Testing nuclear forces in many-body calculations

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ECT* Trento, 20 June 2005

Outline

- Motivation
- *Ab initio* no-core shell model (NCSM)
- ^{6}Li and ^{10}B calculations with the EFT N^{3}LO NN potential
- Importance of three-nucleon interaction (TNI)
- First results with EFT N^{3}LO NN potential plus consistent N^{2}LO TNI
- Results from INOY nonlocal NN potential and a comparison to standard high-precision potentials
- Conclusions

Ab initio approaches to nuclear structure

- **Goal:** Describe nuclei as systems of nucleons that interact by fundamental interactions
  - Non-relativistic point-like nucleons interacting by realistic two- and three-nucleon forces
- Why it has not been solved yet?
  - High-quality nucleon-nucleon potentials constructed only recently
    - Difficult to use in many-body calculations
      - Need sophisticated approaches
      - Big computing power
  - Three-nucleon interaction not well known
    - Even more computing power needed to include it in many-body calculations

- Current status
  - 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)

Ab initio no-core shell-model approach

- **Goal:** Solution of nuclear structure problem for light nuclei
- Many-body Schroedinger equation
  - A-nucleon wave function
- Hamiltonian

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

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

  - Realistic nucleon-nucleon and three-nucleon potentials
    - Coordinate space - Argonne V18, AV8', three-nucleon Tucson-Melbourne
    - Momentum space - CD-Bonn, Chiral N^{3}LO, three-nucleon chiral N^{2}LO
- Modification by center-of-mass harmonic oscillator (HO) potential (Lipkin 1958)

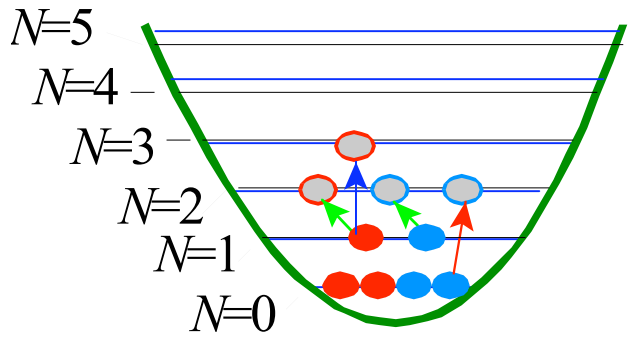
$$\frac{1}{2} A m\Omega^2 \vec{R}^2 = \sum_{i=1}^{A} \frac{1}{2} m\Omega^2 \vec{r}_i^{\,2} - \sum_{i<j}^{A} \frac{m\Omega^2}{2A} (\vec{r}_i - \vec{r}_j)^2$$

  - No influence on the internal motion (in infinite space)
  - Introduces mean field for sub-clusters
  - Convenient to work in the HO basis

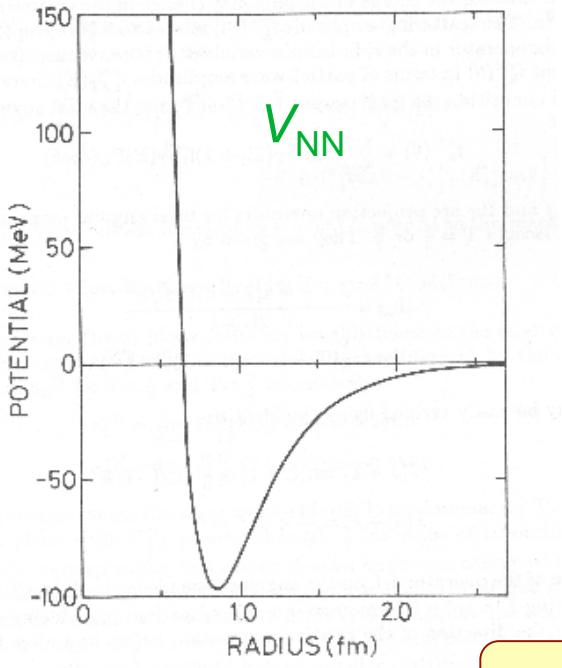
$$H^{\Omega} = \sum_{i=1}^{A} \left[\frac{\vec{p}_i^{\,2}}{2m} + \frac{1}{2} m\Omega^2 \vec{r}_i^{\,2} \right] + \sum_{i<j}^{A} \left[V_{NN}(\vec{r}_i - \vec{r}_j) - \frac{m\Omega^2}{2A} (\vec{r}_i - \vec{r}_j)^2 \right] \quad \left(+ \sum_{i<j<k}^{A} V_{ijk}^{3b} \right)$$

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 $N_{max}\hbar\Omega$ model space



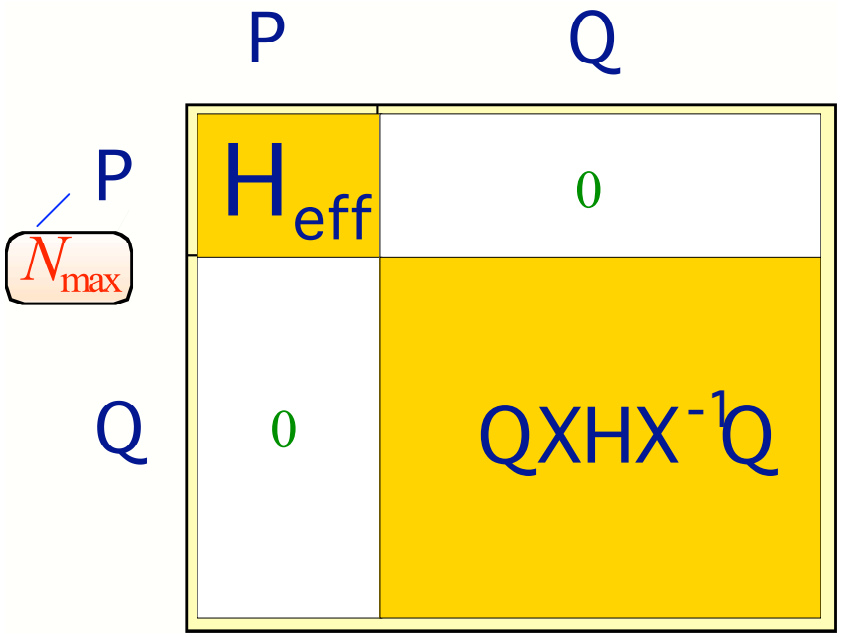
Nucleon-nucleon interaction



Repulsive core in V_{NN} cannot be accommodated in a truncated HO basis

Need for the effective interaction

Effective Hamiltonian in the NCSM



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

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

model space dimension

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

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

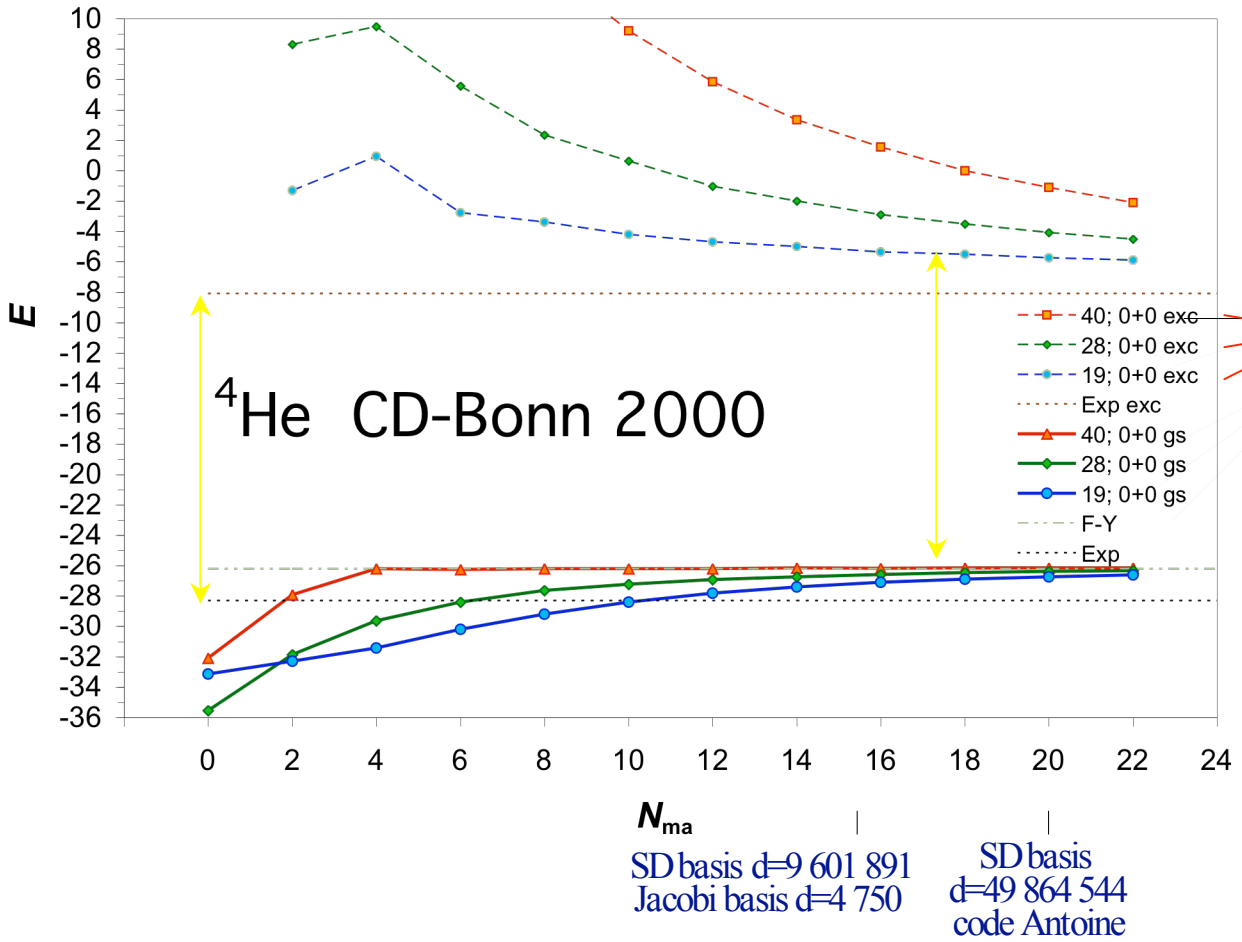
unitary $X = \exp[-\arctan h(\omega^{+} - \omega)]$

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

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

Test of convergence

- ^{4}He with the CD-Bonn 2000 NN interaction
- Dependence of the 0^+ 0 ground state and the 0^+ 0 excited state energies on the basis size (N_{max}) and the HO frequency ($\hbar\Omega$)



