Новое *NN*-взаимодействие JISP: описание *NN*-рассеяния и ядер *s*- и *p*-оболочек в подходе *ab initio*

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Ab initio:

- Без модельных предположений (например, без введения инертного кора)
- *Ab initio* подходы:
- уравнения Фаддеева;
- метод гиперсферических функций;
- Green function’s Monte Carlo;
- no-core shell model;
- coupled-cluster approach

Coupled cluster approach:

$$|\Psi\rangle = \exp(T)|\Phi_0\rangle \ . \tag{1}$$

Here $|\Phi_0\rangle$ is an uncorrelated reference Slater determinant which might be either the Hartree-Fock (HF) state or a naive filling of the oscillator single-particle basis. Correlations are introduced through the exponential $\exp(T)$ operating on $|\Phi_0\rangle$. The operator T is a sum of n-particle–n-hole excitation operators $T = T_1 + T_2 + \ldots$ of the form,

$$T_n = \sum_{a_1\ldots a_n, i_1\ldots i_n} t_{i_1\ldots i_n}^{a_1\ldots a_n} a_{a_1}^\dagger \cdots a_{a_n}^\dagger a_{i_n} \cdots a_{i_1} \ , \tag{2}$$

where $i_1, i_2, \ldots$ are summed over hole states and $a_1, a_2, \ldots$ are summed over particle states. One obtains the algebraic equation for the excitation amplitudes $t_{ij\ldots}^{ab\ldots}$ by left-projecting the similarity-transformed Hamiltonian with an n-particle–n-hole excited Slater determinant giving

$$\langle\Phi_{ij\ldots}^{ab\ldots}| \left(H_N \exp(T)\right)_C |\Phi_0\rangle = 0 \ , \tag{3}$$

Модель оболочек:

- Две основные современные схемы:
- Monte Carlo shell model
- *m*-scheme + Lanczos (в том числе no-core shell model); осцилляторный базис

m-scheme + *Lanczos*:

- Идея: неполная диагонализация в большом базисе быстрее и проще, чем построение “правильного” базиса с определенными *J, L* и т.д.
- Translationary invariant SM (координаты Якоби, *J, L* и т.д.) $\Longrightarrow$

  $\Longrightarrow$ no-core SM (детерминанты Слэтера с фиксированным *m,* но не *J, L* и т.д.); *J* приобретает определенное значение в результате диагонализации.
- Получаем сразу несколько уровней одной четности, но с разными *J.*

Lanczos itterations:

$$\tilde{a}_1 = Ha_0;$$

$$\tilde{a}_1 \Longrightarrow a_1 : \langle a_1 | a_0 \rangle = 0;$$

$$\tilde{a}_2 = Ha_1;$$

$$\tilde{a}_2 \Longrightarrow a_2 : \langle a_2 | a_0 \rangle = \langle a_2 | a_1 \rangle = 0;$$

$$\tilde{a}_3 = Ha_2;$$

$$\cdots\cdots\cdots\cdots$$

$\langle a_i | H | a_j \rangle$ — трехдиагональная матрица.

- Диагонализация сравнительно небольшой трехдиагональной матрицы, дающей хорошее основное и нижайшие возбужденные состояния

Lanczos itterations:

$$a_0 = \alpha_0 x_0 + \alpha_1 x_1 + \alpha_2 x_2 + \ldots$$

$$a_1 = E_0 \alpha_0 x_0 + E_1 \alpha_1 x_1 + E_2 \alpha_2 x_2 + \ldots$$

$$a_2 = E_0^2 \alpha_0 x_0 + E_1^2 \alpha_1 x_1 + E_2^2 \alpha_2 x_2 + \ldots$$

$$\ldots\ldots\ldots\ldots$$

$$a_n = E_0^n \alpha_0 x_0 + E_1^n \alpha_1 x_1 + E_2^n \alpha_2 x_2 + \ldots$$

No-core shell model:

$$H_A = \frac{1}{A}\sum_{i<j}^{A}\frac{(\mathbf{p}_i-\mathbf{p}_j)^2}{2m} + \sum_{i<j}^{A} V_{NN,ij} + \sum_{i<j<k}^{A} V_{NNN,ijk}, \quad (1)$$

where m is the nucleon mass, $V_{NN,ij}$ is the two-nucleon interaction (including both strong and electromagnetic components), and $V_{NNN,ijk}$ is the three-nucleon interaction, should be arranged as spurious-free linear combinations of basis states.

To achieve this, the auxiliary Hamiltonian

$$H_{\rm NCSM} = H_A + \beta\widetilde{Q}_0 \quad (2)$$

is conventionally diagonalized within the NCSM instead of the Hamiltonian (1). Here,

$$\widetilde{Q}_0 \equiv H_{\rm CM} - \frac{3}{2}\hbar\Omega, \quad (3)$$

$$H_{\rm CM} = T_{\rm CM} + U_{\rm CM} \quad (4)$$

is the harmonic oscillator CM Hamiltonian, $T_{\rm CM}$ is the CM kinetic energy operator, and

$$U_{\rm CM} = \frac{1}{2}Am\Omega^2\mathbf{R}^2, \quad (5)$$

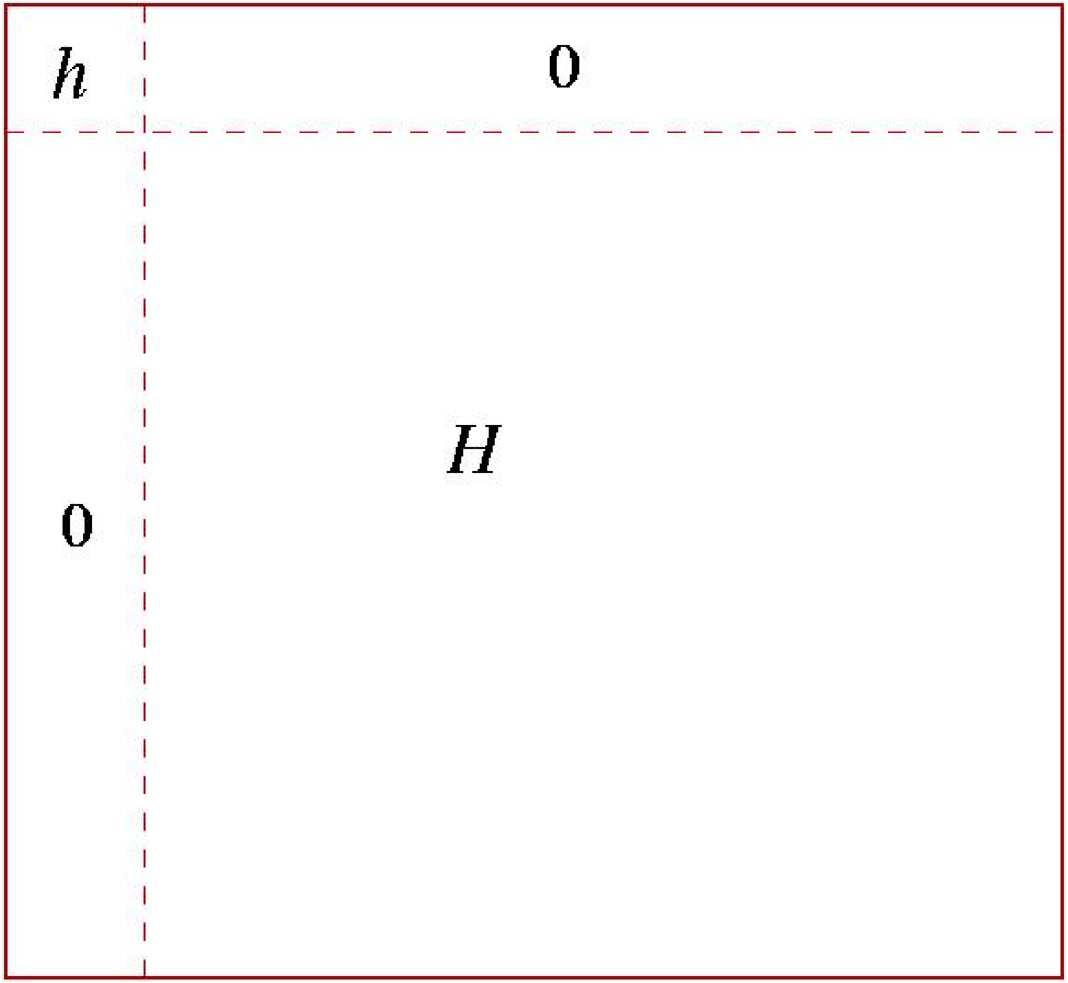
where

$$\mathbf{R} = \frac{1}{A}\sum_{i=1}^{A}\mathbf{r}_i. \quad (6)$$

Effective interactions:

- “Обычная” (с кором) модель оболочек (тяжелые ядра): *G*-матрица или просто феноменология.
- No-core SM: Lee–Suzuki transformation, т.е. *ab initio NN*-взаимодействие, полученное из исходного “гологого” *NN*-взаимодействия.

Lee–Suzuki transformation:



“Кластерное” разложение:

$H \Longrightarrow h_2 + h_3 + \ldots$

Обычно ограничиваются h_2 или $h_2 + h_3$.

Highlights

JISP = J-matrix inverse scattering potential

PETs = phase-equivalent transformations

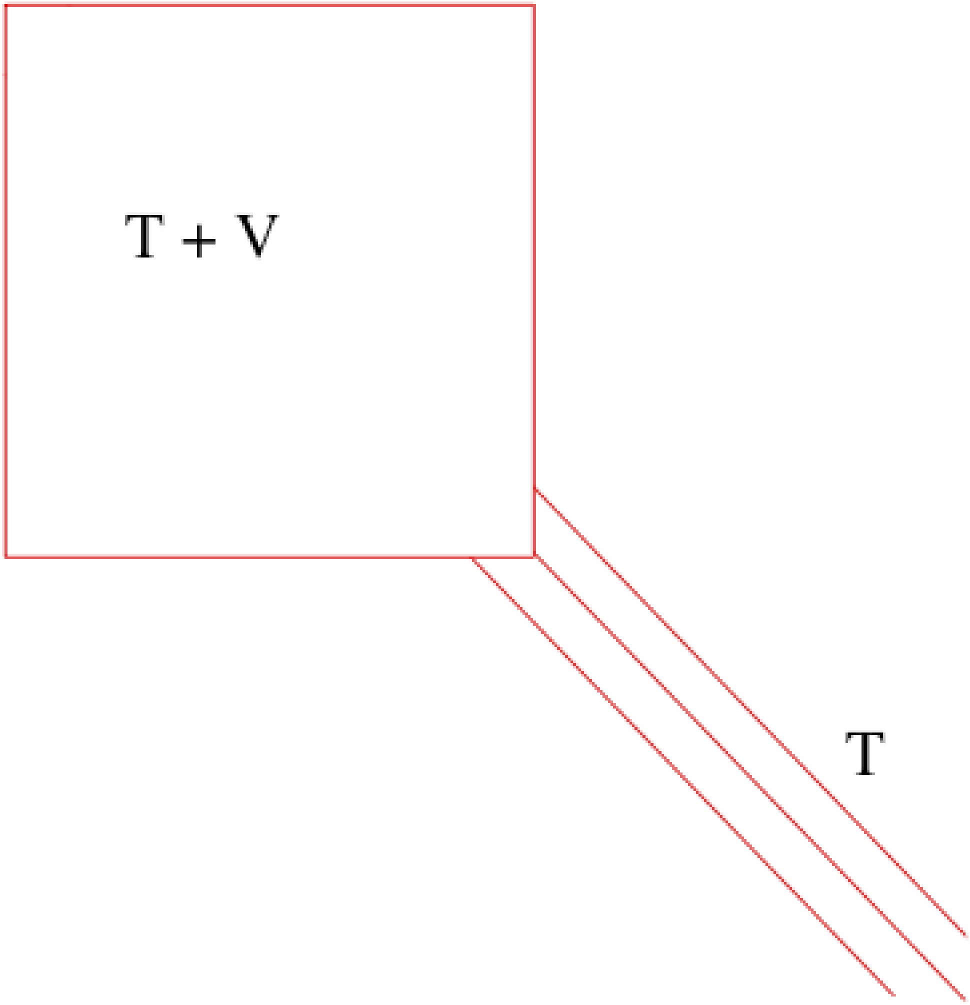
No-core shell model: *ab initio* $\Leftrightarrow$ *ab exitu* approach

