Light Nuclei from chiral EFT interactions

Petr Navratil
Lawrence Livermore National Laboratory*

Collaborators:
V. G. Gueorguiev (UCM), J. P. Vary (ISU), W. E. Ormand (LLNL),
A. Nogga (Julich), S. Quaglioni (LLNL), E. Caurier (Strasbourg)

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Outline

- Motivation
- Introduction to *ab initio* no-core shell model (NCSM)
- *Ab initio* NCSM and interactions from chiral effective field theory (EFT)
  - Determination of NNN low-energy constants
  - Results for mid-*p*-shell nuclei
- Beyond nuclear structure with chiral EFT interactions
  - Photo-disintegration of ^{4}He within NCSM/LIT approach
  - n+^{4}He scattering within the NCSM/RGM approach
  - Preliminary: n+^{7}Li scattering within the NCSM/RGM approach
- Outlook
  - ^{40}Ca within importance-truncated *ab initio* NCSM

Talk by Sofia Quaglioni last week

Motivation

- **Goal:**
  - **Describe nuclei from first principles as systems of nucleons that interact by fundamental interactions**
    - Non-relativistic point-like nucleons interacting by realistic nucleon-nucleon and also three-nucleon forces
- Why it has not been solved yet?
  - High-quality nucleon-nucleon (NN) potentials constructed in last 15 years
    - Difficult to use in many-body calculations
  - NN interaction not enough for $A>2$:
    - Three-nucleon interaction not well known

New developments:
chiral EFT NN+NNN interactions

  - Need sophisticated approaches & big computing power
- *Ab initio* approaches to nuclear structure
  - $A=3,4$ – many exact methods
    - 2001: A=4 benchmark paper: 7 different approaches obtained the same ^{4}He bound state properties
      - Faddeev-Yakubovsky, CRCGV, SVM, GFMC, HH variational, EIHH, NCSM
  - $A>4$ - few methods applicable
    - Green's Function Monte Carlo (GFMC)
      - S. Pieper, R. Wiringa, J. Carlson et al.
    - Effective Interaction for Hyperspherical Harmonics (EIHH)
      - Trento, results for ^{6}Li
    - Coupled-Cluster Method (CCM), Unitary Model Operator Approach (UMOA)
      - Applicable mostly to closed shell nuclei
    - *Ab Initio* No-Core Shell Model (NCSM)

Presently the only method capable
to apply chiral EFT interactions to A>4 systems

Ab Initio No-Core Shell Model (NCSM)

- Many-body Schrodinger equation
  - A-nucleon wave function

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

- Hamiltonian

$$H = \sum_{i=1}^{A} \frac{\vec{p}_i^{\,2}}{2m} + \sum_{i<j}^{A} V_{NN}(\vec{r}_i - \vec{r}_j) \quad \left(+ \sum_{i<j<k}^{A} V_{ijk}^{3b} \right)$$

  - Realistic high-precision nucleon-nucleon potentials
    - Coordinate space – Argonne …
    - Momentum space - CD-Bonn, chiral N^3LO …
  - Three-nucleon interaction
    - Tucson-Melbourne TM', chiral N^2LO
- Modification by center-of-mass harmonic oscillator (HO) potential (Lipkin 1958)

$$\frac{1}{2} Am\Omega^2 \vec{R}^2 = \sum_{i=1}^{A} \frac{1}{2} m\Omega^2 \vec{r}_i^{\,2} - \sum_{i<j}^{A} \frac{m\Omega^2}{2A} (\vec{r}_i - \vec{r}_j)^2$$

  - No influence on the internal motion
  - Introduces mean field for sub-clusters

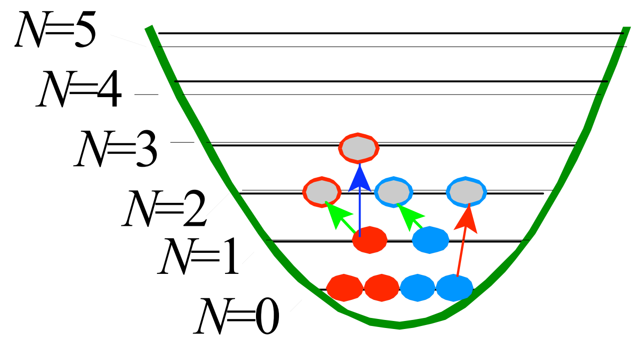
$$H^{\Omega} = \sum_{i=1}^{A} \left[\frac{\vec{p}_i^{\,2}}{2m} + \frac{1}{2} m\Omega^2 \vec{r}_i^{\,2} \right] + \sum_{i<j}^{A} \left[V_{NN}(\vec{r}_i - \vec{r}_j) - \frac{m\Omega^2}{2A} (\vec{r}_i - \vec{r}_j)^2 \right] \quad \left(+ \sum_{i<j<k}^{A} V_{ijk}^{3b} \right)$$

Coordinates, basis and model space

Bound states (and narrow resonances): Square-integrable *A*-nucleon basis

Why HO basis?

- NN (and NNN) interaction depends on relative coordinates and/or momenta
  - Translationally invariant system
  - ⇨ We should use Jacobi (relative) coordinates
- However, if we employ:
  - i) (a finite) **harmonic oscillator basis**
  - ii) a **complete $N_{max}h\Omega$ model space**
- Translational invariance even when Cartesian coordinate Slater determinant basis used
  - Take advantage of powerful second quantization shell model technique
  - Choice of *either* Jacobi *or* Cartesian coordinates according to efficiency for the problem at hand

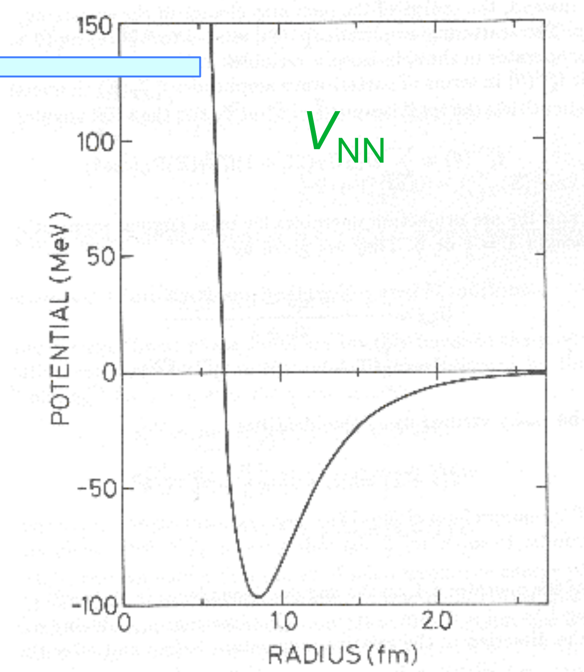


This flexibility is possible only for harmonic oscillator (HO) basis.
A downside: Gaussian asymptotic behavior.

Model space, truncated basis and effective interaction

- **Strategy:** Define Hamiltonian, basis, calculate matrix elements and diagonalize. **But:**
- **Finite** harmonic-oscillator Jacobi coordinate or Cartesian coordinate Slater determinant basis
  - Complete $N_{max}h\Omega$ model space

Nucleon-nucleon interaction



Repulsive core and/or short-range correlations in V_{NN} (and also in V_{NNN}) cannot be accommodated in a truncated HO basis

Need for the effective interaction

Effective Hamiltonian in the NCSM

	P	Q
P (N_{max})	$H^{(n)}_{eff}$	0
Q	0	$Q_n X_n H^{(n)} X_n^{-1} Q_n$

$$H: \quad E_1, E_2, E_3, \ldots E_{d_P}, \ldots E_\infty$$

$$H_{eff}: \quad E_1, E_2, E_3, \ldots E_{d_P}$$

model space dimension

$$QXHX^{-1}P = 0$$

$$H_{eff} = PXHX^{-1}P$$

unitary X=exp[-arctanh(ω^+-ω)]

- Properties of H_{eff} for A-nucleon system
  - A-body operator
    - Even if H two or three-body
  - For $P \rightarrow 1 \quad H_{eff} \rightarrow H$

As difficult as the original problem

- n-body cluster approximation, $2 \leq n \leq A$
- $H^{(n)}_{eff}$ n-body operator
- Two ways of convergence:
  - For $P \rightarrow 1 \quad H^{(n)}_{eff} \rightarrow H$
  - For $n \rightarrow A$ and fixed P: $H^{(n)}_{eff} \rightarrow H_{eff}$

Effective interaction calculation in the NCSM

n-body approximation

$$H^{\Omega} = \sum_{i=1}^{A} h_i + \sum_{i<j}^{A} V_{ij} + \sum_{i<j<k}^{A} V_{ijk}$$

- For ***n*** **nucleons reproduces exactly the full-space results** (for a subset of eigenstates)
  - *n*=2, two-body effective interaction approximation

$$h_1 + h_2 + V_{12} \rightarrow X_2 \rightarrow P_2\left[h_1 + h_2 + V_{2eff,12}\right]P_2 \rightarrow P\left[\sum_{i=1}^{A} h_i + \sum_{i<j}^{A} V_{2eff,ij}\right]P$$

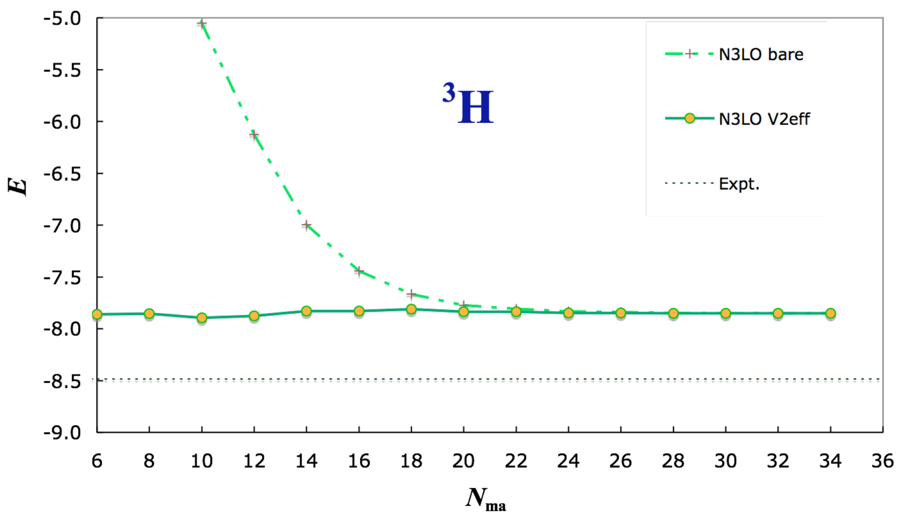
  - *n*=3, three-body effective interaction approximation

$$h_1 + h_2 + h_3 + V_{12} + V_{13} + V_{23} + V_{123} \rightarrow X_3 \rightarrow P_3\left[h_1 + h_2 + h_3 + V^{2b+3b}_{3eff,123}\right]P_3 \rightarrow P\left[\sum_{i=1}^{A} h_i + \frac{1}{A-2}\sum_{i<j<k}^{A} V^{2b}_{3eff,ijk} + \sum_{i<j<k}^{A} V^{3b}_{3eff,ijk}\right]P$$

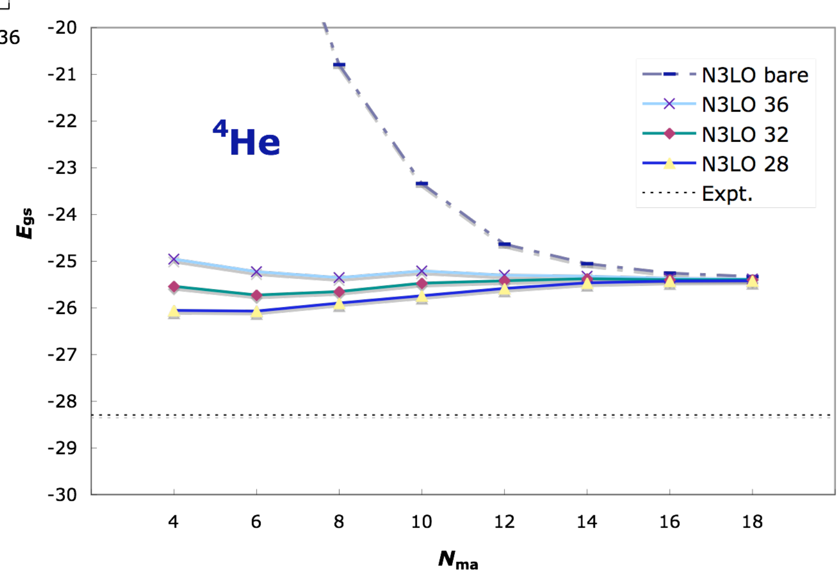
$$Q_n X_n H^{(n)} X_n^{-1} P_n = 0$$

^{3}H and ^{4}He with chiral N^{3}LO NN interaction

- NCSM convergence test
  - Comparison to other methods



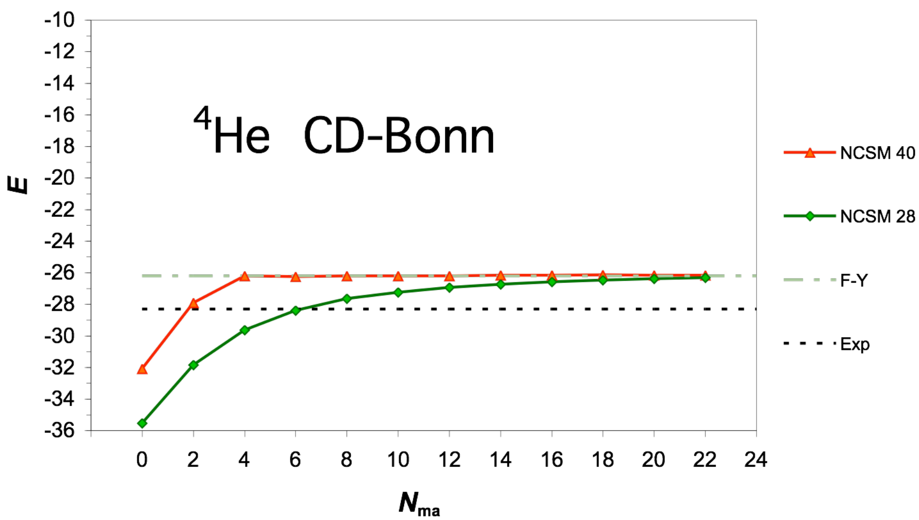
N^{3}LO NN	NCSM	FY	HH
^{3}H	7.852(5)	7.854	7.854
^{4}He	25.39(1)	25.37	25.38

