Chiral 3N Forces in Ab-Initio Nuclear Spectroscopy & Reactions

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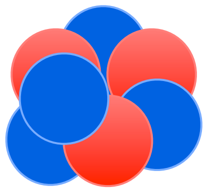
Outline

- Motivation
- Ingredients from Three-Body Technology
- Nuclear Structure within the IT-NCSM
  - Sensitivity of Spectra of *p*-Shell Nuclei on LECs & Cutoff
  - The Oxygen Isotopic Chain
- Nuclear Reactions within the NCSM/RGM approach
  - Formalism Including 3N forces
  - n-^{4}He Scattering
  - Scattering Involving Heavier Nuclei
- Conclusions

What we are aiming for...

Realistic ab-initio description of light nuclei

Bound states
& spectroscopy



A

Using NN+3N forces that are solidly rooted in QCD

Importance-Truncated NCSM

Ab-initio description
of nuclear clusters

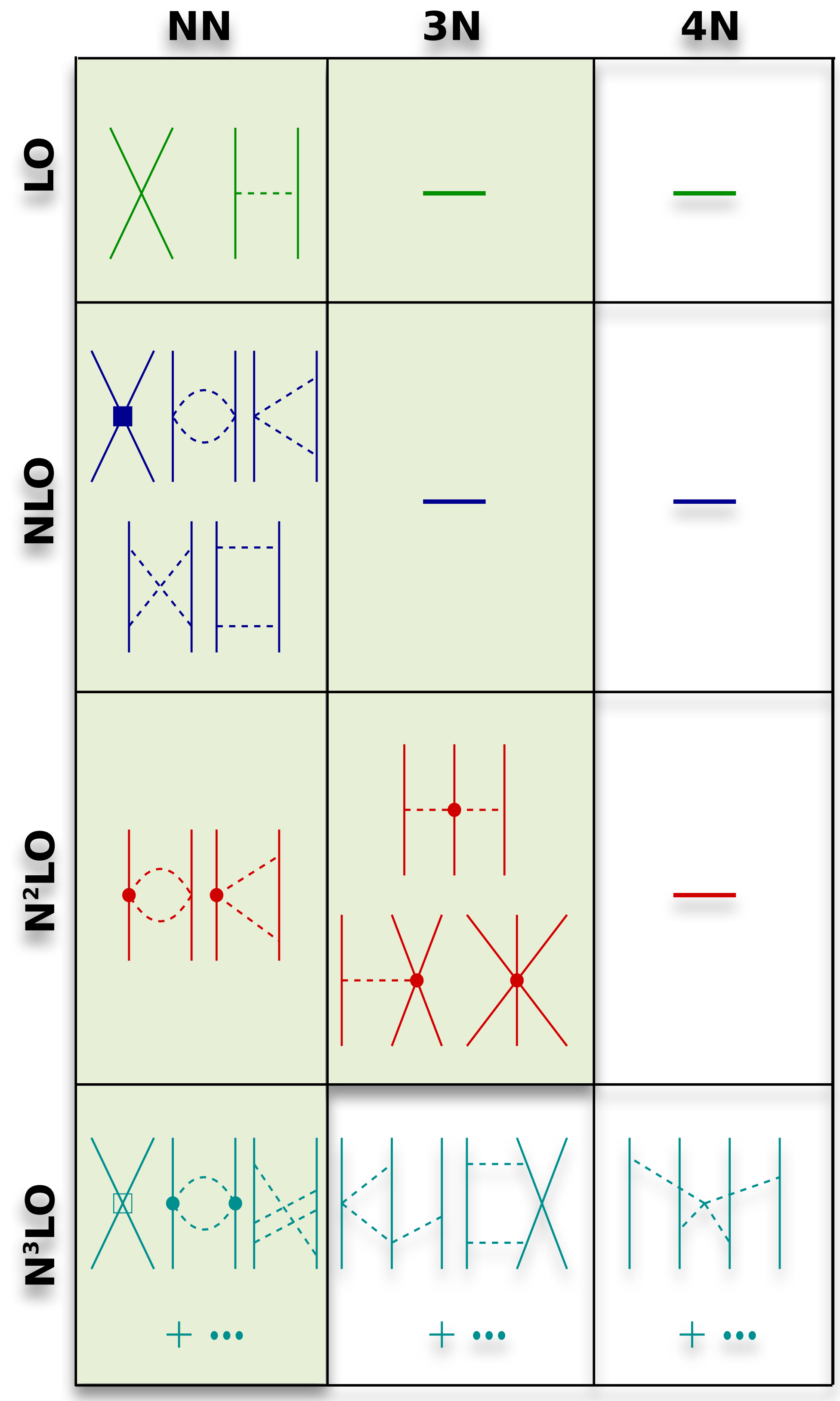
All relevant observables
accessible from the eigenstates

Ingredients from Three-Body Technology

The Chiral NN+3N Hamiltonian

Weinberg, van Kolck, Machleidt, Entem, Meißner, Epelbaum, Krebs, Bernard, Skibinski, Golak...

- Hierarchy of consistent nuclear NN, 3N,... forces (and currents)
- NN interaction @ N^3LO (Λ=500MeV)
  [Entem, Machleidt, Phys.Rev C **68**, 041001(R) (2003)]
- Standard Hamiltonian
  - 3N interaction @ N^2LO(Λ=500MeV)
    - Local form by Navrátil
    - LECs c_D, c_E fitted to β-decay halflife & binding energy of ^3H
      [Gazit et.al., Phys.Rev.Lett. **103**, 102502 (2009)]
- Reduced-Cutoff Hamiltonian
  - 3N interaction @ N^2LO(Λ=400MeV)
    - c_D=-0.2, c_E fitted to ^4He



The Similarity Renormalization Group

Wegner, Glazek, Wilson, Perry, Bogner, Furnstahl, Hergert, Calci, Langhammer, Roth, Jurgenson, Navrátil,...

...yields an evolved Hamiltonian with improved convergence properties in many-body calculations

- Unitary transformation of Hamiltonian $H_\alpha = U_\alpha^\dagger H U_\alpha$

Different SRG-Evolved Hamiltonians

- **NN-only**: start with NN initial Hamiltonian and keep two-body terms only
- **NN+3N-induced**: start with NN initial Hamiltonian and keep two- and three-body terms
- **NN+3N-full**: start with NN+3N initial Hamiltonian and keep two- and three-body terms

Nuclear Structure within the IT-NCSM

Sensitivity on Chiral 3N Forces

- LECs from πn vertices have sizable variations

$$c_1 = (-1.23 \ldots -0.76)\ \mathrm{GeV}^{-1}$$
$$c_3 = (-5.94 \ldots -3.2)\ \mathrm{GeV}^{-1}$$
$$c_4 = (3.4 \ldots 5.4)\ \mathrm{GeV}^{-1}$$

  - Uncertainties may propagate into nuclear structure observables
    ⇒ **quantify theoretical uncertainties**
    ⇒ **provide constraints for next generation chiral forces**

- Some N^3LO contributions can be absorbed into the N^2LO diagrams by shifting the c_i constants:

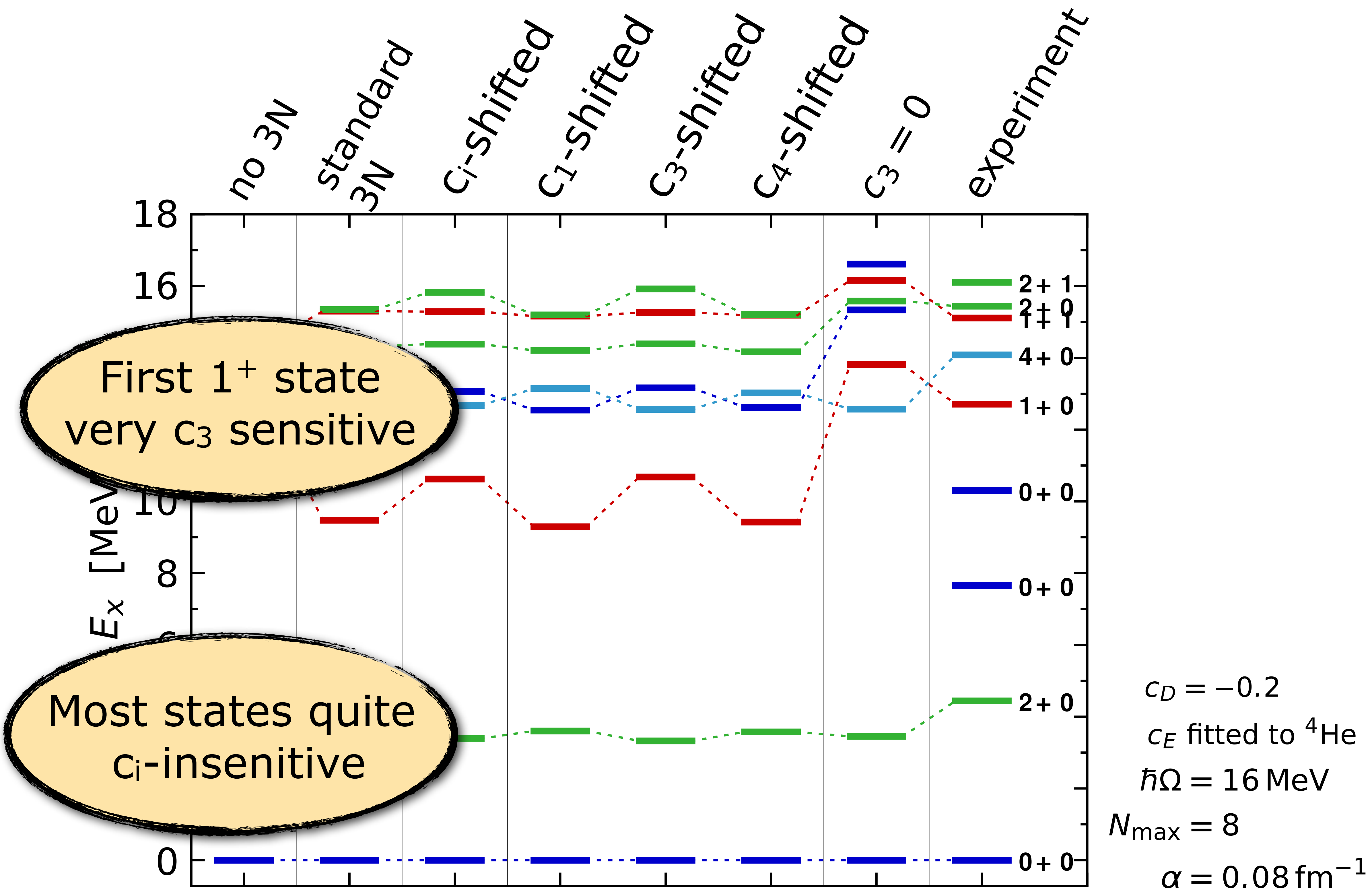
$$\tilde{c}_1 = c_1 - \frac{g_A^2 M_\pi}{64\pi F_\pi^2} \qquad \tilde{c}_3 = c_3 - \frac{g_A^4 M_\pi}{16\pi F_\pi^2} \qquad \tilde{c}_4 = c_4 - \frac{g_A^4 M_\pi}{16\pi F_\pi^2}$$

10-20% change

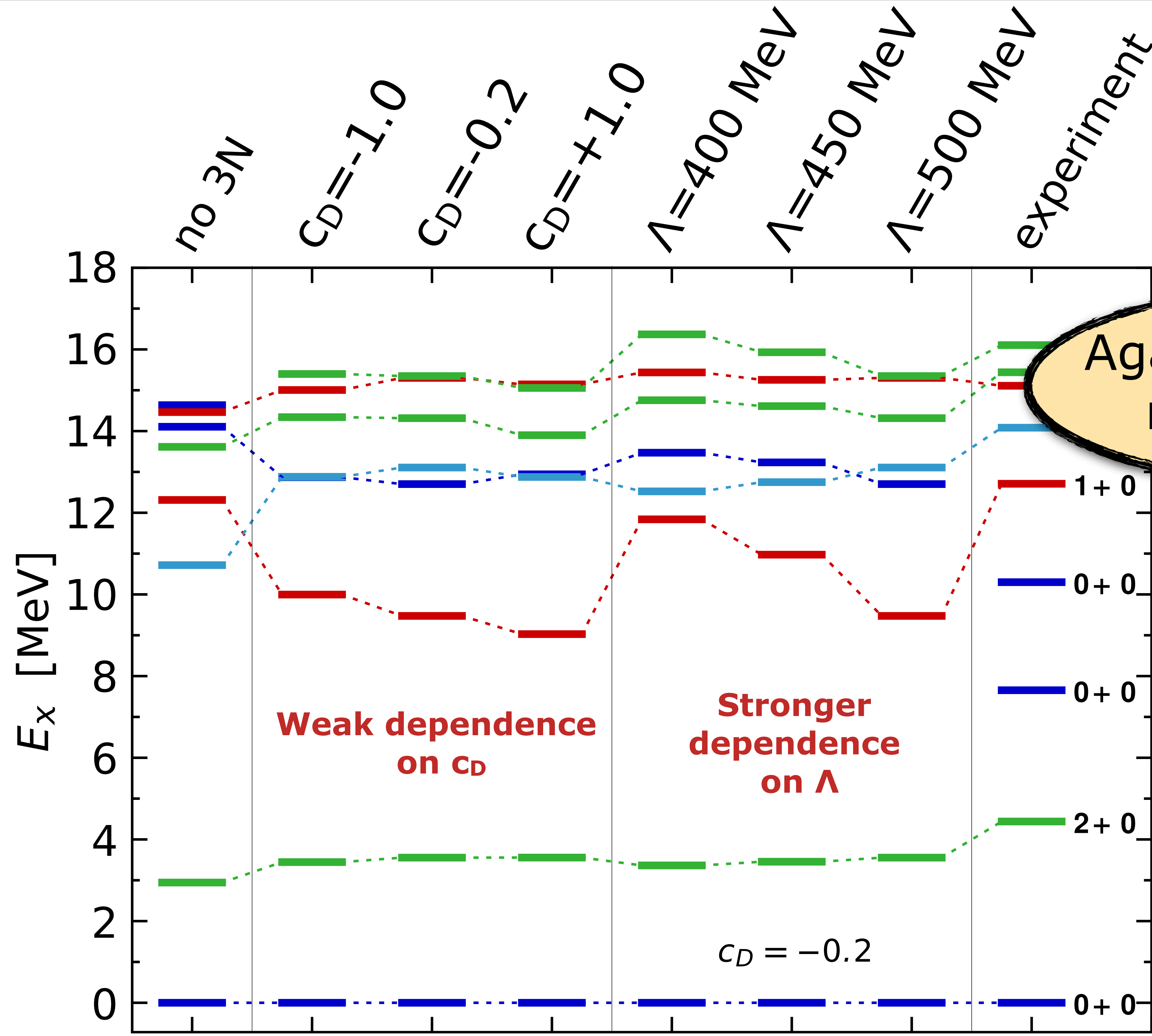
- Does the chosen cutoff Λ affect nuclear structure observables?

