# Nuclear structure from chiral-perturbation-theory two- plus three-nucleon interactions

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# 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
  - $^{7}$Li, $^{10}$B, $^{11}$B, $^{12}$C, $^{13}$C
- 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 $N^3LO$, three-nucleon chiral $N^2LO$
- Modification by center-of-mass harmonic oscillator (HO) potential (Lipkin 1958)

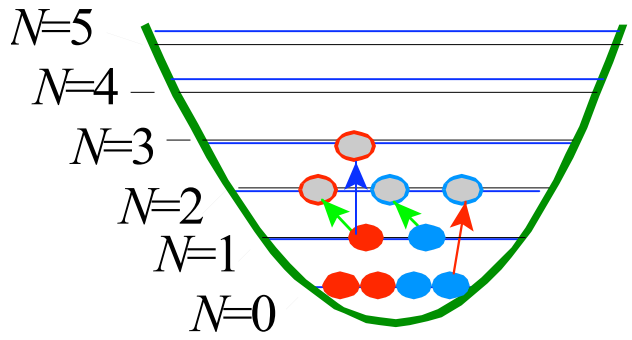
$$\frac{1}{2} A m\Omega^2 \vec{R}^2 = \sum_{i=1}^{A} \frac{1}{2} m\Omega^2 \vec{r}_i^{\,2} - \sum_{i<j}^{A} \frac{m\Omega^2}{2A} (\vec{r}_i - \vec{r}_j)^2$$

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

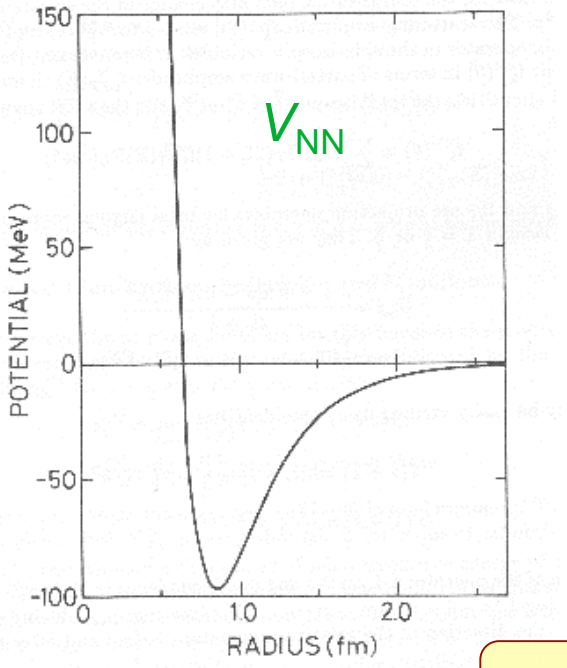
$$H^{\Omega} = \sum_{i=1}^{A} \left[ \frac{\vec{p}_i^{\,2}}{2m} + \frac{1}{2} m\Omega^2 \vec{r}_i^{\,2} \right] + \sum_{i<j}^{A} \left[ V_{NN}(\vec{r}_i - \vec{r}_j) - \frac{m\Omega^2}{2A} (\vec{r}_i - \vec{r}_j)^2 \right] \quad \left( + \sum_{i<j<k}^{A} V_{ijk}^{3b} \right)$$

# 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



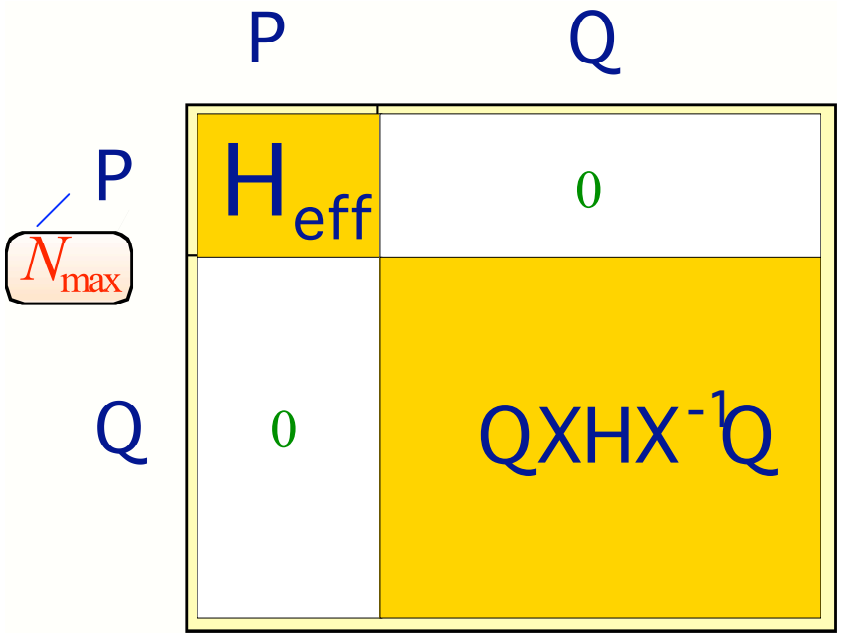

Nucleon-nucleon interaction




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

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

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

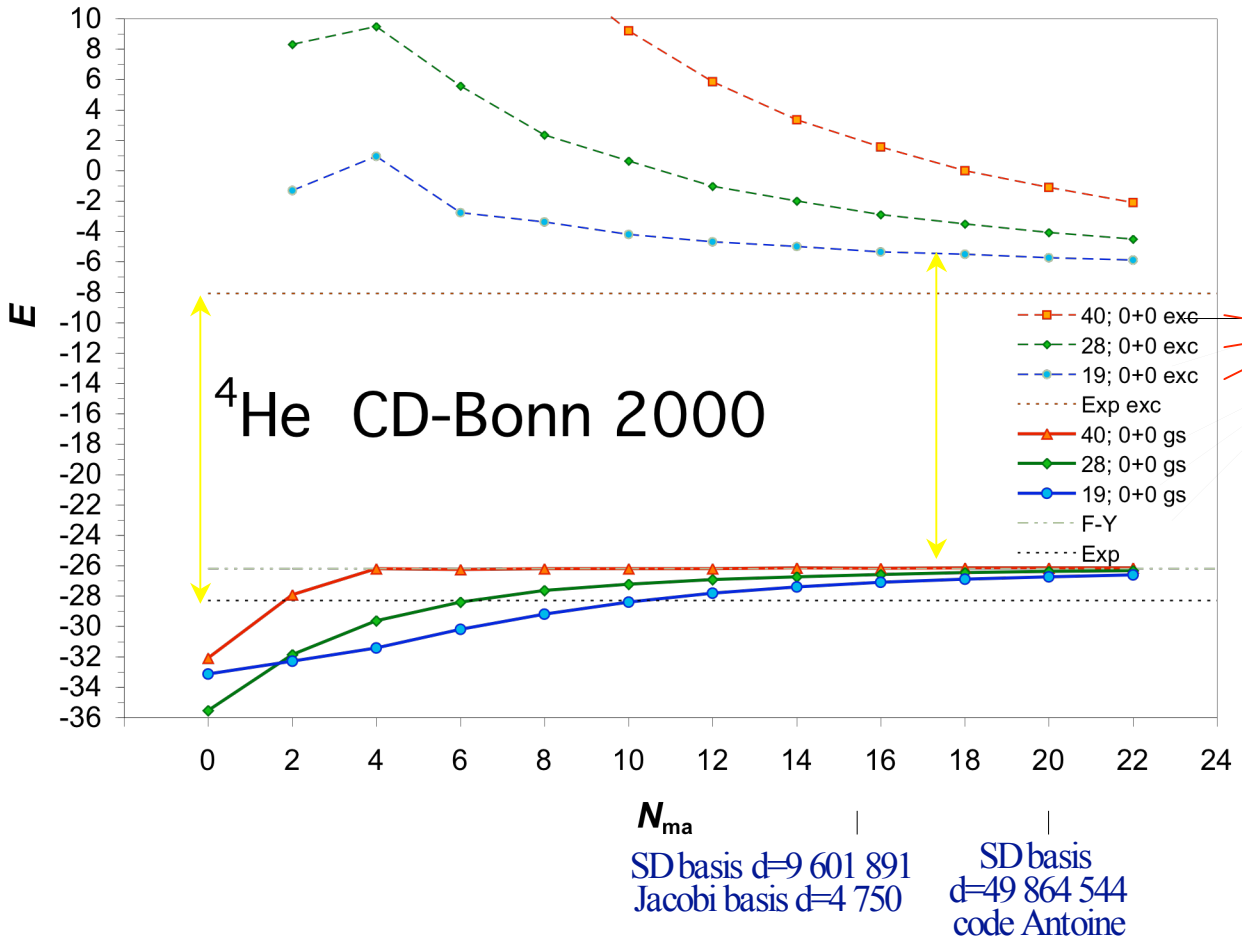
unitary $X = \exp[-\arctan h(\omega^{+} - \omega)]$

- Properties of $H_{\text{eff}}$ 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