No three-nucleon forces

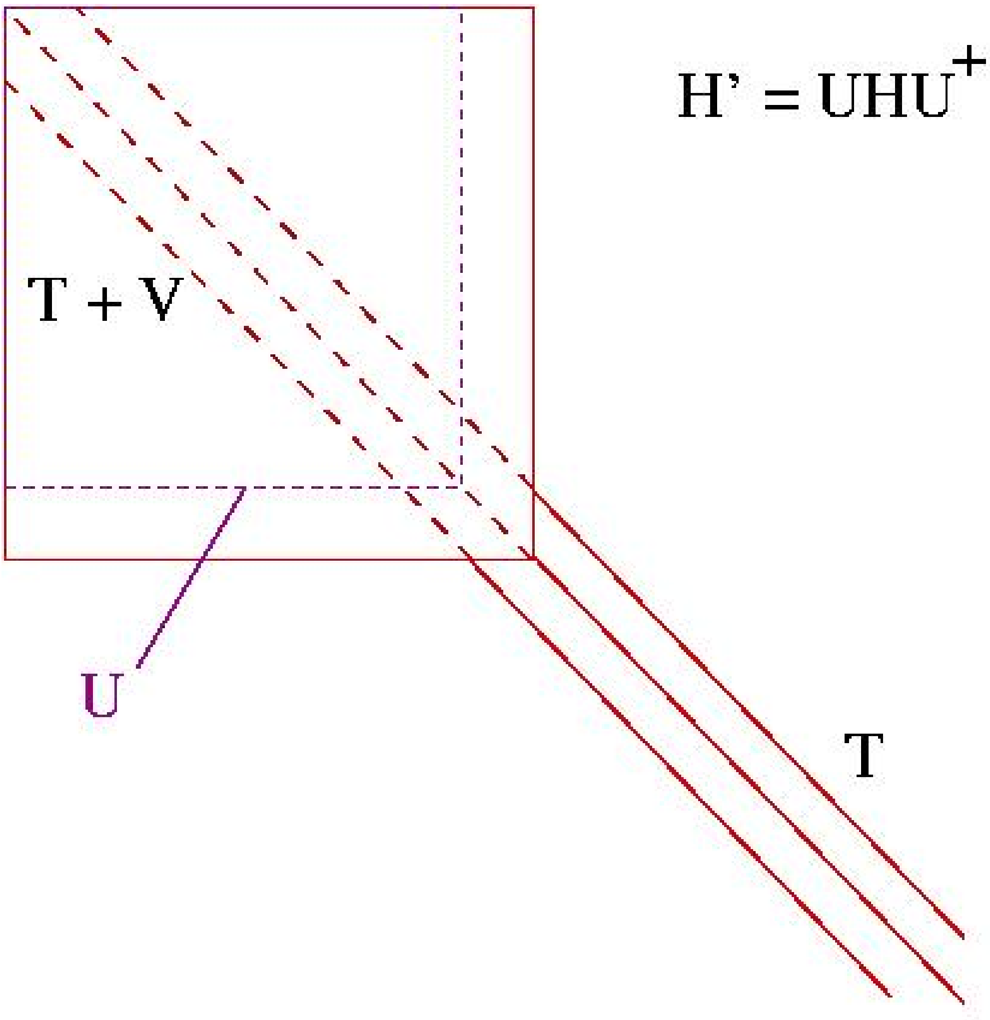
Results for nuclei with $A \leq 16$

J-matrix formalism:

scattering in the oscillator basis



PETs



ab initio ⇔ *ab exitu*

- JISP16: J-matrix inverse scattering 9hΩ *NN* potential with hΩ = 40 MeV fitted to nuclei up through ^{16}O
- Only simplest PETs generated by 2x2 unitary matrix *U* are used
- *Ab exitu* approach:
- PETs: *sd* wave - fitting deuteron properties (rms radius and quadrupole moment)

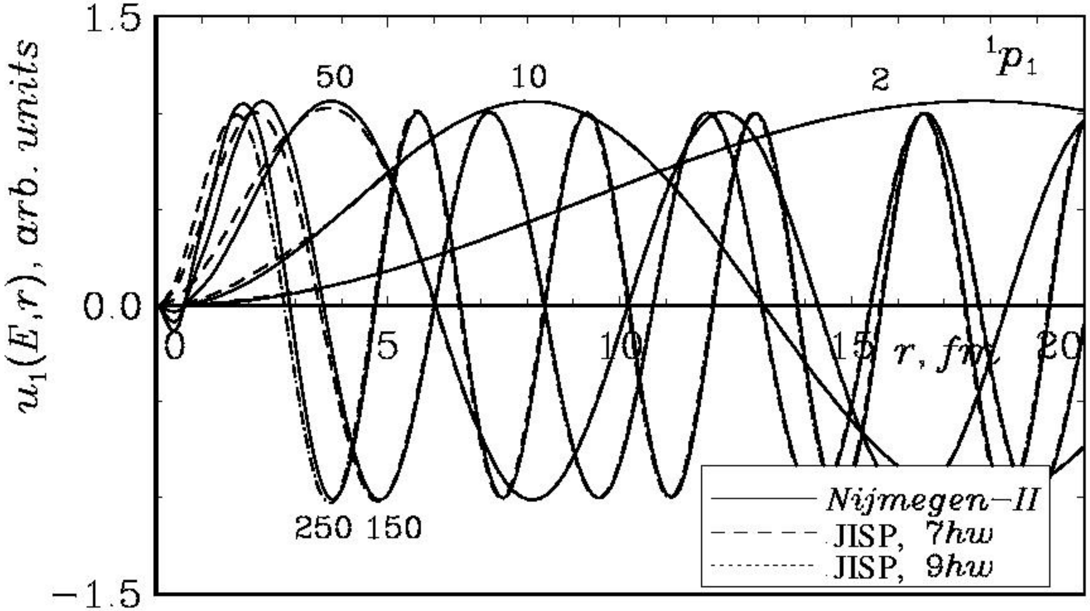
  various *p* and one of *d* waves - fitting few levels of ^{6}Li and binding energy of ^{16}O in relatively small model spaces
- All the rest NCSM results (other nuclei, larger model spaces) are *ab initio*

JISP16 properties

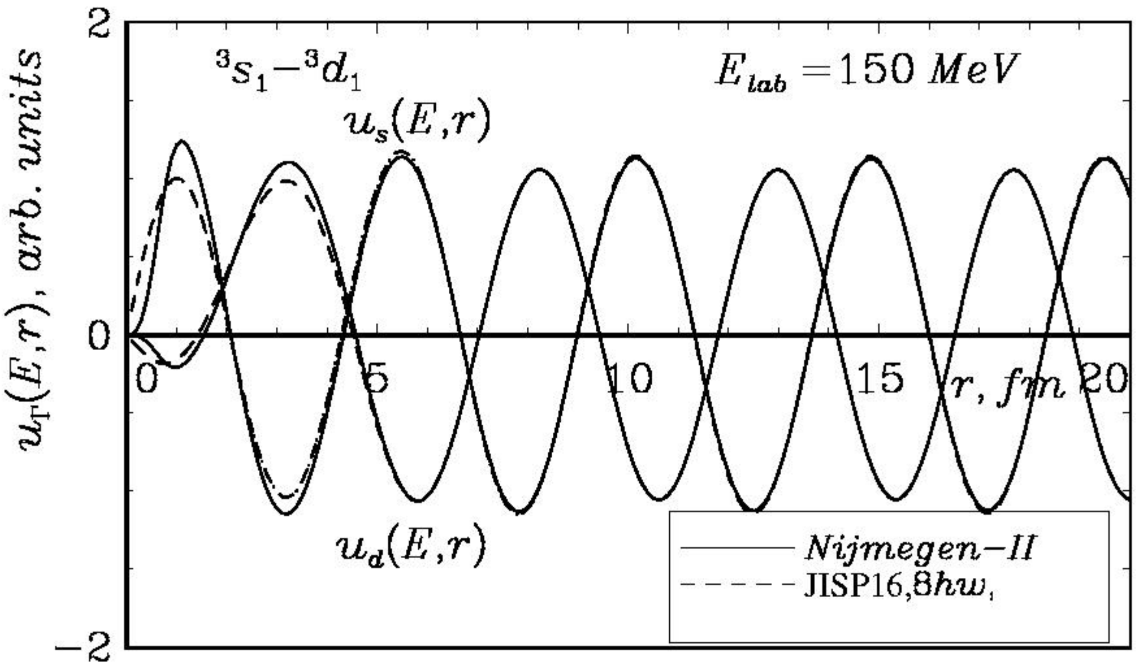
- 1992 *np* data base (2514 data): χ^2/datum = 1.03
- 1999 *np* data base (3058 data): χ^2/datum = 1.05

Table I: Deuteron properties.

