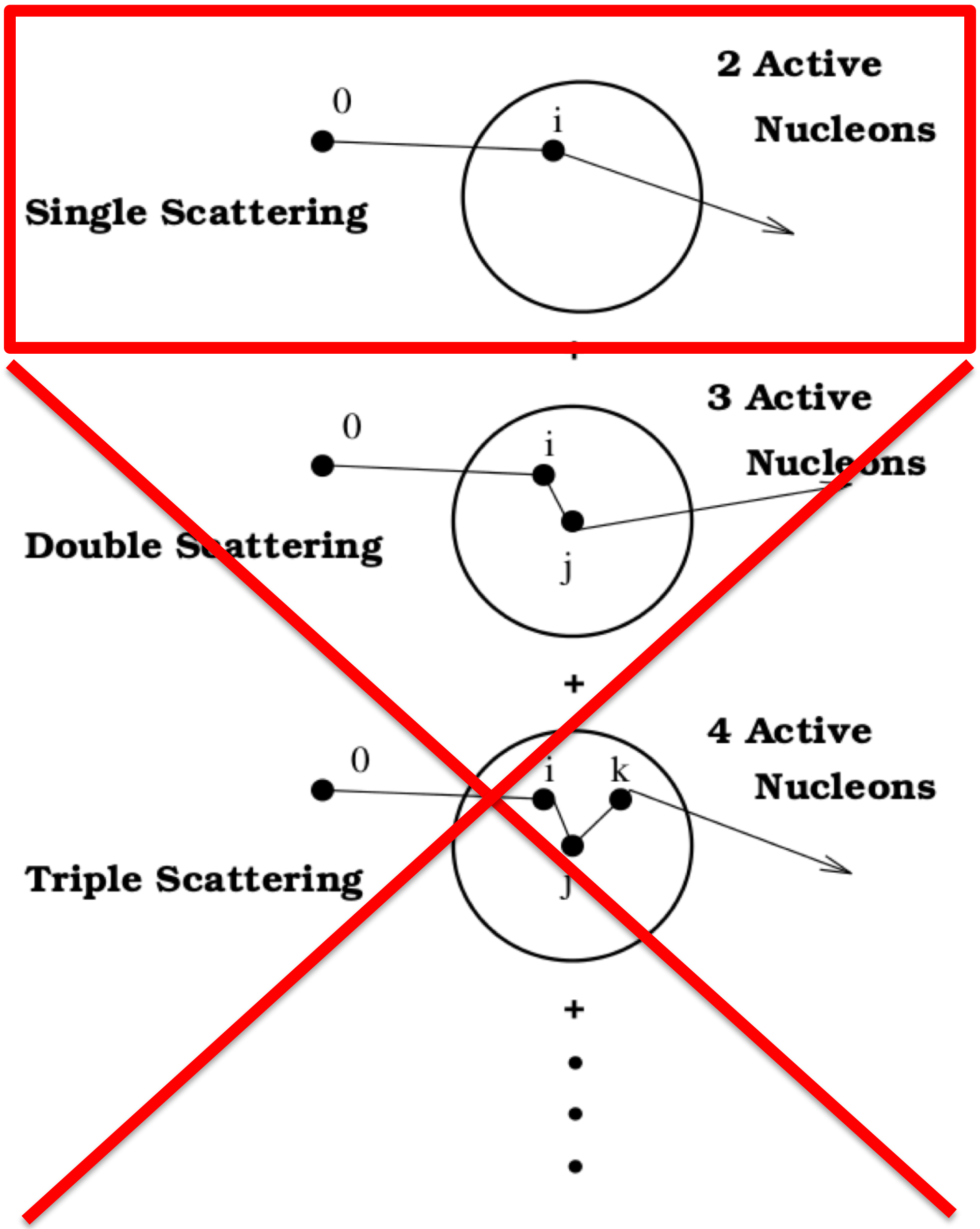
External interaction

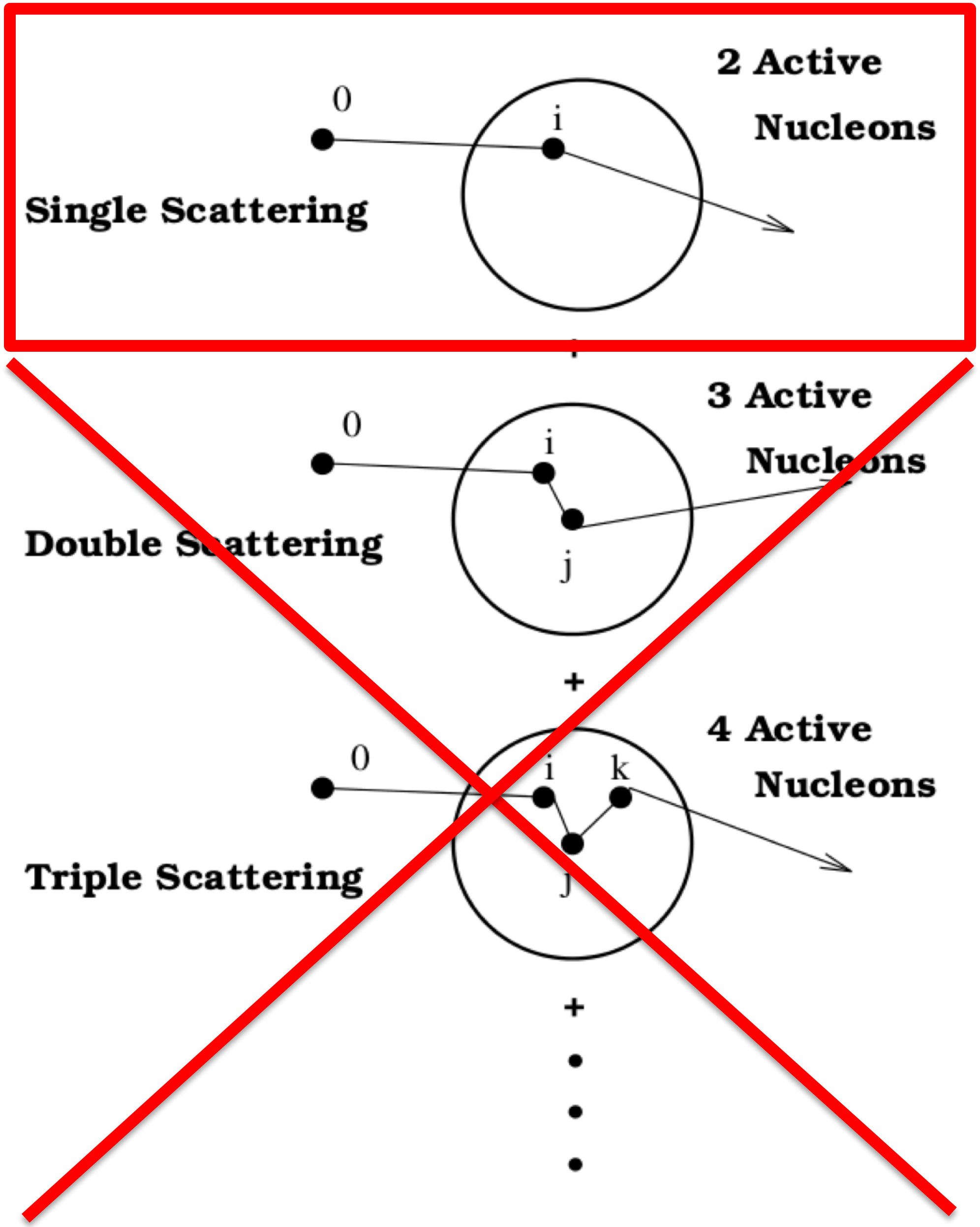
$$V = \sum_{i=1}^{A} v_{0i}$$

Approximations



Approximations





Impulse approximation

- Optical potential operator

$$U = \sum_{i=1}^{A} t_{0i}$$

- The free NN t matrix

$$t_{0i} = v_{0i} + v_{0i} g_i t_{0i}$$

- The free NN propagator

$$g_i = \frac{1}{E - h_0 - h_i + i\epsilon}$$

- The elastic 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

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

Momentum transfer

$$\boldsymbol{q} = \boldsymbol{k}' - \boldsymbol{k}$$

Total momentum

$$\boldsymbol{K} = \frac{1}{2}(\boldsymbol{k}' - \boldsymbol{k})$$

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

- Non-local nuclear density operator

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

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

- Removal of the COM component is required
  - Navratil, PRC **70**, 014317 (2004)

- Recently: Burrows *et al.,* Phys. Rev. C **97**, 024325 (2018)