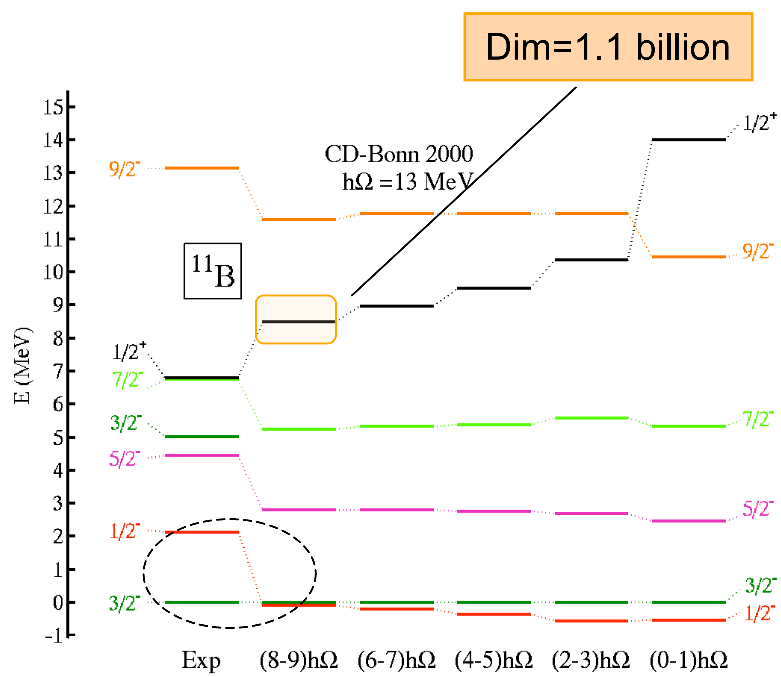


- Short-range correlations ⇒ effective interaction
- Medium-range correlations ⇒ multi-$h\Omega$ model space
- Dependence on
  - size of the model space (N_{max})
  - HO frequency ($h\Omega$)
- Not a variational calculation
- Convergence OK
- NN interaction insufficient to reproduce experiment

Nuclear forces

- Unlike electrons in the atom the interaction between nucleons is not known precisely and is complicated
- Phenomenological NN potentials provide an accurate fit to NN data
  - CD-Bonn 2000
    - One-boson exchange - π, ρ, ω + phenomenological σ mesons
    - χ^2/N_{data}=1.02
- But they are inadequate for A>2 systems
  - Binding energies under-predicted
  - N-d scattering: A_y puzzle; n-^{3}H scattering: total cross section
  - Nuclear structure of p-shell nuclei is wrong





Need to go beyond standard NN potentials

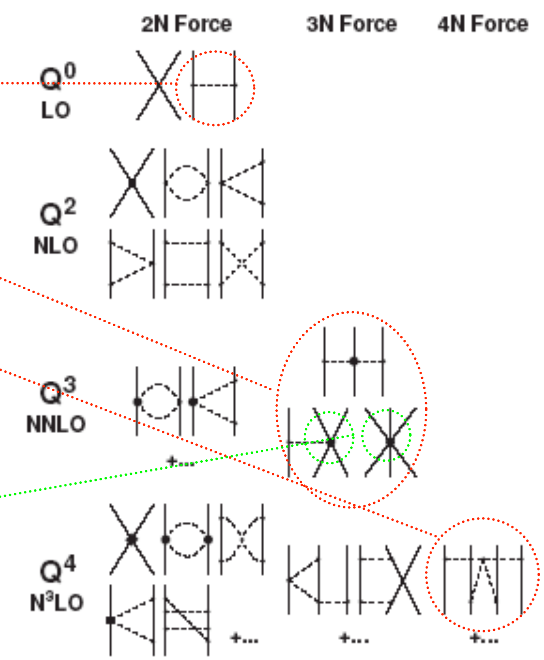
- NNN forces?
  - Consistency between the NN and the NNN potentials
  - Empirical NNN potential models have many terms and parameters
    - Hierarchy?
  - Lack of phase-shift analysis of three-nucleon scattering data
- Predictive theory of nuclei requires a consistent framework for the interaction

Start from the fundamental theory of strong interactions QCD

- QCD non-perturbative in the low-energy regime relevant to nuclear physics
- However, new exciting developments due to Weinberg and others…
  - **Chiral effective field theory (EFT)**
    - Applicable to low-energy regime of QCD
    - Capable to derive systematically inter-nucleon potentials
    - Low-energy constants (LECs) must be determined from experiment

Chiral Effective Field Theory

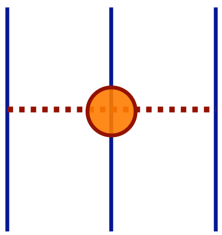
- Chiral symmetry of QCD ($m_u \approx m_d \approx 0$), spontaneously broken with pion as the Goldstone boson
- Systematic low-momentum expansion in $(Q/\Lambda_\chi)^n$; $\Lambda_\chi \approx$ 1 GeV, Q≈100 MeV
  - Degrees of freedom: nucleons + pions
  - Power-counting: Chiral perturbation theory (χPT)
- Describe pion-pion, pion-nucleon and inter-nucleon interactions at low energies
  - Nucleon-nucleon sector - S. Weinberg (1991)
    - Worked out by Van Kolck, Kaiser, Meissner, Epelbaum, Machleidt…
- Leading order (LO)
  - One-pion exchange
- NNN interaction appears at next-to-next-to-leading order (N^2LO)
- NNNN interaction appears at N^3LO order
- Consistency between NN, NNN and NNNN terms
  - NN parameters enter in the NNN terms etc.
- Low-energy constants (LECs) need to be fitted to experiment
- N^3LO is the lowest order where a high-precision fit to NN data can be made
  - Entem and Machleidt (2002) N^3LO NN potential
- Only TWO NNN and NO NNNN low-energy constants up to N^3LO



Challenge and necessity: Apply chiral EFT forces to nuclei

Chiral N^{2}LO NNN interaction

N^{2}LO

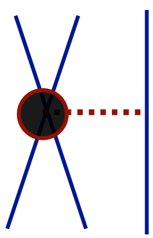


c_1, c_3, c_4

Two-pion exchange

c_1,c_3,c_4 LECs appear in the chiral NN interaction

- Determined in the A=2 system

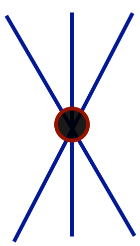


c_D

New!

One-pion-exchange-contact

New c_D LEC



c_E

New!

Contact

New c_E LEC

Must be determined in $A \geq 3$ system

To be used by Pisa group in HH basis

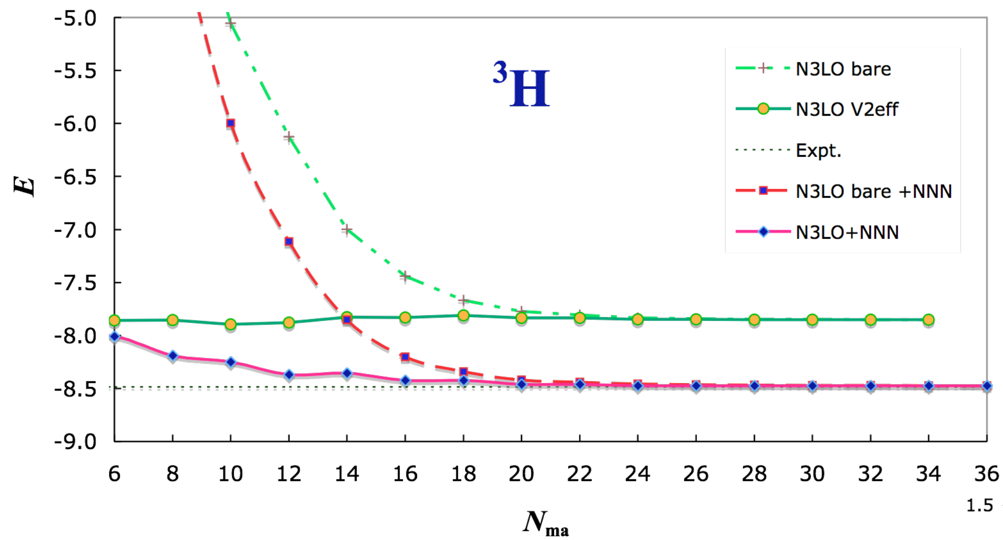
Nontrivial to include in the NCSM calculations

– Regulated with momentum transfer

- local NNN interaction in coordinate space

Application of *ab initio* NCSM to determine c_D, c_E : A=3

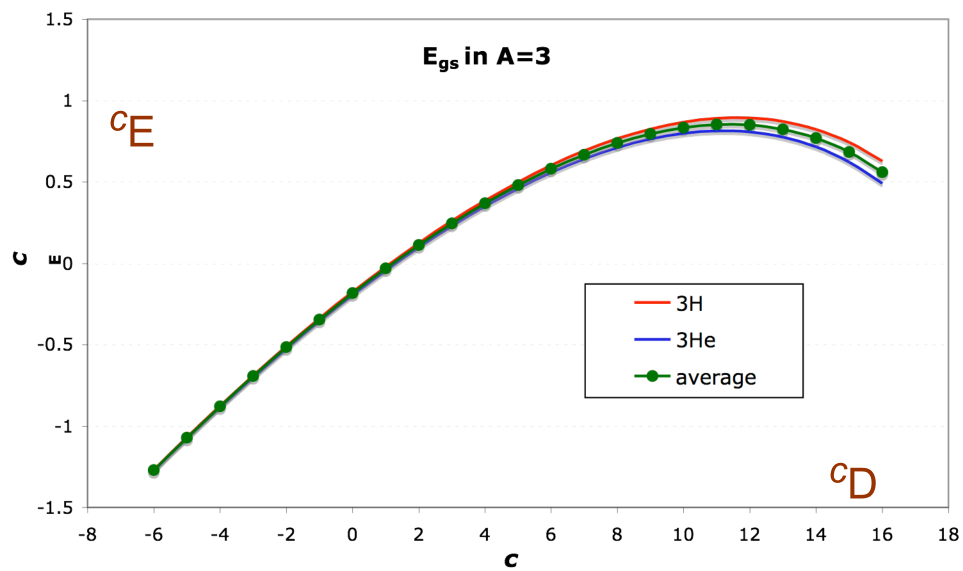
- Fit c_D, c_E to experimental binding energy of ^3H (^3He)



Convergence test for c_D=2 c_E=0.115

NCSM
Jacobi coordinate
HO basis
N^3LO NN ↔ V_{2eff}
N^2LO NNN ↔ bare

c_D - c_E dependence that fits A=3 binding energy

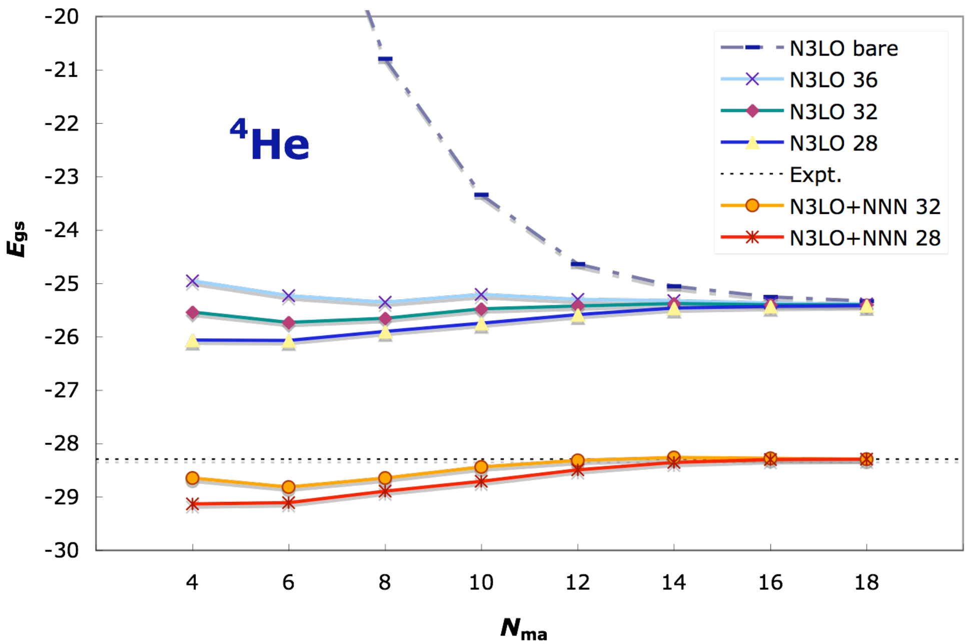


- Another observable needed
  - N-d doublet scattering length
    - Correlated with E_{gs}

Another possibility:
Properties of heavier nuclei

Application of *ab initio* NCSM to determine c_D, c_E : ^{4}He

- Fit constrained c_D, c_E to ^{4}He binding energy



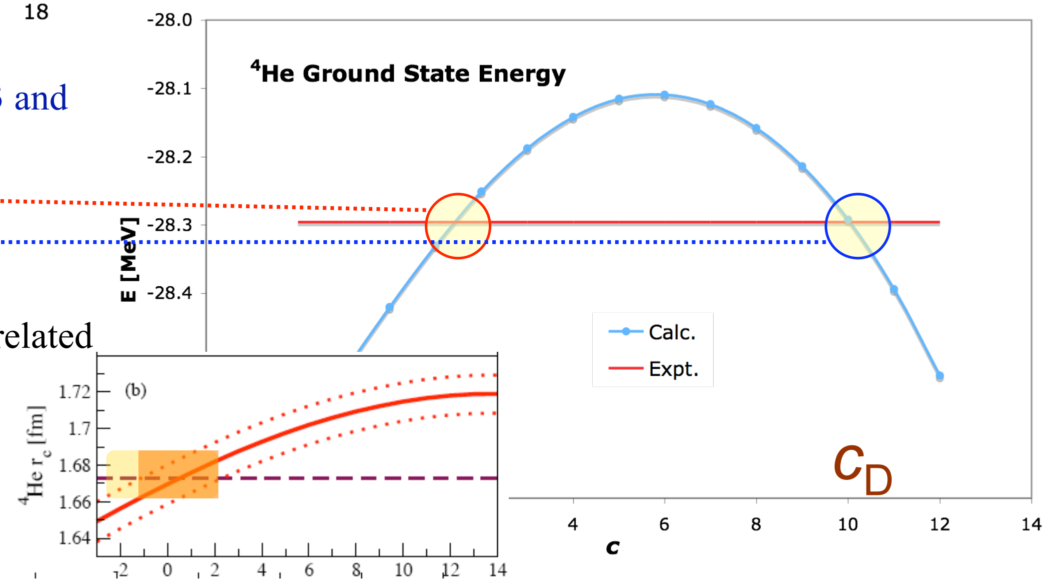
Convergence test for c_D=2 c_E=0.12

NCSM
Jacobi coordinate
HO basis
N^3LO NN $\leftrightarrow V_{3eff}$
N^2LO NNN $\leftrightarrow V_{3eff}$

$c_D \approx -1 \sim 2$ preferred

^{4}He binding energy dependence on c_D

- Two combinations of c_D - c_E that fit both A=3 and ^{4}He binding energies
  - Point A: $c_D \approx 1.5$
  - Point B: $c_D \approx 10$
  - ^{4}He E_{gs} dependence on c_D weak
    - ^{4}He and A=3 binding energies correlated

