The *ab initio* no-core shell model

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Outline

QCD-based nuclear interaction

Low-energy QCD and effective field theory

Unitarily-transformed interactions

Lee-Suzuki (SRG, UCOM)

Computational many-body methods

The *ab initio* no-core shell model

Nuclear structure

Recent NCSM results for $A=12$

Outline

QCD-based nuclear interaction
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Computational many-body methods
The *ab initio* no-core shell model

Extending the model space
The NCSM/RGM

Nuclear Structure and Reactions
Open channels, clustering

Outline

General short-range interaction

Harmonically trapped cold atom gas

↓

Unitarily-transformed interactions

Lee-Suzuki, SRG, UCOM

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Computational many-body methods

The *ab initio* no-core shell model

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Effective interaction approach to the many-boson problem

The nucleon-nucleon interaction

From meson theories to low-energy QCD and effective field theory

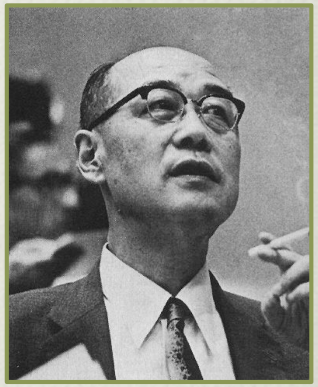
The nucleon-nucleon force

- The interaction between nucleons is complicated.
- In principle, it should be governed by QCD;
  but QCD is non-perturbative at low energies.
- Phenomenological NN potentials provide an accurate fit to NN scattering data
  e.g. CD-Bonn 2000 with χ^2=1.02 is based on one-boson exchange: π, ρ, ω + "σ" mesons
- Missing physics?

  - Underbinding for *A* > 2 systems

  - Fails to reproduce polarized p+d scattering

  - Some nuclear structure in *p*-shell is wrong.



Hideki Yukawa
Meson hypothesis
(1935)

Chiral perturbation theory

- Predictive theory of nuclei requires a consistent framework for the interaction

- QCD at low energies: non-perturbative.
  Effective degrees of freedom are nucleons and pions

Weinberg (1979):

1. Write down the most general Lagrangian consistent with the assumed symmetry principles (in particular broken chiral sym.)

2. Calculate Feynman diagrams (there will be infinitely many…)

3. Find a scheme for assessing the importance of the various diagrams
   Weinberg demonstrated *power counting* in terms of $(Q/\Lambda_\chi)^\nu$

Effective field theory

- Replace heavy-meson degrees of freedom in the low-energy potential by short-range (contact) interactions

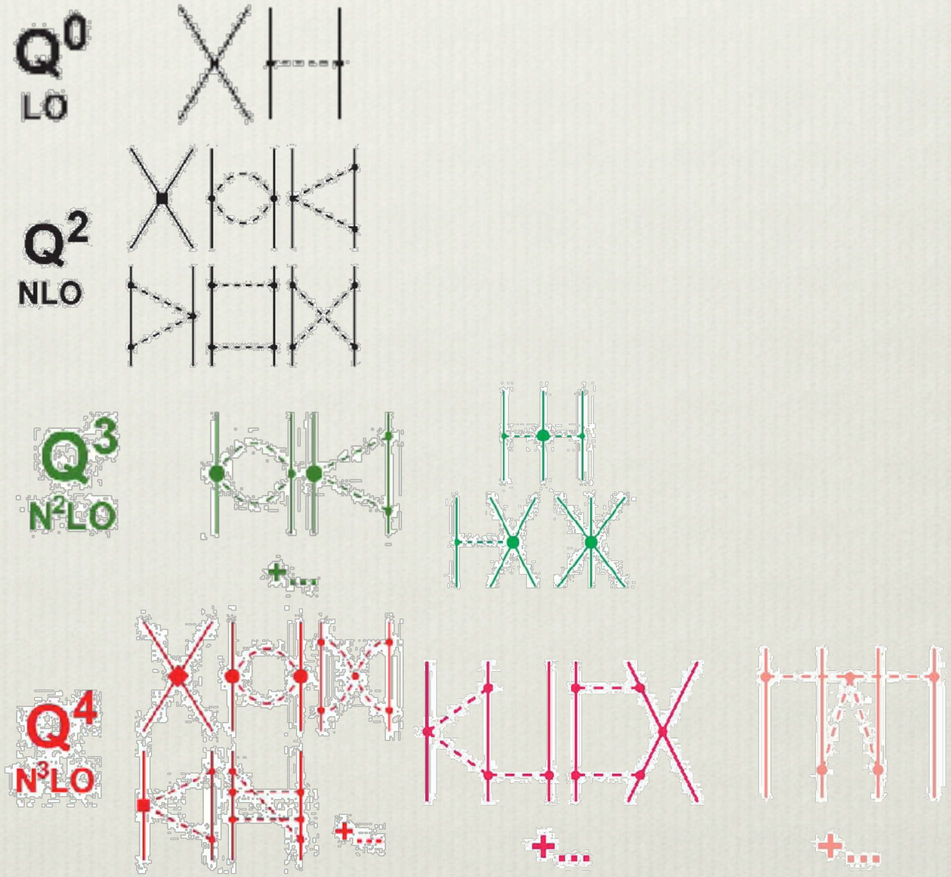
Hierarchy of forces **2N forces** **3N forces** **4N forces**

Leading order

Next-to-leading order

Next-to-next-to-leading order

Next-to-next-to-next-to-leading order



The nuclear many-body problem

From few- to many-body physics – the some-body regime

Microscopic approaches

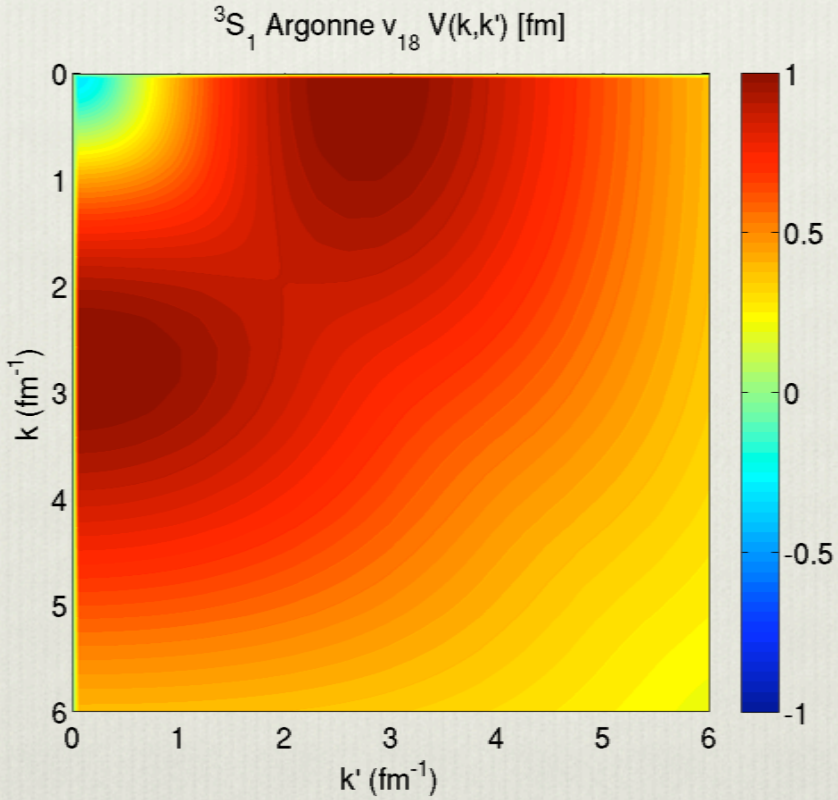
- **A = 3,4: Many exact methods**
  Benchmark paper: Kamada et al, Phys. Rev. C64(2001)044001
  Faddev-Yakubovsky, CRCGV, SVM, GFMC, HH variational, EIHH, NCSM