Ground-state energy agrees with the Faddeev-Yakubovsky result -26.2 MeV

Different HO frequencies

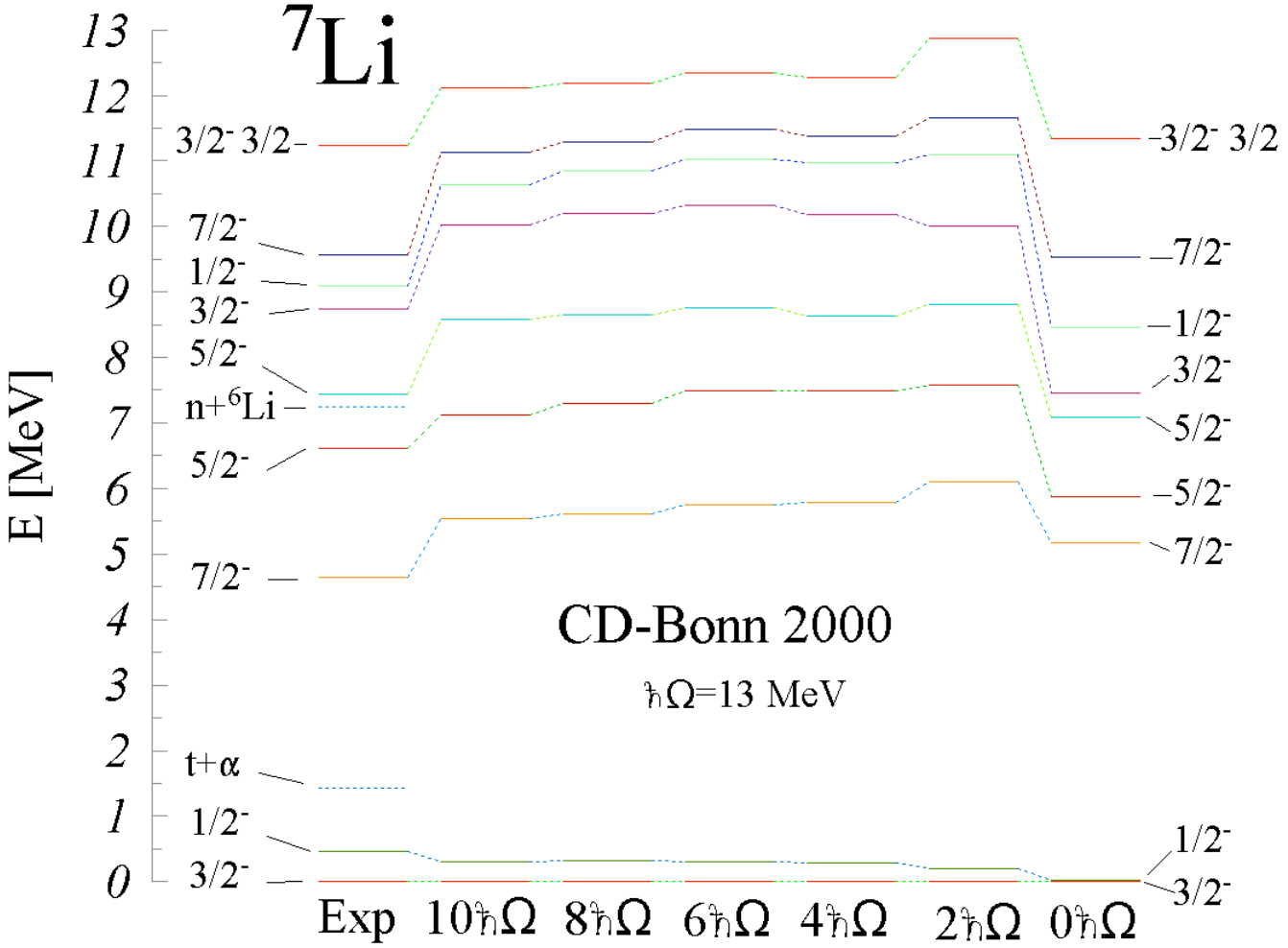
NCSM
Jacobi coordinate *or* Slater determinant HO basis

n=2, two-body effective interaction approximation

not a variational calculation - neglect of three- and four-body correlations

p-shell nuclei with realistic NN forces

- Correct level ordering for light *p*-shell nuclei



Old evaluation NPA**490**,1(1988) No $1/2^-_2$ and $3/2^-_2$, $7/2^-_2$ reversed

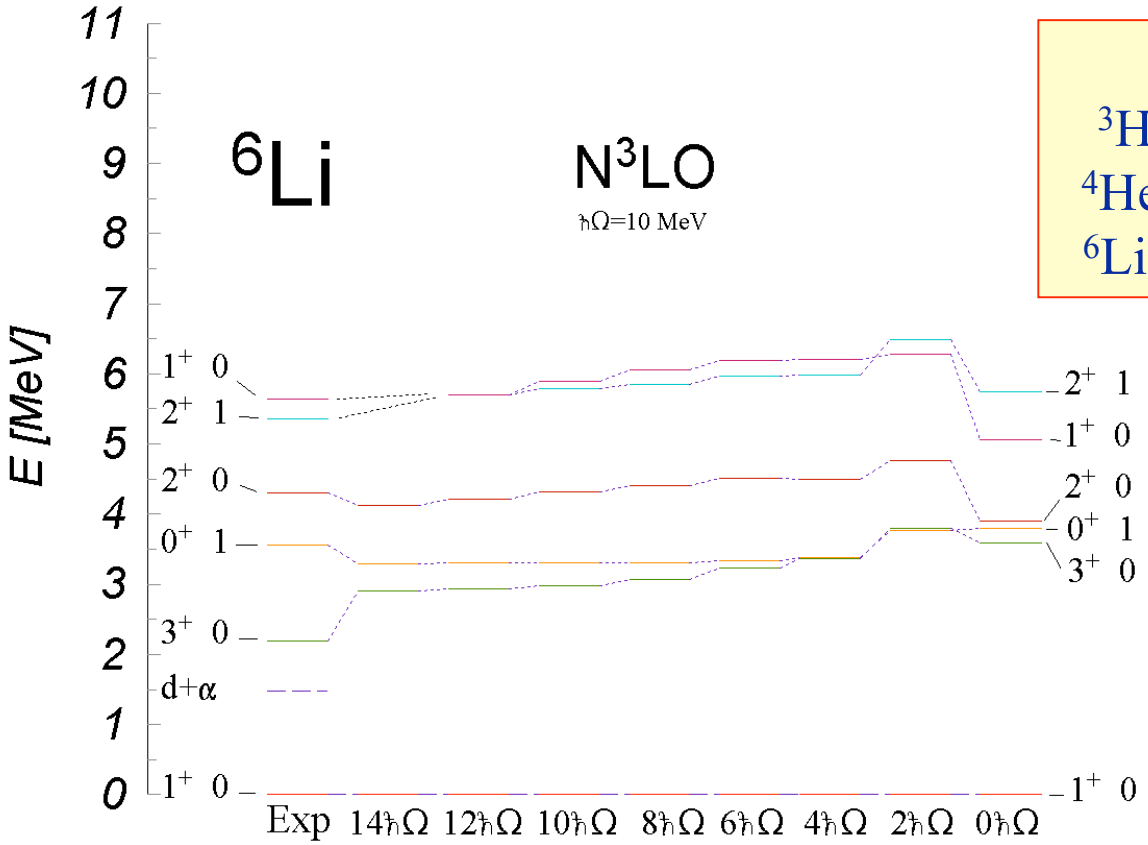
New evaluation NPA**708**,3(2002) introduces $1/2^-_2$ and orders the states as in calculation

Binding energy 35.5(5) MeV

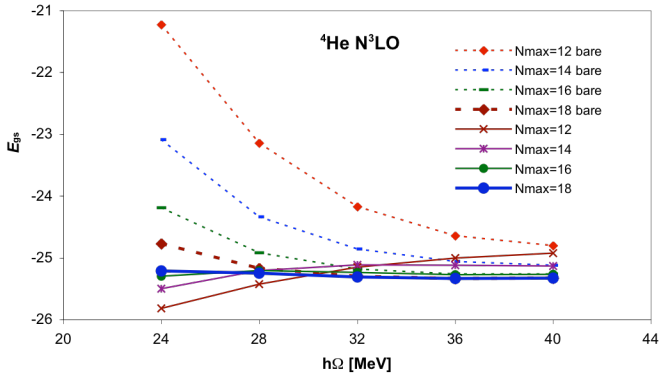
Convergence of excitation energies
Realistic NN interactions provide reasonable description of nuclear structure

NCSM calculations with the EFT N^{3}LO NN interaction

Accurate NN potential at fourth order of chiral-perturbation theory (N^{3}LO)
D. R. Entem and R. Machleidt, Phys. Rev. C **68**, 041001(R) (2003)

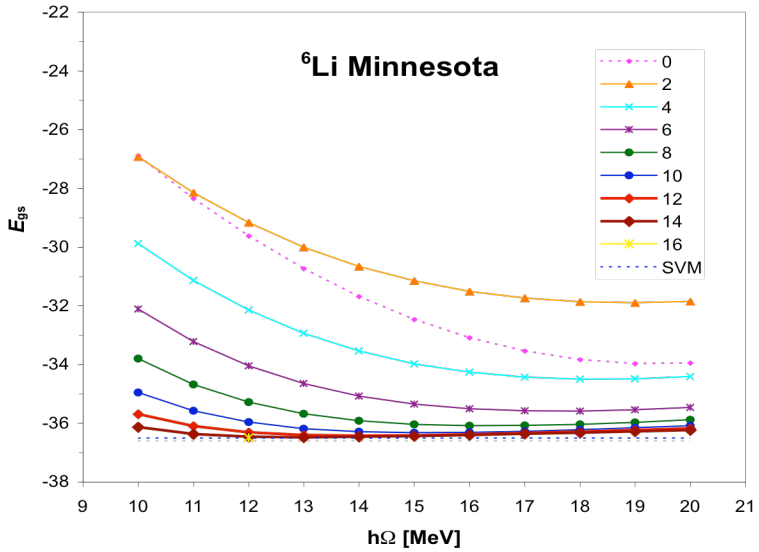


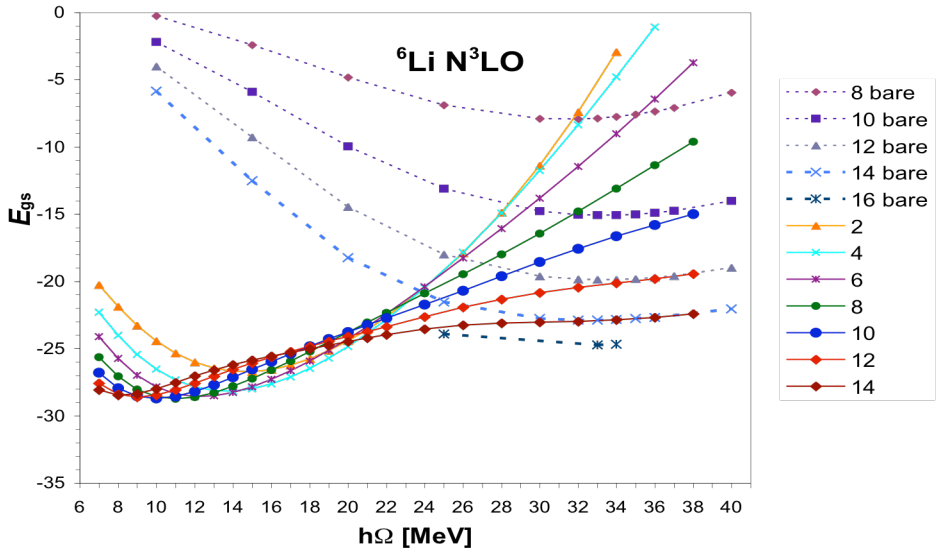
	N^{3}LO	Exp
^{3}H	7.85 MeV	8.48 MeV
^{4}He	25.35(5) MeV	28.30 MeV
^{6}Li	28.5(5) MeV	31.99 MeV

