Lawrence Livermore National Laboratory

From EFT interactions to a unified *ab initio* description of light nuclei

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INT Program on Effective Field Theory and the Many-body Problem, 4/8/2009

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Outline

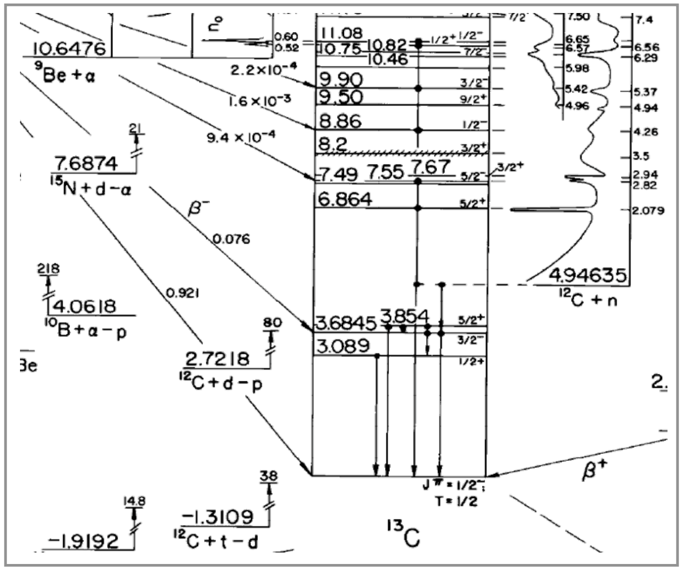
- Motivation
- Chiral NNN interactions and NCSM
- Determination of chiral NNN LECs c_D and c_E
  - A=3 binding energy
  - A=4 binding energy and radius
  - ^{10}B states
  - Triton half life
- p-shell results with chiral NN+NNN
- Scattering and coupling to continuum: Combining NCSM and RGM
  - n-^{4}He
  - p-^{12}C
  - n-^{16}O
- Outlook

Low-Energy nuclear physics

- Overarching goal:

To arrive at a comprehensive and unified microscopic description of all nuclei and their low-energy reactions from the basic interactions between the constituent protons and neutrons

- This is an ambitious goal
  - Nuclei are self-bound, quantum many-fermion system
  - Complicated interaction with at least two- and three-nucleon components
    - Bound states, resonances, scattering states



Our goal is to arrive at an *ab initio* picture for light nuclei and their reactions

Bound-state techniques not sufficient

Where do we start?

- Quantum chromodynamics (QCD) is the underlying theory for the strong interaction
  - Lattice QCD calculations are too difficult to do complex nuclei
    - They are not yet capable of providing an accurate nucleon-nucleon or three-nucleon interaction
      - But they can verify that QCD is the correct theory for the strong interaction between hadrons

- We need a theory with point-like nucleons and an interaction based on QCD
  - Effective field theory (EFT) based on the properties of QCD provides an elegant solution with broad predictive power

Effective Field Theory

- Based on the symmetries of QCD
  - Degrees of freedom: nucleons + pions
  - Describes pion-pion, pion-nucleon and inter-nucleon interactions at low energies
- Systematic low-momentum expansion to a given order

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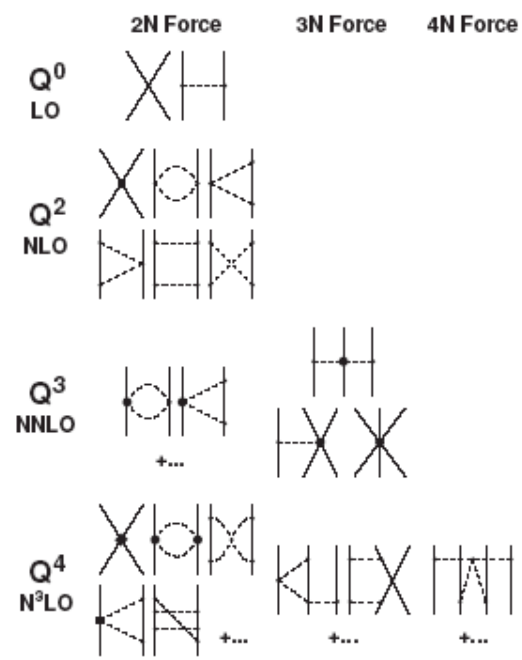

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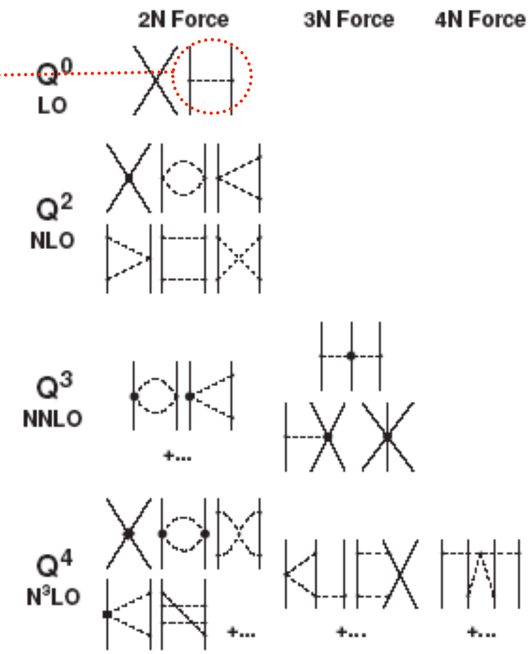
  - One-pion exchange



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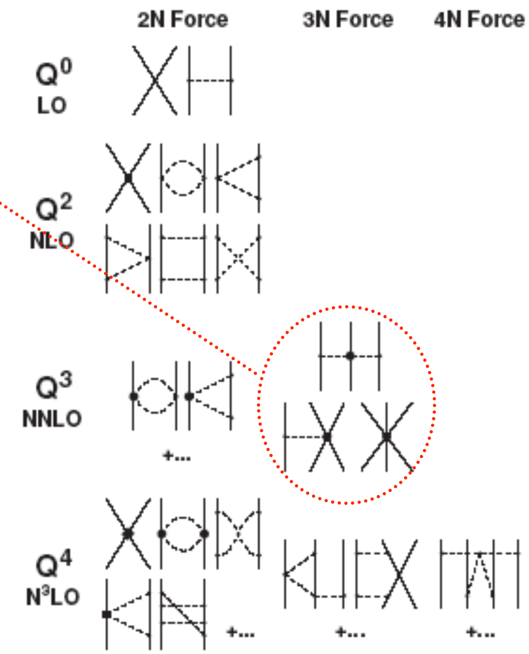

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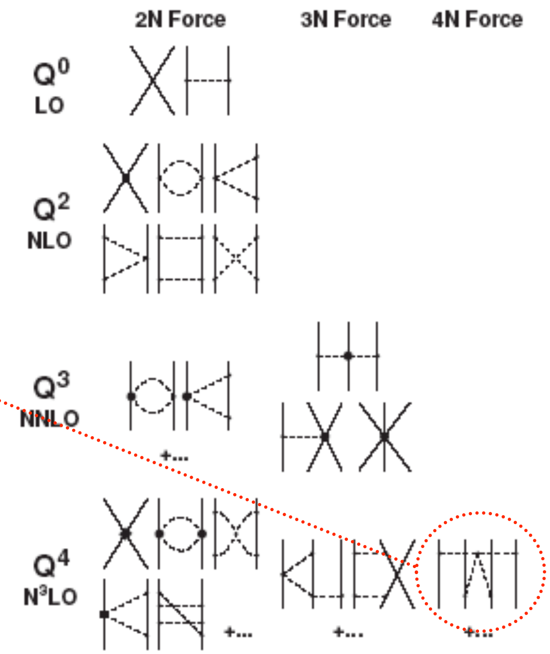

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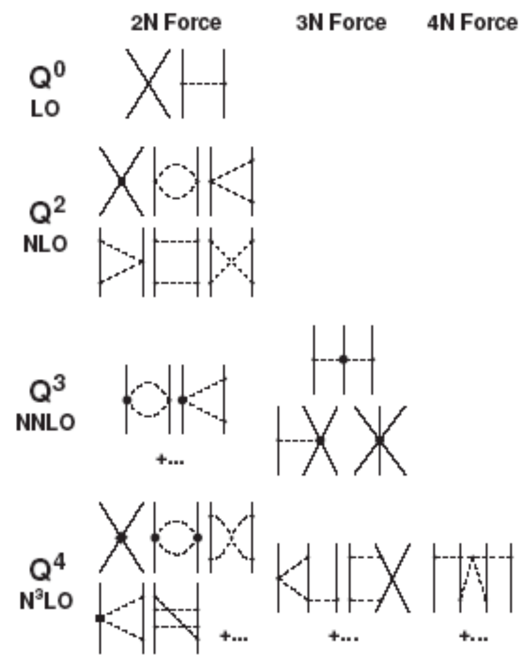
  - NN parameters enter in the NNN terms etc.



Effective Field Theory

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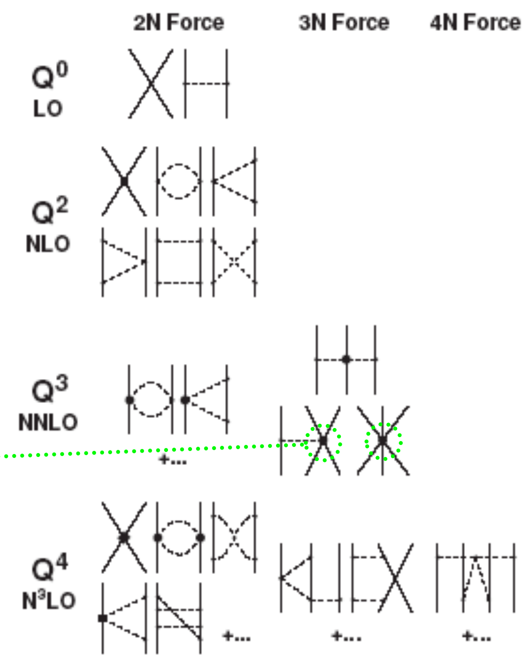
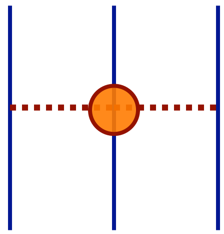
  - NN parameters enter in the NNN terms etc.
- Low-energy constants (LECs)
  - Low-energy theory, integrates out short-range physics
  - Only <u>two</u> NNN and <u>none</u> NNNN low-energy constants up to N^3LO



The NNN interaction

N²LO

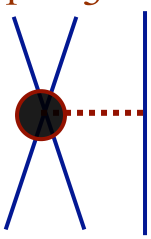


c_1, c_3, c_4

Two-pion exchange

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

- Determined in the A=2 system

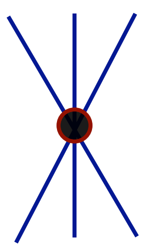


c_D

New!

One-pion-exchange-contact

New c_D LEC



c_E

New!

Contact

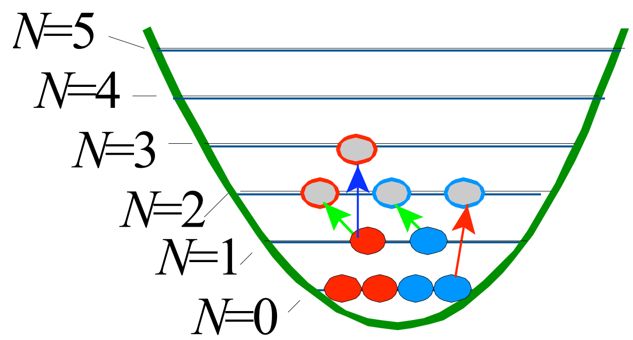
New c_E LEC

Must be determined in $A \geq 3$ system

Nontrivial to include in many-body calculations

The *ab initio* NCSM in brief

- The NCSM is a technique for the solution of the *A*-nucleon bound-state problem
- Hamiltonian (in this talk)
  - Standard high-precision nucleon-nucleon potentials:
    - Idaho chiral N^3LO with 500 MeV cutoff
  - Soft low-momentum interactions
    - SRG-N^3LO
  - Three-nucleon interactions:
    - Local chiral N^2LO



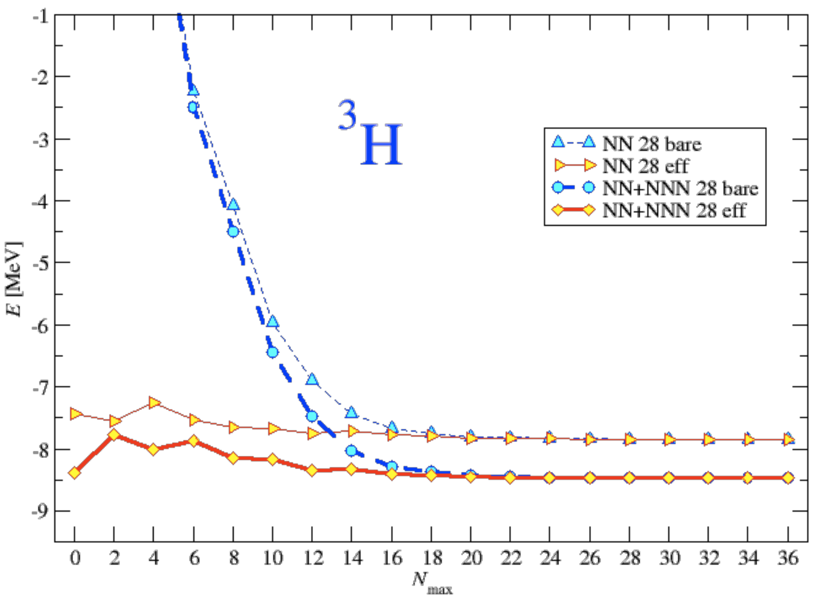
- Finite harmonic oscillator (HO) basis
  - *A*-nucleon HO basis states
    - Jacobi relative coordinates
    - Cartesian single-particle coordinates
  - complete $N_{max}\hbar\Omega$ model space
    - Translational invariance preserved even with single-particle coordinate Slater-determinant (SD) basis
- Effective interaction tailored to model-space truncation for standard potentials
  - Unitary transformation in *n*-body cluster approximation (*n*=2,3)
- Importance-truncated $N_{max}\hbar\Omega$ basis
  - Second-order many-body perturbation theory
  - Dimension reduction from billions to tens of millions
  - Access to nuclei beyond *p*-shell

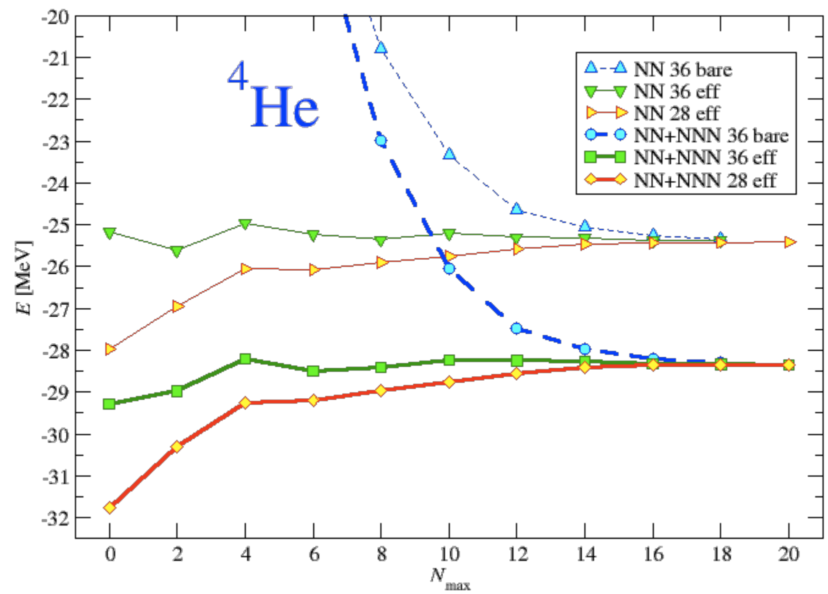
$$\kappa_\nu = -\frac{\langle \Phi_\nu | \mathrm{H}' | \Psi_{\mathrm{ref}} \rangle}{E_\nu^{(0)} - E_{\mathrm{ref}}^{(0)}}$$

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

Convergence to exact solution with increasing N_{max} for bound states.
No coupling to continuum.

