No-core shell model for nuclear structure and reactions

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$$H\,\Psi = E\,\Psi$$

We cannot solve the full problem in the complete Hilbert space, so we must truncate to a finite model space

$\Longrightarrow$ We must use effective interactions and operators!

No Core Shell Model

"*Ab Initio*" approach to microscopic nuclear structure calculations, in which <u>all</u> <u>A</u> nucleons are treated as being active.

Want to solve the A-body Schrödinger equation

$$H_A \Psi^A = E_A \Psi^A$$

Ref: P. Navrátil, J.P. Vary, B.R.B., PRC <u>62,</u> 054311 (2000)

No-Core Shell-Model Approach

- Start with the purely intrinsic Hamiltonian

$$H_A = T_{rel} + \mathcal{V} = \frac{1}{A}\sum_{i<j=1}^{A}\frac{(\vec{p}_i - \vec{p}_j)^2}{2m} + \sum_{i<j=1}^{A} V_{NN} \left(+ \sum_{i<j<k}^{A} V_{ijk}^{3b} \right)$$

Note: There are <u>no</u> phenomenological s.p. energies**!**

Can use <u>any</u> NN potentials

- Coordinate space: Argonne V8', AV18
  Nijmegen I, II
- Momentum space: CD Bonn, EFT Idaho

No-Core Shell-Model Approach

- Next, add CM harmonic-oscillator Hamiltonian

$$H_{CM}^{HO} = \frac{\vec{P}^{\,2}}{2Am} + \frac{1}{2} A m \Omega^2 \vec{R}^{\,2}\,; \quad \vec{R} = \frac{1}{A}\sum_{i=1}^{A} \vec{r}_i\,, \quad \vec{P} = Am\dot{\vec{R}}$$

To H_A, yielding

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

Defines a basis (*i.e.* HO) for evaluating V_{ij}

Effective Interaction

- Must truncate to a finite model space $V_{ij} \rightarrow V_{ij}^{effective}$
- In general, V_{ij}^{eff} is an A-body interaction
- We want to make an a-body cluster approximation

$$\mathcal{H} = \mathcal{H}^{(I)} + \mathcal{H}^{(A)} \quad \underset{a < A}{\gtrapprox} \quad \mathcal{H}^{(I)} + \mathcal{H}^{(a)}$$

Two-body cluster approximation (a=2)

$$\mathcal{H} \approx \mathcal{H}^{(I)} + \mathcal{H}^{(2)}$$

$$H_2^{\Omega} = \underbrace{H_{0_2} + H_2^{CM}}_{h_1+h_2} + V_{12} = \frac{\vec{p}^{\,2}}{2m} + \frac{1}{2} m\Omega^2 \vec{r}^{\,2} + H_2^{CM} + V(\sqrt{2}\vec{r}) - \frac{m\Omega^2}{A} \vec{r}^{\,2}$$

Carry out a unitary transformation on H_2^{Ω}

$$\mathcal{H}_2 = e^{-S^{(2)}} H_2^{\Omega} e^{S^{(2)}} \quad \text{where } S^{(2)} \text{ is anti Hermitian}$$

$S^{(2)}$ is determined from the decoupling condition

$$Q_2 e^{-S^{(2)}} H_2^{\Omega} e^{S^{(2)}} P_2 = 0 \quad \text{where } S^{(2)} = Q_2 S^{(2)} P_2$$

P_2 = model space, Q_2 = excluded space, $P_2 + Q_2 = 1$

$$P_2 S^{(2)} P_2 = Q_2 S^{(2)} Q_2 = 0$$

Two-body cluster approximation (a=2)

It is convenient to write $S^{(2)}$ in terms of another operator "ω" as

$$S^{(2)} = \mathrm{arctanh}(\omega - \omega^\dagger) \quad \text{with} \quad Q_2 \omega P_2 = \omega$$

Then the Hermitian effective operator in the P_2 space can be expressed in the form

$$\mathcal{H}_{\mathrm{eff}}^{(2)} = P_2 \mathcal{H}_2 P_2 = \frac{P_2 + P_2 \omega^\dagger Q_2}{\sqrt{P_2 + \omega^\dagger \omega}} H_2^\Omega \frac{P_2 + Q_2 \omega P_2}{\sqrt{P_2 + \omega^\dagger \omega}}$$

Analogously, <u>any</u> <u>arbitrary</u> operator can be written in the P_2 space as

$$\mathcal{O}_{\mathrm{eff}}^{(2)} = P_2 \mathcal{O}_2 P_2 = \frac{P_2 + P_2 \omega^\dagger Q_2}{\sqrt{P_2 + \omega^\dagger \omega}} O \frac{P_2 + Q_2 \omega P_2}{\sqrt{P_2 + \omega^\dagger \omega}}$$

Exact solution for ω:

Let E_k and $|k\rangle$ be the eigensolutions of H_2^{Ω},

$$H_2^{\Omega}|k\rangle = E_k|k\rangle$$

Let $|\alpha_P\rangle$ and $|\alpha_Q\rangle$ be HO states belonging to the model space P and the excluded space Q, respectively. Then ω is given by:

$$\langle\alpha_Q|k\rangle = \sum_{\alpha_P}\langle\alpha_Q|\omega|\alpha_P\rangle\langle\alpha_P|k\rangle$$

or

$$\langle\alpha_Q|\omega|\alpha_P\rangle = \sum_{k\in K}\langle\alpha_Q|k\rangle\langle\tilde{k}|\alpha_P\rangle$$

NCSM ROAD MAP

1. Choose a NN interaction (or NN + NNN interactions)

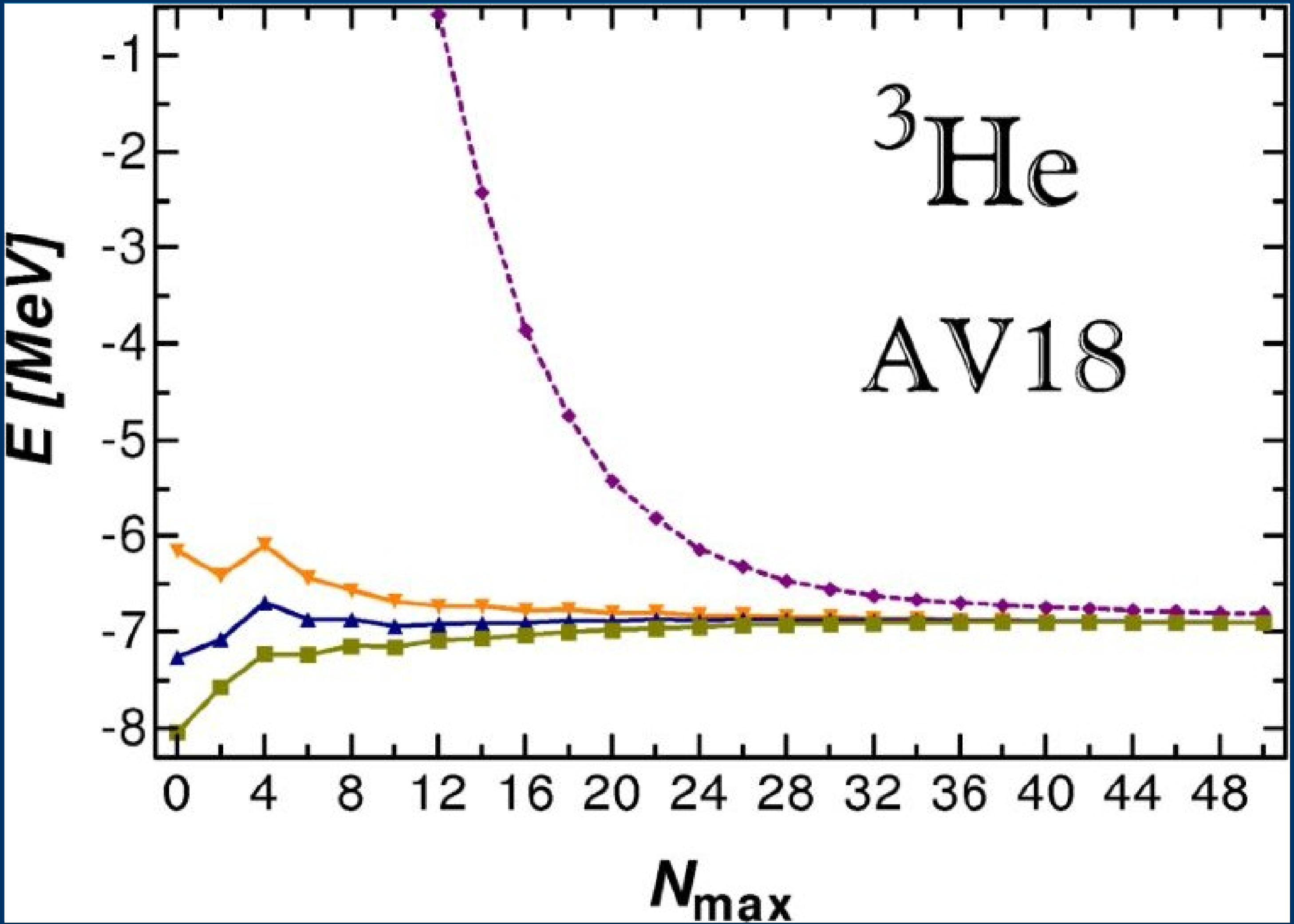
2. Solve $H_n^{\Omega}|k_n\rangle = E_n|k_n\rangle$ for E_n and $|k_n\rangle$ with n=2,3,...