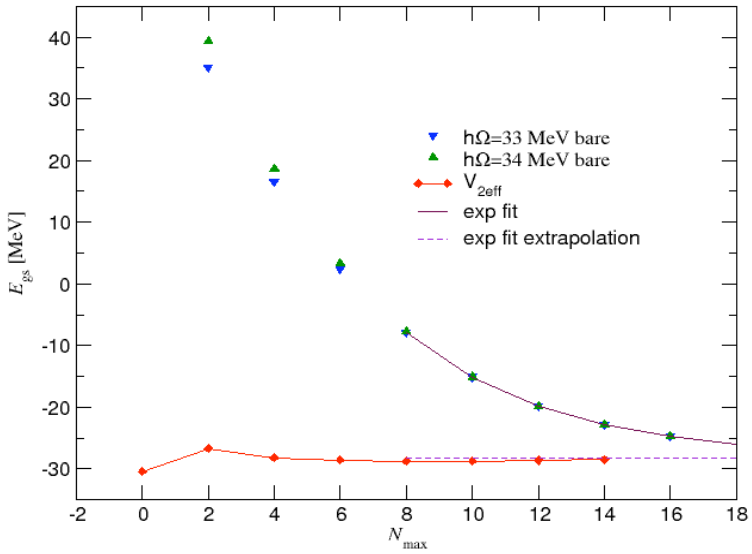


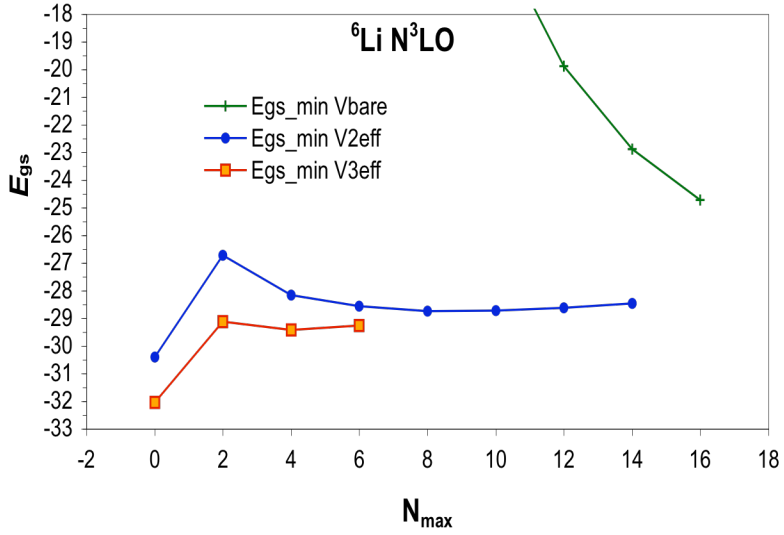
Converged ^{6}Li excitation energies
Correct level ordering, level spacing not right

NCSM calculations with the EFT N^{3}LO NN interaction: ^{6}Li binding energy convergence





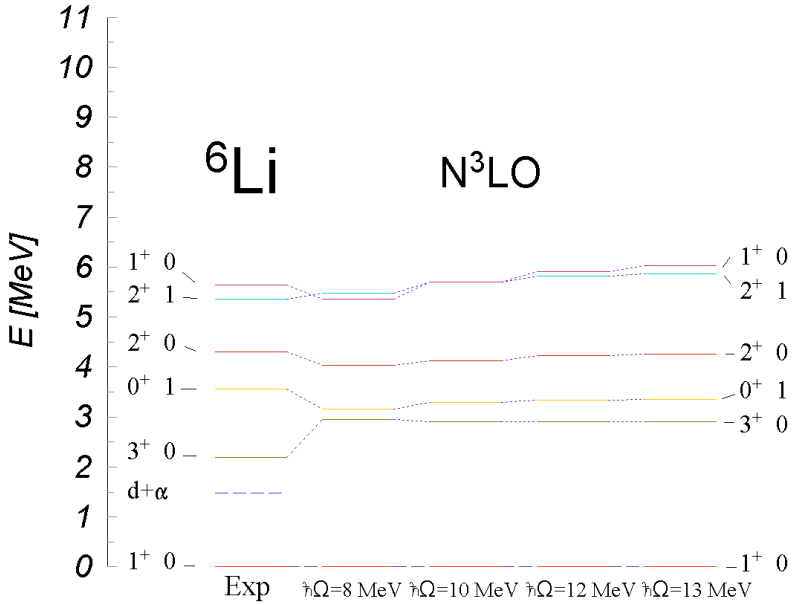


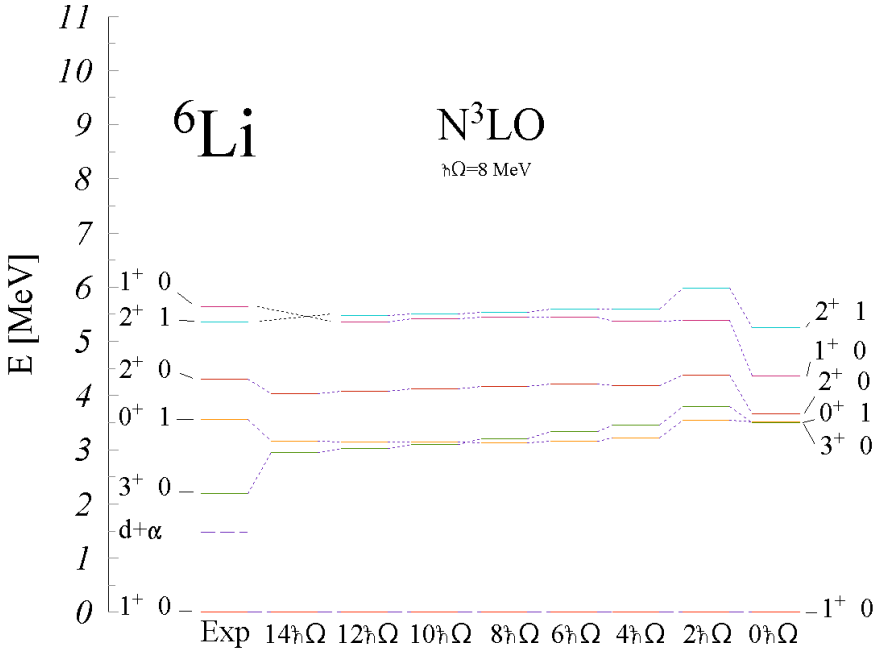


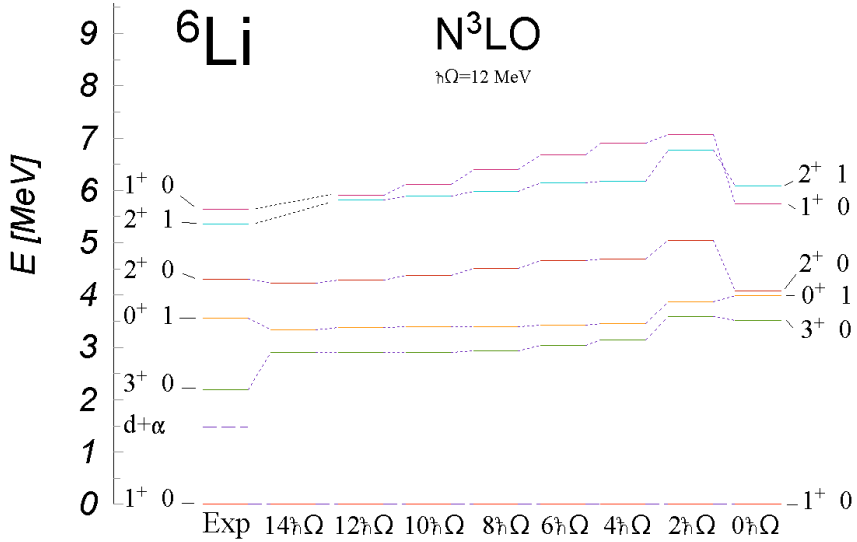
NCSM calculations with the EFT N^{3}LO NN interaction: Convergence of ^{6}Li excitation energies