^{3}H and ^{4}He with chiral interactions



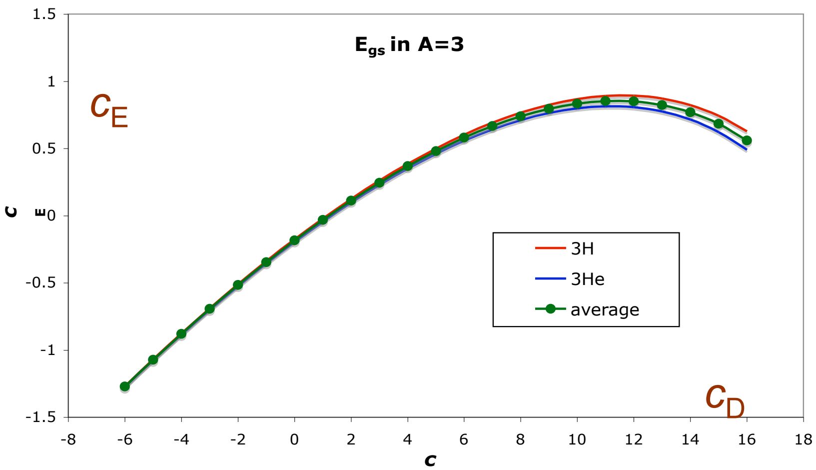


		^{3}H $E_{g.s.}$	^{3}H $\langle r_p^2 \rangle^{1/2}$
NN	NCSM [71]	−7.852(5)	1.650(5)
NN	HH [17]	−7.854	1.655
NN+NNN	NCSM [71]	−8.473(5)	1.608(5)
NN+NNN	HH [17]	−8.474	1.611
Expt.		−8.482	1.60

		^{4}He $E_{g.s.}$	^{4}He $\langle r_p^2 \rangle^{1/2}$
NN	NCSM [71]	−25.39(1)	1.515(2)
NN	HH [17]	−25.38	1.518
NN+NNN	NCSM [71]	−28.34(2)	1.475(2)
NN+NNN	HH [17]	−28.36	1.476
Expt.		−28.296	1.467(13)

Determining the three-nucleon interaction: *A*=3 & ^{4}He

- Constrain c_D, c_E to A=3 binding energy



c_D - c_E dependence that fits *A*=3 binding energy

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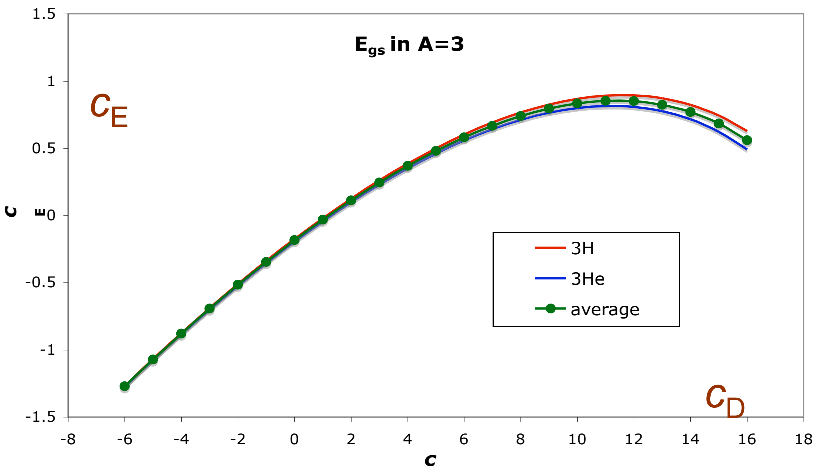
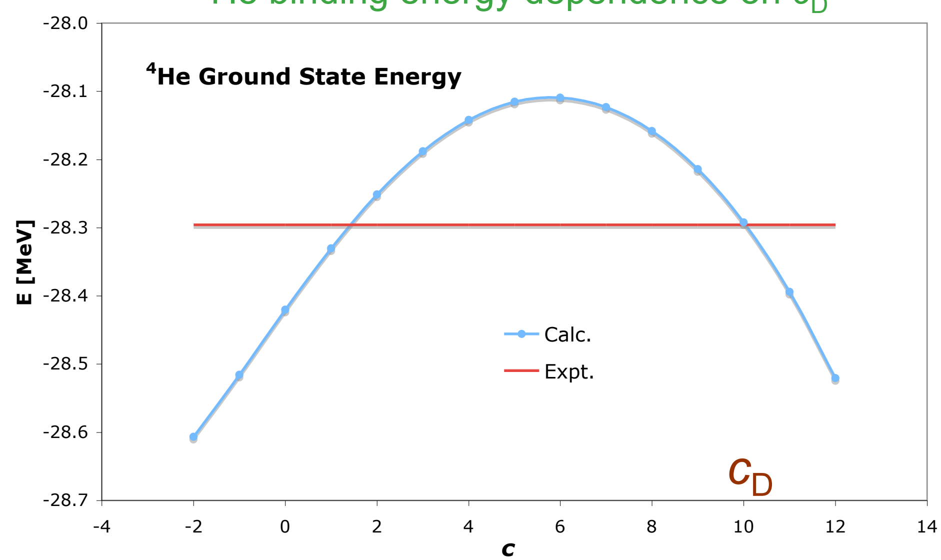


c_D - c_E dependence that fits A=3 binding energy

- Other observables are needed:
  - N-d doublet scattering length
    - Correlated with E_{gs}
- ^{4}He binding energy
- Two combinations of c_D - c_E that fit both A=3 and ^{4}He binding energies
  - ^{4}He E_{gs} dependence on c_D weak
    - ^{4}He and A=3 binding energies correlated

^{4}He binding energy dependence on c_D



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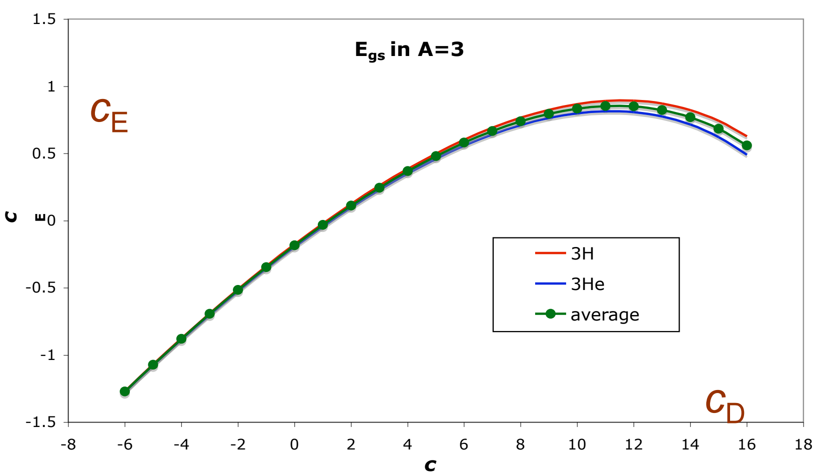

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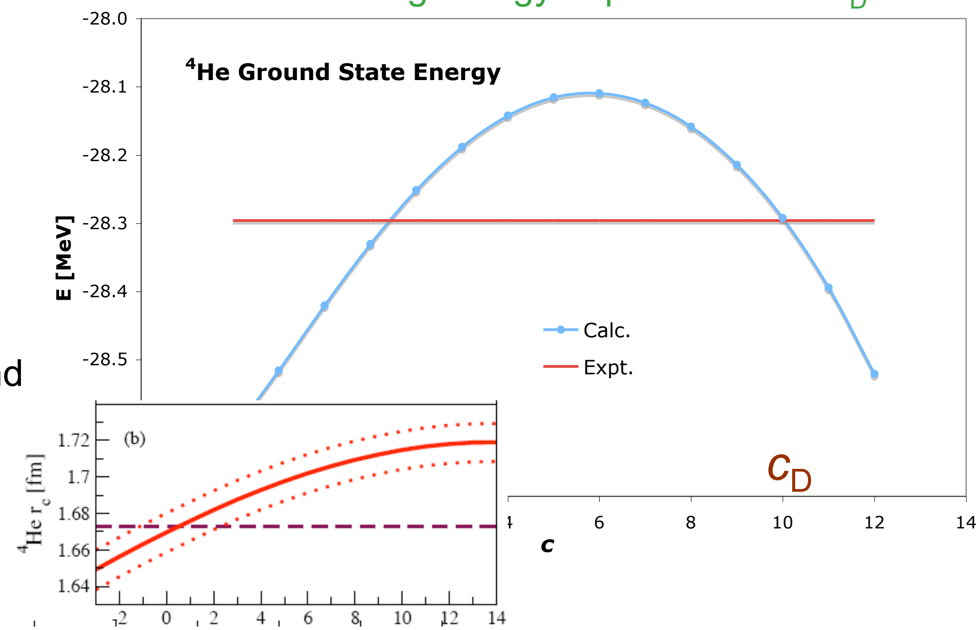

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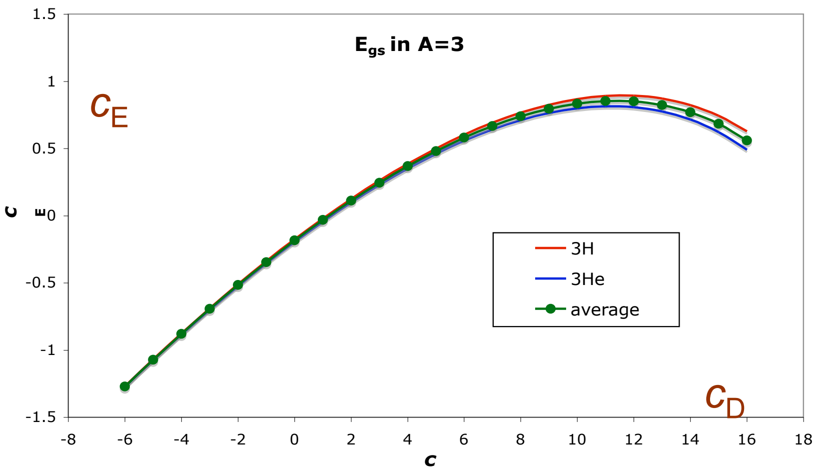

c_D - c_E dependence that fits A=3 binding energy

-2 < c_D < 2
preferred

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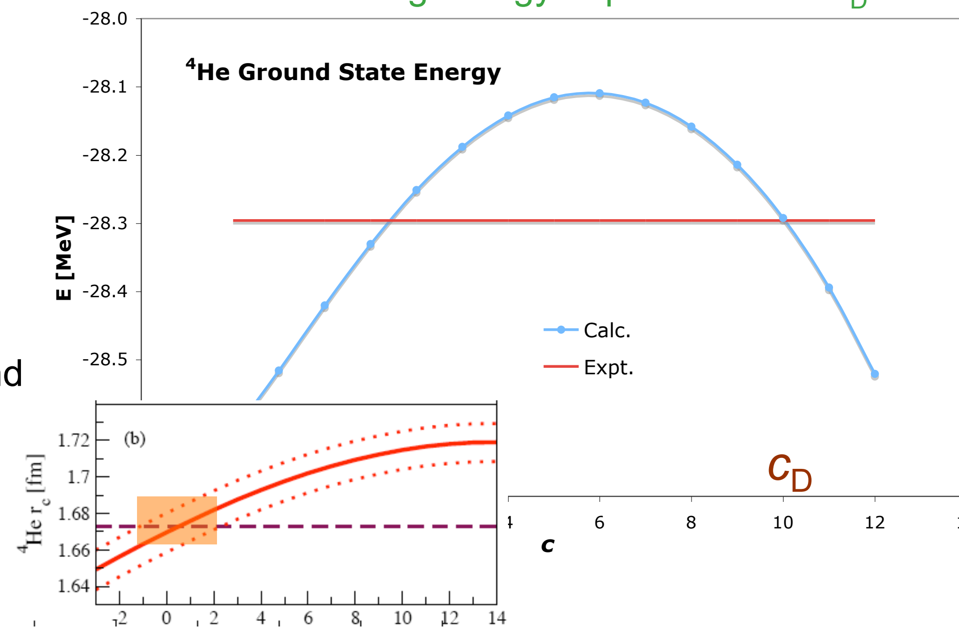