Potential	E_d, MeV	d state probability, %	rms radius, fm	Q, fm^2	As. norm. const. $\mathscr{A}_s$, fm$^{-1/2}$	$\eta = \frac{\mathscr{A}_d}{\mathscr{A}_s}$
JISP16	−2.224575	4.1360	1.9643	0.2886	0.8629	0.0252
Nijmegen-II	−2.224575	5.635	1.968	0.2707	0.8845	0.0252
AV18	−2.224575	5.76	1.967	0.270	0.8850	0.0250
CD–Bonn	−2.224575	4.85	1.966	0.270	0.8846	0.0256
Nature	−2.224575(9)	—	1.971(6)	0.2859(3)	0.8846(9)	0.0256(4)



1.5
0.0
−1.5
$u_1(E,r)$, arb. units
$^1p_1$
50
10
2
250 150
0
5
10
15
20
r, fm
Nijmegen−II
JISP, 7hw
JISP, 9hw



2
0
−2
$u_\Gamma(E,r)$, arb. units
$^3s_1$−$^3d_1$
E_{lab} =150 MeV
$u_s(E,r)$
$u_d(E,r)$
0
5
10
15
20
r, fm
Nijmegen−II
JISP16,8hw,

Table II: The binding energies of ^{3}H, ^{3}He, ^{4}He, ^{6}He and ^{6}Li nuclei.

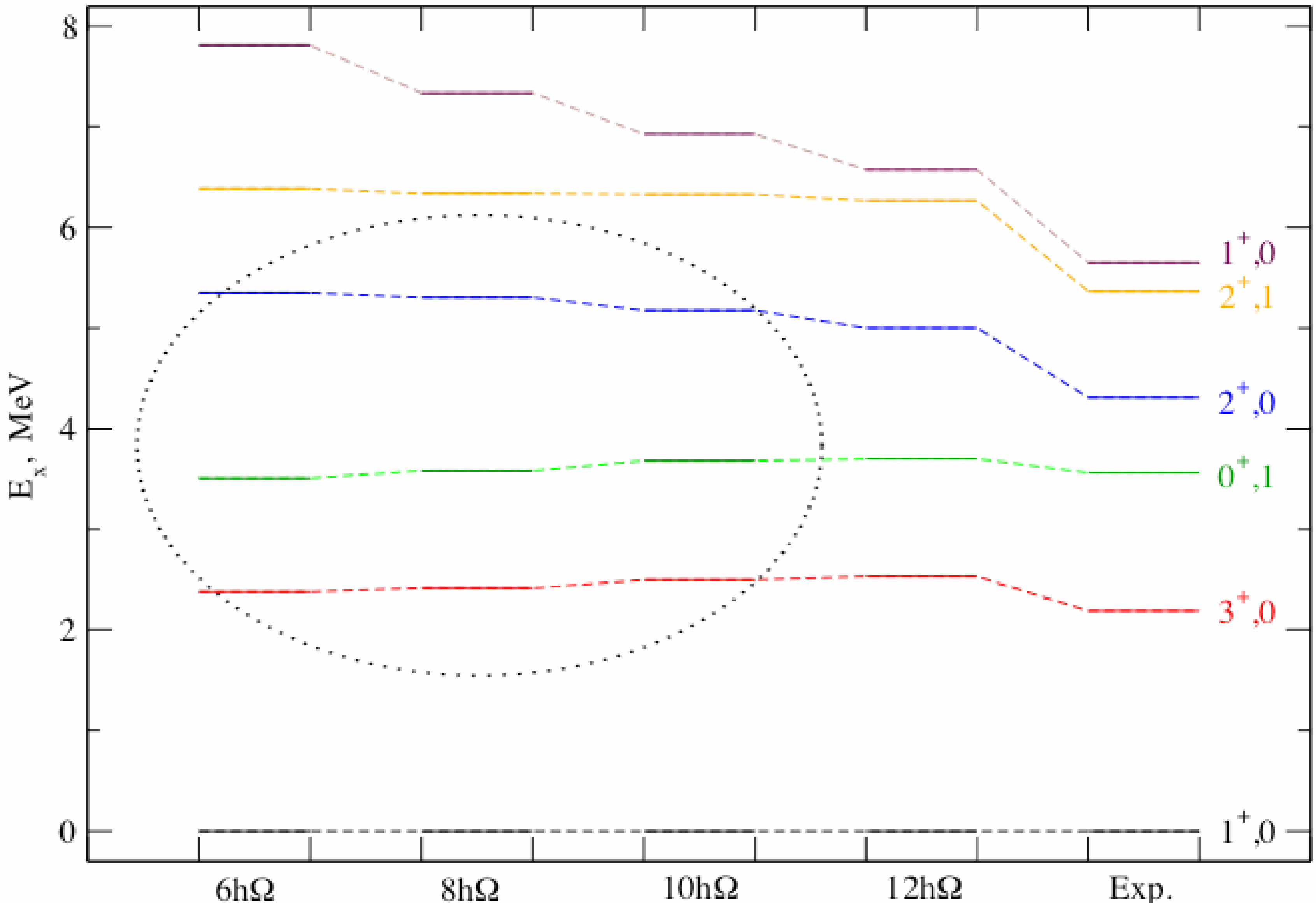
Potential	^{3}H	^{3}He	^{4}He	^{6}He	^{6}Li
JISP16, NCSM	8.496(20)	7.797(17)	28.374(57)	28.32(28)	31.00(31)
CD-Bonn+TM, Faddeev [1]	8.480	7.734	29.15		
AV18+TM, Faddeev [1]	8.476	7.756	28.84		
AV18+TM', Faddeev [1]	8.444	7.728	28.36		
NijmI+TM, Faddeev [1]	8.392	7.720	28.60		
NijmII+TM, Faddeev [1]	8.386	7.720	28.54		
AV18+UrbIX, Faddeev [1]	8.478	7.760	28.50		
AV18+UrbIX, GFMC [2]	8.47(1)		28.30(2)	27.64(14)	31.25(11)
AV8'+TM', NCSM [3]				28.189	31.036
Nature	8.48	7.72	28.30	29.269	31.995

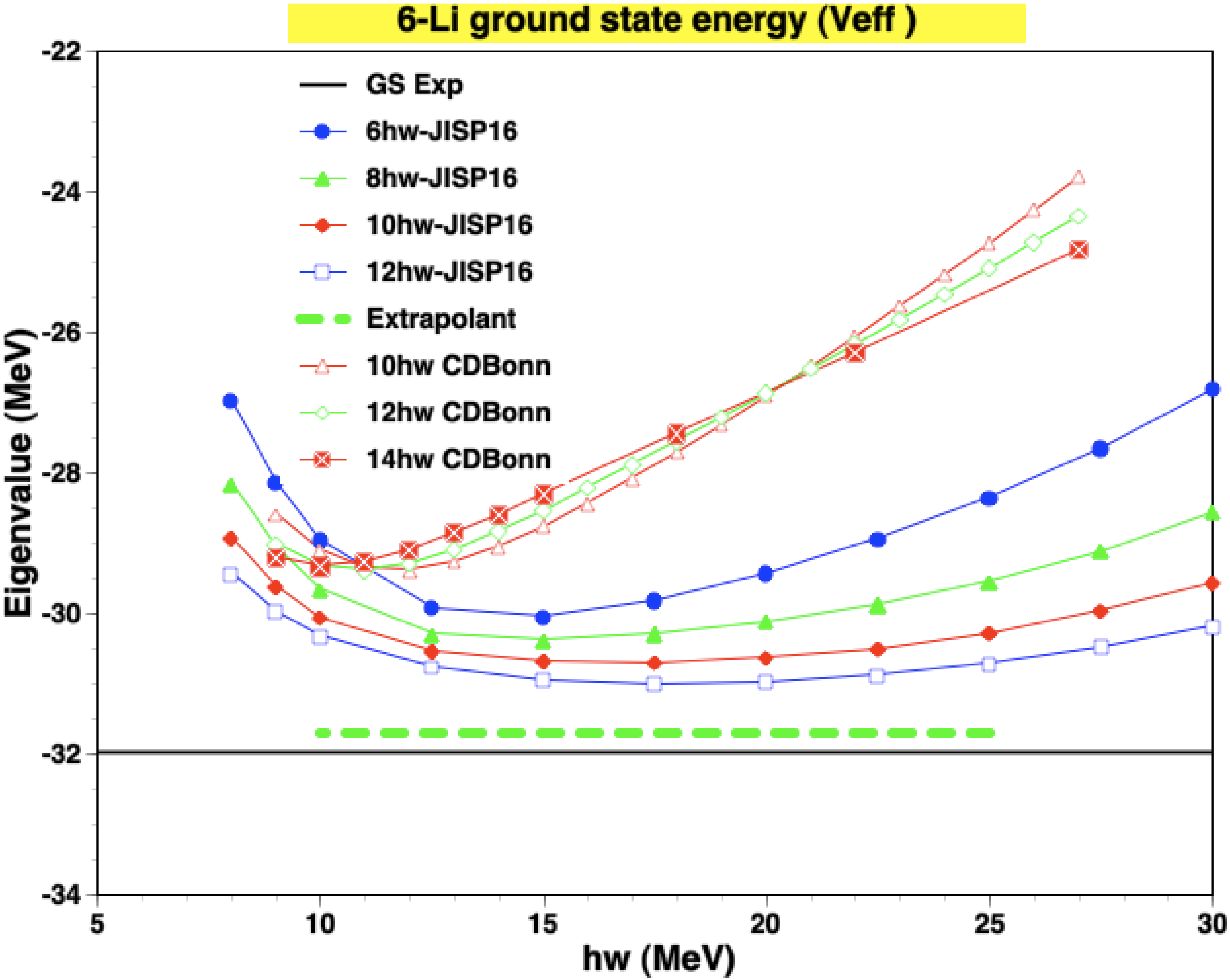
[1] A. Nogga *et al*, Phys. Rev. Lett. **85**, 944 (2000).