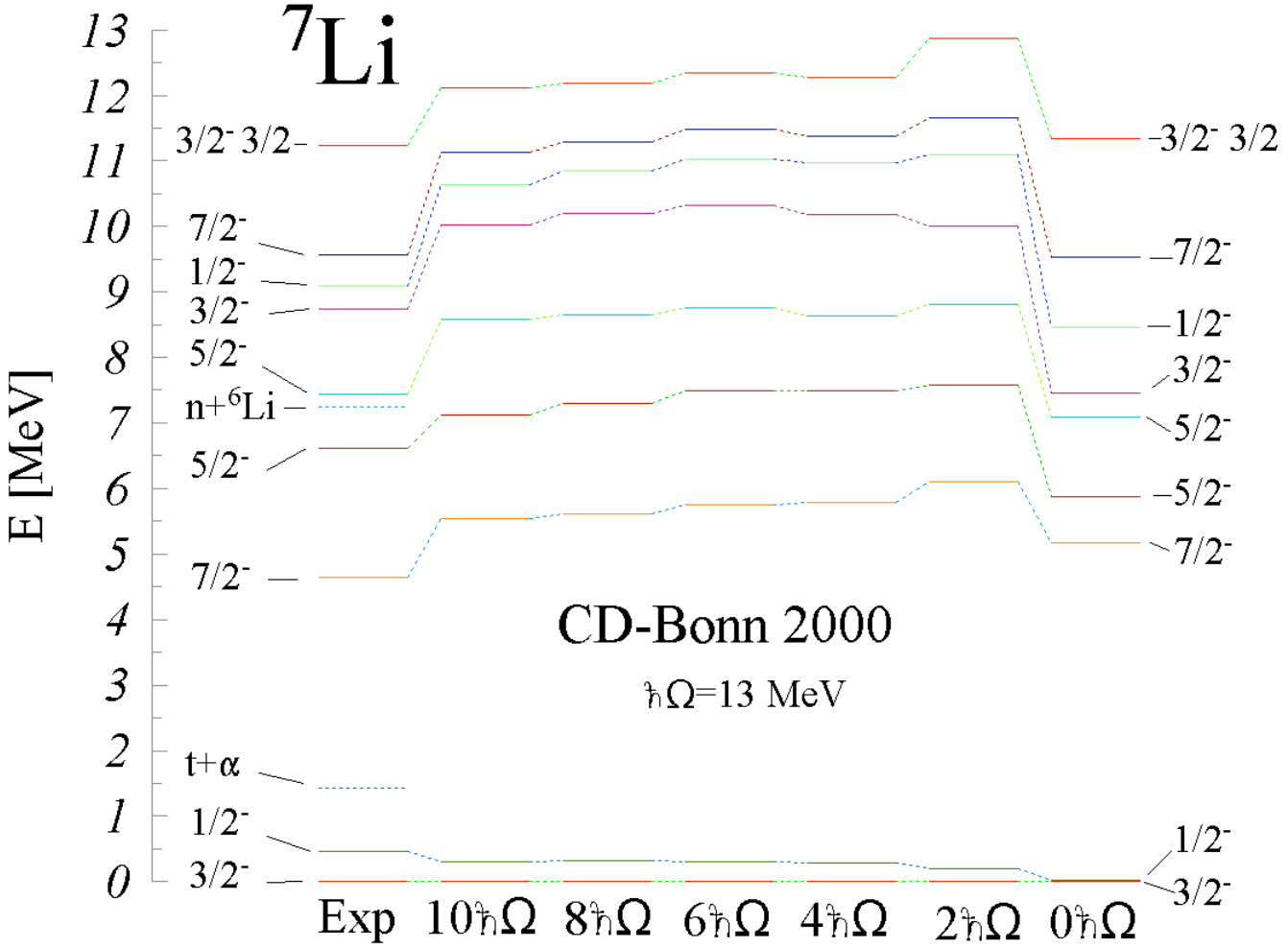
NCSM
Jacobi coordinate *or* Slater determinant HO basis

$n$=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

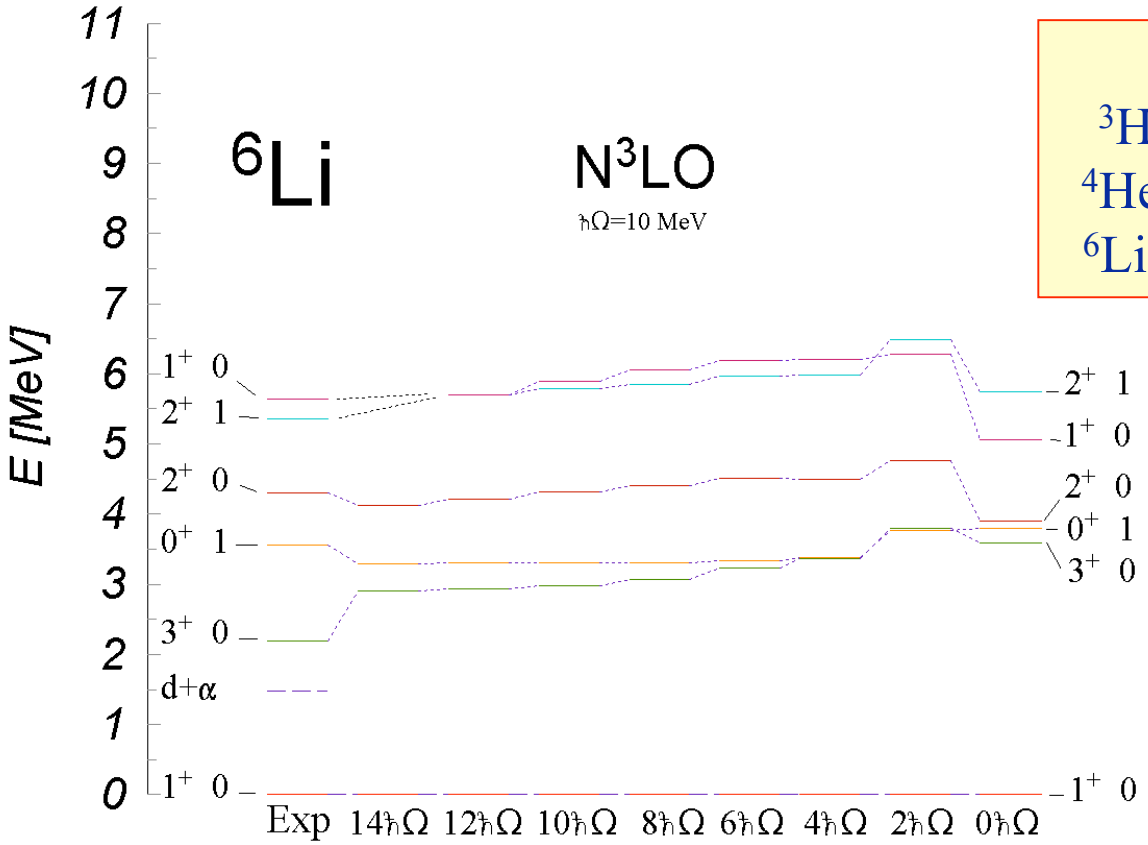
New evaluation NPA**708**,3(2002) introduces $1/2^-_2$ and orders the states as in calculation

Binding energy 35.5(5) MeV

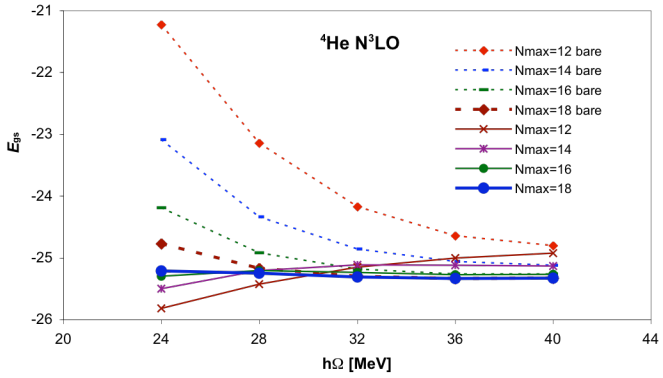
Convergence of excitation energies
Realistic NN interactions provide reasonable description of nuclear structure

# 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)

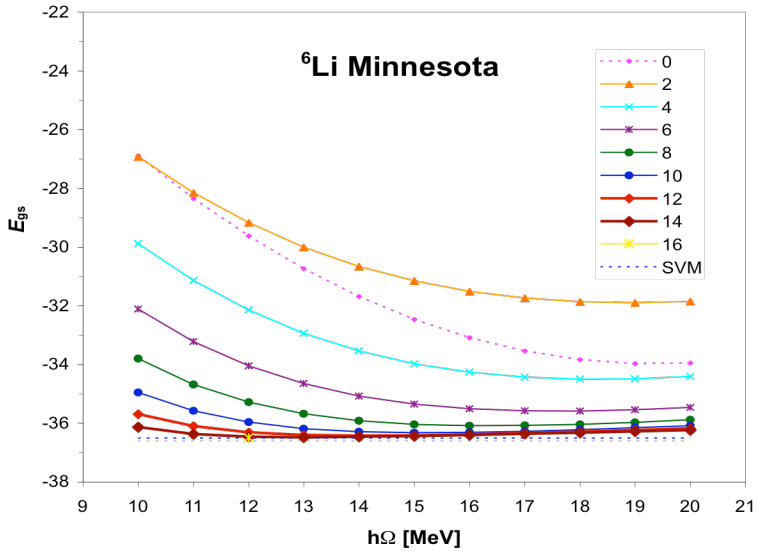


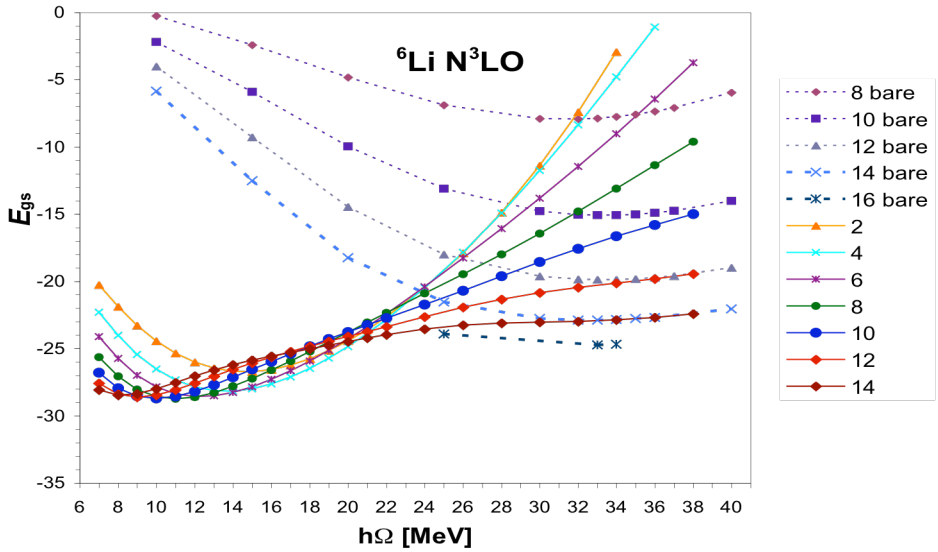

| | N$^3$LO | Exp |
|---|---|---|
| $^3$H | 7.85 MeV | 8.48 MeV |
| $^4$He | 25.35(5) MeV | 28.30 MeV |
| $^6$Li | 28.5(5) MeV | 31.99 MeV |