- **A > 4: Very few (*ab initio*) methods available**
  - Greens Function Monte Carlo (GFMC)
  - Coupled Cluster Method (CCM)
  - Effective Interaction for Hyperspherical Harmonics
  - Fermionic Molecular Dynamics (FMD)
  - Ab initio no-core shell model (NCSM)

Renormalized interaction

- High-momentum components of realistic *NN* forces introduce strong correlations

- Enormously large model spaces required;



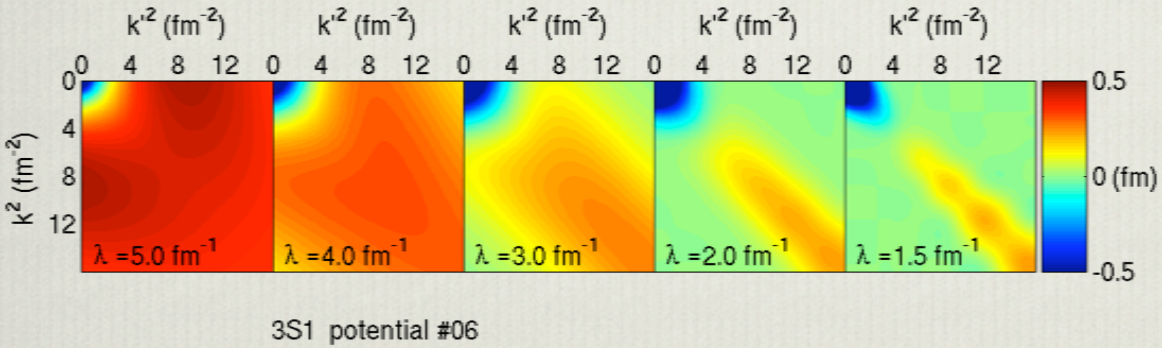
Renormalized interaction

- High-momentum components of realistic *NN* forces introduce strong correlations

- Enormously large model spaces required;

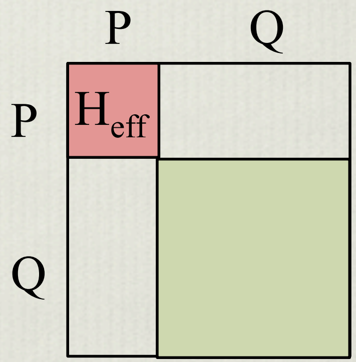
  …or renormalization using a **unitary transformation**:

Similarity Renormalization Group:



V_UCOM, V_low-k

Lee-Suzuki :



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

The *ab initio* no-core shell model

- It is a general approach for studying strongly interacting, quantum many-body systems.
- A matrix diagonalization technique to solve the translational invariant A-body problem in a finite harmonic oscillator basis

P. Navrátil, J.P. Vary and B.R. Barrett, Phys. Rev. C 62, 054311 (2000)
P. Navrátil, J.P. Vary and B.R. Barrett, Phys. Rev. Lett. 84(2000)5728

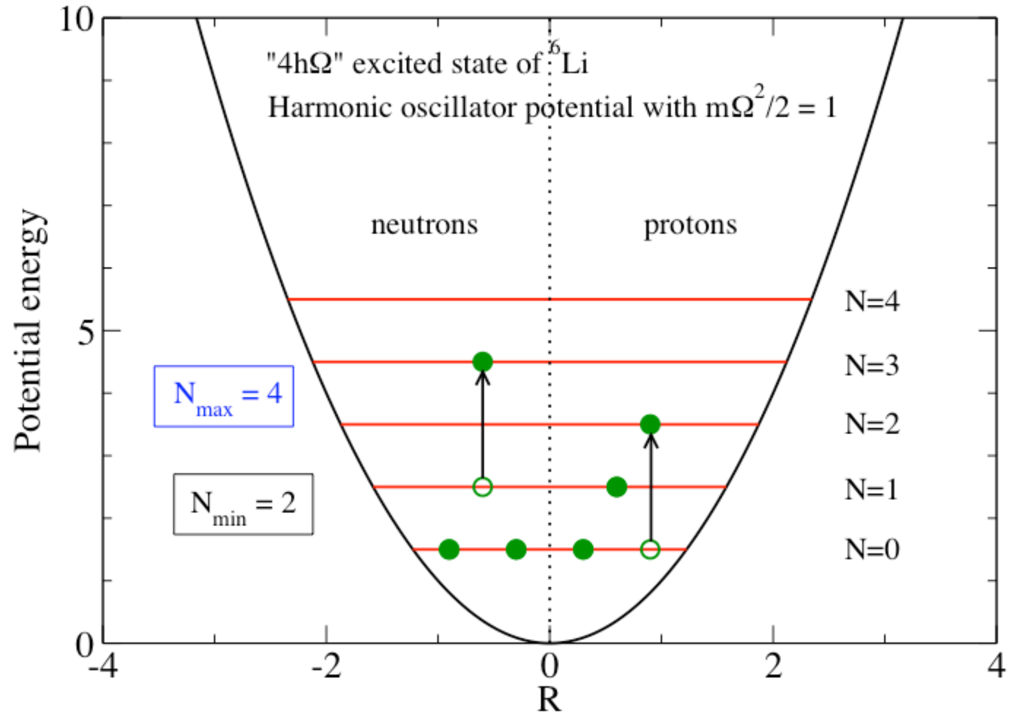
The NCSM model space

The NCSM model space

Define the "$N_{max}h\Omega$" A-particle model space (P-space) as including all HO excitations up to a total energy cutoff:

$$\sum_{i=1}^{A} \varepsilon_i \leq \left(N_m + \frac{3A}{2} \right) \hbar\Omega$$

where $N_m \equiv N_{\min} + N_{\max}$



Definition of P_2 space for computation of two-body effective interaction follows straightforwardly.

$$2n + l \leq N_m - N_{sps\,\min}, \text{ (in this example } N_{sps\,\min} = 0 \text{ and therefore } 2n + l \leq 6)$$

The NCSM effective interaction

Model space: The NCSM solves the Schrödinger equation in a large, but finite model space P.

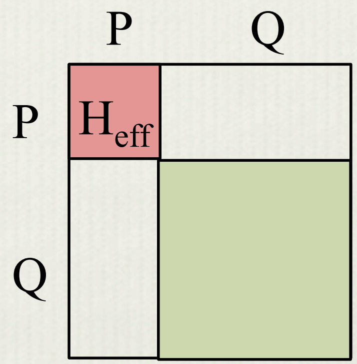
Problem: High-momentum components of high-precision NN interactions require enormously large spaces.

Solution: Follow formal procedure (Lee-Suzuki) to derive an effective interaction acting only in the model space and reproducing exactly a subset of the eigensolutions.

Price: This procedure generates A-body operators and is essentially as difficult to apply as solving the full problem.

Approximation: Generate effective interaction at 2- or 3-body cluster level.

