Chiral Three-Nucleon Interactions
in
Ab Initio Nuclear Structure and Reactions

Joachim Langhammer

TECHNISCHE UNIVERSITÄT DARMSTADT

Outline

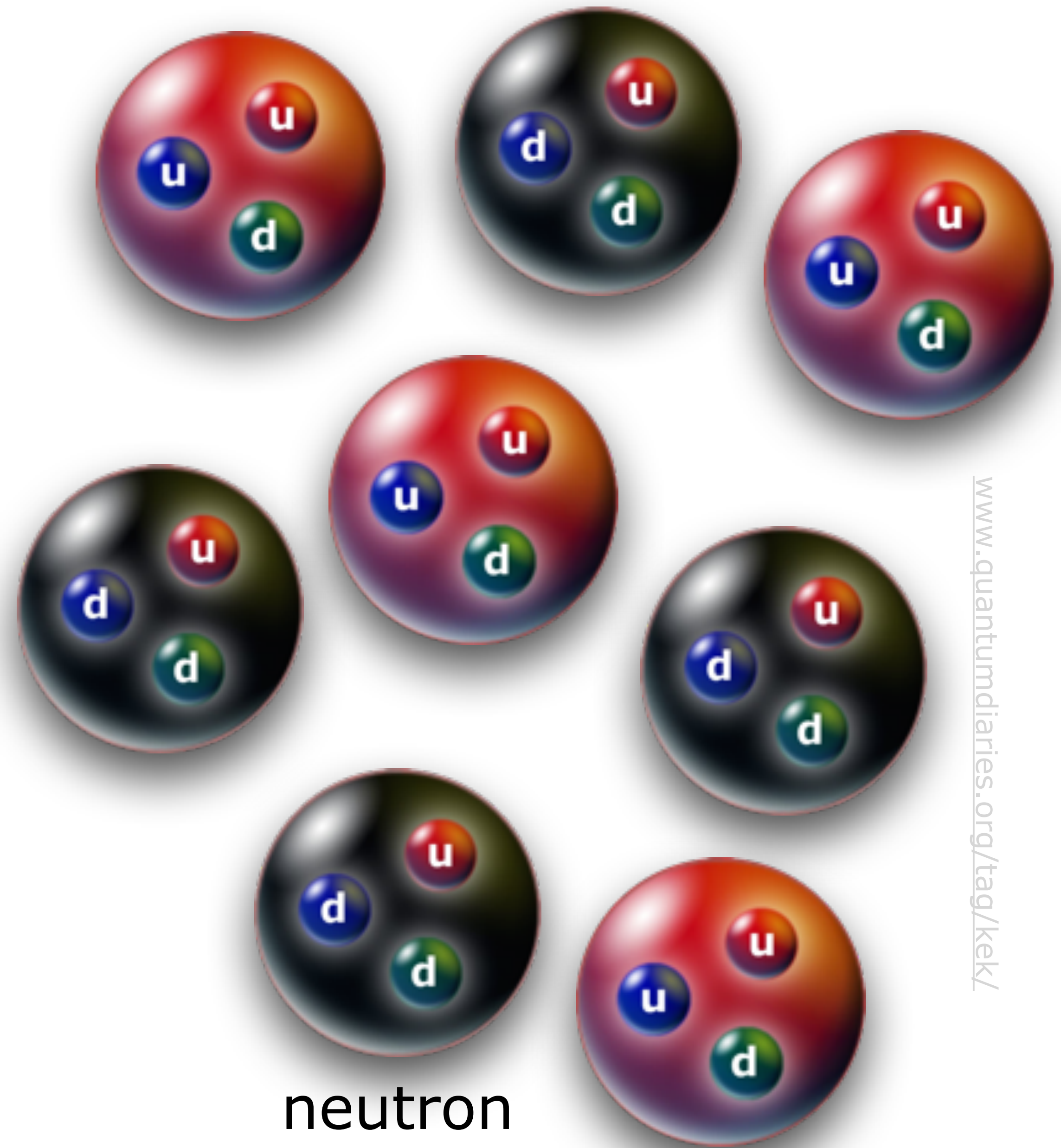
- The Nuclear Many-Body Problem
  - Chiral NN & 3N Interactions
- The No-Core Shell Model / Resonating Group Method
  - 3N Force Effects in Nucleon-^{4}He Scattering
- The No-Core Shell Model with Continuum
  - Continuum & 3N Force Effects on the ^{9}Be Energy Levels
- Summary & Outlook

The Chiral Nuclear Hamiltonian

- Solve the Schrödinger equation for systems of nucleons

$$H\,|\psi^{J\pi T}\rangle = E\,|\psi^{J\pi T}\rangle$$

- Nuclear interaction from effective theory **including nucleons & pions respecting symmetries of QCD**



www.quantumdiaries.org/tag/kek/

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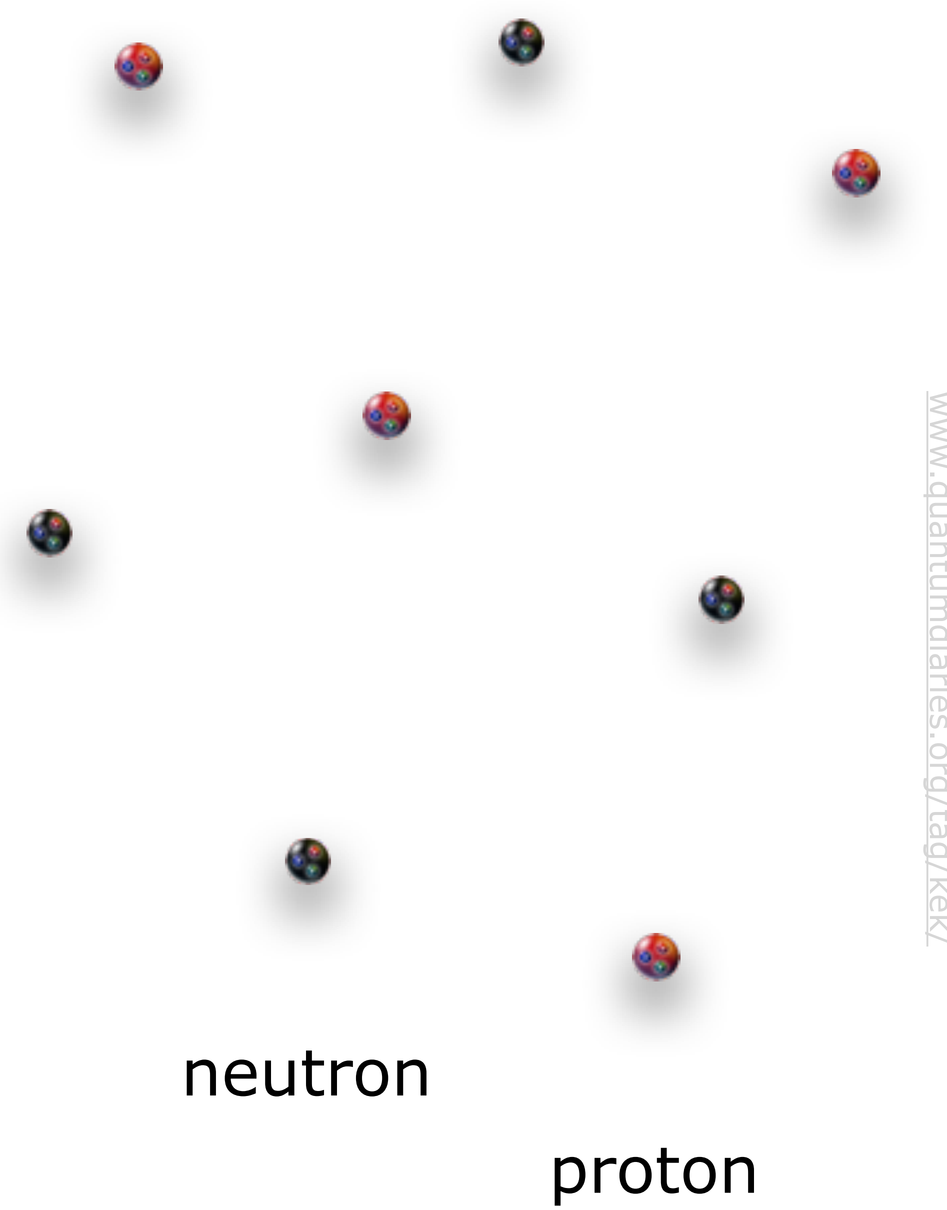

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  - NN interaction @ N^{3}LO
    [Entem, Machleidt, Phys.Rev C **68**, 041001(R) (2003)]
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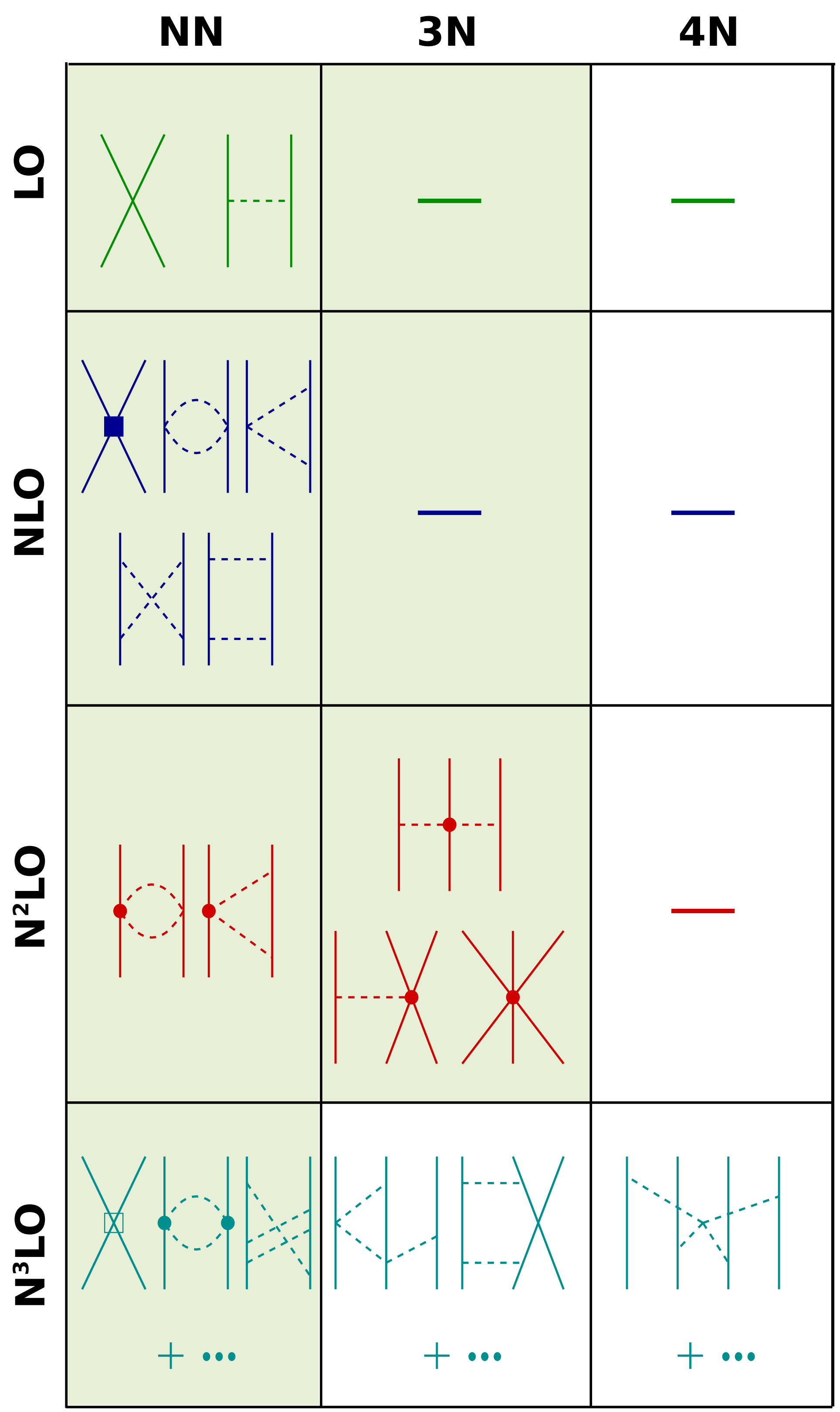