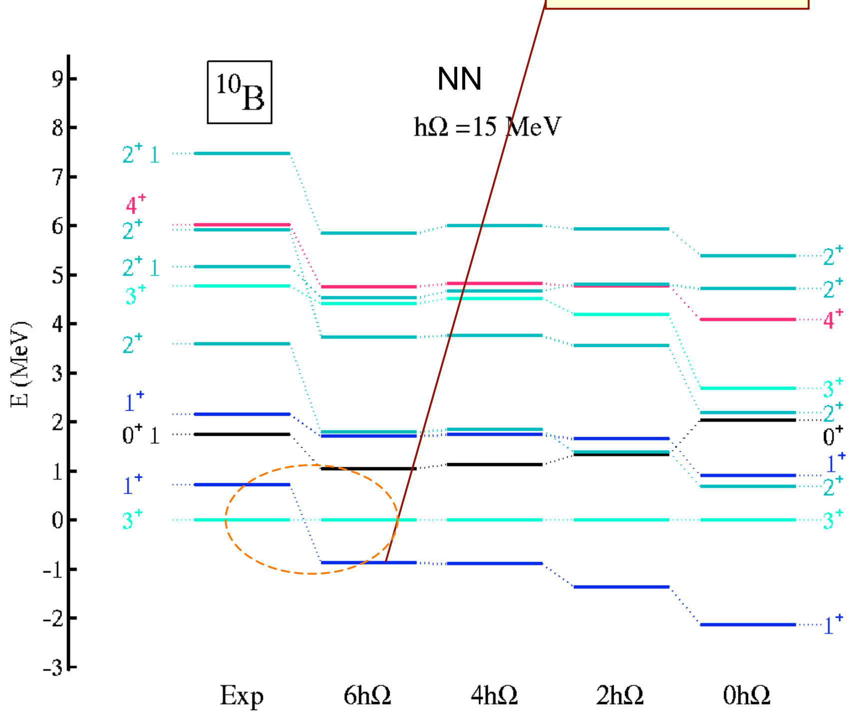


Explore *p*-shell nuclei

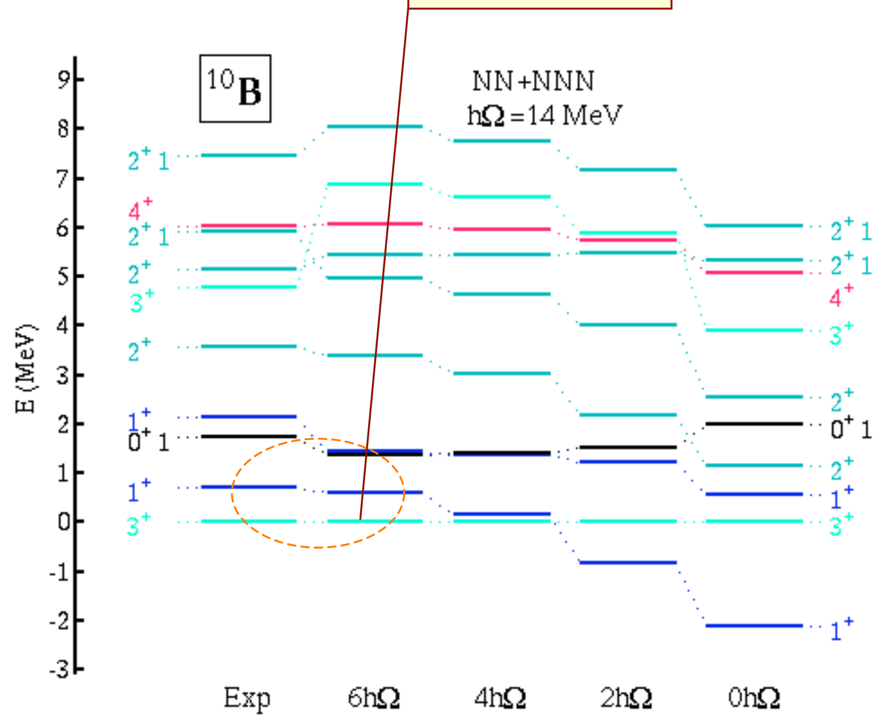
NNN important for heavier *p*-shell nuclei: ^{10}B

- ^{10}B known to be poorly described by standard NN interaction
  - Predicted ground state $1^+ 0$
  - Experiment $3^+ 0$
- Chiral NNN fixes this problem

E_B=56.5 MeV



E_B=65.7 MeV

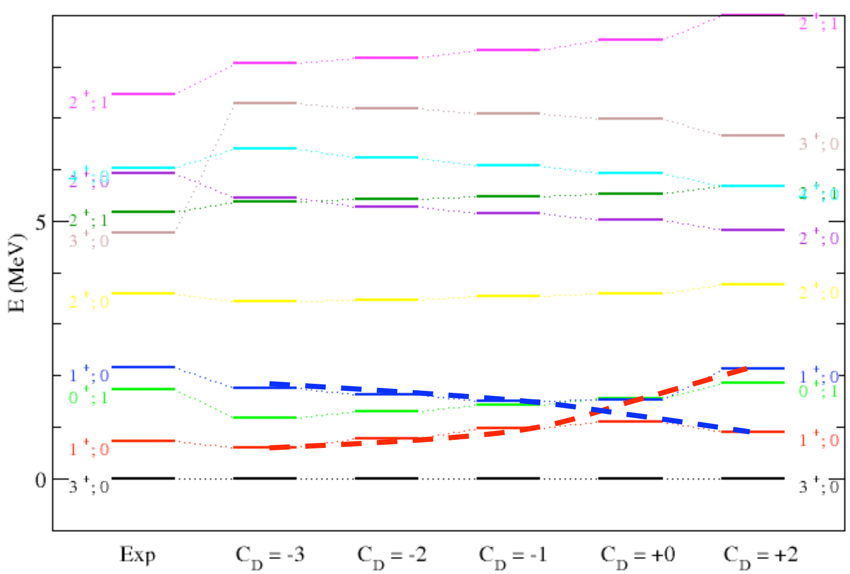


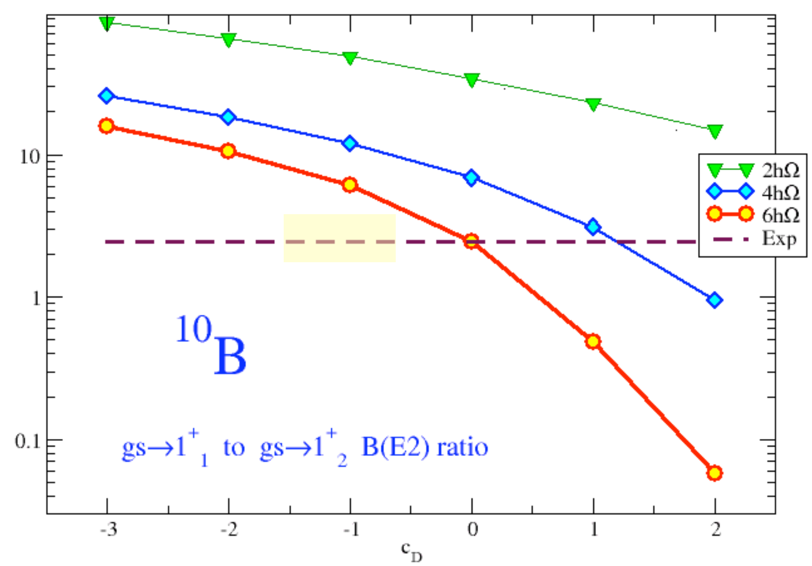
Application of *ab initio* NCSM to determine c_D, c_E : ^{10}B

- ^{10}B properties not correlated with A=3 binding energy
- Spectrum shows weak dependence on c_D
- However: Order of 1^+_1 and 1^+_2 changes depending on c_D
  - This is seen in ratio of E2 transitions from ground state to 1^+_1 and 1^+_2

$c_D \approx$ -1.5 ~ -0.5 preferred

^{10}B NN+NNN c_D dependence for N_{max} = 6, $\hbar\Omega$ =15 MeV

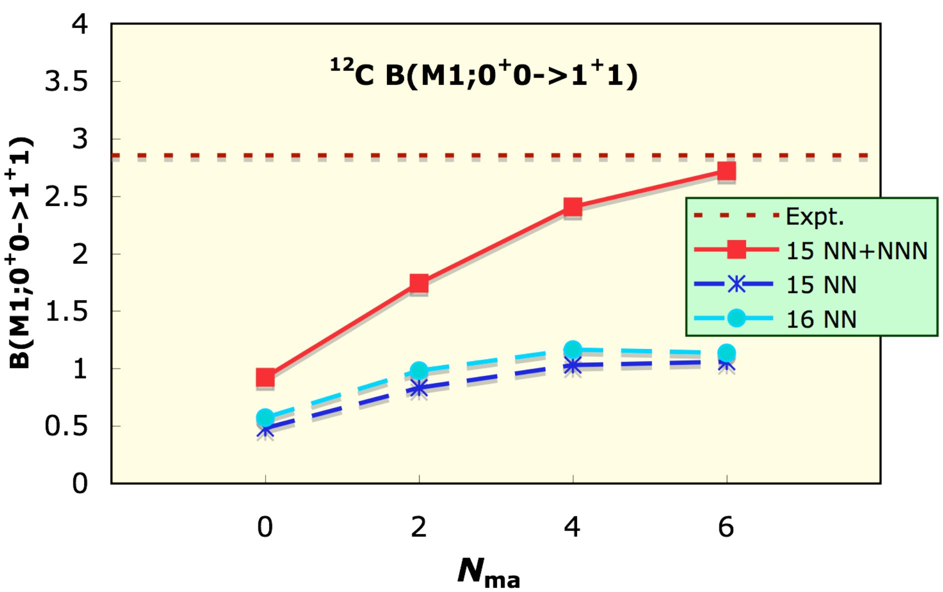


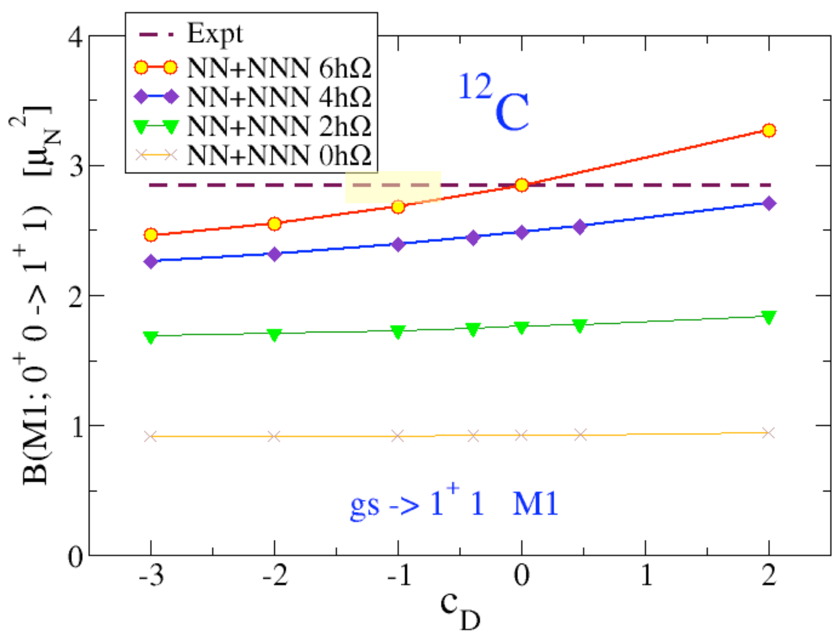


Application of *ab initio* NCSM to determine c_D, c_E : ^{12}C

- Sensitivity of B(M1; $0^+0 \rightarrow 1^+1$) to the strength of spin-orbit interaction
  - Presence of the NNN interaction
  - Choice of the c_D-c_E LECs

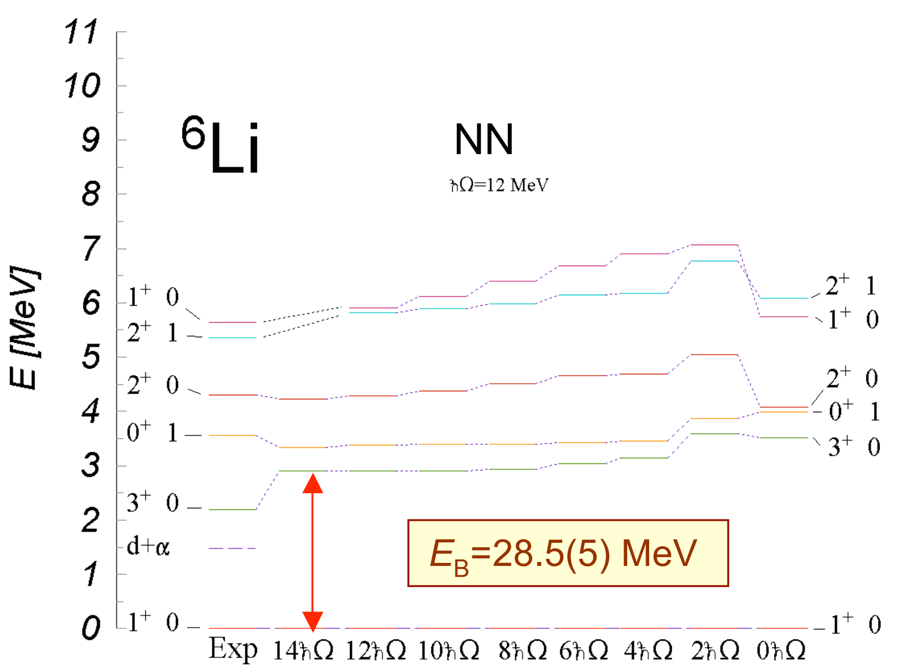
$c_D \approx -1$ preferred

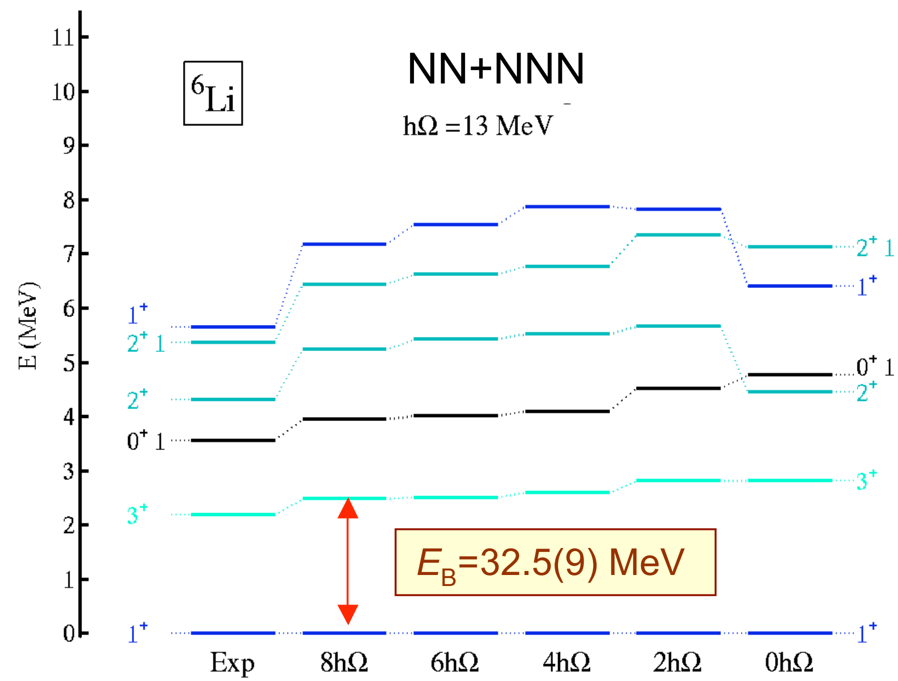




^{6}Li with chiral NN+NNN interactions

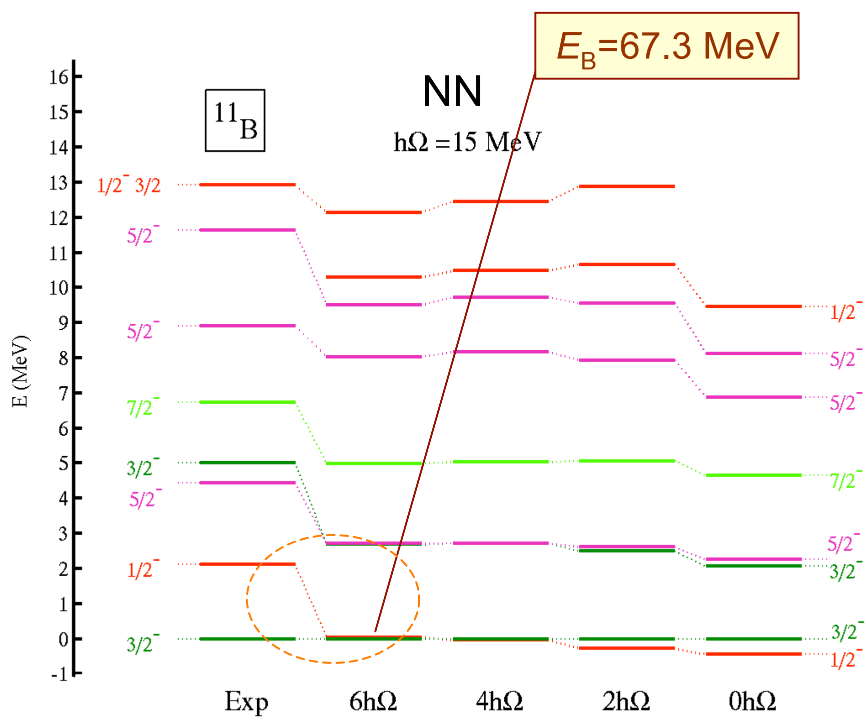
- ^{6}Li calculations with NN can be performed up to 16hΩ
  - Dimensions 10^8
  - Very good convergence of the excitations energies with the chiral N^{3}LO NN
    - Discrepancies in level splitting (e.g. 3^+ 0); binding energy underestimated
- ^{6}Li calculations with NN+NNN performed up to 8hΩ
  - Dimension only 1.5 million, but:
  - 13 GB input file with the three-body effective interaction matrix elements
  - A very challenging calculation performed at the LLNL **up** machine
    - Improvement of the 3^+ 0 state position; binding energy in agreement with experiment