Analyze sensitivity of spectra on LECs and chiral cutoff of the chiral 3N force at N^2LO

^{12}C: Sensitivity on c_i



^{12}C: Sensitivity on c_D and Cutoff



Again First 1^+ state most sensitive

c_E fitted to ^{4}He

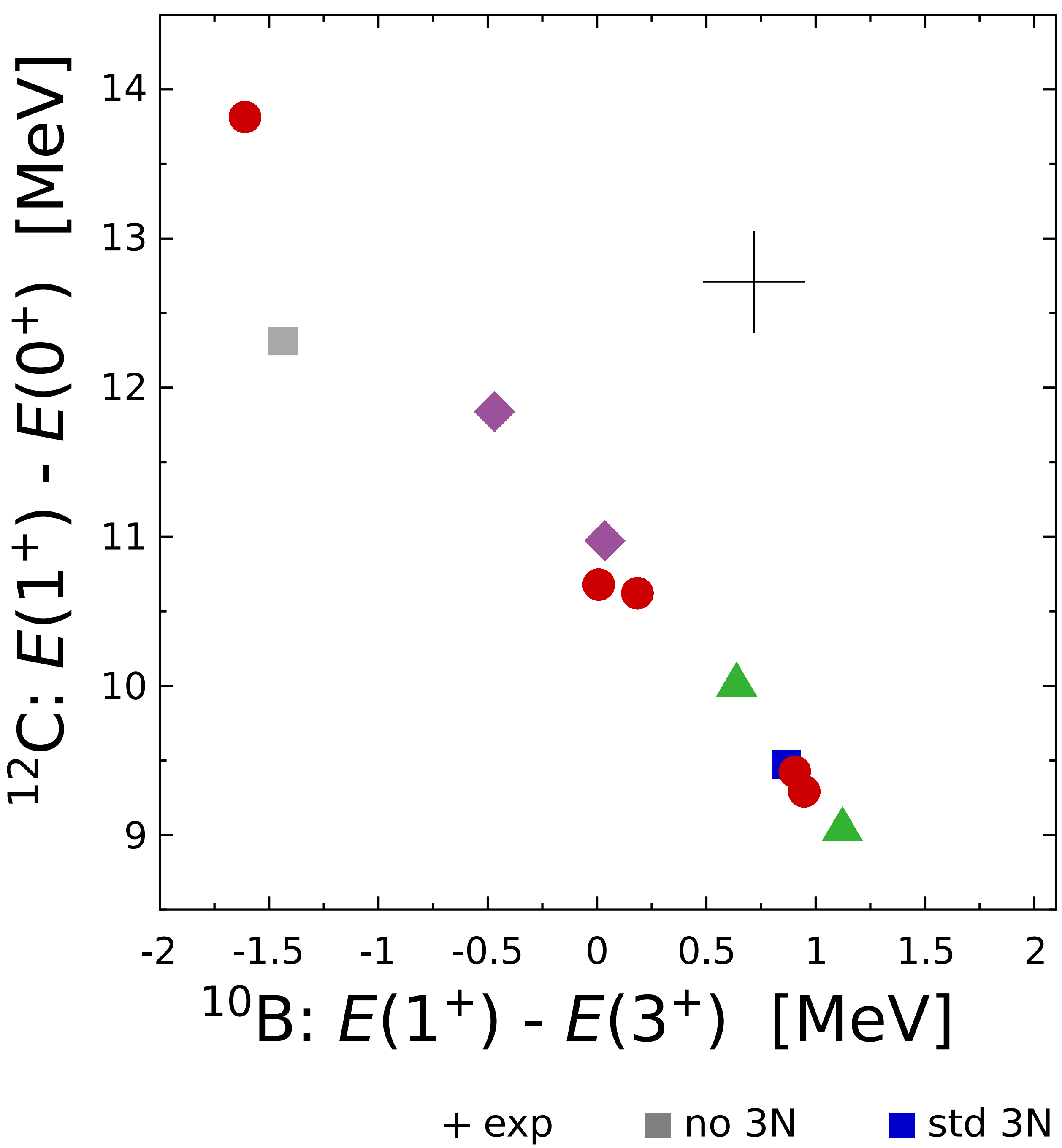
$\hbar\Omega = 16\,\text{MeV}$

$N_{max} = 8$

$\alpha = 0.08\,\text{fm}^{-1}$

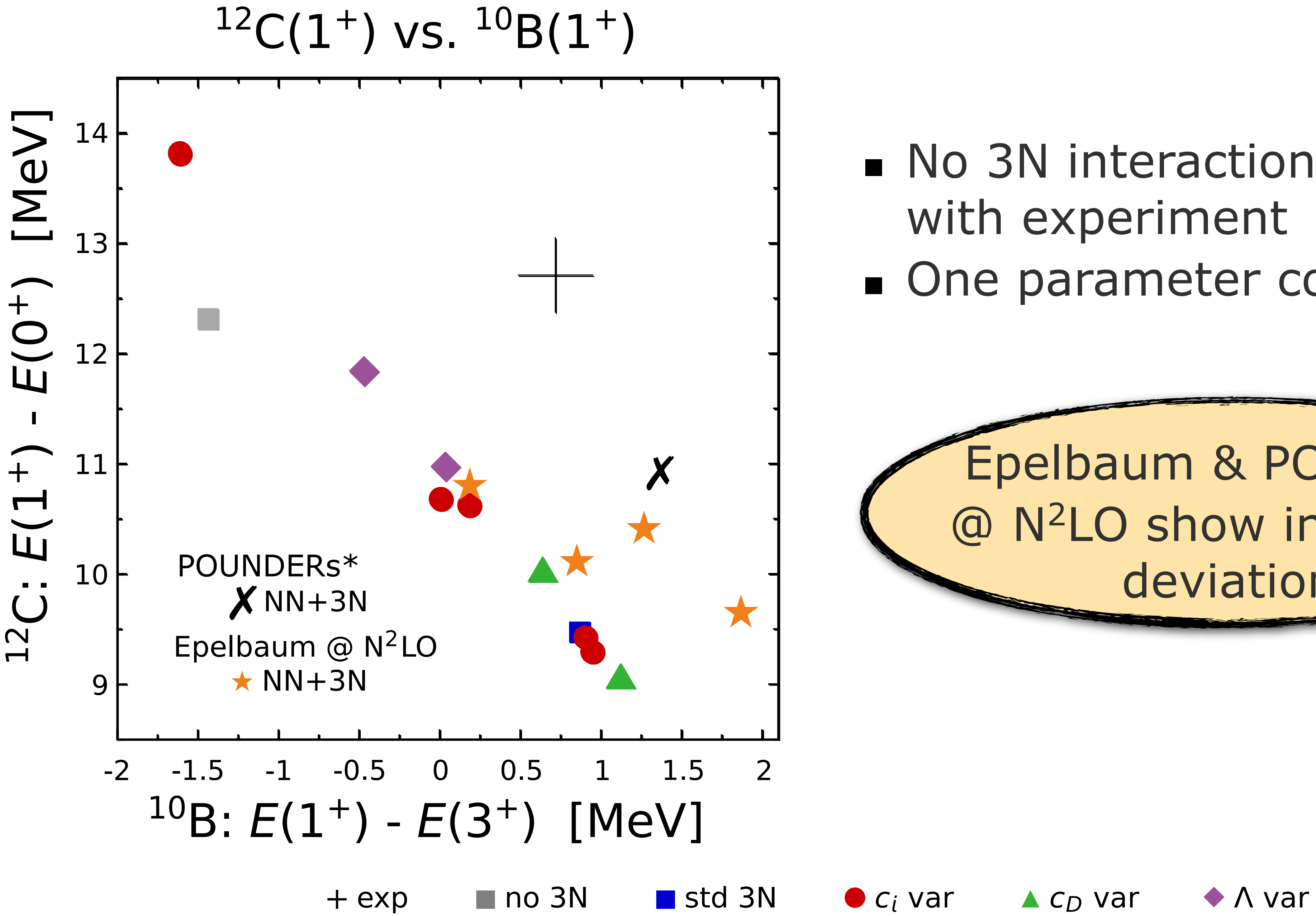
Correlation Analysis

^{12}C(1$^+$) vs. ^{10}B(1$^+$)



- No 3N interaction compatible with experiment
- One parameter correlation

Correlation Analysis

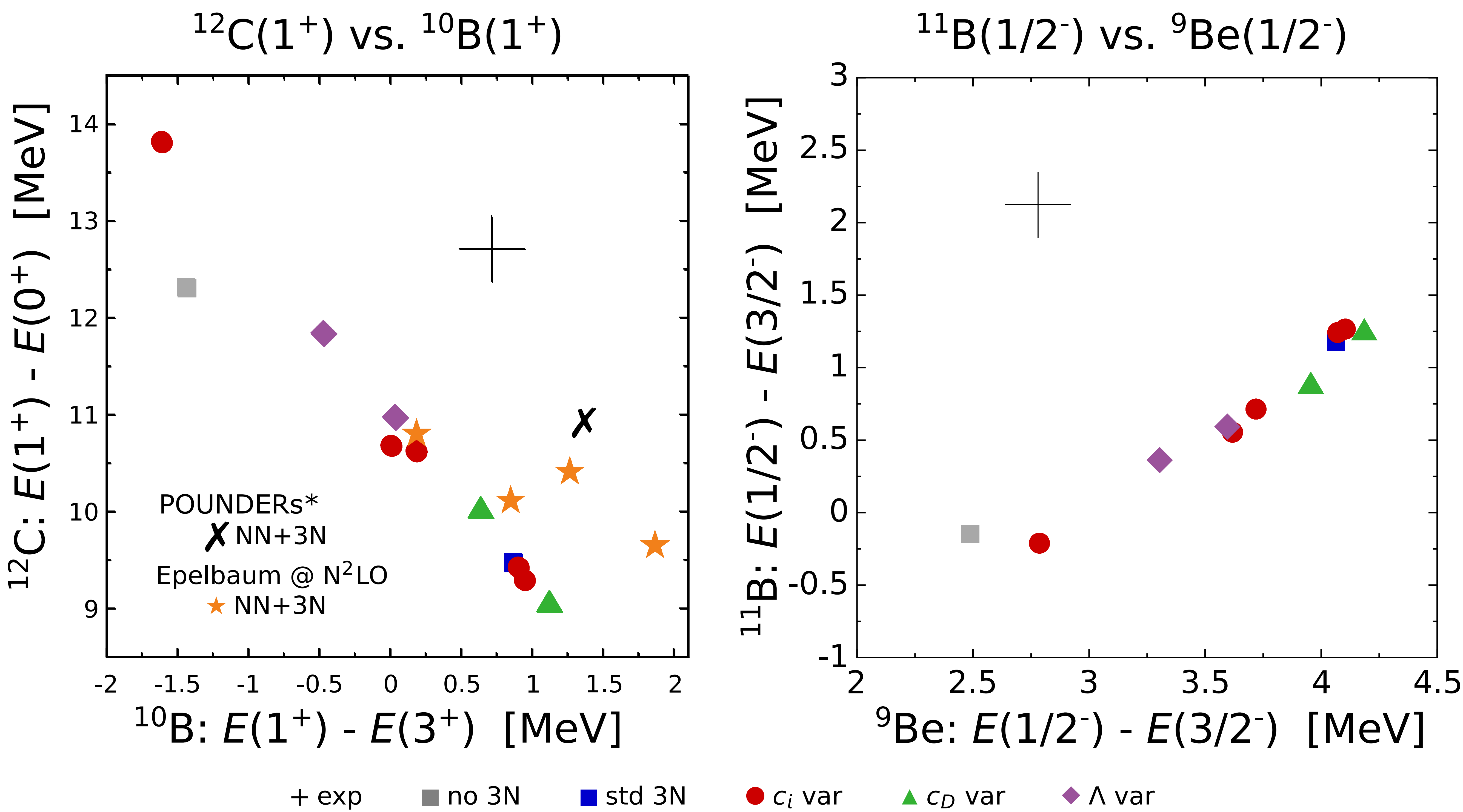


- No 3N interaction compatible with experiment
- One parameter correlation

Epelbaum & POUNDERs @ N^{2}LO show interesting deviations

* Ekström et al., Phys. Rev. Lett. 110, 192502 (2013)
3N fit of c_D and c_E by Navratil & Quaglioni priv. comm.