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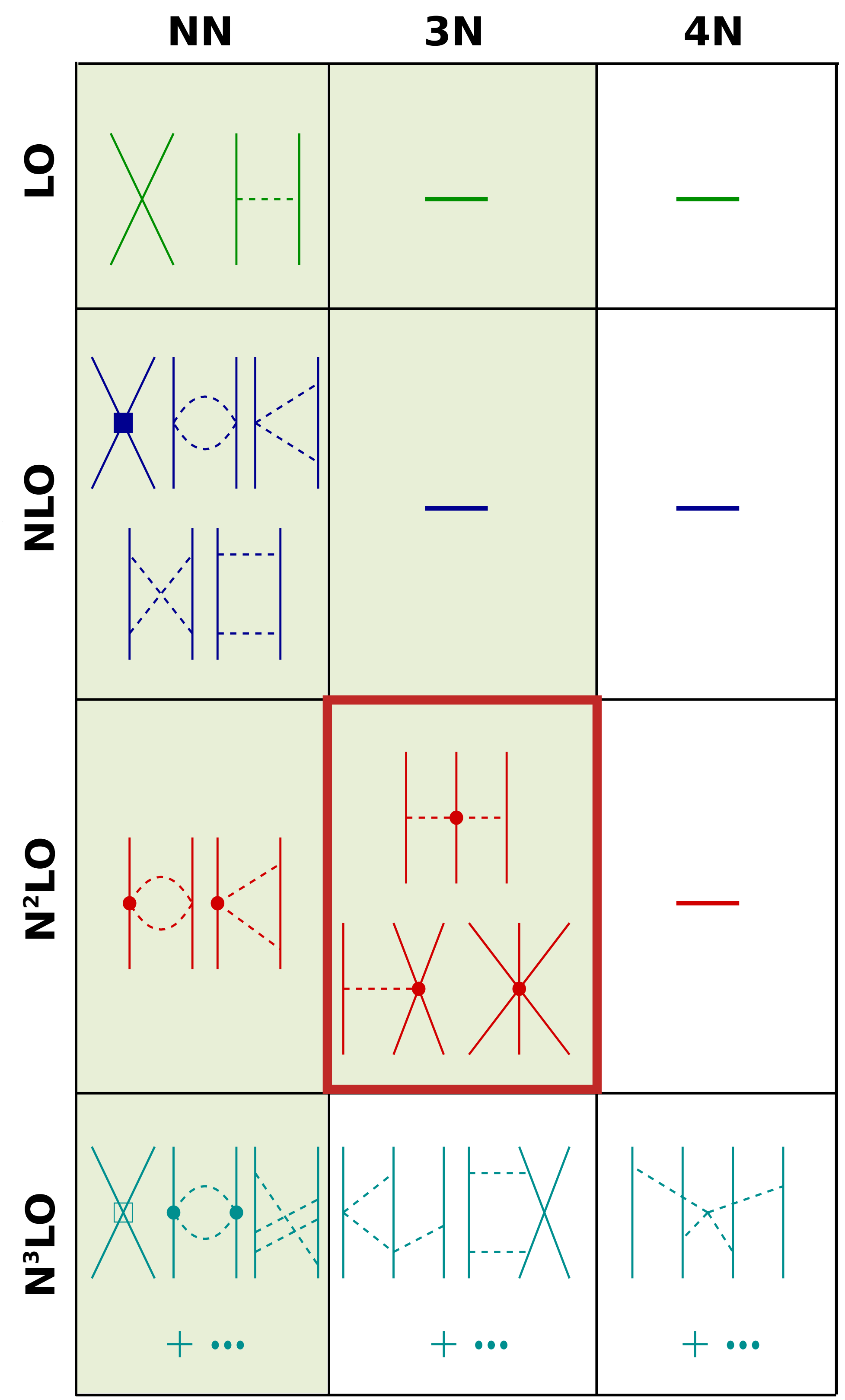
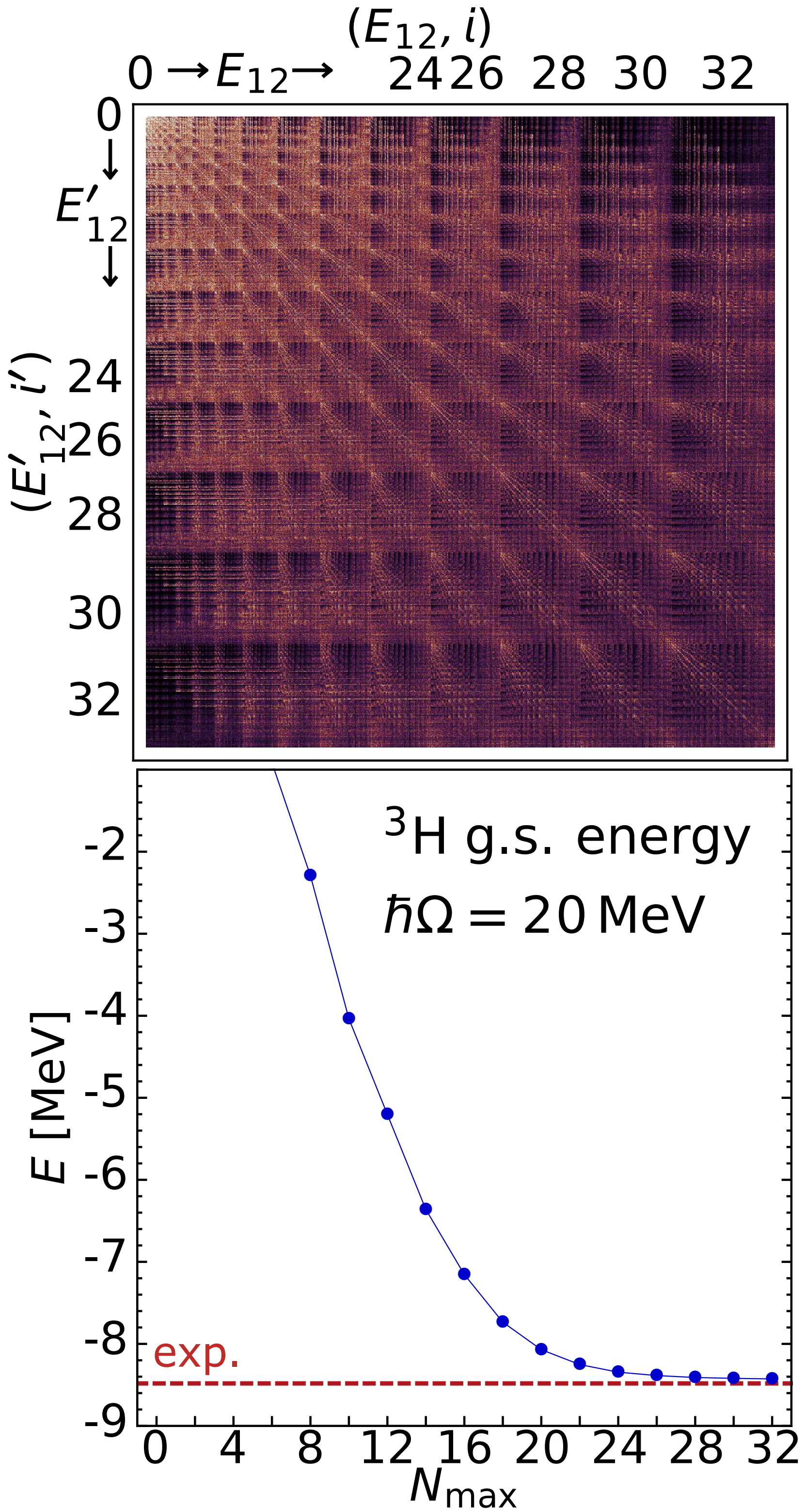


The Similarity Renormalization Group



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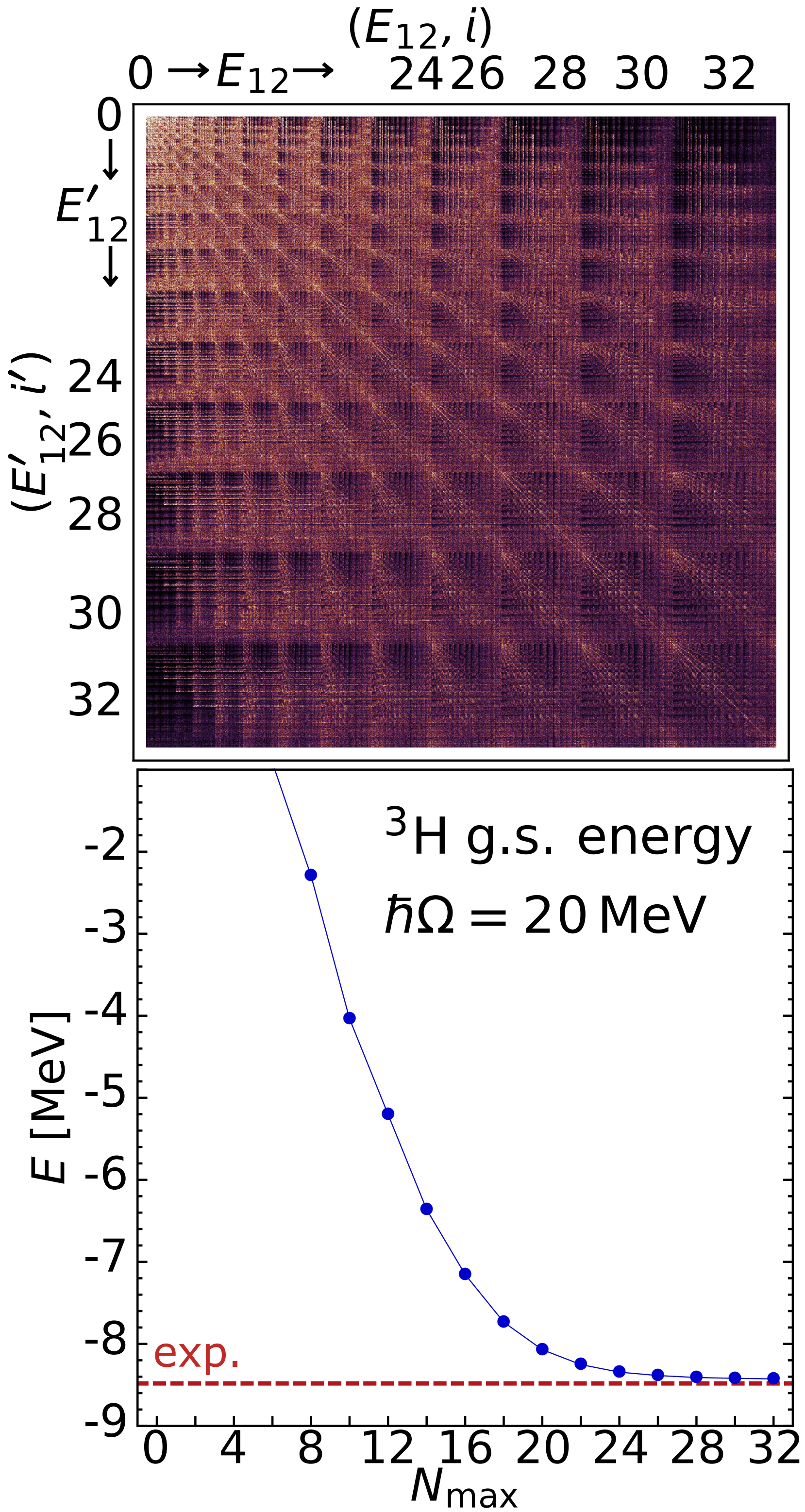
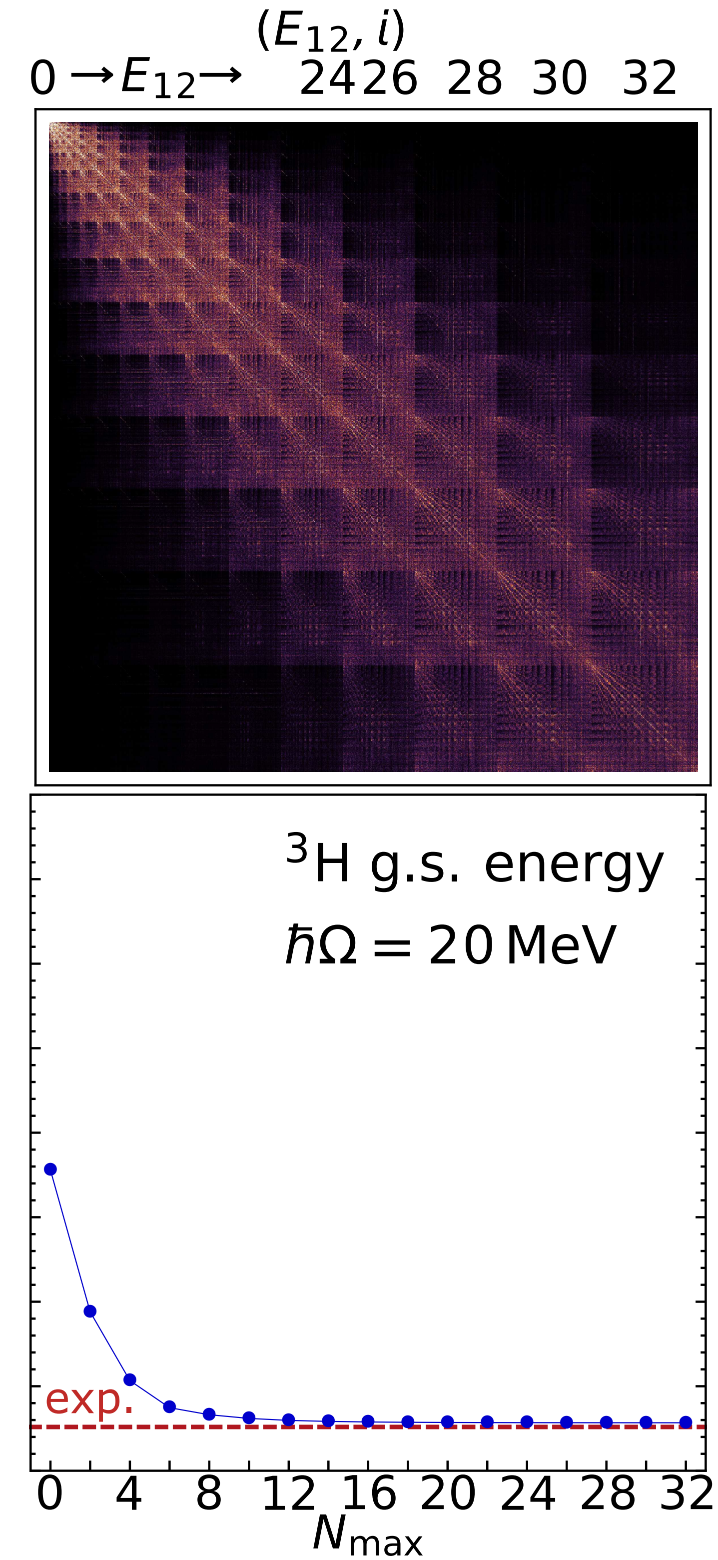