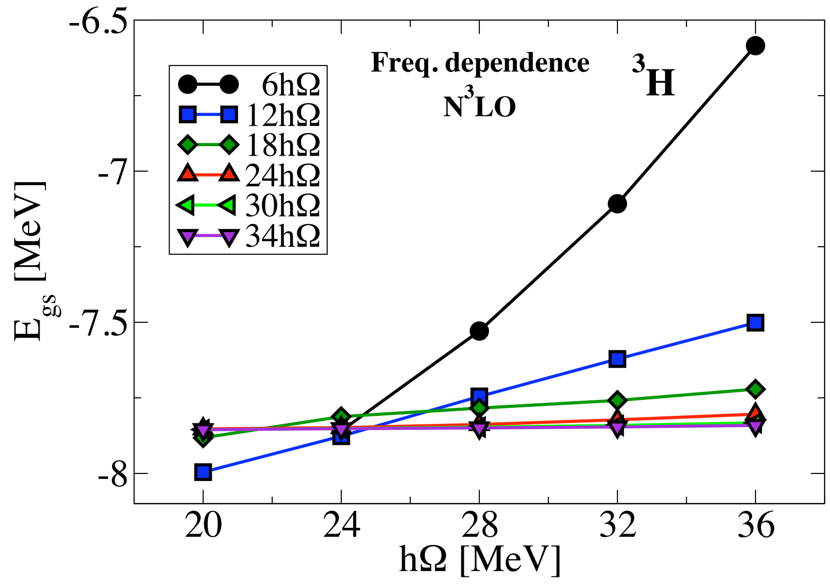
P. Navrátil, J.P. Vary and B.R. Barrett, Phys. Rev. Lett. 84(2000)5728
K. Suzuki and S.Y. Lee, Prog. Theor. Phys. 64(1980)2091



P. Navrátil and W. E. Ormand, Phys. Rev. Lett. 82(2002)152502

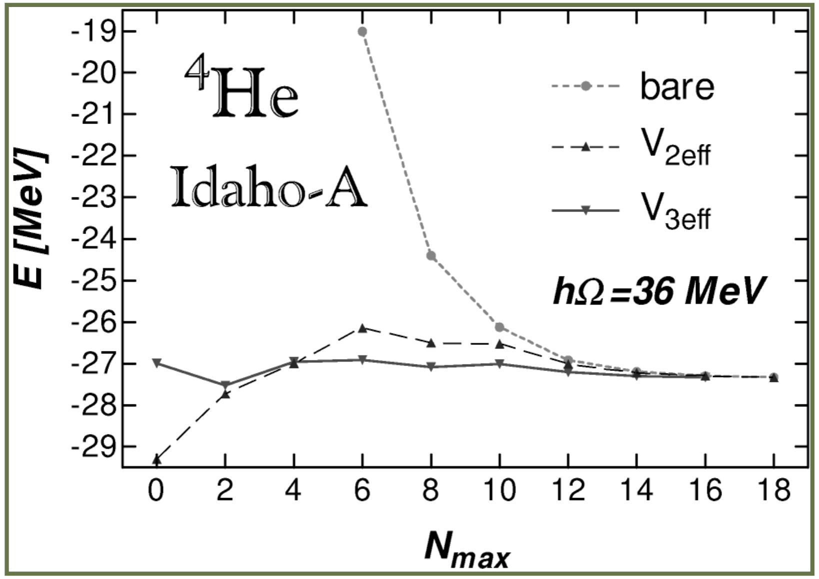
Convergence properties

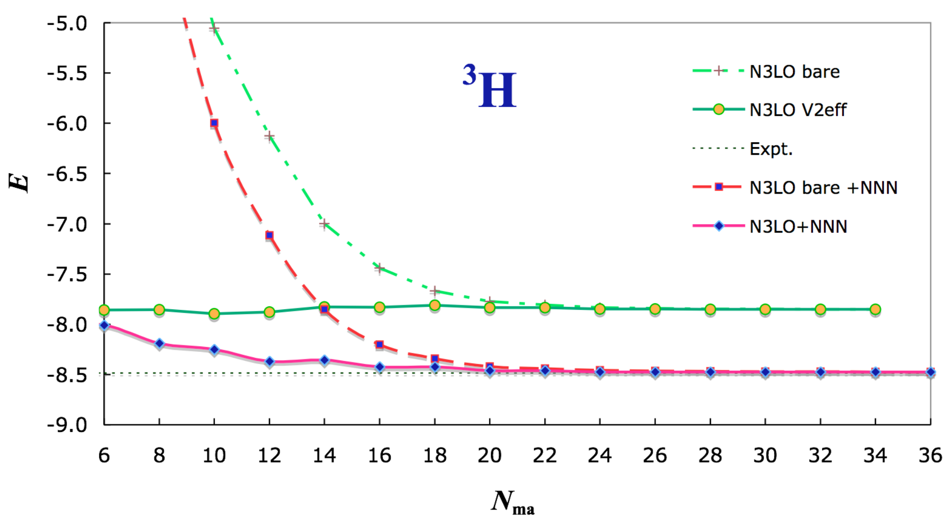
- Independence of Ω when $N_{max} \to \infty$
- It is not a variational calculation (when using effective interactions)



