Scattering and nuclear structure with oscillator basis.

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Nuclear Theory in the Supercomputing Era
June 21, 2012

What are we doing?

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Large-scale *ab initio* No-core Shell Model calculations

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+ new realistic *NN* interaction JISP

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Large-scale *ab initio* No-core Shell Model calculations

+ new realistic *NN* interaction JISP

Can we do also scattering?

Ab initio:

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* No model assumptions (shell model with inert core, cluster model, etc., are not *ab initio*)

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* No model assumptions (shell model with inert core, cluster model, etc., are not *ab initio*)
* *Ab initio* approaches:
* Faddeev ($A \leq 4$)
* hyperspherical ($A \leq 6$)
* Green function's Monte Carlo ($A \leq 13$)
* no-core shell model ($A < 20$)
* coupled-cluster approach
* Symmetry extensions, Monte Carlo no-core shell model

Plan

* Lanczos HORSE: reformulation of the J-matrix approach
* Direct and inverse scattering or what do we obtain with oscillator basis for resonances and scattering states?
* Inverse scattering: JISP *NN* interaction
* No-core shell model, No-core full configuration
* What is next?

Oscillator basis: nuclear structure & reactions

* Searching for links between nuclear structure & reactions
* Oscillator basis: nuclear structure − shell model, Lanczos algorithm
* Oscillator basis: scattering & reactions − can we have something similar?
* HORSE = Harmonic Oscillator Representation of Scattering Equations (*J*-matrix)

* Further discussion: Lanczos HORSE

Lanczos algorithm

$\varphi_0 -$ arbitrary (random) pivot vector

$\varphi_{-1} = 0$

$\beta_0 = 0$

Iterations:

$\phi_{j+1} = H\varphi_j$

orthogonalizing ϕ_{j+1} to φ_j and φ_{j-1} and normalizing:

$\alpha_j = \langle \phi_{j+1} | \varphi_j \rangle$

$\tilde{\phi}_{j+1} = \phi_{j+1} - \alpha_j \varphi_j - \beta_j \varphi_{j-1}$

$\beta_{j+1} = ||\tilde{\phi}_{j+1}||$

$$\varphi_{j+1} = \frac{\tilde{\phi}_{j+1}}{\beta_{j+1}}$$

$$\langle \varphi_i | H | \varphi_j \rangle = \begin{pmatrix} \alpha_0 & \beta_1 & & & \\ \beta_1 & \alpha_1 & \beta_2 & & 0 \\ & \beta_2 & \alpha_2 & \ddots & \\ & & \ddots & \ddots & \beta_{N-1} \\ & 0 & & \beta_{N-1} & \alpha_{N-1} & \beta_N \\ & & & & \beta_N & \alpha_N \end{pmatrix}$$

Oscillator basis

* Matrix of the kinetic energy operator T is tridiagonal in oscillator basis: $T_{nm} = 0$ if $|n - m| > 1$.

$$T\varphi_n = T_{n,n-1}\varphi_{n-1} + T_{nn}\varphi_n + T_{n,n+1}\varphi_{n+1}$$

* Kinetic energy operator T generates oscillator basis
* either from below:

$$\varphi_0, \quad T\varphi_0 \Rightarrow \varphi_1, \quad T\varphi_1 \Rightarrow \varphi_2, \ \ldots$$

* or from above:

$$\ldots, \ \varphi_{M+1}, \ \varphi_M, \quad T\varphi_M \Rightarrow \varphi_{M-1}, \quad T\varphi_{M-1} \Rightarrow \varphi_{M-2}, \ \ldots, \ \varphi_0$$

Free Schrödinger equation

$$T\Psi = E\Psi$$

* Wave function expanded in oscillator basis:

$$\Psi = \sum_{n=0}^{\infty} a_n \varphi_n$$

* The kinetic energy matrix in oscillator basis is tridiagonal, hence a_n are solutions of a three-term recurrent relation (TRR):

$$T_{n,n-1}a_{n-1} + (T_{nn} - E)a_n + T_{n,n+1}a_{n+1} = 0$$

Free Schrödinger equation: TRR solutions

$$T_{n,n-1}a_{n-1} + (T_{nn} - E)a_n + T_{n,n+1}a_{n+1} = 0$$

* Analytical expressions are known for linearly-independent solutions s_n and c_n of this TRR.

* Properties of s_n and c_n:

$$\sum_{n=0}^{\infty} s_n(E)\,\varphi_n = \Psi_E^0 = \sqrt{\frac{2}{\pi}}\,kr\,j_l(kr) \underset{r\to\infty}{\longrightarrow} \sqrt{\frac{2}{\pi}}\sin\left(kr - \frac{\pi l}{2}\right),$$

$$\sum_{n=0}^{\infty} c_n(E)\,\varphi_n \underset{r\to\infty}{\longrightarrow} \Psi_E^{0irreg} = \sqrt{\frac{2}{\pi}}\,kr\,n_l(kr) \underset{r\to\infty}{\longrightarrow} \sqrt{\frac{2}{\pi}}\,\cos\left(kr - \frac{\pi l}{2}\right).$$

* Any TRR solution a_n can be expressed as $a_n = \cos\delta s_n + \sin\delta c_n$ where δ is a scattering phase shift.

Oscillator function at large n

$$n \to \infty, \quad \int f(r)\varphi_n(r)d^3r = ?$$

$$\int f(r)\varphi_n(r)d^3r \sim f(r_n),$$

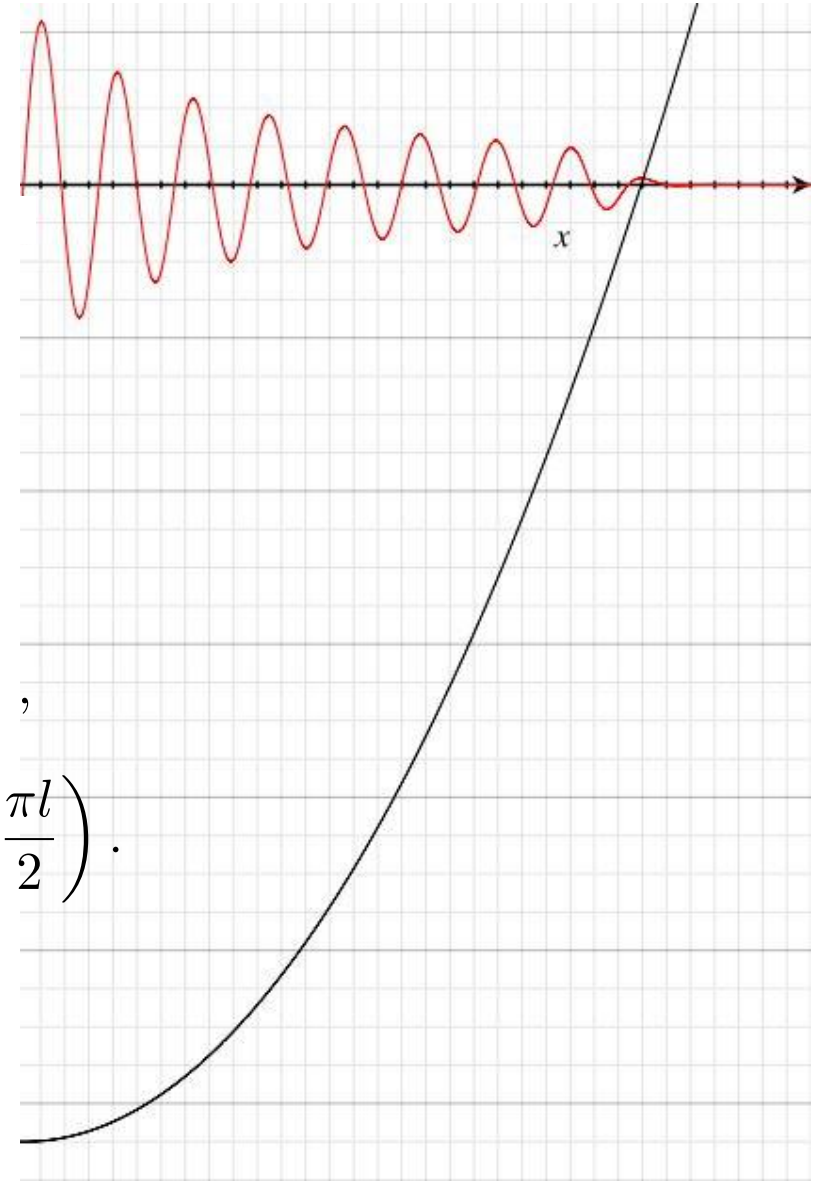
$$r_n = r_0\sqrt{n}, \quad n \to \infty$$

$$\varphi_n(r) \sim \delta(r - r_0\sqrt{n}), \quad n \to \infty$$

At $n \to \infty$:

$$s_n(E) = \int \Psi_E^0 \, \varphi_n \, d^3r \sim \sin\left(kr_0\sqrt{n} - \frac{\pi l}{2}\right),$$

$$c_n(E) = \int \Psi_E^{0irreg} \, \varphi_n \, d^3r \sim \cos\left(kr_0\sqrt{n} - \frac{\pi l}{2}\right).$$