Difficult convergence of the binding energy

Good convergence of the excitation energies

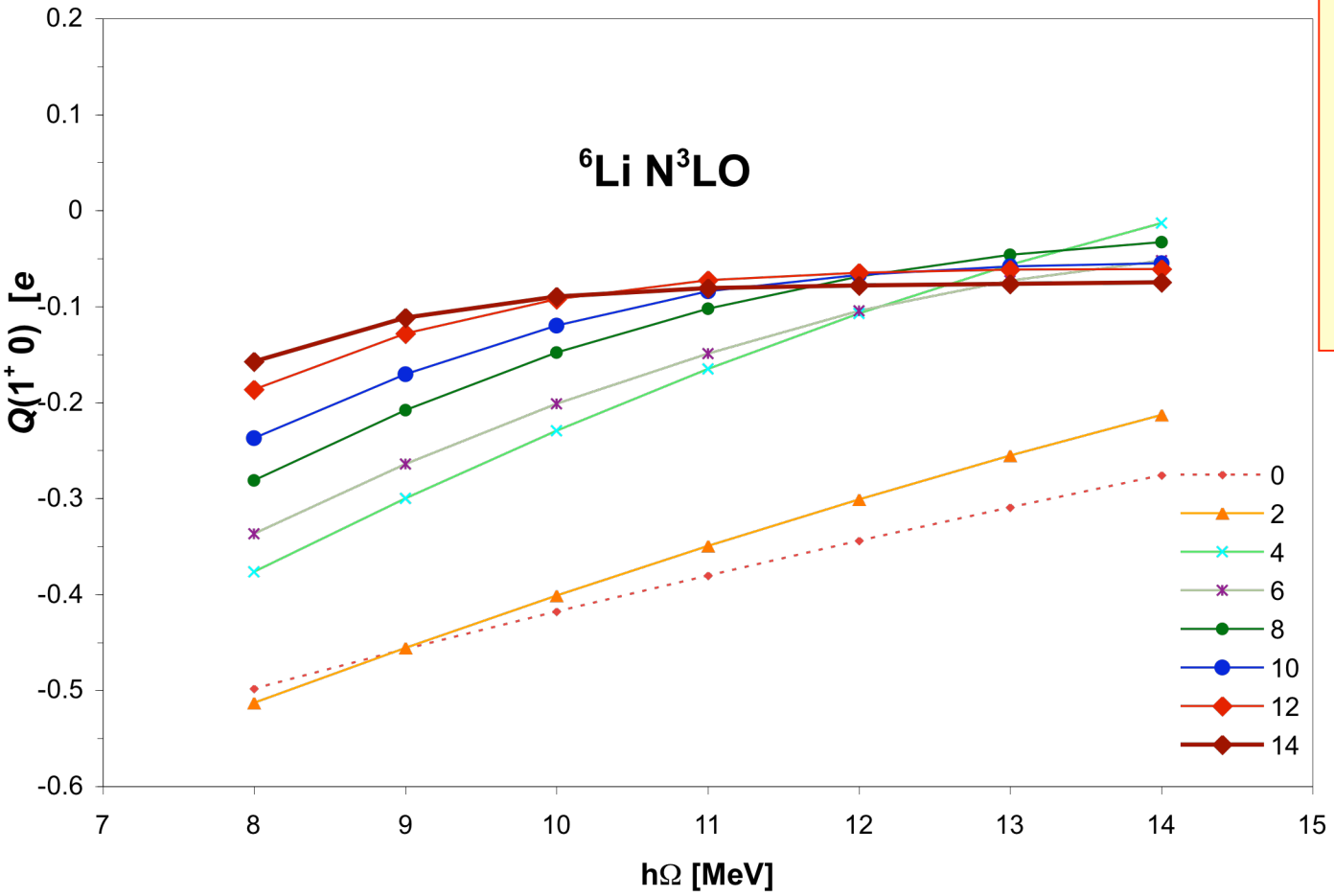






^{6}Li quadrupole moment

EFT N^{3}LO NN potential

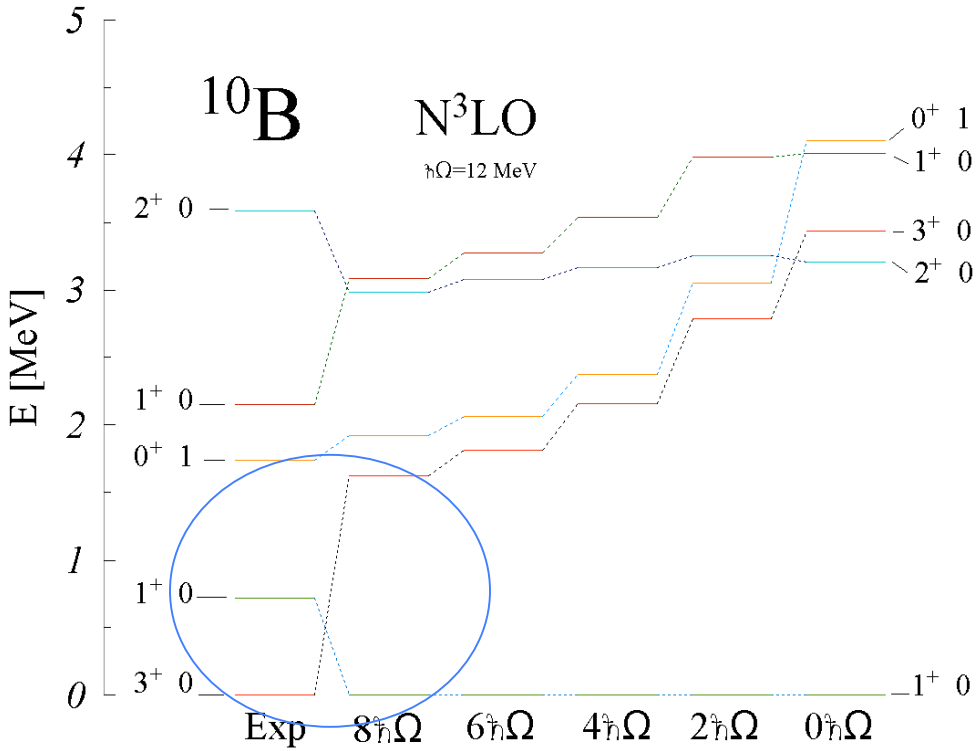


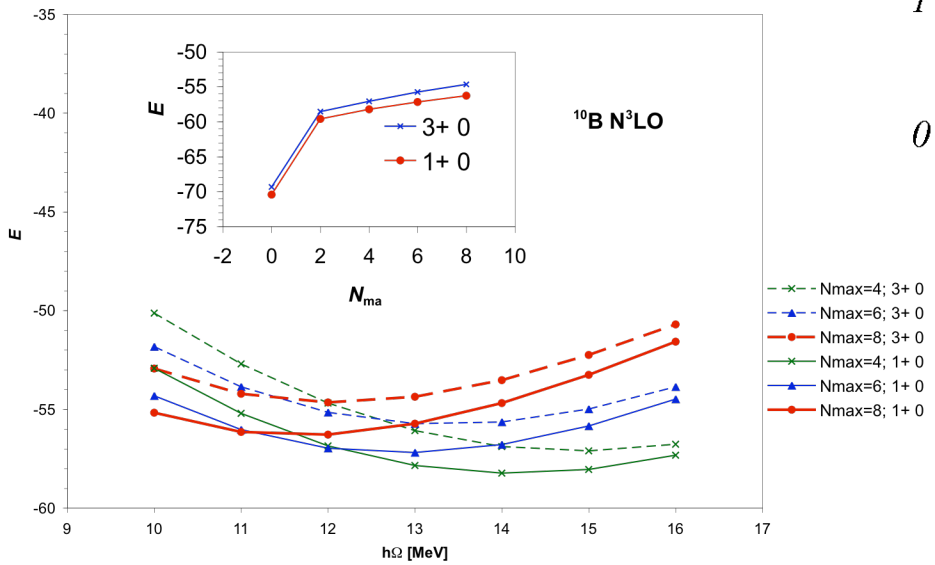
Exp
-0.08 e fm^2

NCSM:
Good convergence
with N_{max}

^{10}B using N^{3}LO NN potential

- Clearly, ground state is incorrectly predicted
- In EFT, three-nucleon interaction appears already at N^{2}LO
  - Should be included in the Hamiltonian
  - c_1,c_3,c_4 parameters of the two-pion term should be the same as those used in the N^{3}LO NN potential
    - c_1=-0.81, c_3=-3.2, c_4= 5.4

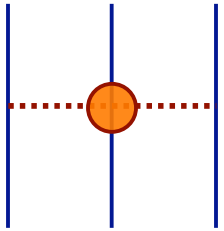


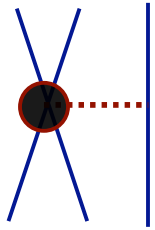


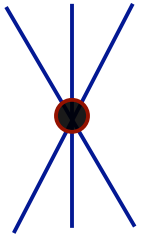
Binding energy
56.3(2.0) MeV

EFT N^{2}LO three-nucleon interaction

- Two-pion exchange term
  - Used in standard TNI models
    - Fujita-Miyazawa
    - Tucson-Melbourne
    - Urbana
    - Illinois
  - Low-energy constants c_1, c_3, c_4
    - Determined by the corresponding EFT NN interaction
      - Consistent NN & TNI
- One-pion exchange plus contact term
  - Low-energy constant c_D
    - Must be determined from experiment
- Contact term
  - Low-energy constant c_E
    - Must be determined from experiment
- A regulator appears in all terms
  - Depends on cutoff parameter Λ
    - Taken consistently from that used in the corresponding EFT NN interaction





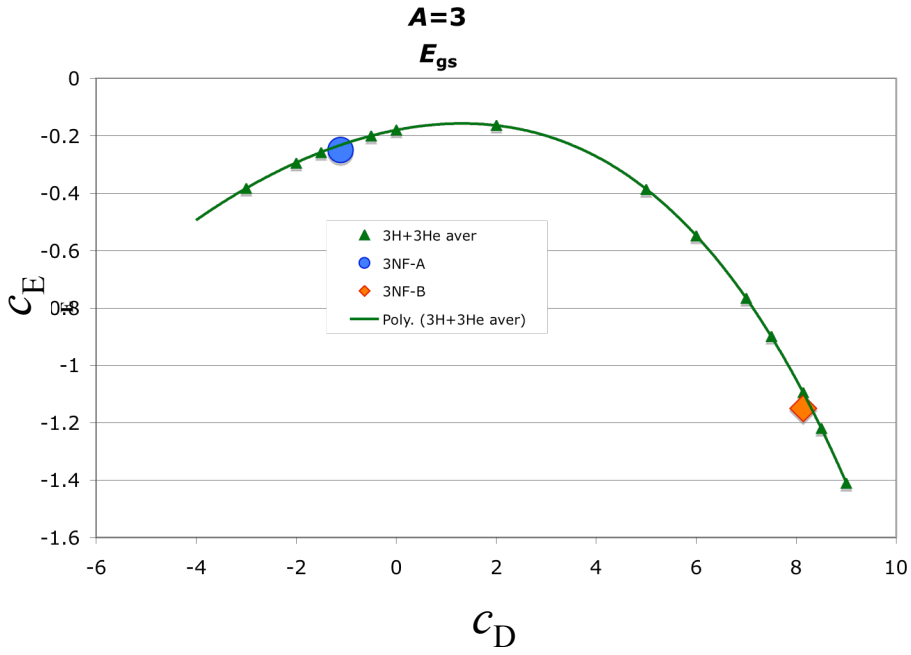


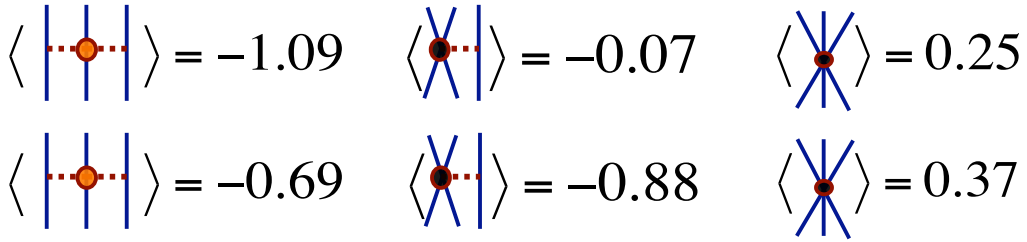
$$\exp[-(Q^2/\Lambda^2)^2]$$

Determination of the c_D and c_E low-energy constants

- Fit the ^{3}H and ^{4}He binding energies
  - Suggested and done by A. Nogga
  - Two solutions
    - 3NF-A
      - c_D=-1.11
      - c_E=-0.66
    - 3NF-B
      - c_D=8.14
      - c_E=-2.02
  - Regulator depending on Jacobi coordinates
- Present work: Two-pion term local in coordinate space
  - Change regulator: depending on momentum transfer
  - Need to re-fit c_D and c_E
    - A=3 done
    - ^{4}He under way
    - Presented results
      - "3NFA": c_D=-1.11, c_E=-0.25
      - "3NFB": c_D=8.14, c_E=-1.15
- 3NFA and 3NFB dominated by different terms
  - 3NFA two-pion term dominant
  - 3NFB one-pion term dominant
  - Contact term repulsive in both cases