- Translationally invariant non-local densities

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

- Translationally invariant non-local densities

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

- 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

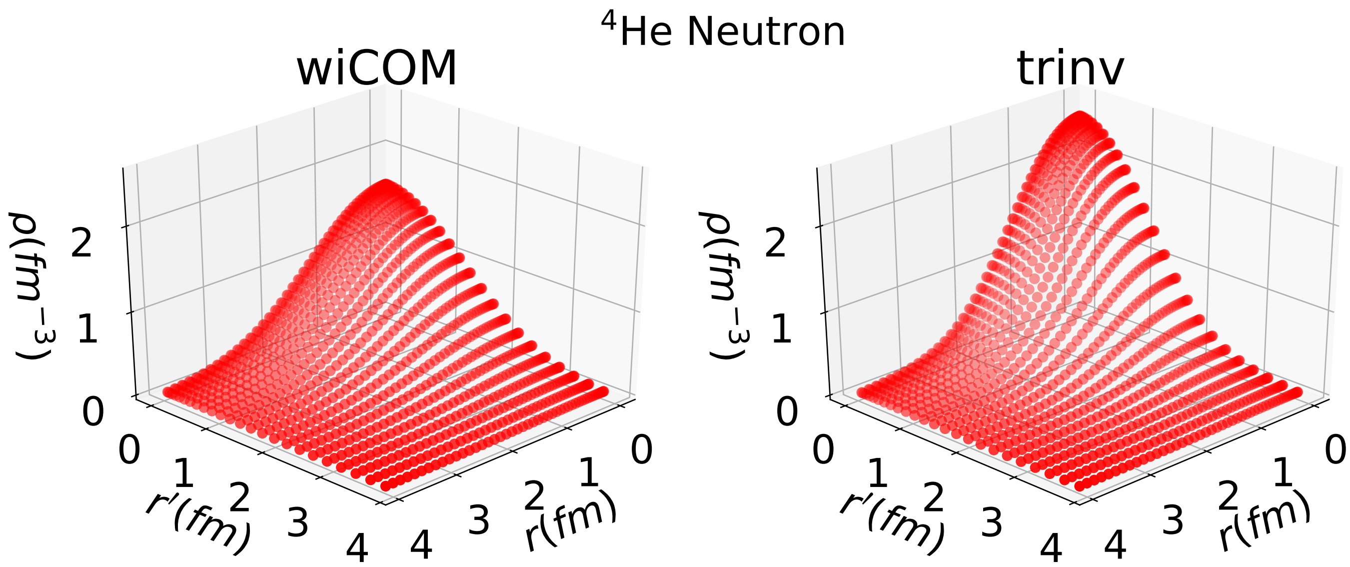
$$\langle A\lambda_j J_j M_j \,|\rho_{op}^{trinv}(\vec{r}-\vec{R},\vec{r}\,'-\vec{R})|\, A\lambda_i J_i M_i\rangle$$
$$= \left(\frac{A}{A-1}\right)^{\frac{3}{2}} \sum \frac{1}{\hat{J}_f}(J_i M_i K k | J_f M_f)$$
$$\times \left(M^K\right)^{-1}_{nln'l',n_1l_1n_2l_2} \left(Y_l^*(\widehat{\vec{r}-\vec{R}})\,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