Correlation Analysis



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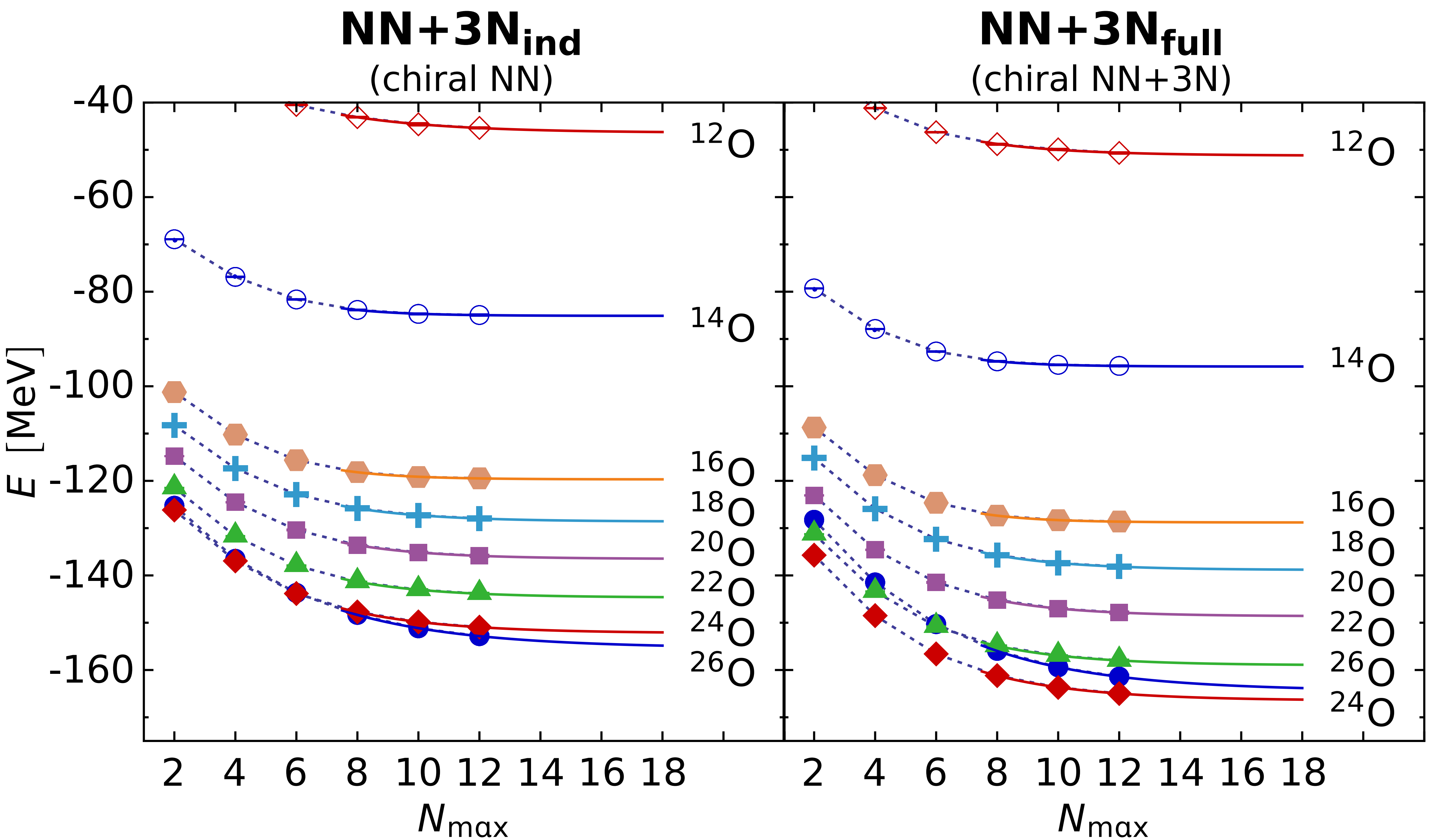
Ab-Initio Study of the Oxygen Chain

Hergert, Binder, Calci, Langhammer, Roth ----- Phys. Rev. Lett. 110 242501 (2013)

Ground-States of Even Oxygen Isotopes

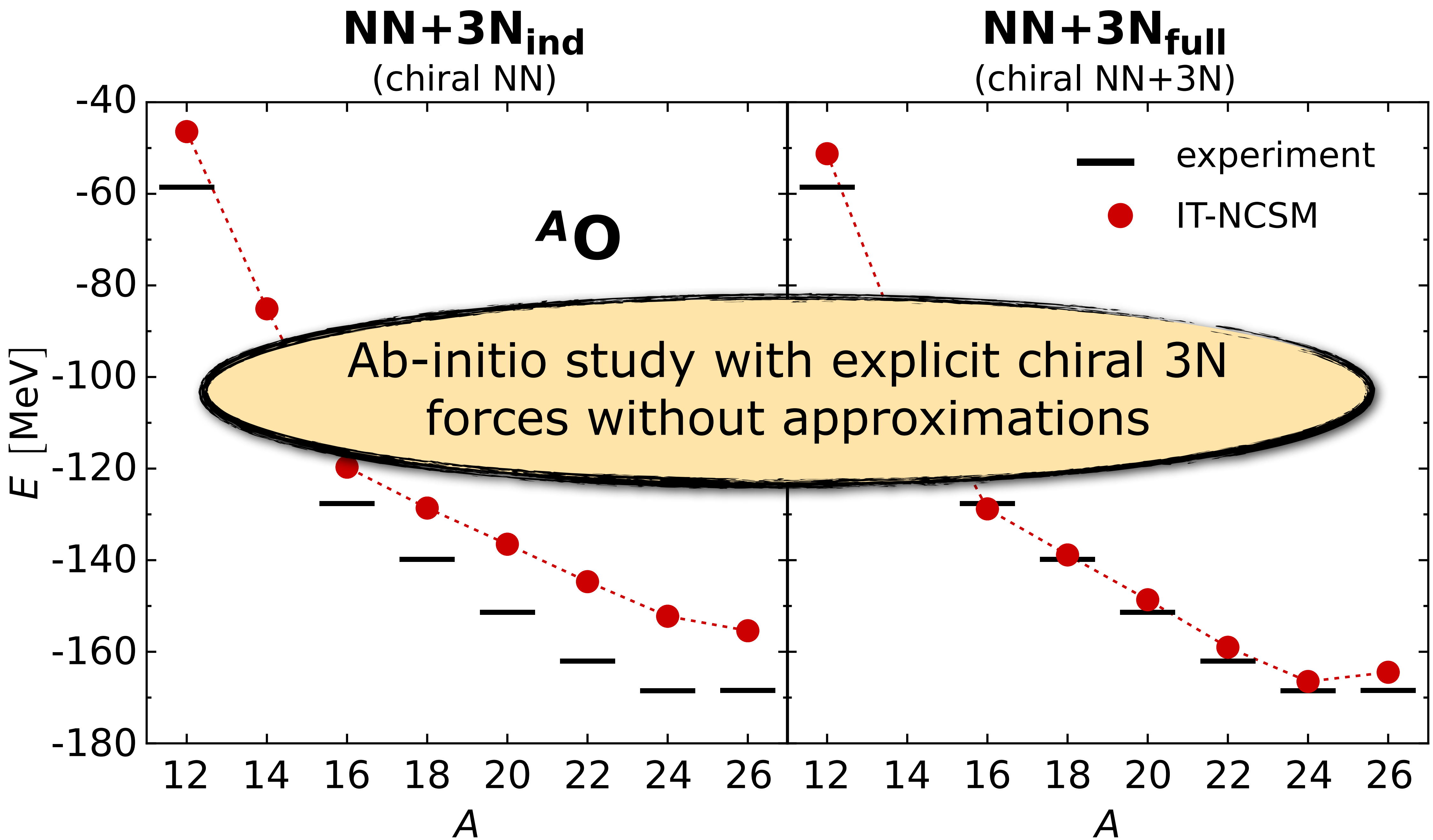
Hergert, Binder, Calci, JL, Roth, PRL ***110*** 242501 (2013)



$\Lambda_{3N} = 400$ MeV, $\alpha = 0.08\,\text{fm}^4$, $E_{3\,max} = 14$, optimal $\hbar\Omega$

Ground-States of Even Oxygen Isotopes

*Hergert, Binder, Calci, JL, Roth, PRL **110** 242501 (2013)*

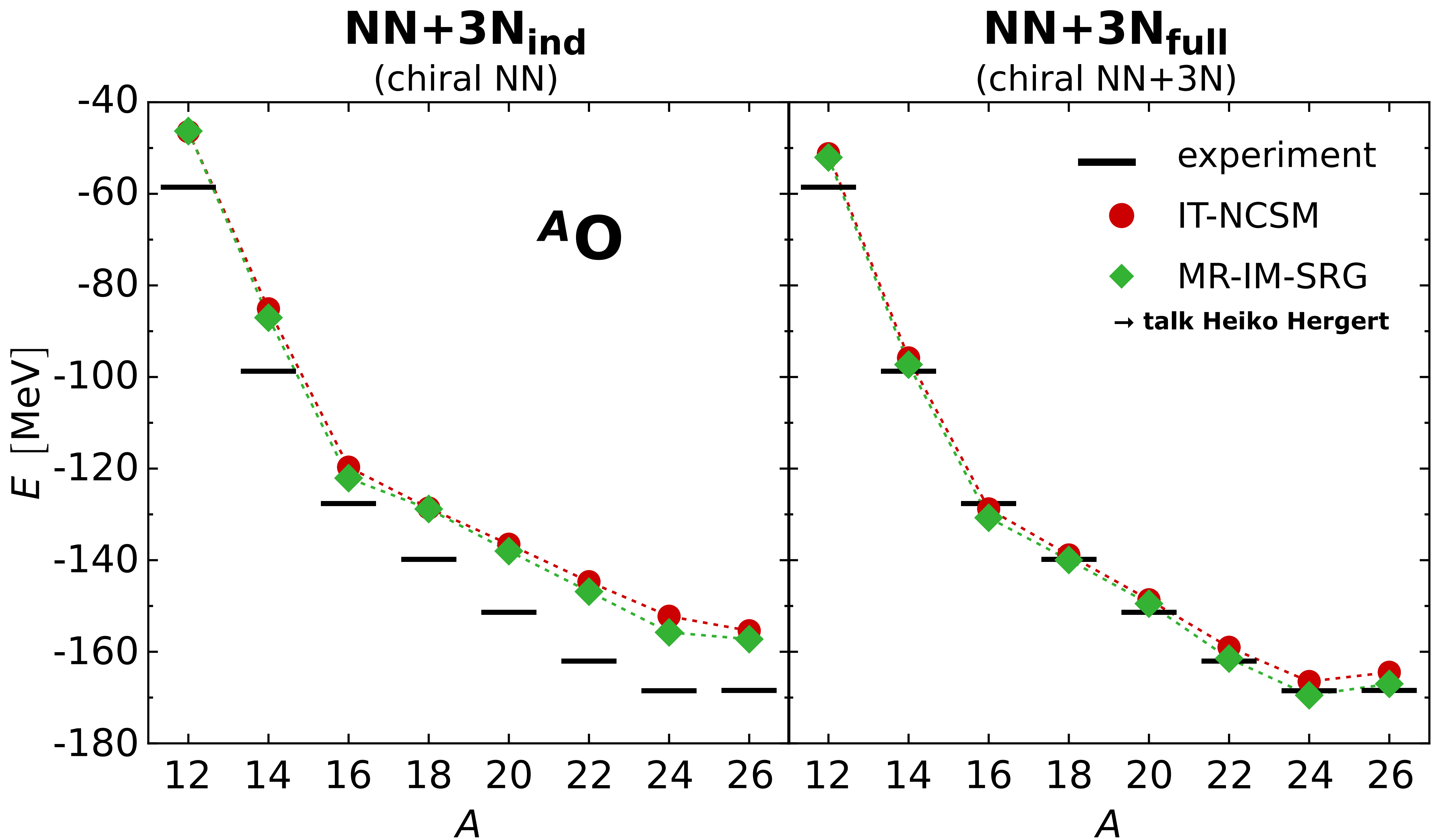


Ab-initio study with explicit chiral 3N forces without approximations

$\Lambda_{3N} = 400$ MeV, $\alpha = 0.08\,\mathrm{fm}^4$, $E_{3\,\mathrm{max}} = 14$, optimal $\hbar\Omega$

Ground-States of Even Oxygen Isotopes

Hergert, Binder, Calci, JL, Roth, PRL **110** 242501 (2013)