Unitary transformation of the Hamiltonian

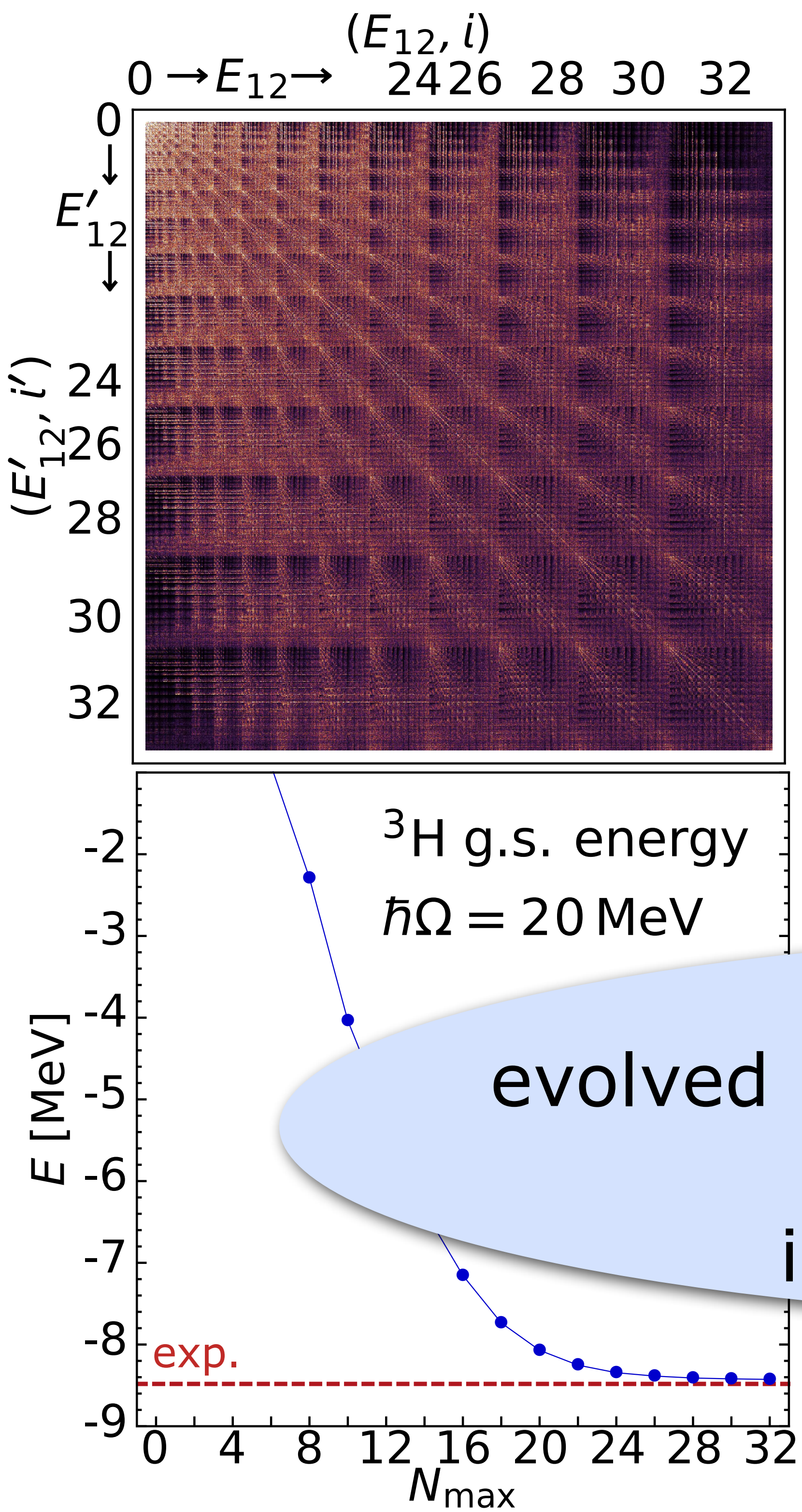
$$H_\alpha = U_\alpha^\dagger H U_\alpha$$



3N interactions consistently included

Dependence on α needs to be checked explicitly

The Similarity Renormalization Group



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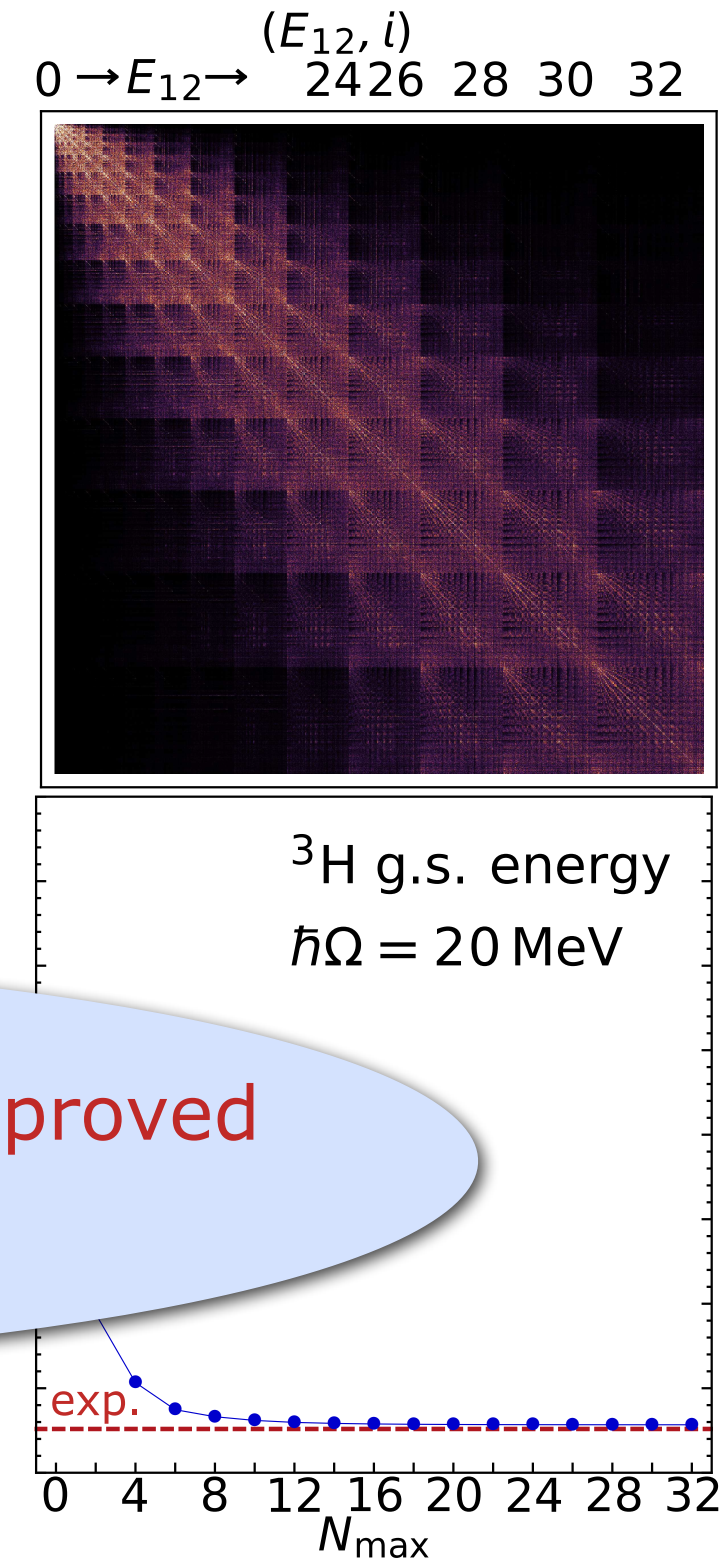

...yields an universal evolved NN+3N interaction with improved convergence properties in many-body calculations

Variety of Developments and Applications

TECHNOLOGY

- Transformation of 3N matrix elements into suitable basis
- Implementation of efficient matrix-element storage scheme (JT-coupled scheme)
- Derivation of reliable, systematically improvable and accurate approximative schemes (Normal-ordering approximation)

STRUCTURE

- Ab-initio nuclear structure with 3N interactions throughout the p-shell
- First ab-initio study of ground states of even oxygen isotopes
- Sensitivity analysis w.r.t. the parameters and cutoff of chiral 3N interactions
- First ab-initio calculations for binding energies of closed-shell nuclei up to heavy tin isotopes

REACTIONS

- Inclusion of 3N interactions into the NCSM/RGM approach
- First ab-initio scatterings with chiral 3N interaction involving more than four nucleons
- Inclusion of 3N interactions into the No-Core Shell Model with Continuum approach
- Investigation of 3N force and continuum effects on ^{9}Be energy levels

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- First [illegible] nuclei up

How to include 3N interactions into a unified ab-initio framework for nuclear structure and reactions?

REACTIONS

- [illegible]
- First ab-initio scatterings with chiral 3N interaction involving more than four nucleons
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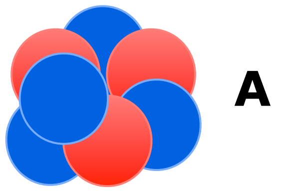
What we are aiming for...

Realistic ab-initio description of nuclei

Bound states
and spectroscopy



Using NN+3N forces that are rooted in QCD

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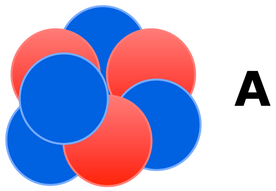

Using NN+3N forces that are rooted in QCD

Importance-Truncated NCSM

Ab-initio description of
nuclear clusters

Computes low-lying eigenvalues of the Hamiltonian
represented in HO Slater determinants

All relevant observables
accessible from the eigenstates

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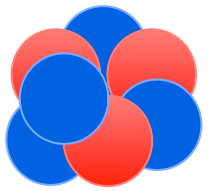

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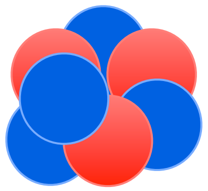

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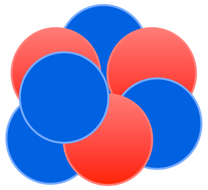

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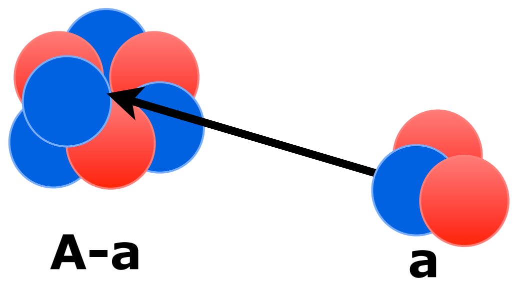

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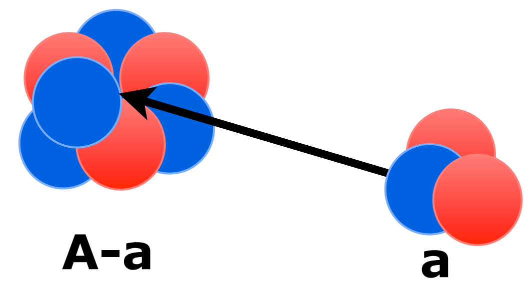

Resonances, scattering states, and halo nuclei

(IT-)NCSM

Ab-initio description of nuclear clusters

Resonating Group Method (RGM)

Describing relative motion of clusters

What we are aiming for...

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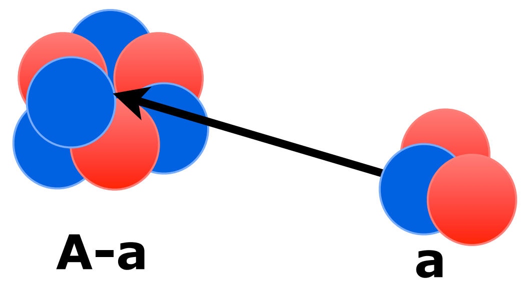


Resonances, scattering states, and halo nuclei

(IT-)NCSM
Ab-initio description nuclear clusters

(IT-)NCSM/RGM or NCSMC approach

Resonating Group Method (RGM)
Describing relative motion of clusters

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

The No-Core Shell Model / Resonating Group Method

—

Inclusion of 3N Interactions

G. Hupin, J. Langhammer et al. ----- Phys. Rev C **88** 054622 (2013)

S. Quaglioni, P. Navrátil, G. Hupin, J. Langhammer et al. ----- Few-Body Syst. **54** 887 (2013)

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

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

General Approach of NCSM/RGM

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

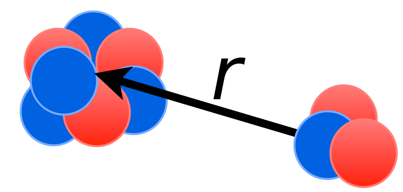
$$|\psi^{J\pi T}\rangle = \sum_{\nu} \int \mathrm{d}r\, r^2\, \frac{g_{\nu}^{J\pi T}(r)}{r}\, \mathcal{A}\, |\phi_{\nu r}^{J\pi T}\rangle$$

$\mathcal{A}$: antisymmetrizer

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

with the **binary-cluster** channel **states**

$$|\phi_{\nu r}^{J\pi T}\rangle = \left\{ |\Phi^{(A-a)}\rangle\, |\Phi^{(a)}\rangle\, |r\, l\rangle \right\}^{J\pi T} \quad \hat{=}$$



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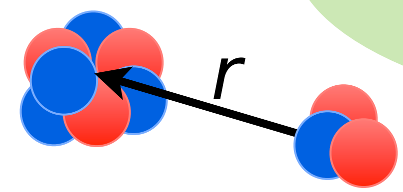

NCSM provides $|\Phi^{(A-a)}\rangle$ and $|\Phi^{(a)}\rangle$

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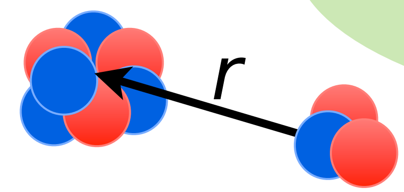

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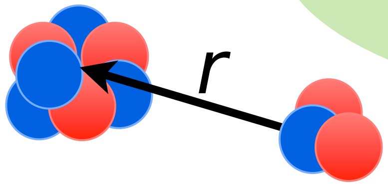

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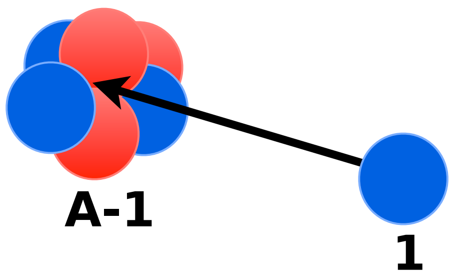
Hamiltonian kernel: **3N interaction causes additional terms**