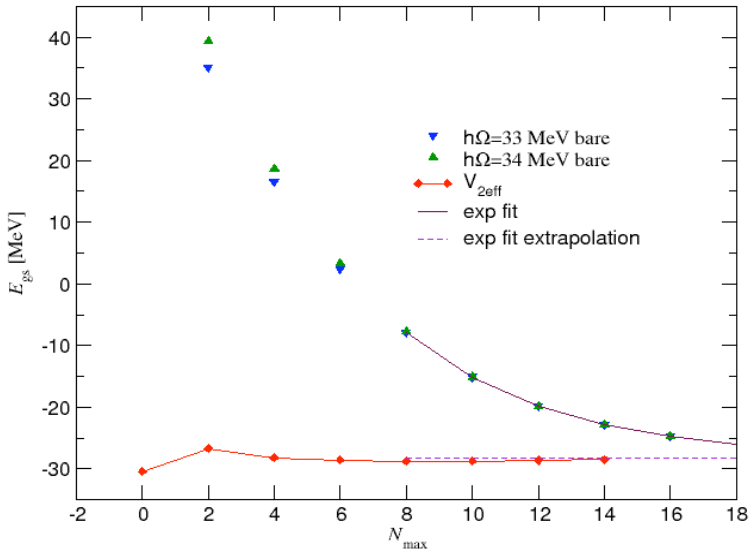


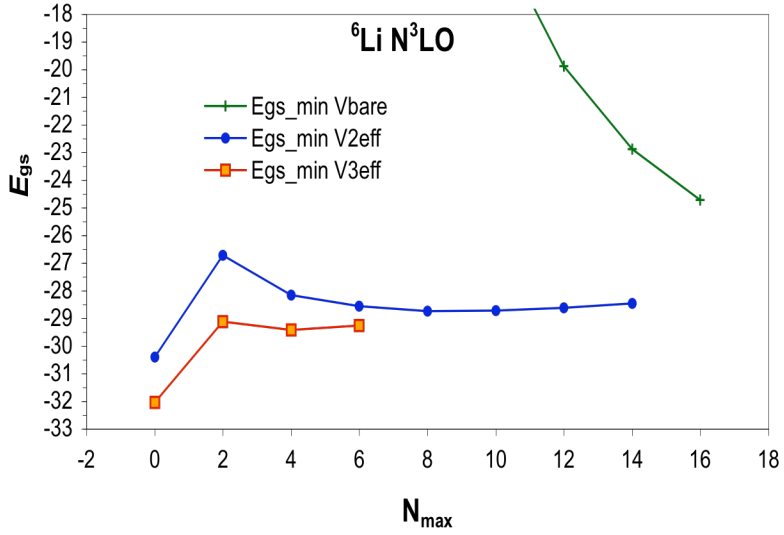

Converged $^6$Li excitation energies
Correct level ordering, level spacing not right

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



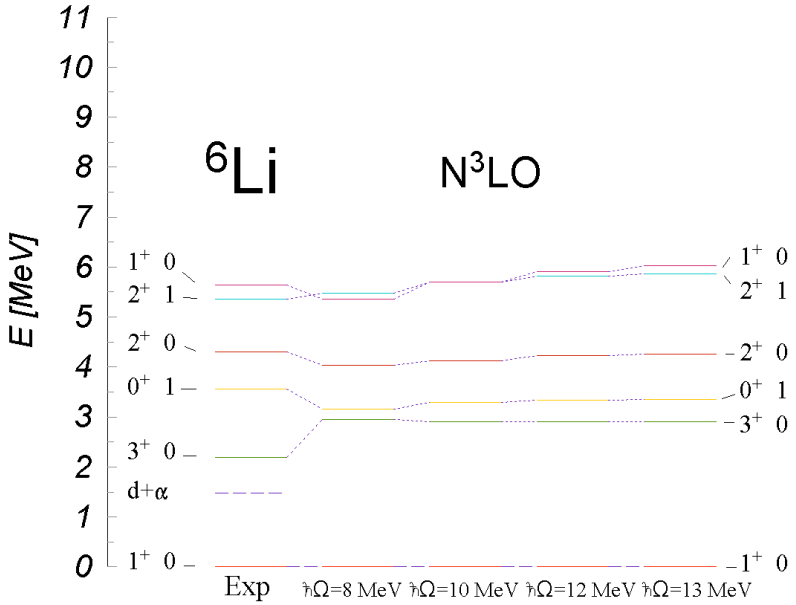



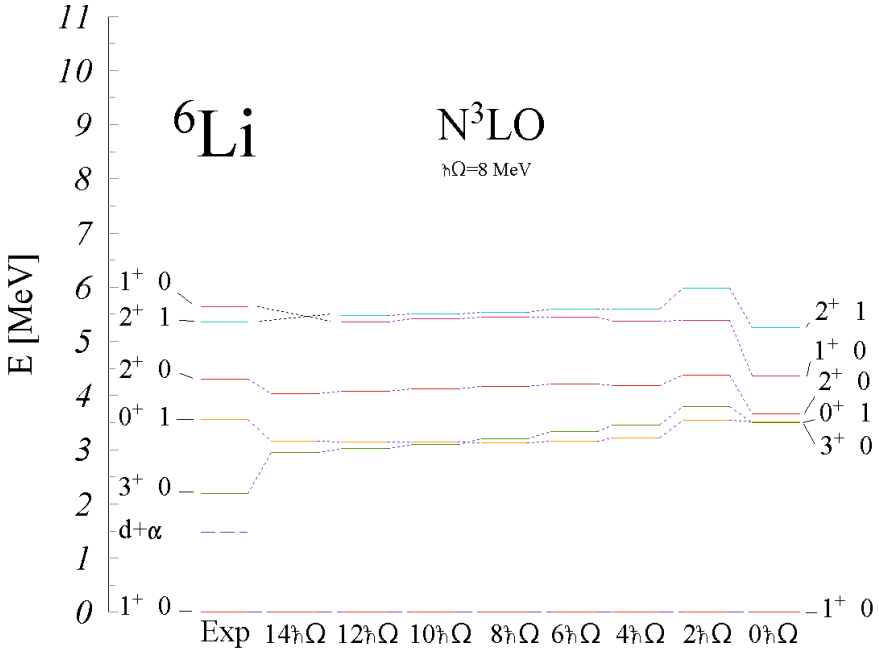



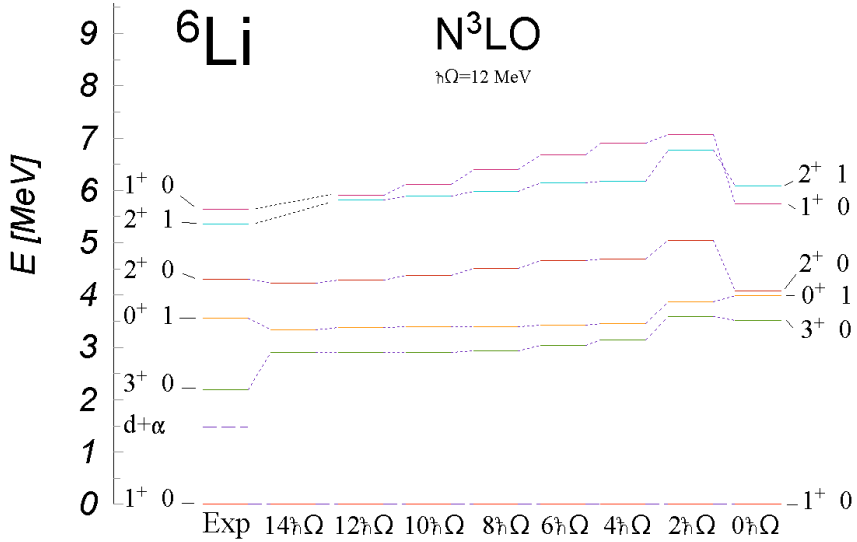
# NCSM calculations with the EFT N$^3$LO NN interaction: Convergence of $^6$Li excitation energies