$$\exp[-((p^2+q^2)/\Lambda^2)^2] \Leftrightarrow \exp[-(Q^2/\Lambda^2)^2]$$

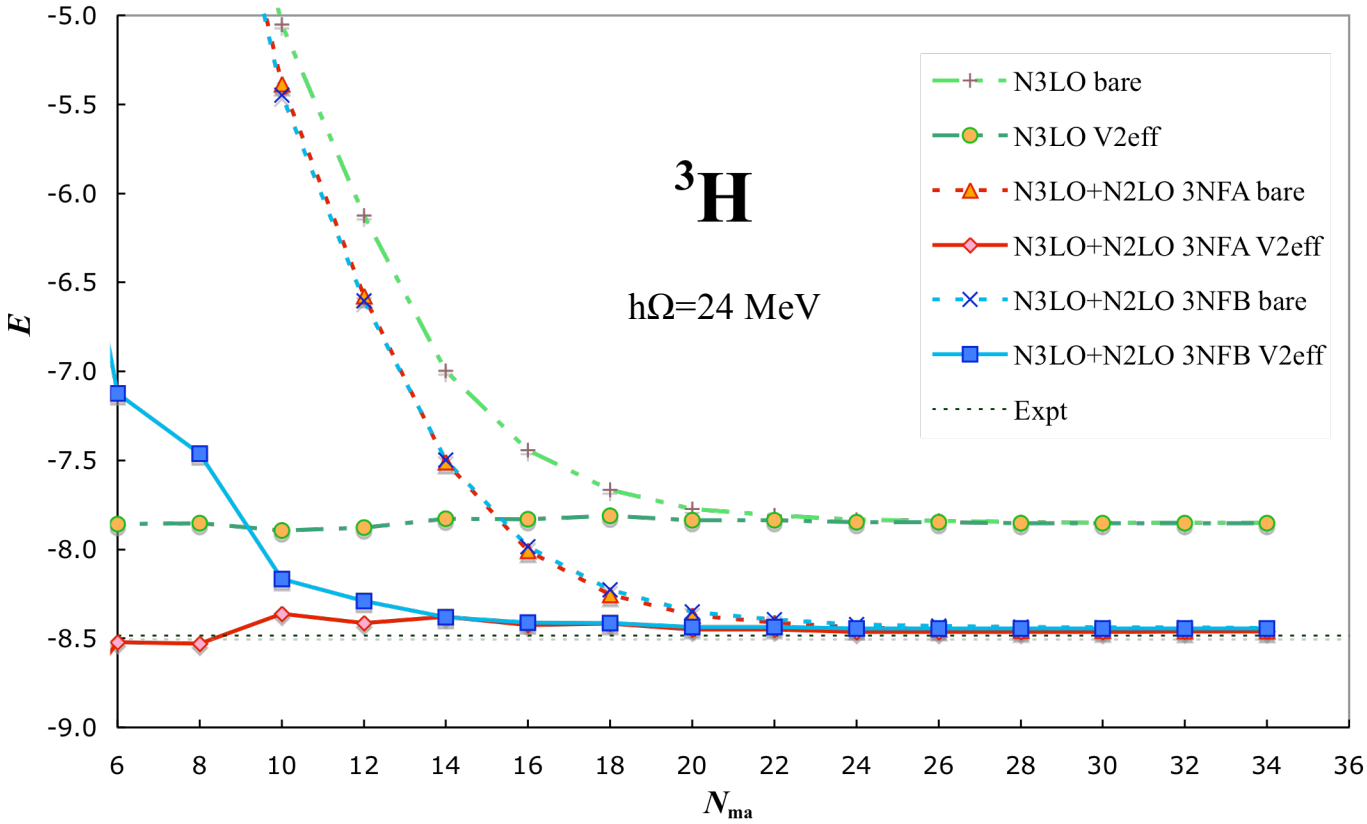




Convergence for ^{3}H with N^{3}LO NN and N^{3}LO NN plus N^{2}LO three-nucleon interaction

N^{2}LO 3NFA and 3NFB

Needed to reproduce experimental binding energy



NCSM
Jacobi coordinate
HO basis

N^{3}LO NN $\leftrightarrow V_{2\text{eff}}$
N^{2}LO 3NF $\leftrightarrow$ bare

Paves the way for including the V_{3b} in the NCSM *p*-shell calculations

Realistic three-nucleon interaction in the NCSM

- The lowest possible approximation n=3 three-body effective interaction
- Calculations performed in four steps
  - 1) Three-nucleon solutions for all relevant n=3 JT channels with and without V_{3b}

$$H^{\Omega} = \sum_{i=1}^{3}\left[\frac{\vec{p}_i^{\,2}}{2m} + \frac{1}{2}m\Omega^2\vec{r}_i^{\,2}\right] + \sum_{i<j}^{3}\left[V_{NN}(\vec{r}_i - \vec{r}_j) - \frac{m\Omega^2}{2A}(\vec{r}_i - \vec{r}_j)^2\right] + V_{123}^{3b}$$

  - 2) Three-body effective interaction by unitary transformation method
    - X_3
  - 3) Effective interaction in Jacobi coordinate HO basis, p-shell nuclei calculations more efficient in Cartesian coordinate Slater determinant basis
    - transformation must be performed
  - 4) A-nucleon calculation performed by a shell model code with a three-body capability
    - MFD, REDSTICK

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

Step 1

Step 2

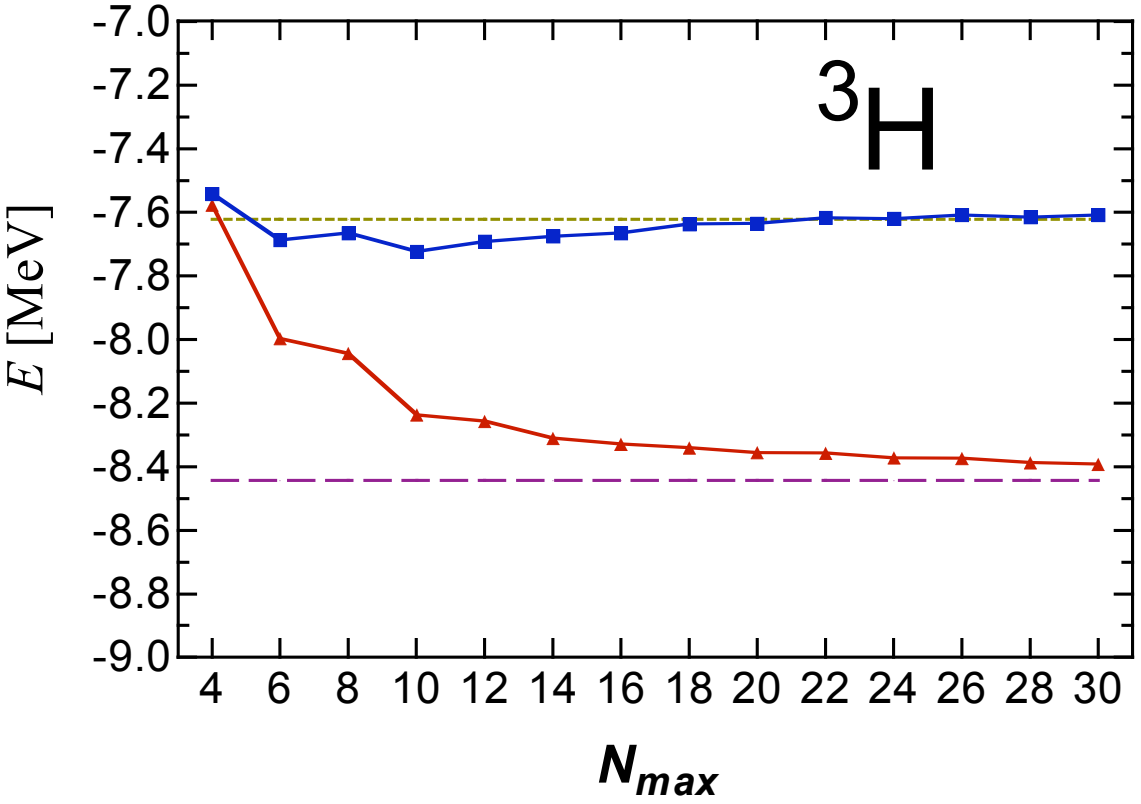
Step 3 Tranformation here

Step 4

Convergence for ^{3}H with a real three-body interaction

Tucson-Melbourne force

Needed to reproduce experimental binding energy



AV18 — NCSM

AV18 +TM'(81) — NCSM

AV18 exact — Faddeev calculation

AV18+TM'(81) exact — Faddeev calculation

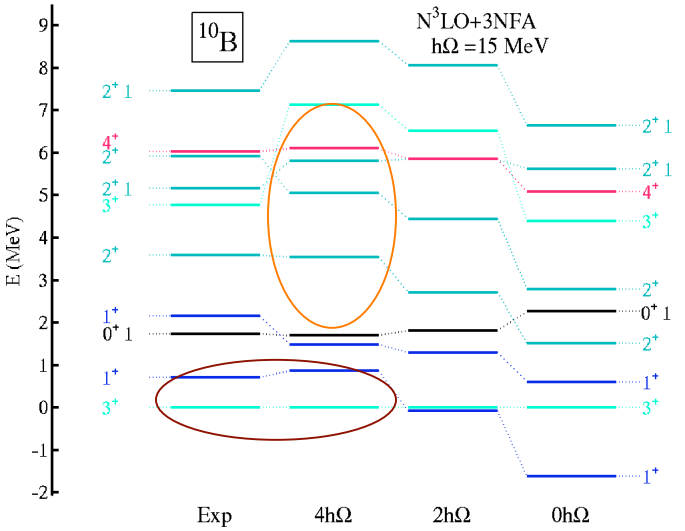
NCSM
Jacobi coordinate HO basis

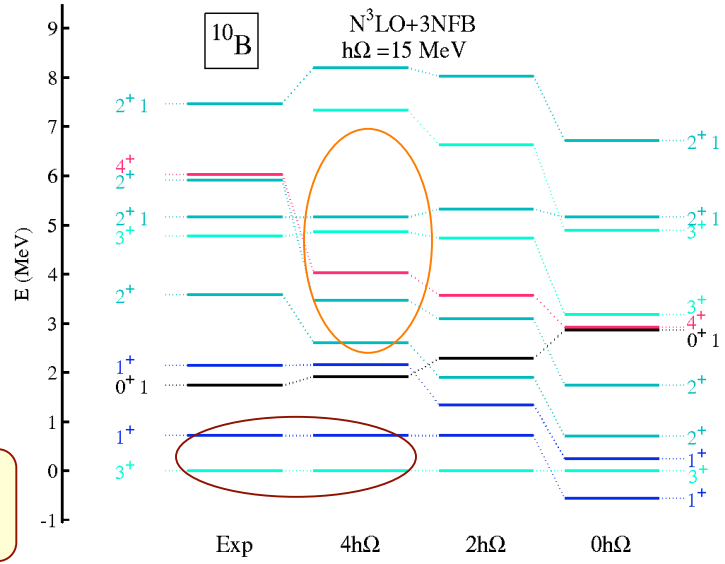
AV18 ↔ V_{2eff}
TM' ↔ bare

Paves the way for including the V3b in the NCSM p-shell calculations

^{10}B using N^{3}LO NN plus consistent N^{2}LO TNI

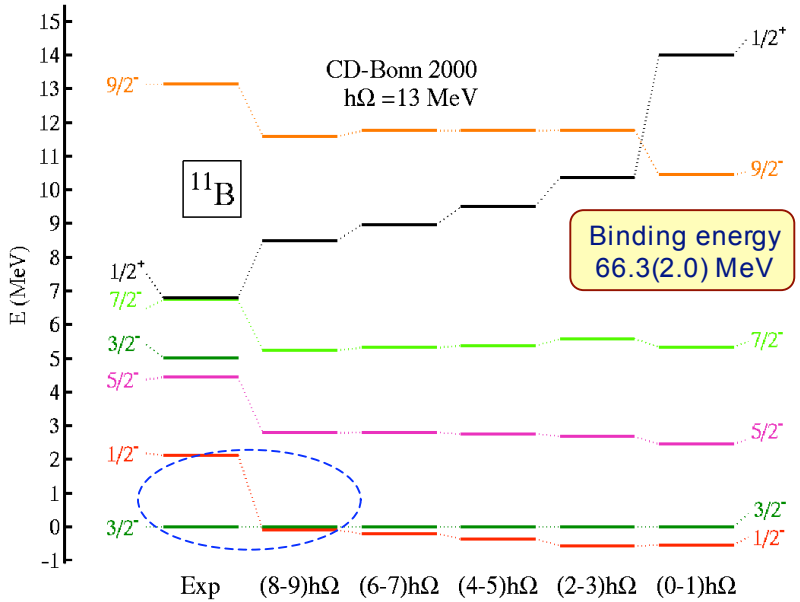
- N^{2}LO TNI 3NF-A dominated by two-pion exchange term
  - Results close to the TM'
  - Smaller radius
  - Larger binding energy
    - E_B=68.36 MeV
- N^{2}LO TNI 3NF-B dominated by one-pion exchange plus contact term
  - Visible difference in particular for higher-lying terms
  - Reasonable radius
  - No overbinding
    - E_B=63.14 MeV
- 6hΩ needed to check convergence of spectra
- Calculation to be re-done after proper fitting to ^{4}He