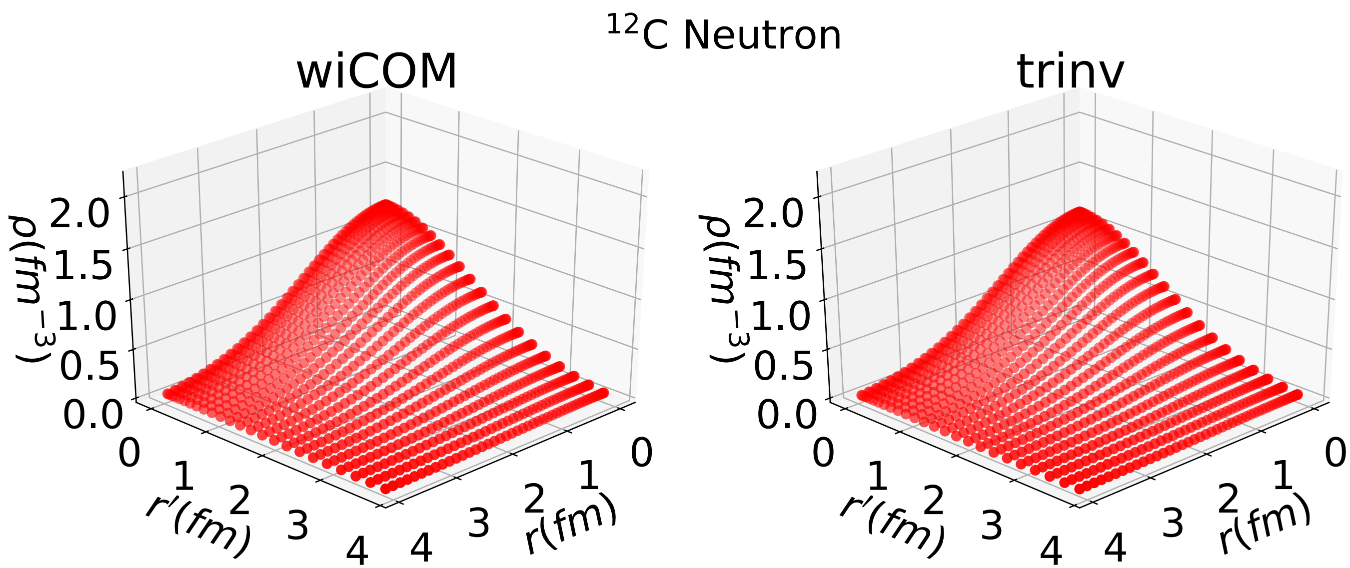
Angular part

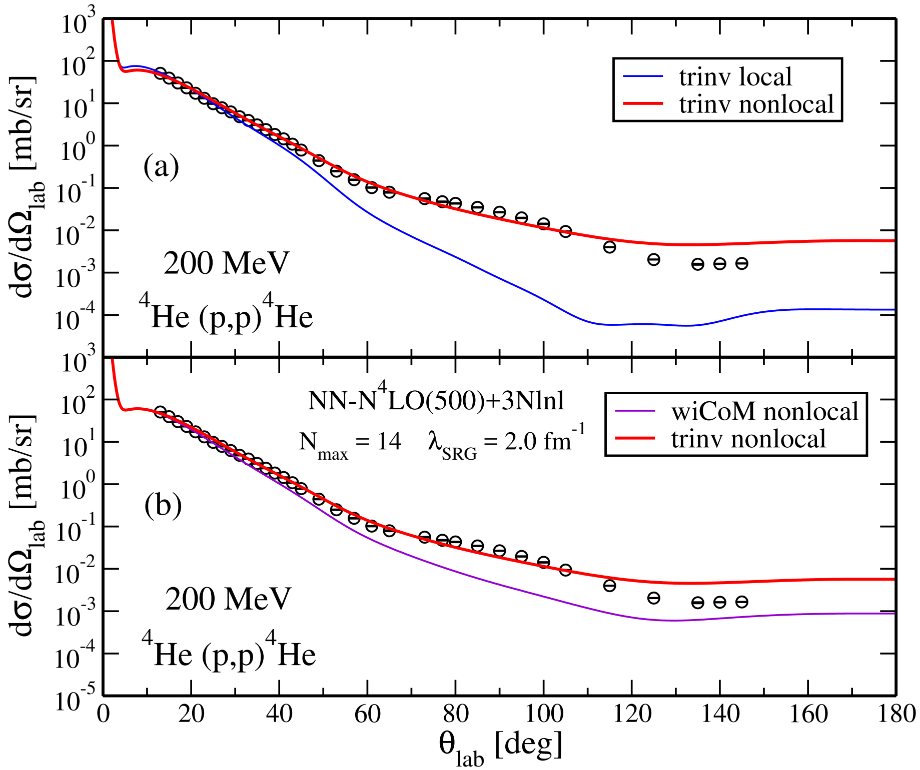
- Ground-state density for even-even nuclei