Difficult convergence of the binding energy

Good convergence of the excitation energies

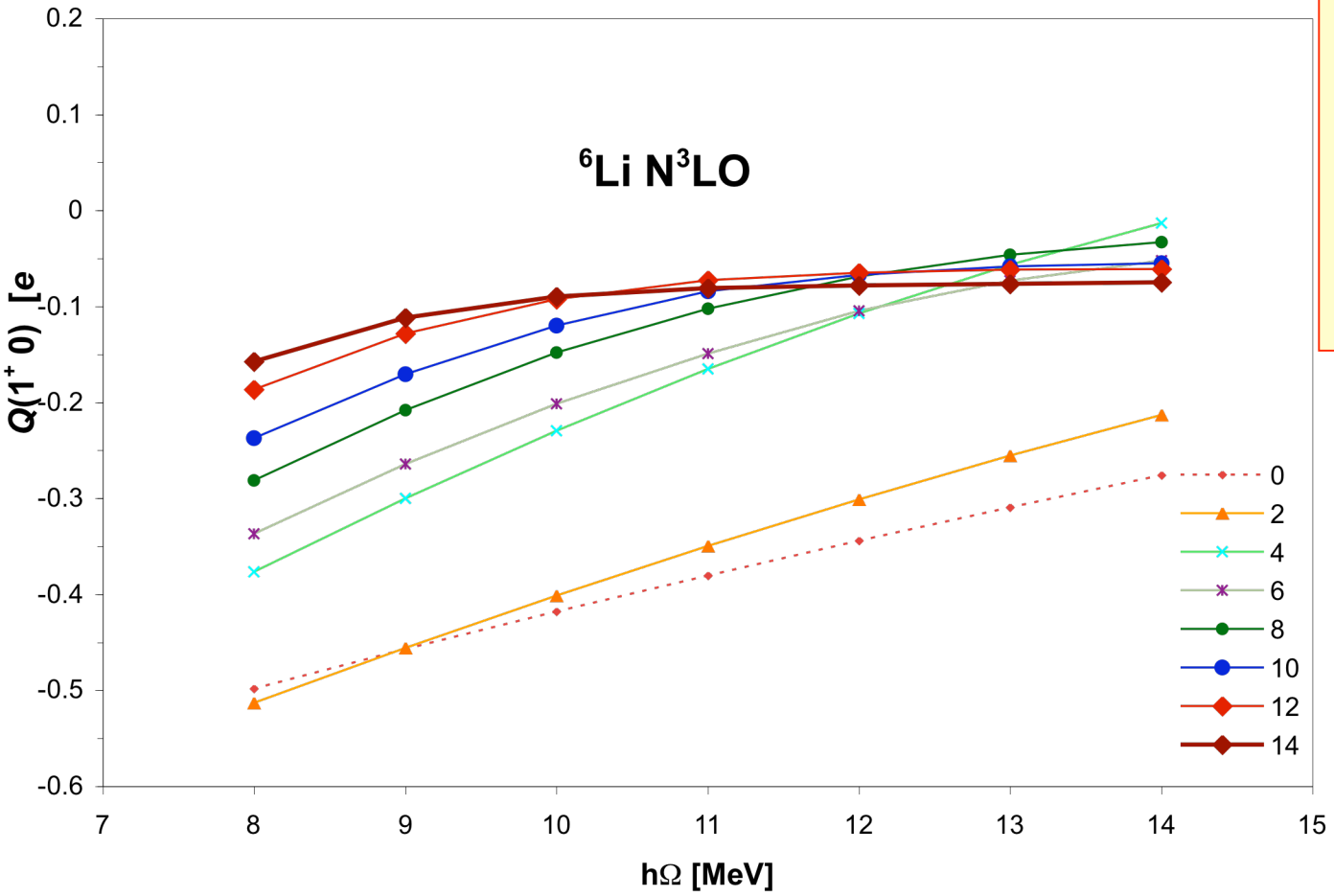


# $^6$Li quadrupole moment

## EFT N$^3$LO NN potential

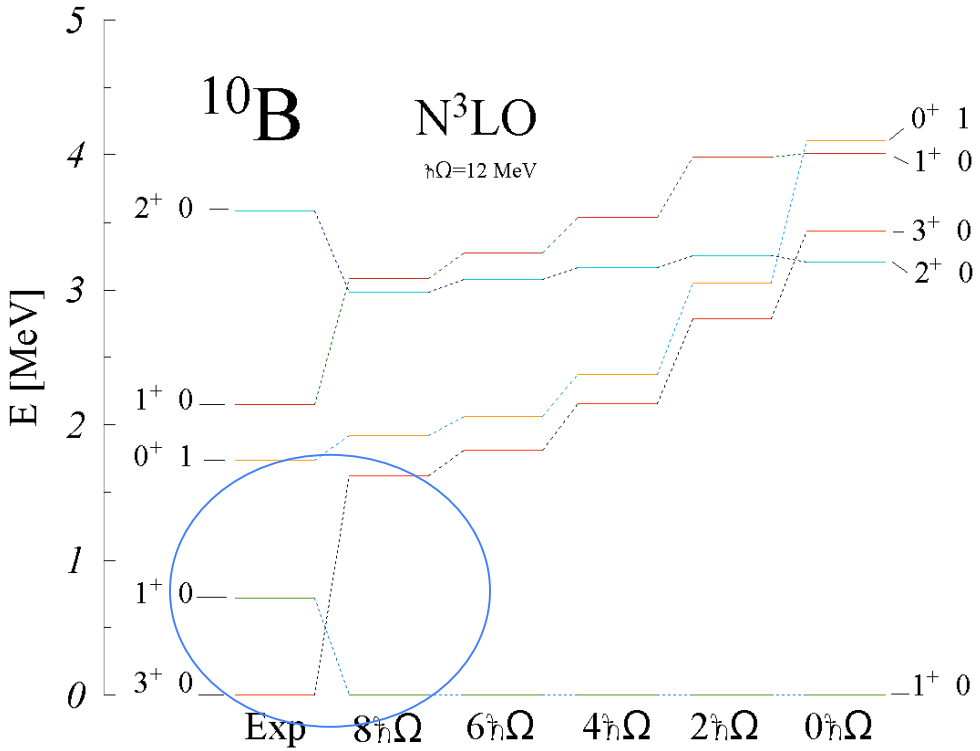


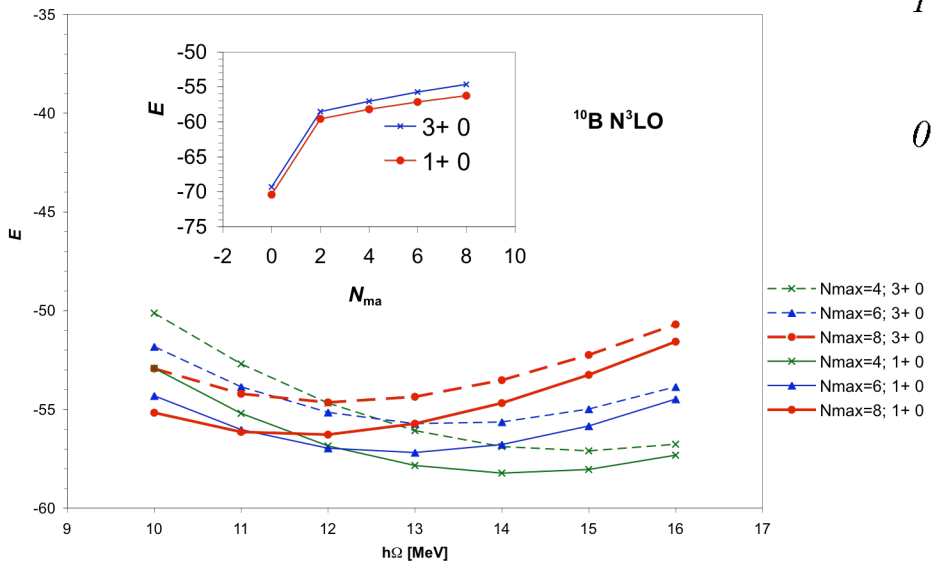

Exp
-0.08 $e$ fm$^2$

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

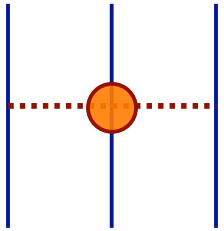


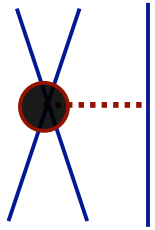



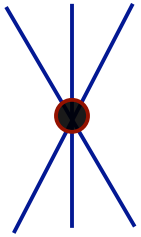

Binding energy
56.3(2.0) MeV

# 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 $\Lambda$
    - Taken consistently from that used in the corresponding EFT NN interaction





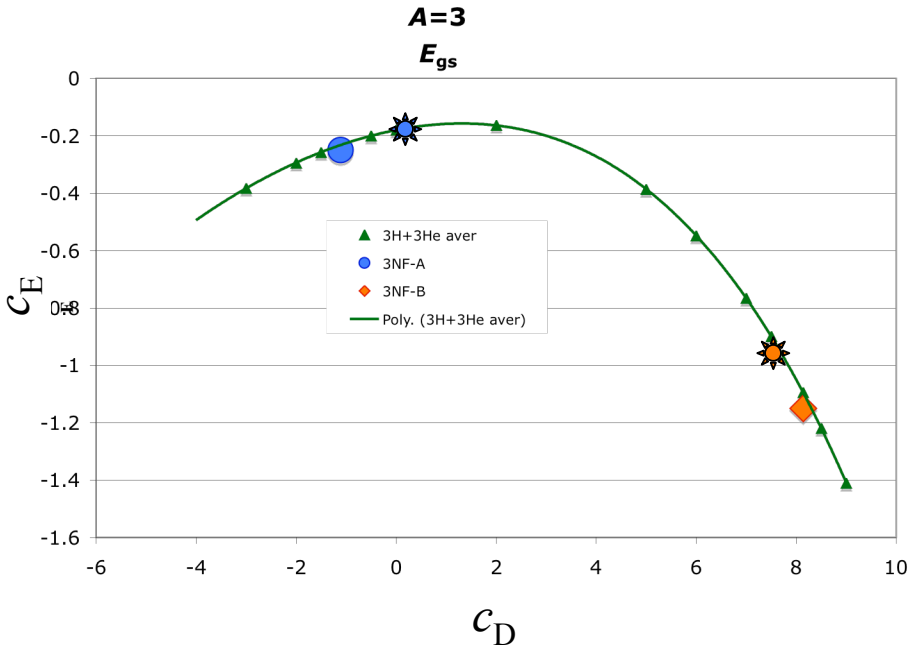


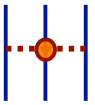
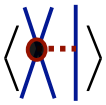
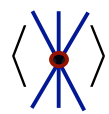
$$\exp[-(Q^2/\Lambda^2)^2]$$