Towards Inclusion of Full 3N Forces

- Contributions of the 3N interaction



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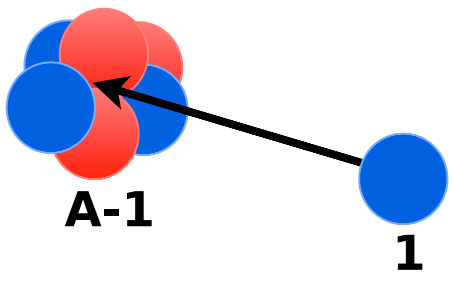

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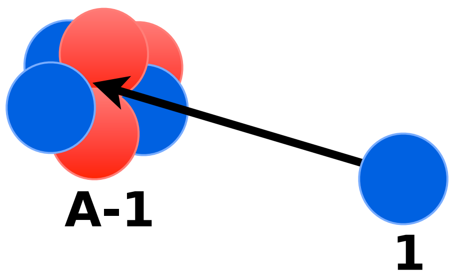

$$\left.\begin{aligned} &= \tfrac{(A-1)(A-2)}{2} \langle \phi^{J\pi T}_{\nu' r'} | V_{A-2,A-1,A} | \phi^{J\pi T}_{\nu r} \rangle \\ &- \tfrac{(A-1)(A-2)}{2} \langle \phi^{J\pi T}_{\nu' r'} | V_{A-2,A-1,A} T_{A-2,A} | \phi^{J\pi T}_{\nu r} \rangle \\ &- \tfrac{(A-1)(A-2)}{2} \langle \phi^{J\pi T}_{\nu'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

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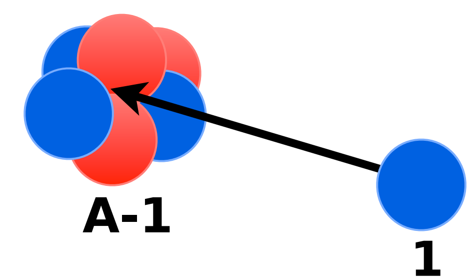

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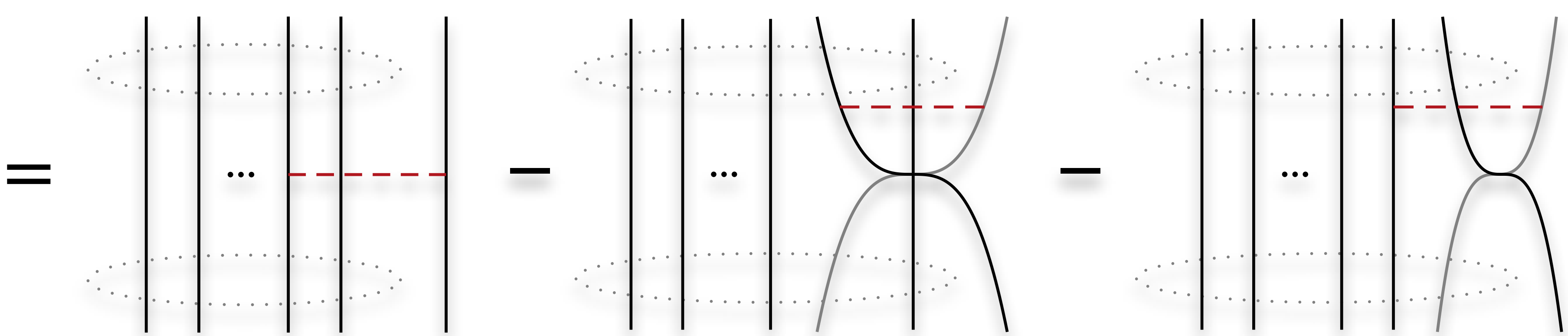

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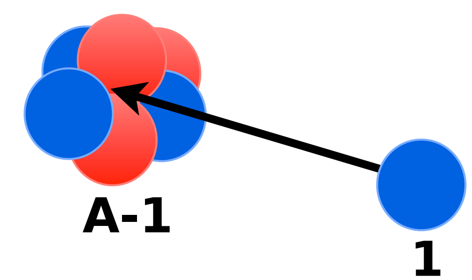

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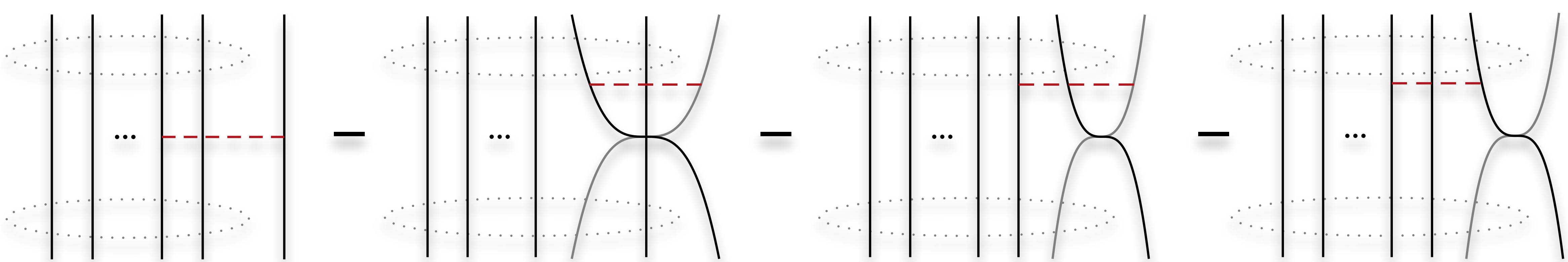
$$- \frac{(A-1)(A-2)(A-3)}{2} \langle \phi^{J\pi T}_{\nu' r'} | V_{A-3,A-2,A} T_{A-1,A} \, | \phi^{J\pi T}_{\nu r} \rangle \qquad \text{“exchange” kernel}$$

$=$ 

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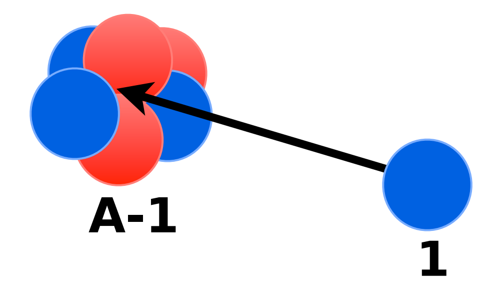

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"direct" kernel

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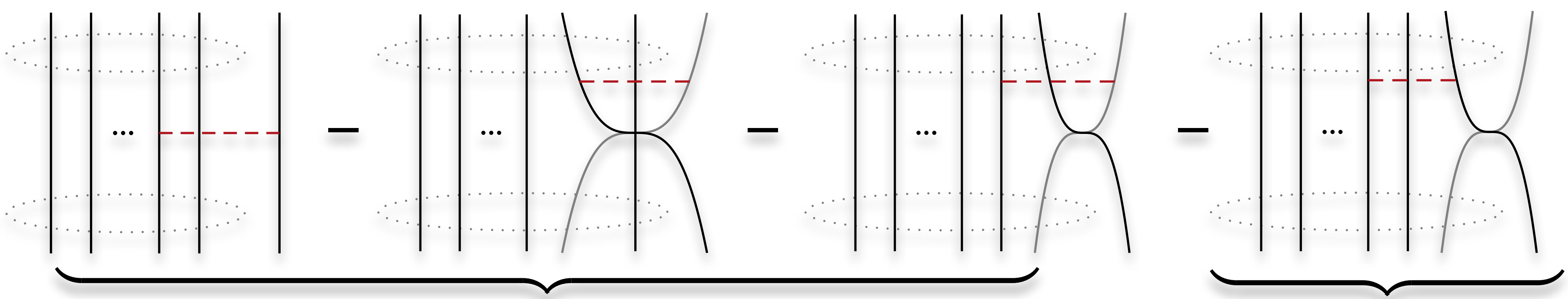

$$\propto \langle \Phi'^{(A-1)} | a^\dagger a^\dagger a a \, | \Phi^{(A-1)} \rangle \qquad \propto \langle \Phi'^{(A-1)} | a^\dagger a^\dagger a^\dagger a a a \, | \Phi^{(A-1)} \rangle$$

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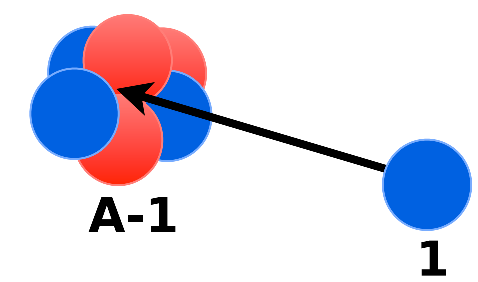
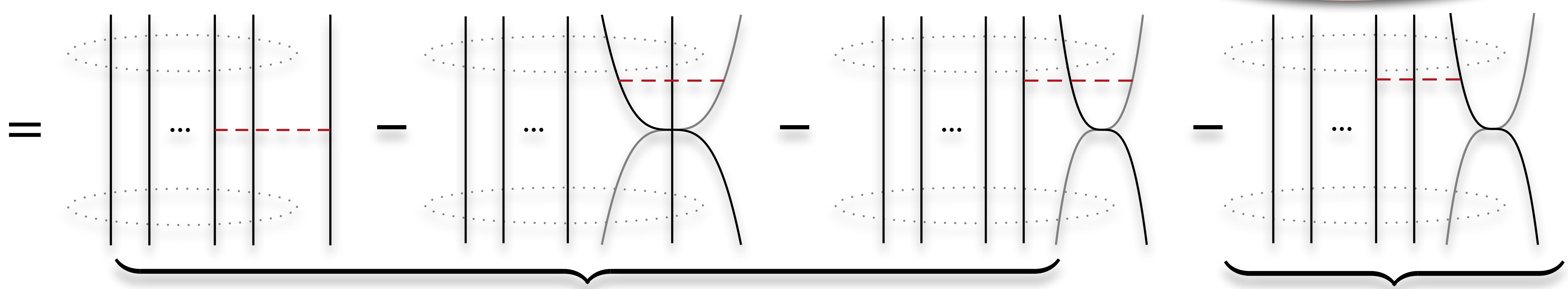
$$\langle \phi^{J\pi T}_{\nu' r'} | V_{3N} \mathcal{A}^2 \, | \phi^{J\pi T}_{\nu r} \rangle = \langle \phi^{J\pi T}_{\nu' r'} | V_{3N} \left[1 - \sum_{i=1}^{A-1} T_{i,A} \right] | \phi^{J\pi T}_{\nu r} \rangle$$



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

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

Handling of 3-body density challenging



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

Handling of the Three-Body Density

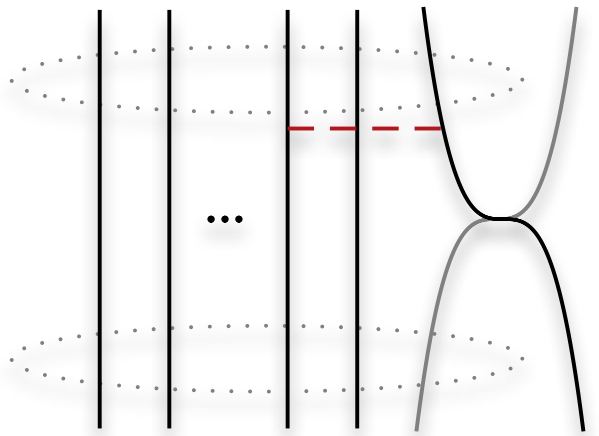
$$\sum_{jj'}\sum_{M_1 m_j}\sum_{M_{T_1} m_t}\sum_{M'_1 m'_j}\sum_{M'_{T_1} m'_t} \tfrac{1}{12}(-1)^{I_1+I'_1+2J+j+j'} \begin{Bmatrix} I_1 & \frac{1}{2} & s \\ l & J & j \end{Bmatrix} \begin{Bmatrix} I'_1 & \frac{1}{2} & s' \\ l' & J & j' \end{Bmatrix}$$

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

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

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

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



- Exploit $|\Phi^{(A-1)} I_1 M_1 T_1 M_{T_1}\rangle = \sum_i c_i \, |\mathrm{SD}\rangle_i$
- **Compute three-body density on the fly**
- Efficient new computational scheme implemented

Handling of the Three-Body Density

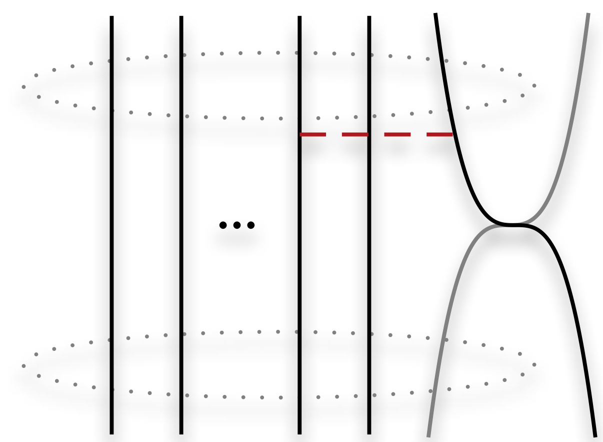
$$\sum_{jj'}\sum_{M_1 m_j}\sum_{M_{T_1} m_t}\sum_{M_1' m_j'}\sum_{M_{T_1}' m_t'} \tfrac{1}{12}(-1)^{I_1+I_1'+2J+j+j'} \begin{Bmatrix} I_1 & \frac12 & s \\ l & J & j\end{Bmatrix}\begin{Bmatrix} I_1' & \frac12 & s' \\ l' & J & j'\end{Bmatrix}$$

$$\left(\begin{array}{cc|c} I_1 & j & J \\ M_1 & m_j & M_J\end{array}\right)\left(\begin{array}{cc|c} T_1 & \frac12 & T \\ M_{T_1} & m_t & M_T\end{array}\right)\left(\begin{array}{cc|c} I_1' & j' & J \\ M_1' & m_j' & M_J'\end{array}\right)\left(\begin{array}{cc|c} T_1' & \frac12 & T \\ M_{T_1}' & m_t' & M_T'\end{array}\right)$$