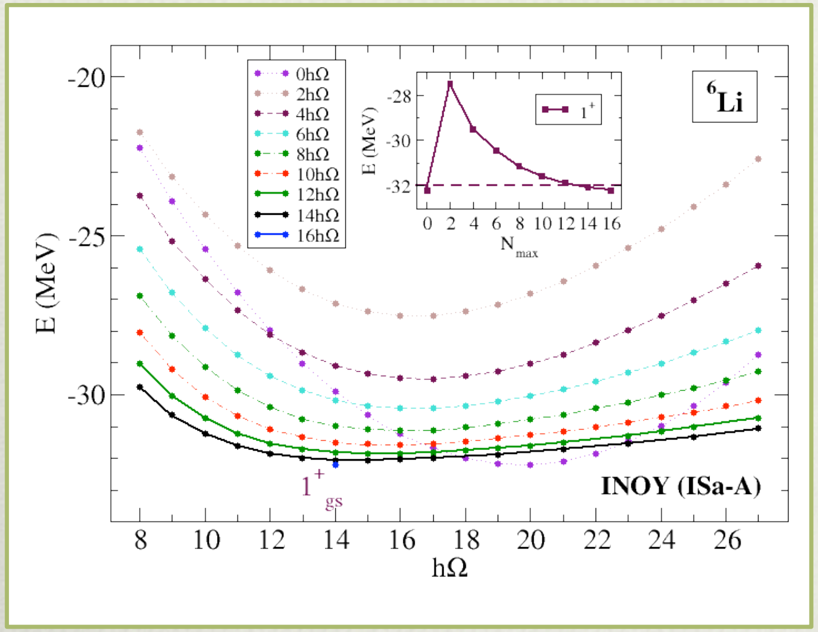
Convergence properties

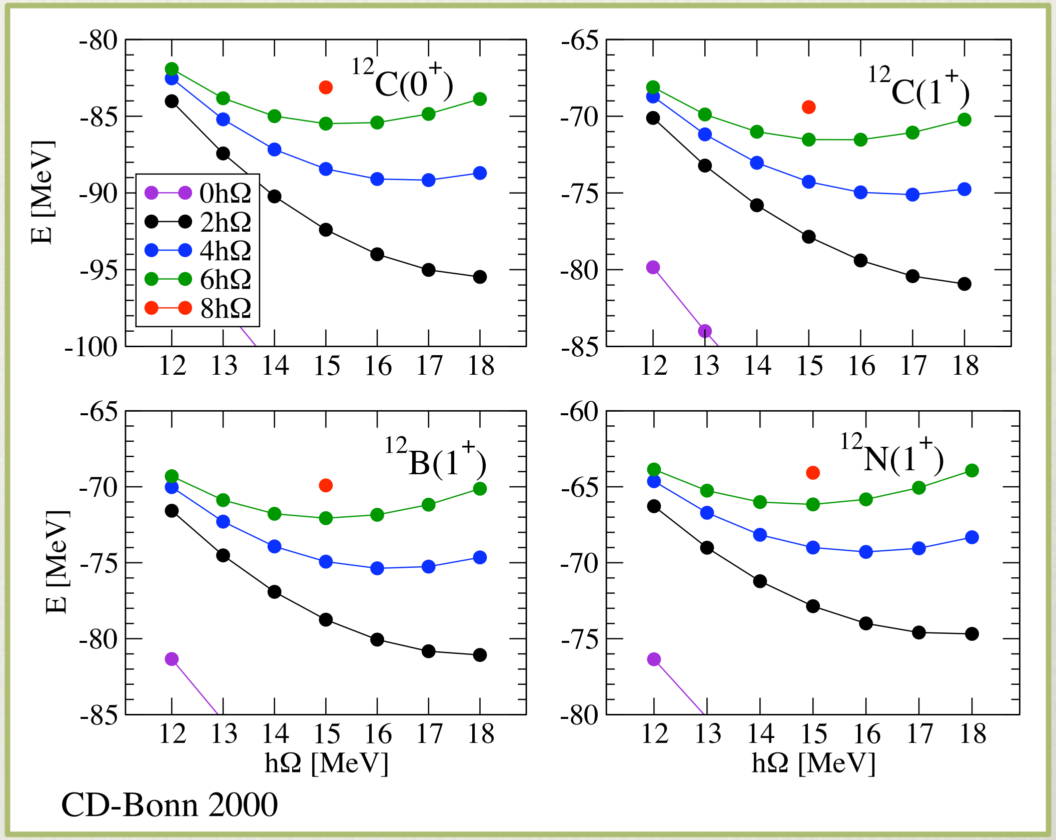
- Independence of Ω when $N_{max} \rightarrow \infty$
- It is not a variational calculation (when using effective interactions)
- **Convergence as $N_{max} \rightarrow \infty$**
- **Convergence as a → A**

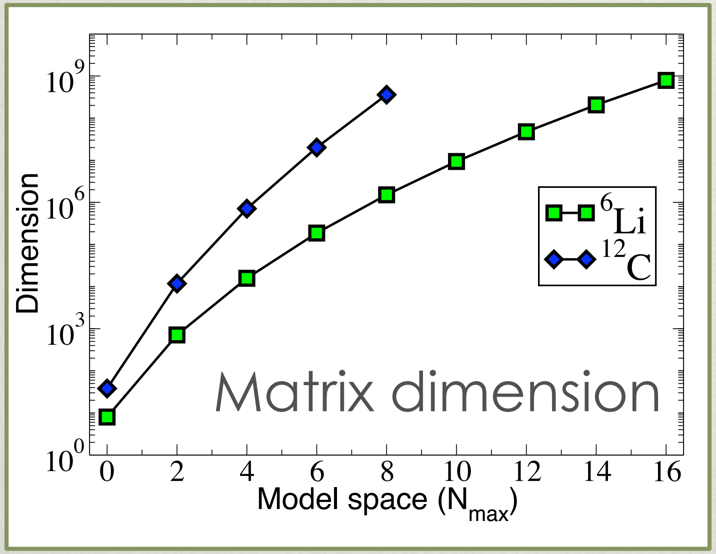




Convergence properties: A=6, 12







NCSM – summary

Some advantages:

- Basically no restrictions regarding the Hamiltonian.
- Preserves the symmetries: Rotational, translational, parity, etc.
- Correct treatment of antisymmetrization.
- Usually very good convergence properties.
- HO basis allows easy transformation between:
  - Jacobi- or single-part. coordinates
  - Coordinate or momentum space
- Lee-Suzuki transformation

Some challenges:

- Dimension grows rapidly with increasing number of nucleons.
- Expansion in bound-state basis functions.
- Slower convergence for $1\hbar\Omega$– and $2\hbar\Omega$-dominated states.
- Lee-Suzuki transformation for observables.
- Cluster limit $a \leq 3$ in eff. int. restricts the description of e.g. α clusterization.
- Sensitivity to thresholds.

Recent NCSM results

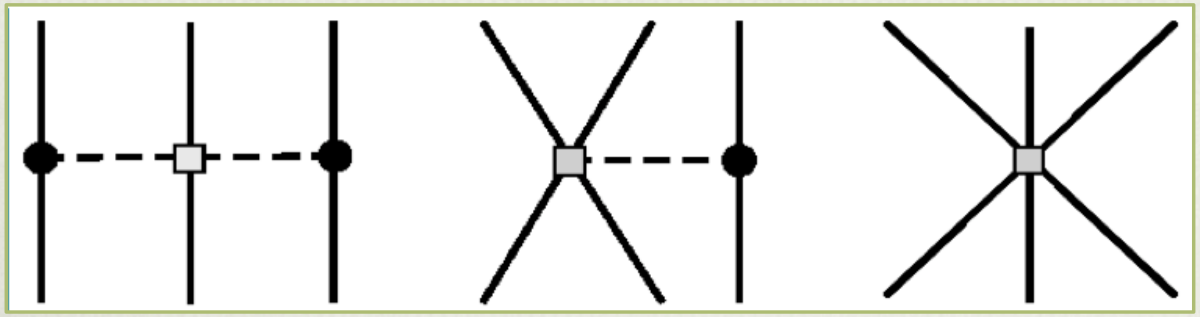
State-of-the-art calculations for A=12 isotopes

Challenge: The A=12 isobar

- Mixture of "cluster" and "shell model" states
- Converged A=12 calculations are very challenging
- Much experimental data is available.
  Allows for precision tests of the wave functions and the Hamiltonian
- ^{12}C as a new benchmark system for different *ab initio* methods and interactions?

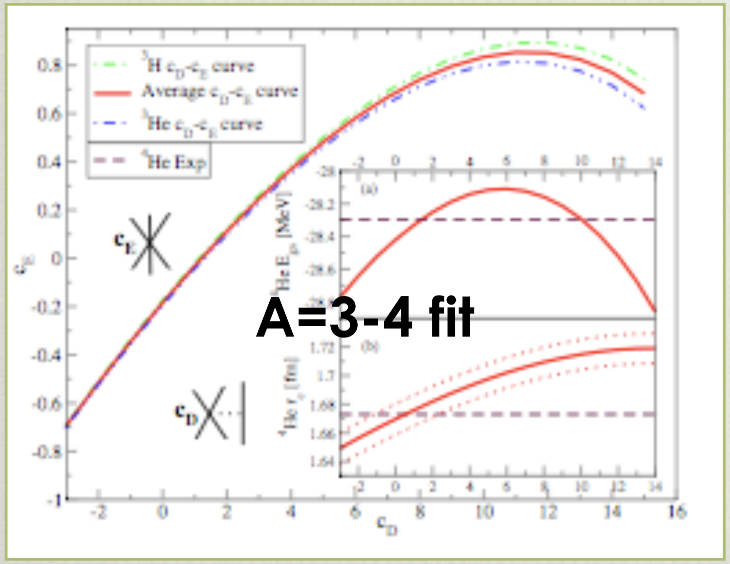
Chiral 3NF in the NCSM

Topology of the leading chiral 3NF (3rd order)