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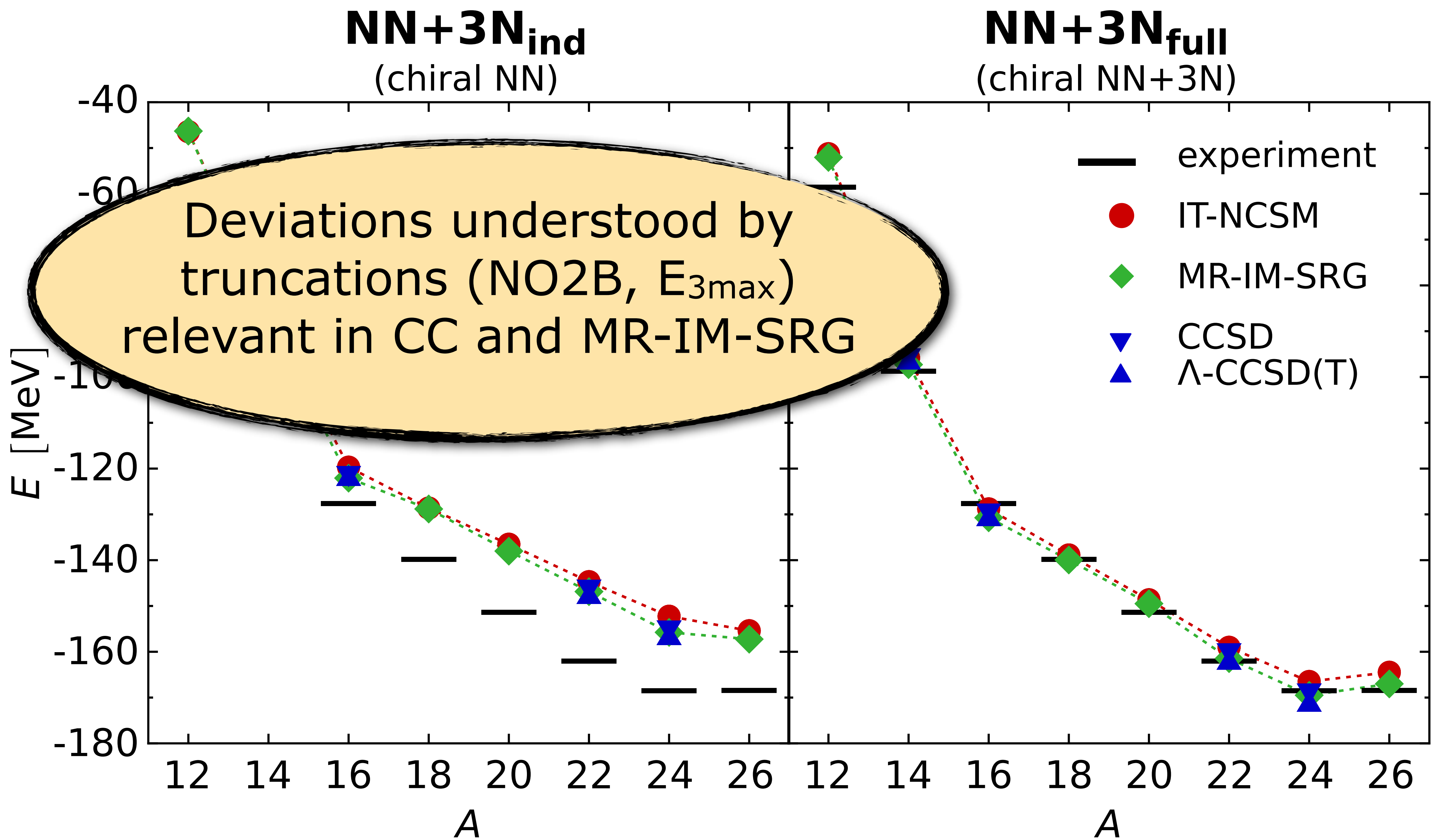

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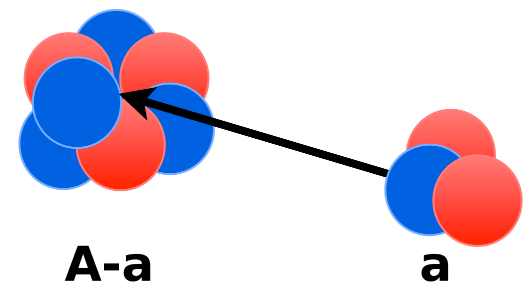


Resonances
& scattering states

(IT-)NCSM
Ab-initio description o
nuclear clusters

(IT-)NCSM/RGM
approach

RGM
Describing relative
motion of clusters

Successfully applied with NN interactions
Now: Inclusion of 3N Forces

Nuclear Reactions within the NCSM/RGM approach

In collaboration with

G. Hupin, S. Quaglioni, P. Navrátil & R. Roth

S. Quaglioni and P. Navrátil ----- Phys. Rev. Lett. 101, 092501 (2008)

P. Navrátil, R. Roth and S. Quaglioni ----- Phys. Rev. C 82, 034609 (2010)

S. Quaglioni, P. Navrátil, G. Hupin, J. Langhammer et al. ----- Few-Body Syst. DOI 10.1007/s00601-012-0505-0 (2012)

S. Quaglioni, P. Navrátil, R. Roth, W. Horiuchi ----- J.Phys.Conf.Ser. 402 (2012)

General Approach of NCSM/RGM

Wildermuth,Thompson, Tang, ..., Navrátil, Quaglioni, Roth, Hupin, Langhammer,...

- Represent $H\,|\psi^{J\pi T}\rangle = E\,|\psi^{J\pi T}\rangle$ using the **over-complete basis**

$$|\psi^{J\pi T}\rangle = \sum_{\nu} \int dr r^2 \frac{g_{\nu}^{J\pi T}(r)}{r} \mathcal{A}_{\nu}\,|\phi_{\nu r}^{J\pi T}\rangle$$

$g_{\nu}^{J\pi T}(r)$ unknown

with the binary-cluster channel states

$$|\phi^{J\pi T}\rangle = \left\{ |\Phi^{(A-a)}\rangle\,|\Phi^{(a)}\rangle \right\}^{J\pi T} \frac{\delta(r - r_{A-a,a})}{r r_{A-a,a}}$$

NCSM delivers $|\Phi^{(A-a)}\rangle$ and $|\Phi^{(a)}\rangle$

- Solve **generalized eigenvalue** problem

$$\sum_{\nu} \int dr r^2 \left[\mathcal{H}_{\nu,\nu'}^{J\pi T}(r',r) - E\mathcal{N}_{\nu,\nu'}^{J\pi T}(r,r')\right] \frac{g_{\nu r}^{J\pi T}}{r} = 0$$

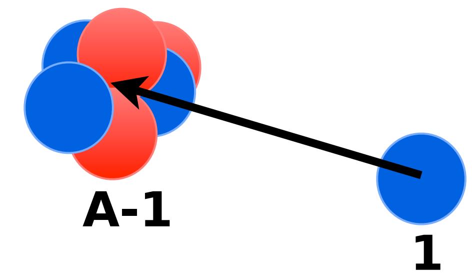
Hamiltonian kernel $\langle\phi_{\nu' r'}^{J\pi T}|\,\mathcal{A}_{\nu'} H \mathcal{A}_{\nu}\,|\phi_{\nu r}^{J\pi T}\rangle$

Norm kernel $\langle\phi_{\nu' r'}^{J\pi T}|\,\mathcal{A}_{\nu'} \mathcal{A}_{\nu}\,|\phi_{\nu r}^{J\pi T}\rangle$

Towards Inclusion of Full 3N Forces

- Derive expressions for 3N-interaction kernel

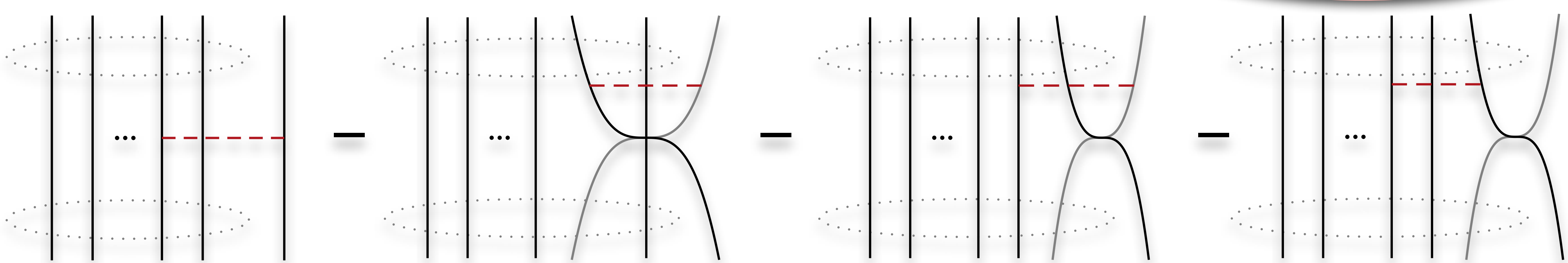
$$\langle \phi^{J\pi T}_{\nu' r'} | V_{3N} \mathcal{A}^2 \, | \phi^{J\pi T}_{\nu r} \rangle = \langle \phi^{J\pi T}_{\nu' r'} | V_{3N} \left[1 - \sum_{i=1}^{A-1} T_{i,A} \right] | \phi^{J\pi T}_{\nu r} \rangle$$



$$\left.\begin{aligned} &= \frac{(A-1)(A-2)}{2} \langle \phi^{J\pi T}_{\nu' r'} | V_{A-2,A-1,A} \, | \phi^{J\pi T}_{\nu r} \rangle \\ &- \frac{(A-1)(A-2)}{2} \langle \phi^{J\pi T}_{\nu' r'} | V_{A-2,A-1,A} T_{A-2,A} \, | \phi^{J\pi T}_{\nu r} \rangle \\ &- \frac{(A-1)(A-2)}{2} \langle \phi^{J\pi T}_{\nu' r'} | V_{A-1,A-2,A} T_{A-1,A} \, | \phi^{J\pi T}_{\nu r} \rangle \end{aligned}\right\} \text{“direct” kernel}$$

$$- \frac{(A-1)(A-2)(A-3)}{2} \langle \phi^{J\pi T}_{\nu' r'} | V_{A-3,A-2,A} T_{A-1,A} \, | \phi^{J\pi T}_{\nu r} \rangle$$

Handling
of 3-body density
challenging

= 

$\propto \langle \Phi'^{(A-1)} | a^\dagger a^\dagger a a \, | \Phi^{(A-1)} \rangle$ $\quad \propto \langle \Phi'^{(A-1)} | a^\dagger a^\dagger a^\dagger a a a \, | \Phi^{(A-1)} \rangle$

Handling of Three-Body Density

Hupin, Quaglioni, Navrátil

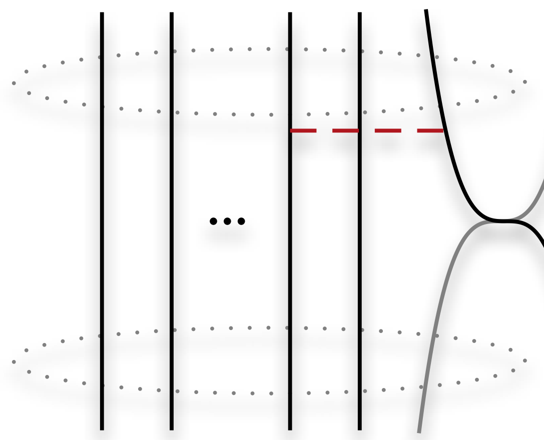
1 Precomputed coupled densities

$$\sum_{\substack{j_0 j'_0\\ K J_0}} \sum_{\substack{t_0 t'_0\\ \tau T_0}} \sum_{\substack{n_a l_a j_a\\ n_b l_b j_b}} \sum_{\substack{n_\alpha l_\alpha j_\alpha\\ n'_a l'_a j'_a}} \sum_{\substack{n'_b l'_b j'_b\\ g' t'_g}} \tfrac{1}{12} \hat{\tau} \hat{K} \hat{J}_0 \hat{T}_0 \hat{g}' \hat{t}'_g (-1)^{j'_a + j'_b - j'_0 + j' + K + I_1 + J} (-1)^{3/2 - t'_0 + j' + \tau + T_1 + T}$$

$$\begin{Bmatrix} I_1 & K & I'_1 \\ j' & J & j \end{Bmatrix} \begin{Bmatrix} j' & K & j \\ g' & j'_0 & J_0 \end{Bmatrix} \begin{Bmatrix} T_1 & \tau & T'_1 \\ \frac{1}{2} & T & \frac{1}{2} \end{Bmatrix} \begin{Bmatrix} \frac{1}{2} & \tau & \frac{1}{2} \\ t'_g & t'_0 & T_0 \end{Bmatrix}$$

$${}_a\langle ((nlj'_a, nlj'_b) j'_0 t'_0, nlj') J_0 T_0 | V_{3N} | ((nlj_\alpha, nlj_a) j_0 t_0, nlj_b) J_0 T_0 \rangle_a$$

$$\left\langle \Phi'^{(A-1)} I'_1 T'_1 \left\| \left[\left(a^\dagger_{nlj} \left(a^\dagger_{nlj'_b} a^\dagger_{nlj'_a} \right)^{j'_0 t'_0} \right)^{g' t'_g} \left(\left(\tilde{a}_{nlj_\alpha} \tilde{a}_{nlj_a} \right)^{j_0 t_0} \tilde{a}_{nlj_b} \right)^{J_0 T_0} \right]^{K\tau} \right\| \Phi^{(A-1)} I_1 T_1 \right\rangle$$