3. Calculate $\langle \alpha_Q^n | \omega | \alpha_P^n \rangle = \sum_{k \in K} \langle \alpha_Q | k_n \rangle \langle \tilde{k}_n | \alpha_P \rangle$

4. Determine $\mathcal{H}_n^{\text{eff}}$ and $\mathcal{O}_n^{\text{eff}}$ in the given model space

5. Diagonalize $\mathcal{H}_n^{\text{eff}}$ in the given model space, *i.e.*,
   $N_{max}\hbar\Omega$ = energy above the ground state

6. To check convergence of results repeat calculations
   for: *i)* increasing N_{max} and/or cluster level
   ii) several values of $\hbar\Omega$



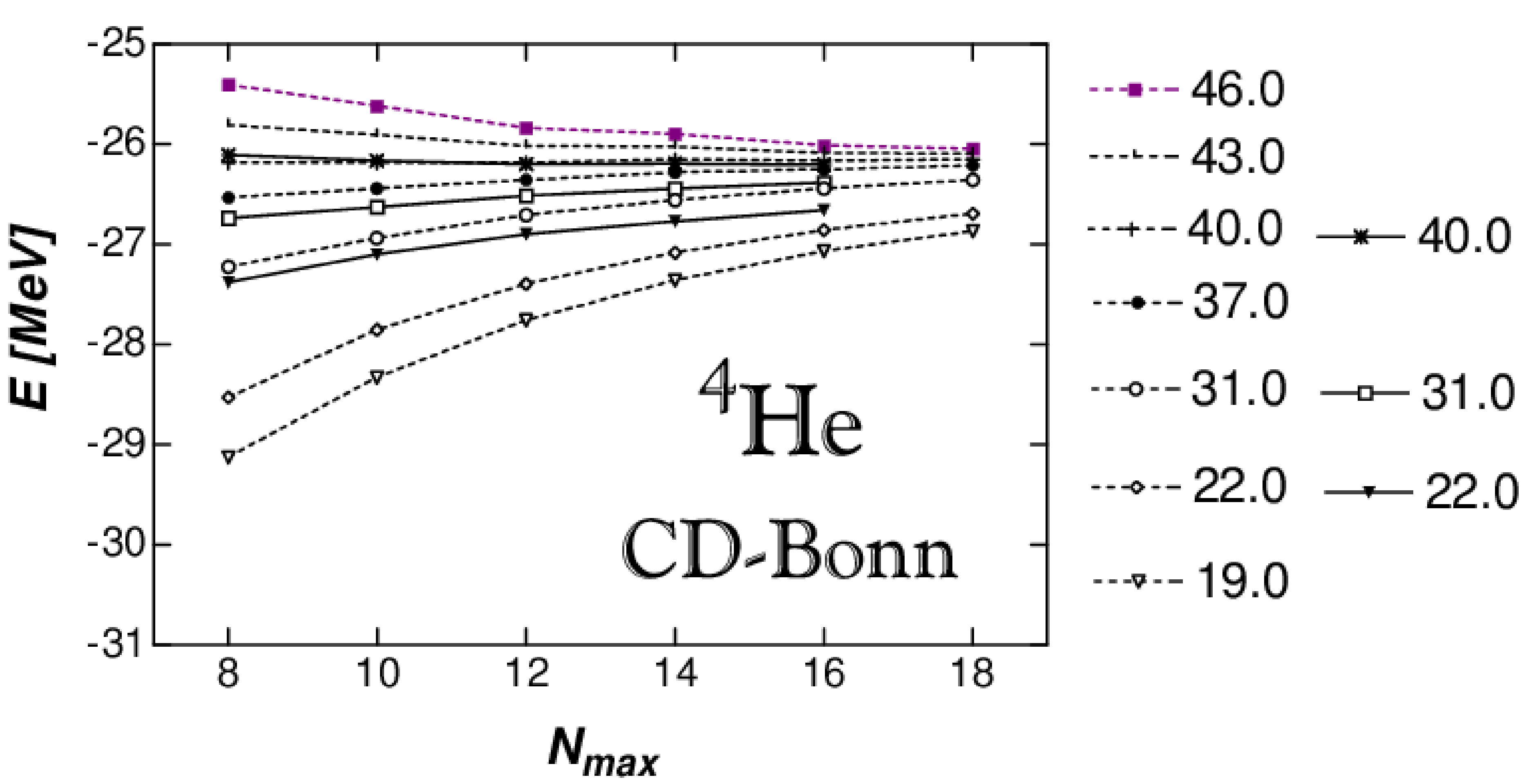
bare

$\hbar\Omega = 32$

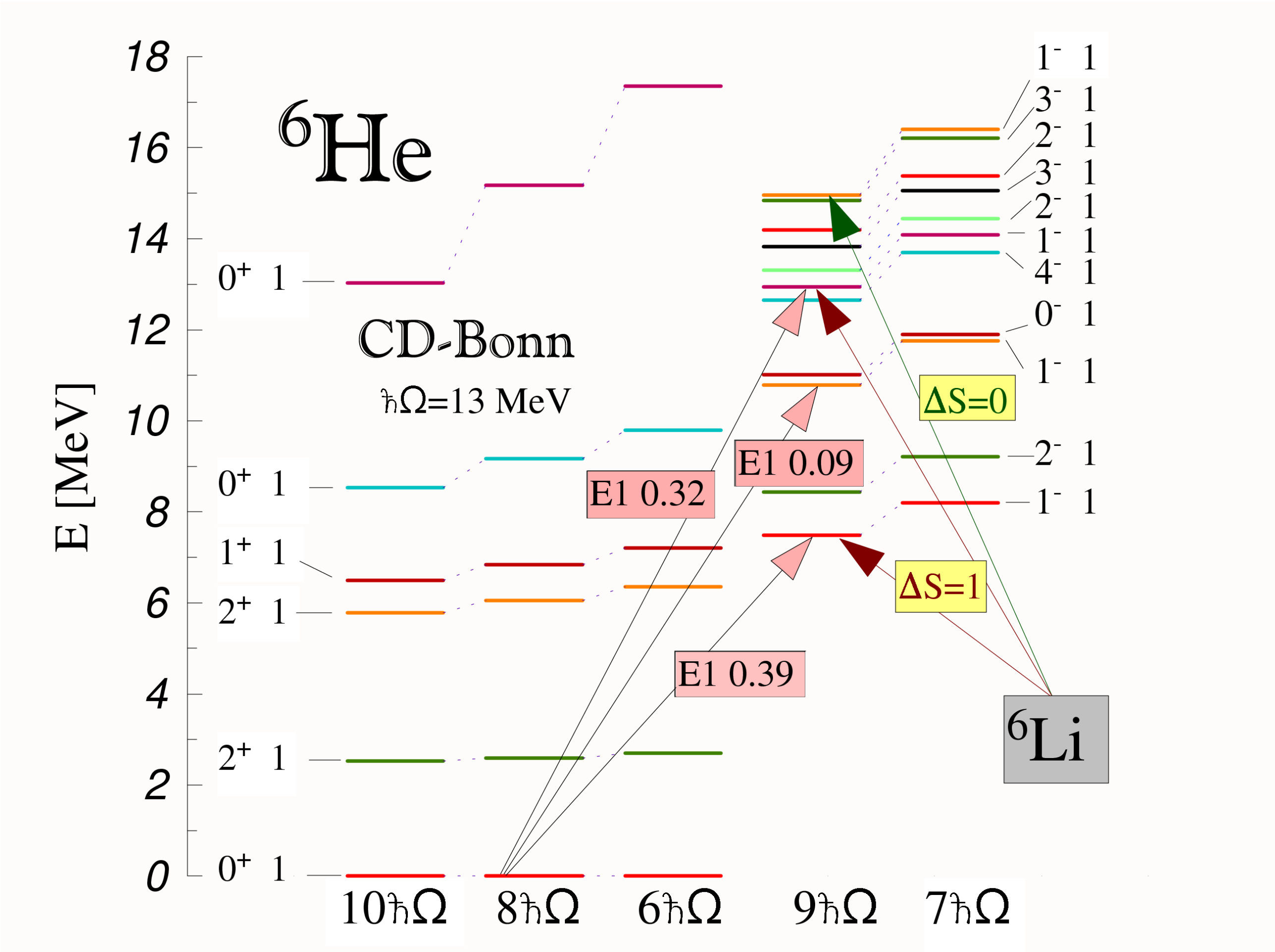
$\hbar\Omega = 28$

$\hbar\Omega = 24$

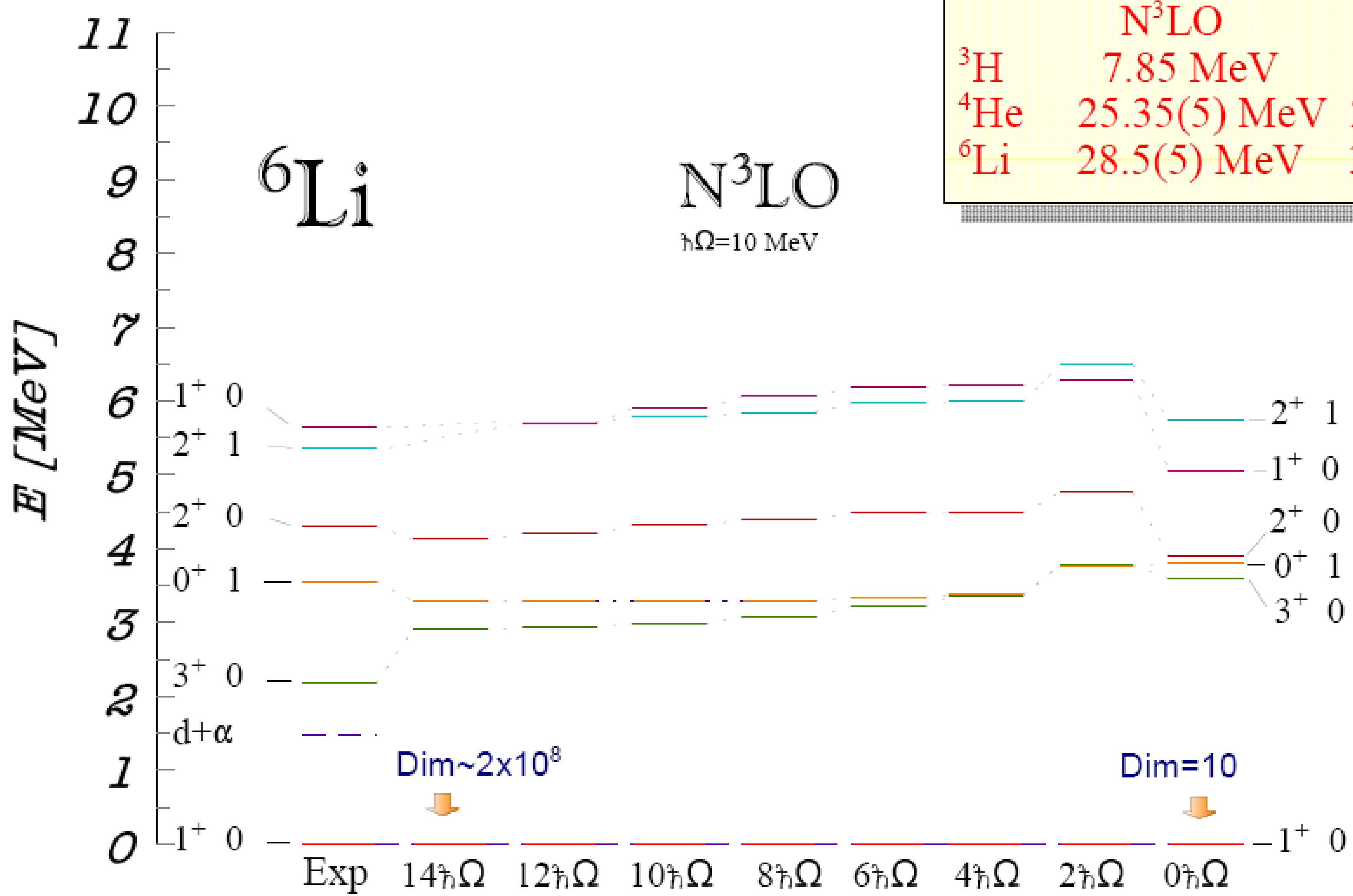
in MeV