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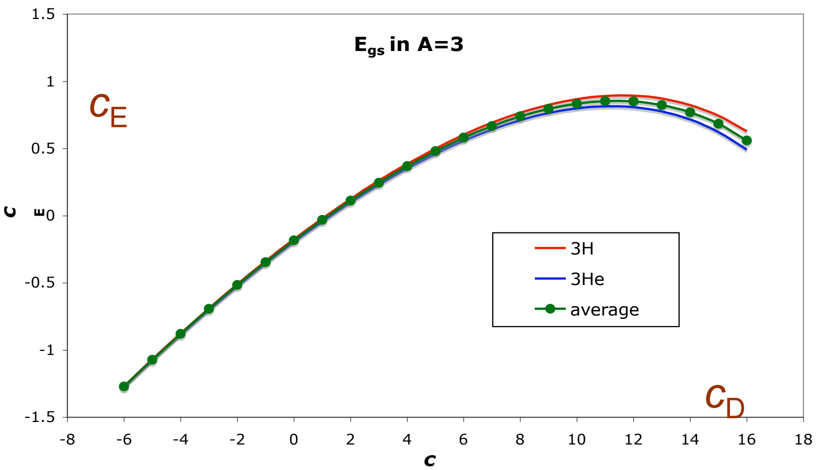

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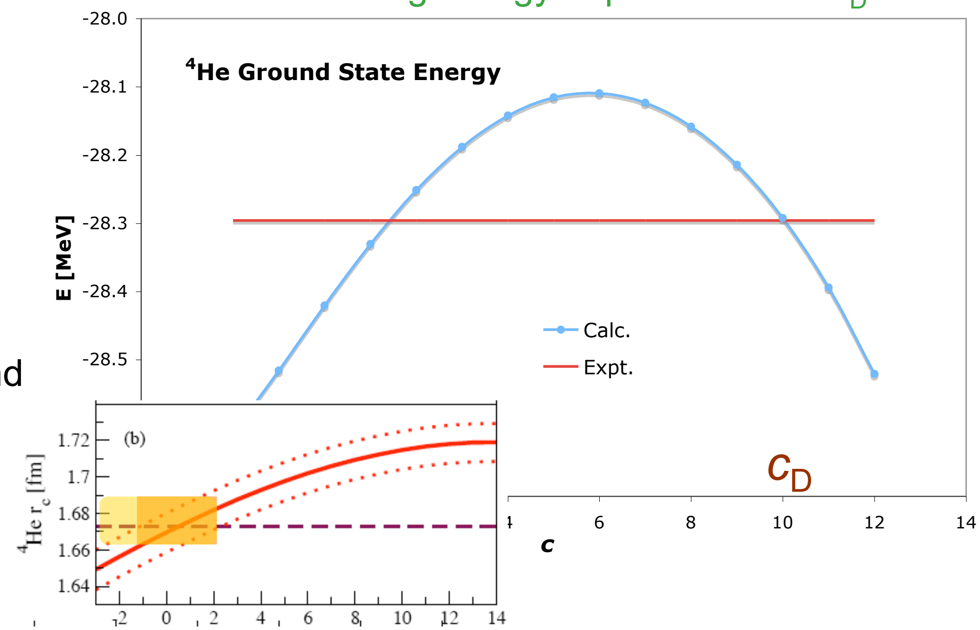
^{4}He binding energy dependence on c_D



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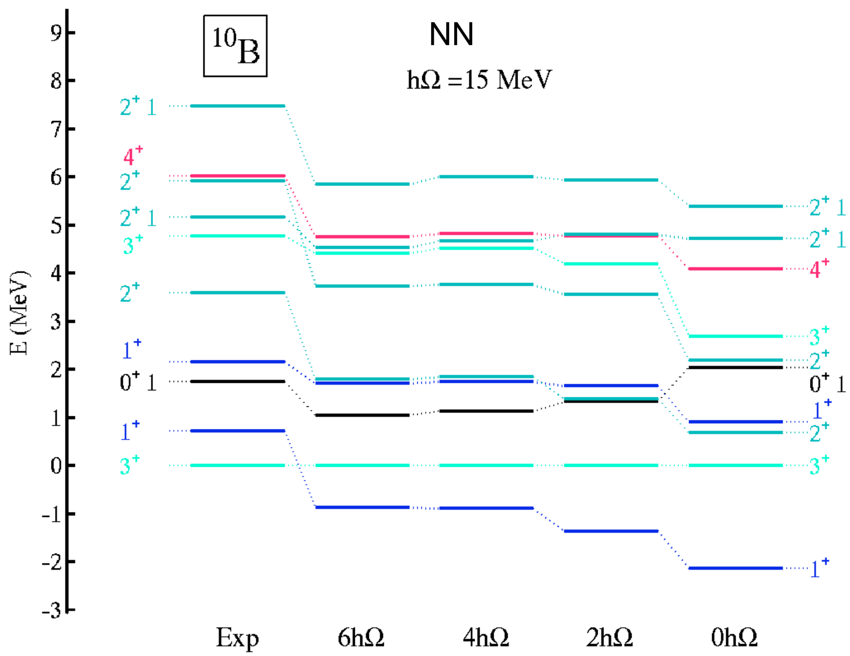
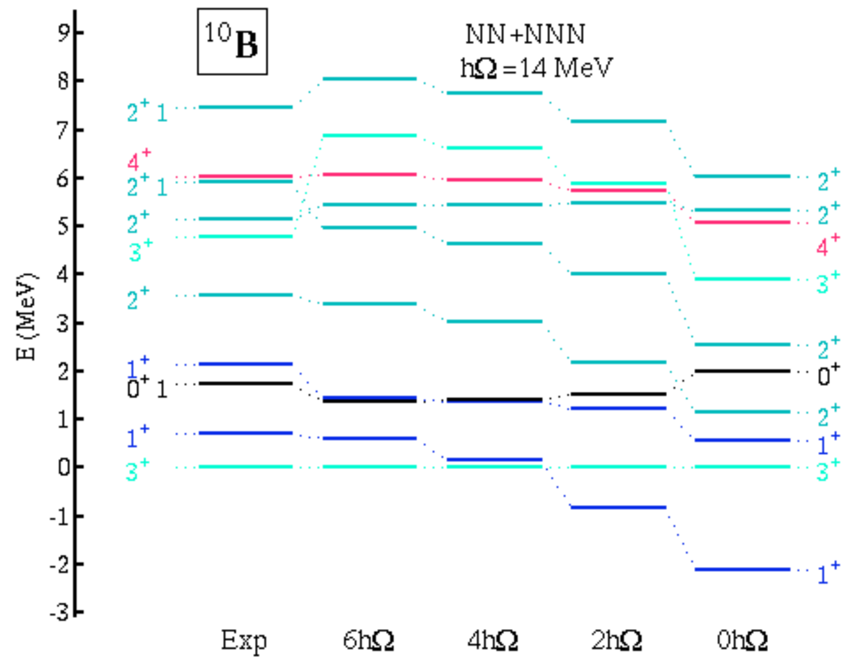
What about the structure of p-shell nuclei?

NNN is 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





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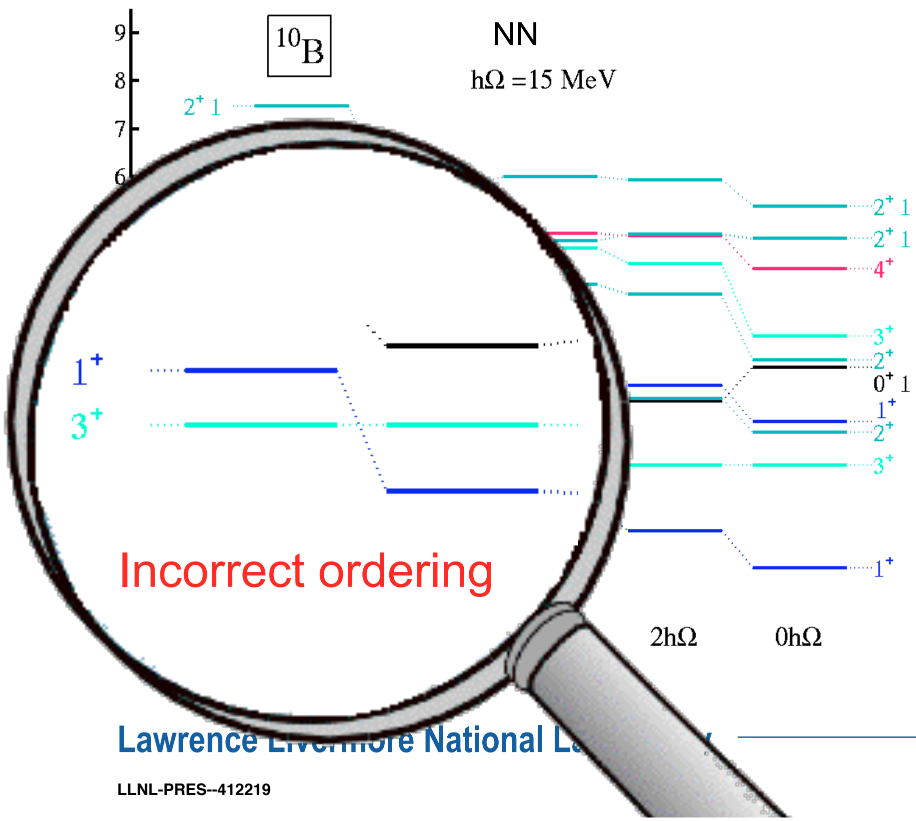

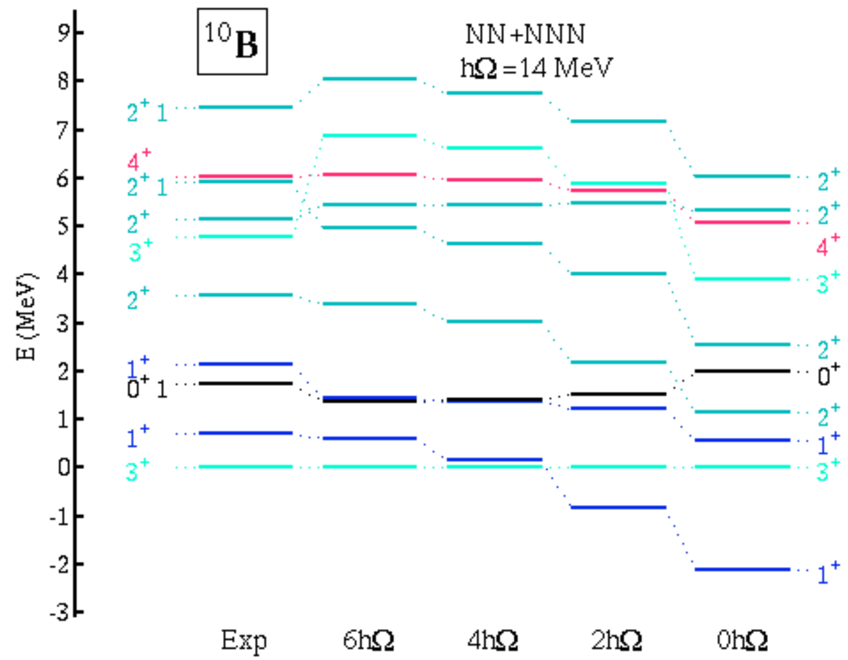

NNN important for heavier *p*-shell nuclei: ^{10}B

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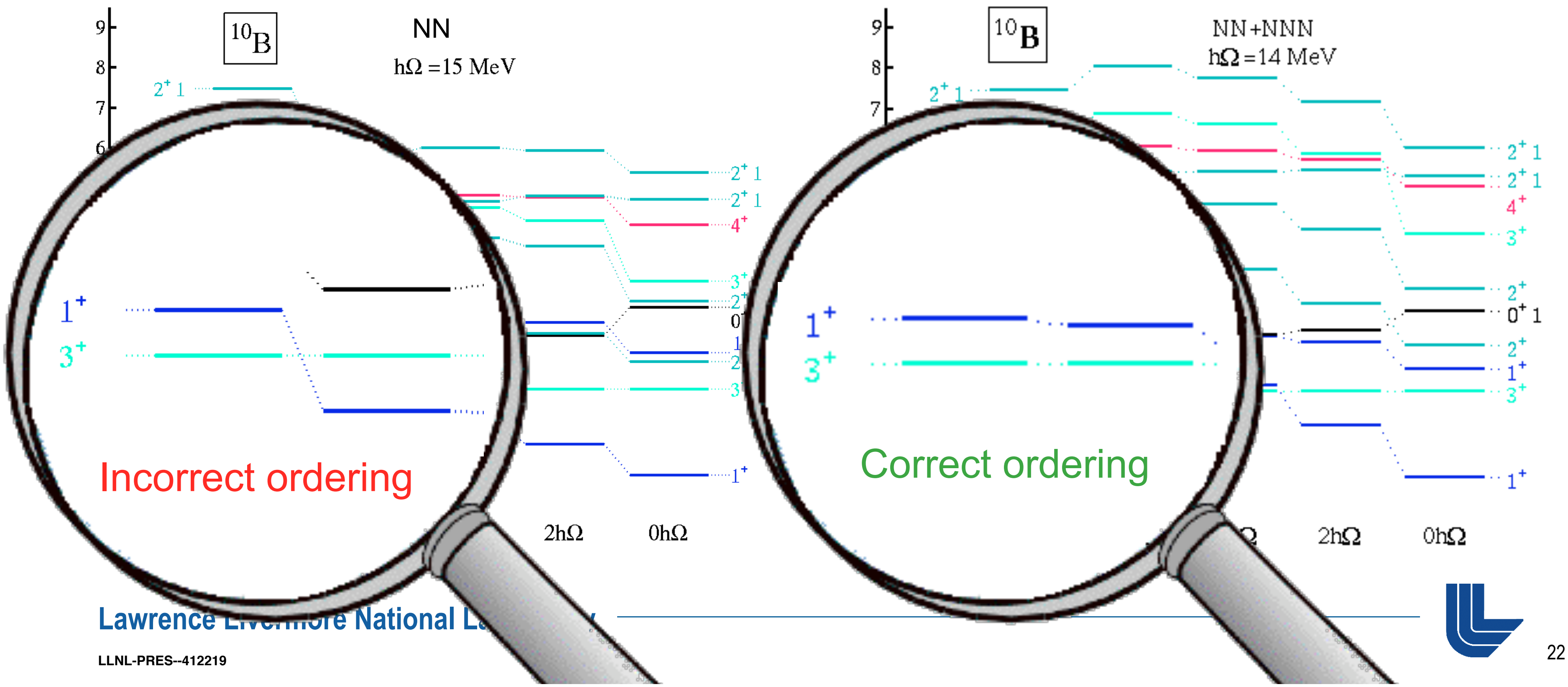
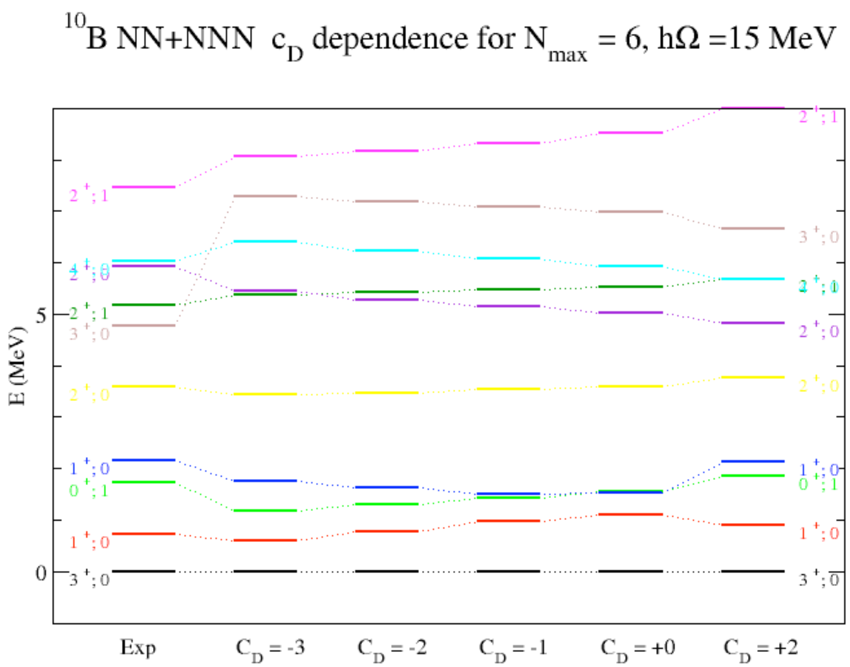
- Chiral NNN fixes this problem