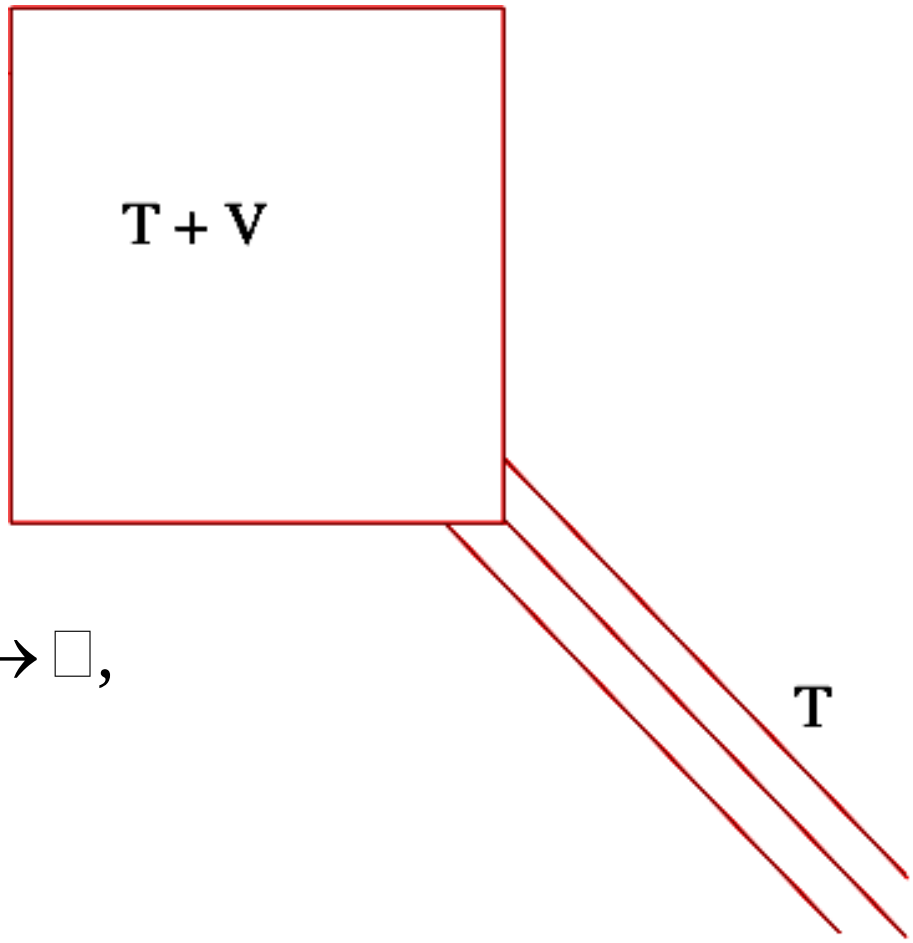
One can calculate s_n and c_n by TRR starting from asymptotically large n.

Hamiltonian

$H = T + V$

A reasonable approximation is to truncate the potential energy matrix: $V_{nm} = 0$ for $n,m > N$, kinetic energy is not truncated.

Justification: kinetic energy m. e. increase with n linearly at large n: $T_{nn} \sim n, \; T_{n,n\pm1} \sim n, \; n \to \infty$, while potential energy m. e. V_{nm} decrease with n and m.



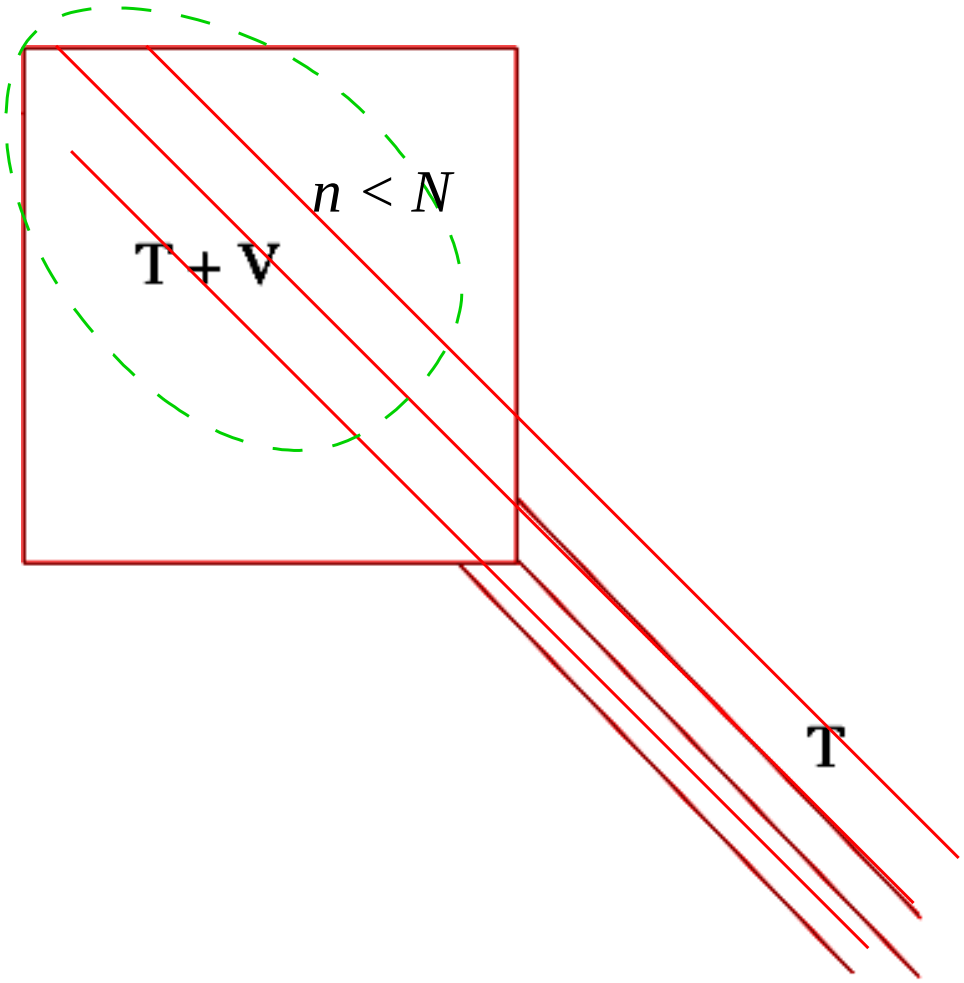
Lanczos algorithm

$H = T + V$

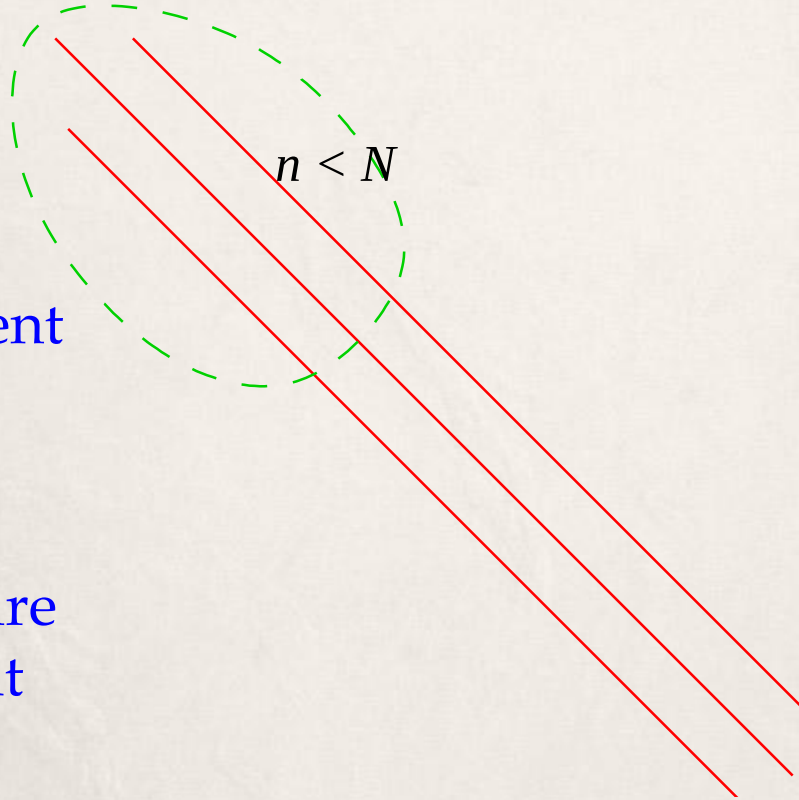
$V_{nm} = 0$ for $n,m > N$, kinetic energy matrix is infinite.

With H we first generate from above the oscillator basis functions Π_i with $n \geq N$.

After that we construct Lanczos basis of states Φ_m which are superpositions of oscillator states Π_i with $n \leq N$. H is tridiagonal in this basis.