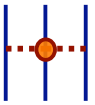
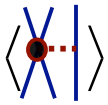
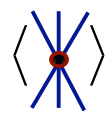
# Determination of the $c_D$ and $c_E$ low-energy constants

- 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 $c_E$
    - Found solutions
      - "3NFA": $c_D$=0.48, $c_E$=-0.17
      - "3NFB": $c_D$=7.69, $c_E$=-0.95
- 3NFA and 3NFB dominated by different terms
  - 3NFA two-pion term dominant
  - 3NFB one-pion term dominant
  - Contact term repulsive in both cases

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




$\langle$  $\rangle = -1.09$ $\langle$  $\rangle = -0.07$ $\langle$  $\rangle = 0.25$

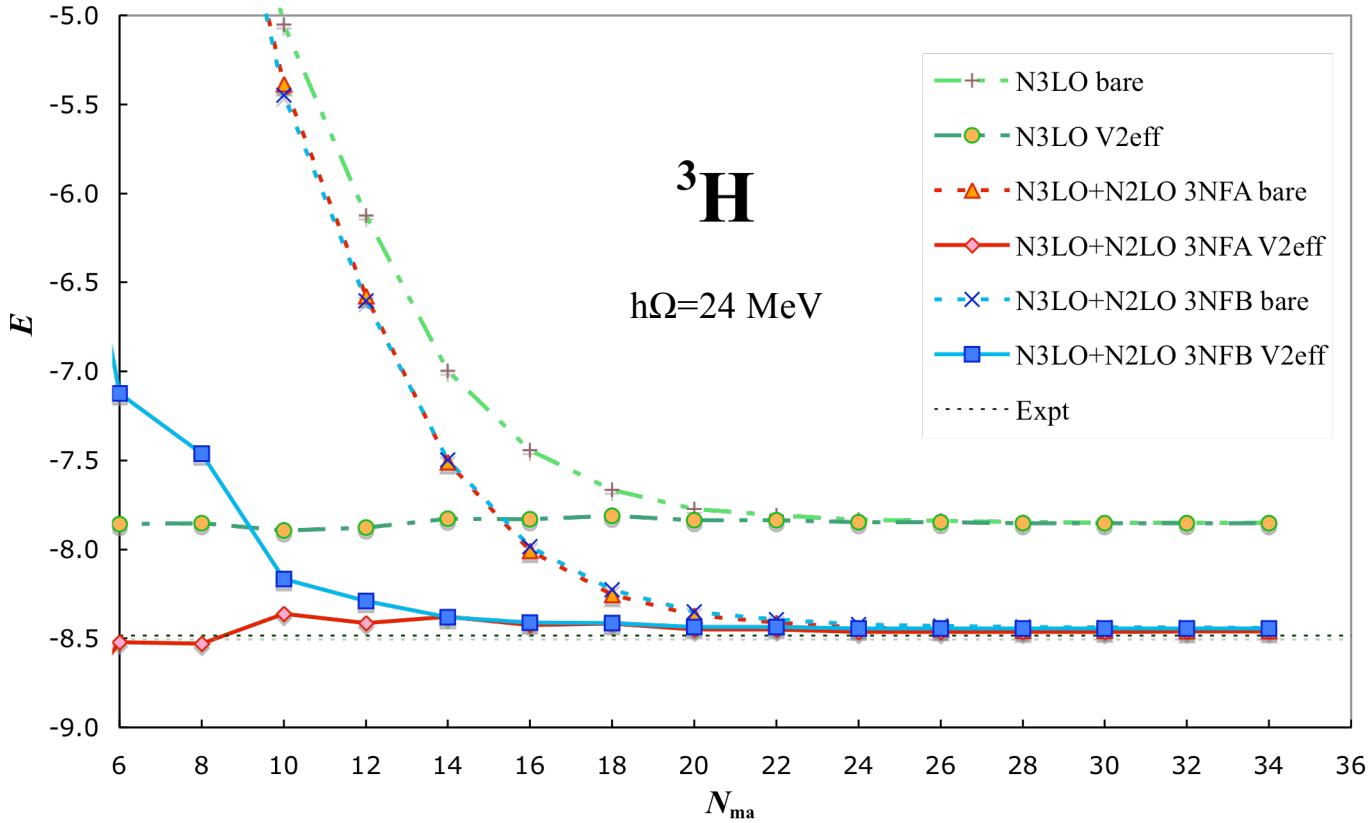
$\langle$  $\rangle = -0.69$ $\langle$  $\rangle = -0.88$ $\langle$  $\rangle = 0.37$