Using the 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



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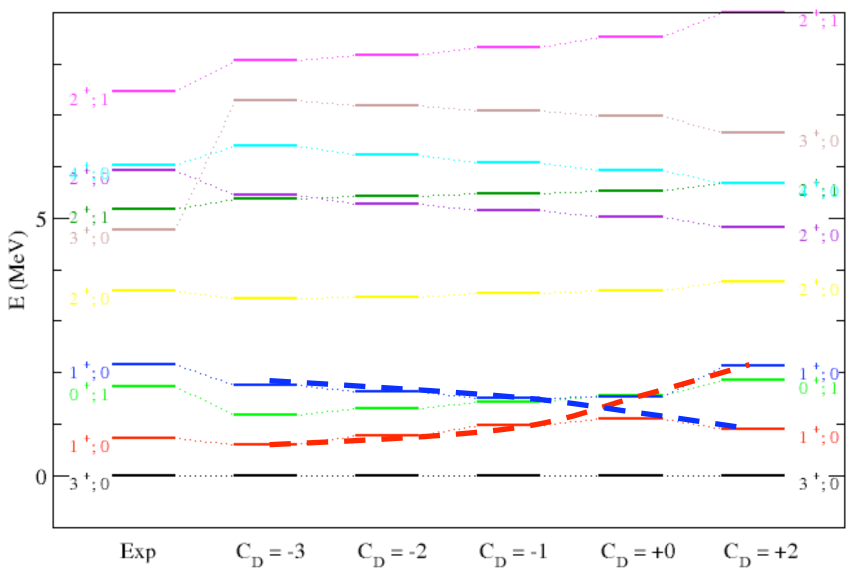
^{10}B NN+NNN c_D dependence for N_{max} = 6, hΩ =15 MeV



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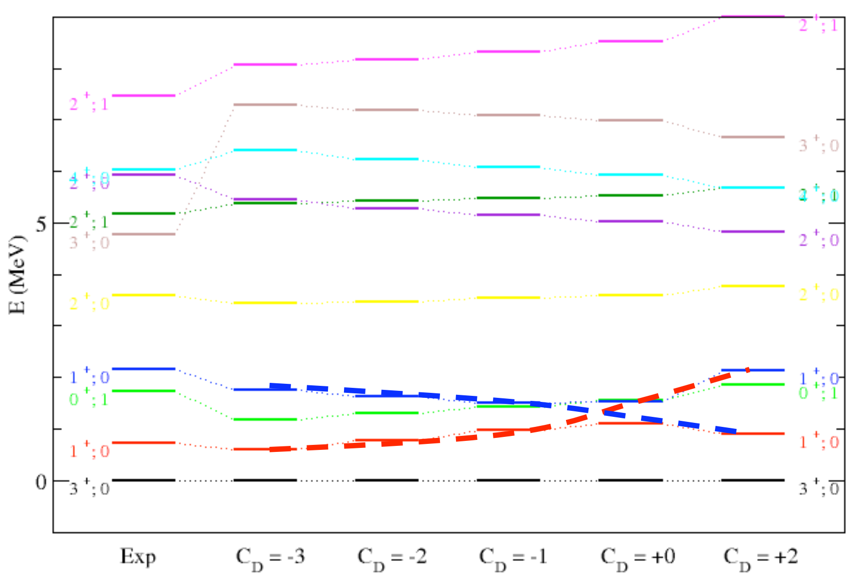

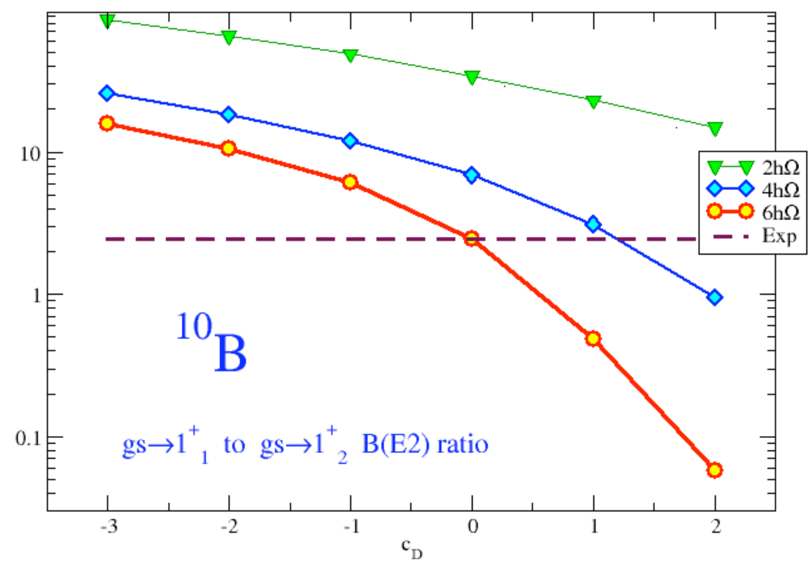

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-2 < c_D < 0 preferred

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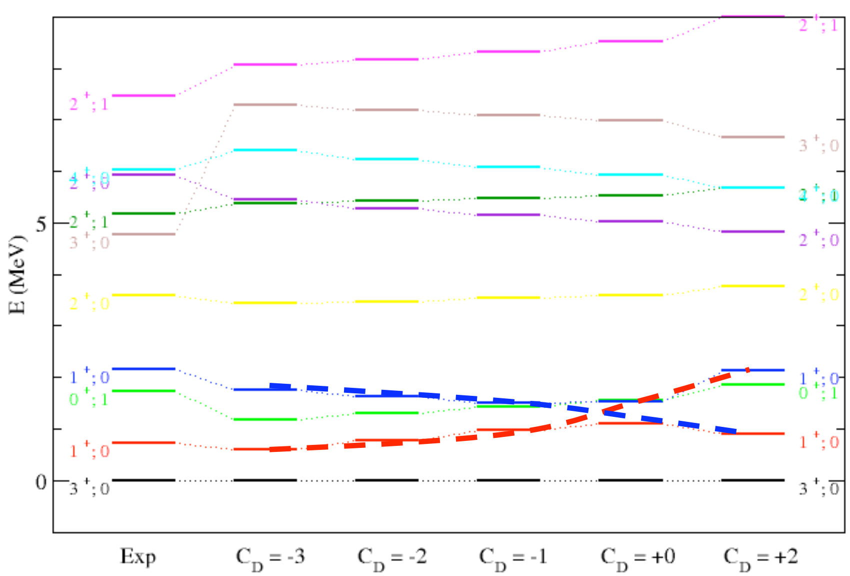
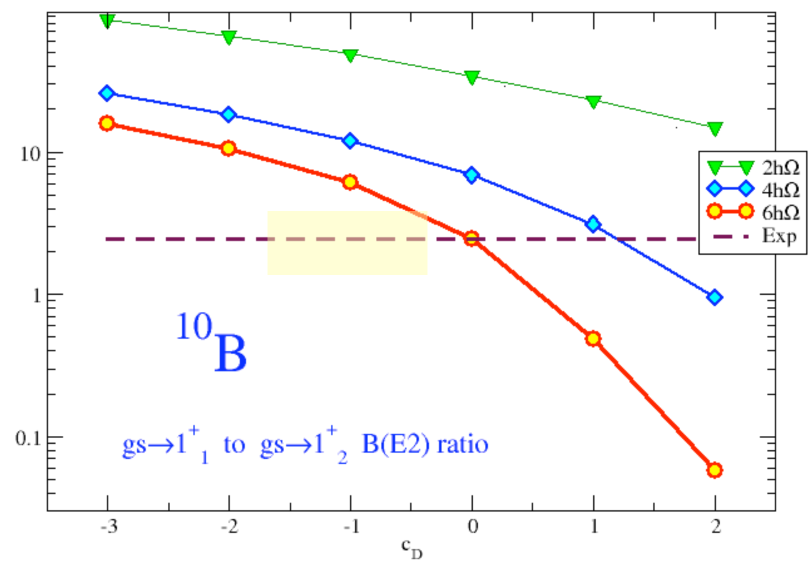




Determination of c_D (and c_E) from the triton half life

- c_D also in the two-nucleon contact vertex with an external probe
- Calculate

$$\langle E_1^A \rangle = |\langle {}^3\mathrm{He}||E_1^A||{}^3\mathrm{H}\rangle|$$

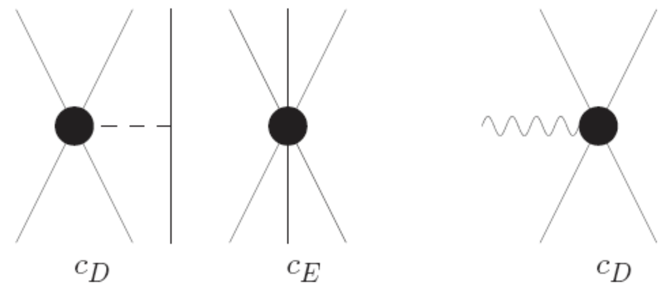
- Leading order GT

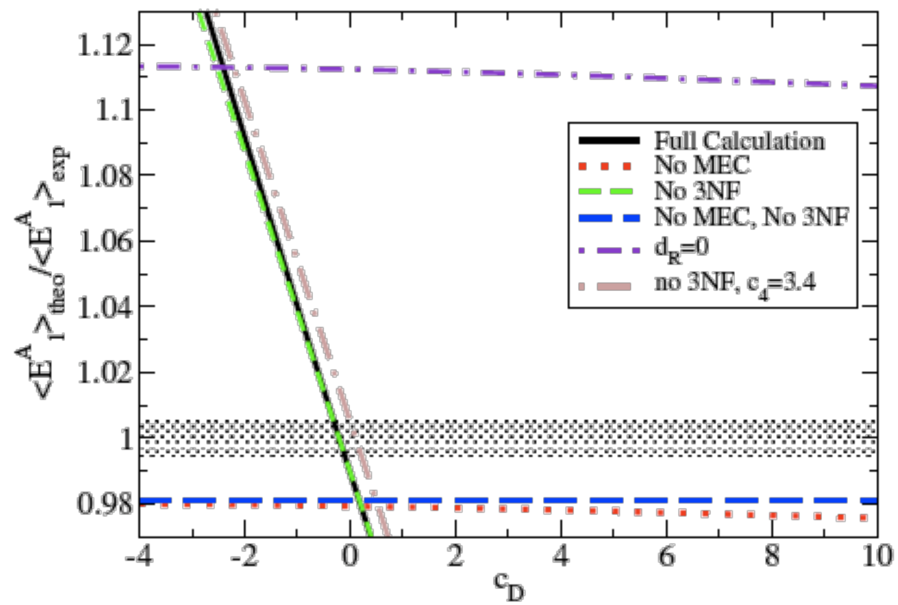
$$E_1^A|_{\mathrm{LO}} = i\, g_A (6\pi)^{-1/2} \sum_{i=1}^{A} \sigma_i \tau_i^+$$

- N^2LO: one-pion exchange plus contact

$$\hat{d}_R \equiv \frac{M_N}{\Lambda_\chi g_A} c_D + \frac{1}{3} M_N (c_3 + 2c_4) + \frac{1}{6}$$

- With the A=3 binding energy constraint a robust determination of c_D=-0.2±0.1 and c_E =-0.205±0.015

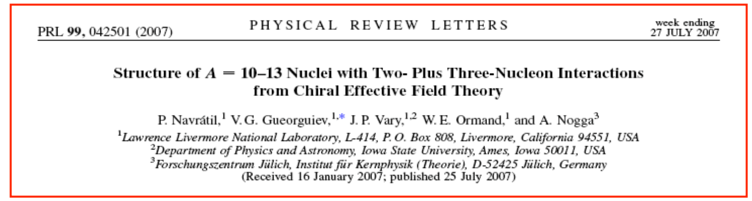




Not inconsistent with the A>3 determination c_D≈ -1 ± 1

Structure of p-shell nuclei with NN+NNN interactions

- NCSM is only method capable to apply the EFT NN+NNN interactions
  - Technically challenging, large-scale computational problem
    - ~4000 processors used in ^{12,13}C calculations
- Applied to constrain the NNN interaction
  - Investigation of A=3, ^{4}He and p-shell nuclei
  - Globally the best results with c_D ~ -1
- NNN interaction essential to describe structure of light nuclei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Structure of A = 10–13 Nuclei with Two- Plus Three-Nucleon Interactions from Chiral Effective Field Theory