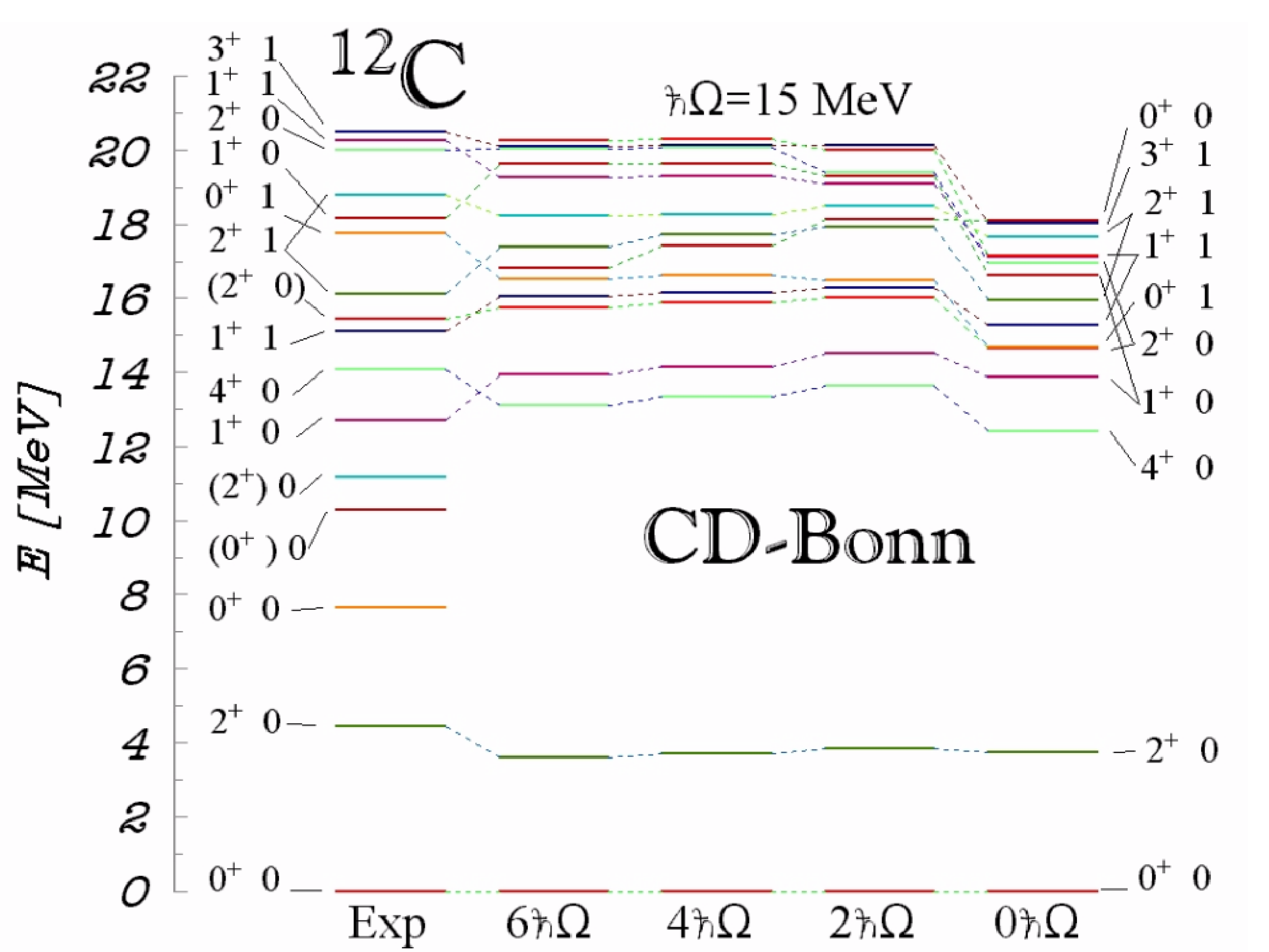
-25
-26
-27
-28
-29
-30
-31
E [MeV]
8
10
12
14
16
18
N_{max}
^{4}He
CD-Bonn
46.0
43.0
40.0
40.0
37.0
31.0
31.0
22.0
22.0
19.0



^{6}He
CD-Bonn
ħΩ=13 MeV
E [MeV]
0
2
4
6
8
10
12
14
16
18
0+ 1
2+ 1
2+ 1
1+ 1
0+ 1
0+ 1
10ħΩ
8ħΩ
6ħΩ
9ħΩ
7ħΩ
1- 1
3- 1
2- 1
3- 1
2- 1
1- 1
4- 1
0- 1
1- 1
2- 1
1- 1
E1 0.32
E1 0.09
E1 0.39
ΔS=0
ΔS=1
^{6}Li



	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



^{12}C
ħΩ=15 MeV
CD-Bonn
E [MeV]
0
2
4
6
8
10
12
14
16
18
20
22
Exp
6ħΩ
4ħΩ
2ħΩ
0ħΩ
3+ 1
1+ 1
2+ 0
1+ 0
0+ 1
2+ 1
(2+ 0)
1+ 1
4+ 0
1+ 0
(2+) 0
(0+) 0
0+ 0
2+ 0
0+ 0
0+ 0
3+ 1
2+ 1
1+ 1
0+ 1
2+ 0
1+ 0
4+ 0
2+ 0
0+ 0

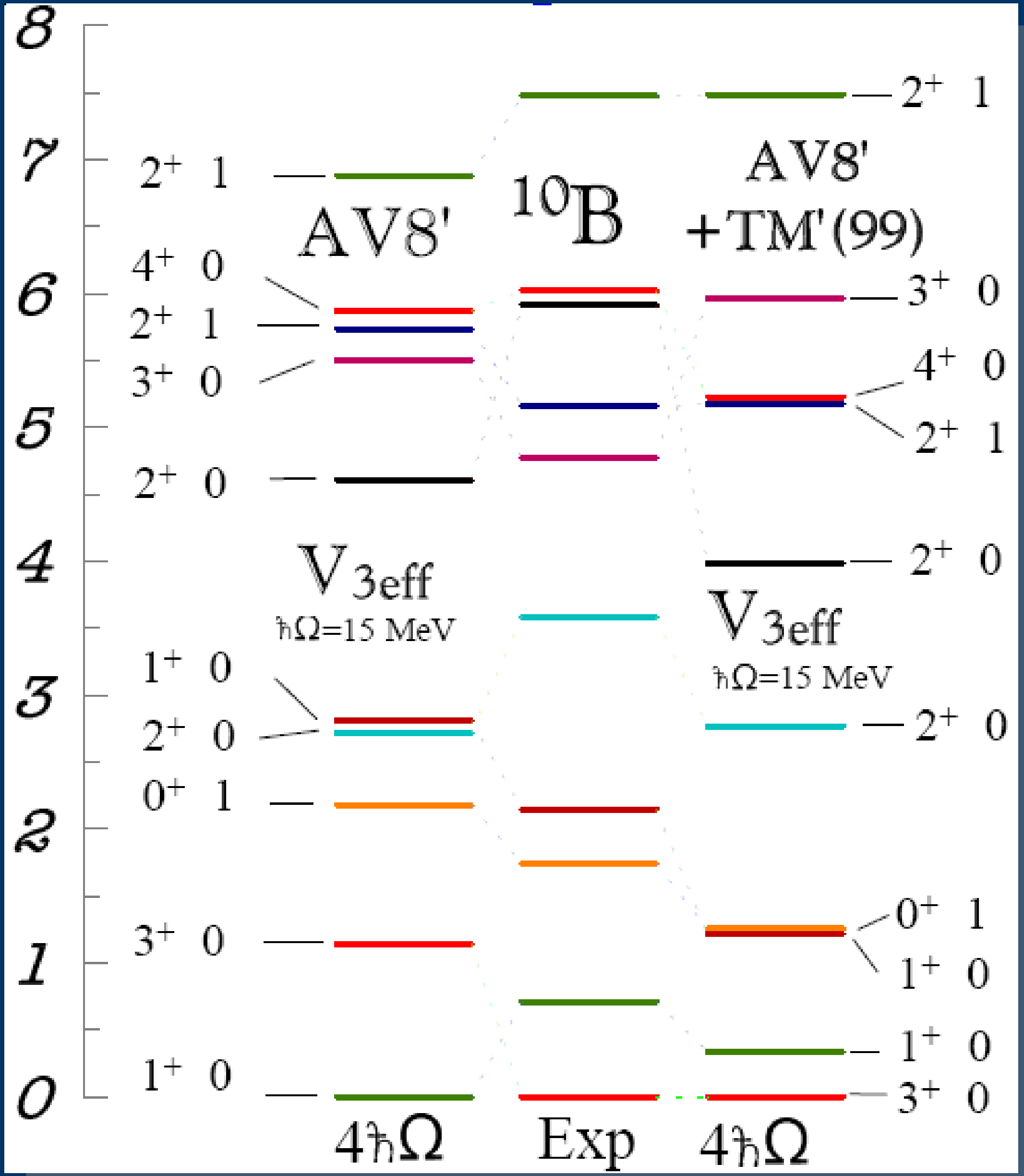
H. Kamada, *et al.*, Phys. Rev. C 64, 044001 (2001)

PHYSICAL REVIEW C, VOLUME 64, 044001

Benchmark test calculation of a four-nucleon bound state

In the past, several efficient methods have been developed to solve the Schrödinger equation for four-nucleon bound states accurately. These are the Faddeev-Yakubovsky, the coupled-rearrangement-channel Gaussian-basis variational, the stochastic variational, the hyperspherical variational, the Green's function Monte Carlo, the no-core shell model, and the effective interaction hyperspherical harmonic methods. In this article we compare the energy eigenvalue results and some wave function properties using the realistic AV8′ *NN* interaction. The results of all schemes agree very well showing the high accuracy of our present ability to calculate the four-nucleon bound state.