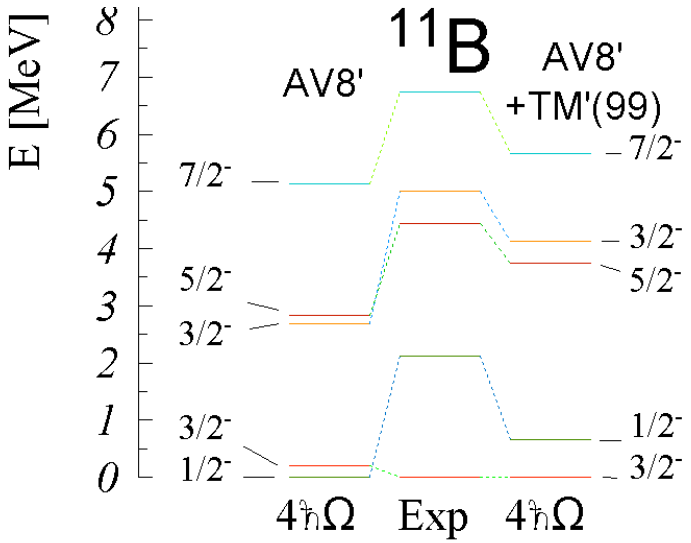




Both 3NF-A and 3NF-B resolve the ^{10}B ground state spin problem
Similarly like TM', Illinois 3NF, but unlike Urbana IX

^{11}B with the CD-Bonn and AV8' plus Tucson-Melbourne force





Gamow-Teller transitions
^{11}B ÷ ^{11}C
B(GT; $3/2^-_1$ ÷ J^-_f)

J^-_f	AV8'	AV8'+TM'(99)	Exp
$3/2^-_1$	0.765	0.315	0.345
$1/2^-_1$	0.909	0.591	0.440
$5/2^-_1$	0.353	0.517	0.526
$3/2^-_2$	0.531	0.741	0.525
$5/2^-_2$	0.197	0.625	0.461

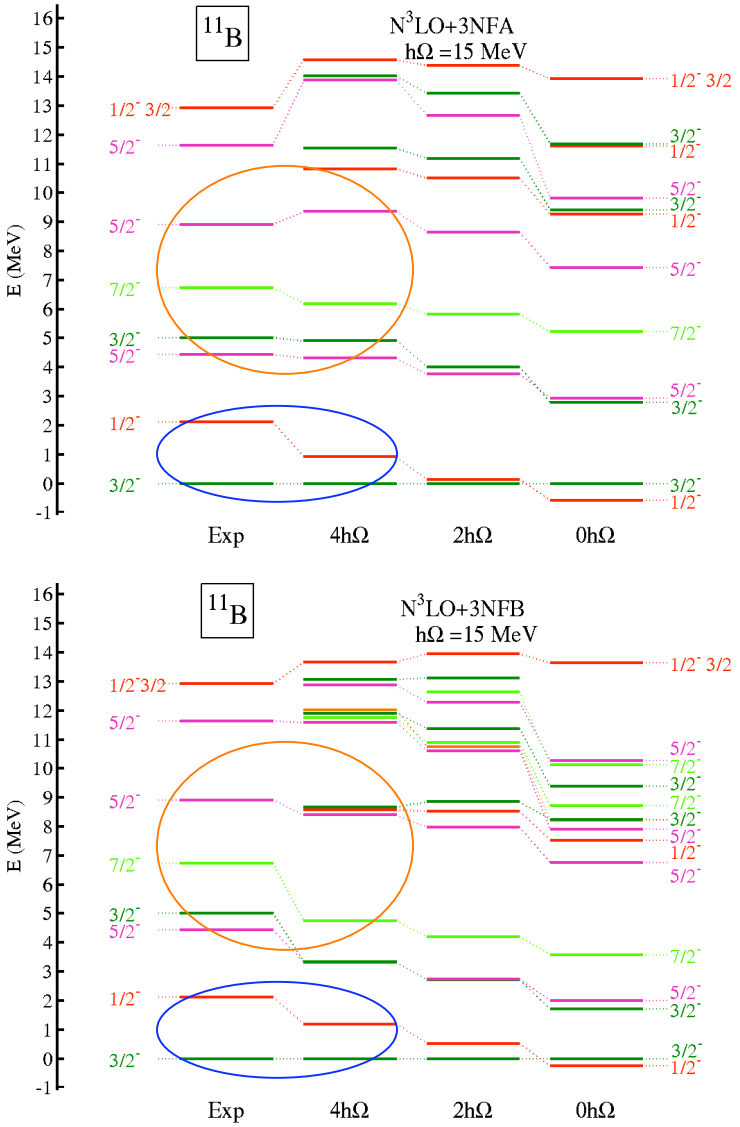
New (^{3}He,t) experiment at RCNP Osaka, Y. Fujita *et al.*, PRC **70**, 011306(R) (2004).

V_{3b} : Bad description of ^{11}B greatly improved

^{11}B using N^{3}LO NN plus consistent N^{2}LO TNI

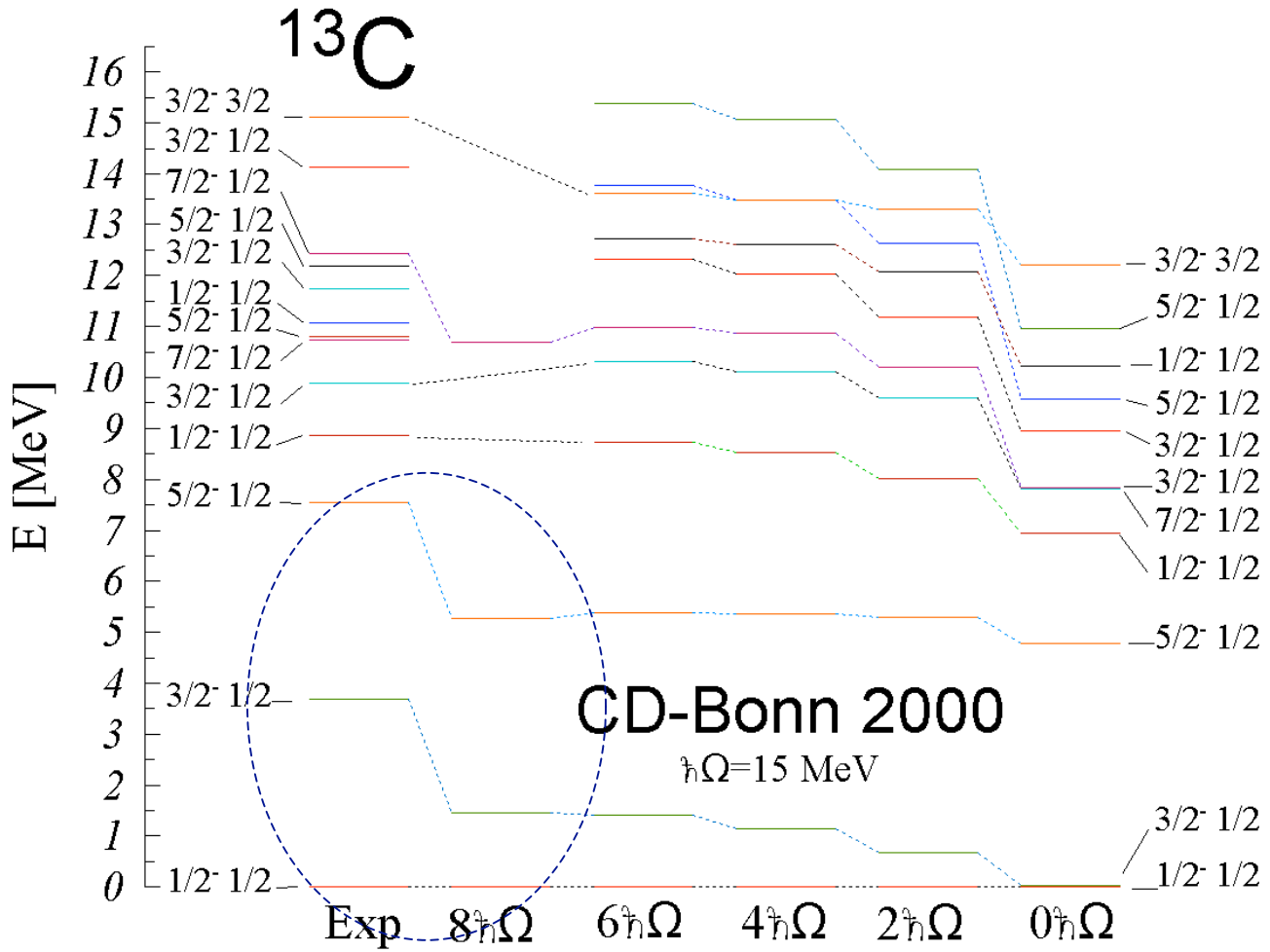
- N^{2}LO TNI 3NF-A dominated by two-pion exchange term
  - Results close to the TM'
  - Better agreement for higher-lying states
  - Smaller radius
  - Larger binding energy
    - E_B=82.68 MeV
- N^{2}LO TNI 3NF-B dominated by one-pion exchange plus contact term
  - Visible difference in particular for higher-lying terms
  - Better agreement for lowest states
  - Reasonable radius
  - No overbinding
    - E_B=76.22 MeV
- 6hΩ needed to check convergence of spectra
- Calculation to be re-done after proper fitting to ^{4}He

Both 3NF-A and 3NF-B predict correct level ordering of lowest states of ^{11}B, similarly like TM'



^{13}C using the CD-Bonn NN potential

- Large basis calculation
- Complex spectrum
- Correct level ordering for 5 lowest states
- Good convergence of excitation energies
- Level spacing incorrect

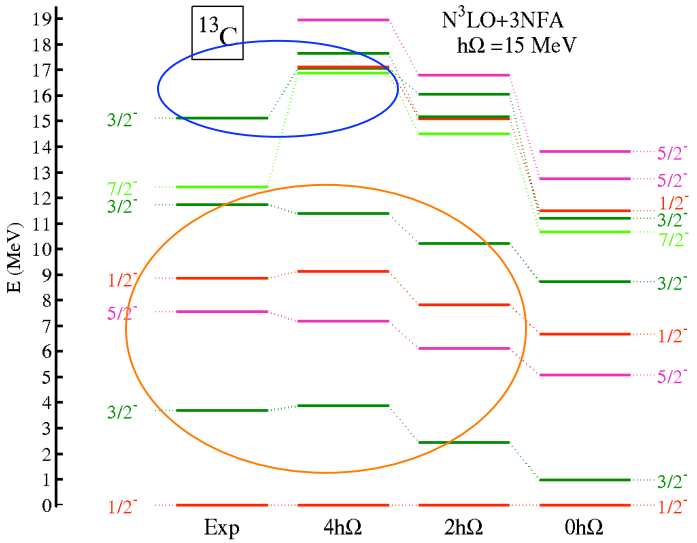


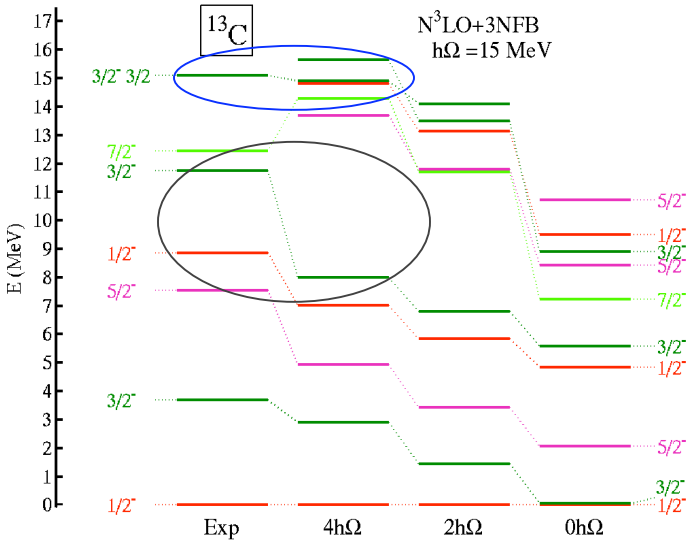
Binding energy
86.5(2.0) MeV

^{13}C using N^{3}LO NN plus consistent N^{2}LO TNI

- N^{2}LO TNI 3NF-A dominated by two-pion exchange term
  - Results close to the TM'
  - Larger binding energy
    - E_B=112.6 MeV
  - Smaller radius
  - Better agreement for low-lying states
    - Issue of convergence
- N^{2}LO TNI 3NF-B dominated by one-pion exchange plus contact term
  - Visible difference in particular for higher-lying terms
  - No overbinding
    - E_B=103.2 MeV
  - Reasonable radius
  - Better agreement for T=3/2 states
  - $3/2^-_2$ appears to be underpredicted
- 6hΩ needed to check convergence of spectra
- Calculation to be re-done after proper fitting to ^{4}He