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

$$_a\langle \beta_{A-3}\beta_{A-2} n l j' m_j' \tfrac12 m_t' |\, V_{3N}\, | \beta_{A-3}'\beta_{A-2}'\beta_{A-1}'\rangle_a$$

$$\langle \Phi'^{(A-1)} I_1' M_1' T_1' M_{T_1}' |\, a^\dagger_{nljm_j\frac12 m_t} a^\dagger_{\beta_{A-2}} a^\dagger_{\beta_{A-3}} a_{\beta_{A-3}'} a_{\beta_{A-2}'} a_{\beta_{A-1}'} | \Phi^{(A-1)} I_1 M_1 T_1 M_{T_1}\rangle$$



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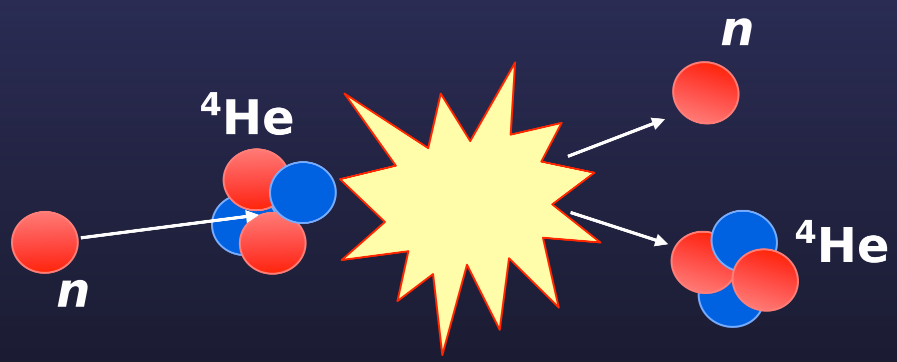
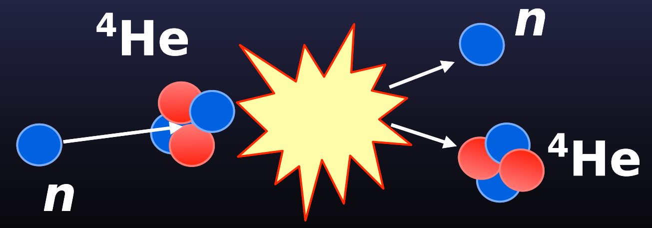
Key to access targets heavier than ^{4}He



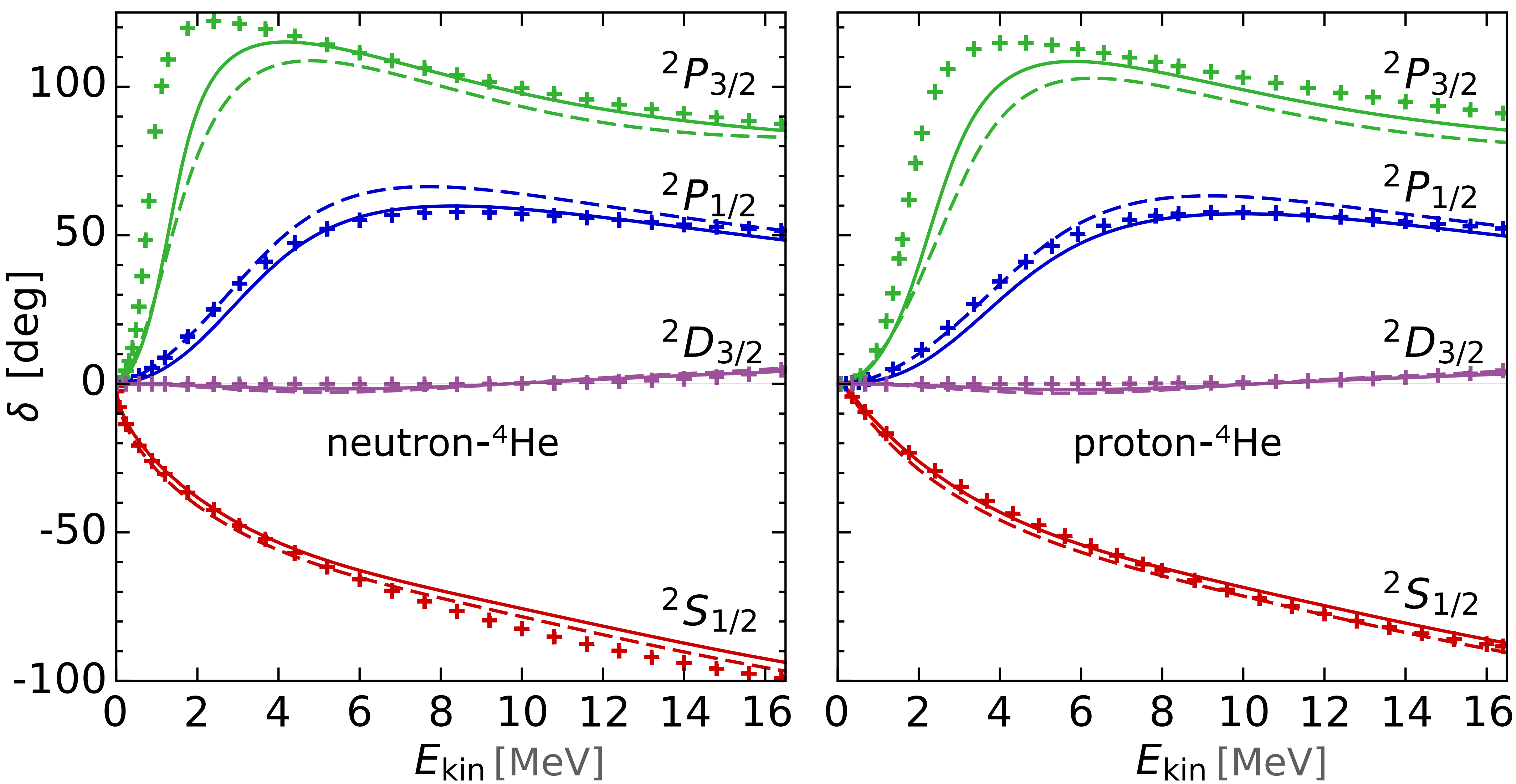
Nucleon-^{4}He Scattering with Chiral 3N Interactions

G. Hupin, J. Langhammer et al. ----- Phys. Rev C **88** 054622 (2013)



3N Force Effects on Phase Shifts

G. Hupin, J. Langhammer et al. - Phys. Rev C **88** 054622 (2013)



$N_{max} = 13$
$E_{3max} = 14$
$\hbar\Omega = 20\,\text{MeV}$
$\alpha = 0.0625\,\text{fm}^4$
$\lambda = 2.0\,\text{fm}^{-1}$

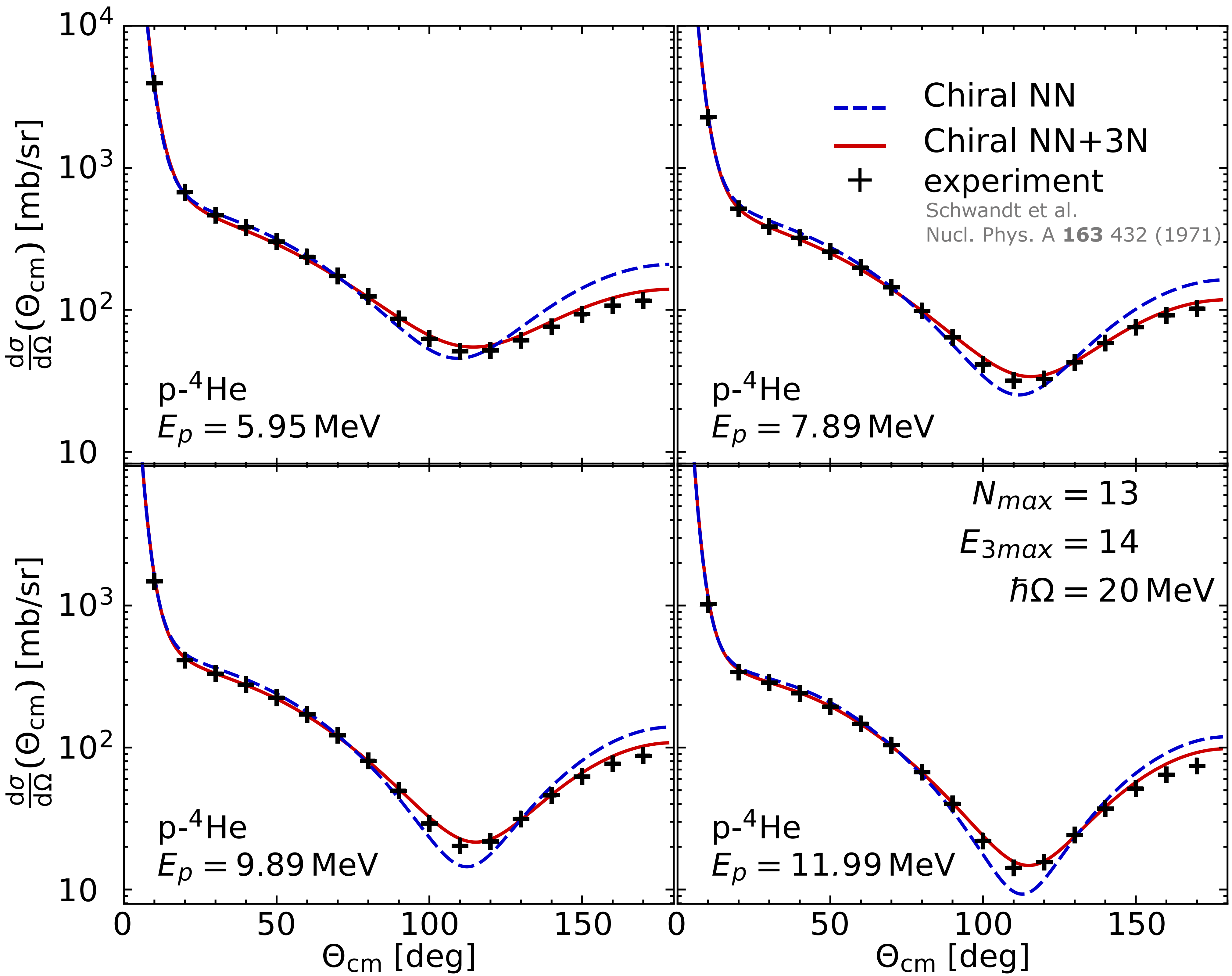
Including seven eigenstates of ^{4}He

+ Experiment
- - - Chiral NN
— Chiral NN+3N

- Good agreement with data for $^2P_{1/2}$, $^2D_{3/2}$ and $^2S_{1/2}$
- 3N interaction increases spin-orbit splitting between P-waves

Differential Cross Section

G. Hupin, J. Langhammer et al. - Phys. Rev C **88** 054622 (2013)



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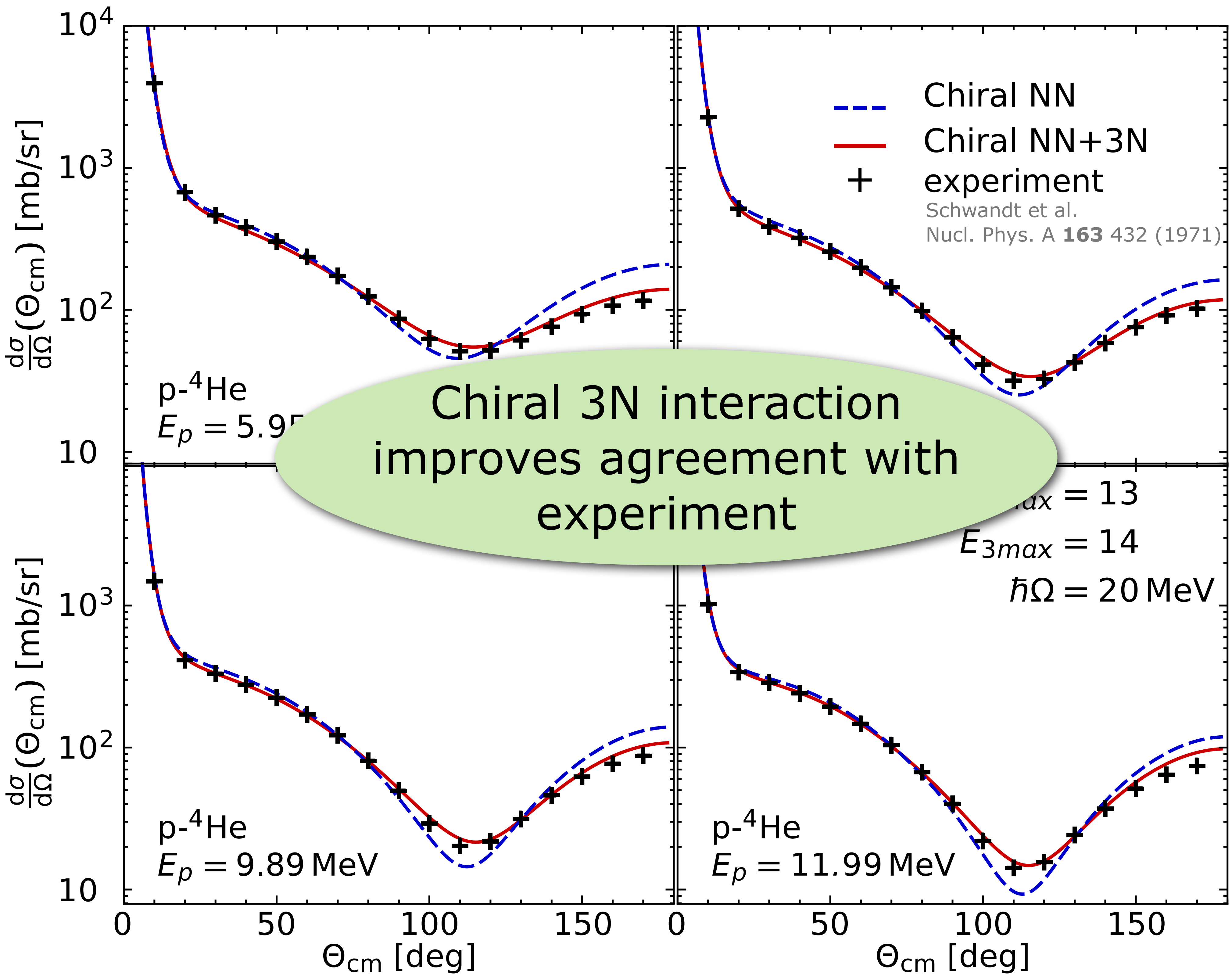