$BE_{th} \approx 25.91$ MeV $\quad$ $BE_{exp} \approx 28.296$ MeV



8
7
6
5
4
3
2
1
0
AV8'
V_{3eff}
ħΩ=15 MeV
4ħΩ
^{10}B
Exp
AV8'
+TM'(99)
V_{3eff}
ħΩ=15 MeV
4ħΩ
2+ 1
4+ 0
2+ 1
3+ 0
2+ 0
1+ 0
2+ 0
0+ 1
3+ 0
1+ 0
2+ 1
3+ 0
4+ 0
2+ 1
2+ 0
2+ 0
0+ 1
1+ 0
1+ 0
3+ 0

Exact solution for ω: 3-body cluster level

Let E_k and $|k\rangle$ be the eigensolutions of H_3^Ω,

$$H_3^\Omega |k\rangle = E_k |k\rangle$$

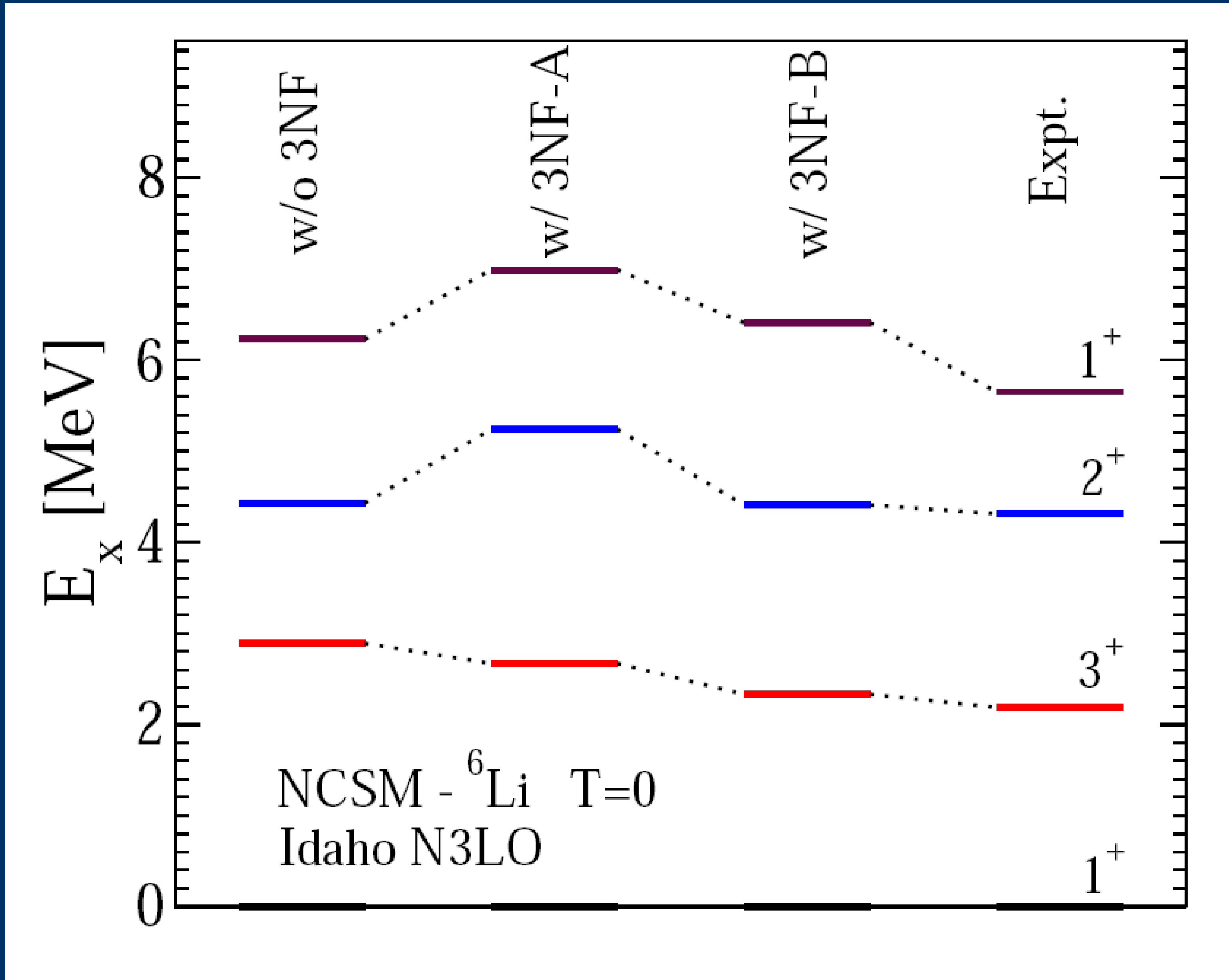
Let $|\alpha_P\rangle$ and $|\alpha_Q\rangle$ be HO states belonging to the model space P and the excluded space Q, respectively. Then ω is given by:

$$\langle\alpha_Q|k\rangle = \sum_{\alpha_P} \langle\alpha_Q|\omega|\alpha_P\rangle\langle\alpha_P|k\rangle$$

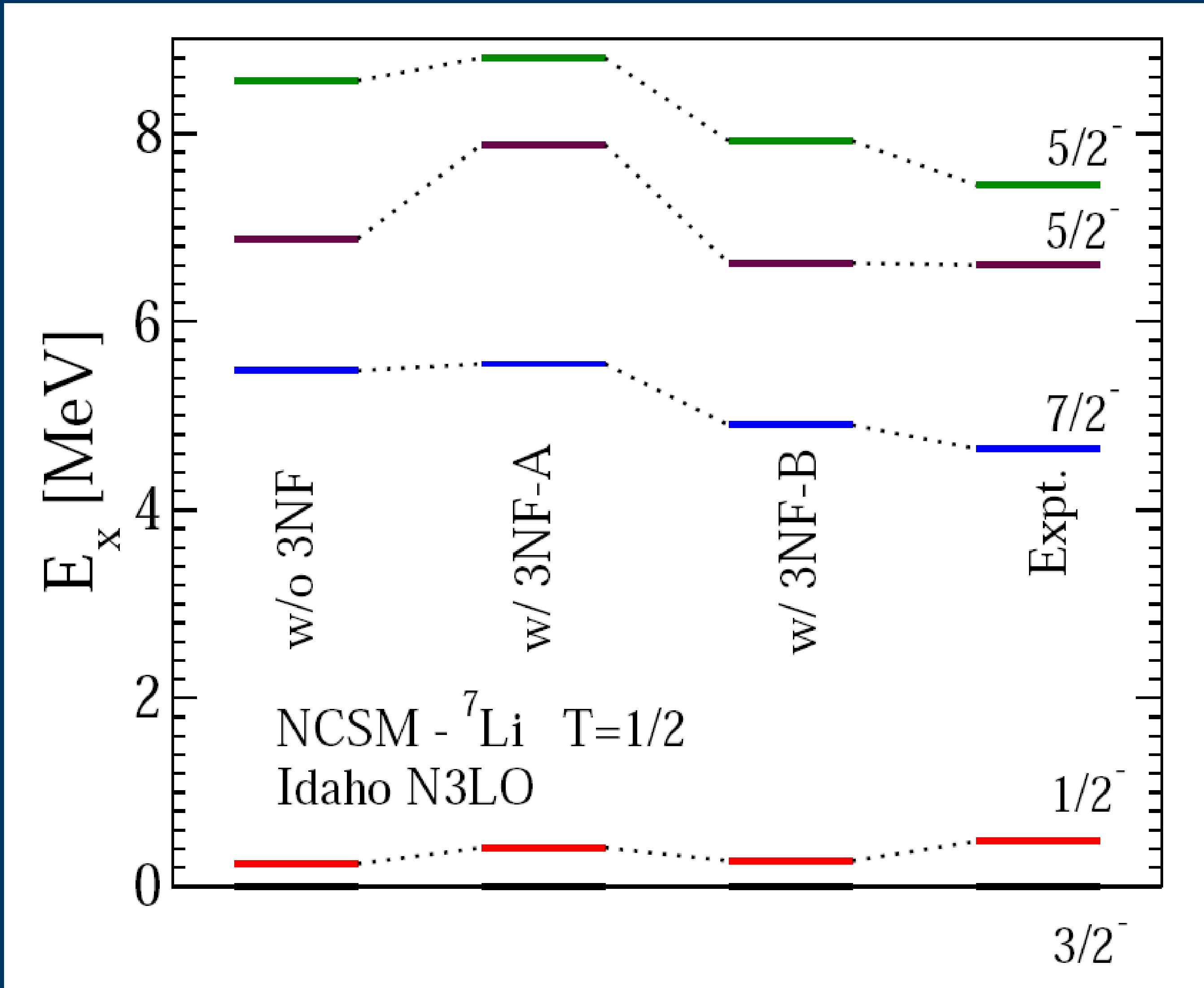
or

$$\langle\alpha_Q|\omega|\alpha_P\rangle = \sum_{k\in K} \langle\alpha_Q|k\rangle\langle\tilde{k}|\alpha_P\rangle$$