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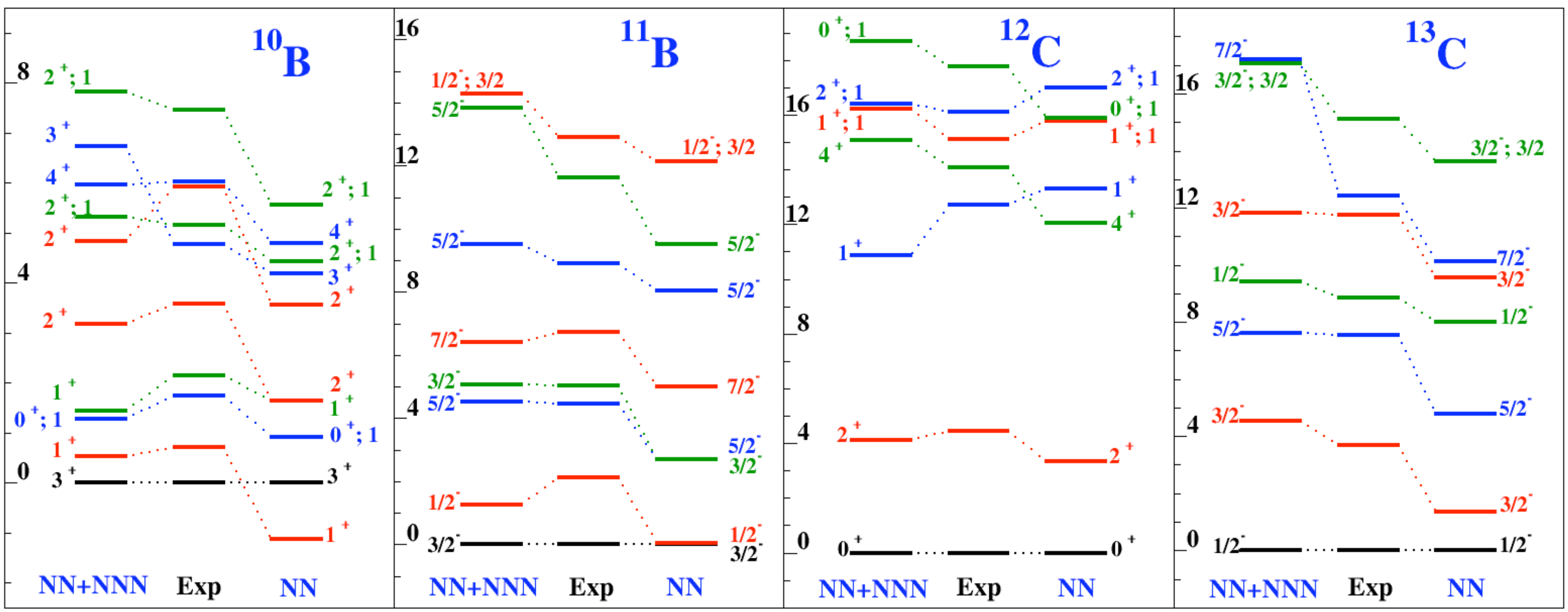
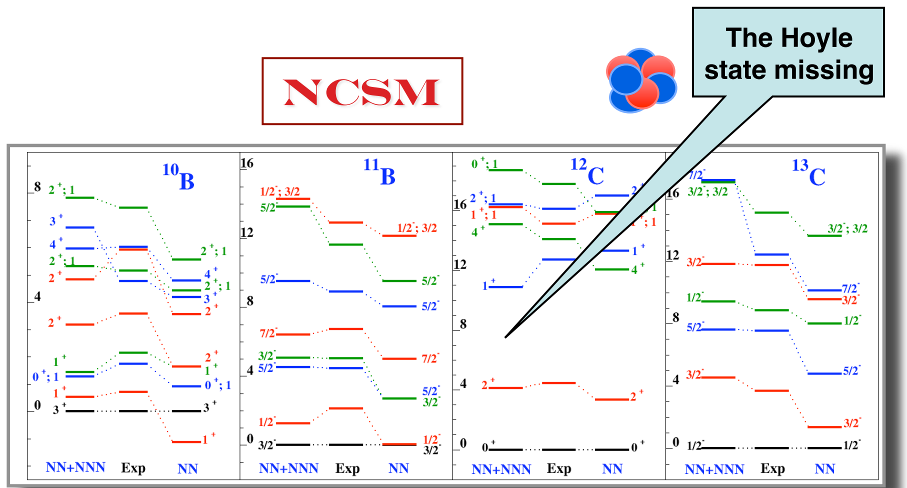


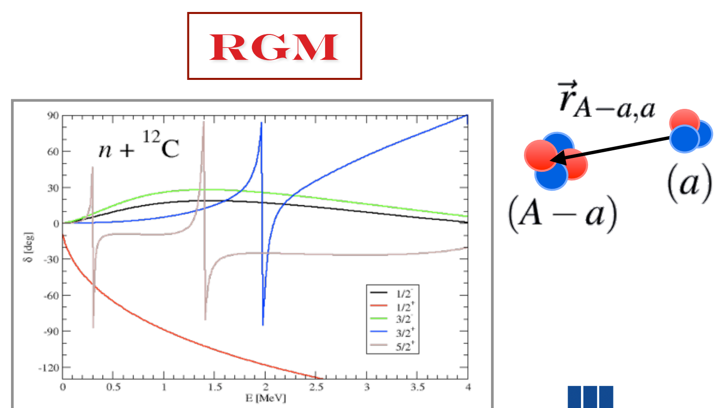
Our goal is to develop an *ab initio* theory to understand nuclear structure….

- … and **reactions** in light nuclei



- How? - Combining the *ab initio* no-core shell model (NCSM) with the resonating group method (RGM)
  - $\Rightarrow$ ***ab initio* NCSM/RGM**
  - NCSM - single-particle degrees of freedom
  - RGM - clusters and their relative motion

- ***Ab initio* theory of nuclear reactions for *A*>4 is new:**
  - **Lisbon**: p+^{3}He scattering published in 2007 (PRL **98**, 162502 (2007)); ***A*=4 is their limit**
  - **ANL**: n+^{4}He scattering published only recently (PRL **99**, 022502 (2007))



- **Our approach: readily extendable**
  - p-^{3}He, n-^{4}He & ***p*-^{4}He** scattering already calculated
  - promising results for p-shell nuclei: n-^{10}Be, p-^{12}C, n-^{16}O
  - Inclusion of d, ^{3}H, ^{3}He and α clusters under way

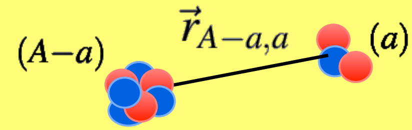
Preserves **Pauli principle** and **translational invariance**

↓

Important as nucleons are fermions and nuclei self-bound

The *ab initio* NCSM/RGM in a snapshot

- Ansatz: $\Psi^{(A)} = \sum_\nu \int d\vec{r}\, \varphi_\nu(\vec{r})\, \hat{\mathcal{A}}\, \Phi^{(A-a,a)}_{\nu\vec{r}}$



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

eigenstates of $H_{(A\text{-}a)}$ and $H_{(a)}$ in the *ab initio* NCSM basis

- Many-body Schrödinger equation:

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

$T_{\rm rel}(r) + \mathcal{V}_{\rm rel} + \bar{V}_{\rm Coul}(r) + H_{(A-a)} + H_{(a)}$

either bare interaction or NCSM effective interaction

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

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

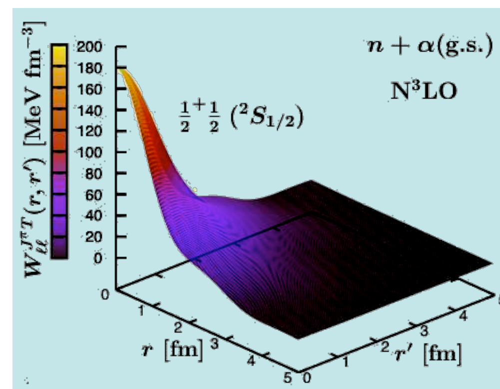
Hamiltonian kernel

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

Norm kernel

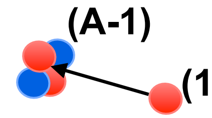
- Non-local integro-differential coupled-channel equations:

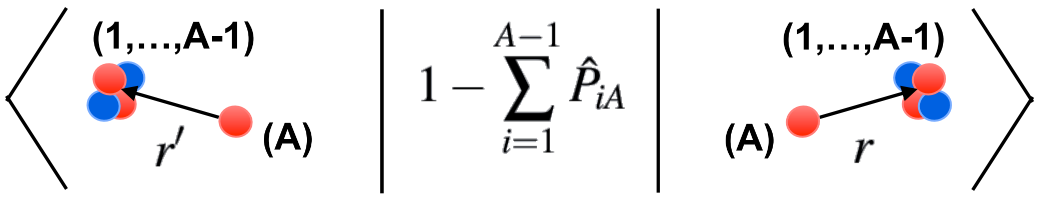
$$[\hat{T}_{\rm rel}(r) + \bar{V}_{\rm C}(r) - (E - E_\nu)]\, u_\nu(r) + \sum_\nu \int dr'\, r'\, W_{\nu\nu'}(r,r')\, u_\nu(r') = 0$$



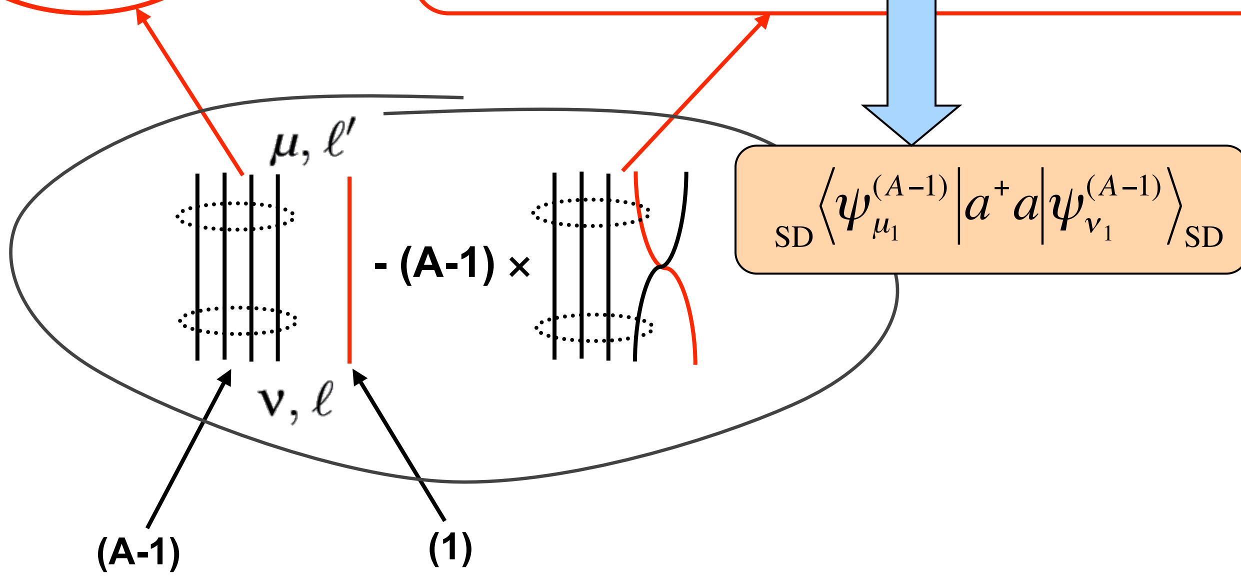
Fully implemented and tested for single-nucleon projectile (nucleon-nucleus) basis

Single-nucleon projectile: the norm kernel

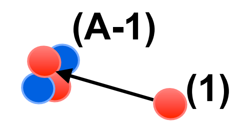


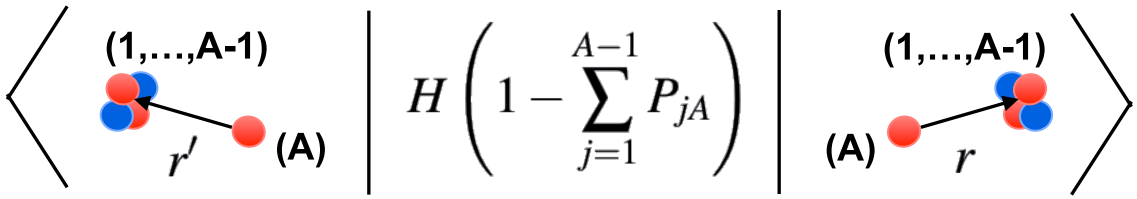


$$\mathcal{N}^{(A-1,1)}_{\mu\ell',\nu\ell}(r',r) = \delta_{\mu\nu}\,\delta_{\ell'\ell}\frac{\delta(r'-r)}{r'r} - (A-1)\sum_{n'n} R_{n'\ell'}(r')\langle\Phi^{(A-1,1)JT}_{\mu n'\ell'}|P_{A,A-1}|\Phi^{(A-1,1)JT}_{\nu n\ell}\rangle R_{n\ell}(r)$$