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

Non-local densities



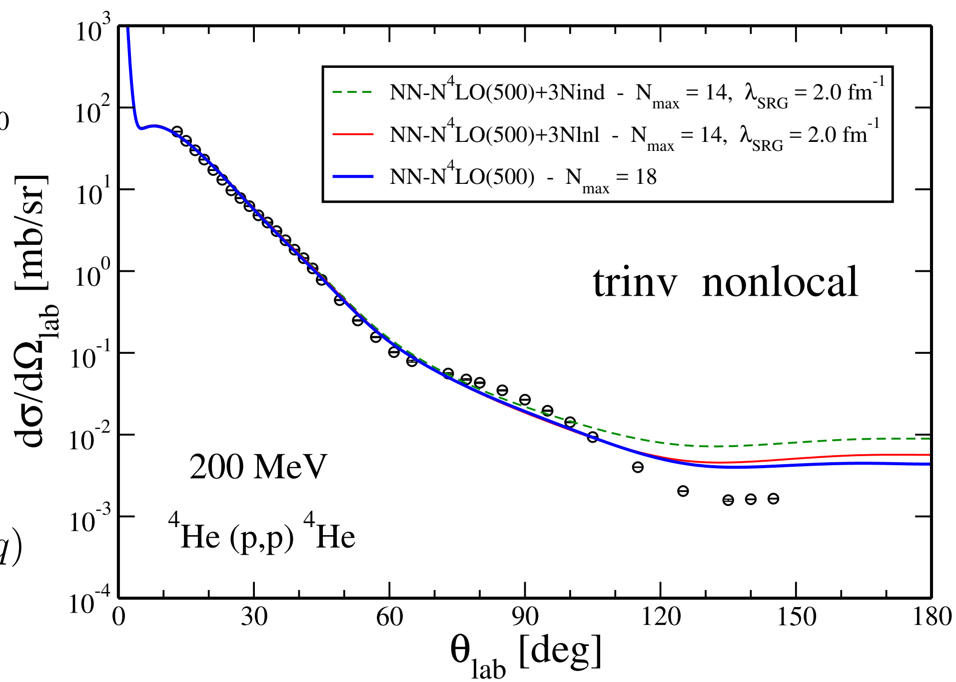




FF from local density

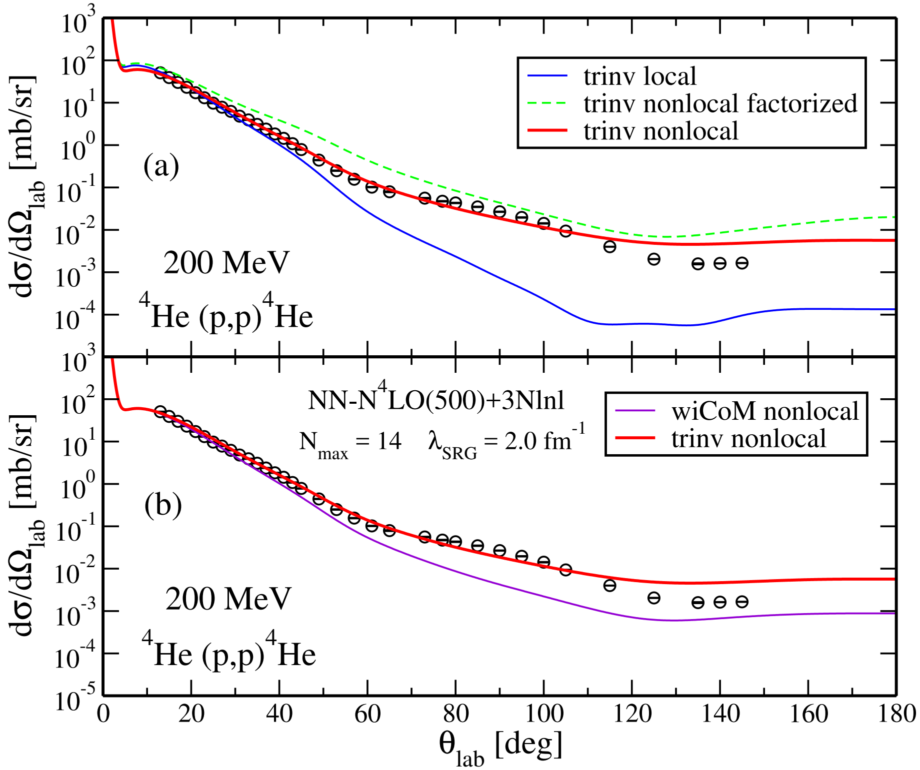
$$\rho_\alpha(q) = 4\pi \int_0^\infty dr r^2 j_0(qr) \rho_\alpha(r)$$