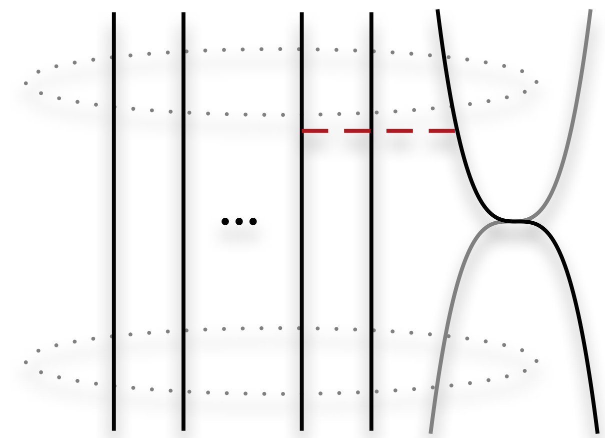
- Make use of *JT*-coupled 3N matrix elements
- Three-body density cannot be stored...use a trick

Handling of Three-Body Density

Hupin, Quaglioni, Navrátil

1 Precomputed coupled densities

$$\sum_{\substack{j_0 j'_0 t_0 t'_0\\ J_0 T_0}} \sum_{\substack{n_a l_a j_a\\ n_b l_b j_b}} \sum_{\substack{n_\alpha l_\alpha j_\alpha\\ n'_a l'_a j'_a}} \sum_{\substack{n'_b l'_b j'_b\\ g' t'_g}} \sum_{\phi'' I_\beta T_\beta} \tfrac{1}{12}\hat{J}_0 \hat{T}_0 \hat{g}' \hat{t}'_g (-1)^{j'_a+j'_b+J_0+g'+I_\beta-I_1+j}(-1)^{3/2+T_0+t'_g-T_1+T_\beta}$$



$$\begin{Bmatrix} I_\beta & g' & I'_1 \\ J_0 & j'_0 & j' \\ J_1 & j & J \end{Bmatrix} \begin{Bmatrix} T_\beta & t'_g & T'_1 \\ T_0 & t'_0 & \frac{1}{2} \\ T_1 & \frac{1}{2} & T \end{Bmatrix}$$

$${}_a\langle ((nlj'_a, nlj'_b)j'_0 t'_0, nlj')J_0 T_0 |\, V_{3N} \,| ((nlj_\alpha, nlj_a)j_0 t_0, nlj_b)J_0 T_0\rangle_a$$

$$\left\langle \Phi'^{(A-1)} I'_1 T'_1 \left\| \left(a^\dagger_{nlj}\left(a^\dagger_{nlj'_b} a^\dagger_{nlj'_a}\right)^{j'_0 t'_0}\right)^{g' t'_g} \right\| \Phi''^{(A-4)} I_\beta T_\beta \right\rangle$$

$$\left\langle \Phi''^{(A-4)} I_\beta T_\beta \left\| \left(\left(\tilde{a}_{nlj_\alpha} \tilde{a}_{nlj_a}\right)^{j_0 t_0} \tilde{a}_{nlj_b}\right)^{J_0 T_0} \right\| \Phi^{(A-1)} I_1 T_1 \right\rangle$$

- Make use of JT-coupled 3N matrix elements
- Three-body density cannot be stored...use a t
- Use reduced density matrix elements

Applicable to ^{4}He targets

Handling of Three-Body Density

Langhammer, Roth, Navrátil

② Compute uncoupled densities on-the-fly

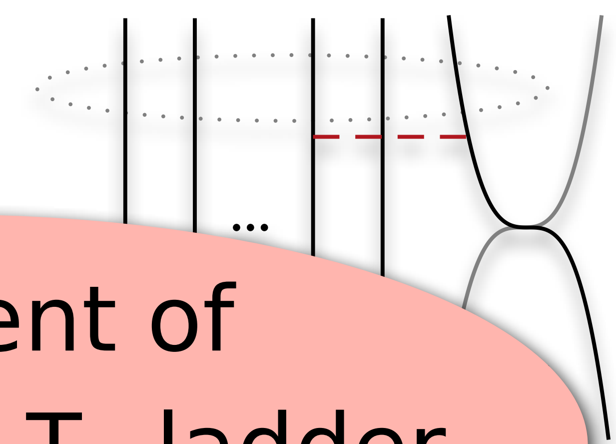
$$\sum_{jj'}\sum_{M_1 m_j}\sum_{M_{T_1} m_t}\sum_{M'_1 m'_j}\sum_{M'_{T_1} m'_t} \tfrac{1}{12}(-1)^{I_1+I'_1+2J+j+j'} \begin{Bmatrix} I_1 & \frac{1}{2} & s \\ l & J & j \end{Bmatrix} \begin{Bmatrix} I'_1 & \frac{1}{2} & s' \\ l' & J & j' \end{Bmatrix}$$

$$\left(\begin{array}{cc|c} I_1 & j & J \\ M_1 & m_j & M_J \end{array}\right) \left(\begin{array}{cc|c} T_1 & \frac{1}{2} & T \\ M_{T_1} & m_t & M_T \end{array}\right) \left(\begin{array}{cc|c} I'_1 & j' & J \\ M'_1 & m'_j & M'_J \end{array}\right) \left(\begin{array}{cc|c} T'_1 & \frac{1}{2} & T \\ M'_{T_1} & m'_t & M'_T \end{array}\right)$$

$$\sum_{\beta_{A-3}}\sum_{\beta_{A-2}}\sum_{\beta'_{A-3}}\sum_{\beta'_{A-2}}\sum_{\beta'_{A-1}}$$

$$_a\langle \beta_{A-3}\beta_{A-2} n l j' m'_j \tfrac{1}{2} m'_t |\, V_{3N}\, | \beta'_{A-3}\beta'_{A-2}\beta'_{A-1}\rangle_a$$

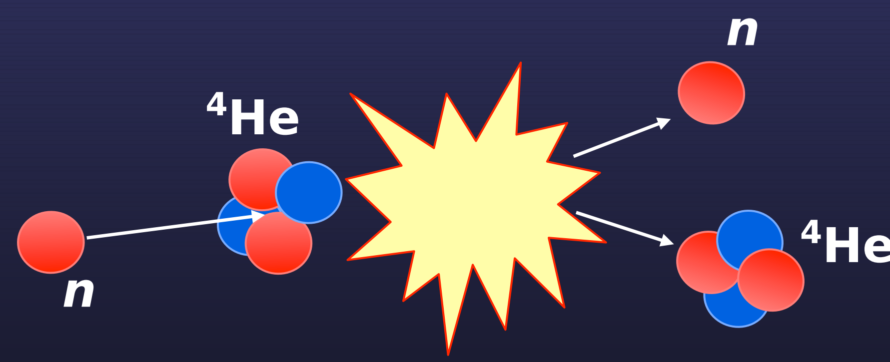
$$\langle \Phi'^{(A-1)} I'_1 M'_1 T'_1 M'_{T_1} |\, a^\dagger_{nljm_j\frac{1}{2}m_t} a^\dagger_{\beta_{A-2}} a^\dagger_{\beta_{A-3}} a_{\beta'_{A-3}} a_{\beta'_{A-2}} a_{\beta'_{A-1}} | \Phi^{(A-1)} I_1 M_1 T_1 M_{T_1}\rangle$$