Single-nucleon projectile basis: the Hamiltonian kernel



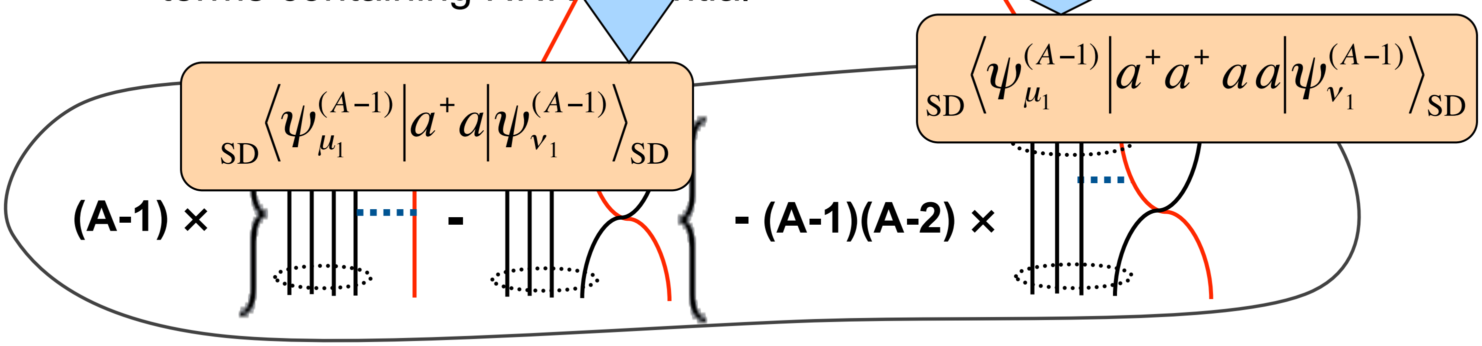


$$\mathcal{H}^{(A-1,1)}_{\mu\ell',\nu\ell}(r',r) = (E_{A-1}+\mathcal{T}_{rel})\,\mathcal{N}^{(A-1,1)}_{\mu\ell',\nu\ell}(r',r)$$

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

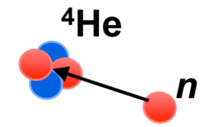
$$-\,(A-1)(A-2)\sum_{n'n} R_{n'\ell'}(r')\langle\Phi^{(A-1,1)JT}_{\mu n'\ell'}|V_{A-2,A}P_{A,A-1}|\Phi^{(A-1,1)JT}_{\nu n\ell}\rangle R_{n\ell}(r)$$

+ terms containing NNN potential

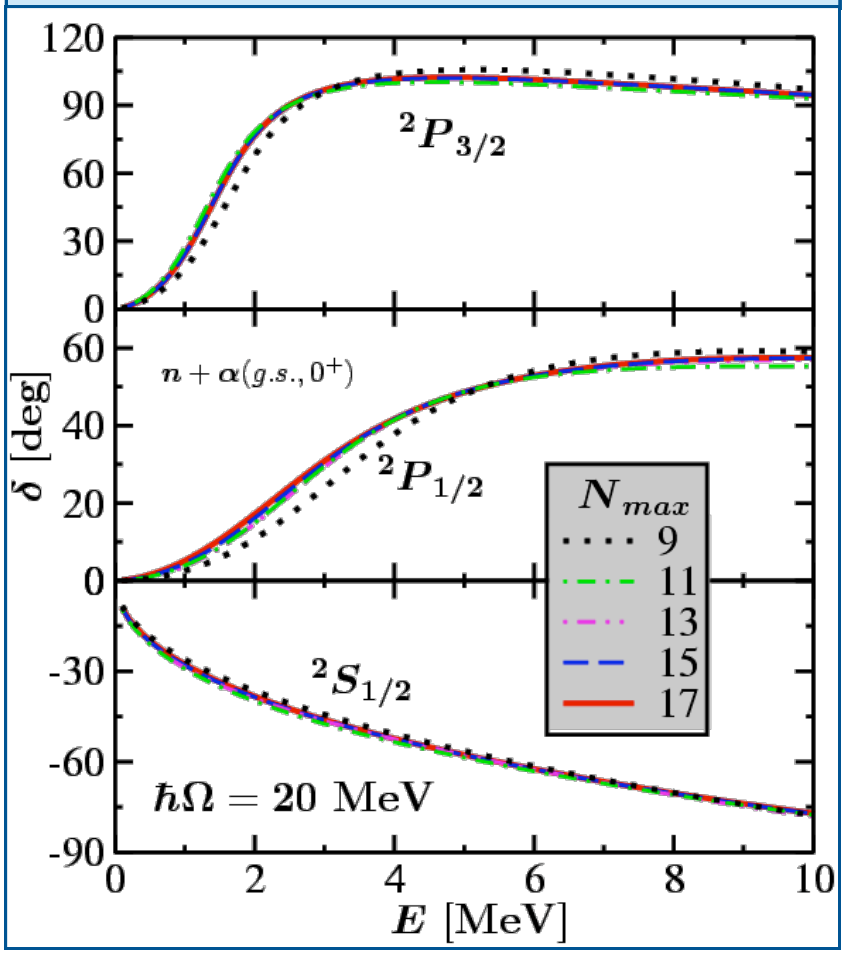


"direct potential" "exchange potential"

NCSM/RGM *ab initio* calculation of n-^{4}He phase shifts



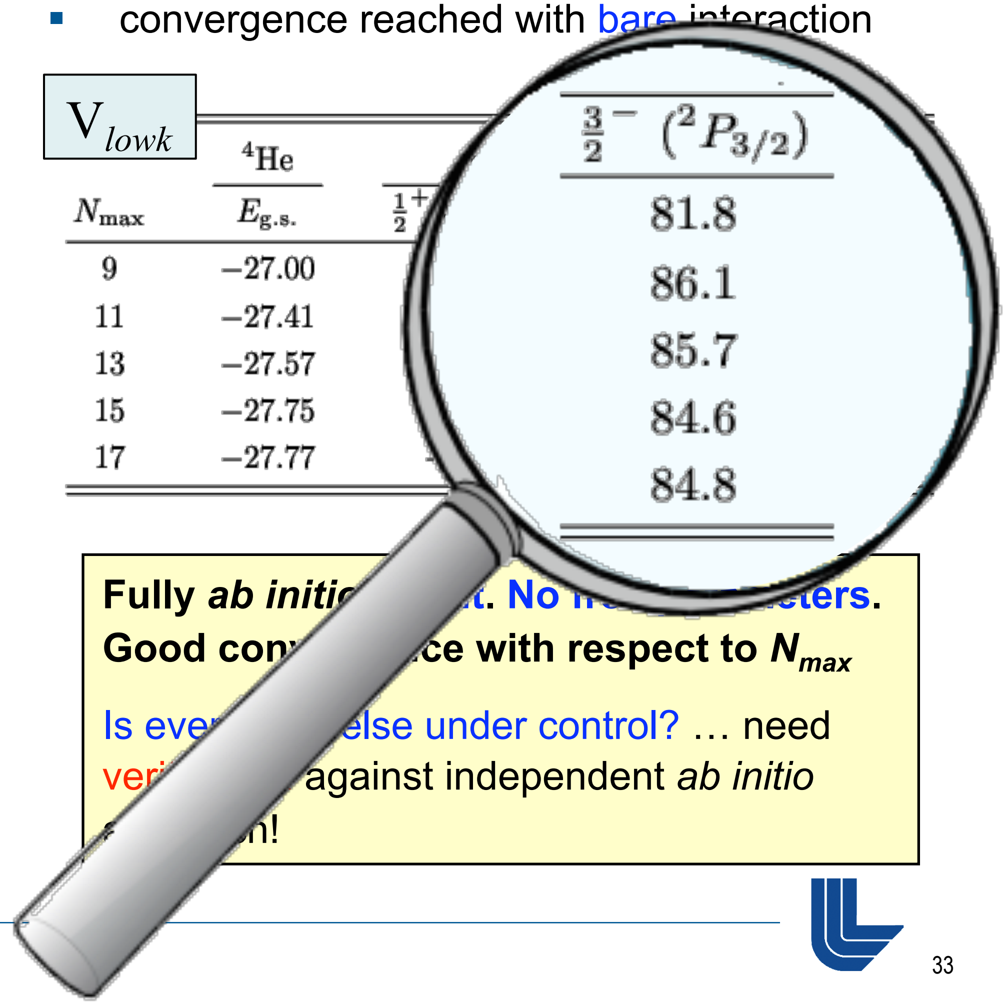
n-^{4}He phase shifts: SRG-N^{3}LO, λ=2.02 fm^{-1}



- Similarity-renormalization-group (SRG) evolved chiral N^{3}LO NN interaction (R. Roth)
- Low-momentum V_{lowk} NN potential
- convergence reached with bare interaction

V_{lowk}

N_{max}	^{4}He $E_{g.s.}$
9	−27.00
11	−27.41
13	−27.57
15	−27.75
17	−27.77

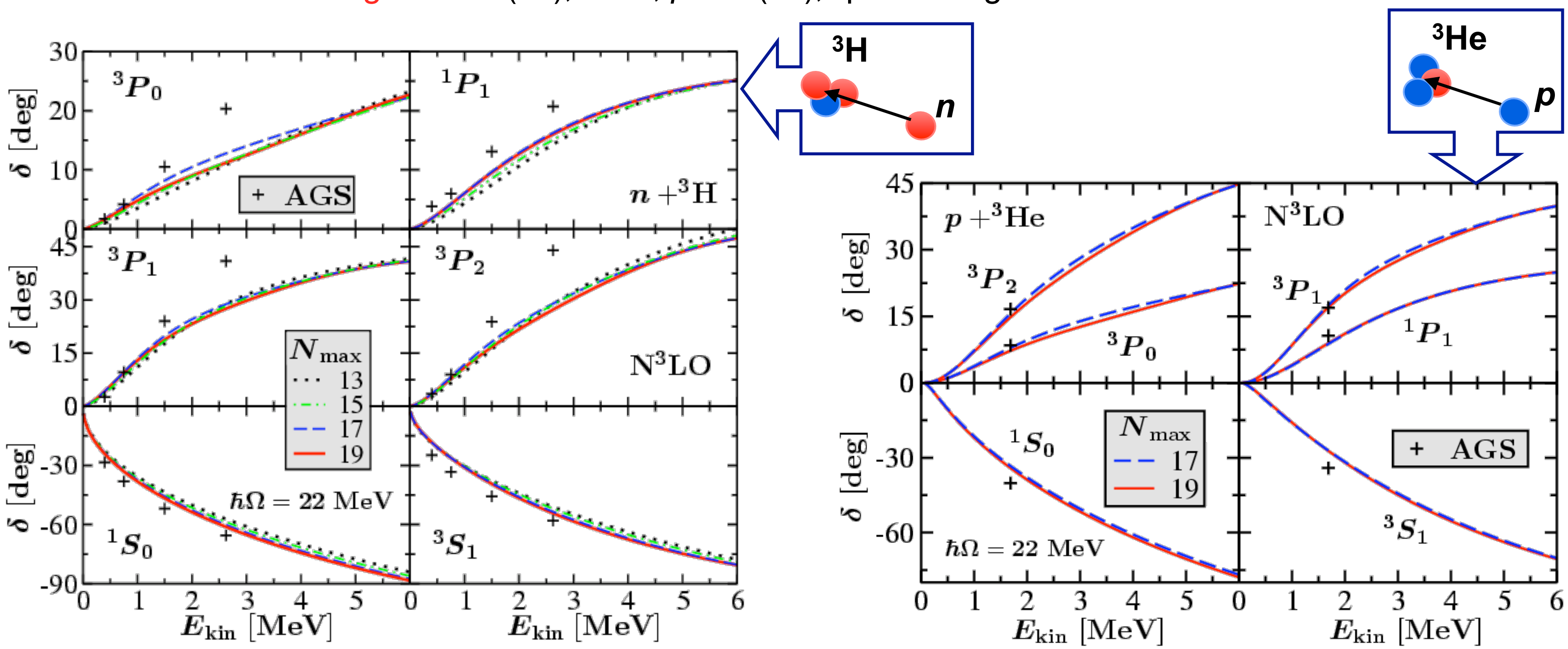


Fully *ab initi*... ...t. No fi... ...eters.
Good con... ...ce with respect to N_{max}

Is eve... ...else under control? … need veri... against independent *ab initio* ...n!

NCSM/RGM *ab initio* calculation of n-^{3}H and p-^{3}He phase shifts

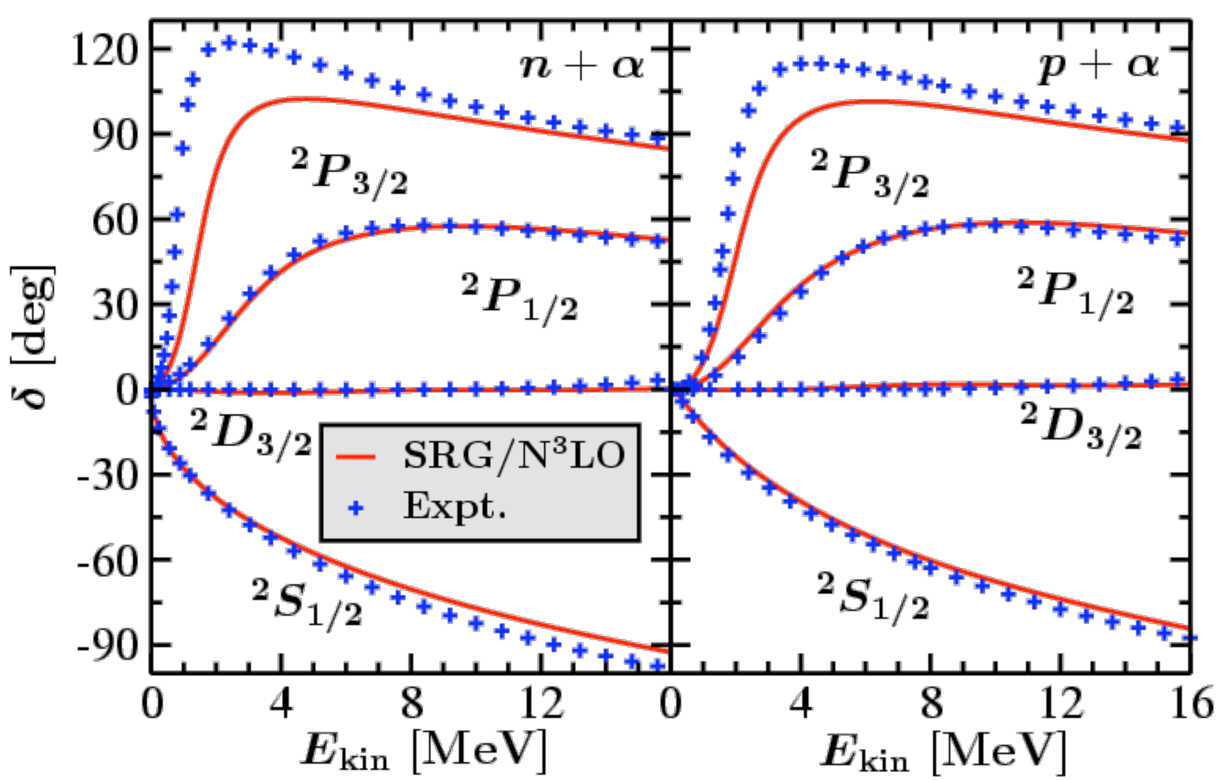
- NCSM/RGM calculations with n+^{3}H(g.s.) and p+^{3}He(g.s.), respectively.
- χEFT N^{3}LO NN potential: convergence reached with two-body effective interaction
- Benchmark with Alt, Grassberger and Sandhas (AGS) results [**PRC75, 014005(2007)**]
  - What is missing? - n+^{3}H(ex), ^2n+d, p-^{3}He(ex), ^{2}p+d configurations