# 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 $V_{3N}$ 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

No transformation for $^4$He
Performed in Jacobi coordinates
Code MANYEFF3b

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

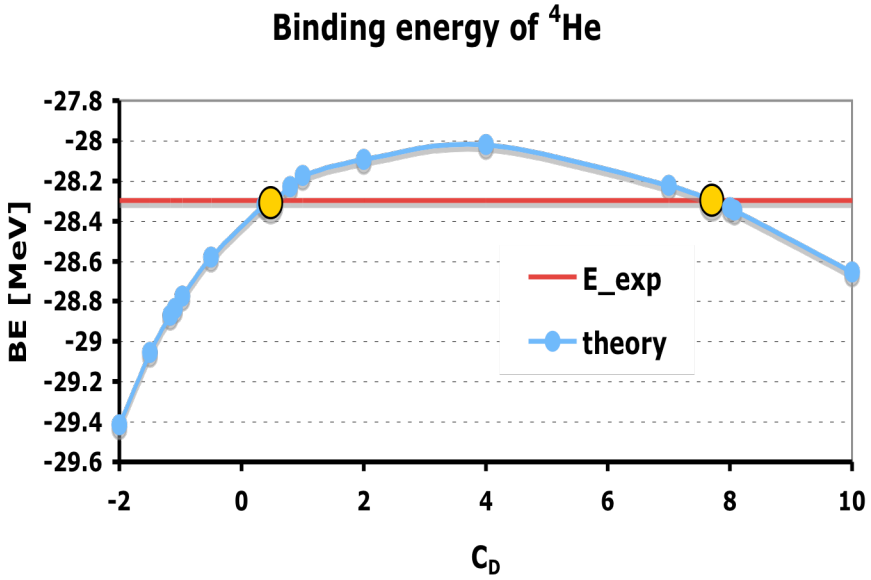
Step 1

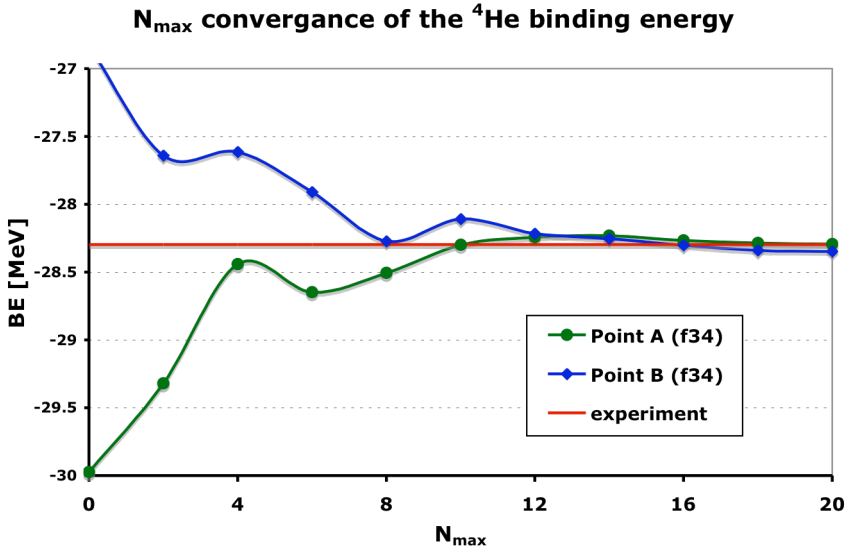
Step 2

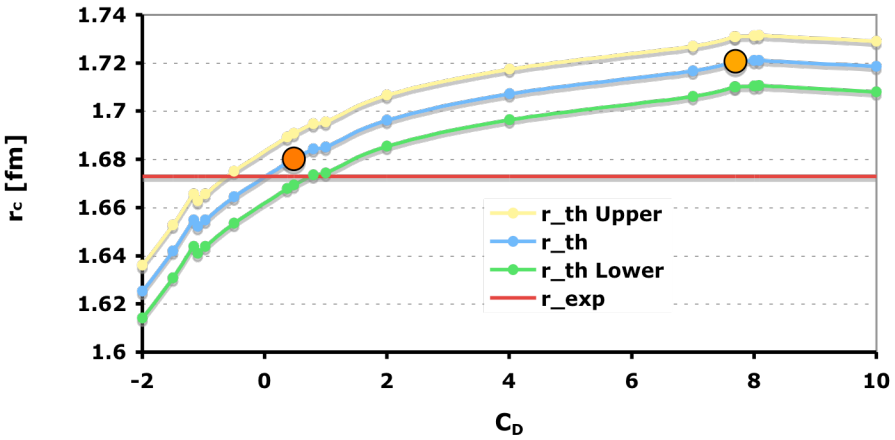
Step 3
Tranformation
here

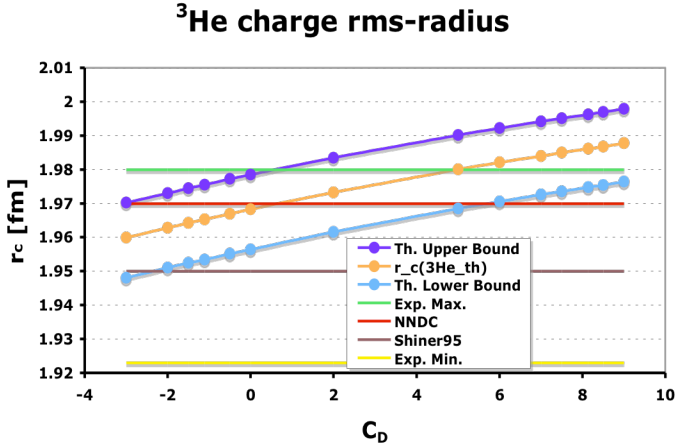
Step 4

# $^4$He binding energy & $^3$He and $^4$He charge radii



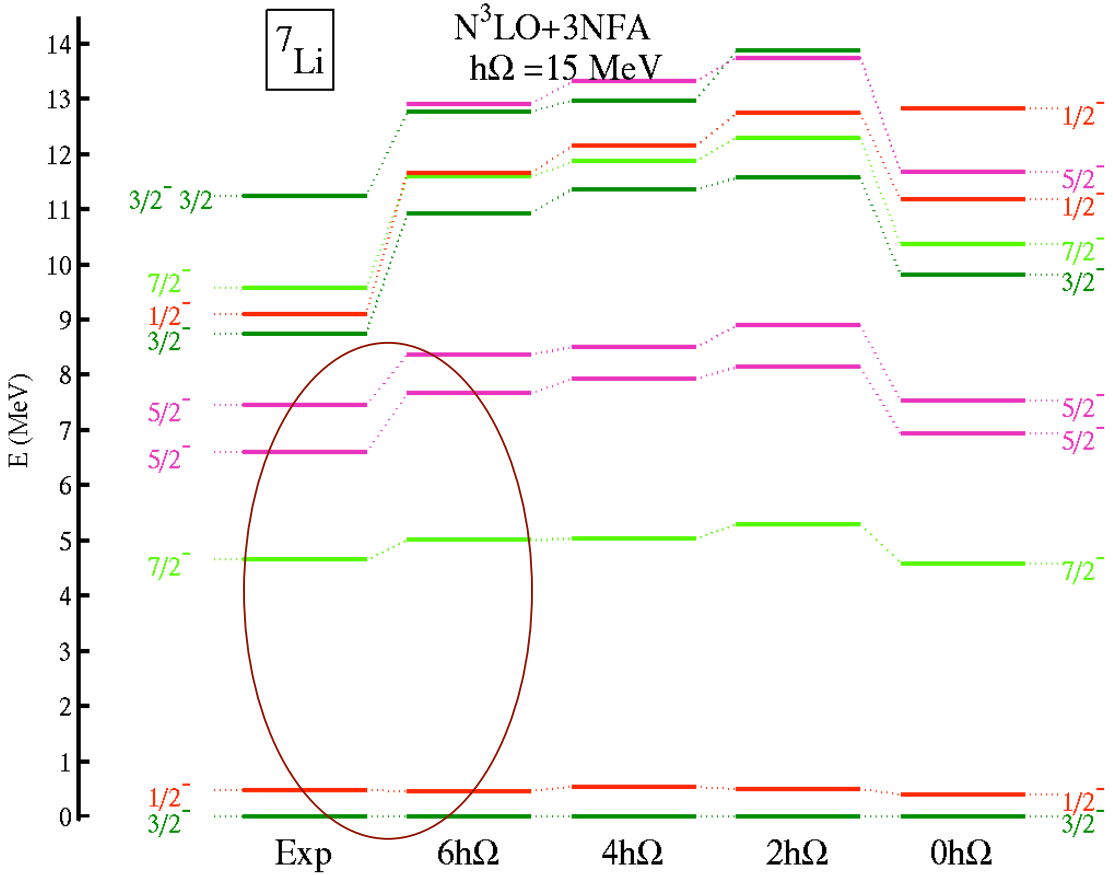




**Solution 3NFA describes charge radii better**

# $^{7}$Li using N$^{3}$LO NN plus consistent N$^{2}$LO TNI

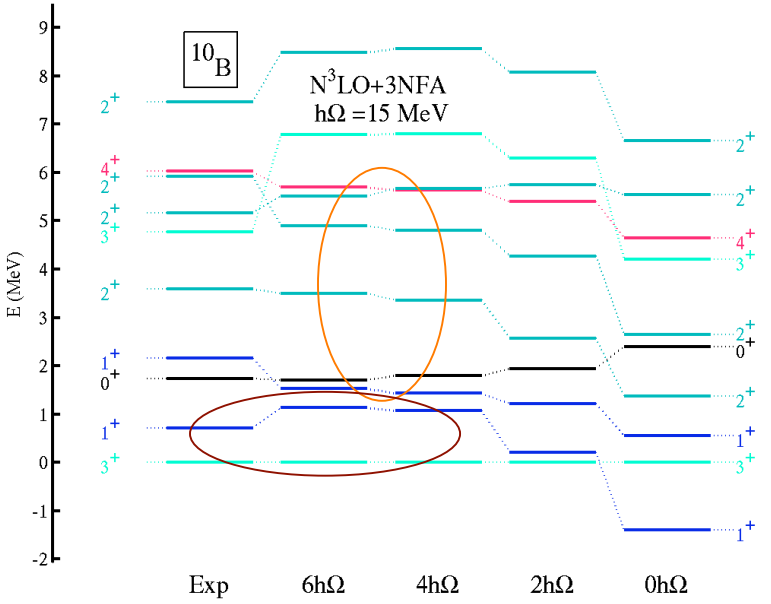
- Very reasonable results obtained using just the NN interaction
  - Some issues concerning level splitting
- What is the effect of the three-nucleon interaction?
- Level ordering remains the same
- Improved level spacing for the lowest five states

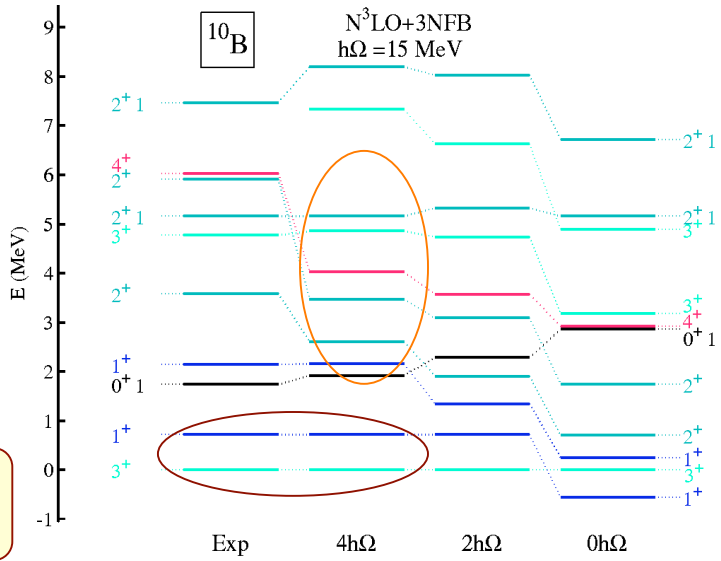



**The N$^{2}$LO three-nucleon interaction does not spoil good description achieved already using the NN interaction**
**Improves on level spacing**

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

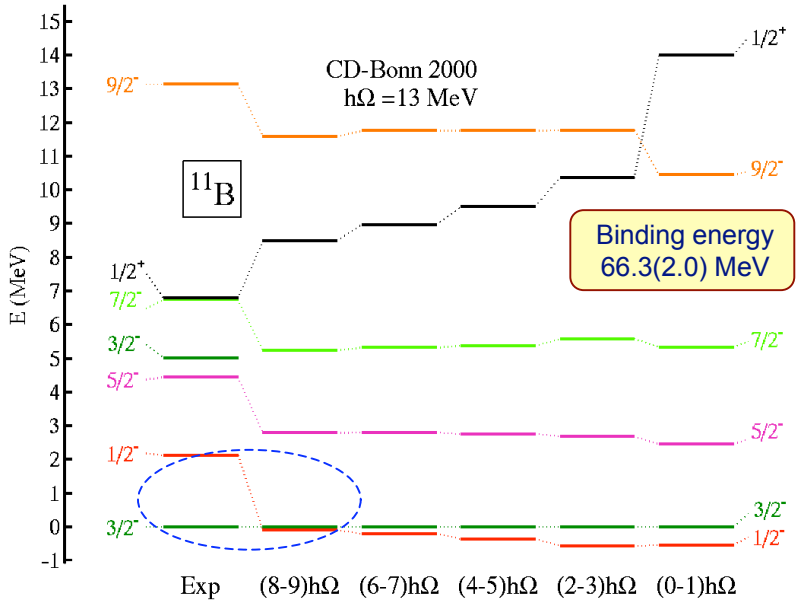
- N$^2$LO TNI 3NF-A dominated by two-pion exchange term
  - The first 6hΩ calculation with $V_{3N}$
    - Dimension 12 million
    - Confirms **convergence of spectra**
  - Results close to the TM'
  - Reasonable binding energy
    - $E_B$=64.03 MeV
- N$^2$LO TNI 3NF-B dominated by one-pion exchange plus contact term
  - Visible difference in particular for higher-lying states
  - No overbinding
    - $E_B$=63.14 MeV
  - Calculation to be re-done after proper fitting to $^4$He