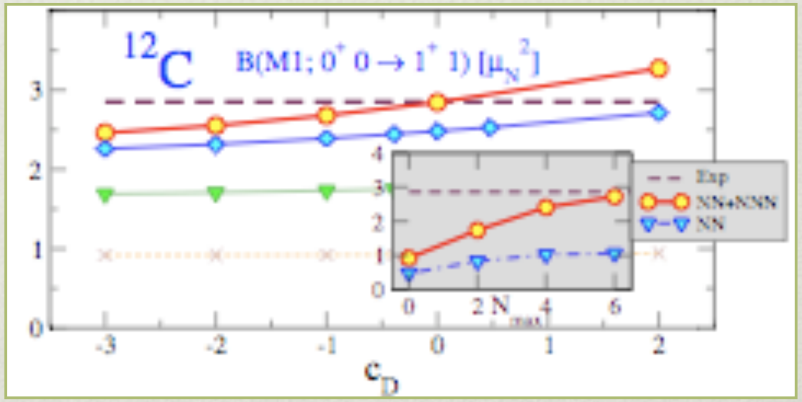
c_D and c_E have to be fitted. Different options for this fit exist.

2π–exchange part (c-terms) | 1π–exchange/contact (D-term) | Pure contact (E-term)

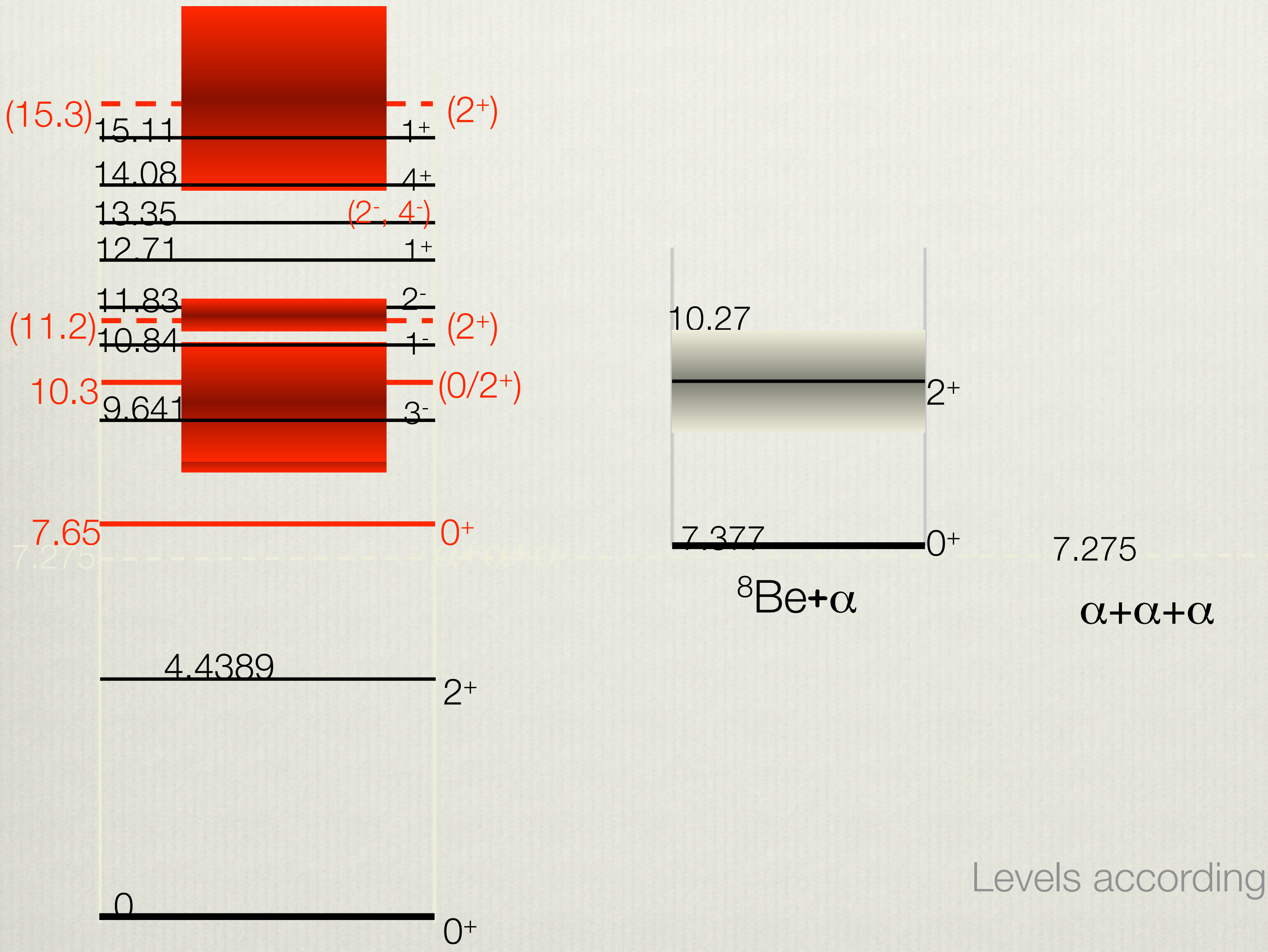


Structure of A=10-13 nuclei with chrial NN+3NF

P. Navrátil et al., Phys. Rev. Lett. **99**(2007)042501



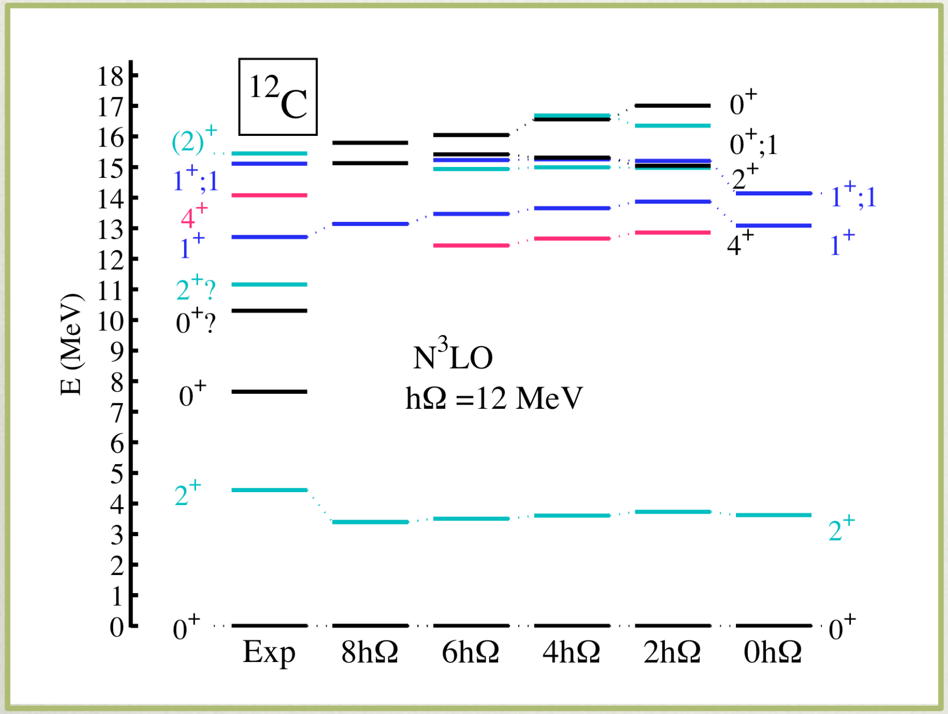
^{12}C by latest evaluation

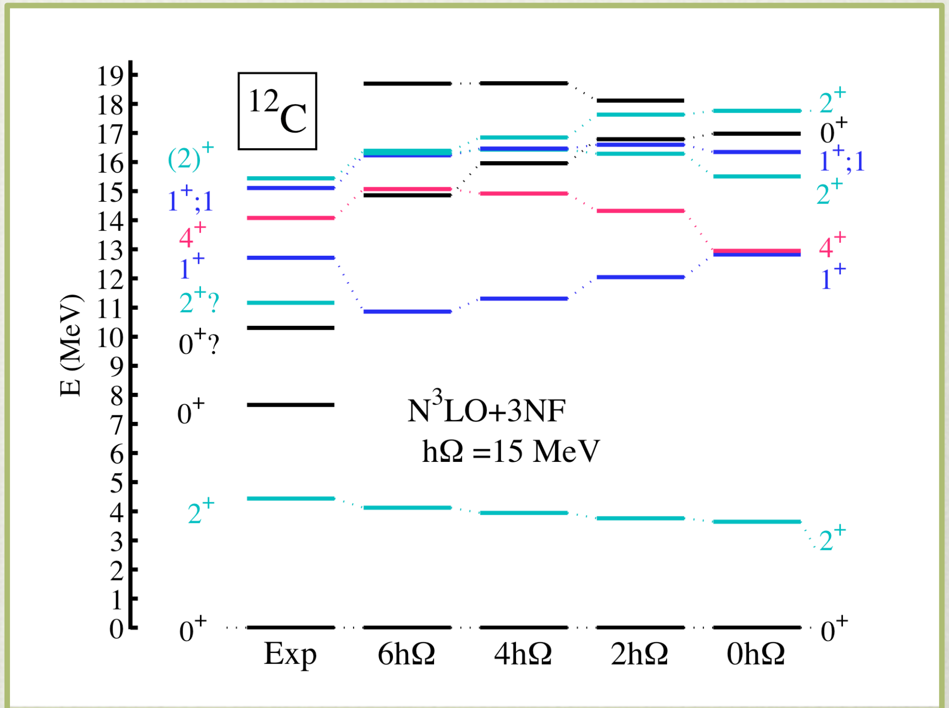


Levels according to TUNL

NCSM: ^{12}C spectrum

Positive-parity energy spectrum obtained with chiral NN and NN+3NF.





P. Navrátil et al., Phys. Rev. Lett. **99**(2007)042501
and C. Forssén et al., work in progress

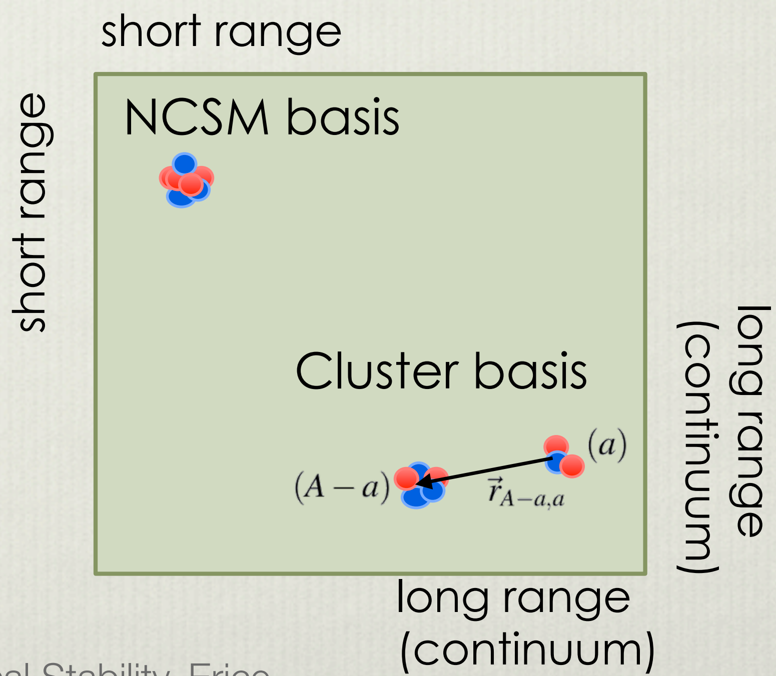
- Improved ordering of states with 3NF included
- "Shell-model" like states well reproduced while "cluster states" appear too high in the spectrum.

Ab initio description of open (nuclear) quantum systems

NCSM with RGM

Need to extend the basis space

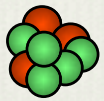
- The finite HO basis used in the NCSM has two main shortcomings:
  - Insufficient description of long-range correlations