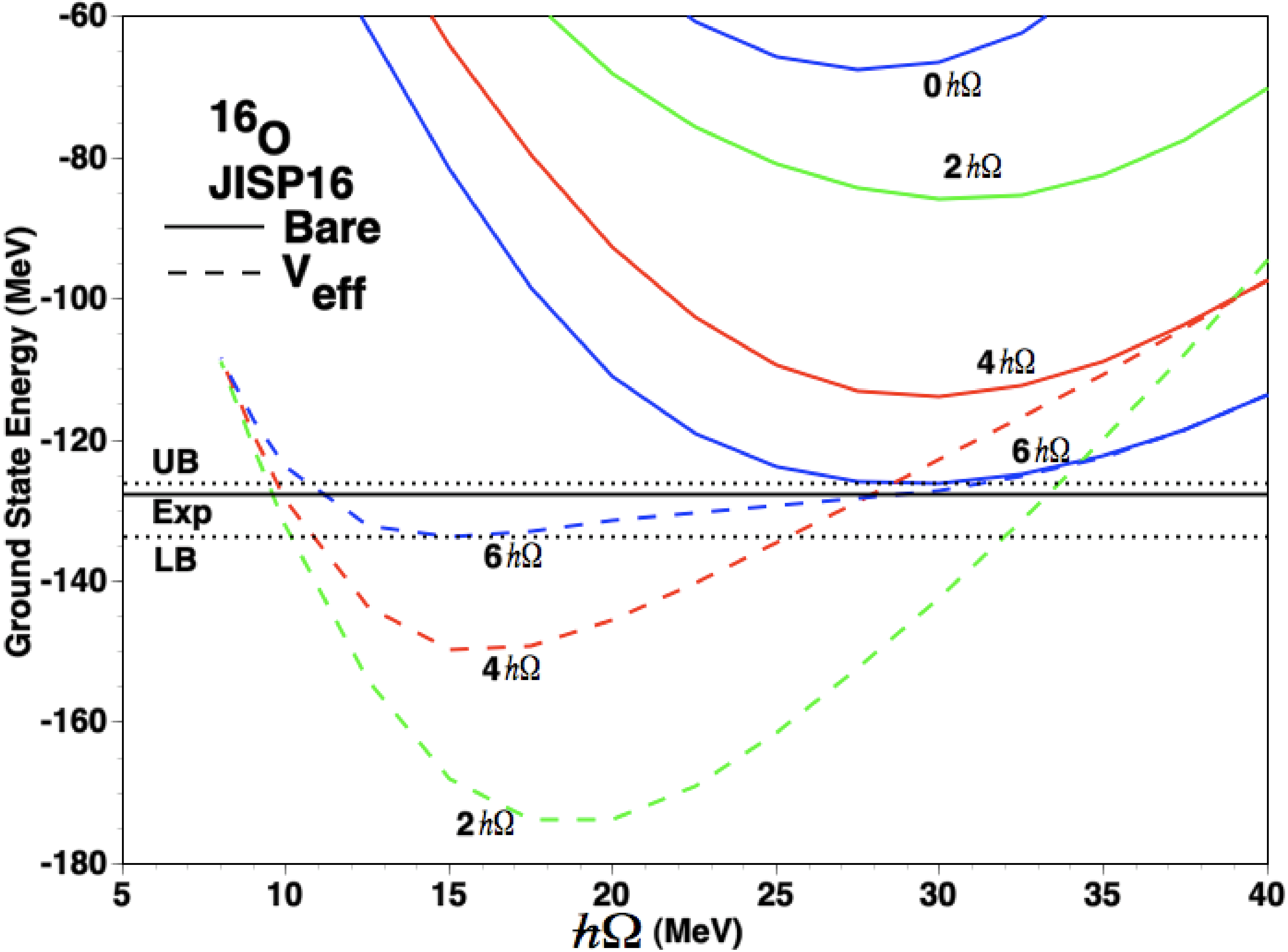
[2] B. S. Pudliner *et al.*, Phys. Rev. **C 56**, 1720 (1997).

[3] P. Navrátil and E. Ormand, Phys. Rev. **c 68**, 034305 (2003).

^{6}Li spectrum with JISP16 NN interaction, hΩ=17.5 MeV



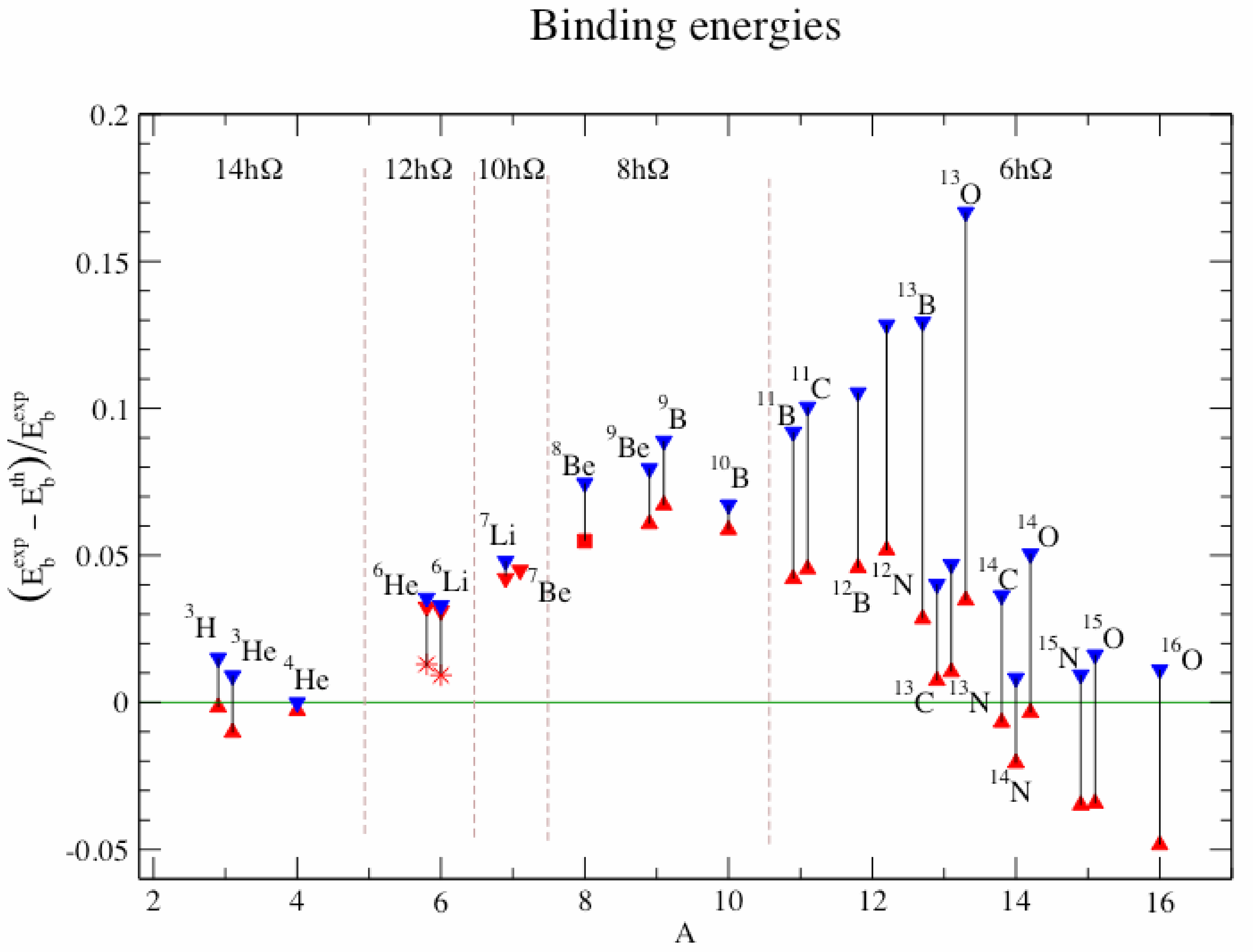

6-Li ground state energy (Veff)
GS Exp
6hw-JISP16
8hw-JISP16
10hw-JISP16
12hw-JISP16
Extrapolant
10hw CDBonn
12hw CDBonn
14hw CDBonn
Eigenvalue (MeV)
hw (MeV)
-22
-24
-26
-28
-30
-32
-34
5
10
15
20
25
30



16O
JISP16
Bare
Veff
Ground State Energy (MeV)
ħΩ (MeV)
-60
-80
-100
-120
-140
-160
-180
5
10
15
20
25
30
35
40
0 ħΩ
2 ħΩ
4 ħΩ
6 ħΩ
UB
Exp
LB
6 ħΩ
4 ħΩ
2 ħΩ

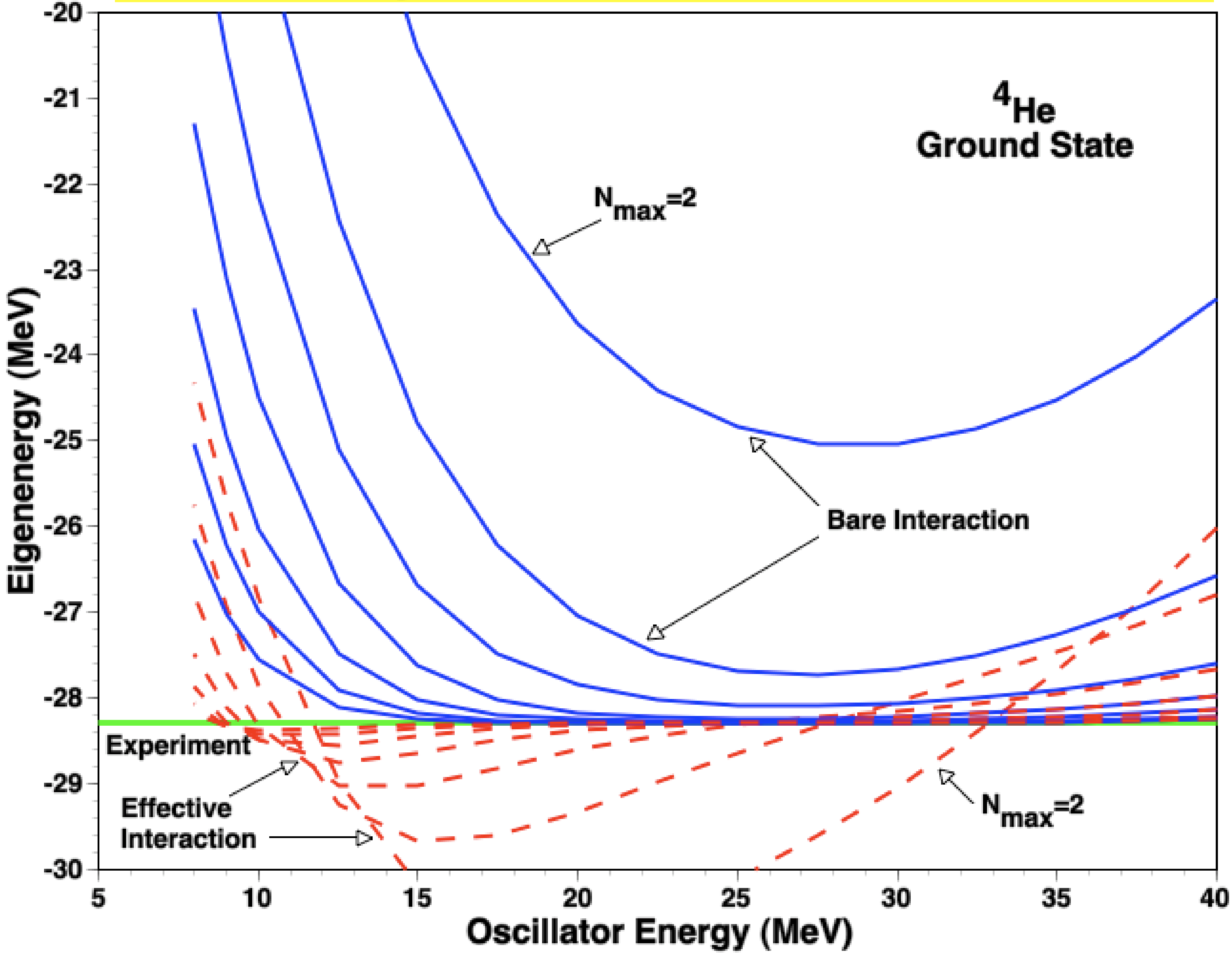
Nucleus	Nature	Bare	Effective	$\hbar\omega$ (MeV)	Model space
^{3}H	8.482	8.354	8.496(20)	7	$14\hbar\omega$
^{3}He	7.718	7.648	7.797(17)	7	$14\hbar\omega$
^{4}He	28.296	28.297	28.374(57)	10	$14\hbar\omega$
^{6}He	29.269		28.32(28)	17.5	$12\hbar\omega$
^{6}Li	31.995		31.00(31)	17.5	$12\hbar\omega$
^{7}Li	39.245		37.59(30)	17.5	$10\hbar\omega$
^{7}Be	37.600		35.91(29)	17	$10\hbar\omega$
^{8}Be	56.500		53.40(10)	15	$8\hbar\omega$
^{9}Be	58.165	53.54	54.63(26)	16	$8\hbar\omega$
^{9}B	56.314	51.31	52.53(20)	16	$8\hbar\omega$
^{10}Be	64.977	60.55	61.39(20)	19	$8\hbar\omega$
^{10}B	64.751	60.39	60.95(20)	20	$8\hbar\omega$
^{10}C	60.321	55.26	56.36(67)	17	$8\hbar\omega$
^{11}B	76.205	69.2	73.0(31)	17	$6\hbar\omega$