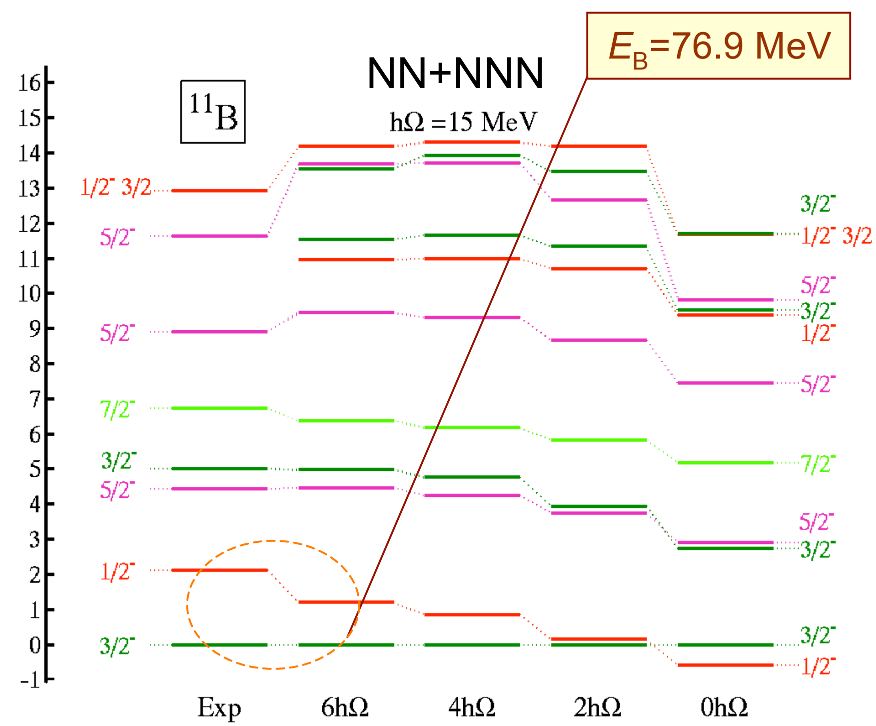




^{11}B with chiral NN+NNN interactions

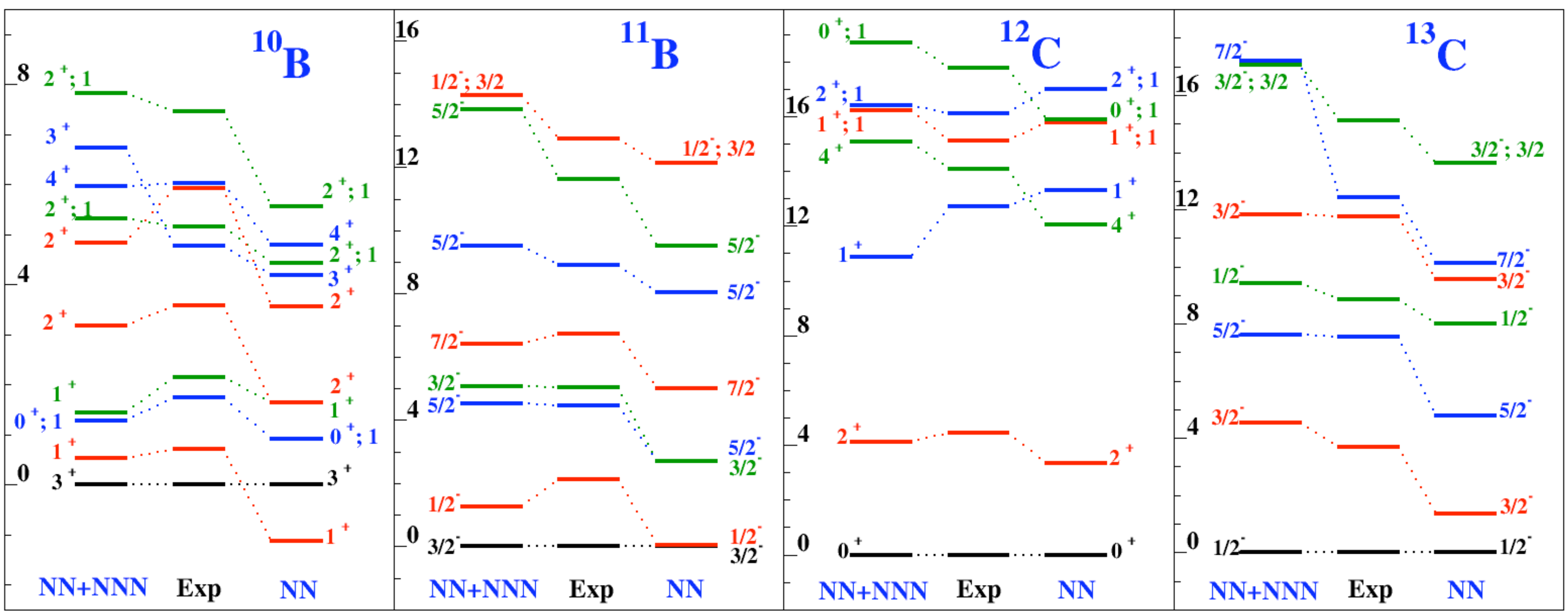
- ^{11}B also poorly described by standard NN interactions
  - Excitation energies
  - Gamow-Teller transitions
- Chiral NNN improves on both
  - Results using c_D=-1





Ab initio NCSM calculations with chiral EFT NN+NNN interactions: Summary

- *Ab initio* NCSM presently the only method capable to apply the chiral EFT NN+NNN interactions to *p*-shell nuclei
  - Technically challenging, large-scale computational problem
    - ~3000 processors used in ^{12,13}C calculations
- Applied to determine the NNN contact interaction LECs
  - Investigation of A=3, ^{4}He and *p*-shell nuclei
  - Globally the best results with $c_D \sim -1$
- NNN interaction essential to describe structure of light nuclei



Applications to nuclear reactions

- *Ab initio* description of nuclear reactions
  - Even stricter test of NN and NNN interactions
  - Important for nuclear astrophysics
    - Understanding of the solar model, big-bang nucleosynthesis, star evolution
    - Low-energy reactions difficult or impossible to measure experimentally
      - Need theory with predictive power
- In general, need to go beyond bound states
  - clustering
  - resonant and non-resonant continuum
- However, for a certain type of reactions bound-state techniques can be used
  - Photo-disintegration

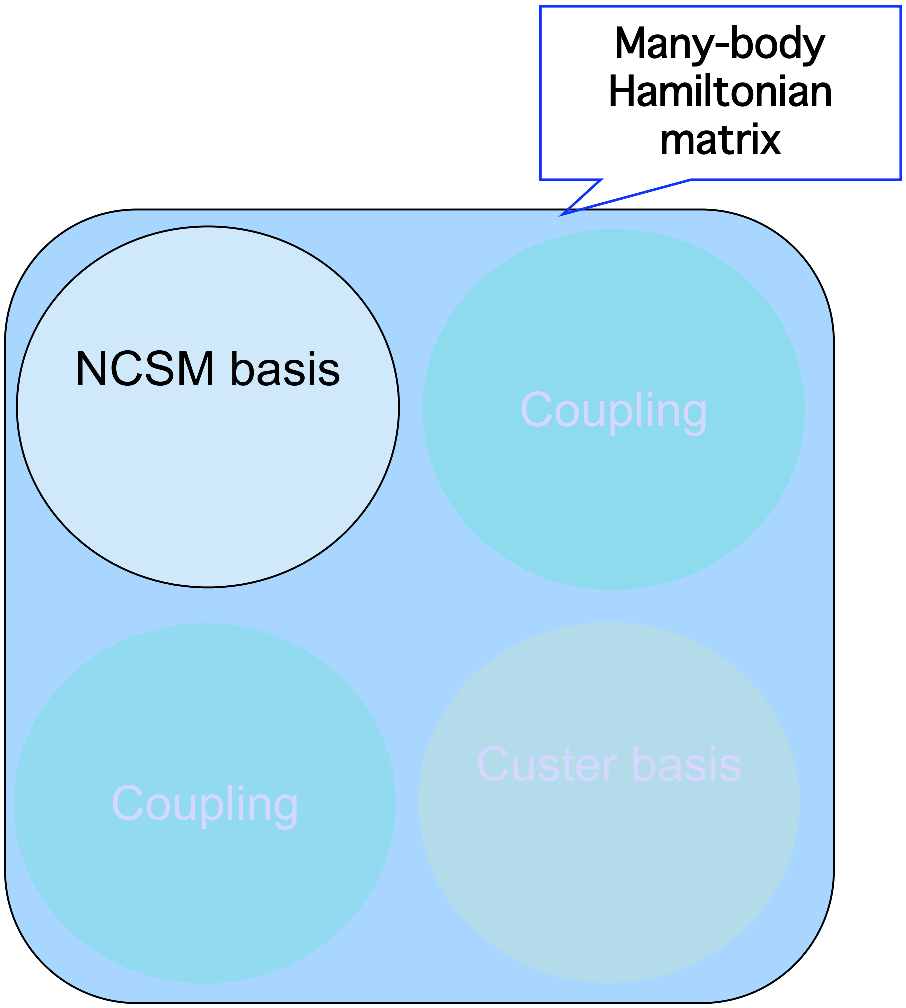


Photo-disintegration of the α-particle: LIT method

- Photo-absorption cross section

$$\sigma_\gamma(\omega) = 4\pi^2 \frac{e^2}{\hbar c}\omega R(\omega) \leftarrow \sum_f \left|\langle \Psi_f | \hat{D} | \Psi_0 \rangle\right|^2 \delta(E_f - E_0 - \omega)$$

Inclusive response function

- LIT method:
  - solve the many-body Schrödinger equation for $|\Psi_0\rangle$
  - apply the Lanczos algorithm to the Hamiltonian starting from:

$$|\varphi_0\rangle = \langle \Psi_0 | \hat{D}^\dagger \hat{D} | \Psi_0 \rangle^{-\frac{1}{2}} \hat{D} | \Psi_0 \rangle$$

  - calculate the LIT of $R(\omega)$

$$L(\sigma_R, \sigma_I) = \int R(\omega) \frac{1}{(\omega - \sigma_R)^2 + \sigma_I^2} d\omega = -\frac{1}{\sigma_I} Im \left\{ \langle \psi_0 | \hat{D}^\dagger \frac{1}{E_0 + \sigma_R + i\sigma_I - \hat{H}} \hat{D} | \psi_0 \rangle \right\}$$

$\sigma_I \sim 10 - 20$ MeV!

  - invert the LIT and calculate the cross section

Continued fraction of Lanczos coefficients

$$-\frac{1}{\sigma_I} Im \frac{\langle \Psi_0 | \hat{D}^\dagger \hat{D} | \Psi_0 \rangle}{(z - a_0) - \frac{b_i^2}{(z-a_1) - \frac{b_2^2}{(z-a_2) - \frac{b_3}{\ddots}}}}$$

- Ingredients:
  - NCSM ^{4}He wave functions obtained from NN+NNN χEFT

The LIT method is a microscopic approach to perturbation-induced reactions (also exclusive!). The continuum problem is mapped onto a bound-state-like problem.

Numerical accuracy and NNN effects

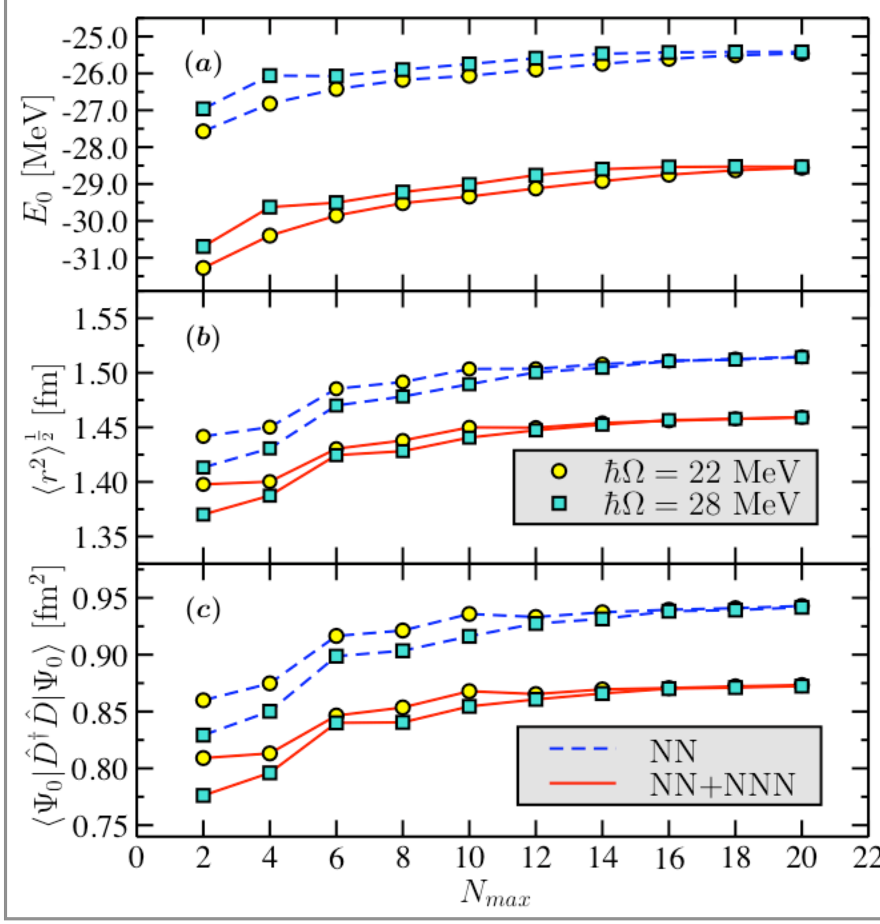
- effective interaction at the three-body cluster level for both NN and NN+NNN
  - similar patterns
  - accurate convergence
- NNN force effects:
  - more binding
  - reduced size
  - reduced dipole strength

$$\langle \Psi_0 | \hat{D}^\dagger \hat{D} | \Psi_0 \rangle \simeq \frac{ZN}{3(A-1)} \langle r_p^2 \rangle$$

pure symmetric spatial wave functions

(8% off)