Treatment of M_J, M_T via J±, T± ladder operators

- Use m-scheme matrix elements ⇒ effici
- Perfectly parallel

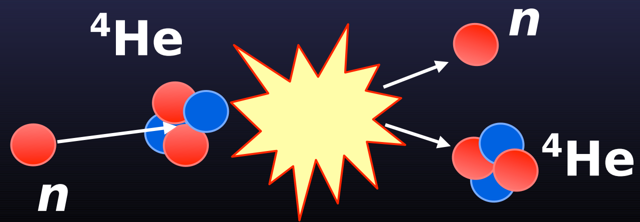
Access to heavier targets



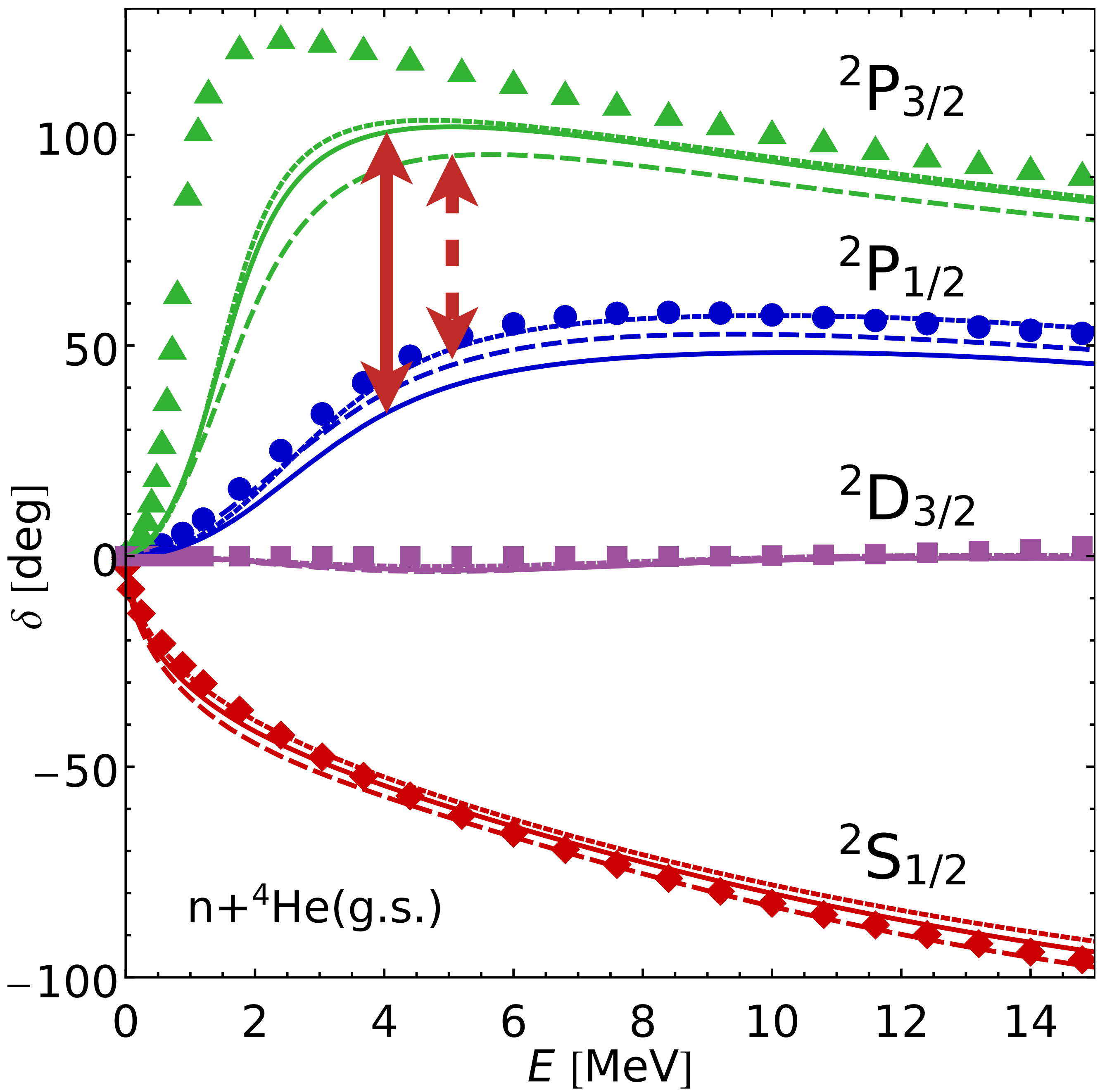
n+^{4}He Scattering

In collaboration with
G. Hupin, S. Quaglioni, P. Navrátil & R. Roth

G. Hupin, J. Langhammer et al. ----- in prep.



3N Force Effects on Phase Shifts



◆▲●■ Experiment

······ NN-only

----- 3N-induced

—— 3N-full

3N increases spin-orbit splitting

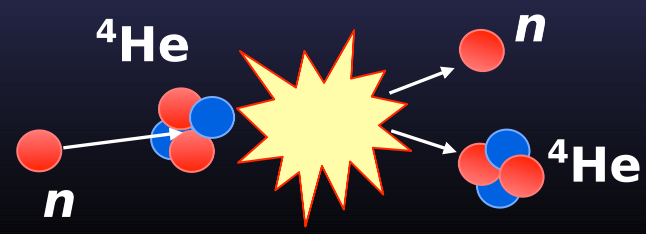
$N_{max} = 12$

$E_{3max} = 14$

$\hbar\Omega = 20\,\mathrm{MeV}$

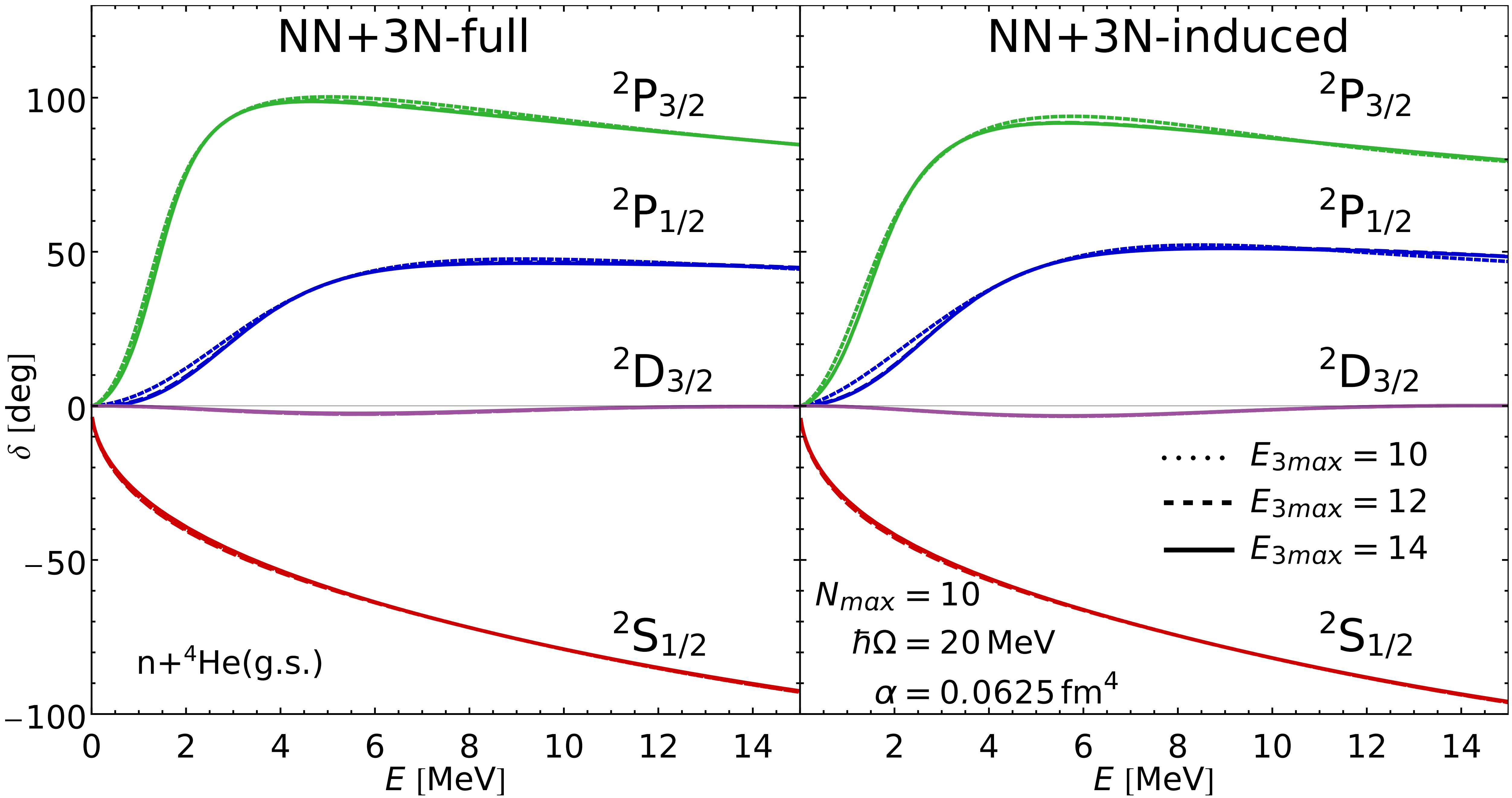
$\alpha = 0.0625\,\mathrm{fm}^4$

$\lambda = 2.0\,\mathrm{fm}^{-1}$



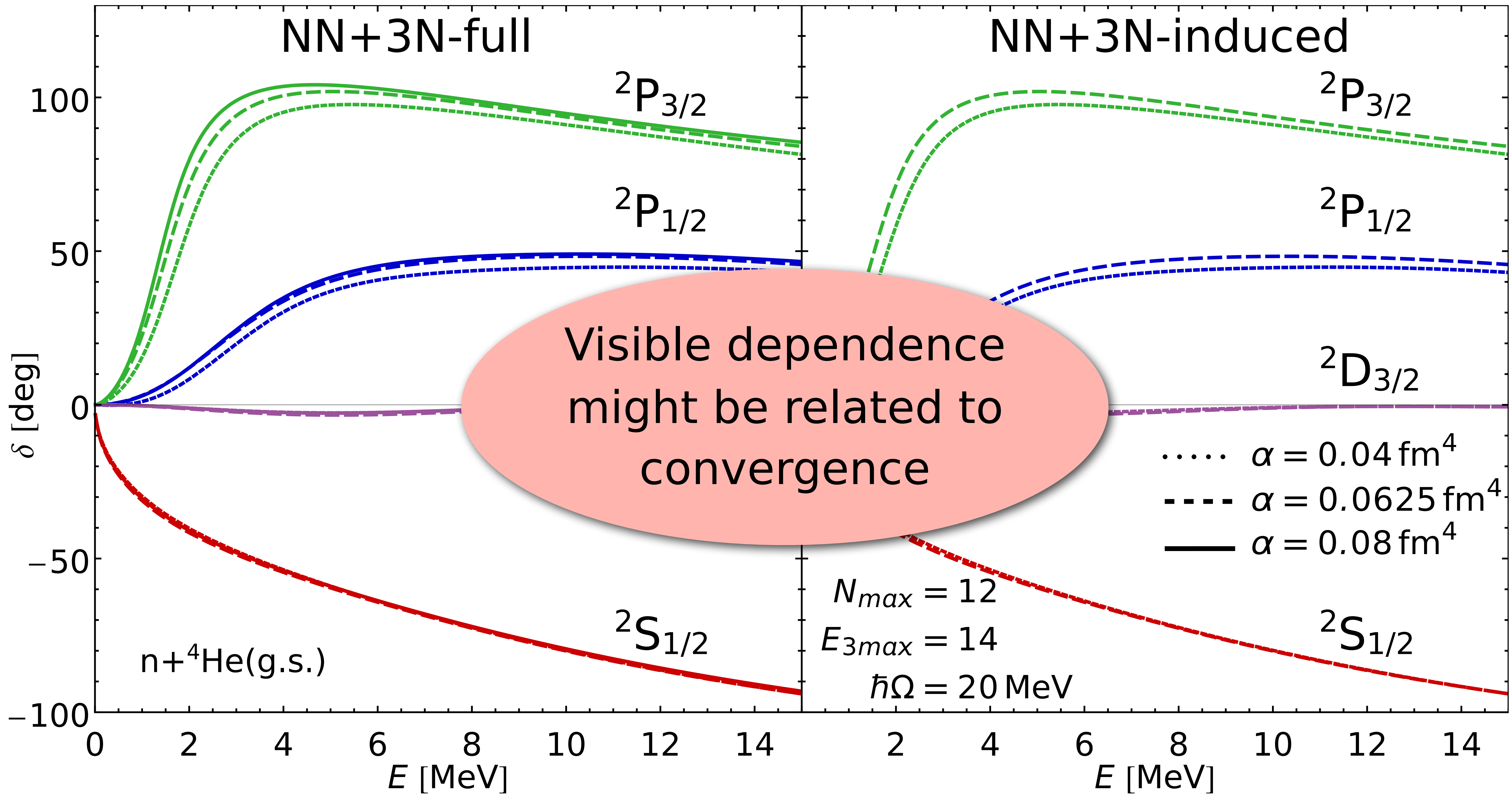
3N Force Effects on Phase Shifts

Study dependence on E_{3max} parameter

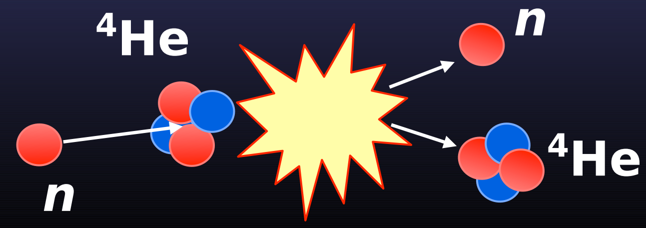


3N Force Effects on Phase Shifts

Study dependence on SRG parameter

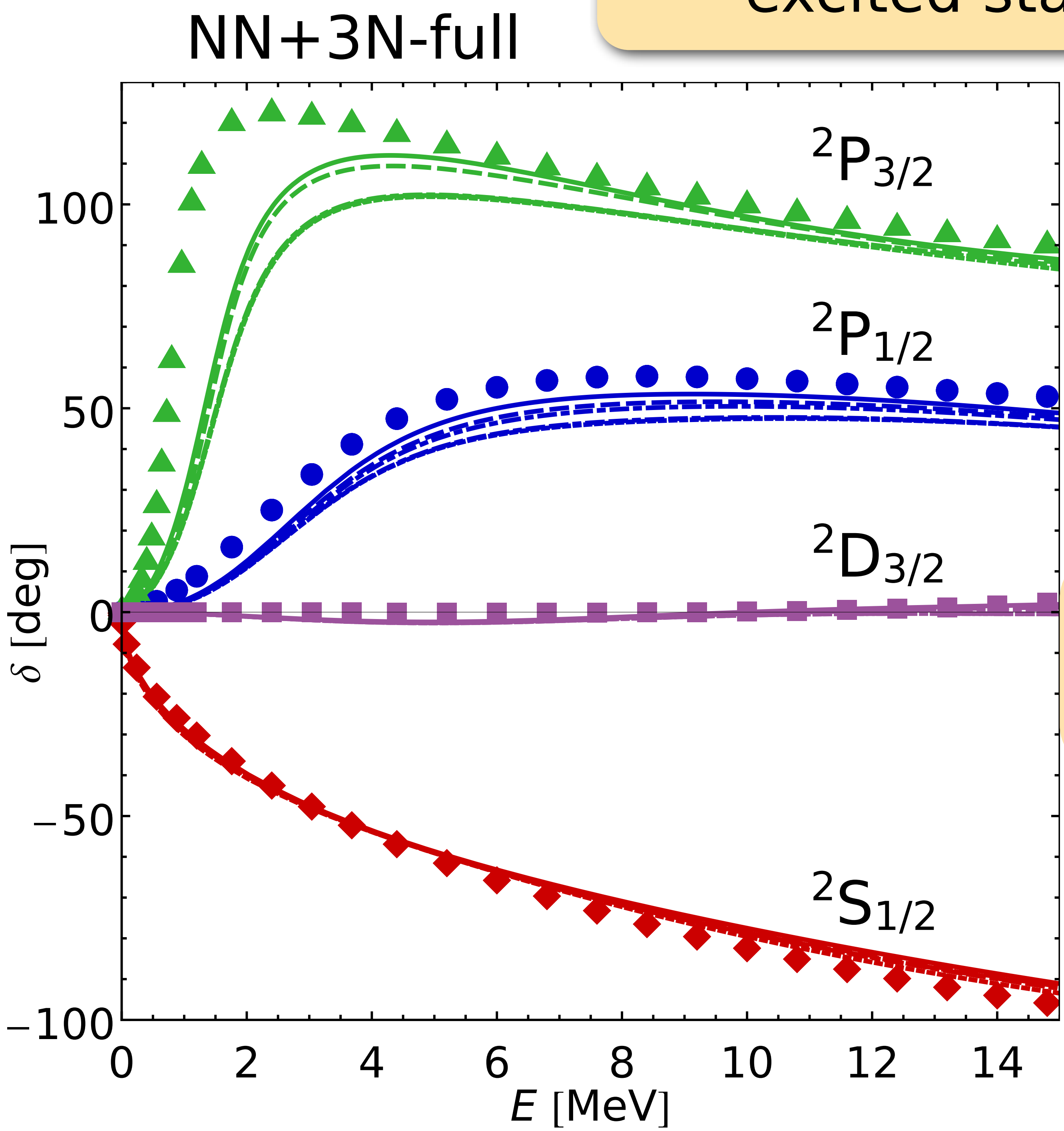


Visible dependence might be related to convergence



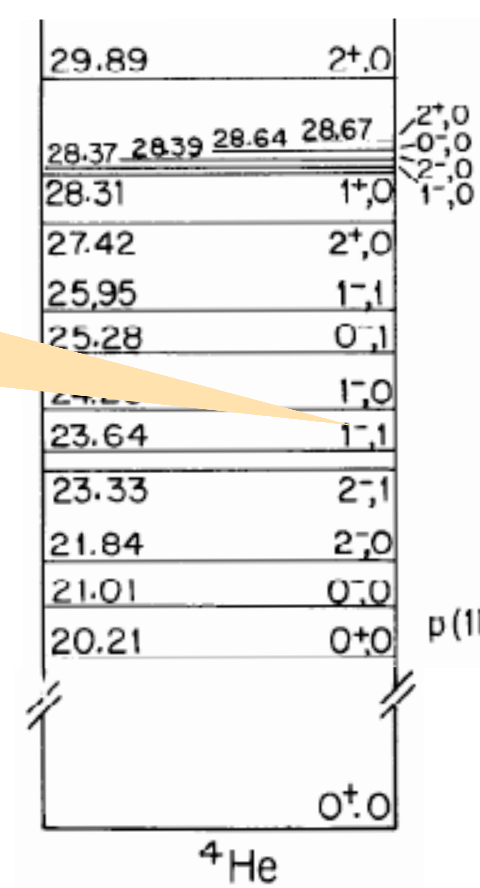
3N Force Effects on Phase Shifts

Inclusion of more excited states



n+^{4}He(g.s.)
n+^{4}He(g.s., 0^+)
n+^{4}He(g.s., 0^+, 0^-)
n+^{4}He(g.s., 0^+, 0^-, 2^-)
n+^{4}He(g.s., 0^+, 0^-, 2^-, 2^- T=1)
Experiment