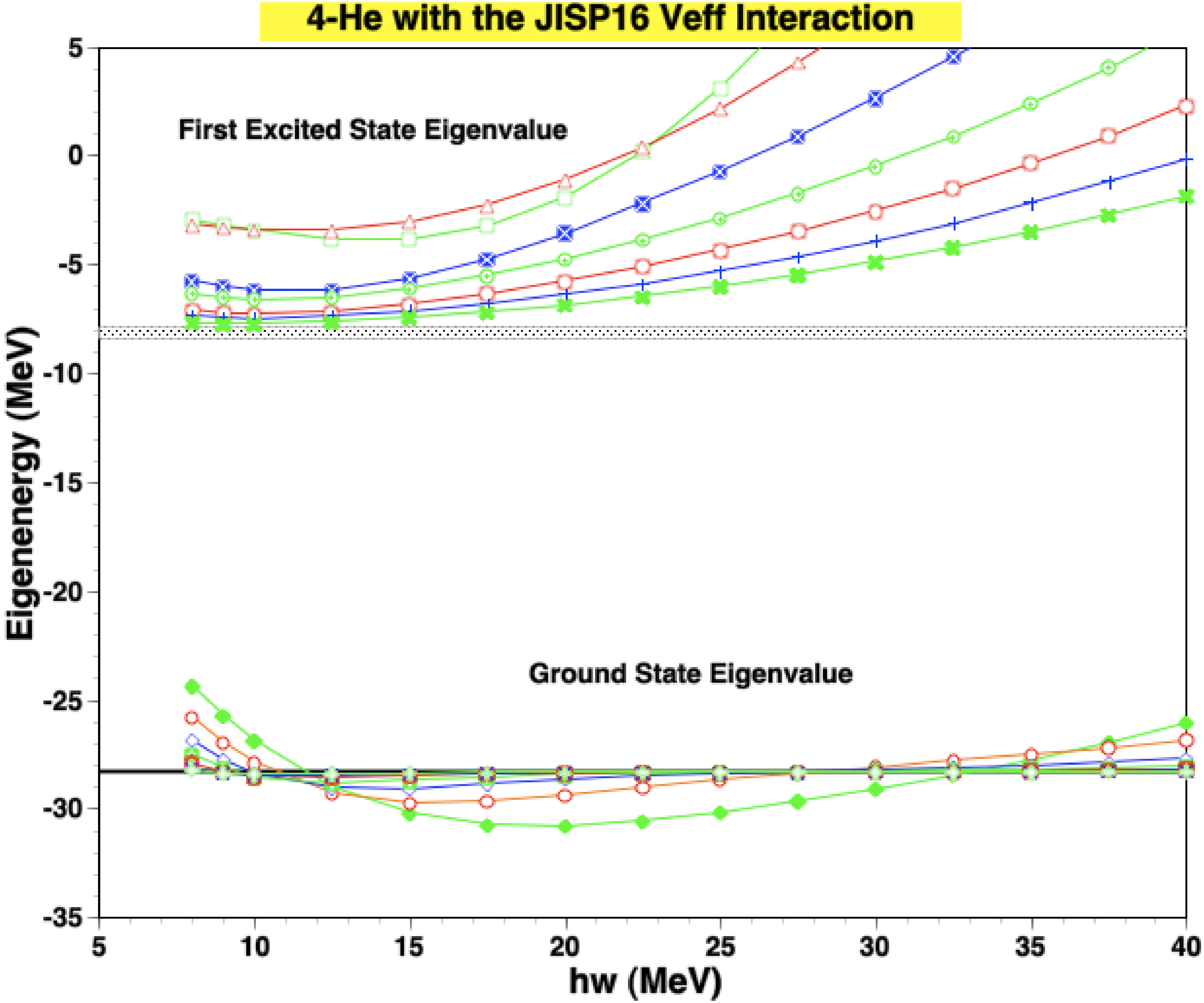
Nucleus	Nature	Bare	Effective	$\hbar\omega$ (MeV)	Model space
^{11}C	73.440	66.1	70.1(32)	17	$6\hbar\omega$
^{12}B	79.575	71.2	75.9(48)	15	$6\hbar\omega$
^{12}C	92.162	87.4	91.0(49)	17.5	$6\hbar\omega$
^{12}N	74.041	64.5	70.2(48)	15	$6\hbar\omega$
^{13}B	84.453	73.5	82.1(67)	15	$6\hbar\omega$
^{13}C	97.108	93.2	96.4(59)	19	$6\hbar\omega$
^{13}N	94.105	89.7	93.1(62)	18	$6\hbar\omega$
^{13}O	75.558	63.0	72.9(62)	14	$6\hbar\omega$
^{14}C	105.285	101.5	106.0(93)	17.5	$6\hbar\omega$
^{14}N	104.659	103.8	106.8(77)	20	$6\hbar\omega$
^{14}O	98.733	93.7	99.1(92)	16	$6\hbar\omega$
^{15}N	115.492	114.4	119.5(126)	16	$6\hbar\omega$
^{15}O	111.956	110.1	115.8(126)	16	$6\hbar\omega$
^{16}O	127.619	126.2	133.8(158)	15	$6\hbar\omega$



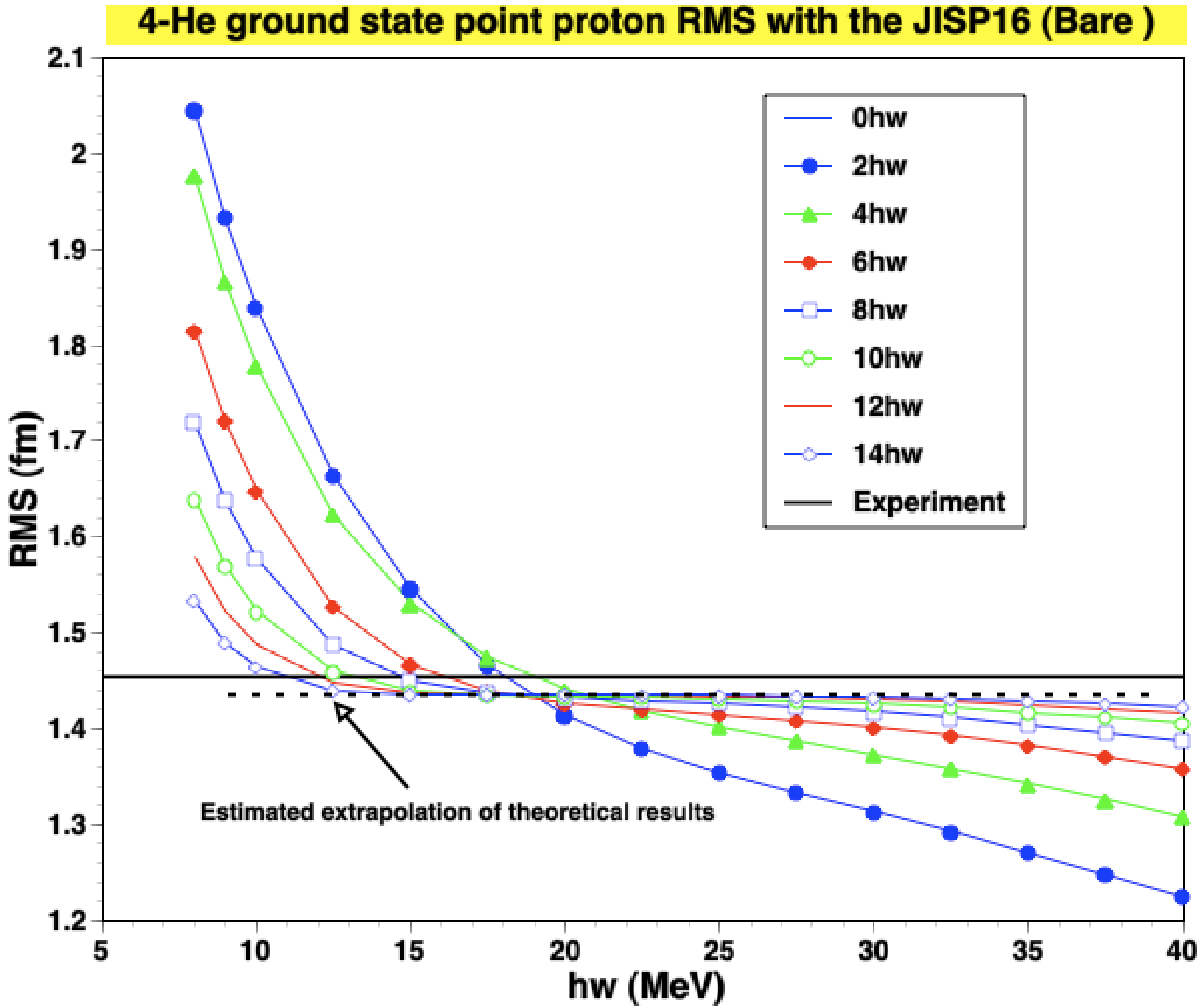
Binding energies
14hΩ
12hΩ
10hΩ
8hΩ
6hΩ
3H
3He
4He
6He
6Li
7Li
7Be
8Be
9Be
9B
10B
11B
11C
12B
12N
13B
13C
13N
13O
14C
14N
14O
15N
15O
16O
0.2
0.15
0.1
0.05
0
-0.05
2
4
6
8
10
12
14
16
A
$(E_b^{exp} - E_b^{th})/E_b^{exp}$