Chiral 3N interaction improves agreement with experiment

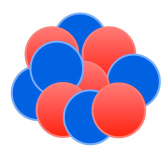
3N Interactions in the No-Core Shell Model with Continuum

The No-Core Shell Model with Contiuum

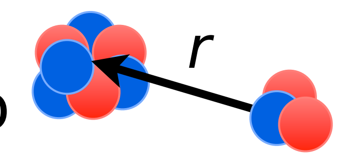
- Representing $H|\psi^{J\pi T}\rangle = E|\psi^{J\pi T}\rangle$ using the **basis expansion**

$$|\Psi^{J\pi T}\rangle = \sum_{\lambda} c_\lambda |\Psi_A E_\lambda J^\pi T\rangle + \sum_{\nu} \int \mathrm{d}r\, r^2 \frac{\chi_\nu(r)}{r} |\xi_{\nu r}^{J\pi T}\rangle$$

Expansion in A-body
(IT-)NCSM eigenstates



Identically equal to
NCSM/RGM expansion



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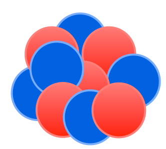

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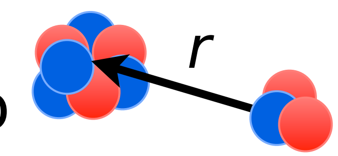


leads to the NCSMC equations

$$\begin{pmatrix} H_{\mathrm{NCSM}} & h \\ h & \mathscr{H} \end{pmatrix} \begin{pmatrix} c \\ \chi(r)/r \end{pmatrix} = E \begin{pmatrix} \mathbb{1} & g \\ g & \mathbb{1} \end{pmatrix} \begin{pmatrix} c \\ \chi(r)/r \end{pmatrix}$$

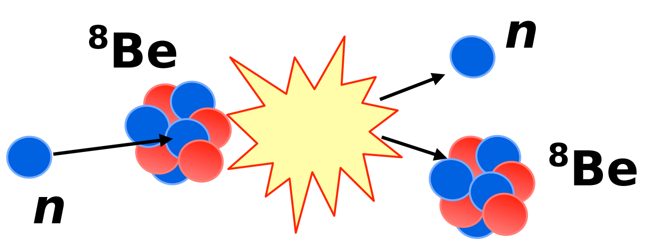
3N forces contribute in

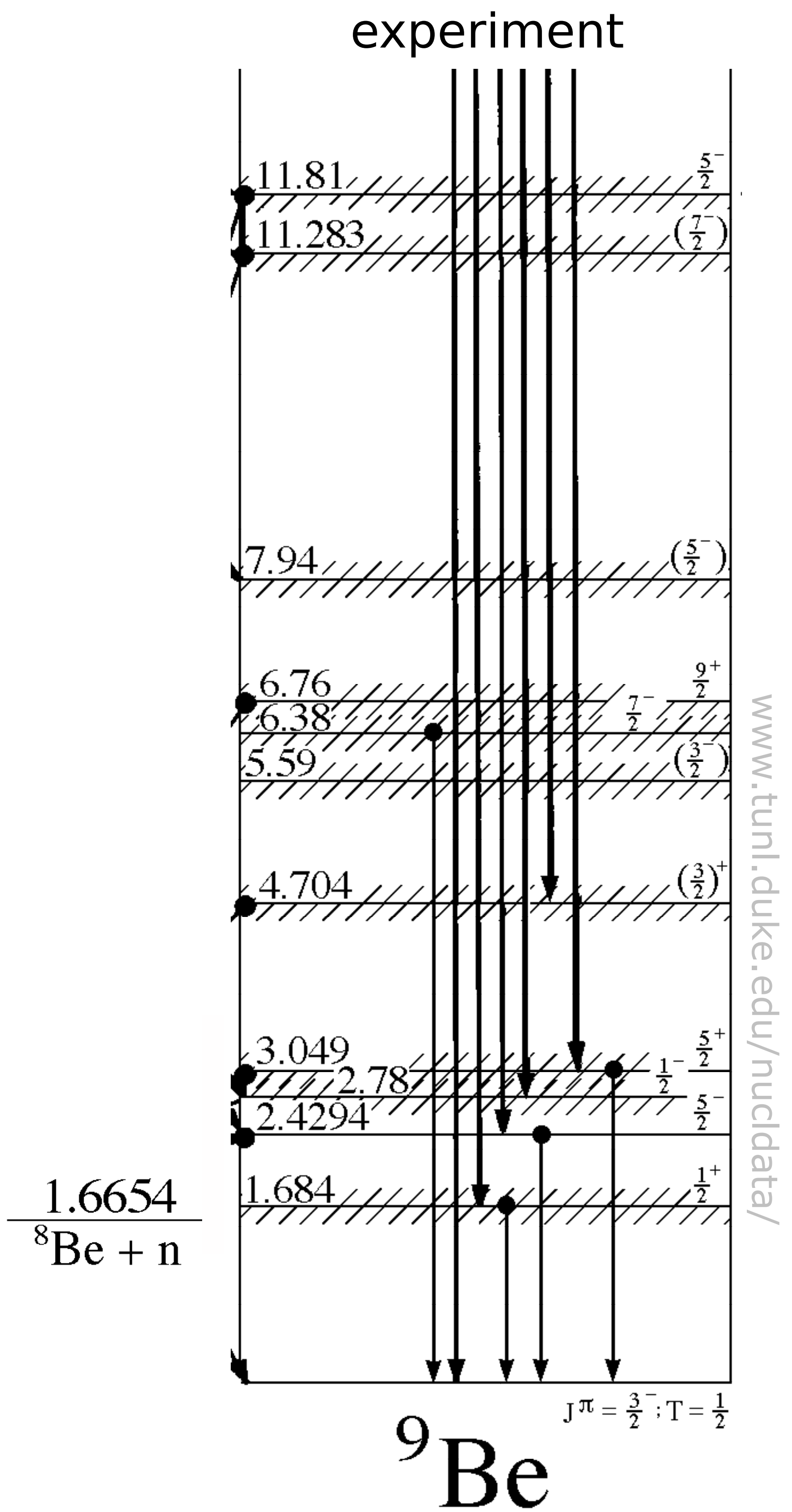
Again use new computational scheme

H_{NCSM}	h	$\mathscr{H}$
Covered by (IT-)NCSM	Given by $\langle \Psi_A E_{\lambda'} J^{\pi} T \vert \hat{H} \vert \xi^{J\pi T}_{\nu r}\rangle$	Contains the NCSM/RGM Hamiltonian kernel

Ab-initio Description of ^{9}Be via NCSMC

- All excited states are resonances
- Study the impact of the continuum by investigating neutron-^{8}Be scattering





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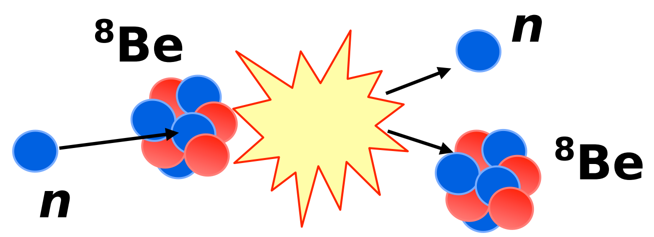

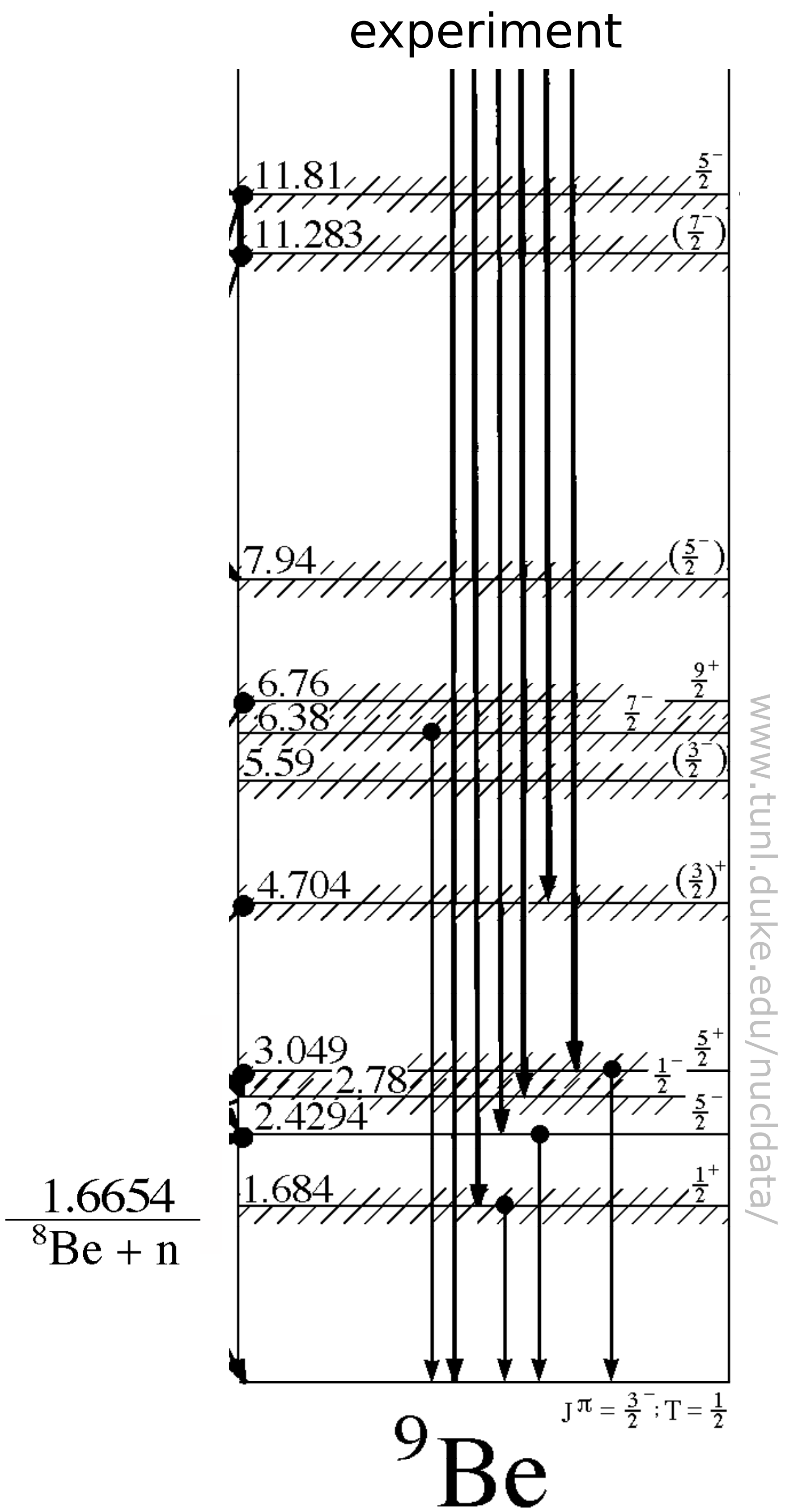

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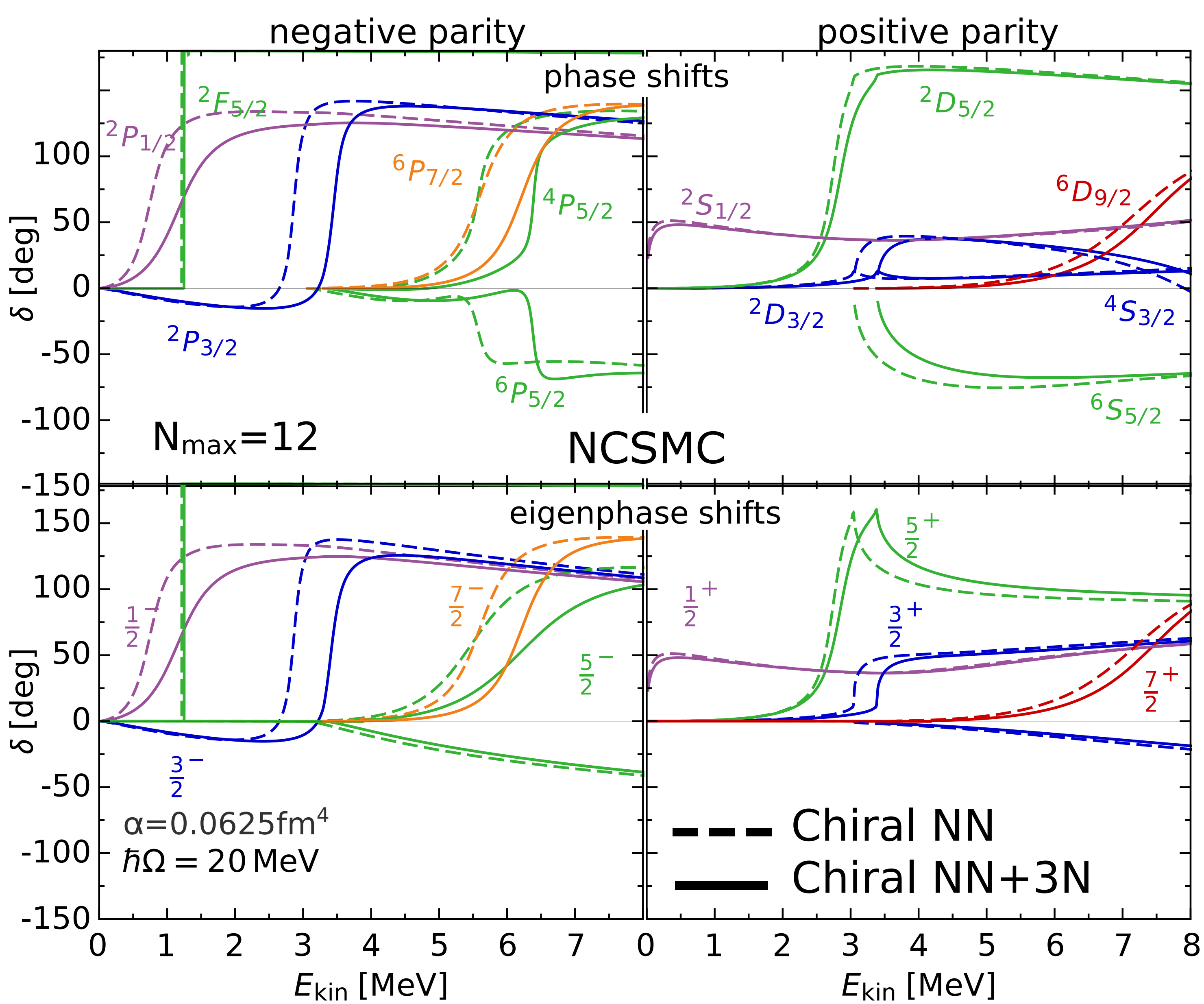