Further inclusion of 1-,1 & 1-,0 states necessary



$$N_{max} = 12$$
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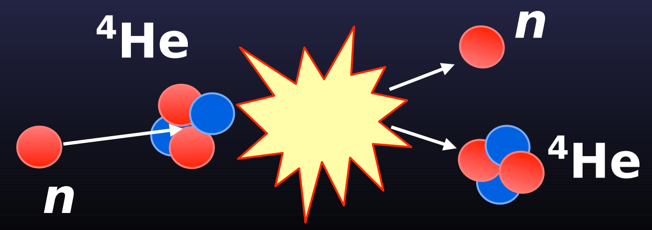
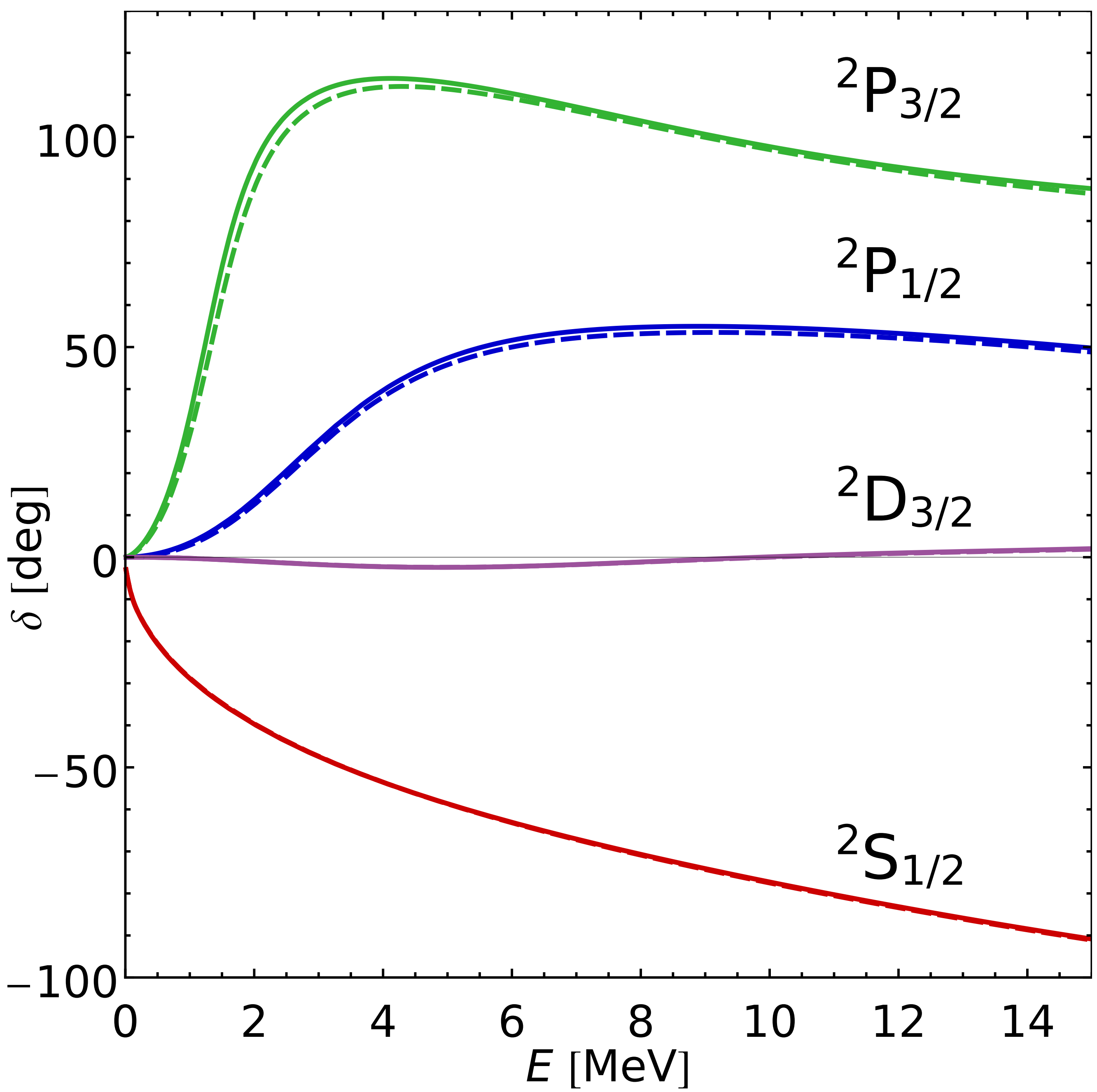


3N Force Effects on Phase Shifts

SRG parameter dependence with more excited states

NN+3N-full



n+^{4}He(g.s., 0^+,0^-,2^-,2^- T=1)

- - - - $\alpha = 0.0625\,\mathrm{fm}^4$

—— $\alpha = 0.08\,\mathrm{fm}^4$

Minimal dependence on SRG parameter

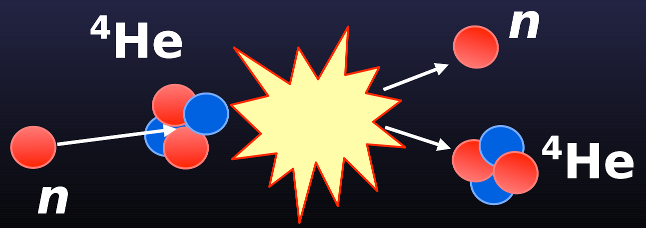
$N_{max} = 12$

$E_{3max} = 14$

$\hbar\Omega = 20\,\mathrm{MeV}$

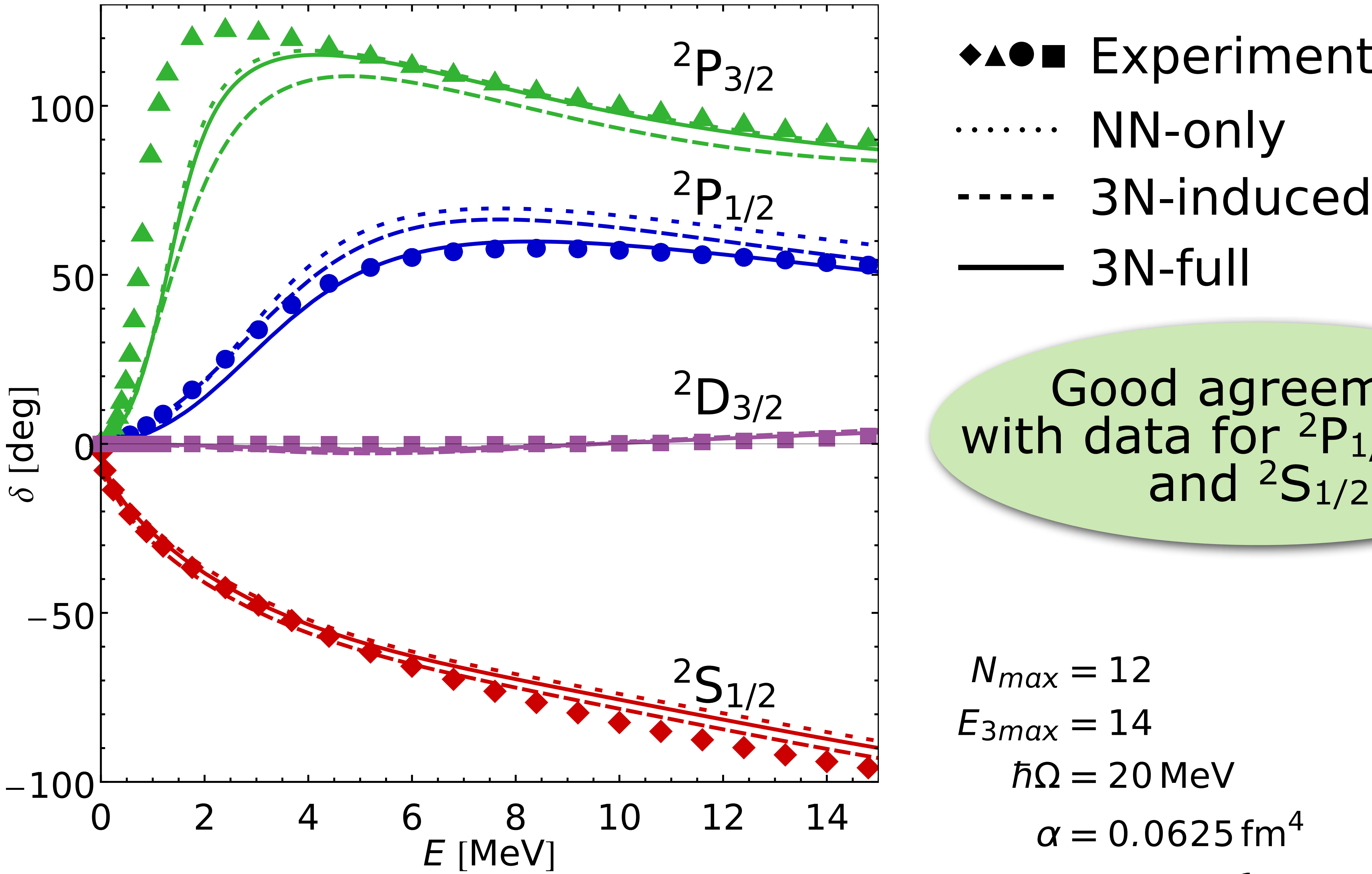
$\alpha = 0.0625\,\mathrm{fm}^4$

$\lambda = 2.0\,\mathrm{fm}^{-1}$



3N Force Effects on Phase Shifts

n+^{4}He(g.s., 0^+,0^-,2^-,2^- T=1, 1^-, 1^- T=1)