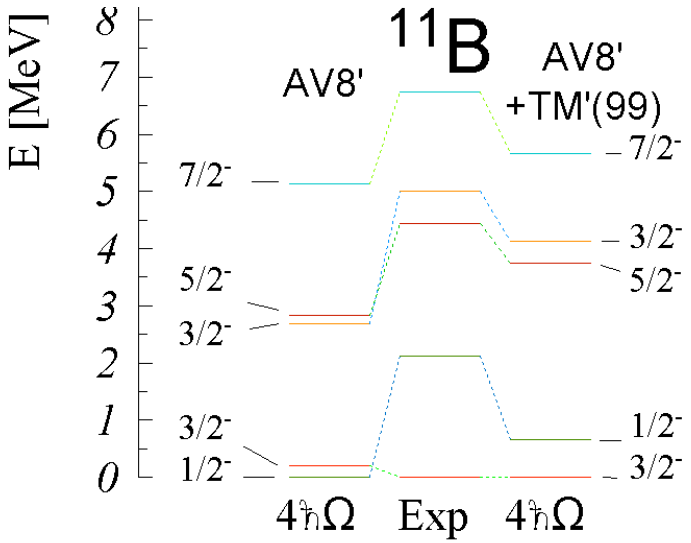



**Both 3NF-A and 3NF-B resolve the $^{10}$B ground state spin problem**
**Similarly like TM', Illinois 3NF, but unlike Urbana IX**

# $^{11}$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 |

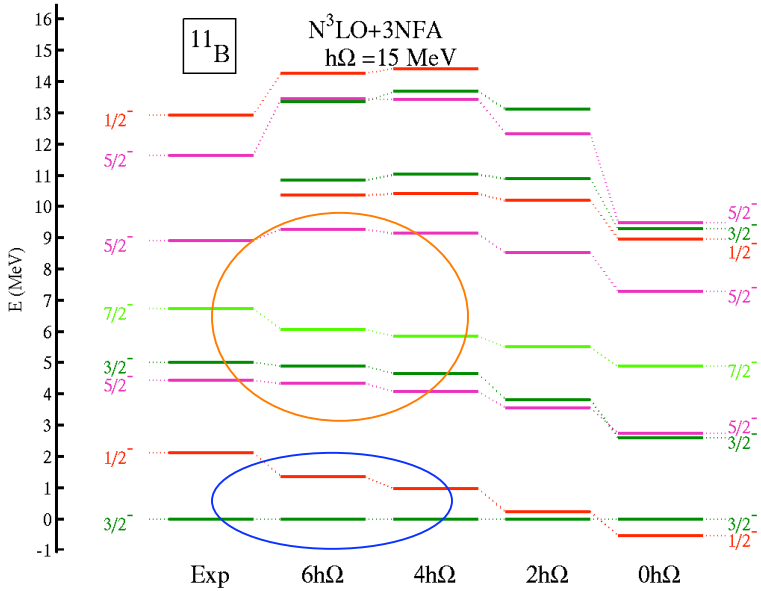
New ($^3$He,t) experiment at RCNP Osaka, Y. Fujita *et al.*, PRC **70**, 011306(R) (2004).

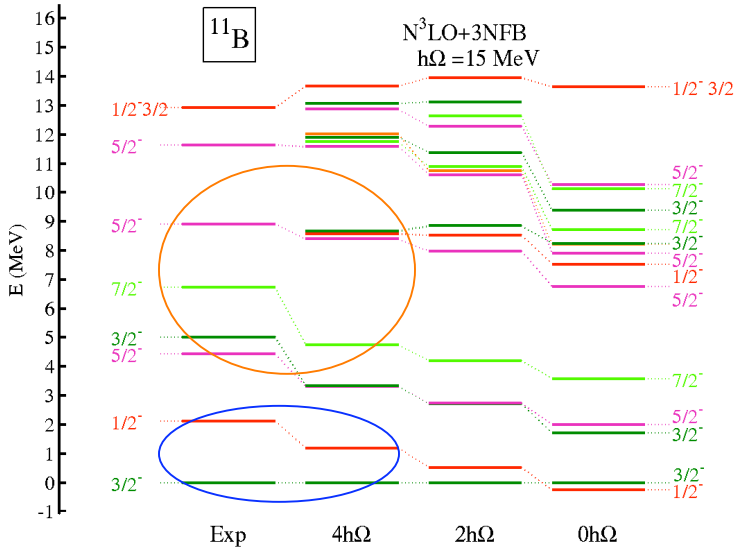
$V_{3b}$ : Bad description of $^{11}$B greatly improved

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

- N$^2$LO TNI 3NF-A dominated by two-pion exchange term
  - A large-scale 6hΩ calculation with the $V_{3N}$
    - Dimension 20 million
    - Confirms convergence of spectra
  - Results close to the TM'
  - Good agreement for higher-lying states
  - Reasonable binding energy
    - $E_B$=76.70 MeV
- N$^2$LO TNI 3NF-B dominated by one-pion exchange plus contact term
  - Visible difference in particular for higher-lying states
  - No overbinding
    - $E_B$=76.22 MeV
  - Calculation to be re-done after proper fitting to $^4$He

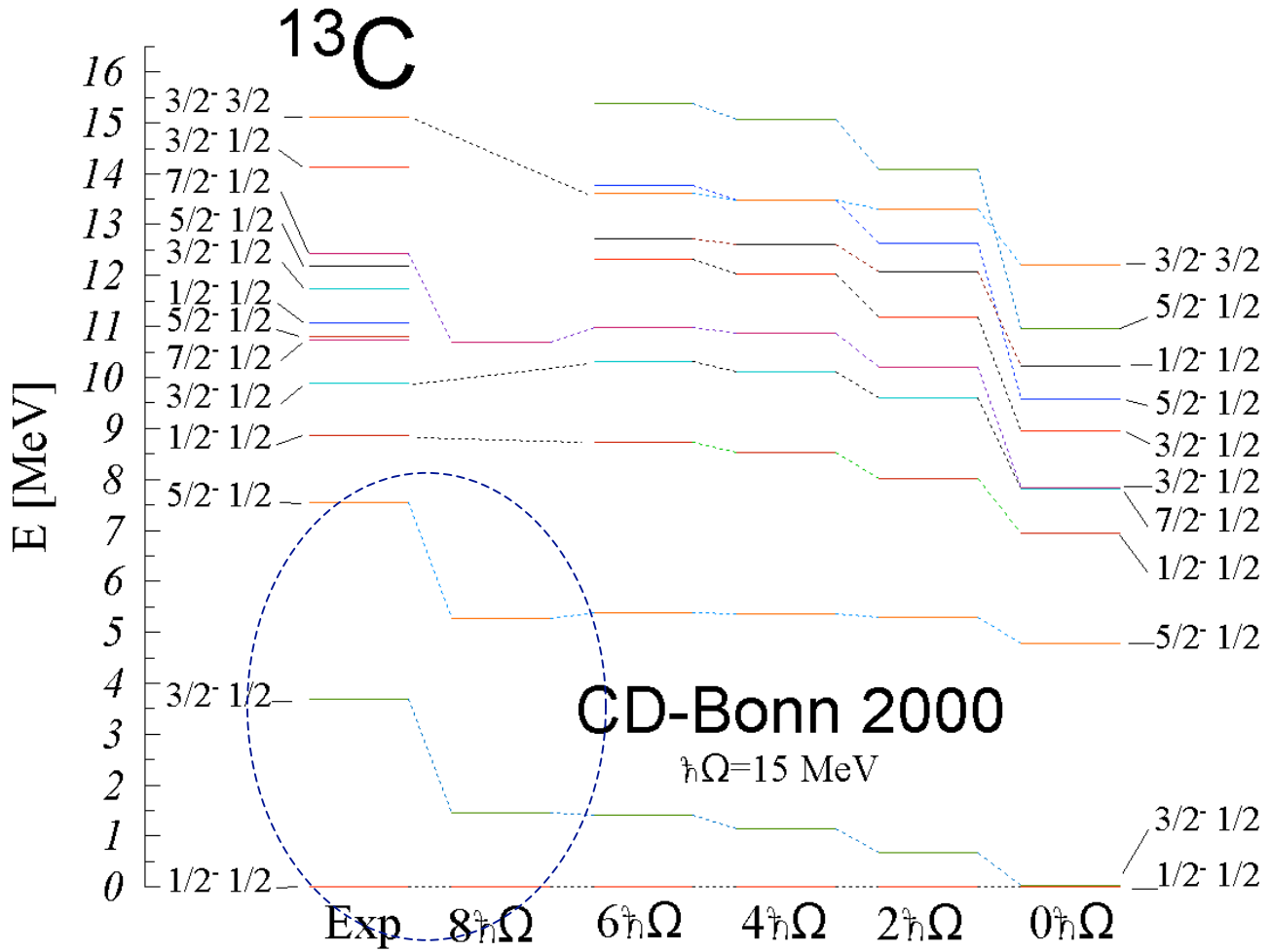
**Both 3NF-A and 3NF-B predict correct level ordering of lowest states of $^{11}$B, similarly like TM'**