  - Lack of coupling to continuum
- Need to go beyond the standard NCSM



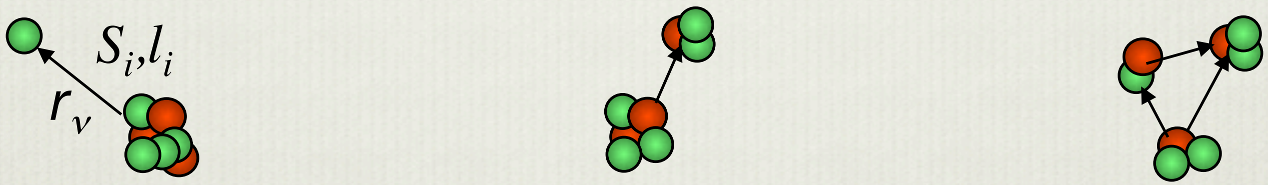
Resonating Group Method

$$(H - E)\,\Phi^{(A)} = 0$$

Time-independent Schrödinger equation for A-body scattering.

The A-body system:  J, π

is decomposed into various “channels” ν:



Here, we focus on two-cluster channels:

$$\Phi^{(A)} = \sum_\nu \mathcal{A}_\nu \left\{ \Phi_{1\nu} \Phi_{2\nu} \varphi_\nu(\vec{r}_\nu) \right\} = \sum_\nu \int d^3 r \varphi_\nu(\vec{r}) \mathcal{A}_\nu \Phi_\nu^{(A)}(\vec{r})$$

expansion coefficient

basis functions: $\Phi_\nu^{(A)}(\vec{r}) = \Phi_{1\nu} \Phi_{2\nu} \delta(\vec{r} - \vec{r}_\nu)$

RGM equations of motion

RGM equations: coupled integro-differential equations:

$$\sum_{\nu'} \int d^3r' \left[H_{\nu\nu'}\left(\vec{r},\vec{r'}\right) - E N_{\nu\nu'}\left(\vec{r},\vec{r'}\right) \right] \varphi_{\nu'}(\vec{r'}) = 0$$

- The RGM basis functions are non-orthogonal (at short distances):

$$\mathcal{N}_{\nu\nu'}(\vec{r},\vec{r'}) = \langle \Phi_{\nu}^{(A)}(\vec{r}) | \mathcal{A}_{\nu} \mathcal{A}_{\nu'} | \Phi_{\nu'}^{(A)}(\vec{r'}) \rangle$$