A. Nogga, *et al.*, NPA 737, 236 (2004)



A. Nogga, *et al.*, nucl-th/0511082 (2005)



H. Kamada, *et al.*, Phys. Rev. C 64, 044011 (2001)

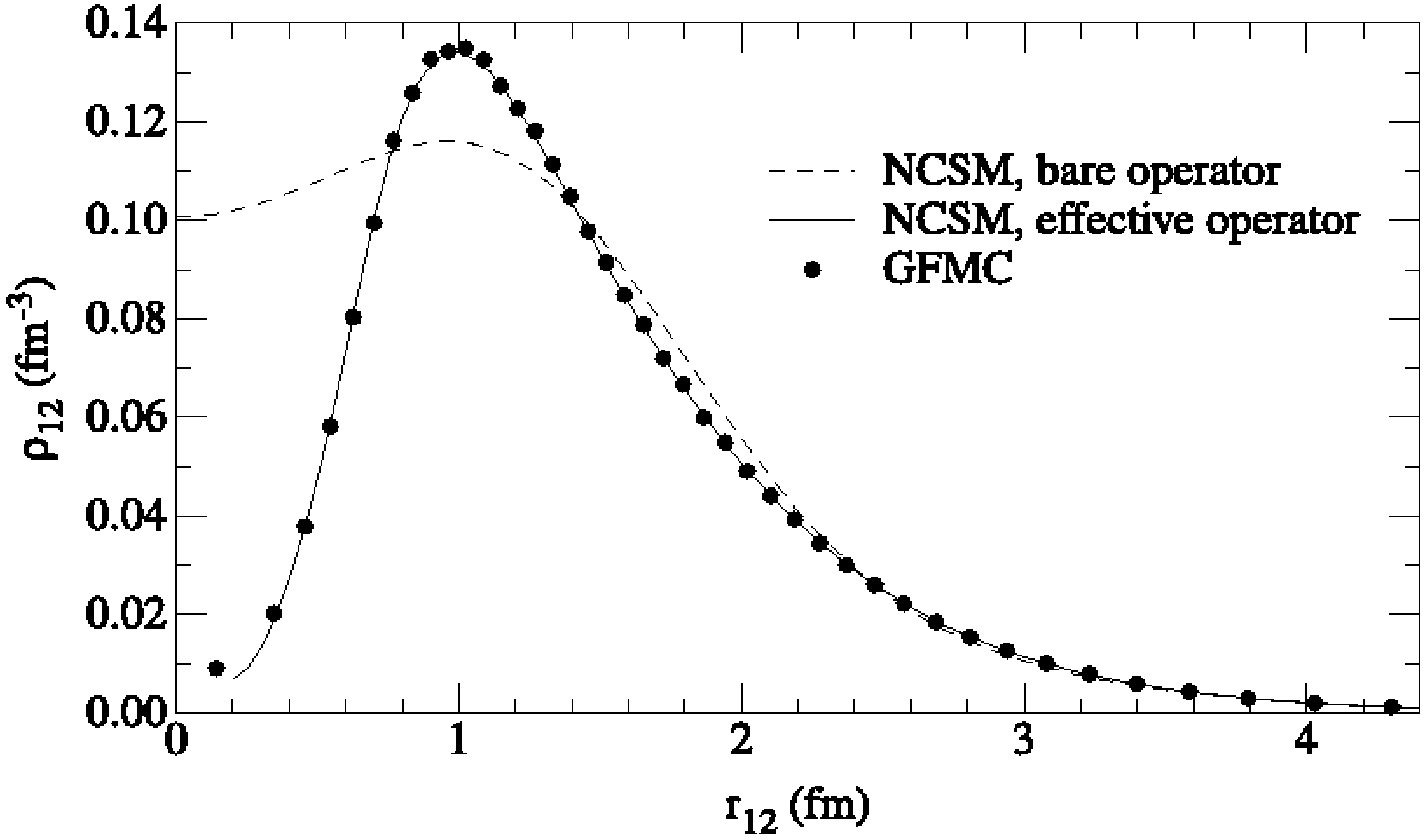


Figure 2. *NCSM and GFMC NN pair density in ^4He.*

Renormalization of other physical operators

$$\mathcal{H}_{eff}^{(2)} = P_2 \mathcal{H}_2 P_2 = \frac{P_2 + P_2 \omega^\dagger Q_2}{\sqrt{P_2 + \omega^\dagger \omega}} H_2^\Omega \frac{P_2 + Q_2 \omega P_2}{\sqrt{P_2 + \omega^\dagger \omega}}$$

$$\mathcal{O}_{eff}^{(2)} = P_2 \mathcal{O}_2 P_2 = \frac{P_2 + P_2 \omega^\dagger Q_2}{\sqrt{P_2 + \omega^\dagger \omega}} O \frac{P_2 + Q_2 \omega P_2}{\sqrt{P_2 + \omega^\dagger \omega}}$$

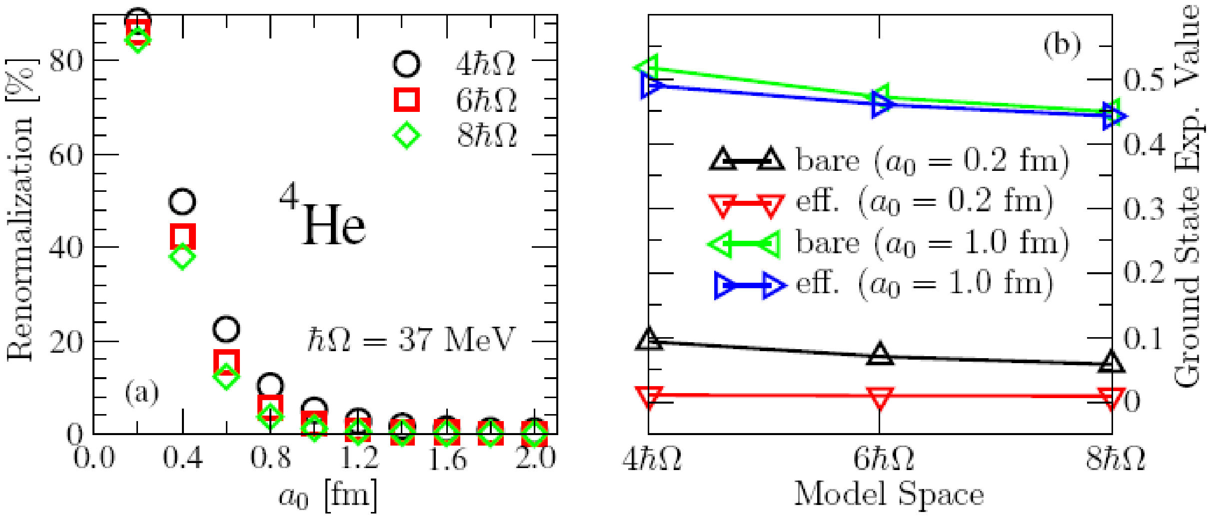
Nucleus	Observable	Model Space	Bare operator	Effective operator
^{2}H	Q_0	$4\hbar\Omega$	0.179	0.270
^{6}Li	$B(E2, 1^+0 \rightarrow 3^+0)$	$2\hbar\Omega$	2.647	2.784
^{6}Li	$B(E2, 1^+0 \rightarrow 3^+0)$	$10\hbar\Omega$	10.221	-
^{6}Li	$B(E2, 2^+0 \rightarrow 1^+0)$	$2\hbar\Omega$	2.183	2.269
^{6}Li	$B(E2, 2^+0 \rightarrow 1^+0)$	$10\hbar\Omega$	4.502	-
^{10}C	$B(E2, 2_1^+0 \rightarrow 0^+0)$	$4\hbar\Omega$	3.05	3.08
^{12}C	$B(E2, 2_1^+0 \rightarrow 0^+0)$	$4\hbar\Omega$	4.03	4.05
^{4}He	$\langle g.s.\vert T_{rel}\vert g.s.\rangle$	$8\hbar\Omega$	71.48	154.51