NCSM Convergence with bare and effective JISP16 Potentials

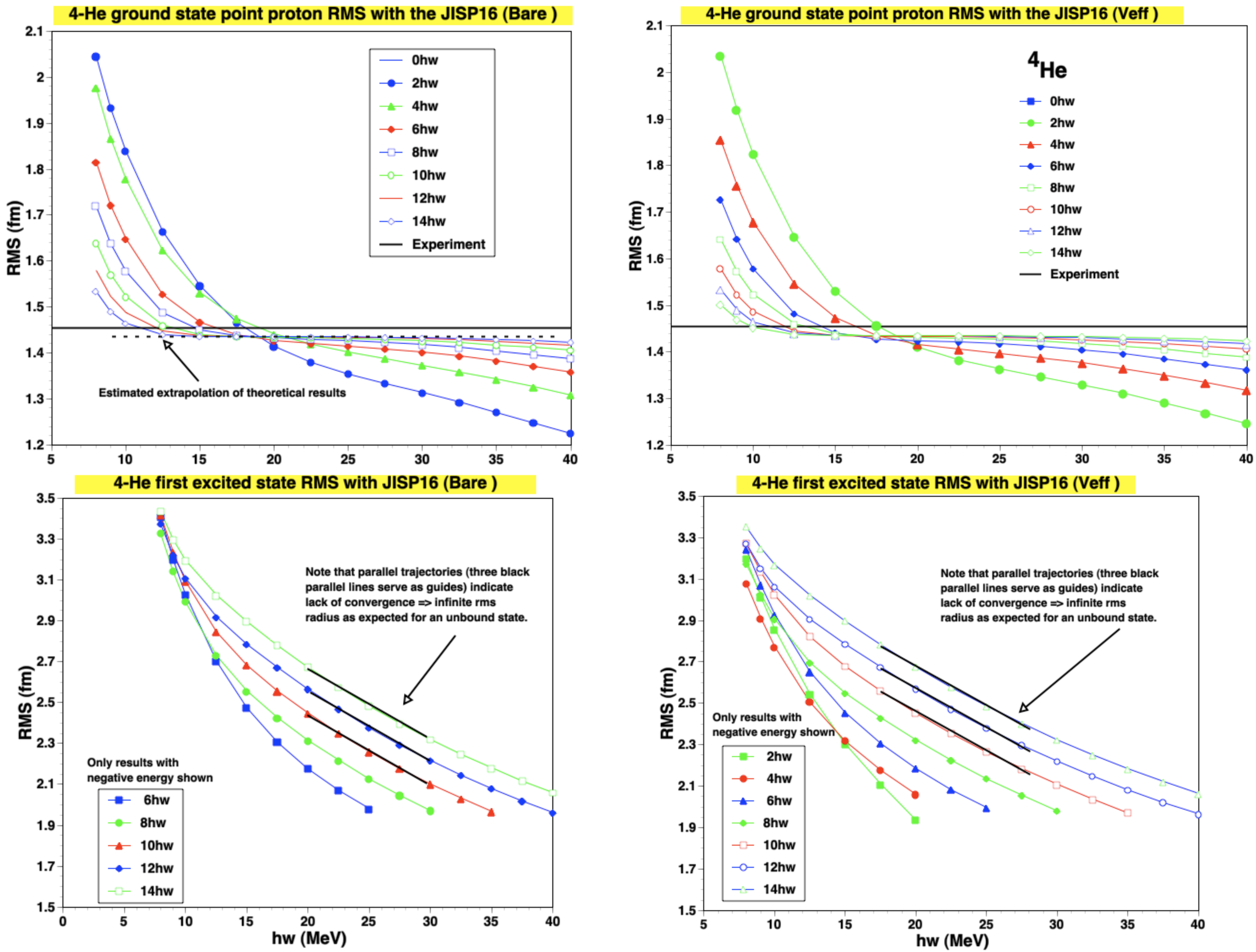




4-He with the JISP16 Veff Interaction
First Excited State Eigenvalue
Ground State Eigenvalue
Eigenenergy (MeV)
hw (MeV)
5
0
-5
-10
-15
-20
-25
-30
-35
5
10
15
20
25
30
35
40



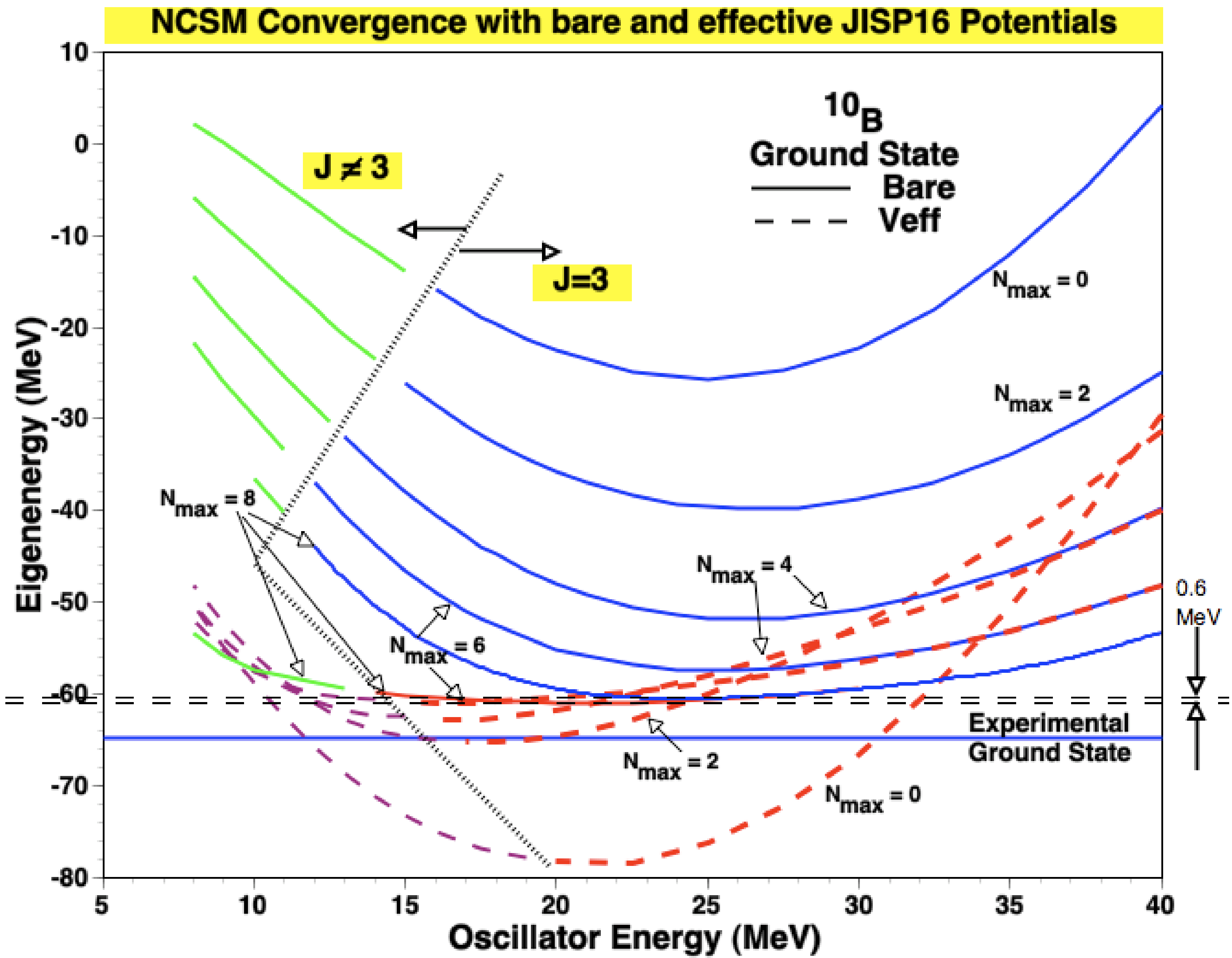
4-He ground state point proton RMS with the JISP16 (Bare)
RMS (fm)
hw (MeV)
0hw
2hw
4hw
6hw
8hw
10hw
12hw
14hw
Experiment
Estimated extrapolation of theoretical results
2.1
2
1.9
1.8
1.7
1.6
1.5
1.4
1.3
1.2
5
10
15
20
25
30
35
40