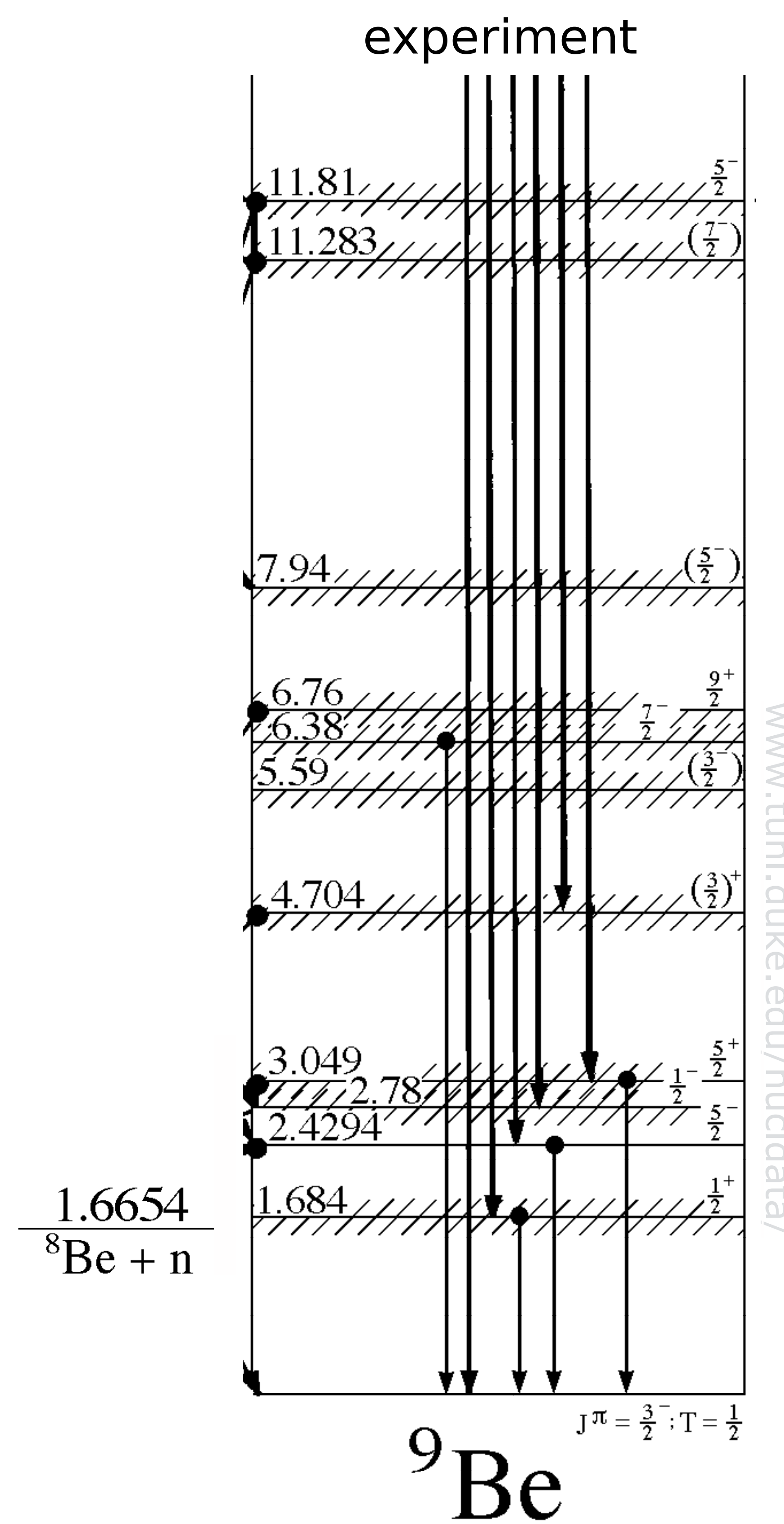

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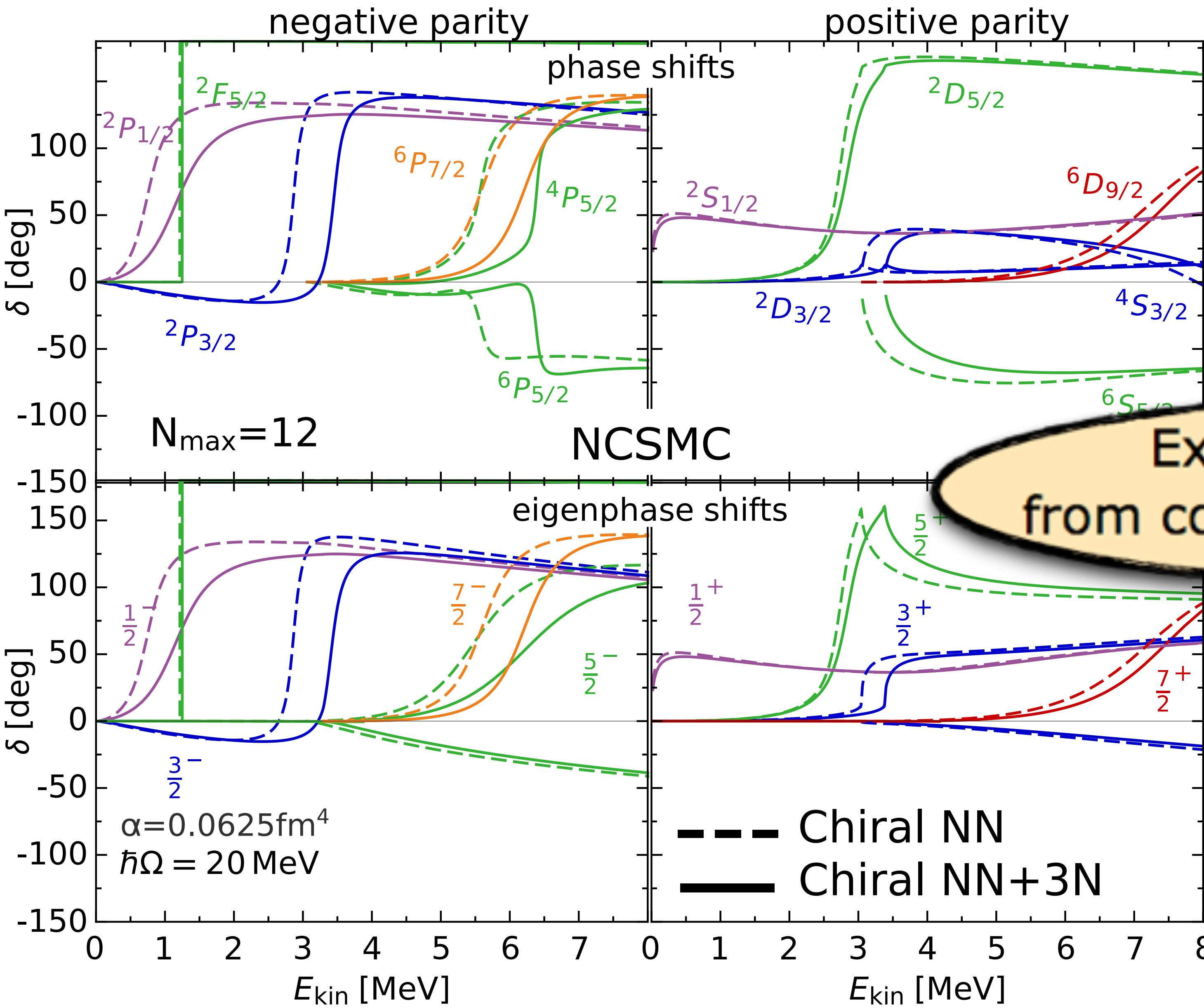
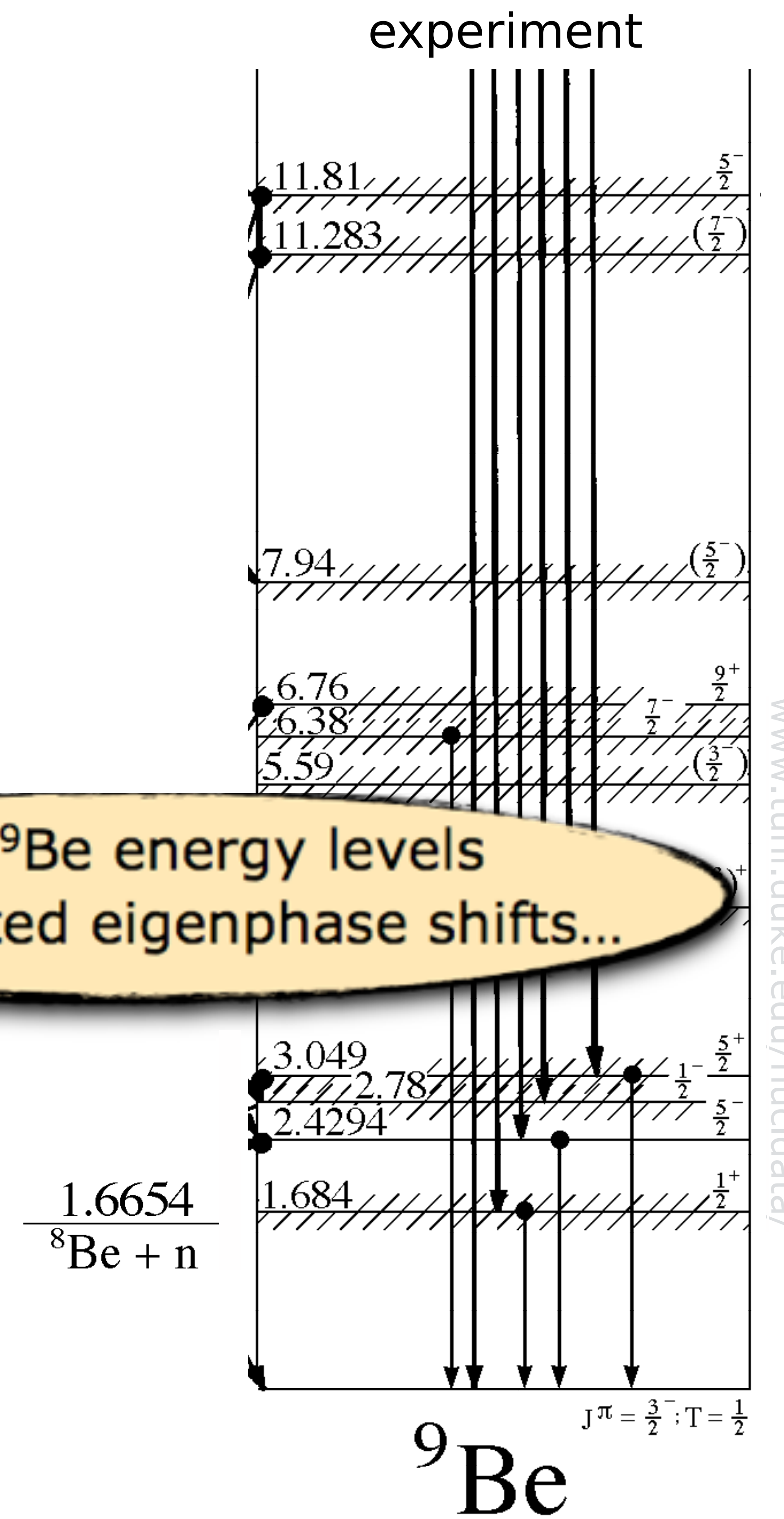
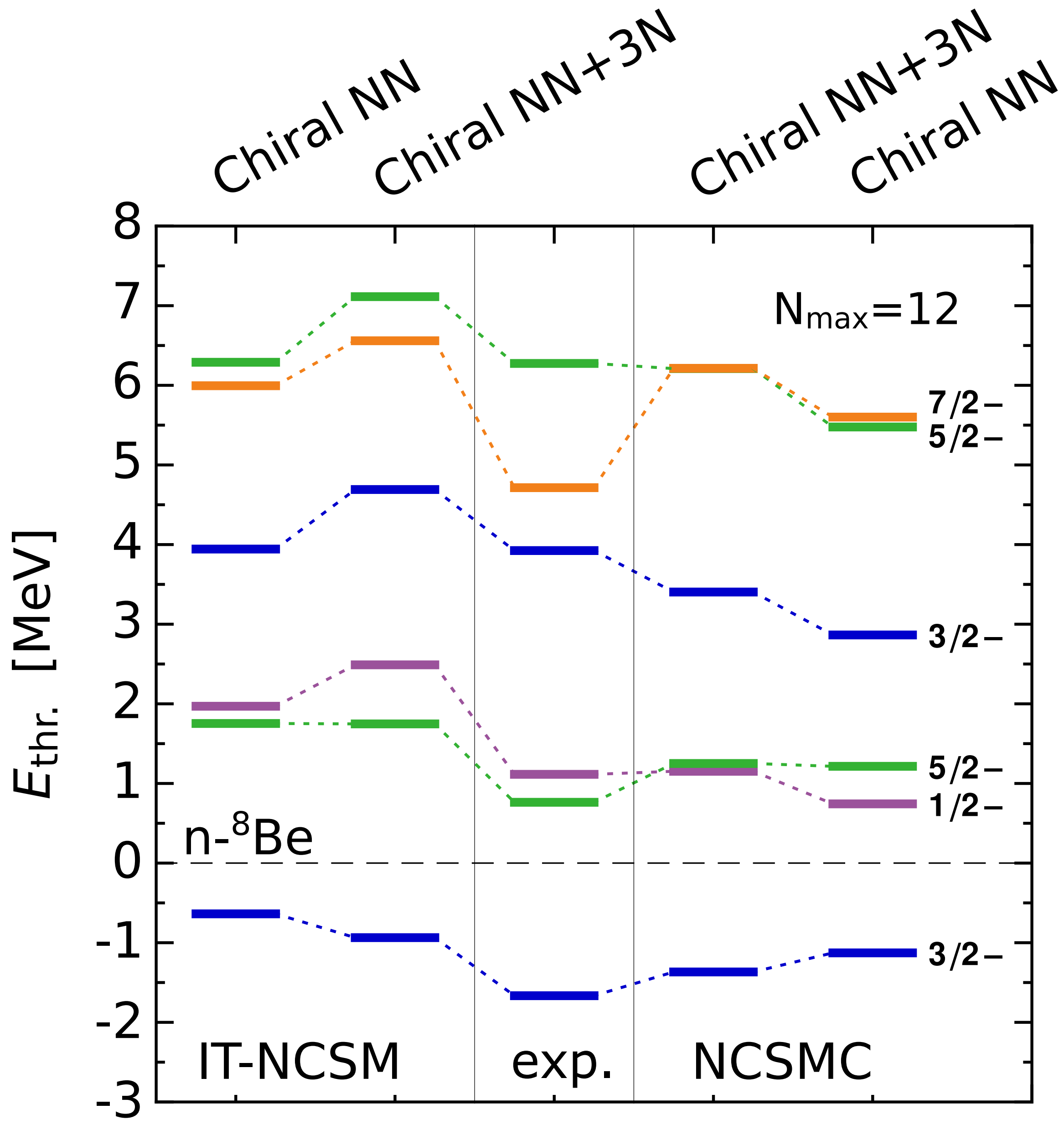


Extract ^{9}Be energy levels from computed eigenphase shifts...