Stetcu, Barrett, Navratil, Vary, Phys. Rev. C 71, 044325 (2005)

- small model space: expect larger renormalization
- large variation with the model space
- three-body forces: might be important, but not the issue

- $a \rightarrow A$ for fixed model space;
- $P \rightarrow \infty$ for fixed cluster.

Range dependence

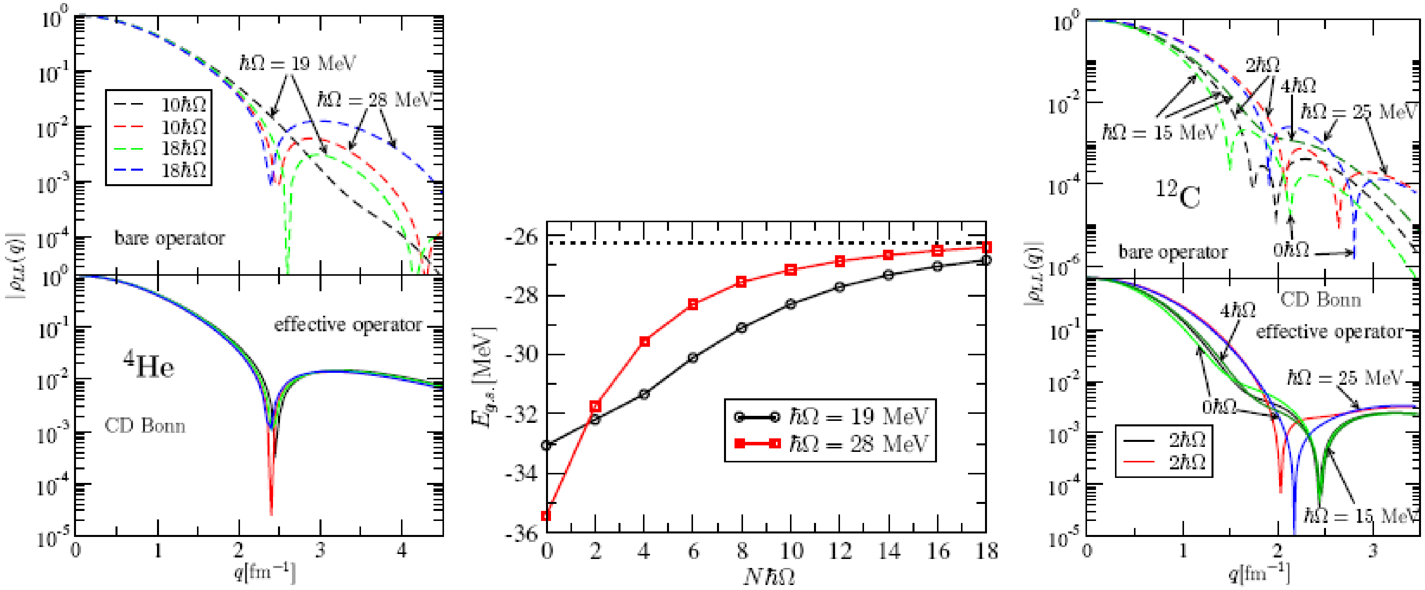


$$O \sim \exp\left[-\frac{(\vec{r}_1 - \vec{r}_2)^2}{a_0^2}\right]$$

Stetcu, Barrett, Navratil, Vary, Phys. Rev. C **71**, 044325 (2005)

Longitudinal-longitudinal distribution function

$$\rho_{LL}(q) = \frac{1}{4Z} \sum_{j \neq i} (1 + \tau_z(i))(1 + \tau_z(j)) \langle g.s. | j_0(q|\vec{r}_i - \vec{r}_j|) | g.s. \rangle$$



Stetcu, Barrett, Navratil, Vary, nucl-th/0601076

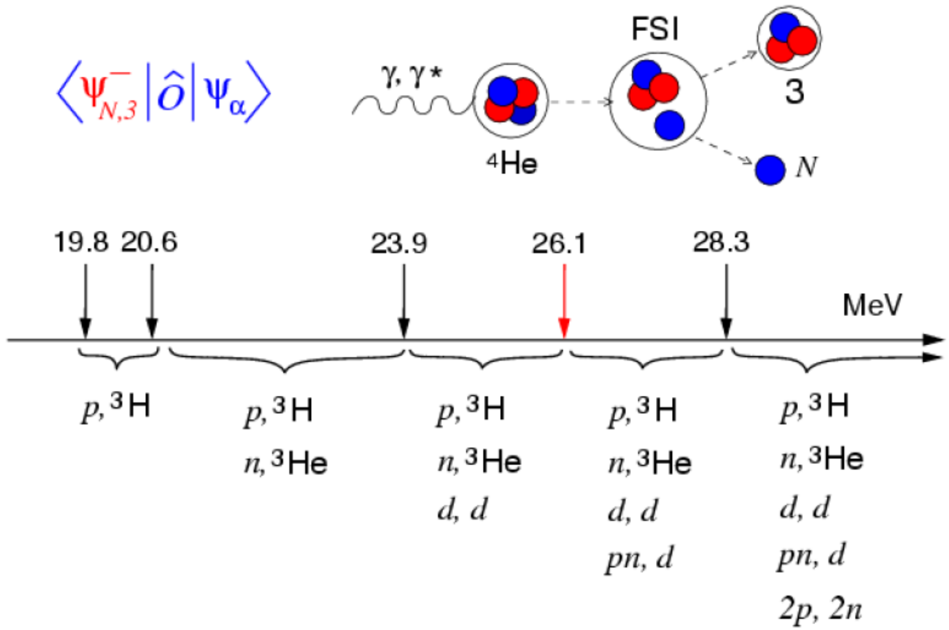
Model space independence at high momentum transfer: good renormalization at the two-body cluster level

Microscopic approach to nuclear reactions

Where is the challenge?