Lanczos HORSE = *J*-matrix

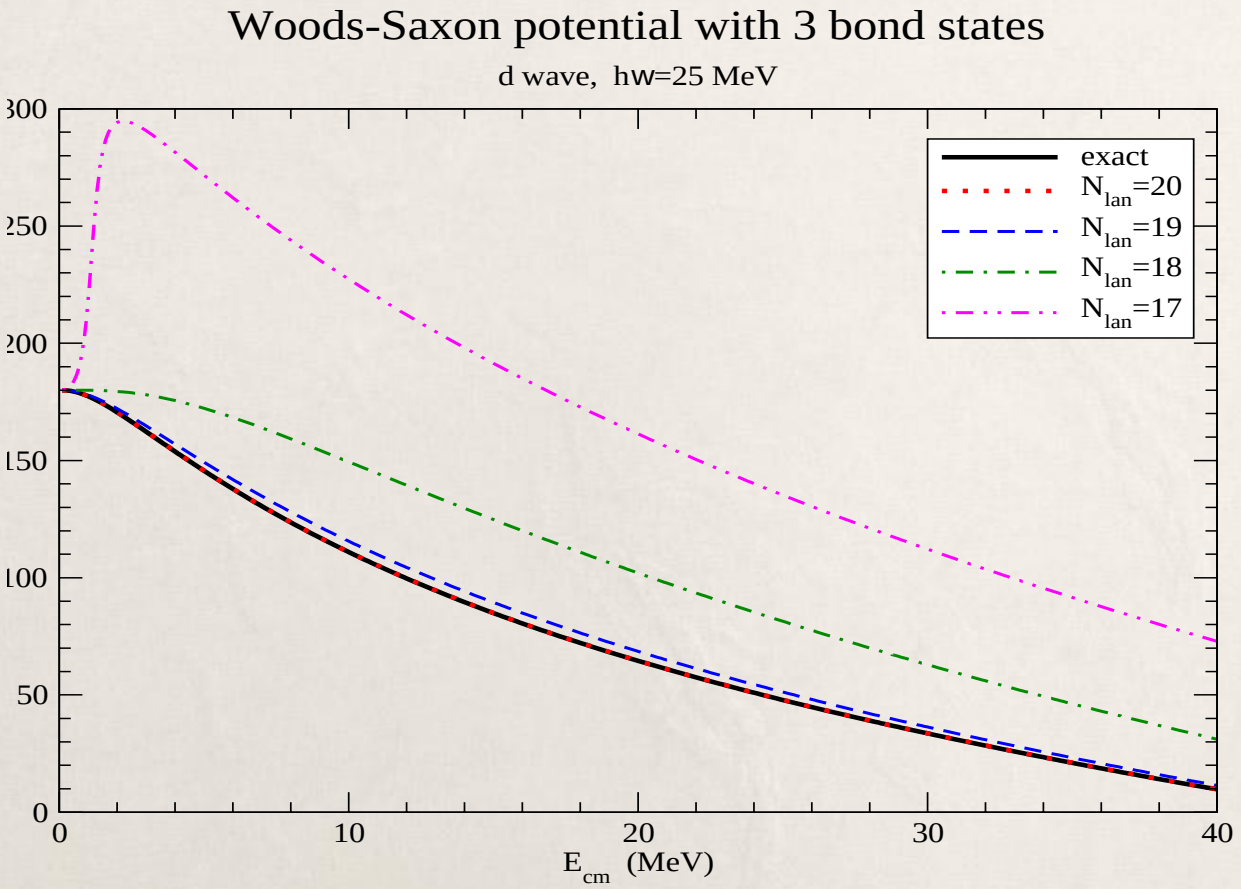


This is a reformulation of the *J*-matrix formalism. Hopefully it is more convenient for the shell model and *ab initio* no-core shell model applications.

We just extended usual Lanczos procedure in many-body applications and will use it with different boundary conditions: (i) scattering $a_n = \cos\delta s_n + \sin\delta c_n$ or (ii)decreasing a_n at large n.

How does it work and does it work at all?

Scattering



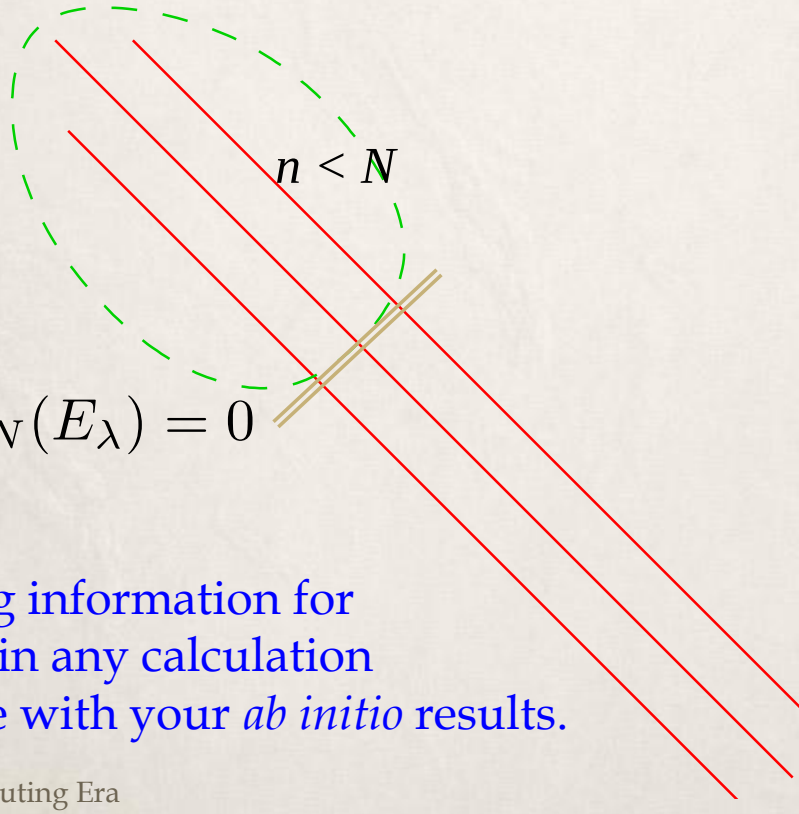
Hamiltonian eigenstates

$$H_{n,n-1}a_{n-1} + (H_{nn} - E)a_n + H_{n,n+1}a_{n+1} = 0$$

Boundary condition: $H_{N,N-1}a_{N-1}(E_\lambda) + (H_{NN} - E)a_N(E_\lambda) = 0$

or $a_{N+1}(E_\lambda) = 0$

If the phase shifts are known experimentally, it is easy to solve numerically:

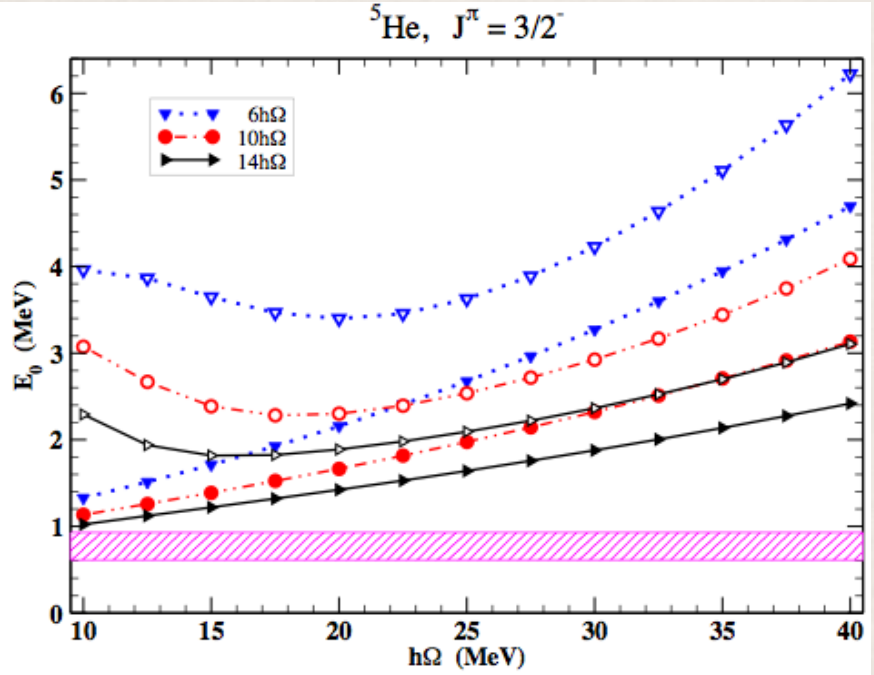


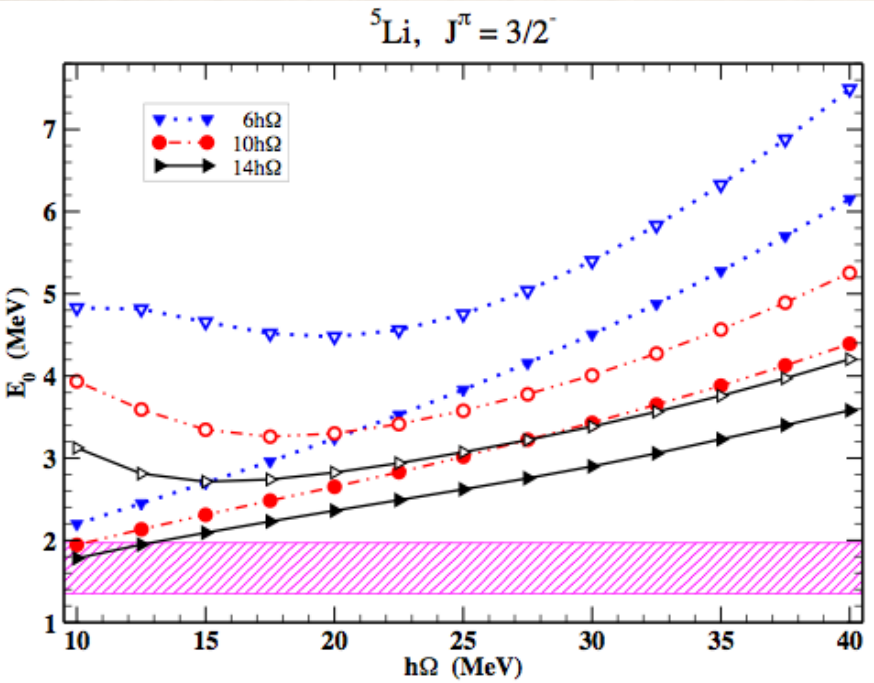
Scattering:

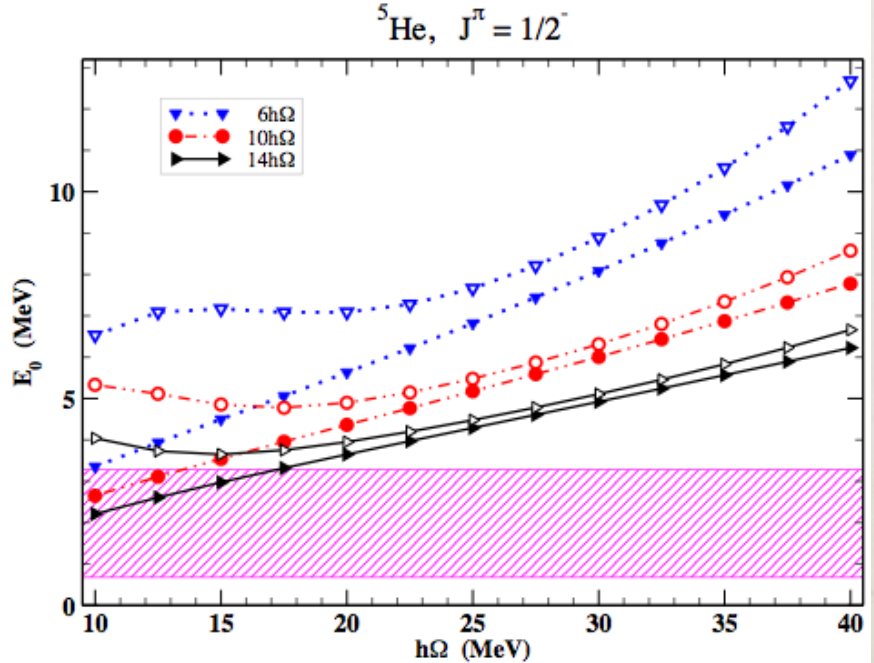
$$a_{N+1}(E_\lambda) = \cos\delta(E_\lambda)s_N(E_\lambda) + \sin\delta(E_\lambda)c_N(E_\lambda) = 0$$

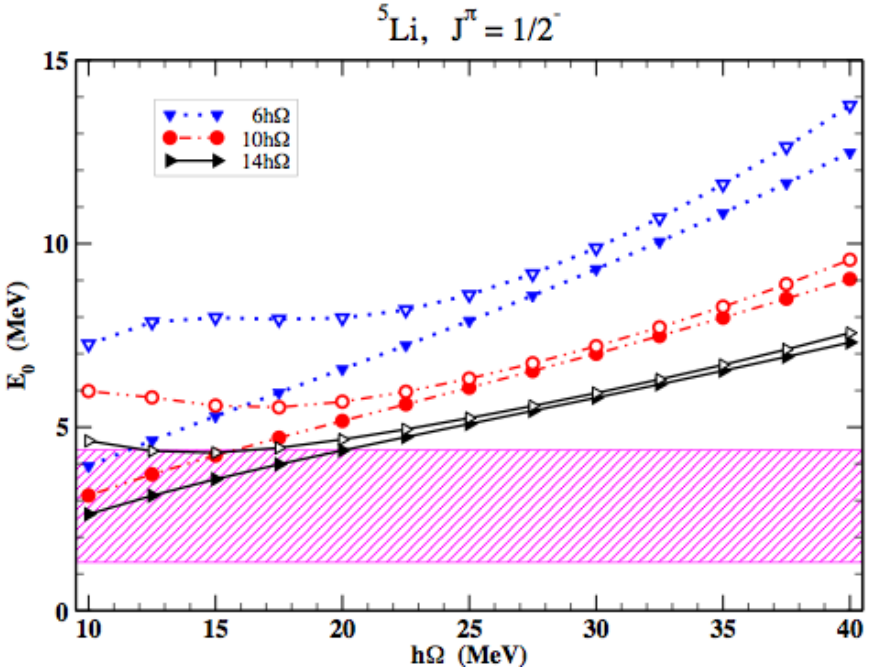
E_λ are eigenstates that are consistent with scattering information for given $\hbar\Omega$ and N_{max}; this is what you should obtain in any calculation with oscillator basis and what you should compare with your *ab initio* results.