- Full microscopic Hamiltonian and the Hamiltonian Kernel

$$H = T_{\rm rel}(r) + \mathcal{V}_{\rm rel} + \bar{V}_{\rm Coul}(r) + H_{1\nu} + H_{2\nu}$$

$$\mathcal{H}_{\nu\nu'}(\vec{r},\vec{r'}) = \langle \Phi_{\nu}^{(A)}(\vec{r}) | \mathcal{A}_{\nu} H \mathcal{A}_{\nu'} | \Phi_{\nu'}^{(A)}(\vec{r'}) \rangle$$

See **S. Quaglioni and P. Navrátil** arXiv: 0804.1560 [nucl-th] (2008); accepted for PRL

A=5: The n+^{4}He scattering problem

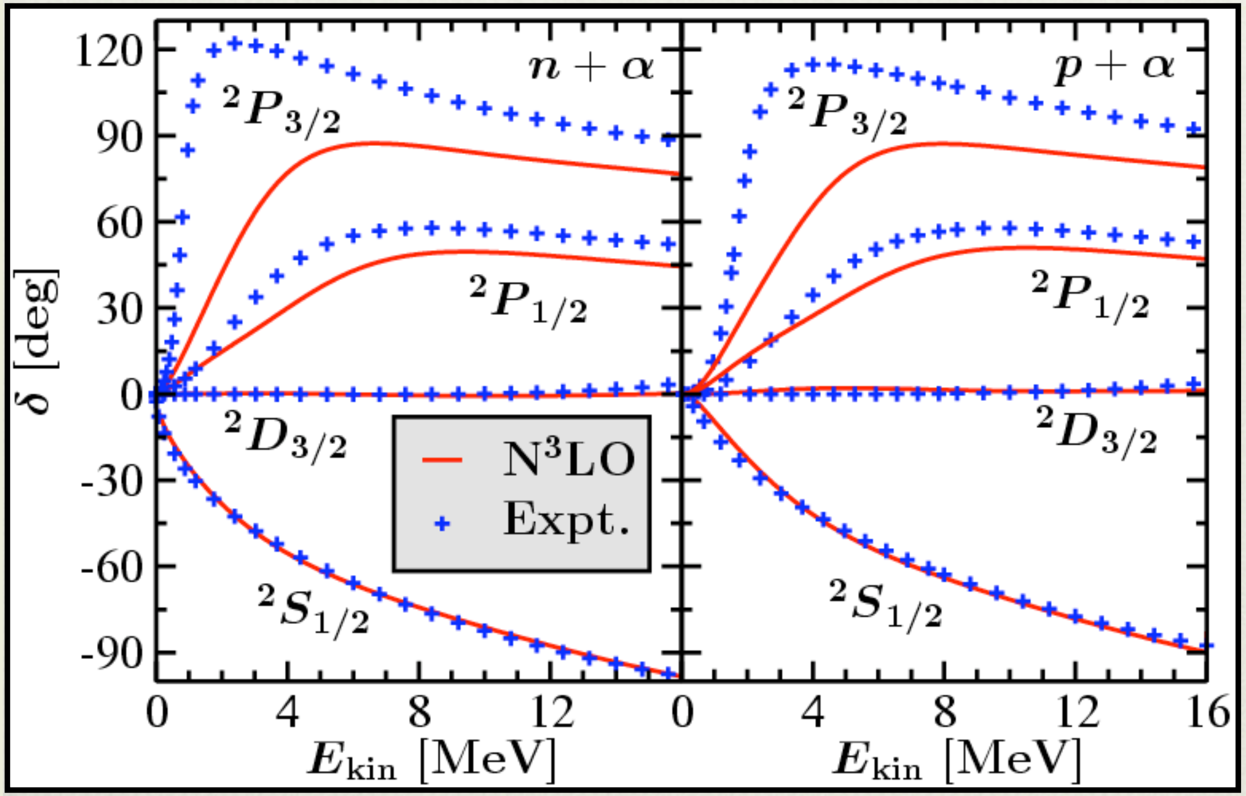
Ideal test ground for many-body scattering theory:

- The A=5 system does not have a bound state
- ^{4}He is tightly bound: single-channel scattering is valid up to ~20 MeV
- Two low-lying p-wave resonances ($3/2^-$ and $1/2^-$)
  Non-resonant s-wave scattering ($1/2^+$)
- Large effects of the Pauli exclusion principle
- Studied with GFMC, NCSM/RGM, rRGM (prelim.)

A=5: NCSM/RGM

χEFT N^{3}LO NN potential convergence reached with two-body effective interaction

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



- ^{4}He states: g.s., 0^+0, 0^-0, 2^-0, 2^-1, 1^-1, 1^-0
- $^2S_{1/2}$ is in agreement with experiment. Dominated by N-α repulsion due to Pauli exclusion.
- $^2P_{1/2}$ and $^2P_{3/2}$ present insufficient spin-orbit splitting. Sensitive to Interaction model.

S. Quaglioni and P. Navratil, arXiv: 0804.1560 [nucl-th] (2008)

The first n-^{4}He and p-^{4}He phase shifts calculation within the NCSM/RGM approach. Fully *ab initio*, very promising results. The resonances are sensitive to 3NF interaction.

Cold atom gases

Effective interaction approach to the many-boson problem

New arena for nuclear physics tools

- System of harmonically trapped, spinless bosons.
- Strong short-range interactions ⇒
  Description beyond the mean field desirable.
- Exact diagonalizatoin with Lee-Suzuki effective
  interaction à la NCSM.

See:
J. Christensson, C.Forssén, S. Åberg, and S.M. Reimann
arXiv: 0802.2811 [cond-mat.other](2008)

(Quasi) 2D-trap

- $\omega_x = \omega_y = \omega \ll \omega_z$ length scale $b=(\hbar/m\omega)^{1/2}$
- Short-range, repulsive interaction

$$H = \sum_{i=1}^{N} \left[\frac{\mathbf{p}_i^2}{2m} + \frac{1}{2} m\omega^2 \mathbf{r}_i^2 \right] + \frac{1}{2} \sum_{i \neq j}^{N} \frac{g}{2\pi\sigma^2} \exp\left(-\frac{|\mathbf{r}_i - \mathbf{r}_j|^2}{2\sigma^2} \right)$$