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



Factorized optical potential

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

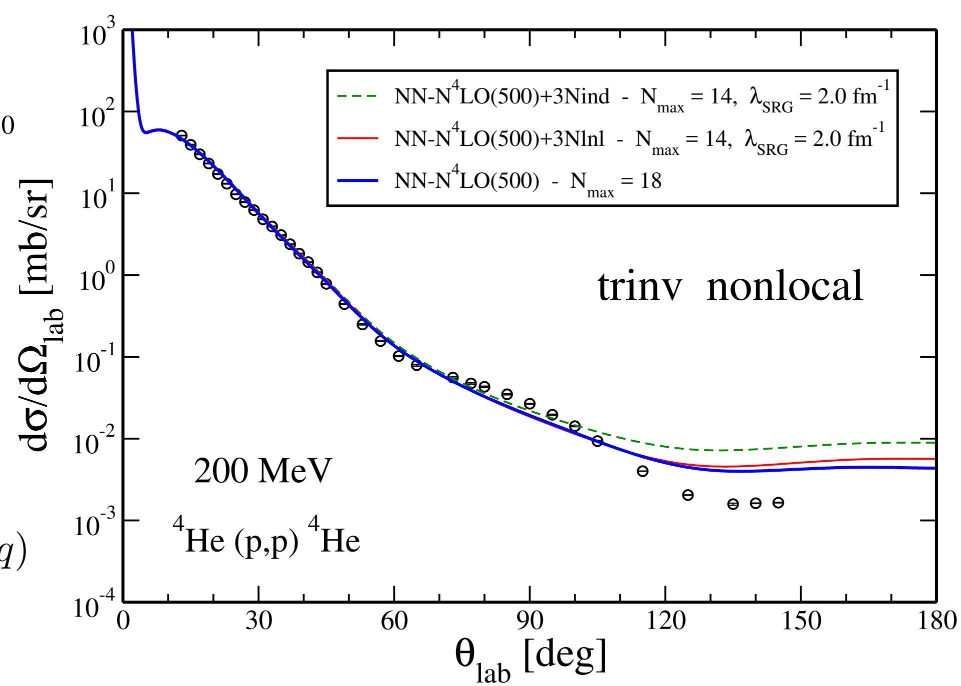


FF from nonlocal density

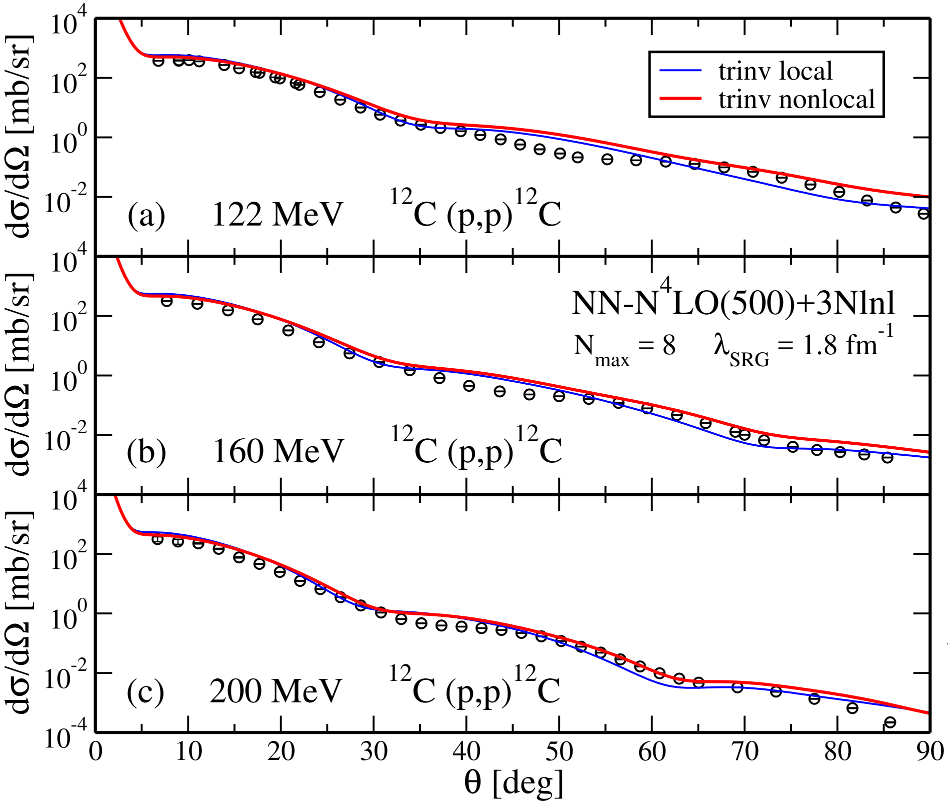
$$\rho_\alpha(q) = \int d\boldsymbol{P}\ \rho_\alpha\left(\boldsymbol{P} - \frac{A-1}{2A}\boldsymbol{q}, \boldsymbol{P} + \frac{A-1}{2A}\boldsymbol{q}\right)$$

Factorized optical potential

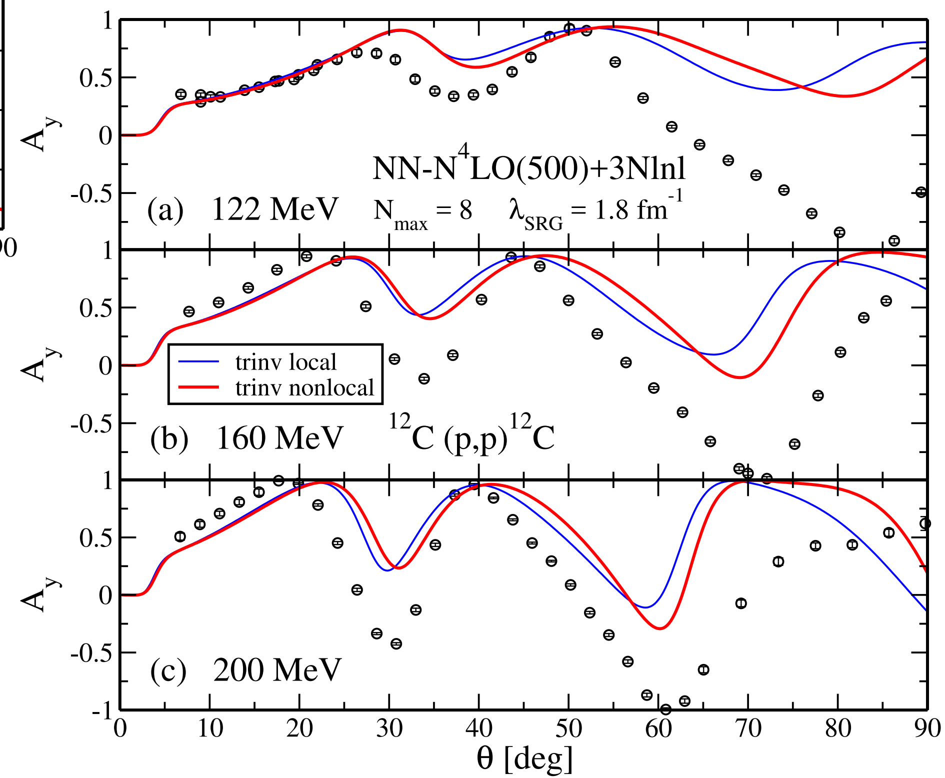
$$U(\boldsymbol{q}, \boldsymbol{K}; E) = \eta(\boldsymbol{q}, \boldsymbol{K}) \sum_{\alpha=n,p} t_{p\alpha}\left[\boldsymbol{q}, \frac{A+1}{2A}\boldsymbol{K}; E\right]\ \rho_\alpha(q)$$