Nα inverse scattering and NCSM

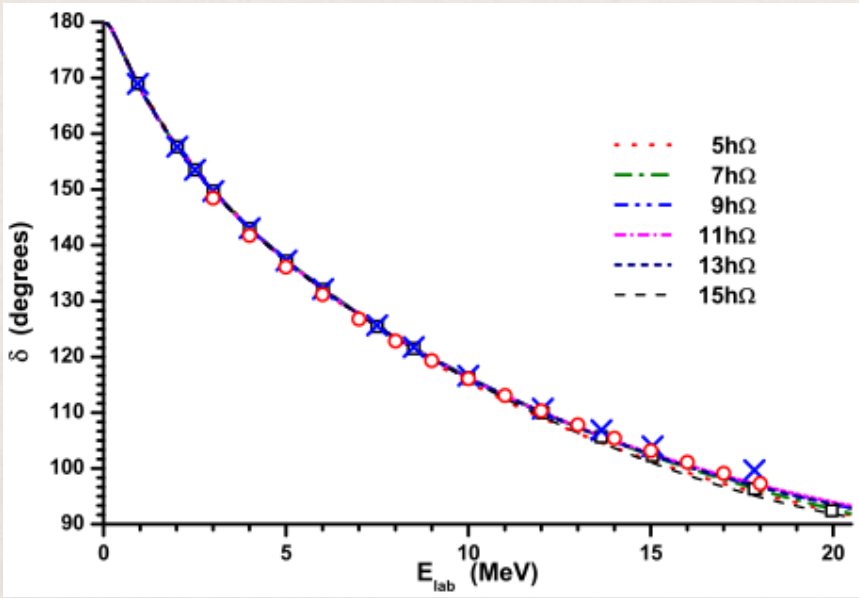


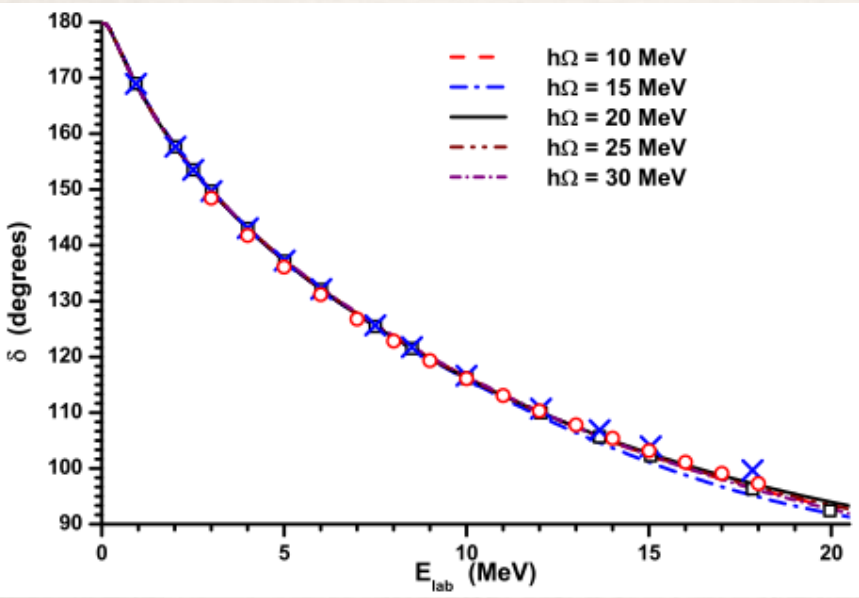


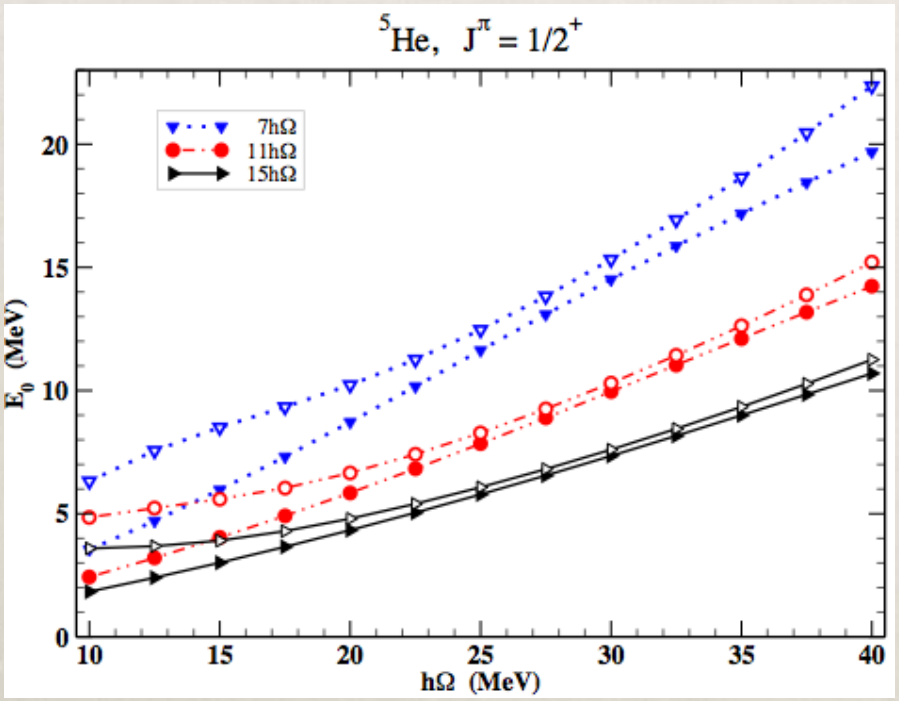


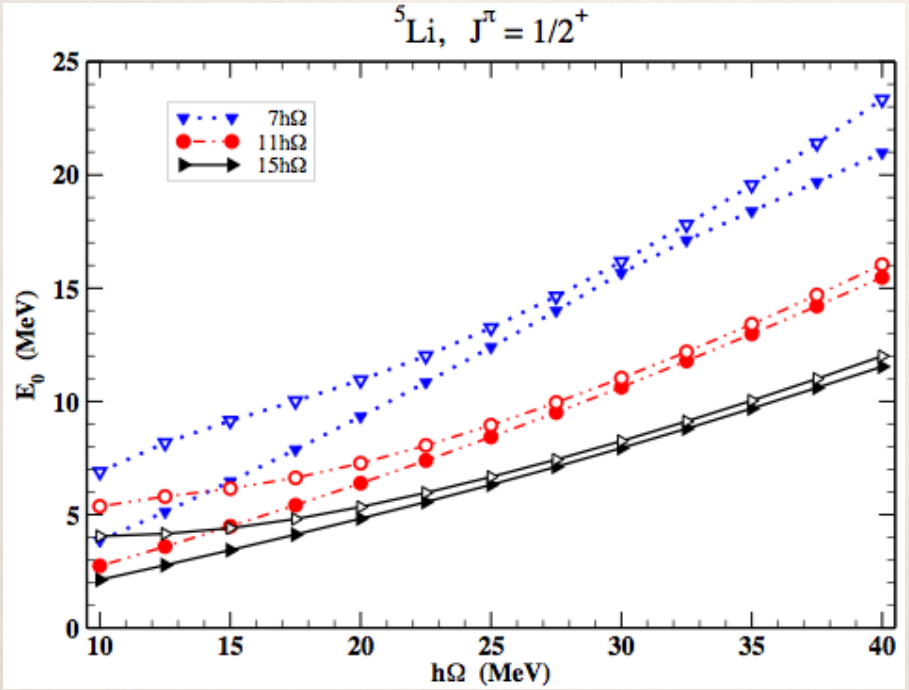


Nα non-resonant inverse scattering and NCSM







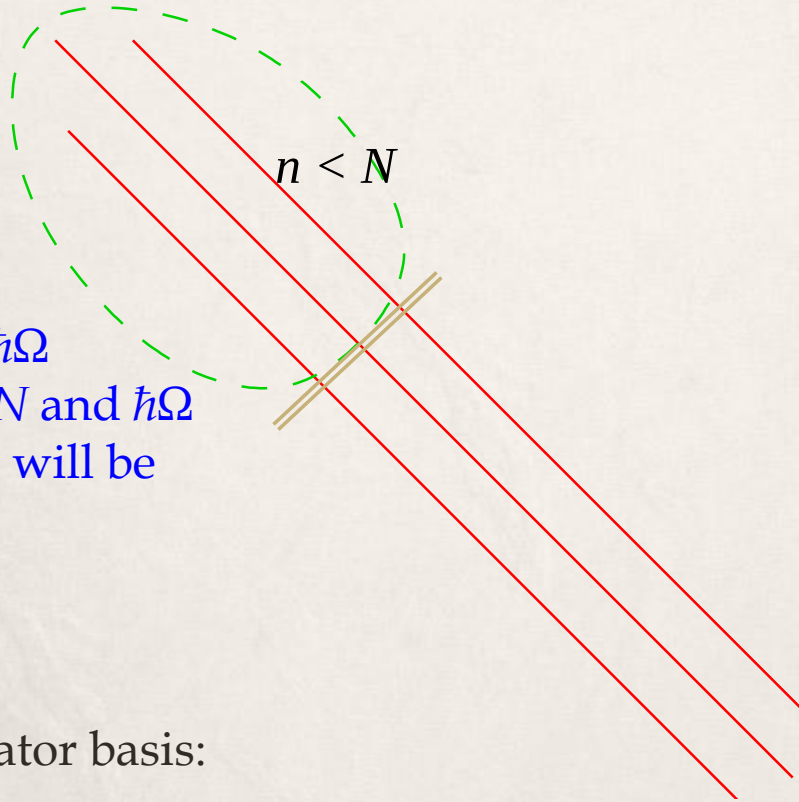


Inverse scattering

$$H_{n,n-1}a_{n-1} + (H_{nn} - E)a_n + H_{n,n+1}a_{n+1} = 0$$

S. Zaytsev was the first to study the *J*-matrix inverse scattering.

One can obtain not only E_λ but restore completely the tridiagonal matrix with $n \le N$ for given N and $\hbar\Omega$ provided that the phase shifts are known. Larger N and $\hbar\Omega$ larger is the energy interval where the phase shifts will be described.



JISP = *J*-matrix inverse scattering potential

NN interaction is a small matrix of the in the oscillator basis:
9ħΩ truncation, ħΩ = 40 MeV
Fast convergence of shell model calculations
Good description of *NN* data

Modern *NN* interaction models:

* Realistic (phenomenological) meson-exchange *NN* potentials (Nijmegen, Bonn, Argonne)