Both 3NF-A and 3NF-B improve level spacing of lowest states of ^{13}C, compared to CD-Bonn





First *p*-shell nuclei results with EFT based NN plus consistent NNN interaction

- N^{3}LO NN potential by D. Entem and R. Machleidt
- N^{2}LO three-nucleon interaction with consistent c_1, c_3, c_4 and Λ
  - c_D and c_E terms determined as suggested by A. Nogga to reproduce A=3,4 binding energies
- Two solutions: 3NF-A, 3NF-B
  - Predict different spectra as well as binding energies, radii, and electromagnetic properties
  - Both solve major issues like level ordering of lowest states
  - Neither give a perfect agreement with experiment and it is not straightforward to judge which is preferable at this point
  - Most important issue is improvement of convergence
    - 6hΩ calculations within reach
- One-pion and contact terms important: 3NF-A and 3NF-B improves TM' results
  - No overbinding, larger radii
  - Level ordering of lowest states the same
  - Fine details: Spectra similarly (in)accurate
- N^{3}LO LEC c_1, c_3, c_4 different from those used in TM'(99), also different from those given by Rentmeester *et al.*
  - Worth-investigating different sets of LEC in the TNI

TM' $\Leftrightarrow$ N^{2}LO

$$a' = \frac{4m_\pi^2 c_1}{f_\pi^2}$$

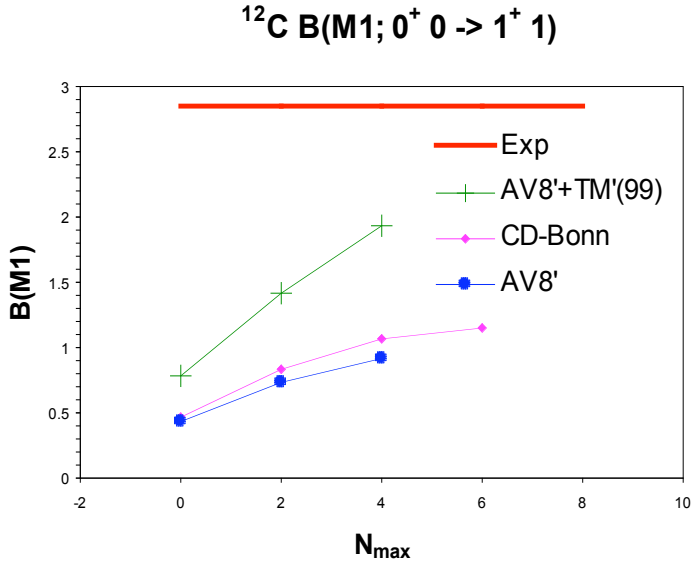
$$b = \frac{2c_3}{f_\pi^2}$$

$$d = -\frac{c_4}{f_\pi^2}$$

	c_1	c_3	c_4
Entem	-0.81	-3.20	5.40
Rentmeester	-0.76	-4.78	3.96
TM'(99)	-0.93	-4.55	2.44

Neutrino scattering on ^{12}C

- Exclusive $0^+\ 0 \rightarrow 1^+\ 1$ cross section & transistions
- Extremely sensitive to the spin-orbit interaction strength
  - B(GT) (B(M1)) - $\sigma\tau$,
    - No spin-orbit $0^+\ 0$ and $1^+\ 1$ in different SU(4) irreps
      - no transition
    - ^{12}C ground state 8 nucleons in $p_{3/2}$
      - Transition overestimated by a factor of six
- NCSM - no fit, no free parameters
  - V_{2b} up to 6hΩ - saturation
    - Underestimates by a factor of 2-3
  - $V_{2b}+V_{3b}$ up to 4hΩ
    - Significant improvement
  - Different processes dominated by different Q
    - Correlation with M1 transverse form factor

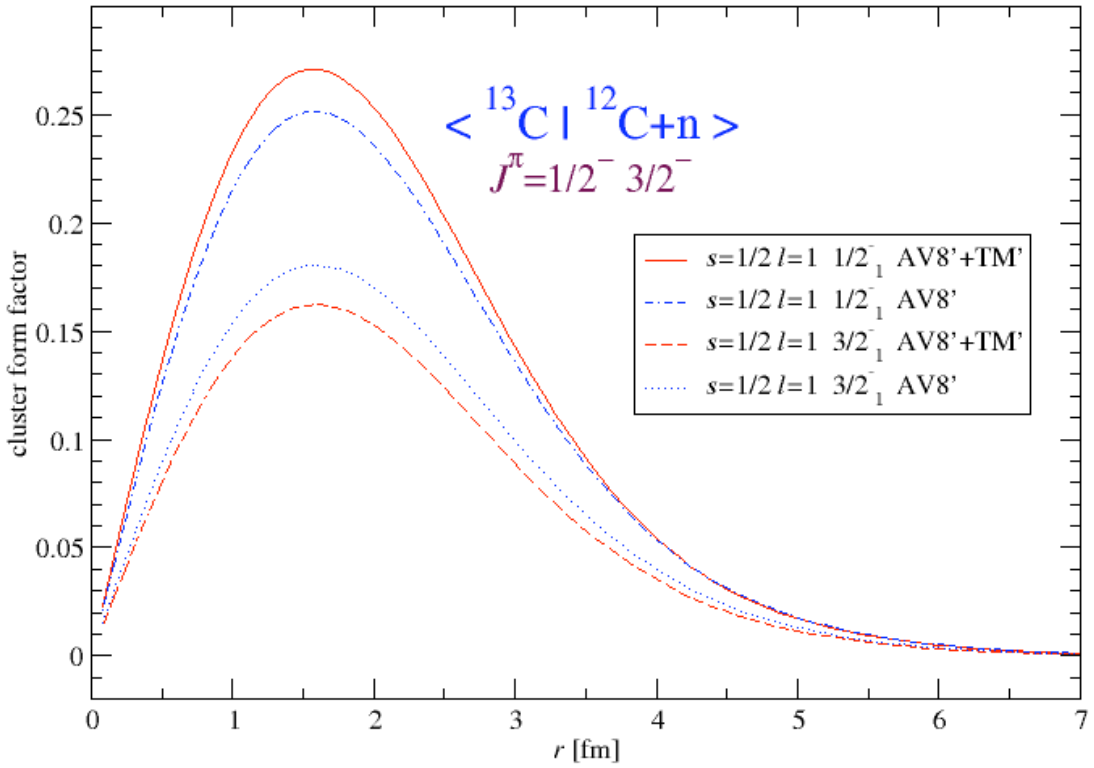


	AV8'	AV8'+TM'(99)	Exp
B(GT)	0.26	0.67	0.88
	CD-Bonn	AV8'+TM'(99)	Exp
(ν e^-)	3.69	6.8	8.9±0.3±0.9
(ν μ^-)	0.312	0.537	0.56±0.08±0.1
μ-capture	2.38	4.43	6.0±0.4

V_{3b} increases the strength of the spin-orbit force

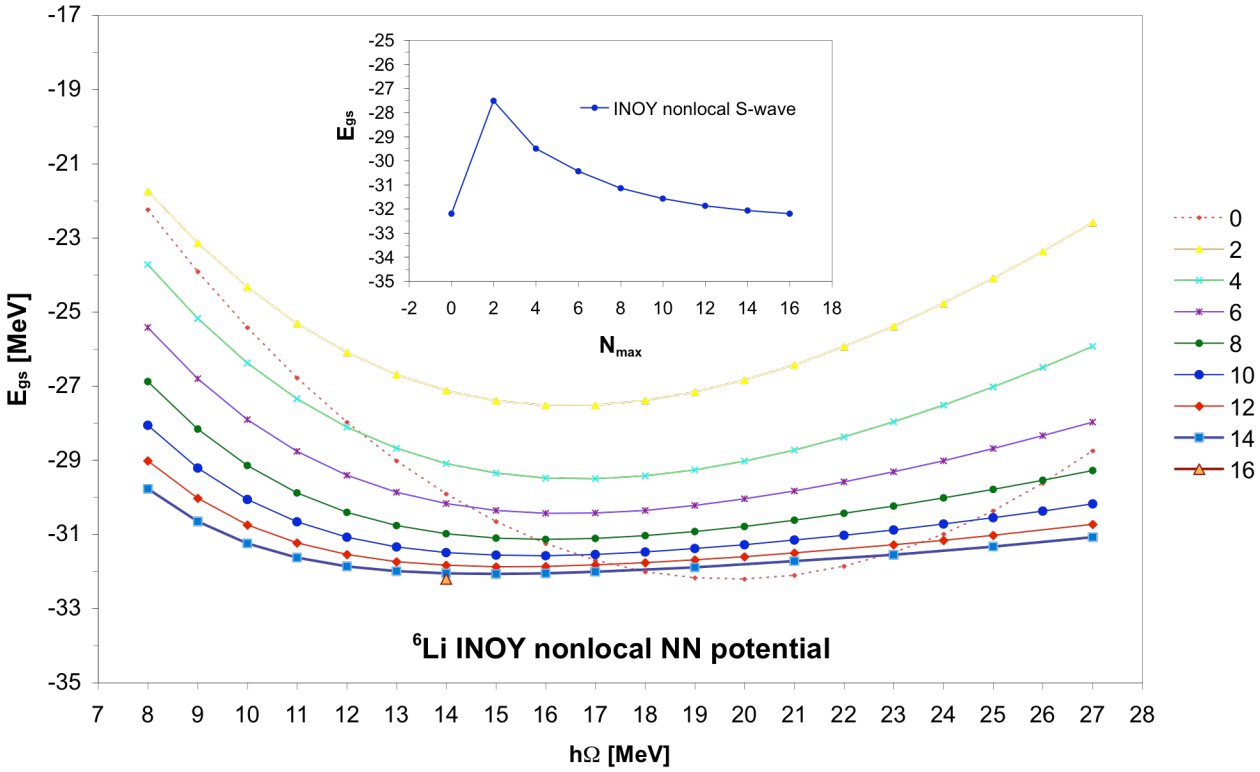
Cluster form factors for $\langle {}^{13}\mathrm{C} \,|\, {}^{12}\mathrm{C}+\mathrm{n} \rangle$