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

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

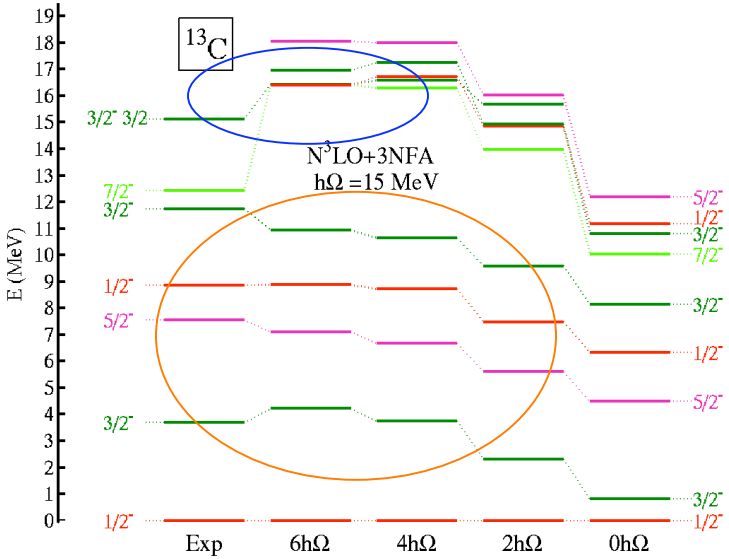


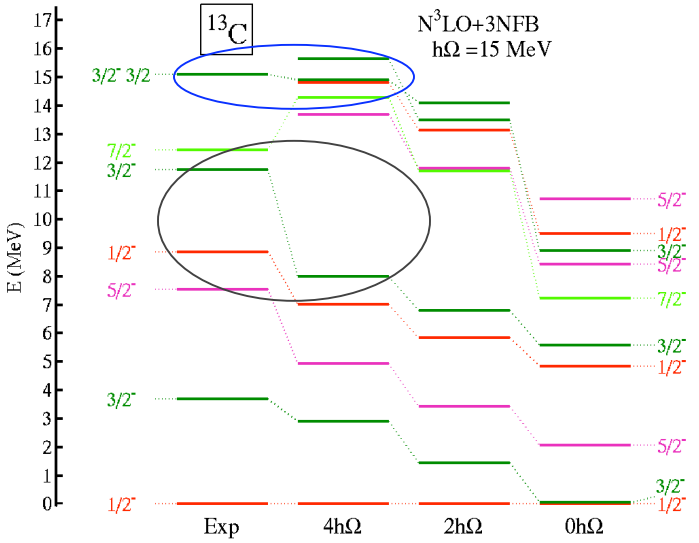

Binding energy
86.5(2.0) MeV

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

- N$^2$LO TNI 3NF-A dominated by two-pion exchange term
  - The 6hΩ $^{13}$C
    - One of the two biggest calculation with the TNI so far
    - Dimension 38 million
    - 3 GB TNI input file
    - MFD code on 3160 processors of Thunder in 4.6 hours
    - Confirms convergence of the excitation energies
    - Significant improvement for lowest states compared to the NN interaction only
    - Reasonable binding energy $E_B$=98.7 MeV
  - Results close to the TM'
- N$^2$LO TNI 3NF-B dominated by one-pion exchange plus contact term
  - Visible difference in particular for low-lying states
    - Worse agreement with experiment compared to 3NF-A
  - Better agreement for T=3/2 states
  - $3/2^-_2$ appears to be under-predicted
  - Binding energy at 4hΩ
    - $E_B$=103.2 MeV
  - Calculation to be re-done after proper fitting to $^4$He
  - 6hΩ needed to check convergence of spectra

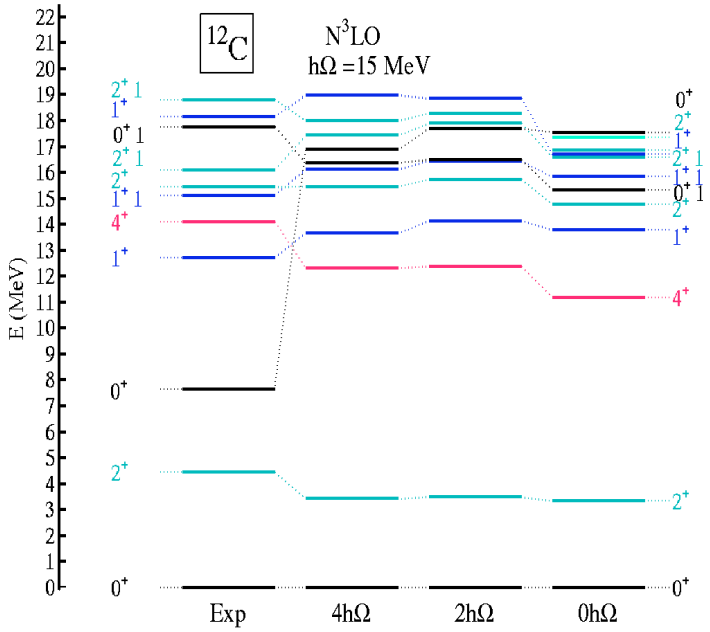
**Both 3NF-A and 3NF-B improve level spacing of lowest states of $^{13}$C, compared to CD-Bonn**

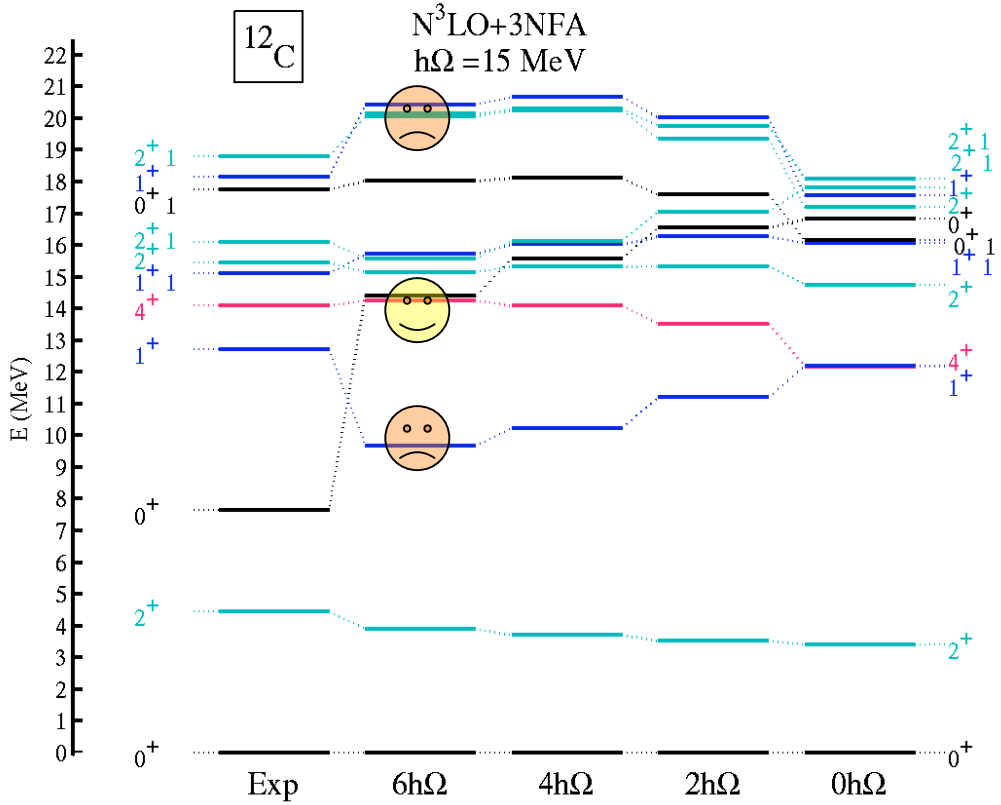


# $^{12}$C using N$^3$LO NN plus consistent N$^2$LO TNI

- The $^{12}$C 6hΩ, one of the two biggest calculation with the TNI so far
  - Dimension 32 million
  - 3 GB TNI input file
  - MFD code on 3160 processors of Thunder in 4.5 hours
- The 6hΩ stabilizes the spectrum
  - Move in the right direction
  - Overdone for $1^+$ 0, $2^+$ 1
  - The second $0^+$ 0 coming down
  - Binding energy 94.3 MeV

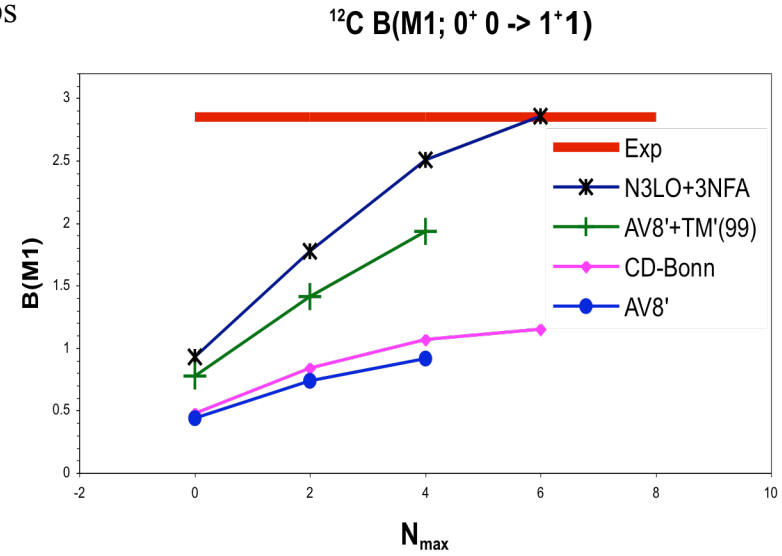



**Testing of $c_3$, $c_4$?**

# 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 6h$\Omega$ - saturation
    - Underestimates by a factor of 2-3
  - $V_{2b}$+$V_{3b}$ up to 6h$\Omega$
    - 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 |
| ( $\nu$ e$^-$) | 3.69 | 6.8 | 8.9±0.3±0.9 |
| ( $\nu$ $\mu^-$) | 0.312 | 0.537 | 0.56±0.08±0.1 |
| $\mu$-capture | 2.38 | 4.43 | 6.0±0.4 |

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

# 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 $\Lambda$
  - $c_D$ 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
    - 3NF-A describes better the $^4$He charge radius
  - Most important issue is to verify the convergence
    - 6hΩ calculations now possible for the whole *p*-shell
- 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 |

# 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