Ground-state convergence

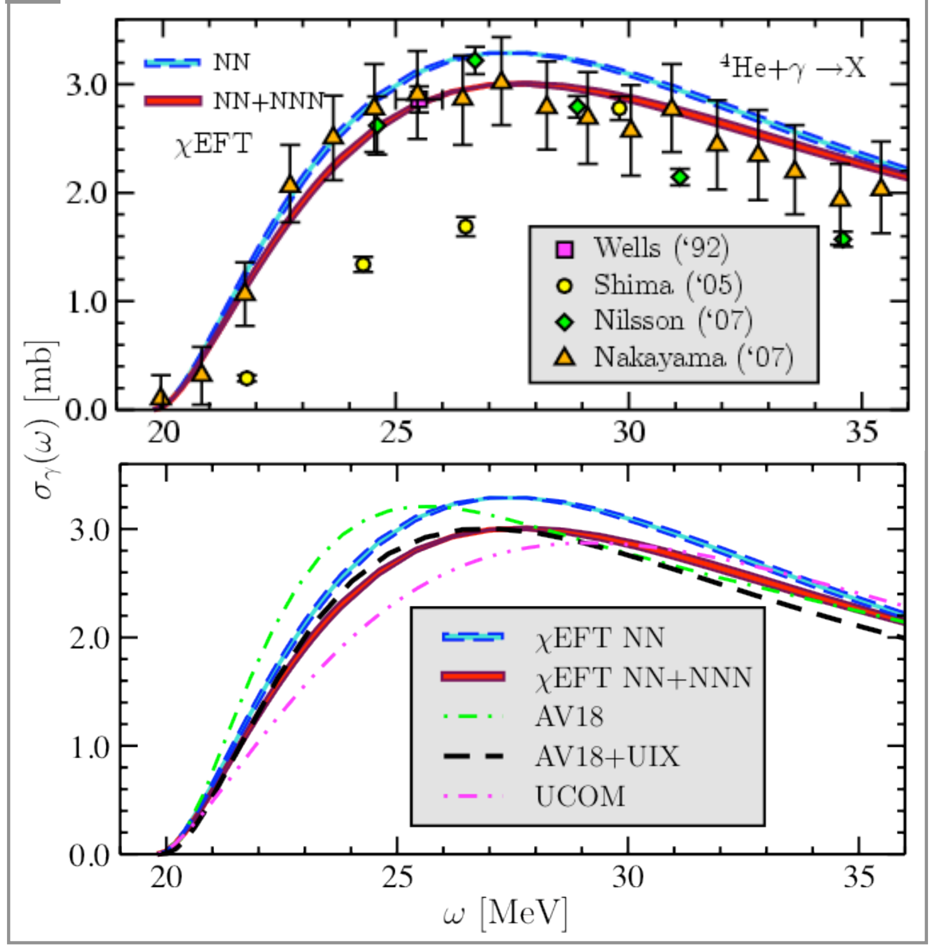


The ground-state properties present very similar smooth convergence patterns

Photo-disintegration of the α-particle: χEFT NN+NNN interactions

- Still large discrepancies between different experimental data
  - up to 100% disagreement on the peak-height
- The NNN force induces a suppression of the peak
  - not enough to explain data from Shima *et al.*!
- In the peak region χEFT NN+NNN and AV18+UIX curves are relatively close:
  - weak sensitivity to the details of NNN force
  - expect larger effects in *p*-shell nuclei!

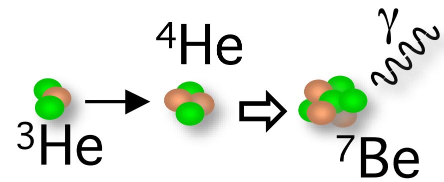
^{4}He photo-absorption cross section

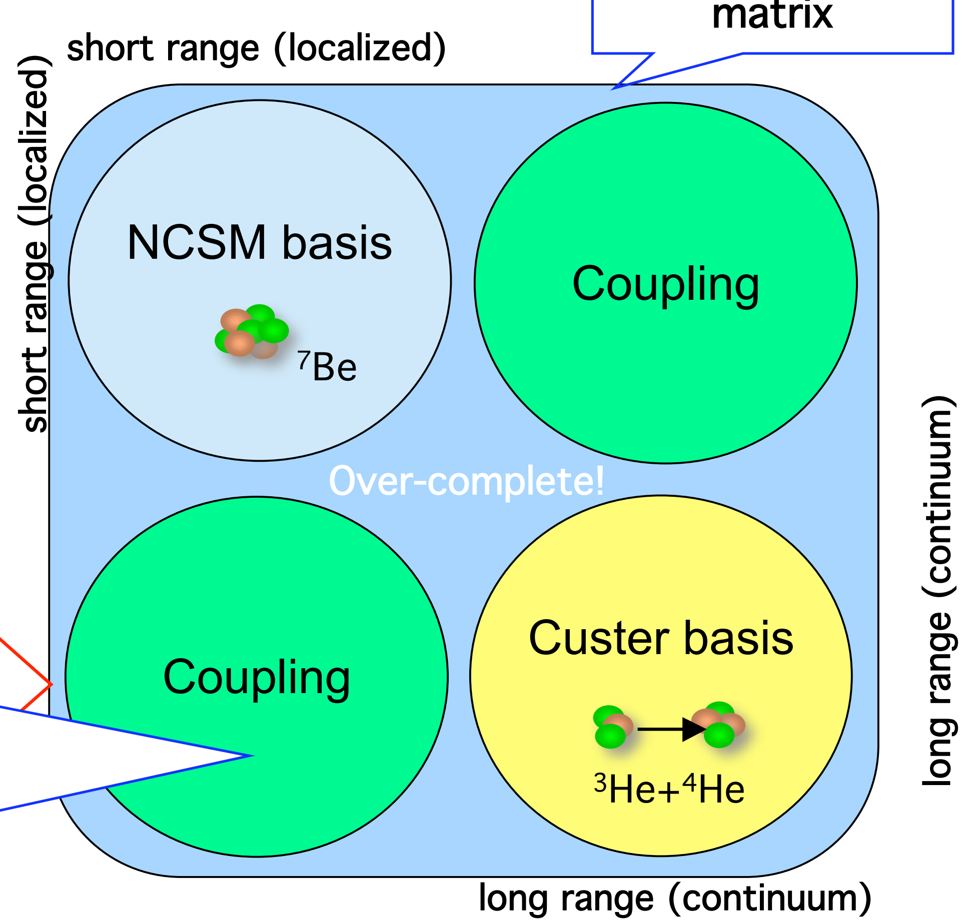


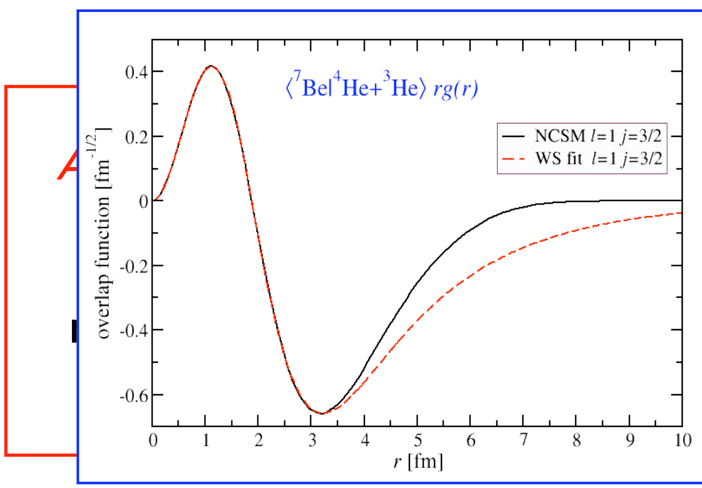
The differences in the realistic calculations are far below the experimental uncertainties: urgency for further experimental activity to clarify the situation.

Proper treatment of long-range properties: Towards *ab initio* reaction theory

- Need to go beyond NCSM and include
  - clustering
  - resonant and non-resonant continuum
- We can build upon *ab initio* NCSM to describe
  - discrete spectrum
  - continuum spectrum
  - coupling between them





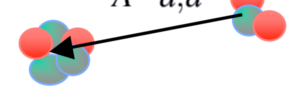


Resonating group method (RGM)

- Ansatz:

$$\Psi^{(A)} = \sum_\nu \hat{\mathcal{A}} \left[\psi_{1\nu}^{(A-a)} \psi_{2\nu}^{(a)} \varphi_\nu(\vec{r}_{A-a,a}) \right] = \sum_\nu \int d\vec{r}\, \varphi_\nu(\vec{r})\, \hat{\mathcal{A}}\, \Phi_{\nu\vec{r}}^{(A-a,a)}$$

$$\Phi_{\nu\vec{r}}^{(A-a,a)} = \psi_{1\nu}^{(A-a)} \psi_{2\nu}^{(a)} \delta(\vec{r} - \vec{r}_{A-a,a})$$



- The many-body problem is mapped onto various channels of nucleon clusters and their relative motion:

$$H\Psi^{(A)} = E\Psi^{(A)} \longrightarrow \sum_\nu \int d\vec{r} \left[\mathcal{H}_{\mu\nu}^{(A-a,a)}(\vec{r}\,', \vec{r}) - E\mathcal{N}_{\mu\nu}^{(A-a,a)}(\vec{r}\,', \vec{r}) \right] \varphi_\nu(\vec{r}) = 0$$

Hamiltonian kernel

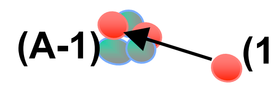
$$\langle \Phi_{\mu\vec{r}\,'}^{(A-a,a)} | \hat{\mathcal{A}} H \hat{\mathcal{A}} | \Phi_{\nu\vec{r}}^{(A-a,a)} \rangle$$

$$\langle \Phi_{\mu\vec{r}\,'}^{(A-a,a)} | \hat{\mathcal{A}}^2 | \Phi_{\nu\vec{r}}^{(A-a,a)} \rangle$$

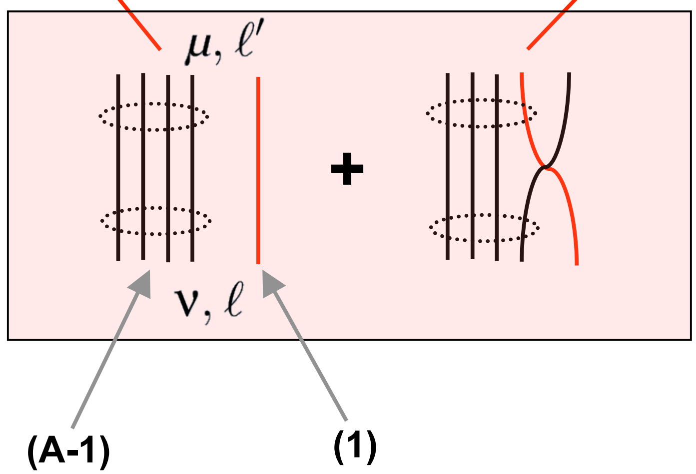
Norm kernel

To treat clustering and continuum we extend the RGM approach by using NCSM *ab initio* wave functions for the clusters involved, and effective interactions derived from realistic two- and three-nucleon forces.

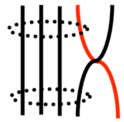
Single-nucleon projectile: the norm kernel



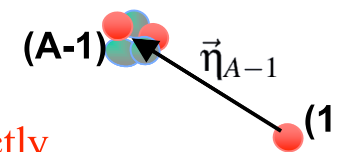
$$\mathcal{N}^{(A-1,1)}_{\mu\ell',\nu\ell}(r',r) = \delta_{\mu\nu}\,\delta_{\ell'\ell}\frac{\delta(r'-r)}{r'r} - (A-1)\sum_{n'n} R_{n'\ell'}(r')\langle\Phi^{(A-1,1)JT}_{\mu n'\ell'}|P_{A,A-1}|\Phi^{(A-1,1)JT}_{\nu n\ell}\rangle R_{n\ell}(r)$$



Jacobi or single-particle coordinates? Both …

- An example:  $= \sum_{n'n} R_{n'\ell'}(r') \langle \Phi^{(A-1,1)JT}_{\mu n'\ell'} | P_{A,A-1} | \Phi^{(A-1,1)JT}_{\nu n\ell} \rangle R_{n\ell}(r)$

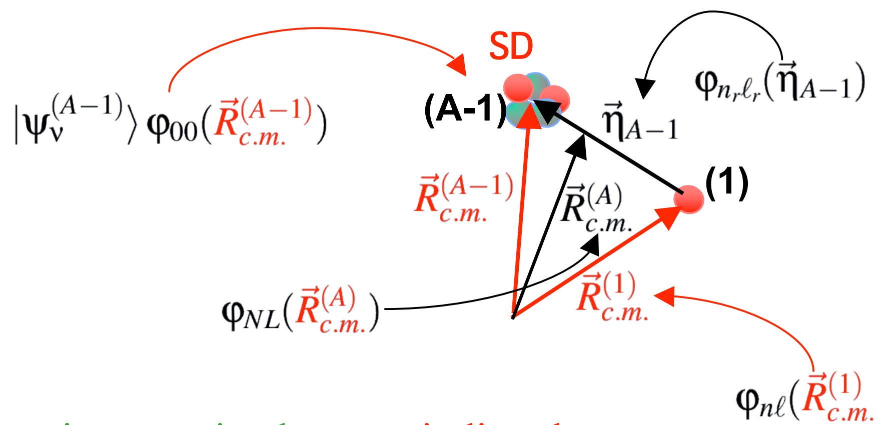
- Jacobi coordinate basis



  ➡ Intrinsic motion only! Translational invariant matrix elements directly

- Slater determinant (SD) basis:

$$\left[\varphi_{00}(\vec{R}^{(A-1)}_{c.m.}) \otimes \varphi_{n\ell}(\vec{R}^{(1)}_{c.m.})\right]^{\ell}$$
$$= \sum_{n_r\ell_r,NL} \langle n_r\ell_r, NL, \ell | 00, n\ell, \ell \rangle_{\frac{1}{A-1}} \times \left[\varphi_{n_r\ell_r}(\vec{\eta}_{A-1}) \otimes \varphi_{NL}(\vec{R}^{(A)}_{c.m.})\right]^{\ell}$$