- Effects of the TNI on the $\langle {}^{13}\mathrm{C} \,|\, {}^{12}\mathrm{C}+\mathrm{n} \rangle$ overlap integrals
  - Increases $J^{\pi}= 1/2^{-}$ cluster form factor and spectroscopic factor
  - Reduces $J^{\pi}= 3/2^{-}$ cluster form factor and spectroscopic factor
- Stronger spin-orbit interaction due to the TNI



NCSM binding energy calculations with INOY NN potentials

P. Doleschall *et al.*, Phys. Rev. C 67, 064005 (2003)

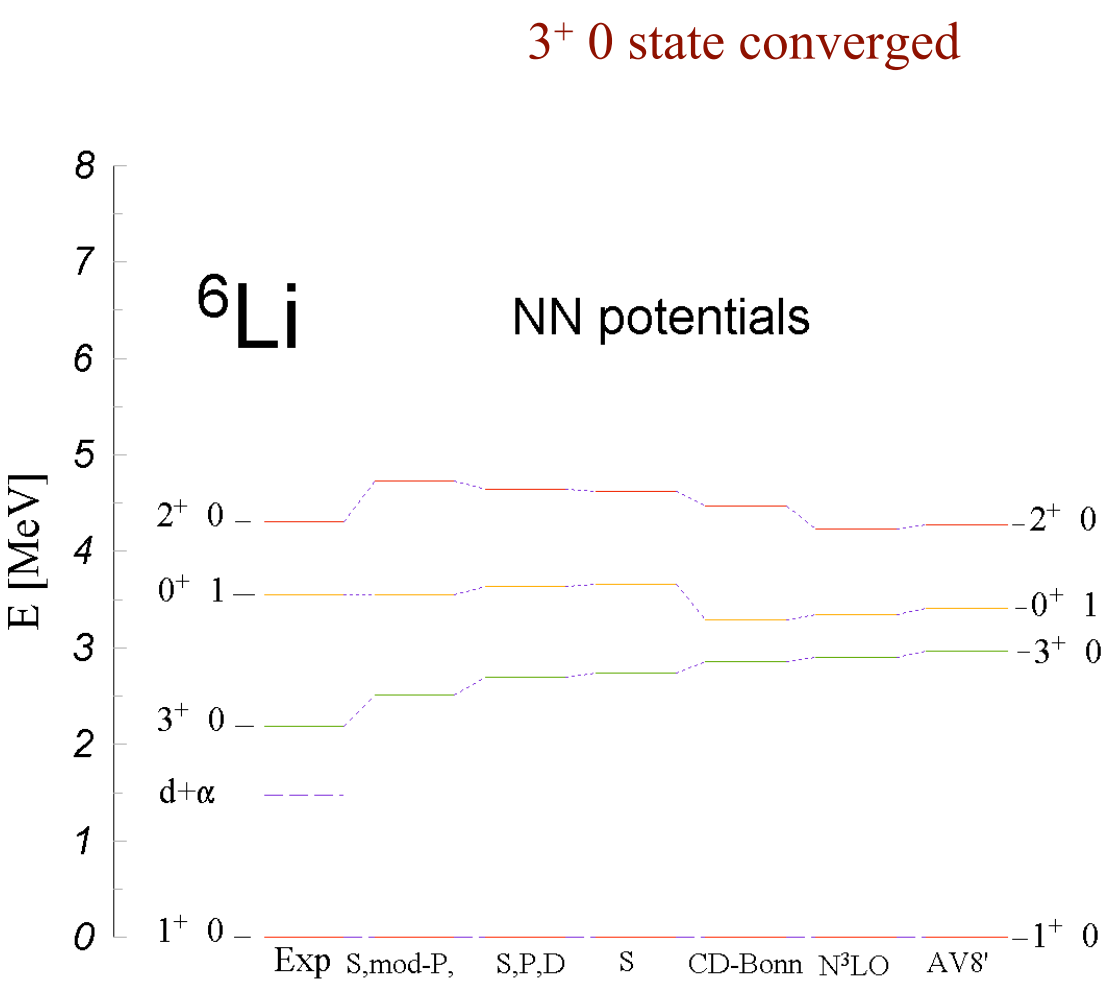


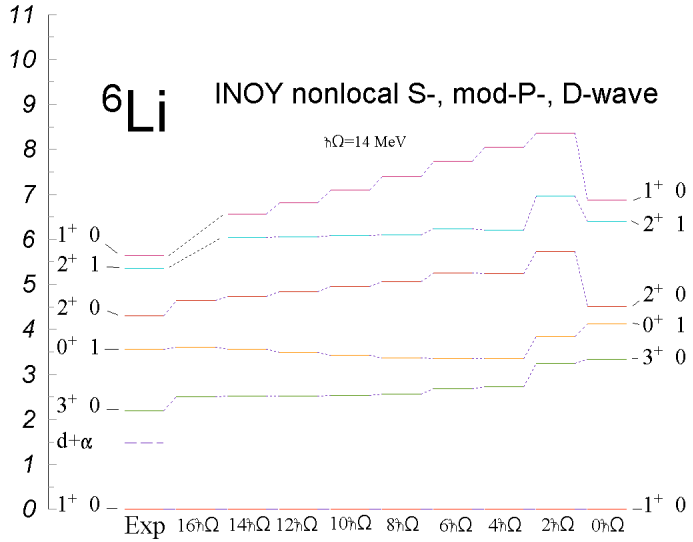
E[MeV]	INOY S	Exp
^{3}H	8.47(1)	8.48
^{3}He	7.71(1)	7.72
^{4}He	29.1(2)	28.30
^{6}Li	32.3(3)	31.99
^{6}He	29.1(5)	29.27
^{7}Li	38.9(8)	39.25
^{7}Be	37.2(8)	37.60
^{8}Li	39.9(1.2)	41.28
^{8}B	36.1(1.2)	37.74
^{9}Be	56.1(1.5)	58.16
^{10}B	62.5(2.0)	64.75
^{12}C	93.5(2.5)	92.16
^{16}O	138.0(4.0)	127.6

Binding energies much closer to experiment than for standard NN potentials
However, isospin dependence problematic: ^{4}He, ^{12}C, ^{16}O overbound; ^{8}B, ^{8}Li underbound
Radii typically underestimated (^{4}He: r=1.39 fm)

^{6}Li spectrum sensitive to the NN potential

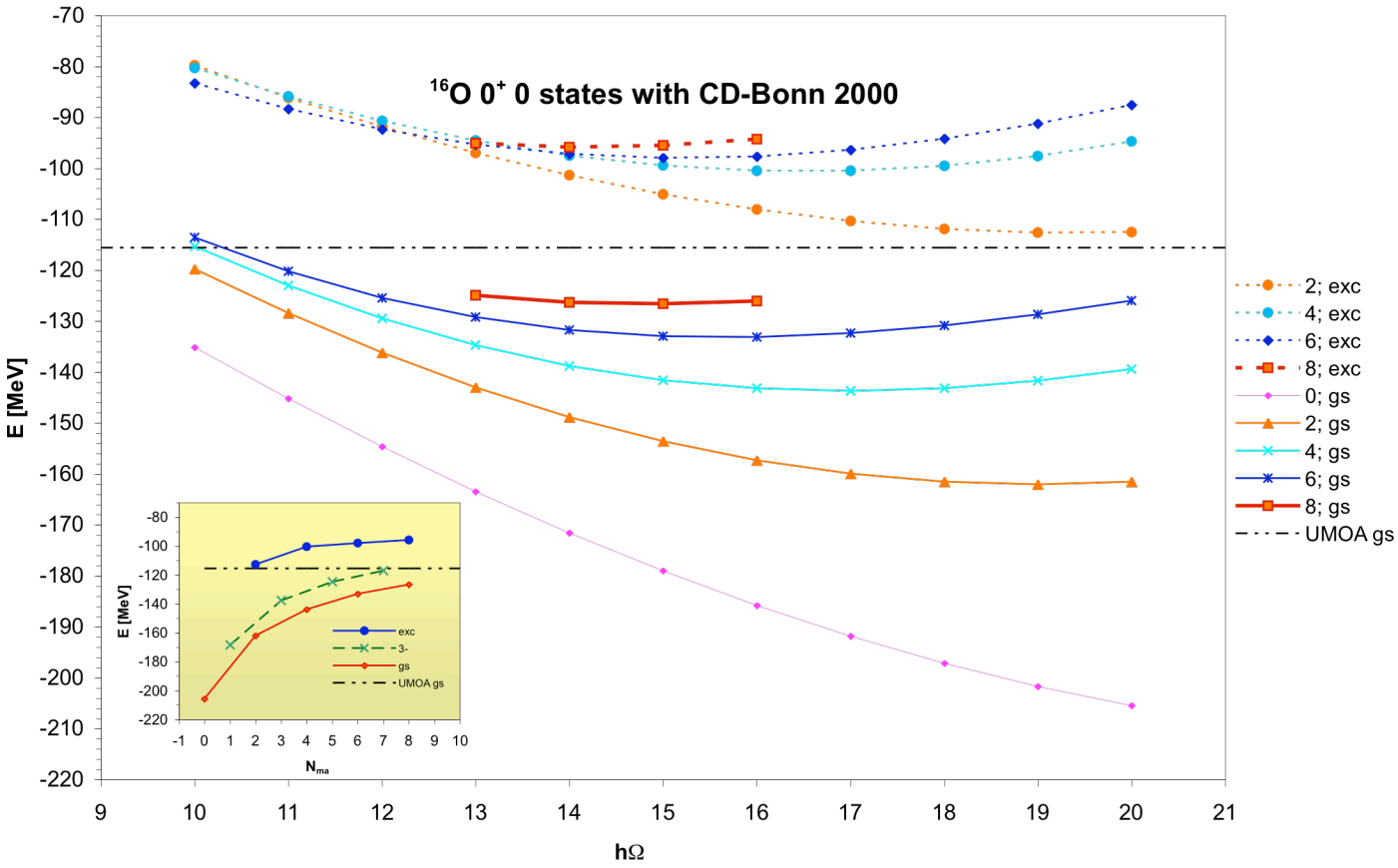
3^+ 0 state converged





INOY nonolocal NN potential with modified triplet P-waves:
Best agreement with experiment
Very similar effect as adding three-nucleon interaction to standard NN potentials

^{16}O ground and excited 0^+ 0 and 3^- 0 states



- Ground state changes structure
  - 0hΩ less than 50%, large 2hΩ and 4hΩ components
  - Energy consistent with the UMOA result
- Excited 3^- 0 state dominated by 1hΩ; follows the ground state
- Excited 0^+ 0 state 2hΩ dominated; stable
- The 4hΩ dominated state still higher in the 8hΩ model space

Conclusions and outlook

- *Ab initio* no-core shell model
  - Method for solving the nuclear structure problem for light nuclei
  - Apart from the GFMC the only working method for $A>4$ at present
  - Advantages
    - applicable for any NN potential
    - Presently the only method capable to apply the QCD χPT NN+NNN interactions to *p*-shell nuclei
    - Easily extendable to heavier nuclei
    - Calculation of complete spectra at the same time
  - Success - importance of three-nucleon forces for nuclear structure

Work in progress

- Calculations with realistic three-body forces in the *p*-shell
  - Better determination of the three-body force itself
- Coupling of the NCSM to nuclear reactions theories
  - Direct reactions
    - Density from NCSM plus folding approaches
  - Low-energy resonant and nonresonant reactions
    - RGM-like approach
      - Exotic nuclei: RIA
      - Thermonuclear reaction rates: Astrophysics

Future plans

- Extensions to heavier nuclei
  - Effective interaction for valence nucleons
    - RIKEN, RIA