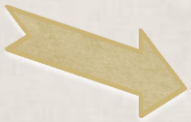
  \+ *NNN* phenomenological potentials

* EFT (ChPT) *NN* potentials

  \+ *NNN* EFT (ChPT) potentials

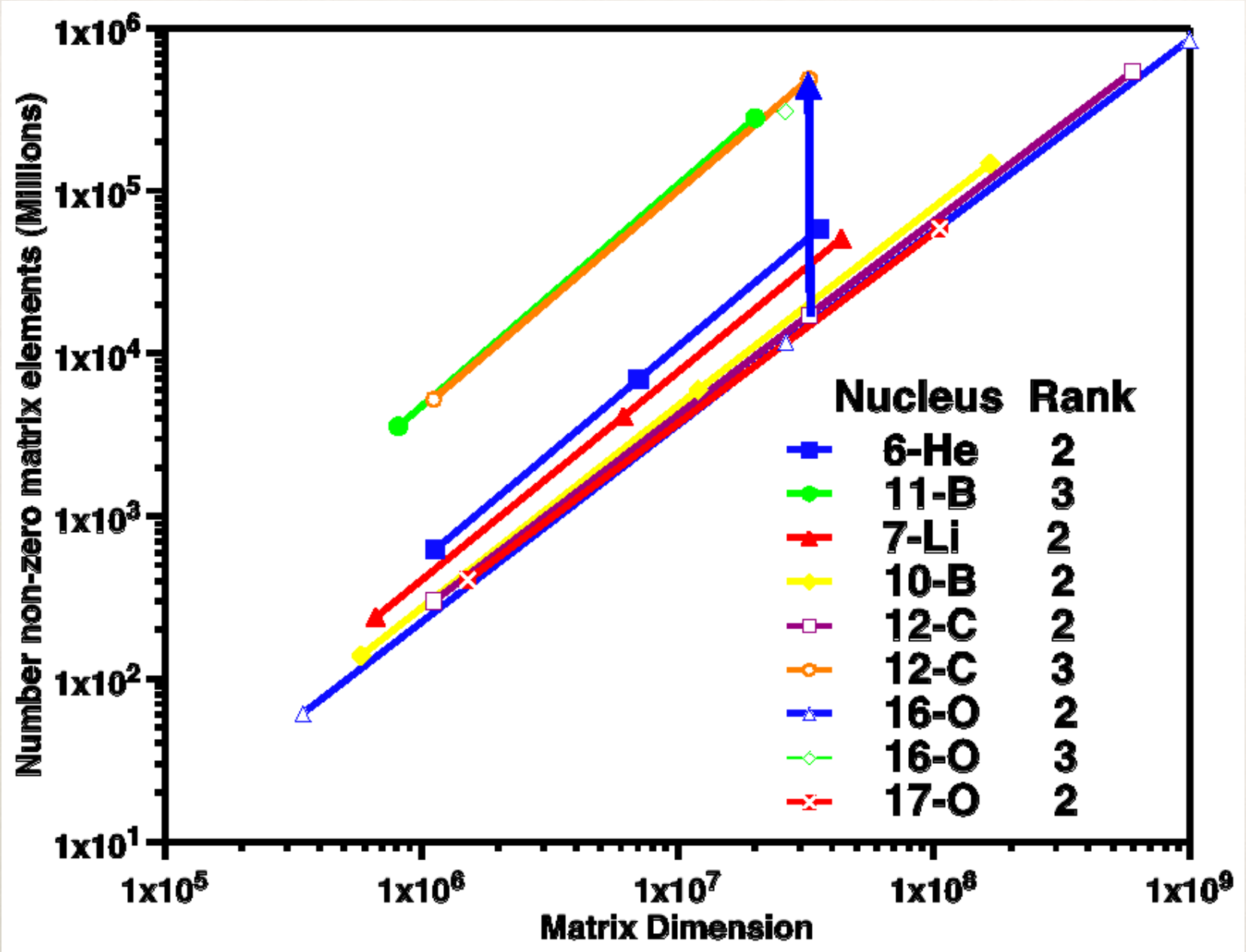
* JISP16 *NN* interaction

  no *NNN* interaction



fitted to light nuclei

Why would be nice to avoid *NNN* forces?



Role of *NNN* force?

* W. Polyzou and W. Glöckle theorem (Few-body Syst. **9**, 97 (1990)): $H=T+V_{ij} \rightarrow H'=T+V'_{ij}+V_{ijk'}$

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

  Hope:

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

  with (approximately) isospectral H and H' .

  JISP type interaction seems to be *NN* interaction minimizing *NNN* force.

  Without *NNN* force calculations are simpler, calculations are faster, larger model spaces become available; hence predictions are more reliable.

Ambiguity of JISP *NN* interaction

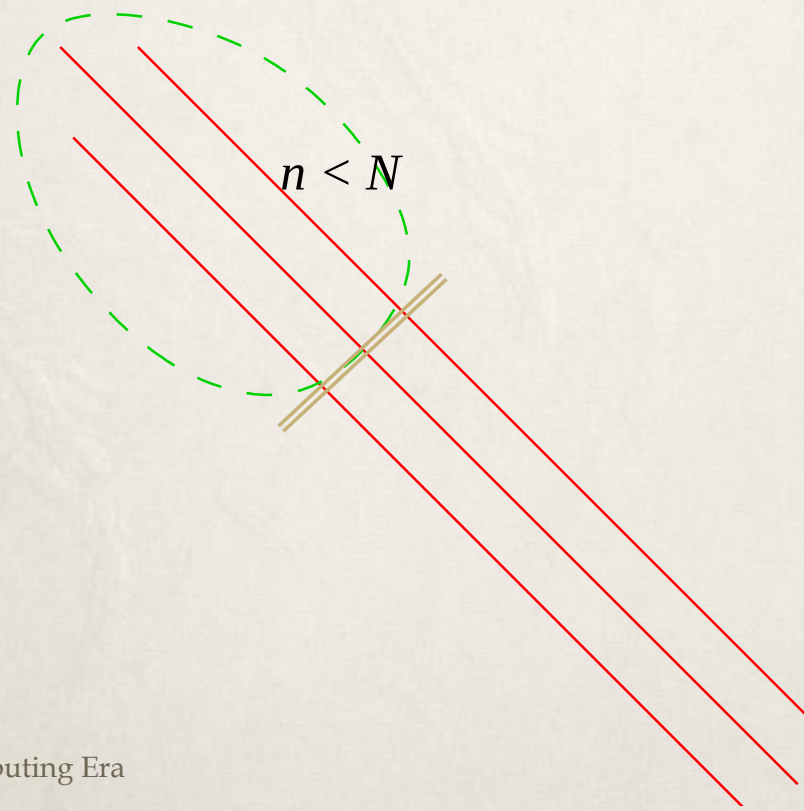
$$H_{n,n-1}a_{n-1} + (H_{nn} - E)a_n + H_{n,n+1}a_{n+1} = 0$$

We construct *NN* potential as a tridiagonal matrix in oscillator basis. However the basis functions with $n \le N$ can be any mixture of oscillator functions (unitary transformations, phase-equivalent transformations).

We use this ambiguity trying to fit JISP to binding energies and spectra of *s* and *p* shell nuclei.

JISP6 – fitted to $A \le 6$ nuclei.

JISP16 – fitted to $A \le 16$ nuclei.