Full and consistent treatment of the FSI also beyond the 3-body breakup threshold

Channels up to the π−production threshold



Lorentz integral transform 101

Efros, Leidemann, Orlandini, Phys. Lett. B338, 130 (1994).

$$R(E) = \sum_{\nu} |\langle \psi_0 | O | \psi_\nu \rangle|^2 \delta(E - E_\nu)$$

LIT approach: calculate the transform of $R(E)$ and then invert:

$$\Phi[R](\sigma) = \int R(E) K(\sigma, E) dE$$

Lorentz kernel:

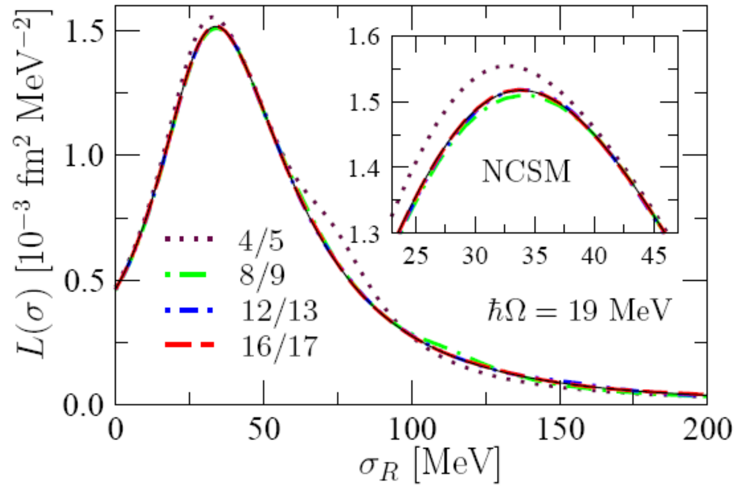
$$K(\sigma, E) = \frac{1}{(E - \sigma_R)^2 + \sigma_I^2}$$

$$\Phi[R](\sigma) = \langle \phi | \phi \rangle$$

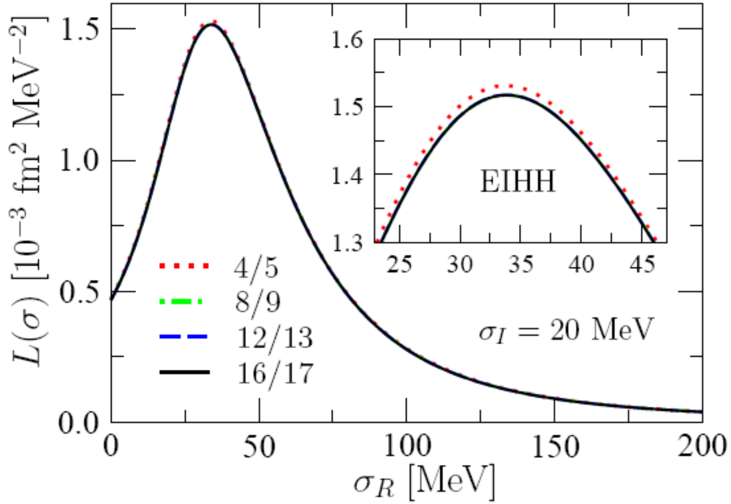
$$(H - \sigma_R - i\sigma_I)|\phi\rangle = O|\psi_0\rangle$$

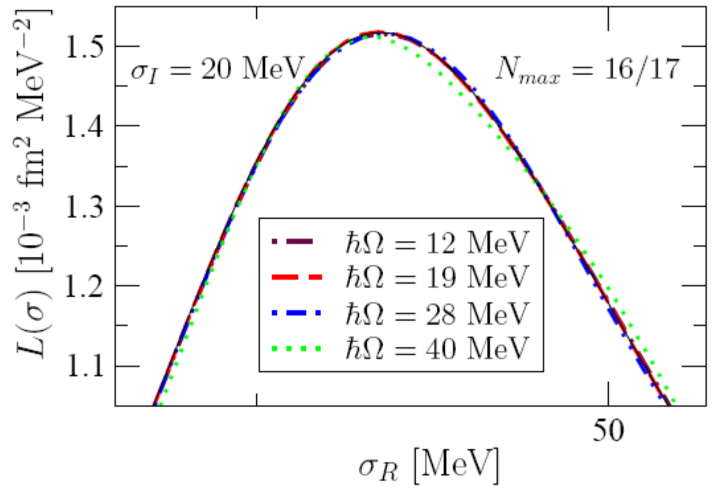
LIT convergence: ^{4}He

NCSM: model space dependence (N_{max}) ▶



Dipole transition





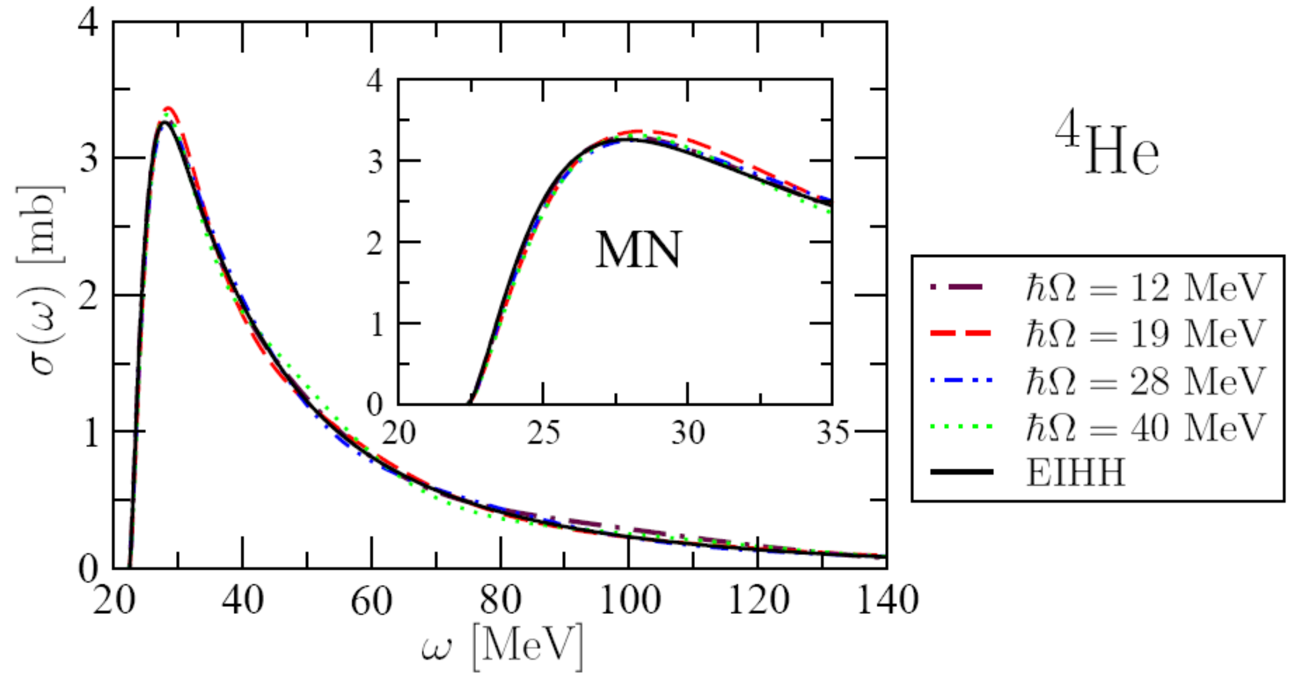
▲ EIHH: model space dependence (K_{max})

▲NCSM: Ω-dependence

Bacca, Stetcu, Quaglioni *et al.*

The ^{4}He photoabsorption cross section

within EIHH and NCSM through LIT
(test calculation with semirealistic interaction)



Bacca, Stetcu, Quaglioni *et al.*

Towards a unified decription of the nucleus

RIA:

probe medium and heavy mass nuclei off the line of stability

The goal of nuclear theory:

exact treatment of nuclei based on NN and NNN interactions

⇨ need to build a bridge between:

- *ab initio* few-body & light nuclei calculations: A $\lesssim$ 24
- $0\hbar\Omega$ Shell Model calculations: 16 $\lesssim$ A $\lesssim$ 60
- Density Functional Theory calculations: A $\gtrsim$ 60

The NCSM and RIA

The NCSM provides a microscopic understanding of light nuclei, based on the properties of the NN + NNN interactions.

As such, the NCSM will serve in a supporting role to RIA, by providing the benchmark calculations for input to investigations for heavier nuclei, *e.g.*, density functional calculations, standard shell model calculations, *etc*.

By investigating the intersections between these theoretical strategies, RIA will provide the experimental tool for developing the unified description of the nucleus.

The NCSM builds the bridge to predictive power for these approaches for heavier mass nuclei as well as tying the microscopic theory to the basic hadron physics of the nuclear Hamiltonian.