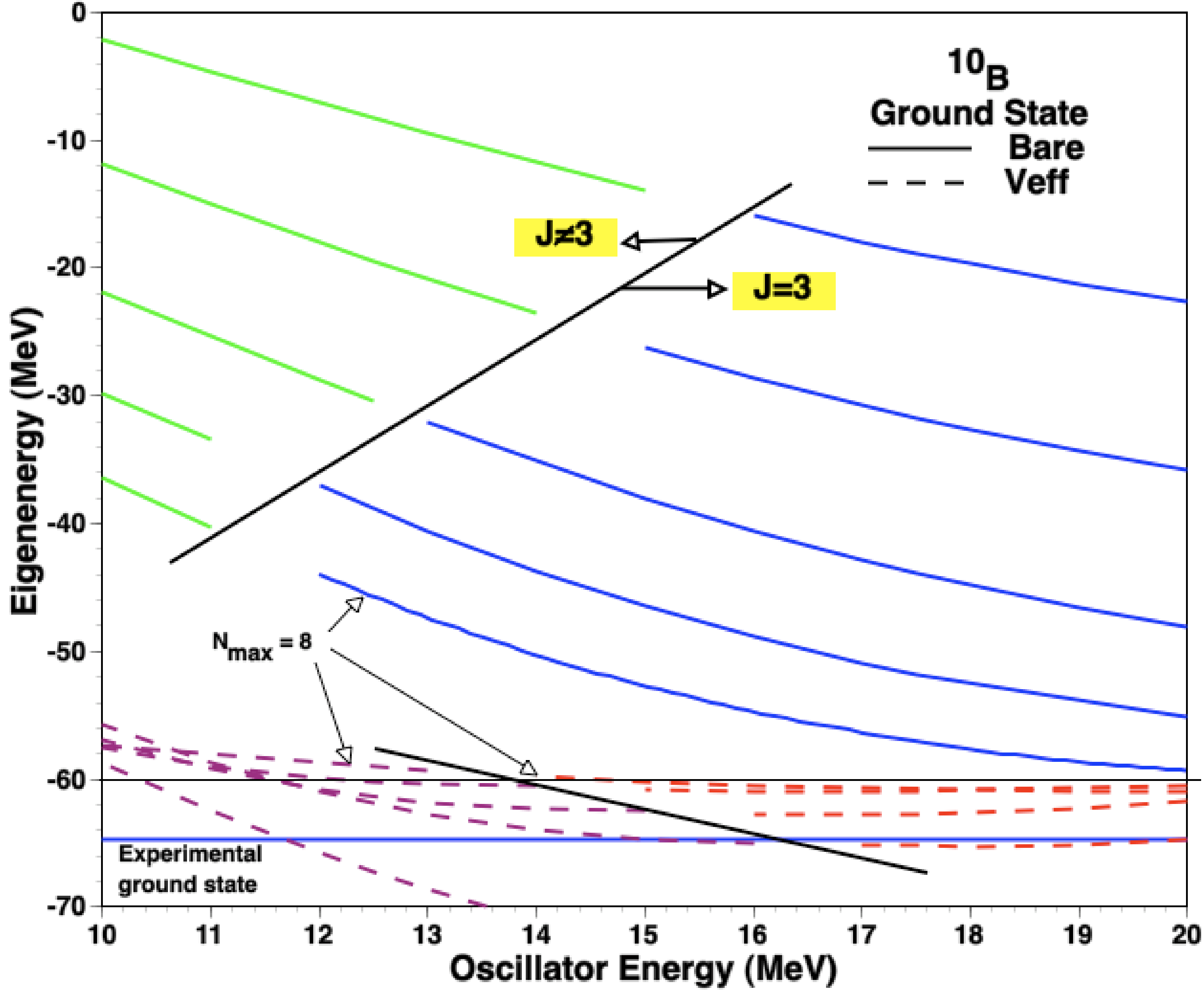


4-He ground state point proton RMS with the JISP16 (Bare)
RMS (fm)
0hw
2hw
4hw
6hw
8hw
10hw
12hw
14hw
Experiment
Estimated extrapolation of theoretical results
4-He ground state point proton RMS with the JISP16 (Veff)
4He
0hw
2hw
4hw
6hw
8hw
10hw
12hw
14hw
Experiment
4-He first excited state RMS with JISP16 (Bare)
Note that parallel trajectories (three black parallel lines serve as guides) indicate lack of convergence => infinite rms radius as expected for an unbound state.
Only results with negative energy shown
6hw
8hw
10hw
12hw
14hw
hw (MeV)
4-He first excited state RMS with JISP16 (Veff)
Note that parallel trajectories (three black parallel lines serve as guides) indicate lack of convergence => infinite rms radius as expected for an unbound state.
Only results with negative energy shown
2hw
4hw
6hw
8hw
10hw
12hw
14hw
hw (MeV)

Ground state energy E_{gs} and excitation energies E_x (in MeV), ground state point-proton rms radius r_p (in fm) and quadrupole moment Q (in $e \cdot \mathrm{fm}^2$) of the ^{6}Li nucleus; $\hbar\omega = 17.5$ MeV.

Interaction Method	Nature	JISP6 NCSM, $10\hbar\omega$ [6]	JISP16 NCSM, $12\hbar\omega$	AV8'+TM' NCSM, $6\hbar\omega$ [2]	AV18+UIX GFMC [8,15]	AV18+IL2 GFMC [10,15]
$E_{gs}(1_1^+, 0)$	-31.995	-31.48	-31.00	-31.04	$-31.25(8)$	$-32.0(1)$
r_p	2.32(3)	2.083	2.151	2.054	2.46(2)	2.39(1)
Q	$-0.082(2)$	-0.194	-0.0646	-0.025	$-0.33(18)$	$-0.32(6)$
$E_x(3^+, 0)$	2.186	2.102	2.529	2.471	2.8(1)	2.2
$E_x(0^+, 1)$	3.563	3.348	3.701	3.886	3.94(23)	3.4
$E_x(2^+, 0)$	4.312	4.642	5.001	5.010	4.0(1)	4.2
$E_x(2^+, 1)$	5.366	5.820	6.266	6.482		5.5
$E_x(1_2^+, 0)$	5.65	6.86	6.573	7.621	5.1(1)	5.6


NCSM Convergence with bare and effective JISP16 Potentials
^{10}B
Ground State
Bare
Veff
J ≠ 3
J=3
N_{max} = 0
N_{max} = 2
N_{max} = 4
N_{max} = 6
N_{max} = 8
N_{max} = 2
N_{max} = 0
Experimental
Ground State
0.6
MeV
Eigenenergy (MeV)
Oscillator Energy (MeV)
10
0
-10
-20
-30
-40
-50
-60
-70
-80
5
10
15
20
25
30
35
40



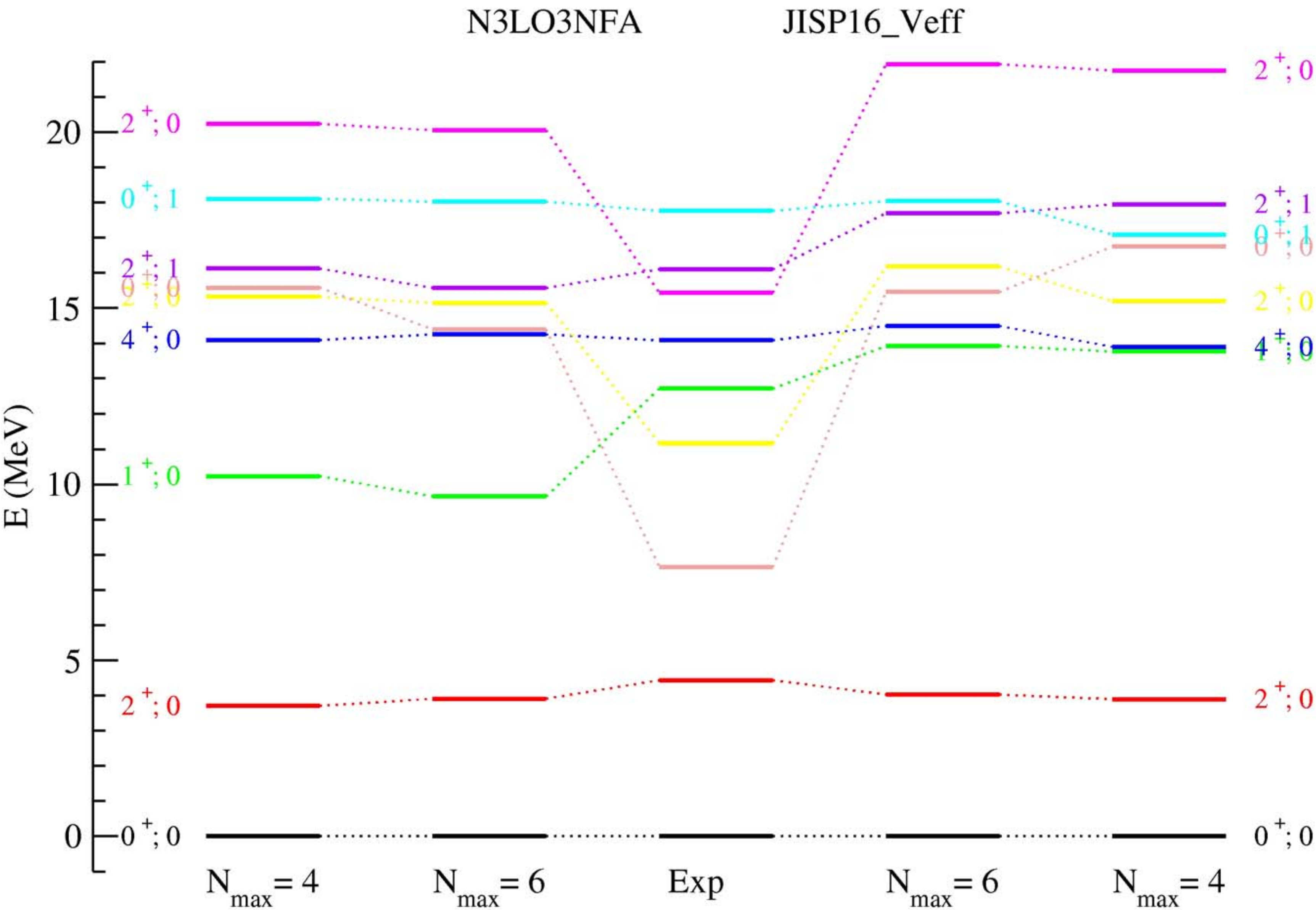
^{10}B
Ground State
Bare
Veff
J≠3
J=3
N_{max} = 8
Experimental
ground state
Eigenenergy (MeV)
Oscillator Energy (MeV)
0
-10
-20
-30
-40
-50
-60
-70
10
11
12
13
14
15
16
17
18
19
20

Same as in Table 4 but for the ^{10}B nucleus; $\hbar\omega = 15$ MeV.

Interaction Method	Nature	JISP16 NCSM, $8\hbar\omega$	AV8'+TM' NCSM, $4\hbar\omega$ [2]	AV18+IL2 GFMC [16]
$E_{gs}(3_1^+, 0)$	-64.751	-60.14	-60.57	$-65.6(5)$
r_p	2.30(12)	2.168	2.168	2.33(1)
Q	+8.472(56)	6.484	+5.682	+9.5(2)
$E_x(1_1^+, 0)$	0.718	0.555	0.340	0.9
$E_x(0^+, 1)$	1.740	1.202	1.259	
$E_x(1_2^+, 0)$	2.154	2.379	1.216	
$E_x(2_1^+, 0)$	3.587	3.721	2.775	3.9
$E_x(3_2^+, 0)$	4.774	6.162	5.971	
$E_x(2_1^+, 1)$	5.164	5.049	5.182	
$E_x(2_2^+, 0)$	5.92	5.548	3.987	
$E_x(4^+, 0)$	6.025	5.775	5.229	5.6
$E_x(2_2^+, 1)$	7.478	7.776	7.491	

^{10}B Basis space	Exp -	JISP16 $8\hbar\Omega$	JISP16 $6\hbar\Omega$	$N3LO+NNN_B$ $6\hbar\Omega$	$N3LO+NNN_A$ $6\hbar\Omega$	$N3LO$ $6\hbar\Omega$
$\lvert E(3^+,0)\rvert$ [MeV]	64.751	60.138	60.800	60.167	64.027	55.613
r_p [fm]	2.30(12)	2.167	2.173	2.248	2.168	2.224
$Q(3_1^+,0)$ [e fm^2]	+8.472(56)	6.483	6.239	6.101	6.104	6.665
$\mu(3_1^+,0)[\mu_N]$	+1.8006	N/A	N/A	N/A	N/A	N/A
$\mu(1_1^+,0)[\mu_N]$	+0.63(12)	N/A	N/A	N/A	N/A	N/A
$E_x(3_1^+0)$ [MeV]	0.0	0.0	0.0	0.0	0.0	0.0
$E_x(1_1^+0)$ [MeV]	0.718	0.555	0.345	0.728	1.131	-0.877
$E_x(0_1^+1)$ [MeV]	1.740	1.202	1.000	1.662	1.704	1.049
$E_x(1_2^+0)$ [MeV]	2.154	2.379	2.189	2.077	1.529	1.706
$E_x(2_1^+0)$ [MeV]	3.587	3.721	3.323	2.762	3.498	1.797
$E_x(3_2^+0)$ [MeV]	4.774	6.162	5.896	5.093	6.785	4.406
$E_x(2_1^+1)$ [MeV]	5.164	5.049	4.863	4.982	5.518	4.530
$E_x(2_2^+0)$ [MeV]	5.92	5.548	4.992	3.675	4.900	3.732
$E_x(4_1^+0)$ [MeV]	6.025	5.775	5.428	4.398	5.699	4.763
$E_x(2_2^+1)$ [MeV]?	7.478	7.776	7.586	7.998	8.480	5.848
$rms(Exp-Th)$ [MeV]	-	0.539	0.609	0.988	0.875	1.333
B(E2;$1_1^+0 \to 3_1^+0$)	4.13(6)	3.317	3.151	0.227	0.356	4.003
B(E2;$1_2^+0 \to 3_1^+0$)	1.71(0.26)	0.627	0.540	2.514	2.771	N/A
B(M1;$2_1^+0 \to 3_1^+0$)	0.0015(3)	0.0022	0.0022	0.0048	0.0008	N/A
B(M1;$2_1^+1 \to 3_1^+0$)	0.041(4)	0.086	0.097	0.002	0.091	N/A
B(M1;$2_2^+0 \to 3_1^+0$)	0.050(12)	0.056	0.044	0.031	0.044	N/A
B(M1;$4_1^+0 \to 3_1^+0$)	0.043(7)	0.005	0.002	0.002	0.003	N/A
B(M1;$2_2^+1 \to 3_1^+0$)	-	3.899	4.113	2.635	3.580	N/A
B(GT;$2_1^+1 \to 3_1^+0$)	0.083(3)	0.042	0.041	0.010	0.061	N/A
B(GT;$2_2^+1 \to 3_1^+0$)	0.95(13)	1.652	1.745	1.212	1.559	N/A