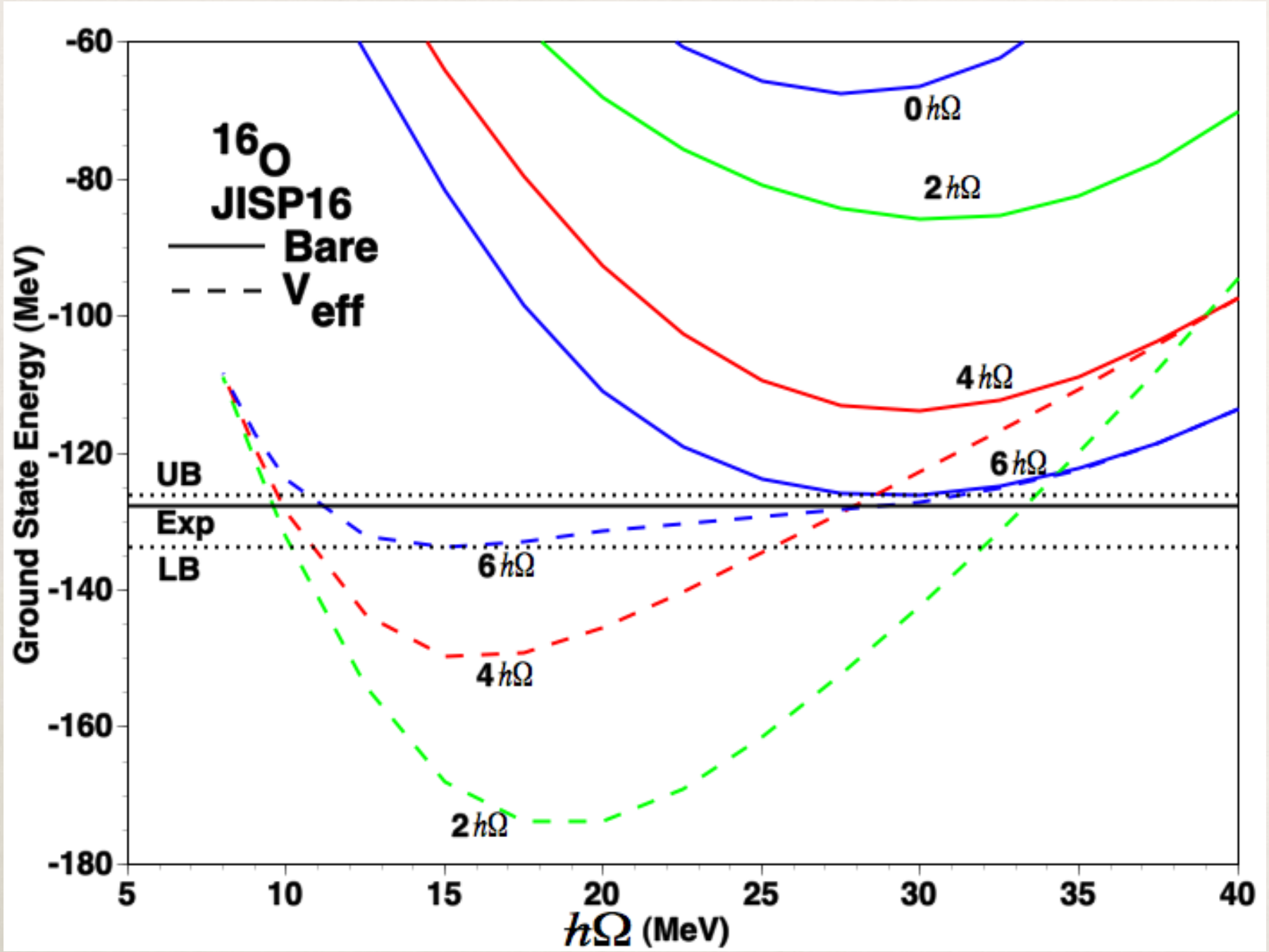
JISP16 properties

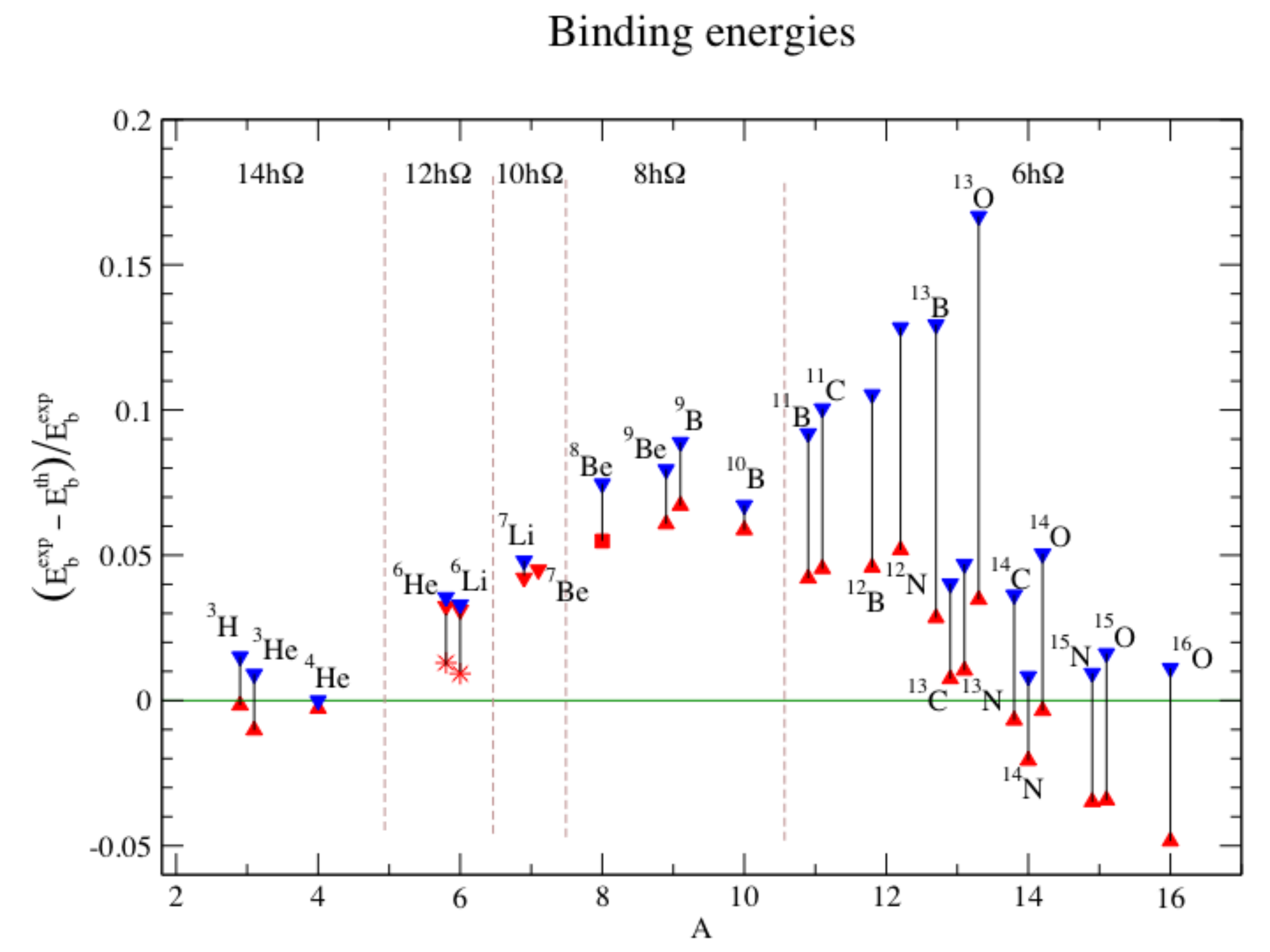
* 1992 *np* data base (2514 data): χ^2/datum = 1.03
* 1999 *np* data base (3058 data): χ^2/datum = 1.05

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)

How it was done initially


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


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

JISP16

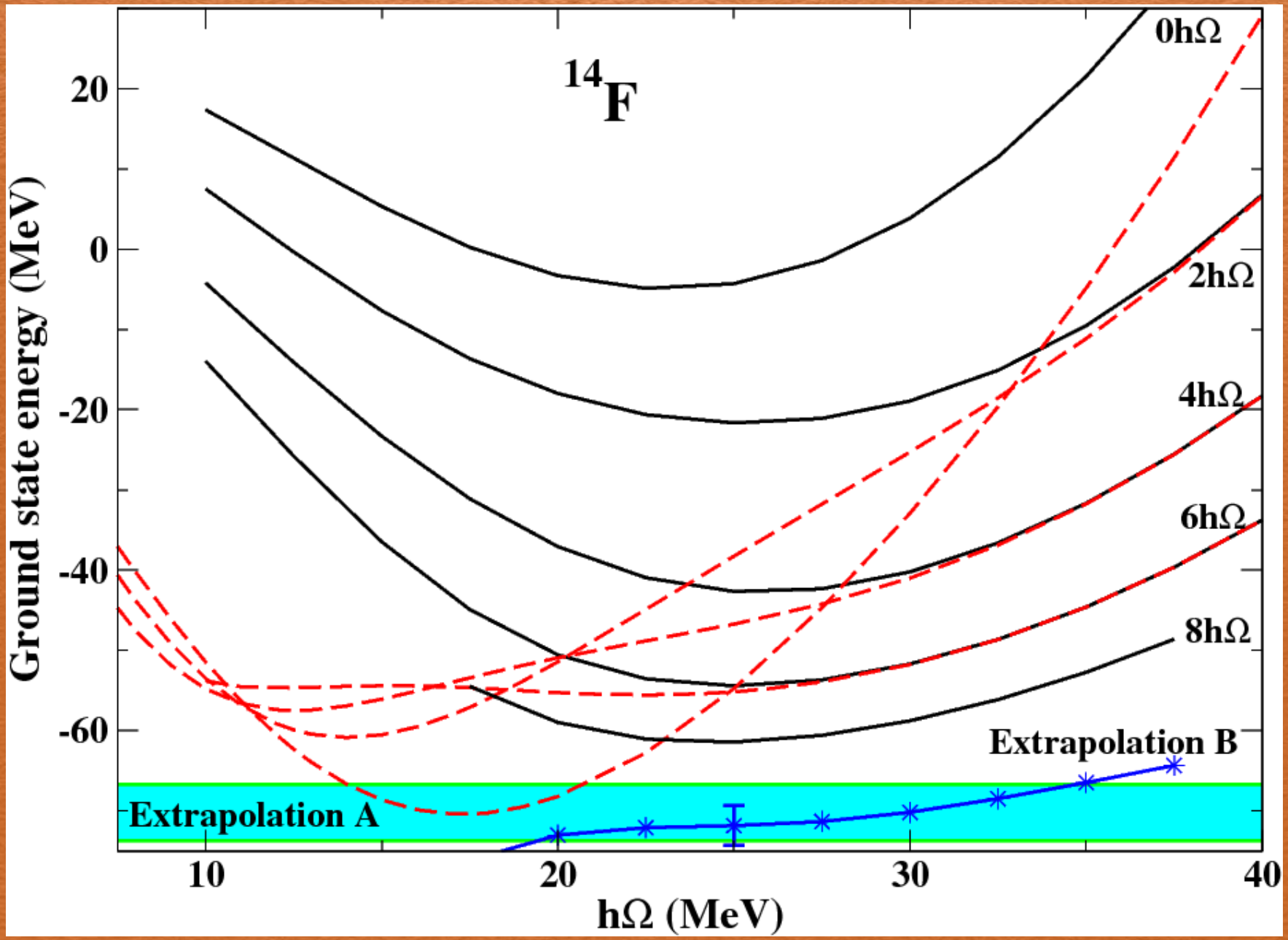
Ground state energy E_{gs} and excitation energies E_x (in MeV), ground state point-proton rms radius r_p (in fm) and quadrupole moment Q (in $e \cdot \mathrm{fm}^2$) of the ^{6}Li nucleus; $\hbar\omega = 17.5$ MeV.