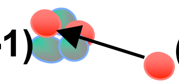


  ➡ Spurious c.m. motion! Translational invariant matrix elements indirectly

$$_{SD}\langle \Phi^{(A-1,1)JT}_{\mu n'\ell'} | P_{A,A-1} | \Phi^{(A-1,1)JT}_{\nu n\ell} \rangle_{SD} = \sum_{n_r\ell_r n'_r\ell'_r J_r} \langle \Phi^{(A-1,1)J_rT}_{\mu n'_r\ell'_r} | P_{(A-1,1)} | \Phi^{(A-1,1)J_rT}_{\nu n_r\ell_r} \rangle$$
$$\times \sum_{NL} \hat{\ell}\hat{\ell}' \hat{J}_r^2 (-1)^{s+\ell_r-s'-\ell'_r} \begin{Bmatrix} s & \ell_r & J_r \\ L & J & \ell \end{Bmatrix} \begin{Bmatrix} s' & \ell'_r & J_r \\ L & J & \ell' \end{Bmatrix} \times \langle n_r\ell_r NLl | 00n\ell\ell \rangle_{\frac{1}{A-1}} \langle n'_r\ell'_r NL\ell' | 00n'\ell'\ell' \rangle_{\frac{1}{A-1}}$$

Procedure generally applicable if projectile (a) is obtained in the Jacobi coordinate basis

Single-nucleon projectile: the norm kernel



$$\mathcal{N}^{(A-1,1)}_{\mu\ell',\nu\ell}(r',r) = \delta_{\mu\nu}\,\delta_{\ell'\ell}\frac{\delta(r'-r)}{r'r} - (A-1)\sum_{n'n} R_{n'\ell'}(r')\langle\Phi^{(A-1,1)JT}_{\mu n'\ell'}|P_{A,A-1}|\Phi^{(A-1,1)JT}_{\nu n\ell}\rangle R_{n\ell}(r)$$

$$\langle\Phi^{(A-1,1)JT}_{\mu n'\ell'}|P_{A,A-1}|\Phi^{(A-1,1)JT}_{\nu n\ell}\rangle$$

$$= \sum_{n'_{A-1}\ell'_{A-1}\mathcal{J}'_{A-1}} \langle A-1\alpha' I'_1 T'_1|[N_{A-2}i_{A-2}J_{A-2}T_{A-2};n'_{A-1}\ell'_{A-1}\mathcal{J}'_{A-1}]\,I'_1T'_1\rangle$$

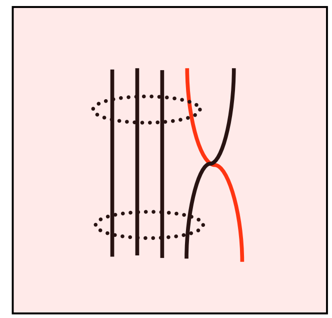
$$\times \sum_{n_{A-1}\ell_{A-1}\mathcal{J}_{A-1}} \langle[N_{A-2}i_{A-2}J_{A-2}T_{A-2};n_{A-1}\ell_{A-1}\mathcal{J}_{A-1}]\,I_1T_1|A-1\alpha I_1T_1\rangle$$

$$\times\, \hat{T}'_1\hat{T}_1(-)^{1+T'_1+T_1}\begin{Bmatrix}\frac{1}{2} & T_{A-2} & T_1\\ \frac{1}{2} & T & T'_1\end{Bmatrix}\hat{s}'\hat{s}\hat{I}'_1\hat{I}_1\hat{\mathcal{J}}'_{A-1}\hat{\mathcal{J}}_{A-1}(-)^{s'+s+\ell+\ell'_{A-1}}$$

$$\times \sum_{L,Z}\hat{L}^2\hat{Z}^2(-)^L\begin{Bmatrix}\mathcal{J}'_{A-1} & J_{A-2} & I'_1\\ \mathcal{J}_{A-1} & Z & I_1\end{Bmatrix}\begin{Bmatrix}\ell'_{A-1} & \frac{1}{2} & \mathcal{J}'_{A-1}\\ I_1 & Z & s\end{Bmatrix}\begin{Bmatrix}\ell_{A-1} & \frac{1}{2} & \mathcal{J}_{A-1}\\ I'_1 & Z & s'\end{Bmatrix}$$

$$\times \begin{Bmatrix}L_2 & \ell'_{A-1} & \ell'\\ \ell_{A-1} & Z & s'\\ \ell & s & J\end{Bmatrix}\langle n'\ell',n'_{A-1}\ell'_{A-1},L|n_{A-1}\ell_{A-1},n\ell,L\rangle_{A(A-2)}$$

Jacobi coordinate derivation

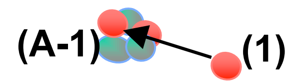


$A > 3$

$\mu = \{\alpha' I'_1 T'_1 s'\}$

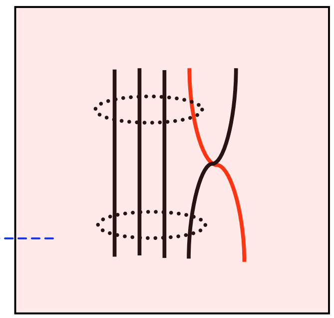
$\nu = \{\alpha I_1 T_1 s\}$

Single-nucleon projectile: the norm kernel



$$\mathcal{N}^{(A-1,1)}_{\mu\ell',\nu\ell}(r',r) = \delta_{\mu\nu}\,\delta_{\ell'\ell}\frac{\delta(r'-r)}{r'r} - (A-1)\sum_{n'n} R_{n'\ell'}(r')\langle\Phi^{(A-1,1)JT}_{\mu n'\ell'}|P_{A,A-1}|\Phi^{(A-1,1)JT}_{\nu n\ell}\rangle R_{n\ell}(r)$$

Single-particle coordinate SD derivation



$${}_{SD}\langle\Phi^{(A-1,1)JT}_{\mu n'\ell'}|P_{A,A-1}|\Phi^{(A-1,1)JT}_{\nu n\ell}\rangle_{SD} = \sum_{n_r\ell_r n'_r\ell'_r J_r}\langle\Phi^{(A-1,1)J_rT}_{\mu n'_r\ell'_r}|P_{(A-1,1)}|\Phi^{(A-1,1)J_rT}_{\nu n_r\ell_r}\rangle$$
$$\times\sum_{NL}\hat{\ell}\hat{\ell}'\hat{J}_r^2(-1)^{s+\ell_r-s'-\ell'_r}\begin{Bmatrix} s\,\ell_r J_r \\ L\,J\,\ell\end{Bmatrix}\begin{Bmatrix} s'\ell'_r J_r \\ L\,J\,\ell'\end{Bmatrix}$$
$$\times\langle n_r\ell_r NLl|00n\ell\ell\rangle_{\frac{1}{A-1}}\langle n'_r\ell'_r NL\ell'|00n'\ell'\ell'\rangle_{\frac{1}{A-1}}$$

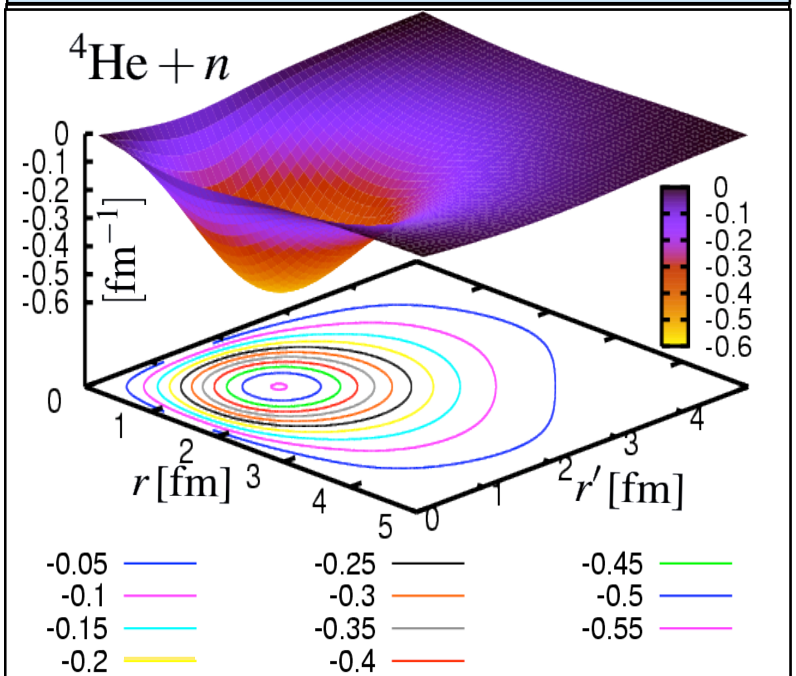
$${}_{SD}\langle\Phi^{(A-1,1)JT}_{\mu n'\ell'}|P_{A,A-1}|\Phi^{(A-1,1)JT}_{\nu n\ell}\rangle_{SD} = \frac{1}{A-1}\sum_{jj'K\tau}\begin{Bmatrix} I_1\frac{1}{2}s \\ \ell\,J\,j\end{Bmatrix}\begin{Bmatrix} I'_1\frac{1}{2}s' \\ \ell' J\,j'\end{Bmatrix}\begin{Bmatrix} I_1 K I'_1 \\ j'\,J\,j\end{Bmatrix}\begin{Bmatrix} T_1\,\tau\,T'_1 \\ \frac{1}{2}\,T\,\frac{1}{2}\end{Bmatrix}$$
$$\times\hat{s}\hat{s}'\hat{j}\hat{j}'\hat{K}\hat{\tau}(-1)^{I'_1+j'+J}(-1)^{T_1+\frac{1}{2}+T}$$
$$\times{}_{SD}\langle A-1\alpha' I'_1 T'_1|||(a^\dagger_{n\ell j\frac{1}{2}}\tilde{a}_{n'\ell' j'\frac{1}{2}})^{(K\tau)}|||A-1\alpha I_1 T_1\rangle_{SD}$$

$$\mu = \{\alpha' I'_1 T'_1 s'\}$$
$$\nu = \{\alpha I_1 T_1 s\}$$

This formalism will allow the application of the NCSM+RGM approach to *p*-shell nuclei

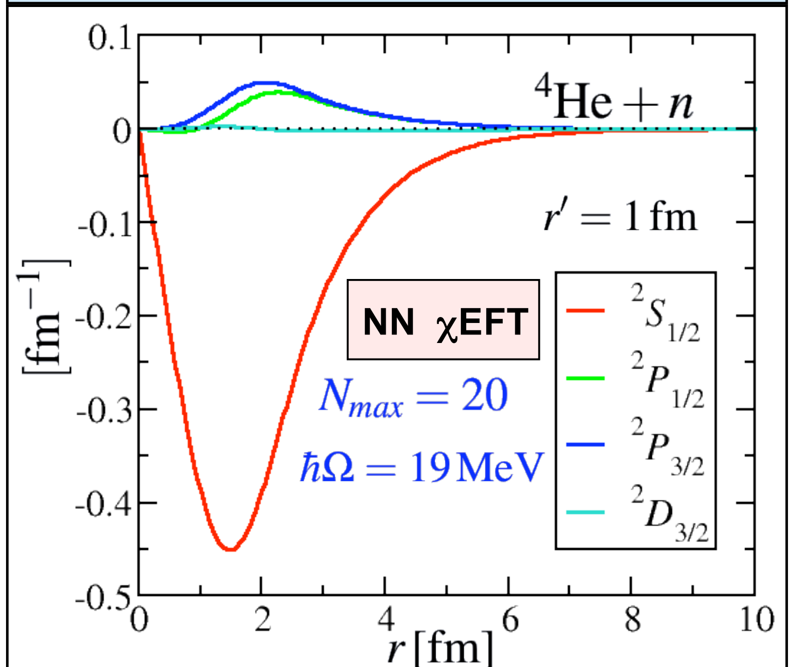
Exchange part of the norm kernel: (^{4}He,n) basis

: the $^2S_{1/2}$ channel



The non-orthogonality is short-ranged

: channels relative contribution



The $^2S_{1/2}$ channel shows large effects of the Pauli exclusion principle

First step towards coherent picture: describe correctly low-energy neutron scattering on ^{4}He. Jacobi and single-particle SD algorithm lead to results in complete agreement for the norm and Hamiltonian kernel.

Single-nucleon projectile: the Hamiltonian kernel

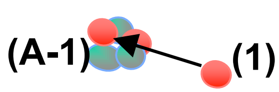
$$\mathcal{H}^{(A-1,1)}_{\mu\ell',\nu\ell}(r',r) = (E_{A-1} + \mathcal{T}_{rel})\,\mathcal{N}^{(A-1,1)}_{\mu\ell',\nu\ell}(r',r)$$

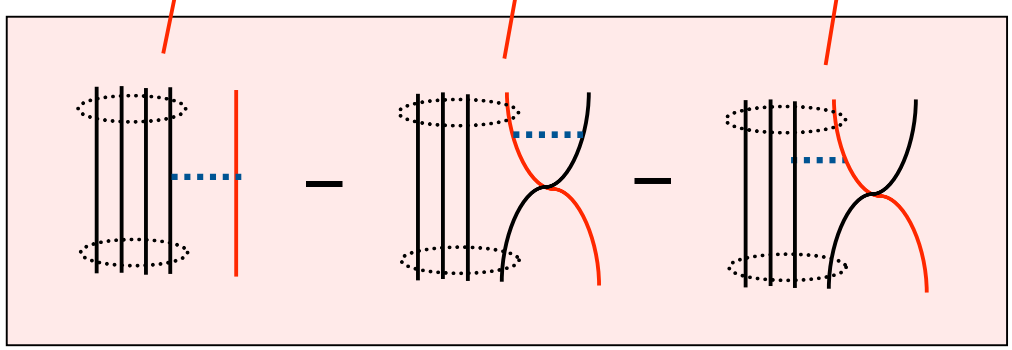
$$+ (A-1)\sum_{n'n} R_{n'\ell'}(r')\left\langle \Phi^{(A-1,1)JT}_{\mu n'\ell'} \right| V_{A-1,A} \left| \Phi^{(A-1,1)JT}_{\nu n\ell} \right\rangle R_{n\ell}(r)$$

$$- (A-1)\sum_{n'n} R_{n'\ell'}(r')\ \langle \Phi^{(A-1,1)JT}_{\mu n'\ell'} | V_{A-1,A} P_{A,A-1} | \Phi^{(A-1,1)JT}_{\nu n\ell} \rangle R_{n\ell}(r)$$

$$- (A-1)(A-2)\sum_{n'n} R_{n'\ell'}(r')\ \langle \Phi^{(A-1,1)JT}_{\mu n'\ell'} | V_{A-2,A} P_{A,A-1} | \Phi^{(A-1,1)JT}_{\nu n\ell} \rangle R_{n\ell}(r)$$