Scattering observables – Stable nuclei

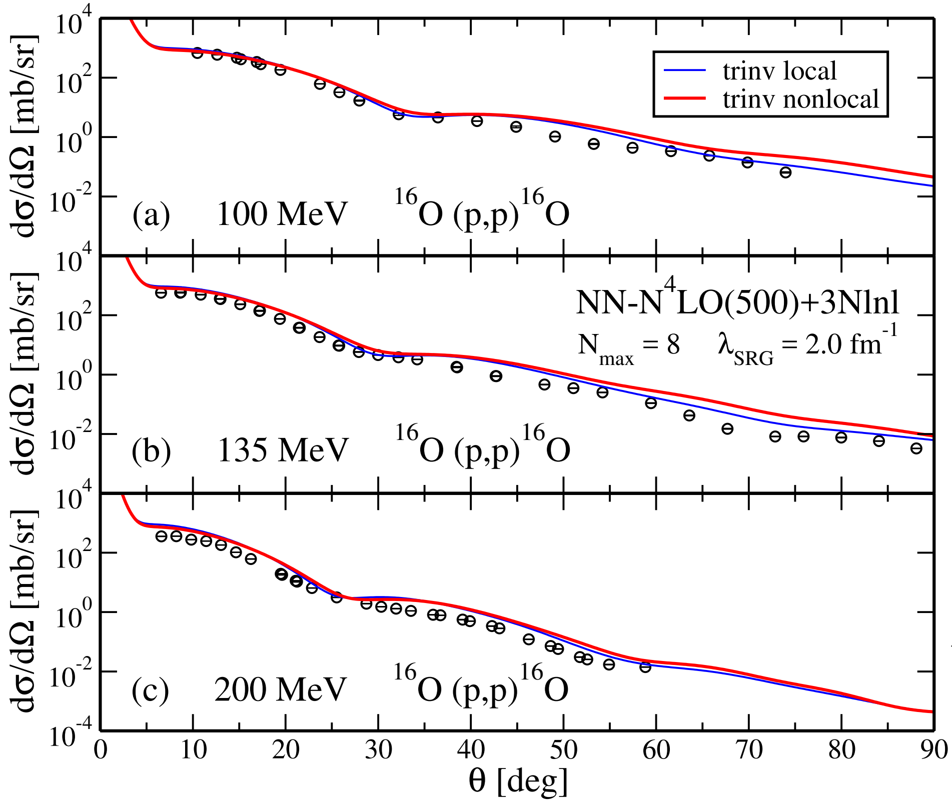


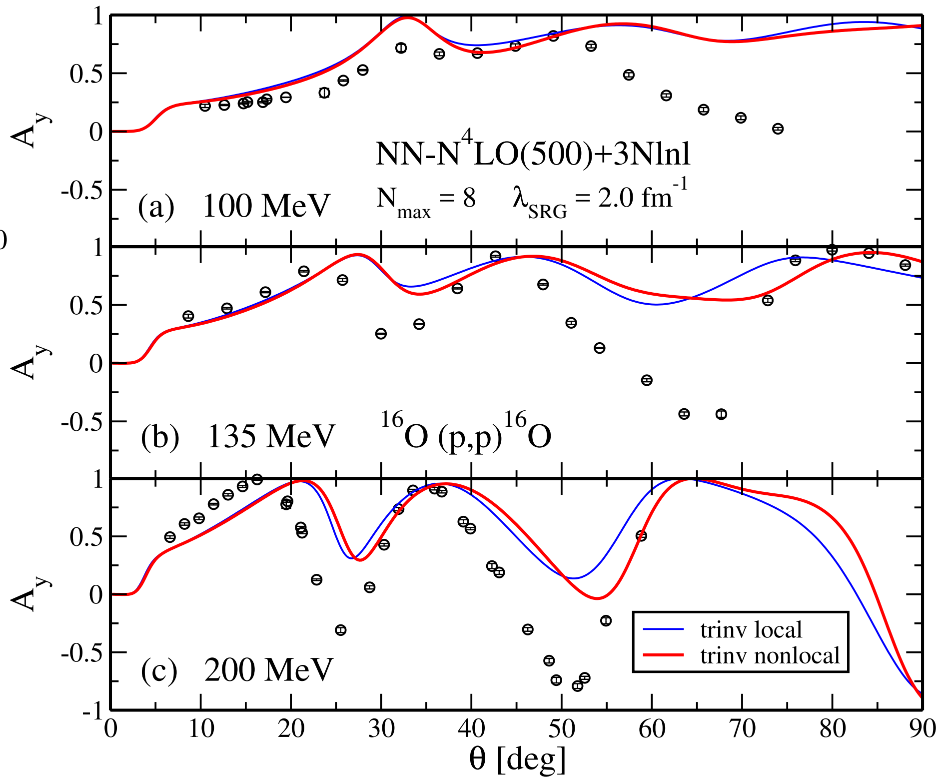
Good description of differential cross sections