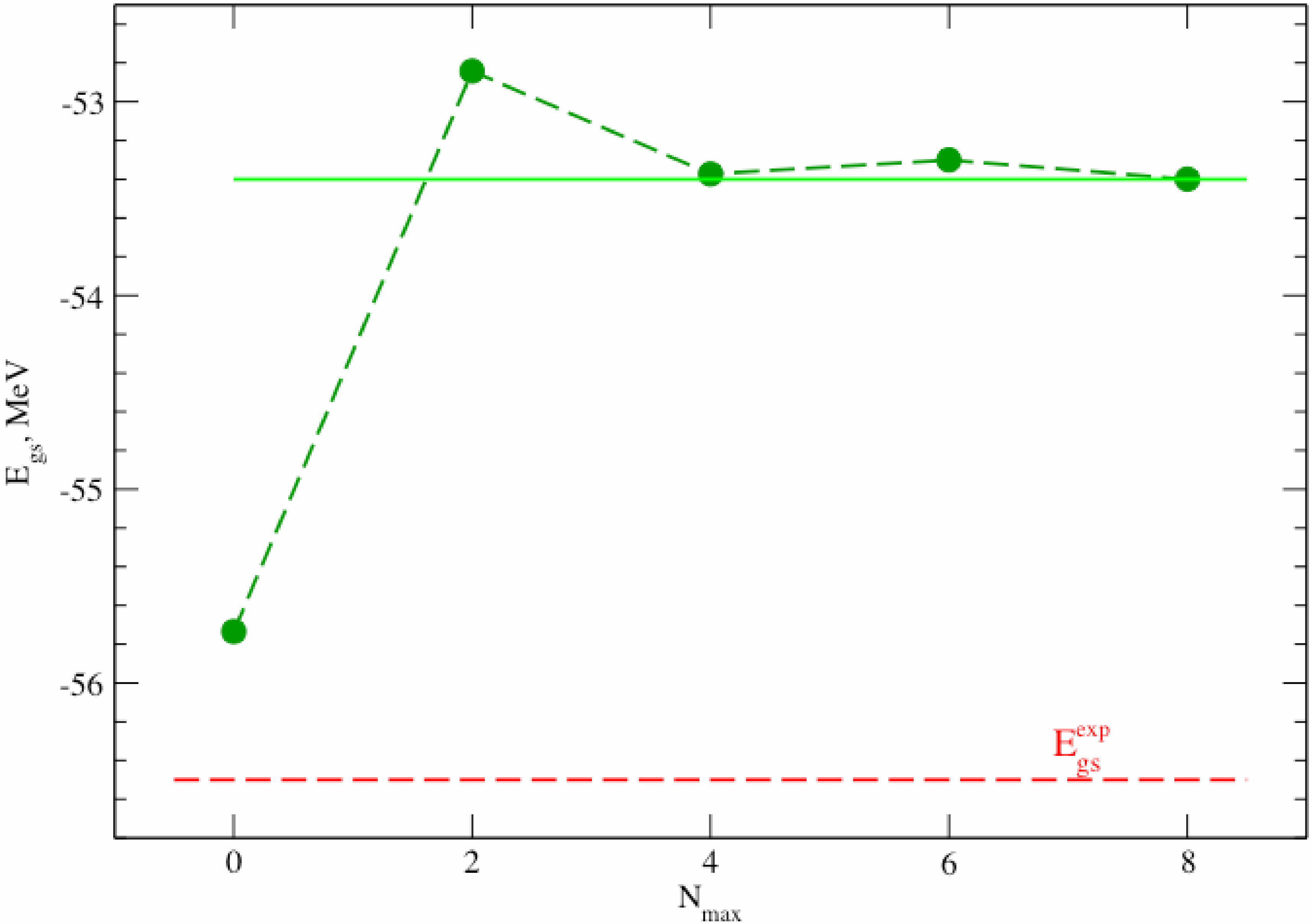
^{12}C Spectral Convergence for $\hbar\Omega$ = 15 MeV

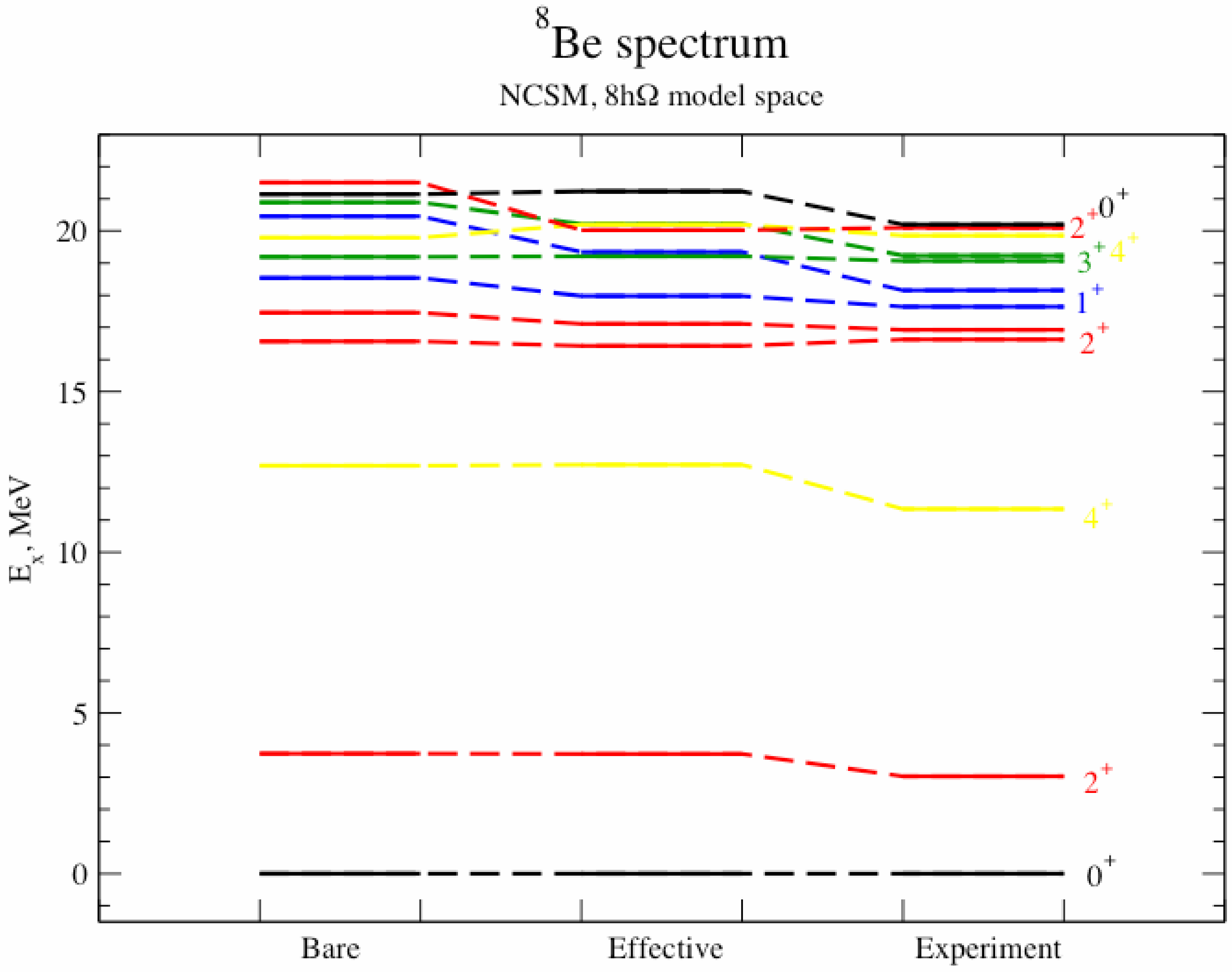


distance (MeV)		1.510		9.642		11.693		2.035
(10 states)	3.329		3.049		rmsd		3.698	3.868

^{8}Be g.s. convergence with $N_{max}h\Omega$

$h\Omega = 15$ MeV





^{8}Be spectrum
NCSM, 8hΩ model space
E_x, MeV
0
5
10
15
20
Bare
Effective
Experiment
0^+
2^+
4^+
2^+
1^+
3^+
4^+
2^+
0^+

Role of *NNN* force?

- W. Polyzou and W. Glöckle theorem (Few-body Syst. **9**, 97 (1990)):

$$H=T+V_{ij} \Longrightarrow H'=T+V'_{ij}+V_{ijk},$$

*w*here V_{ij} and V'_{ij} are phase-equivalent, H and H' are isospectral.

Hope:

$$H'=T+V'_{ij}+V_{ijk} \Longrightarrow H=T+V_{ij}$$

with (approximately) isospectral H and H' .

JISP16 seems to be *NN* interaction minimizing *NNN* force.

Without *NNN* force calculations are simpler, calculations are faster, larger model spaces become available.

Conclusions

- JISP16 provides a realistic description of two-body and many-body properties, comparable with modern realistic *NN* + *NNN* forces
- Convergence of NCSM calculations with JISP16 is faster, even the bare JISP16 calculation convergence is reasonable, I.e. the results are more reliable. A confidence region of the binding energy predictions can be obtained for many nuclei by comparing the bare and effective interaction results

Plans

- JISP16 improvement by the fit to the same nuclei
- Charge-dependent JISP16
- Extending the calculations to the *sd* shell
- Scattering calculations: NCSM + J-matrix