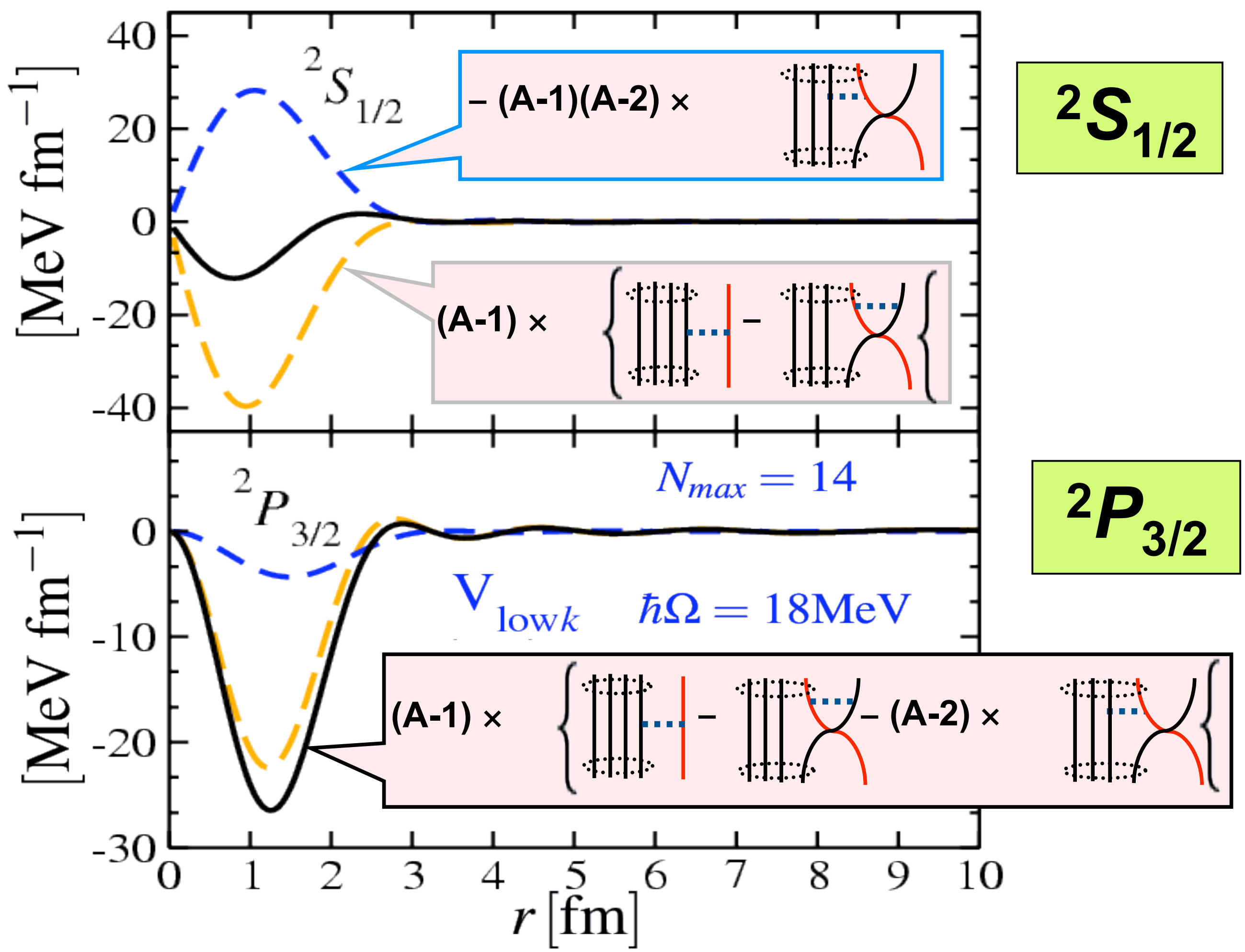
+ terms containing NNN potential





Pauli principle effects in the NN potential kernel: (^{4}He,n) basis

$V(r,r')$
r'=1 fm



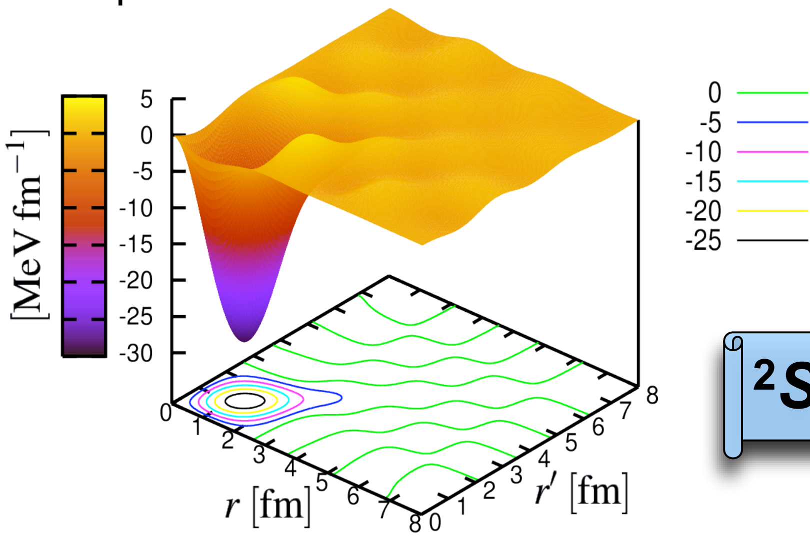
$^2S_{1/2}$

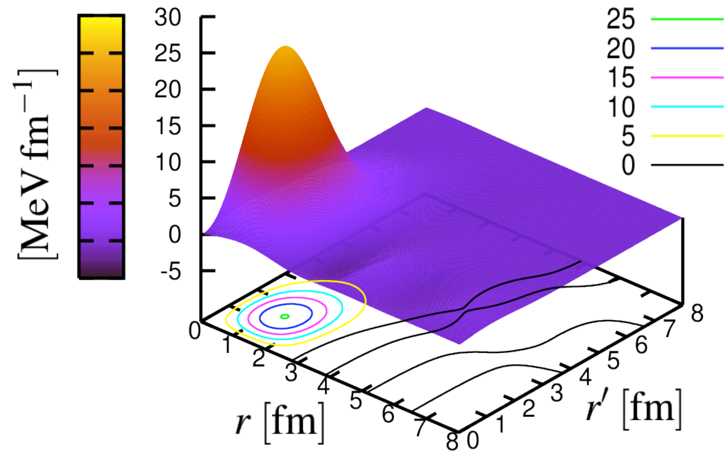
$^2P_{3/2}$

Pauli principle effects in the NN potential kernel: (^{4}He,n) basis

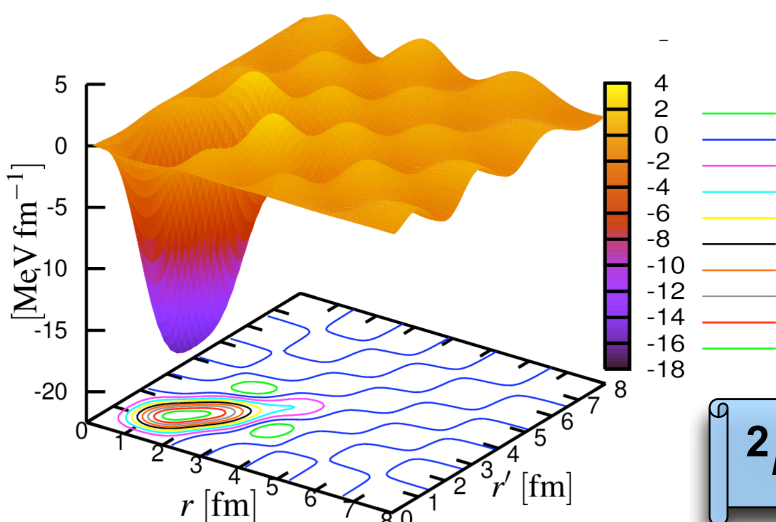
NN potential-direct

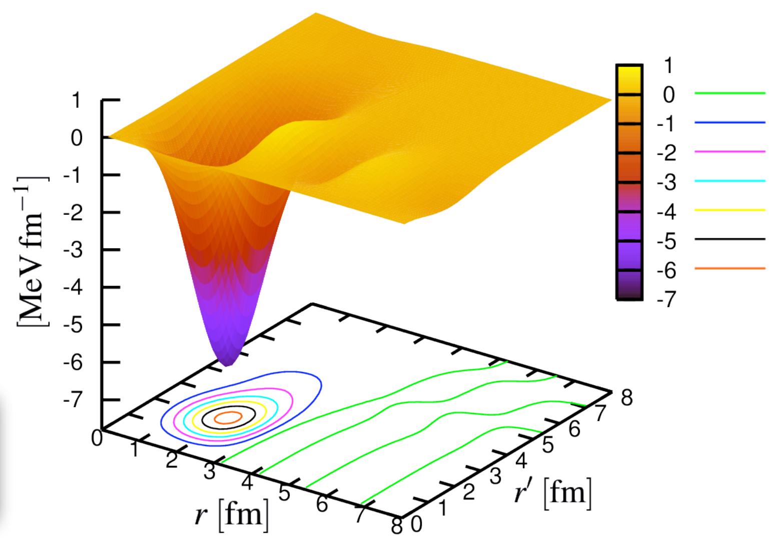
NN potential-exchange





$^2S_{1/2}$

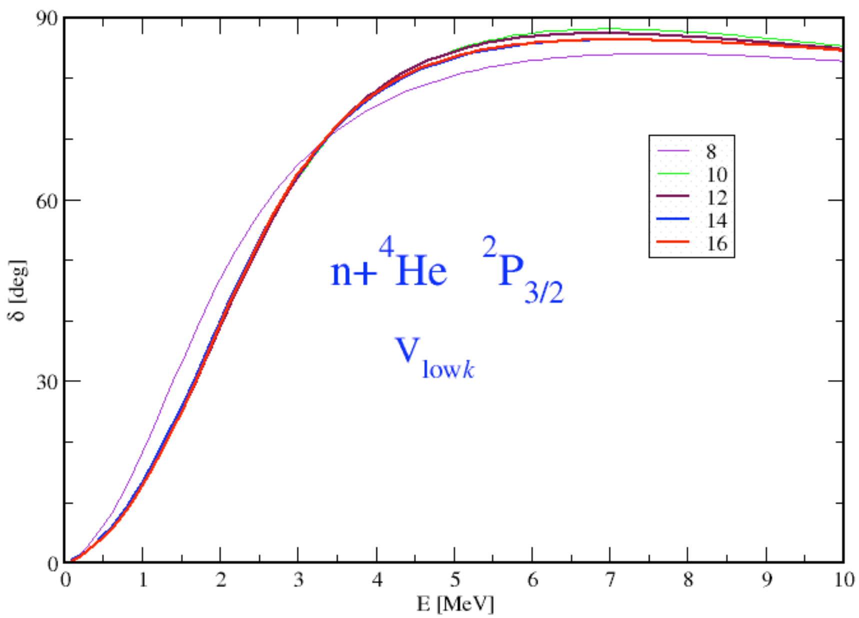


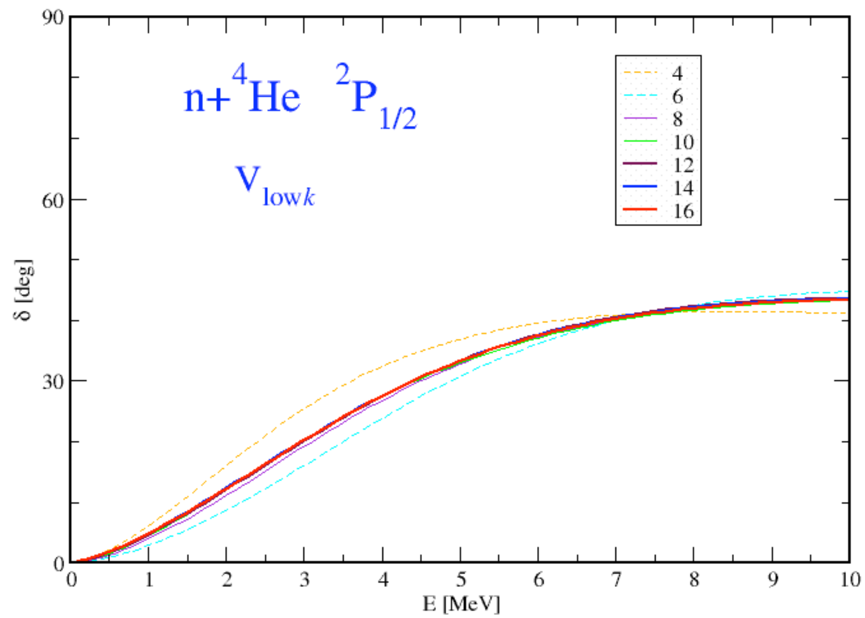


$^2P_{3/2}$

n+^{4}He scattering in an *ab initio* approach

- The first n+^{4}He phase-shift calculations within the *ab initio* NCSM/RGM
  - Convergence tests with the low-momentum $V_{\mathrm{low}k}$ NN potential
    - Calculations up to 16hΩ

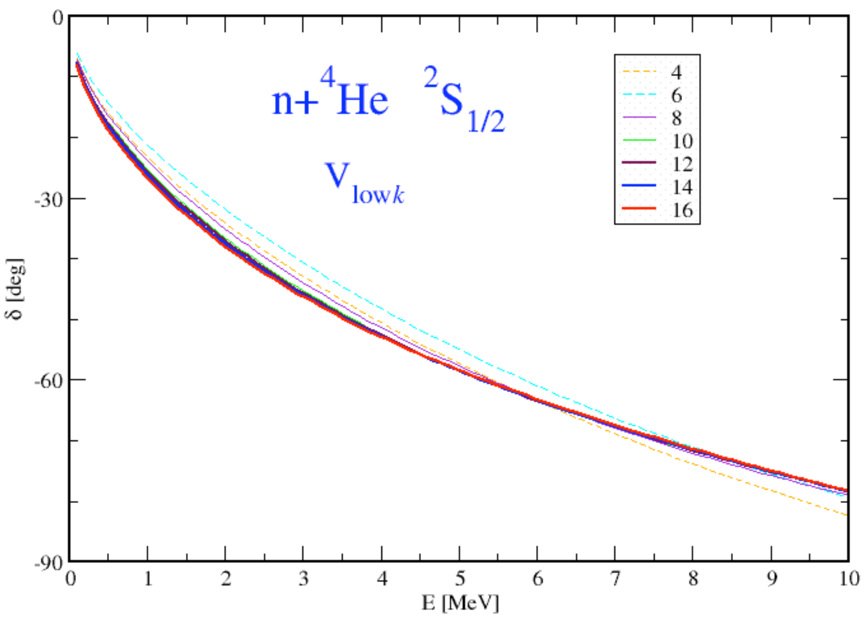


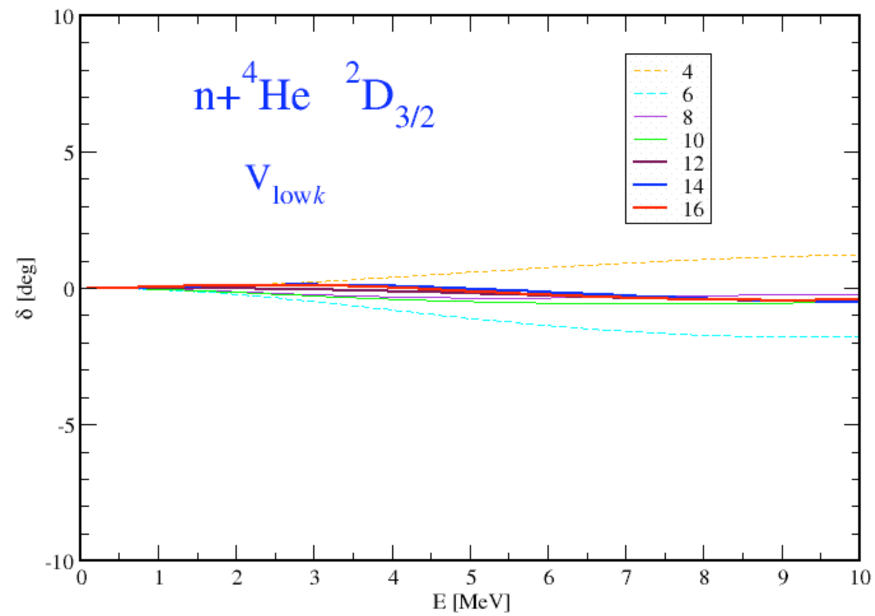


Convergence reached with the $V_{\mathrm{low}k}$ interaction

n+^{4}He scattering in an *ab initio* approach

- The first n+^{4}He phase-shift calculations within the *ab initio* NCSM/RGM
  - Convergence tests with the low-momentum V_{lowk} NN potential
    - Calculations up to 16ħΩ