Good agreement with data for $^2P_{1/2}$, $^2D_{3/2}$ and $^2S_{1/2}$

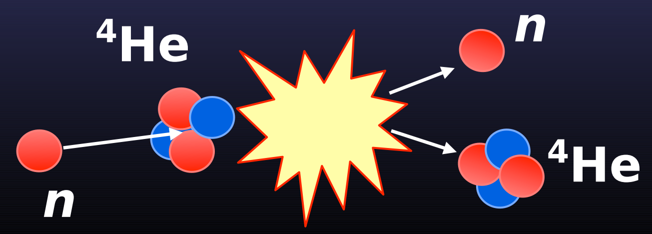
$N_{max} = 12$

$E_{3max} = 14$

$\hbar\Omega = 20\,\mathrm{MeV}$

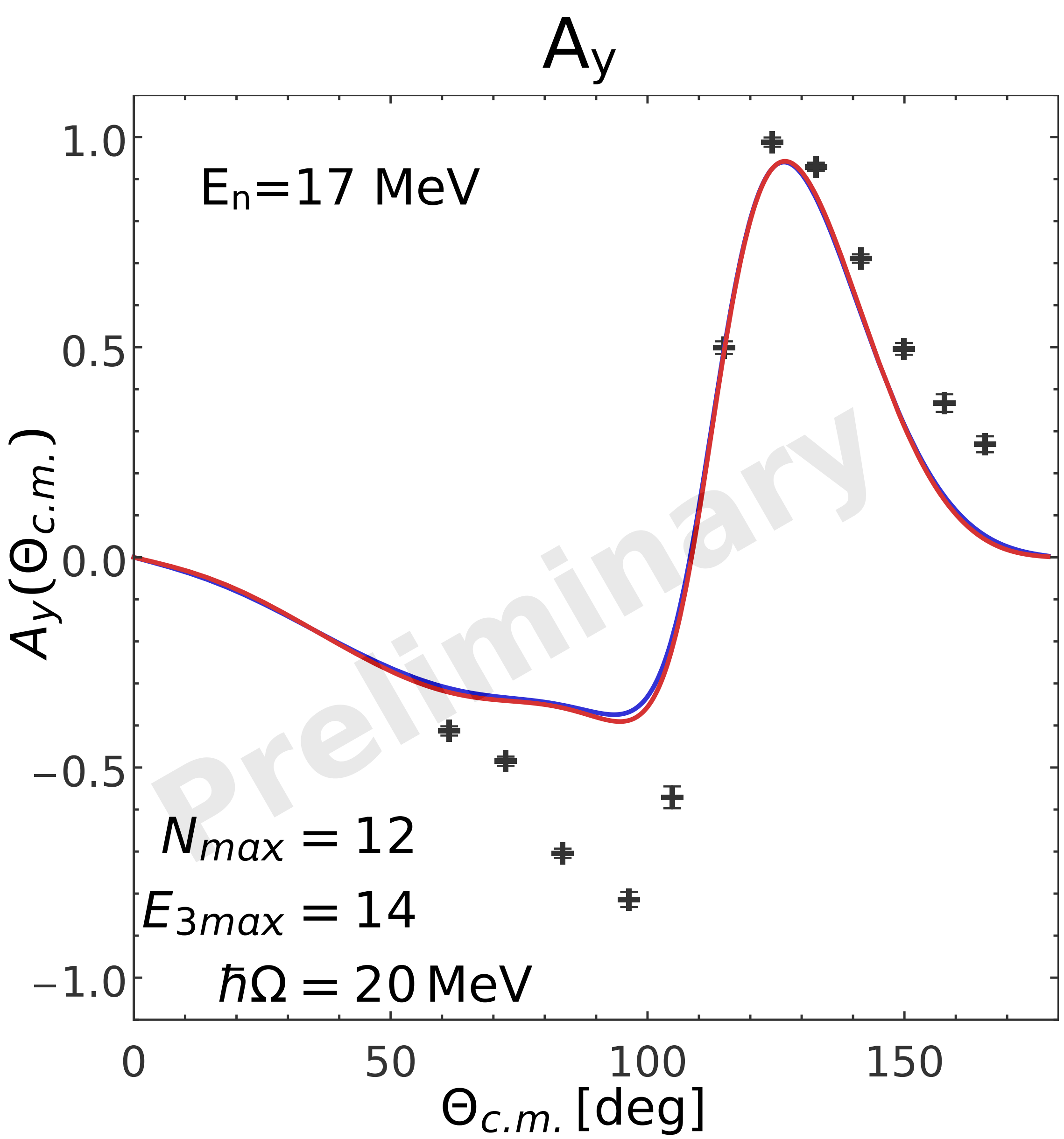
$\alpha = 0.0625\,\mathrm{fm}^4$

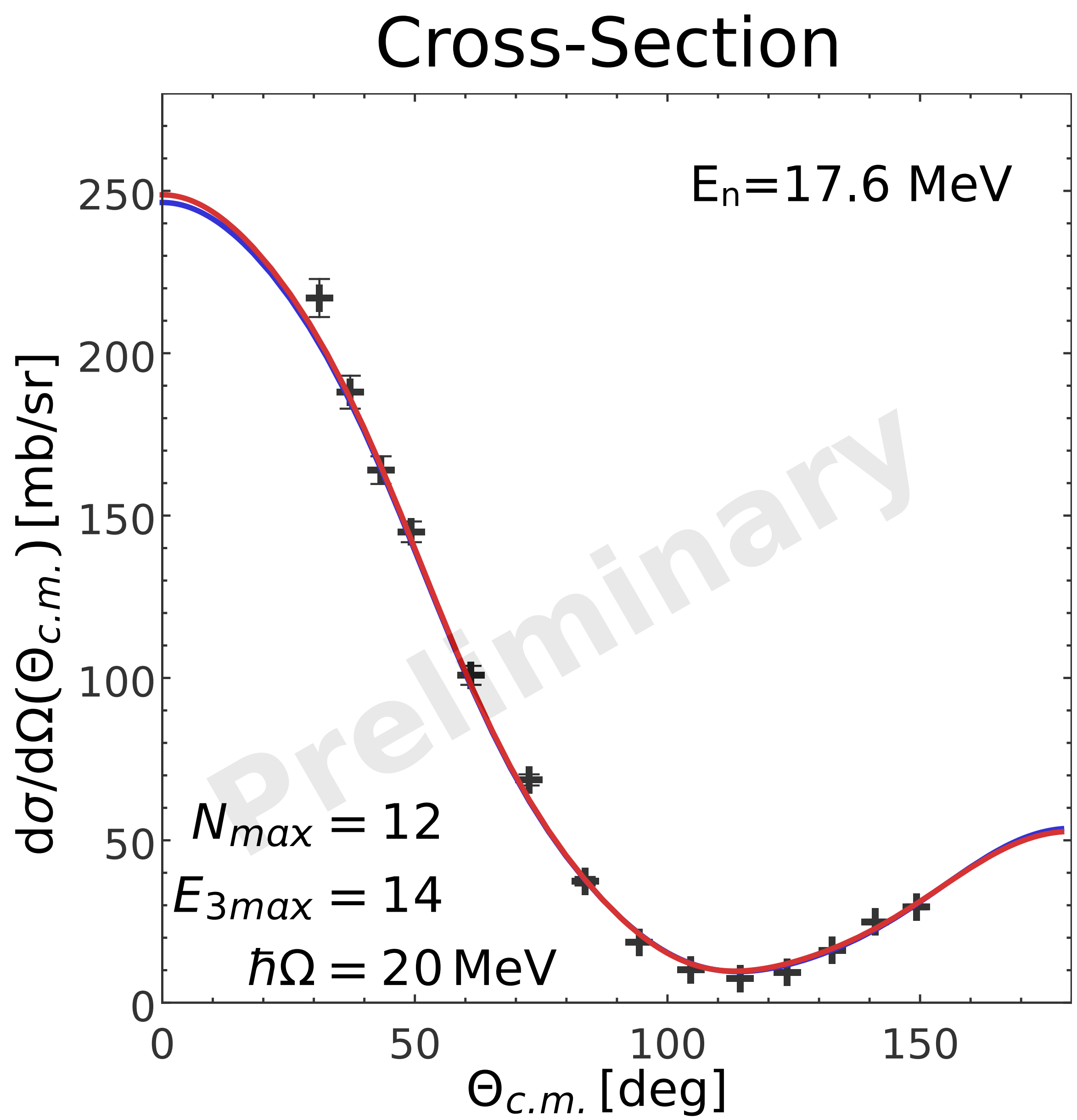
$\lambda = 2.0\,\mathrm{fm}^{-1}$



Cross Section & Analyzing Power

n+^{4}He(g.s., 0^+,0^-,2^-,2^- T=1)





$\alpha = 0.0625\,\mathrm{fm}^4$, $\lambda = 2.0\,\mathrm{fm}^{-1}$ (blue)

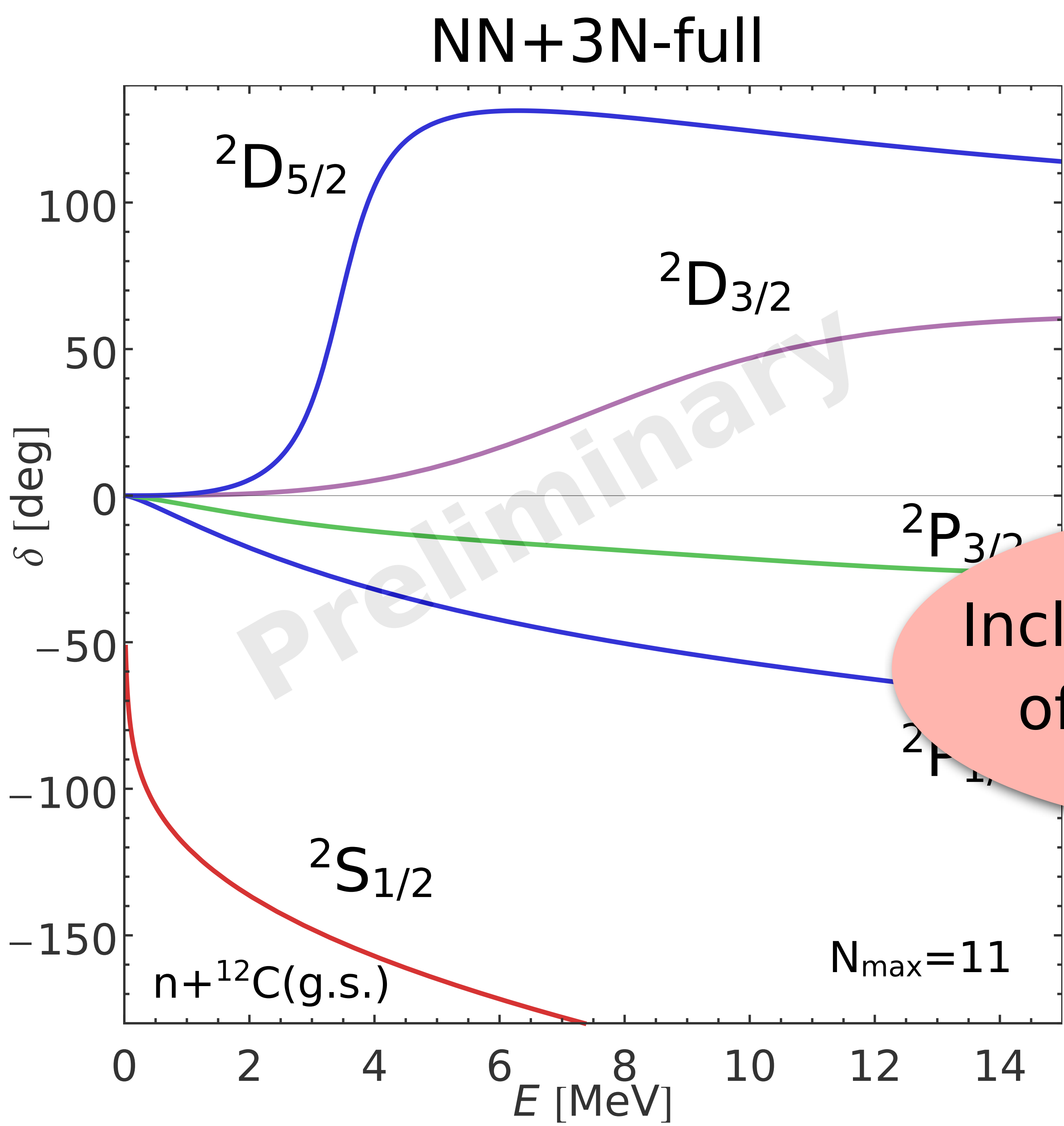
$\alpha = 0.08\,\mathrm{fm}^4$, $\lambda = 1.88\,\mathrm{fm}^{-1}$ (red)

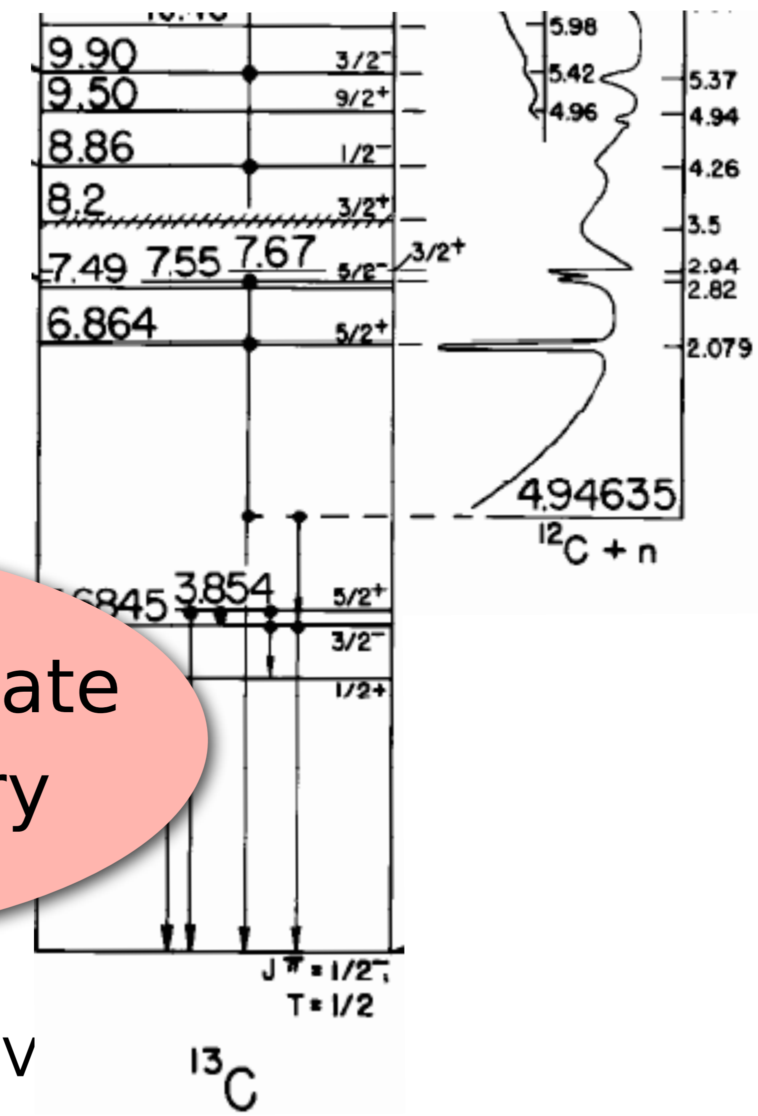
\+ Exp.

[Krupp et al., Phys.Rev.C **30**, 1810]
[M. Drosg, Los Alamos Scientific Laboratory Report, LA-7269-MS]

$n + {}^{12}C$ Scattering

- Accessible due to new computational scheme





Inclusion of 2^+ state of ${}^{12}C$ necessary

$$\hbar\Omega = 20\,\text{MeV}$$
$$\alpha = 0.0625\,\text{fm}^4$$
$$\lambda = 2.0\,\text{fm}^{-1}$$
$$E_{3max} = 14$$

Conclusions

Conclusions

Nuclear spectroscopy with chiral NN+3N forces via IT-NCSM

- **Propagate uncertainties** to nuclear spectra **and provide feedback**
- Importance of LEC c_3 for certain states in *p*-shell nuclei
- **Reach** of exact methods **extended**, ***e.g.* Oxygen isotopes** in very good agreement with experiments and dripline reproduced

Nuclear reactions with full 3N treatment via NCSM/RGM

- **Inclusion of 3N forces** challenging but **completed**
- n+^{4}He scattering phase shifts show **enhanced spin-orbit splitting**
- New computational scheme $\Longrightarrow$ **heavier targets accessible**

Strict tests of chiral interactions in both, nuclear structure and reactions possible

Epilogue

- **thanks to my group & collaborators**
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  IP…

Thanks for your attention!

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