The omission of three-nucleon partial waves with 1/2 < J ≤ 5/2 leads to effects of comparable magnitude on the AGS results. Need to include target excited states!

n-^{4}He phase shifts from SRG-evolved NN interactions

n-^{4}He and p-^{4}He phase shifts

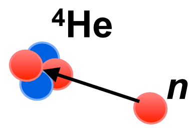


- SRG-evolved interactions (R. Roth)
  - SRG-N^{3}LO
  - SRG-AV18
- convergence reached with bare interaction
- ^{4}He states: g.s., 0^+0
- SRG-AV18 phase shifts present unphysical oscillations

Insufficient spin-orbit strength: $^2P_{3/2}$ underestimated ➔ **NNN needed**

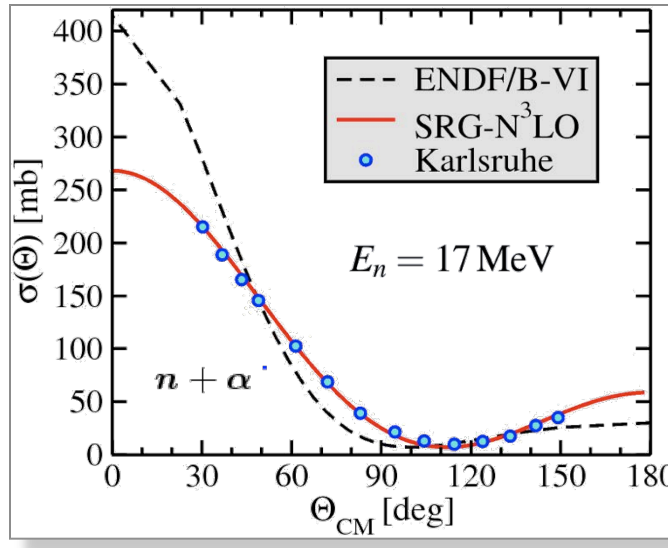
n+^{4}He differential cross section and analyzing power

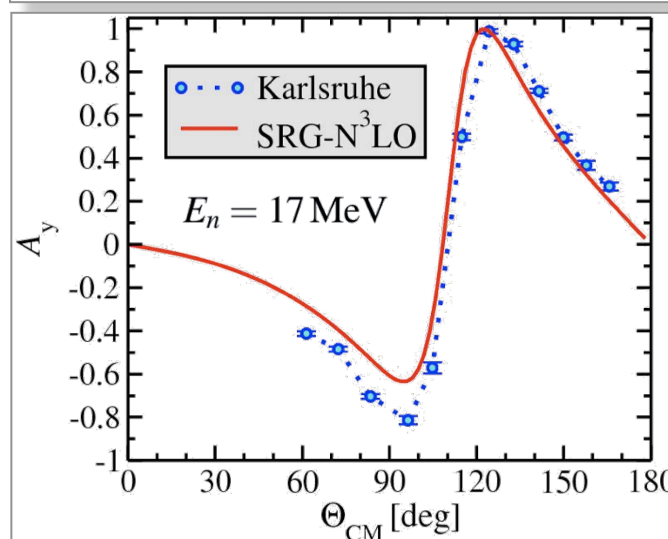
- Neutron energy of 17 MeV
  - beyond low-lying resonances
- Polarized neutron experiment at Karlsruhe
- NCSM/RGM calculations



  - n+^{4}He(g.s,0+0)
  - SRG-evolved N^{3}LO NN potential
- Good agreement for angular distribution
- Differences for analyzing power
  - A_y puzzle for A=5?

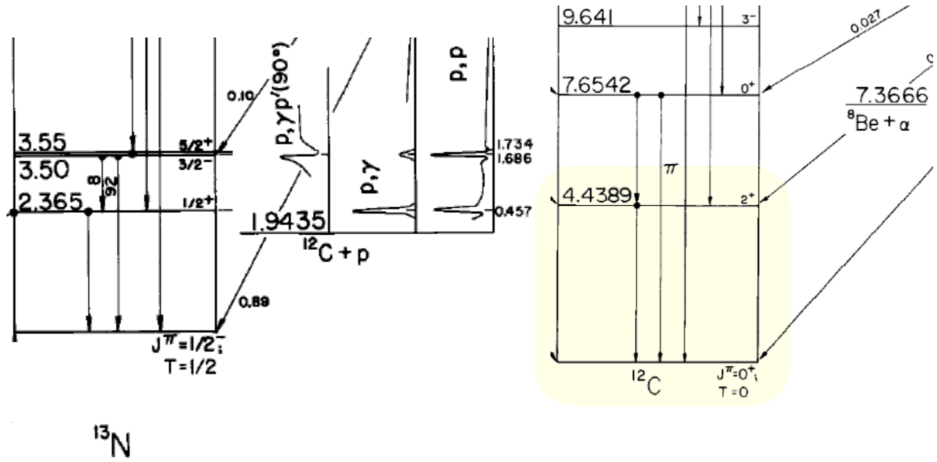
First ever *ab initio* calculation of A_y in for a A=5 system. Strict test of inter-nucleon interactions.

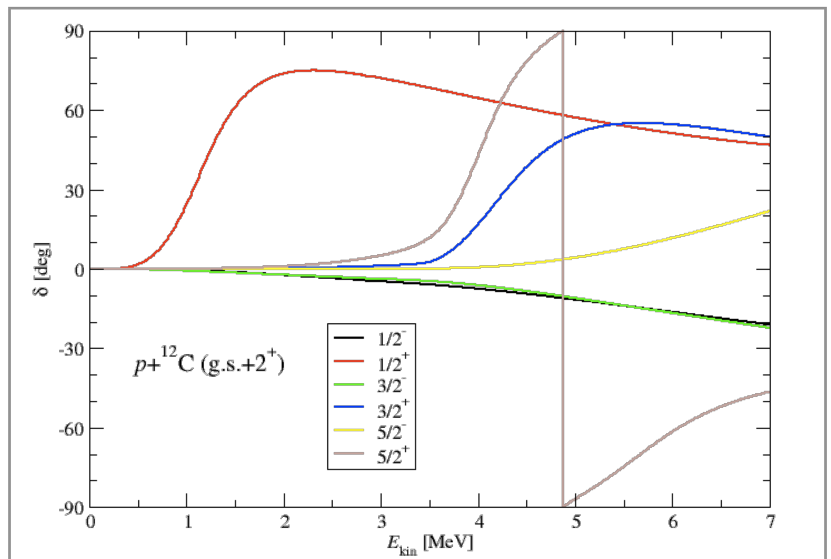




p-^{12}C scattering with SRG-N^{3}LO NN potential

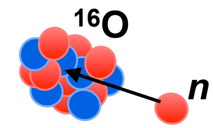
- ^{12}C
  - Full NCSM up to N_{max}=8
  - IT NCSM up to N_{max}=18(!)
- ^{13}N, ^{13}C within the NCSM
  - 1/2$^+$ state ~ 3 MeV too high
- p+^{12}C
  - Experiments with a polarized proton target under way
  - NCSM/RGM up N_{max}=14 so far
    - ^{12}C g.s. and 2$^+$ included
    - 1/2$^-$ state bound by 2.9 MeV
      - ^{13}N ground state
    - Other states unbound
    - 1/2$^+$ resonance at ~1.2 MeV
    - 5/2$^+$ resonance
    - Good stability: Moderate changes from N_{max}=6 to N_{max}=14



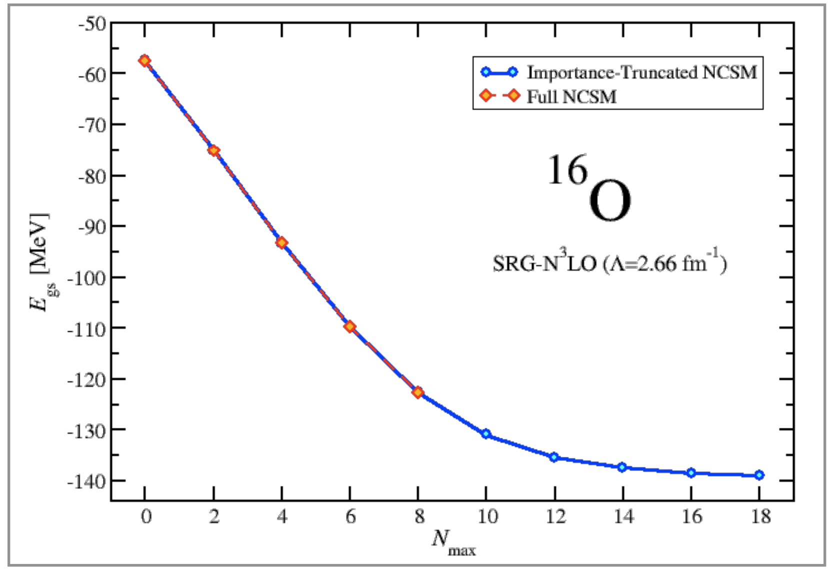


Qualitative agreement with experiment

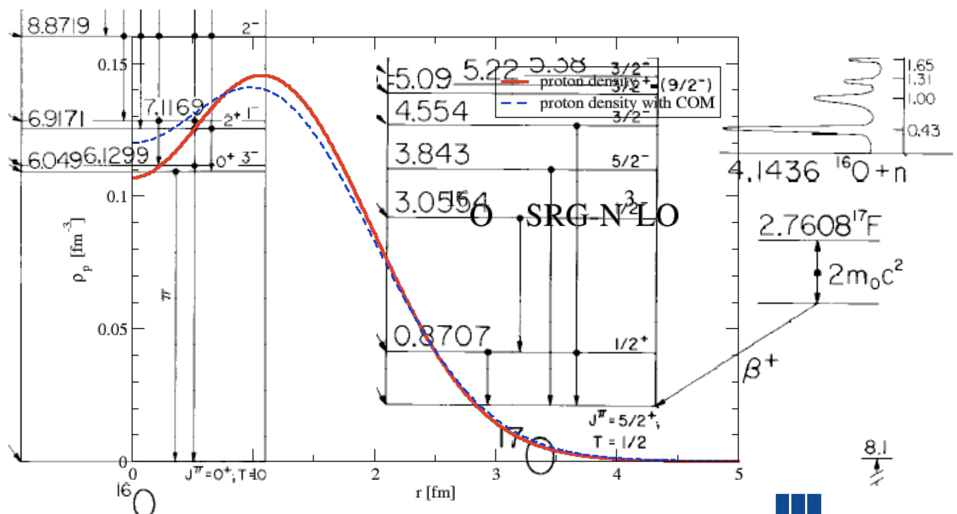
^{16}O ground state, ^{17}O bound states



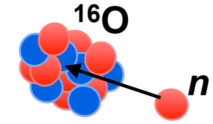
- ^{16}O ground state calculated within importance-truncated NCSM
  - ≥4p-4h up to N_{max}=18 (N_{max}=22 possible!?), $h\Omega$=24 MeV
  - SRG-N^{3}LO with Λ=2.66 fm^{-1}
    - Less overbinding: $E_\infty \approx$ -140 MeV
  - Benchmarking with full NCSM
    - ^{16}O binding energy up to N_{max}=8
    - **Perfect agreement**



- ^{17}O within *ab initio* NCSM/RGM
  - 1/2$^+$ bound: E_b=-0.88 MeV wrt ^{16}O
  - 5/2$^+$ bound: E_b=-0.41 MeV wrt ^{16}O
    - N_{max}=19, $h\Omega$=24 MeV
    - Only ^{16}O ground-state included

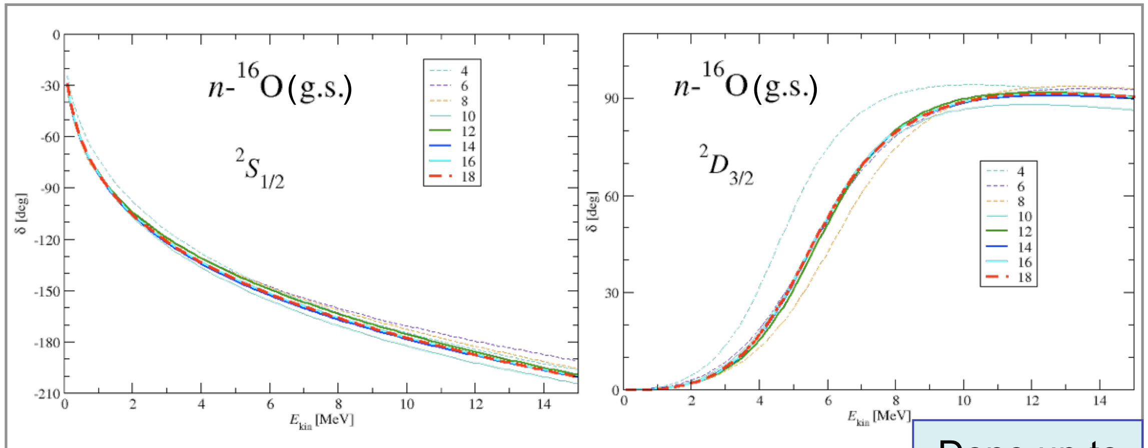


n-^{16}O scattering with SRG-N^{3}LO NN potential

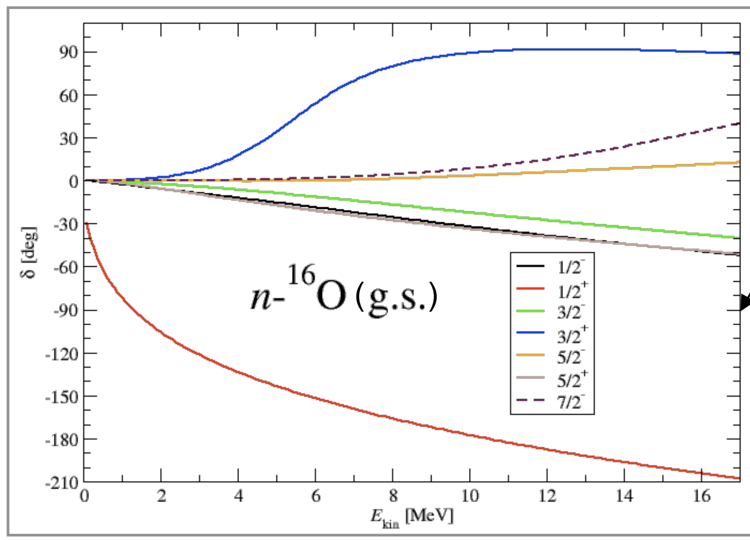


- ^{16}O ground state only
- Phase-shift convergence very good
- Essential to use **large N_{max}**
  - Target wave function
  - Expansion of short-range parts of kernels
  - **IT NCSM** for the target makes it possible