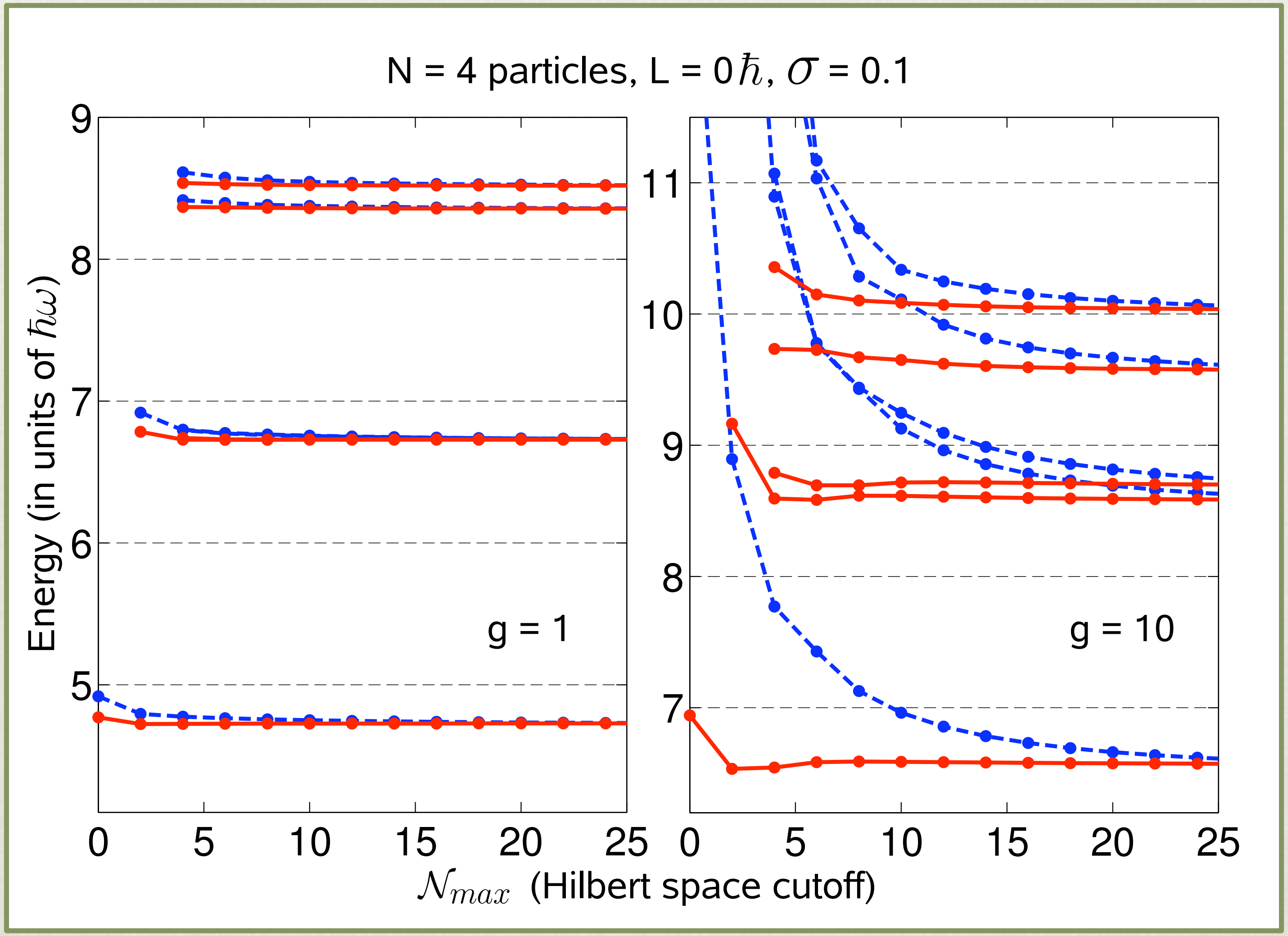
$\sigma \sim 0.1$, $g \sim 1$ (tunable)

- Many-body basis states are permanents

- *P*-space defined by $E \leq \hbar\omega\ (N + \mathcal{N}_{max})$

- *L* good quantum number

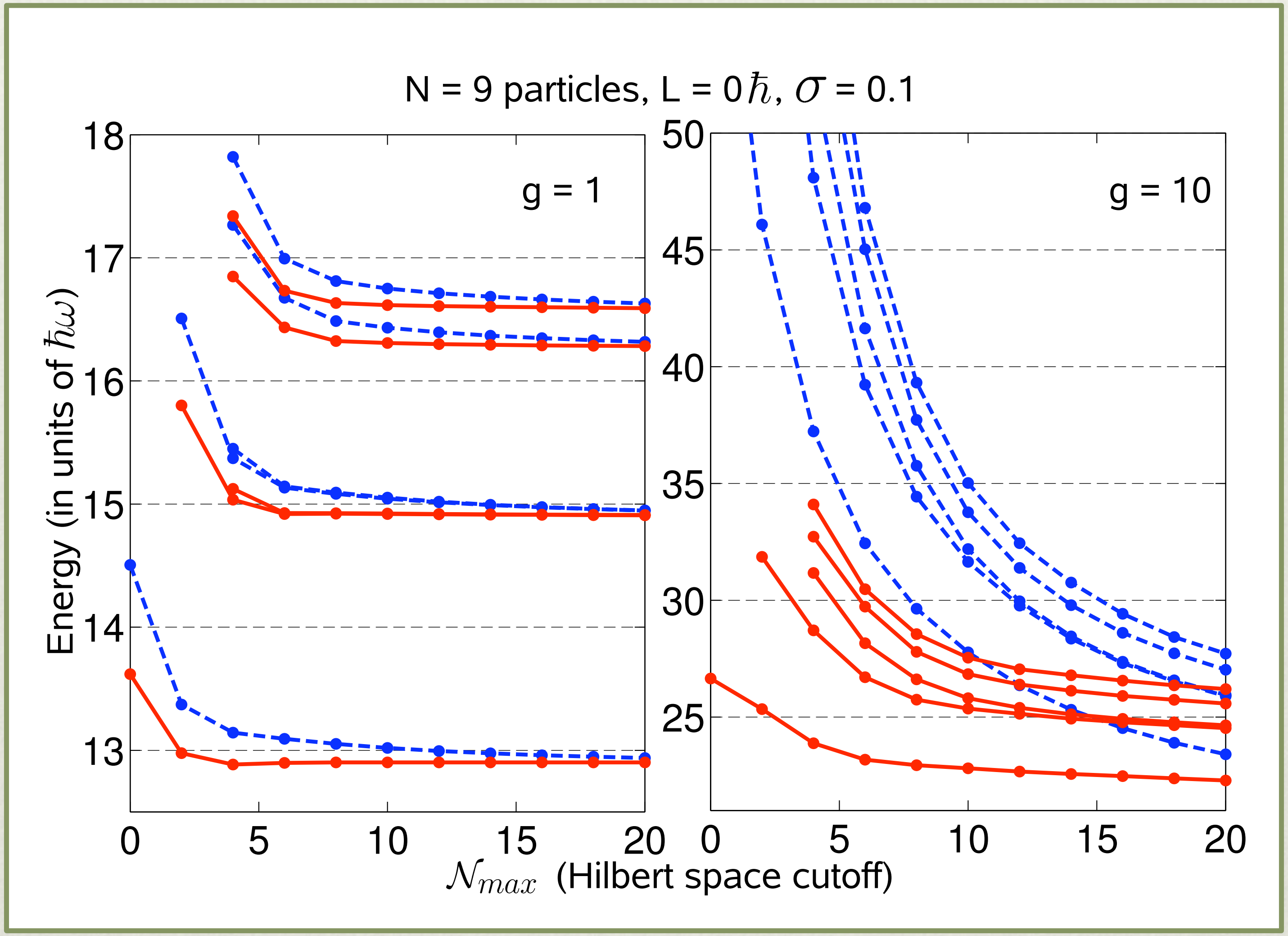
Results: $N = 4$



Blue-dashed = Standard CI

Red solid = two-body Lee-Suzuki effective interaction

Results: N = 9



Blue-dashed = Standard CI

Red solid = two-body Lee-Suzuki effective interaction

Summary

- From QCD to effective nuclear interactions
- Chiral 3NF in *p*-shell nuclei using NCSM
- Towards an extended basis space:
  clustering + continuum
- NCSM/RGM first steps:
  single-nucleon scattering calculations
- Effective interaction approach to the
  many-boson systems