^{9}Be Energy Levels: NCSM vs. NCSMC



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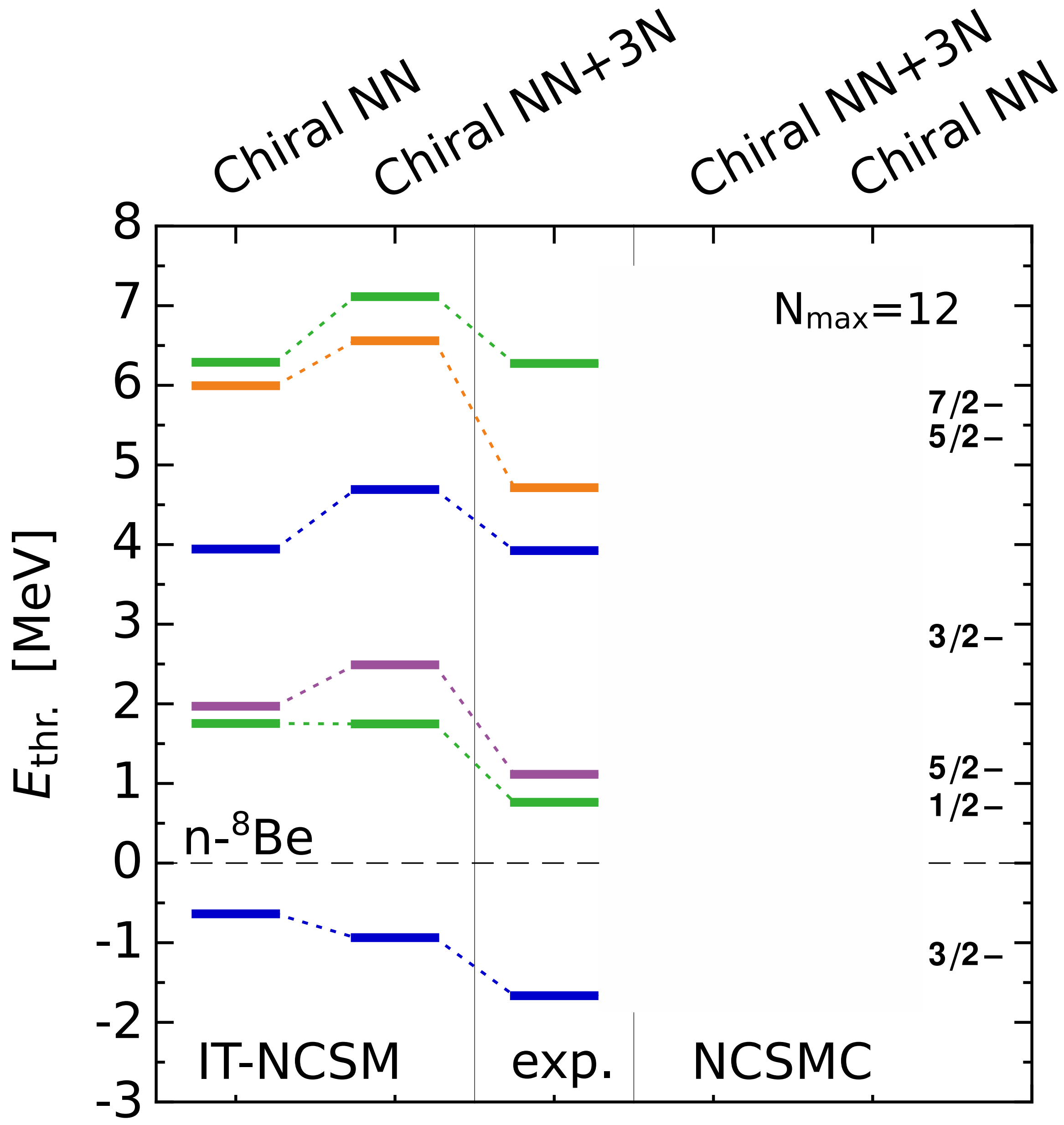

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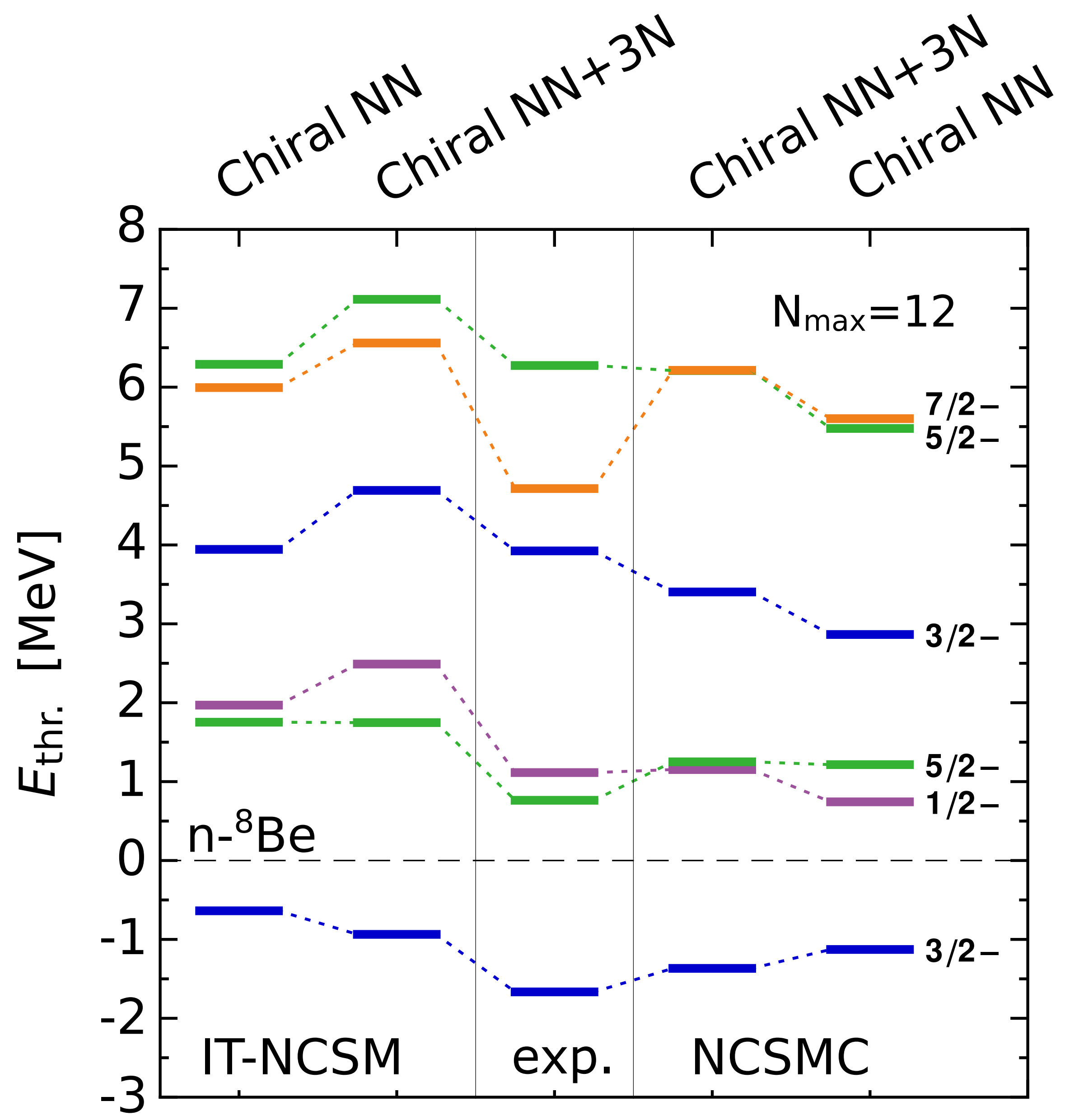
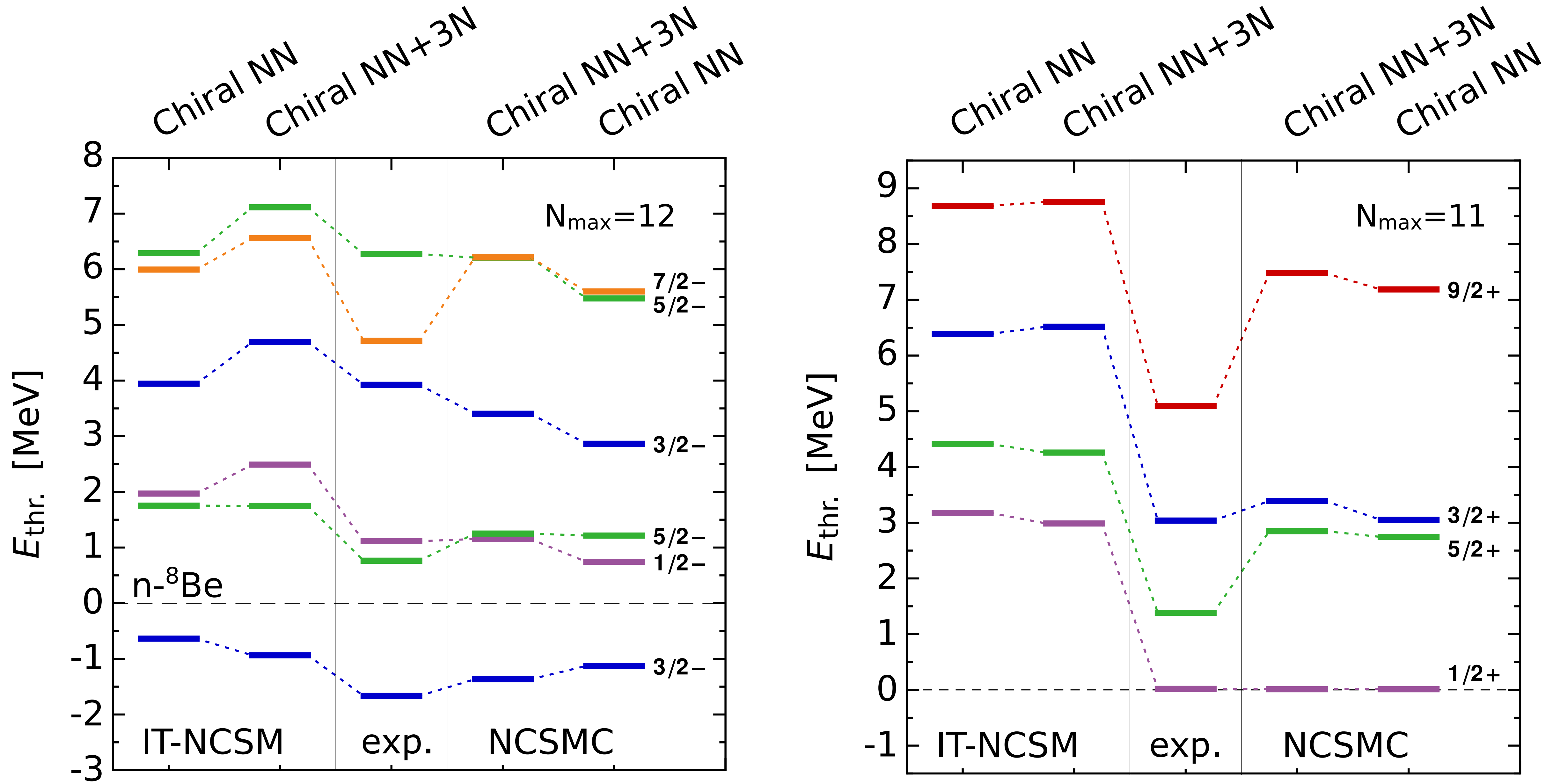


Treatment of continuum indispensable for conclusions about 3N interactions

^{9}Be Energy Levels: NCSM vs. NCSMC



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Summary & Outlook

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Nuclear structure and reactions
accessible within a unified ab-initio
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- Proper **treatment of continuum vital** for validation of and predictions with chiral 3N interactions
- Computational scheme allows study of **p- & sd-shell targets**
- Chiral NN+3N forces yield promising results for ground- and excited-state energies

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- Application of NCSMC to halo nuclei

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Thank you for your kind attention!