Combining the *ab initio* NCSM/RGM with the importance-truncated NCSM highly **promising. Access to medium mass nuclei.**

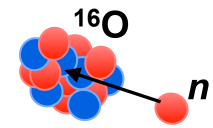


Done up to N_{max}=18 **converged**



N_{max}=18

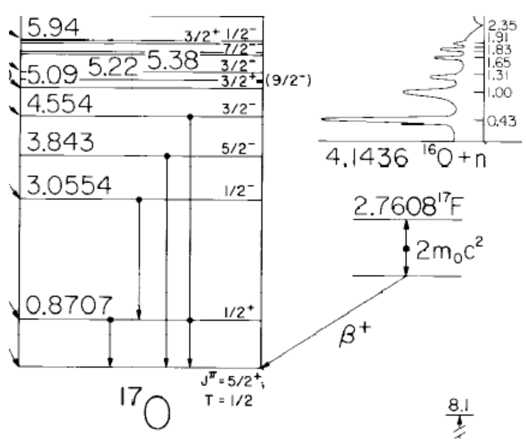
n-^{16}O scattering: Effect of ^{16}O excited states

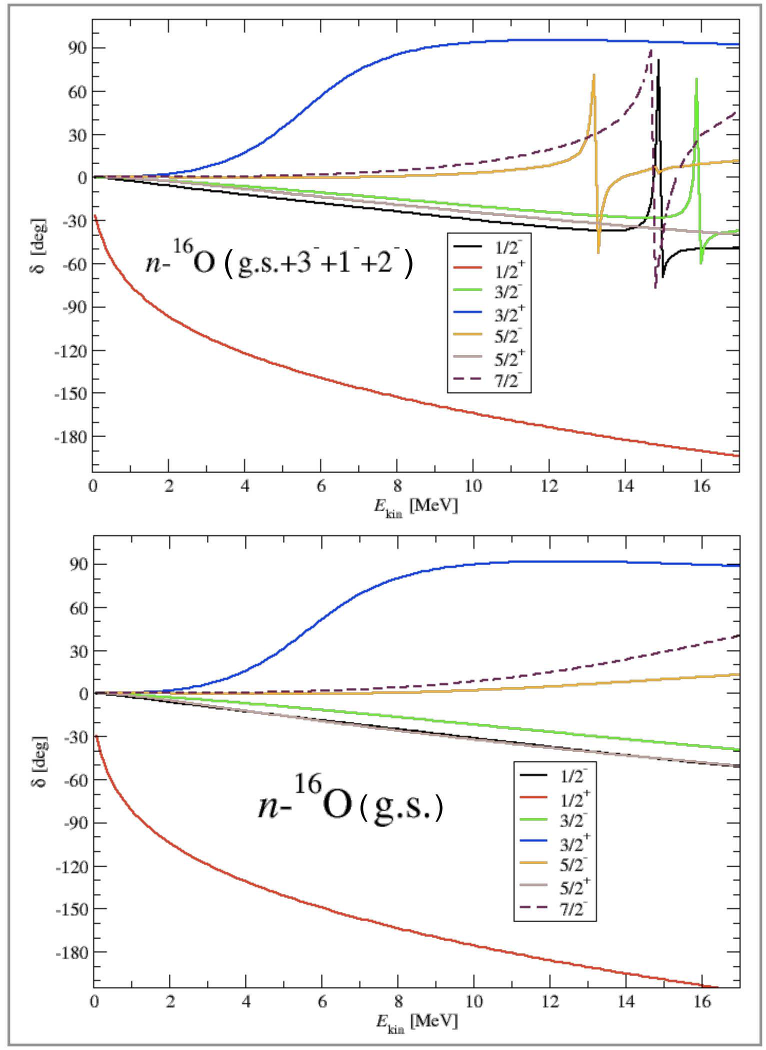


- **Need to include ^{16}O excited states** (1p-1h…)
- **IT NCSM for both the ground state & excited states**
- Done up to N_{max}=12/13
  - g.s. in N_{max}=12
  - 3^-, 1^-, 2^- in N_{max}=13
  - Significant increase of binding energies
    - $1/2^+$: -0.78 → -1.03
    - $5/2^+$: -0.37 → -1.32
  - Appearance of sharp resonances

Good stability

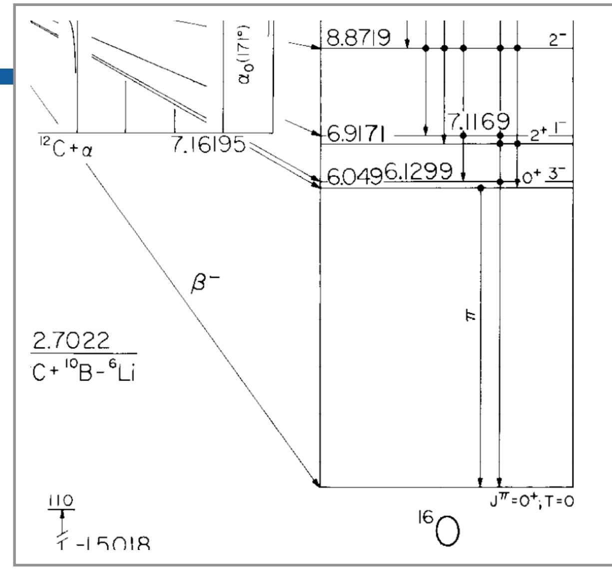
Correct order



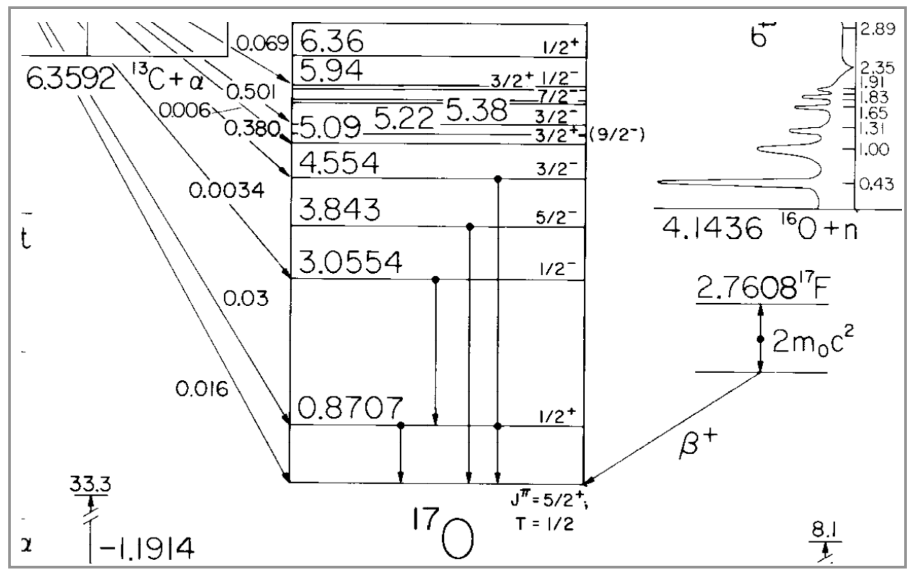


n-^{16}O scattering: Open issues

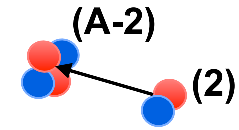
- ^{16}O excited states with the SRG-N^{3}LO NN potential too high
  - 3^-, 1^-, 2^- calculated: ≈13.3, 15.9, 16.3 MeV
  - 3^-, 1^-, 2^- experiment: 6.13, 7.12, 8.87 MeV
    - Importance of 3-body force?
    - Density too high?
  - ^{12}C+alpha not included at present



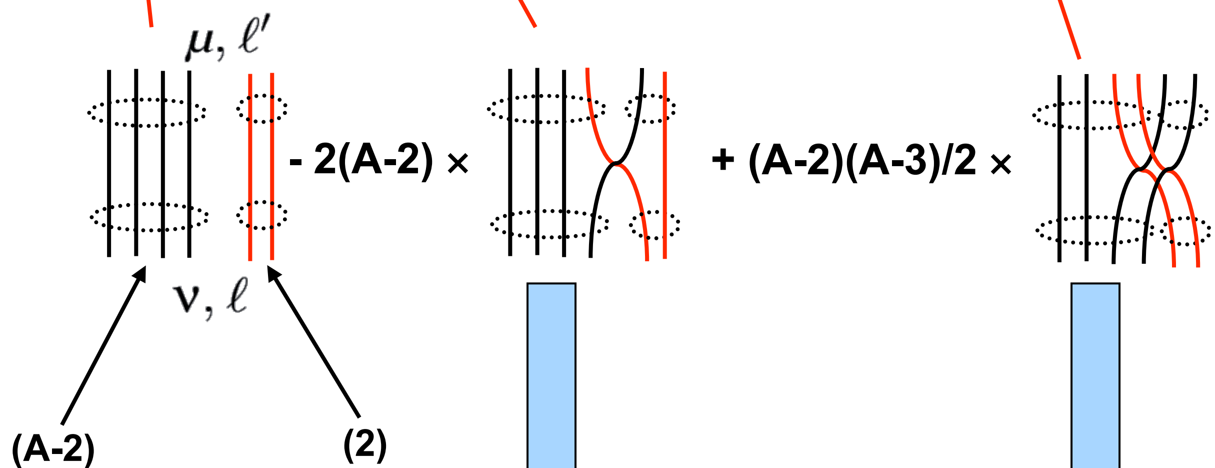
- n+^{16}O with the SRG-N^{3}LO NN potential
  - $5/2^+$, $1/2^+$ underbound
  - $1/2^-$, $5/2^-$ not bound
  - Resonances too high
    - Impact of incomplete ^{16}O description
    - ^{13}C+alpha not taken into account



The deuteron projectile: Norm kernel



$$\left\langle \underset{(A-1,A)}{\overset{(1,\dots,A-2)}{r'}} \right| 1 - 2(A-2)\hat{P}_{A-2,A-1} + \tfrac{1}{2}(A-2)(A-3)\hat{P}_{A-2,A}\hat{P}_{A-3,A-1} \left| \underset{(A-1,A)}{\overset{(1,\dots,A-2)}{r}} \right\rangle$$

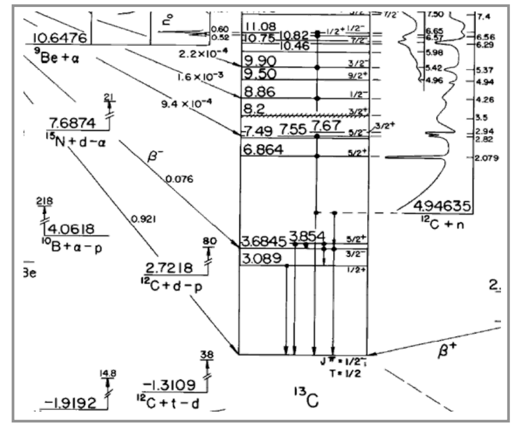


$${}_{SD}\left\langle \psi_{\mu_1}^{(A-2)} \middle| a^{+} a \middle| \psi_{\nu_1}^{(A-2)} \right\rangle_{SD}$$

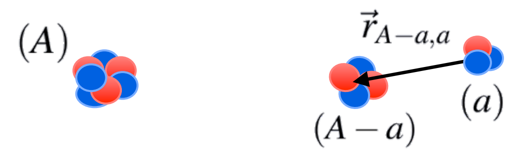
$${}_{SD}\left\langle \psi_{\mu_1}^{(A-2)} \middle| a^{+} a^{+} a\, a \middle| \psi_{\nu_1}^{(A-2)} \right\rangle_{SD}$$

Conclusions and outlook

- We are extending the *ab initio* NCSM to treat low-energy light-ion reactions
- Our recent achievements:
  - n-^{3}H, n-^{4}He, n-^{10}Be and p-^{3,4}He scattering phase-shifts with realistic NN potentials (**PRL 101, 092501 (2008)**)
- n-^{16}O under way:
  - Breakthrough due to the importance-truncated NCSM approach
- Coming next:
  - inclusion of NNN potential terms
  - *d,* ^{3}H and ^{3}He, ^{4}He projectiles



- Nuclei - complex open many-body systems
  - Bound states, resonances, continuum
- A correct and efficient theoretical description must include all these features
  - Coupling of bound-state theory with cluster theory



$$\left|\Psi_A^J\right\rangle = \sum c_\lambda \left|A\lambda J\right\rangle + \sum \int d\vec{r}\,\varphi_\nu(\vec{r})\hat{\mathcal{A}}\Phi_{\nu\vec{r}}^{(A-a,a)}$$

$$\begin{pmatrix} H & h \\ h & \mathcal{H} \end{pmatrix}\begin{pmatrix} c \\ \varphi \end{pmatrix} = E\begin{pmatrix} 1 & g \\ g & \mathcal{N} \end{pmatrix}\begin{pmatrix} c \\ \varphi \end{pmatrix}$$

***Ab Initio* No-Core Shell Model with Continuum**