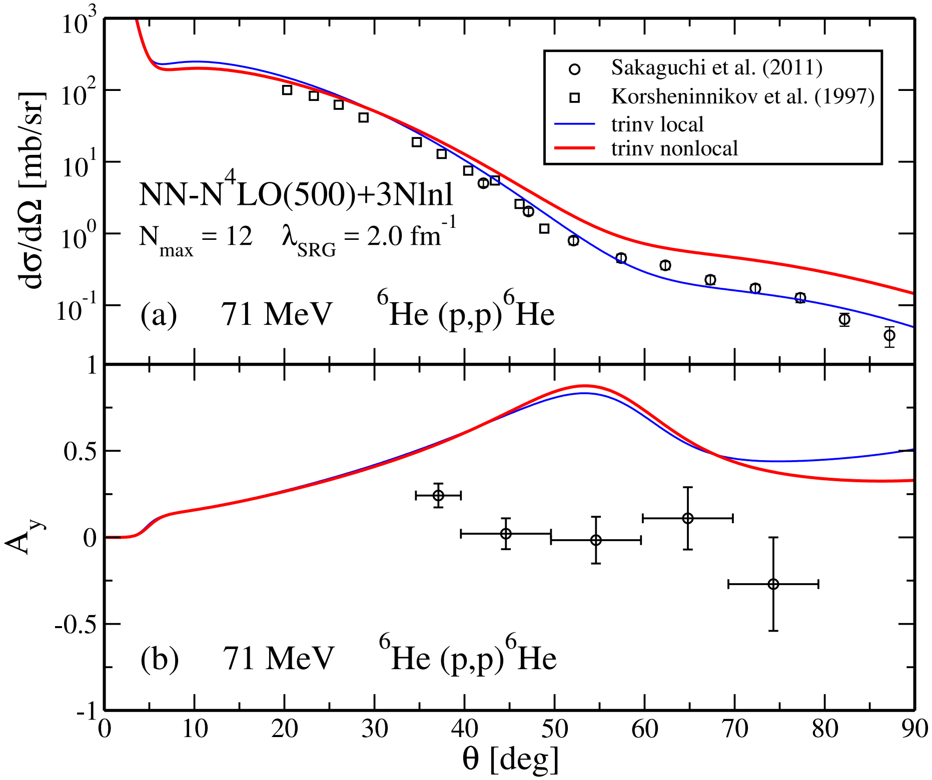
Reproduction of the general trend of the A_y

Scattering observables – Stable nuclei

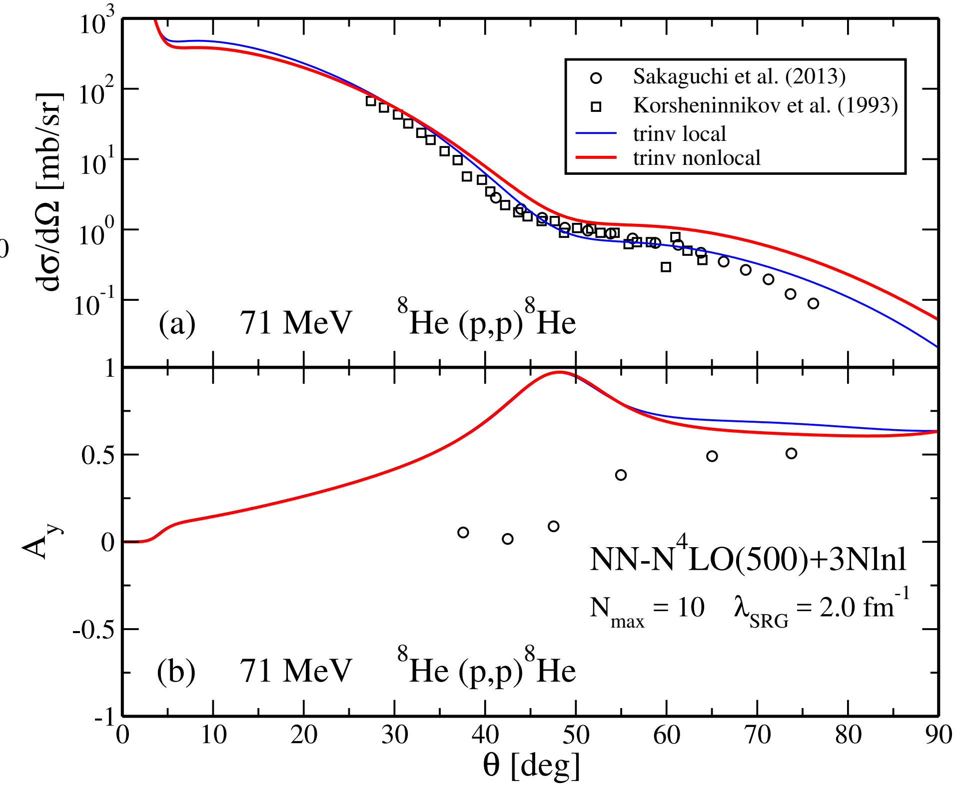




Scattering observables – Halo nuclei



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
- 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