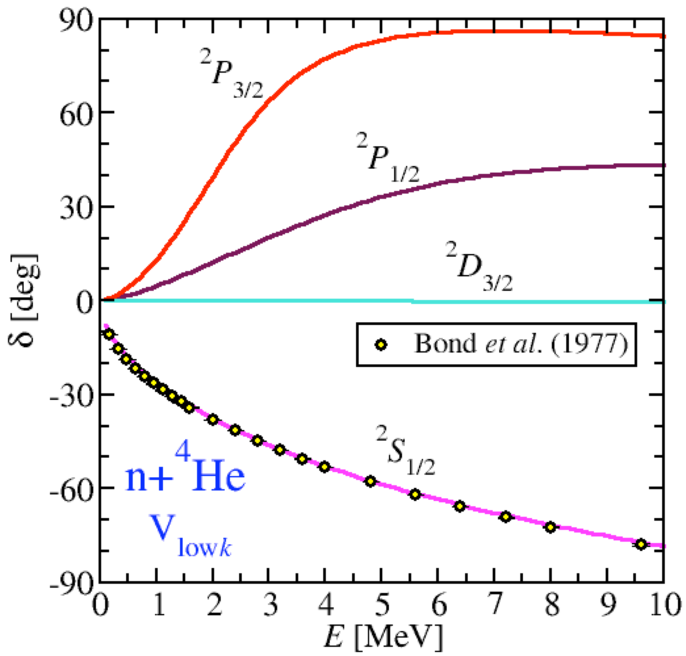


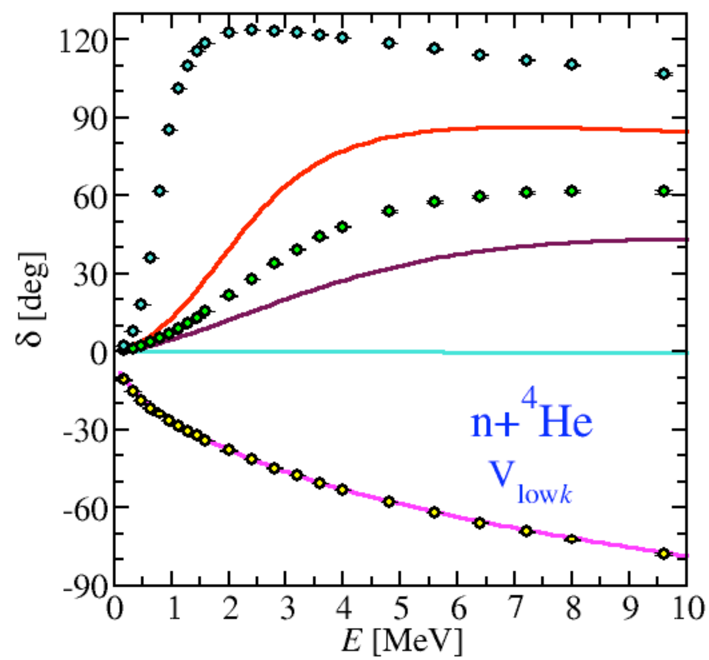


Convergence reached with the V_{lowk} interaction

$n+^4He$ scattering in an *ab initio* approach

- The first $n+^4He$ phase-shift calculations within the *ab initio* NCSM/RGM
  - Low-momentum V_{lowk} NN potential
    - $^2S_{1/2}$ in perfect agreement with experiment
      - Known to be insensitive to the NNN interaction
    - $^2P_{3/2}$ and $^2P_{1/2}$ underestimate the data ⇔ threshold incorrect with the V_{lowk} NN potential
      - Resonances sensitive to NNN interaction

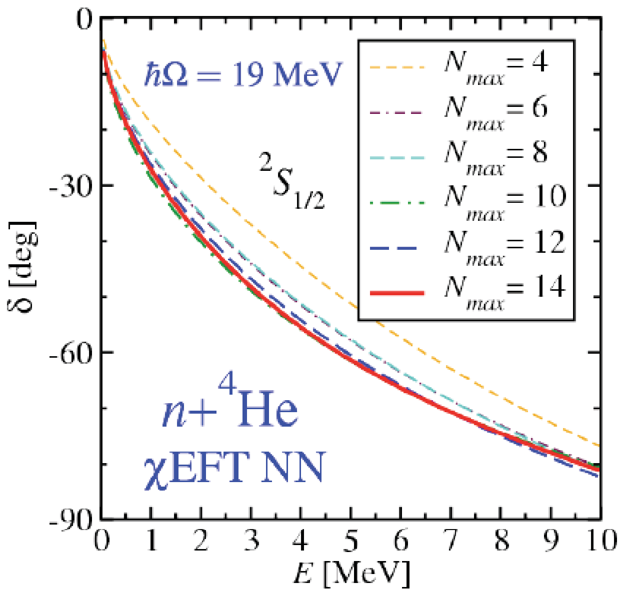


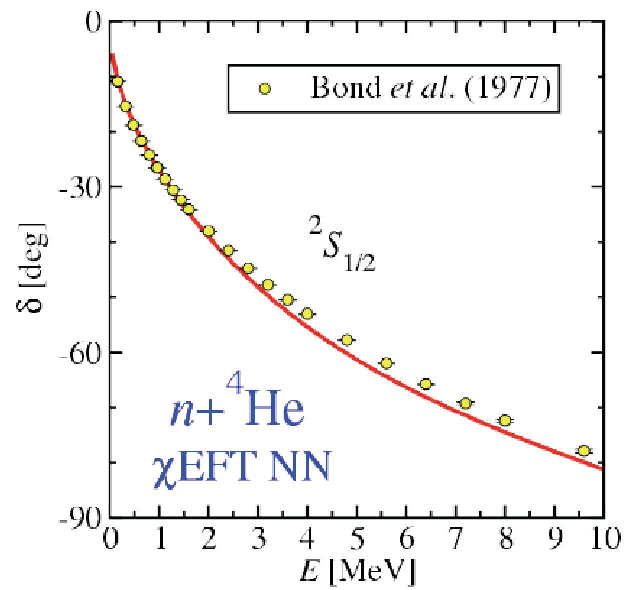


Fully *ab initio*. No fit. No free parameters.
Very promising results…

n+^{4}He scattering in an *ab initio* approach

- The first n+^{4}He phase-shift calculations within the *ab initio* NCSM/RGM
  - Chiral EFT N^{3}LO NN potential
    - Convergence in the $^2S_{1/2}$ channel
      - Model space up to 16hΩ
      - Effective interaction used
      - Open questions on how to apply the effective interaction theory

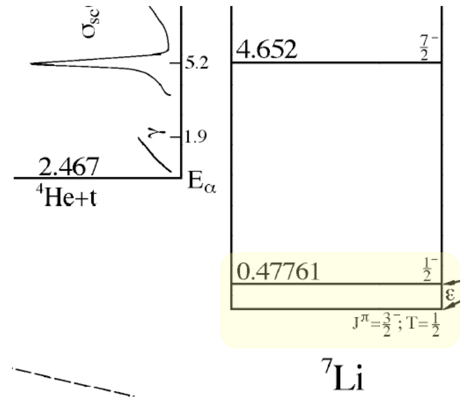


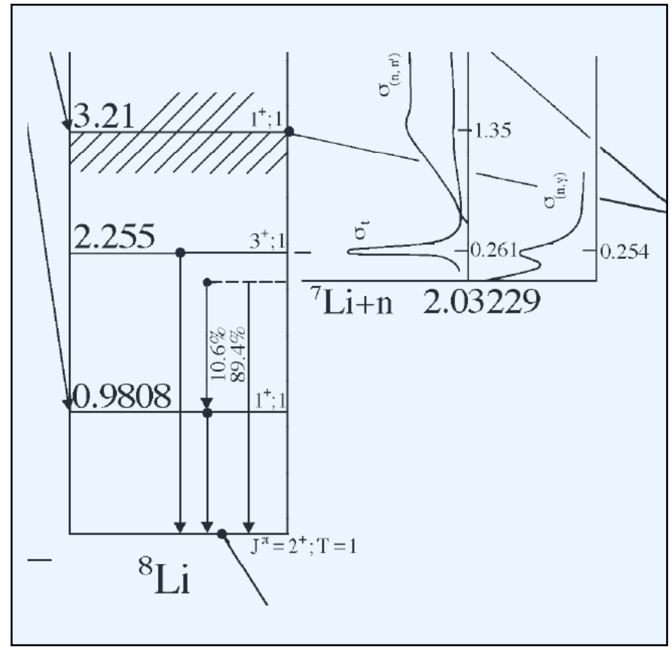


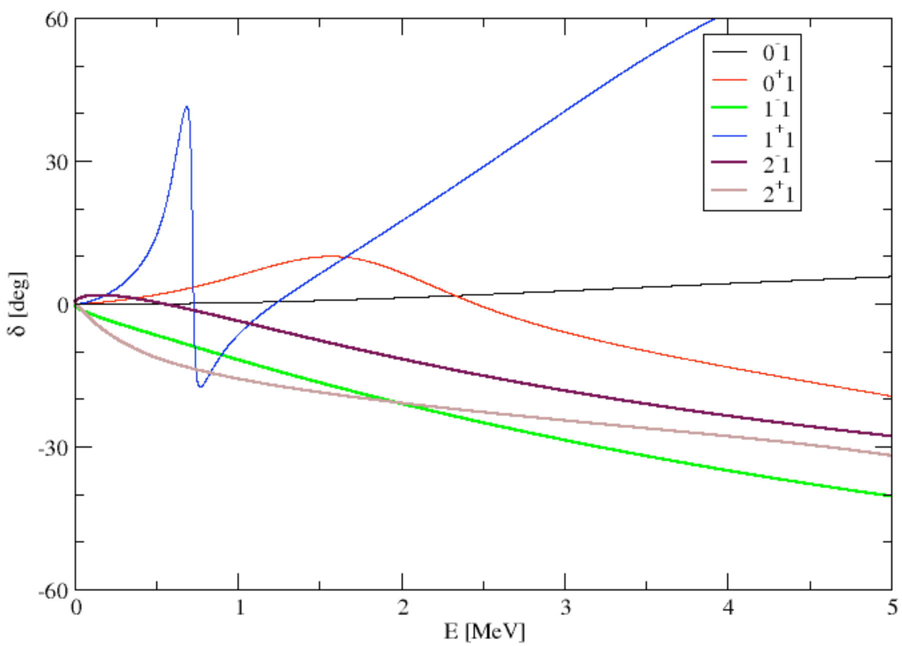
The first scattering calculation with chiral EFT interaction for *A*>4

n+^{7}Li scattering in an *ab initio* approach

- Multiple coupled channels
  - Both closed and open
    - Included ^{7}Li 3/2$^-$ and 1/2$^-$
  - Solved by microscopic R-matrix on a Langrange mesh
- $V_{low\text{-}k}$ interaction
  - Preliminary (last week)
  - 8hΩ
  - 2$^+$ bound state







S-wave scattering length

Expt: a_{01}=0.87(7) fm

a_{02}=-3.63(5) fm

Calc: a_{01}=0.55 fm

a_{02}=-0.59 fm

Outlook: Extension to heavier nuclei

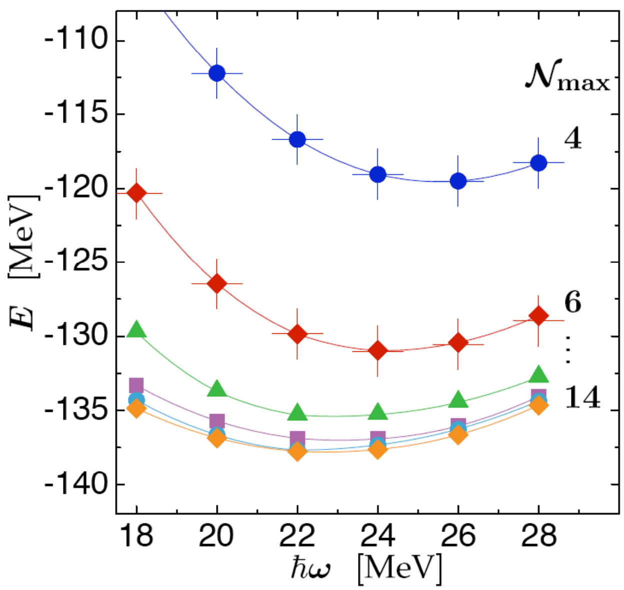
- Importance-truncated NCSM (with R. Roth, TU Darmstadt)
  - Based on many-body perturbation theory
  - Dimension reduction from billions to ~10 million

$$\kappa_\nu = -\frac{\langle \Phi_\nu | H' | \Psi_{\rm ref} \rangle}{E_\nu^{(0)} - E_{\rm ref}^{(0)}}$$

$$|\kappa_\nu| \geq \kappa_{\min}$$

$V_{\text{low-}k}$ (AV18, $\Lambda = 2.1\ \text{fm}^{-1}$)

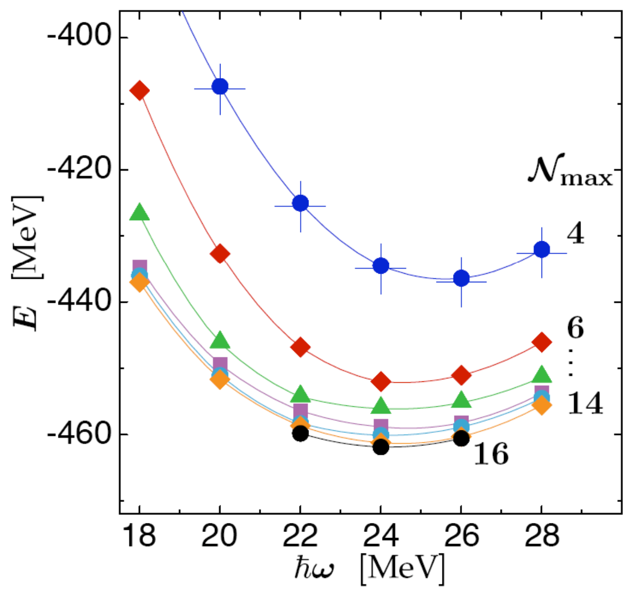
^{16}O (up to 4p4h)



E_∞(4p4h) ≈ -138 MeV

$R_{\rm rms}$(4p4h) $= 2.03$ fm

^{40}Ca (up to 3p3h)



E_∞(3p3h) ≈ -463 MeV

$R_{\rm rms}$(3p3h) $= 2.27$ fm

Convergence feasible for A=40 system: ^{40}Ca with $V_{\text{low-}k}$ up to 4p4h E=-471 MeV

New tool for *ab initio* calculations beyond *p*-shell

Outlook

- *p*-shell and light *sd*-shell calculations with χEFT NN+NNN interactions
  - Include χEFT N^3LO NNN terms
- *Ab initio* NCSM with continuum (NCSMC)
  - Augmenting the *ab initio* NCSM by the RGM technique to include clustering and resonant plus non-resonant continuum (with Sofia Quaglioni)
    - Description of cluster states
    - Low-energy nuclear reactions important for astrophysics
- Extension to heavier nuclei: Importance truncated NCSM (with Robert Roth)
  - ^{40}Ca