Interaction	Nature	JISP6	JISP16	AV8'+TM'	AV18+UIX	AV18+IL2
Method		NCSM, $10\hbar\omega$ [6]	NCSM, $12\hbar\omega$	NCSM, $6\hbar\omega$ [2]	GFMC [8,15]	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

^{10}B

Potential Approach	Nature	JISP16 NCSM, $8\hbar\omega$ [a]	AV8'+TM' NCSM, $4\hbar\omega$ [b]	AV18+IL2 GFMC [c]	ChPT NCSM, $6\hbar\omega$ [d]
$E_{gs}(3_1^+,0)$	−64.751	−60.14	−60.57	−65.6(5)	−64.78
r_p	2.30(12)	2.168	2.168	2.33(1)	2.197
Q	+8.472(56)	6.484	+5.682	+9.5(2)	+6.327
$E_x(1_1^+,0)$	0.718	0.555	0.340	0.9	0.523
$E_x(0^+,1)$	1.740	1.202	1.259		1.279
$E_x(1_2^+,0)$	2.154	2.379	1.216		1.432
$E_x(2_1^+,0)$	3.587	3.721	2.775	3.9	3.178
$E_x(3_2^+,0)$	4.774	6.162	5.971		6.729
$E_x(2_1^+,1)$	5.164	5.049	5.182		5.315
$E_x(2_2^+,0)$	5.92	5.548	3.987		4.835
$E_x(4^+,0)$	6.025	5.775	5.229	5.6	5.960
$E_x(2_2^+,1)$	7.478	7.776	7.491		7.823
$B(E2;1_1^+0 \to 3_1^+0)$	4.13(6)	3.317	1.959		3.05
$B(E2;1_2^+0 \to 3_1^+0)$	1.71(26)	0.627	1.010		0.50
$B(\mathrm{GT};3_1^+0 \to 2_1^+1)$	0.083(3)	0.042	0.066		0.07
$B(\mathrm{GT};3_1^+0 \to 2_2^+1)$	0.95(13)	1.652	1.291		1.22

[a] A.M.Shirokov, J.P.Vary, A.I.Mazur, T.A.Weber, Phys. Lett. **B644**, 33 (2007).
[b] P. Navrátil, W. E. Ormand, Phys. Rev. **C 68**, 034305 (2003).
[c] S. C. Pieper, K. Varga, R. B. Wiringa, Phys. Rev. **C 66**, 044310 (2002).
[d] P. Navrátil, V. G. Gueorguiev, J. P. Vary, W. E. Ormand, A. Nogga, Phys. Rev. Lett. **99**, 042501 (2007).


^{14}F
0hΩ
2hΩ
4hΩ
6hΩ
8hΩ
Extrapolation A
Extrapolation B
Ground state energy (MeV)
hΩ (MeV)
20
0
-20
-40
-60
10
20
30
40

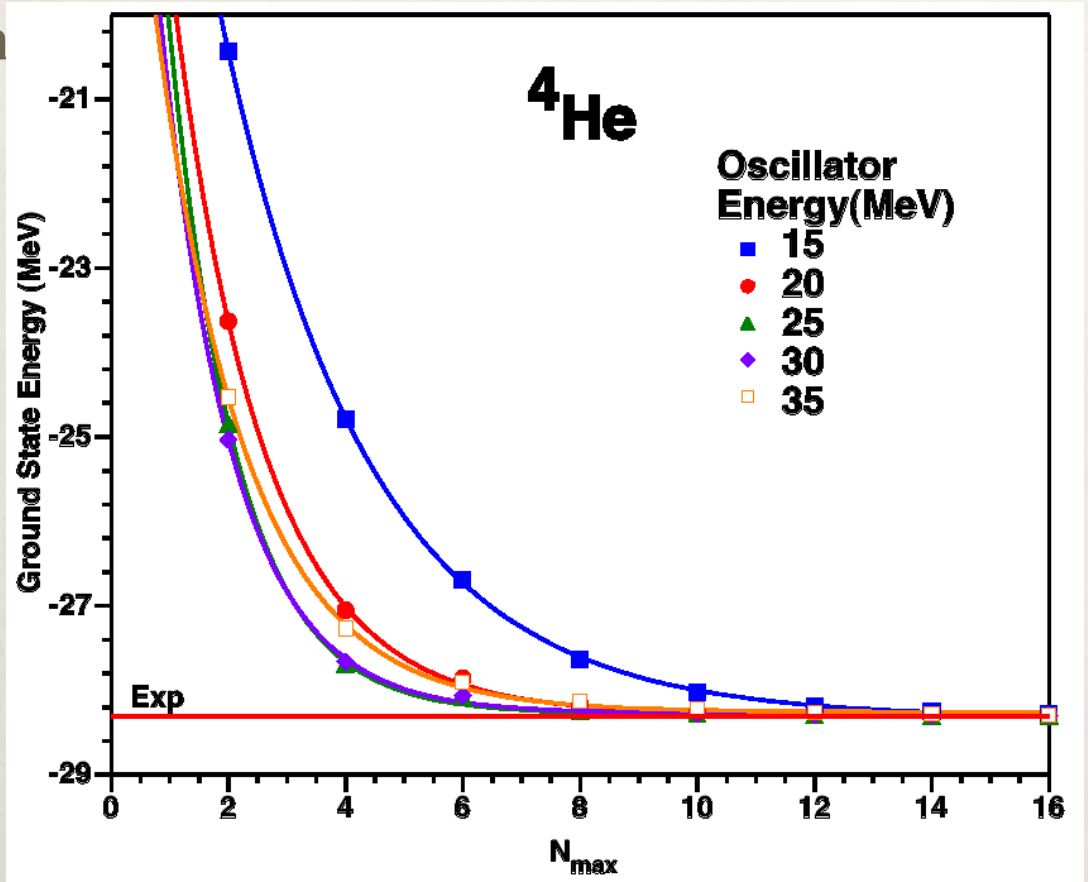
From effective interactions to full configuration calculations

* Extrapolation:

$$E_{gs}(N_{max}) = ae^{-bN_{max}} + E_{gs}(\infty)$$

* Works with bare in

* Example:



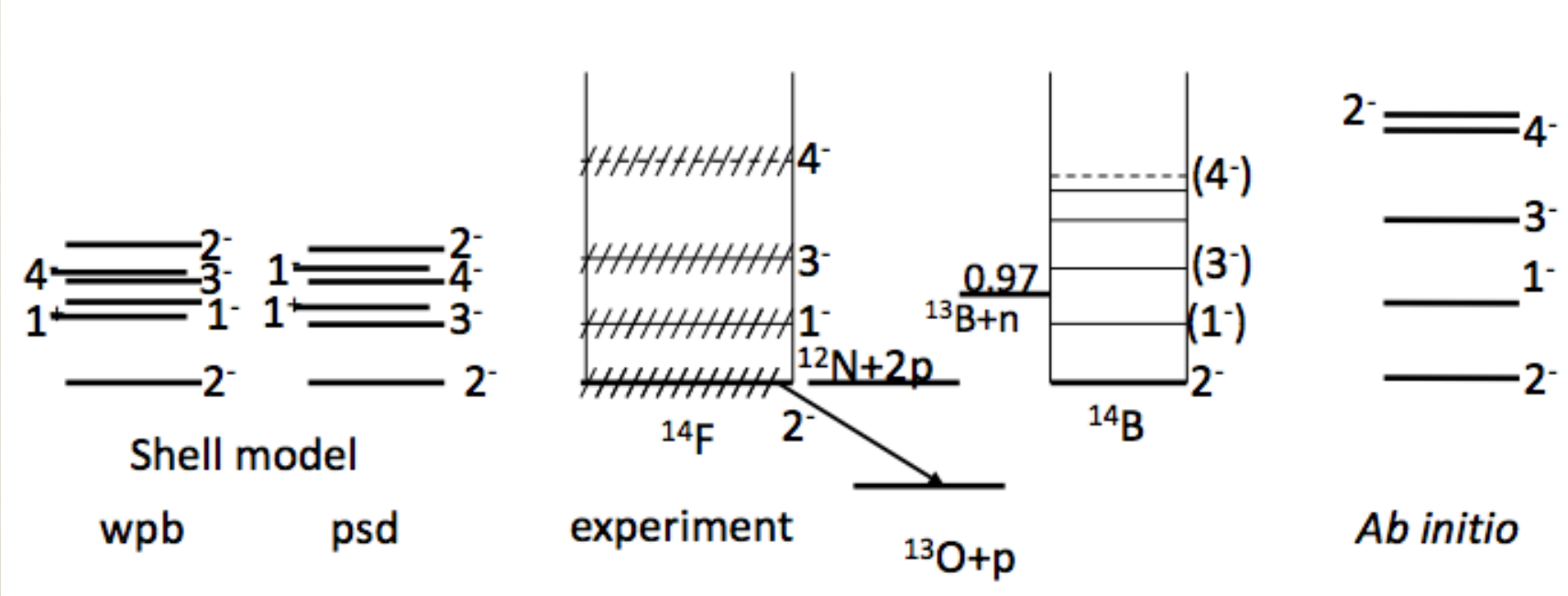
P. Maris, J. P. Vary, A. M. Shirokov, Phys. Rev. C **79**, 014308 (2009)

^{14}F

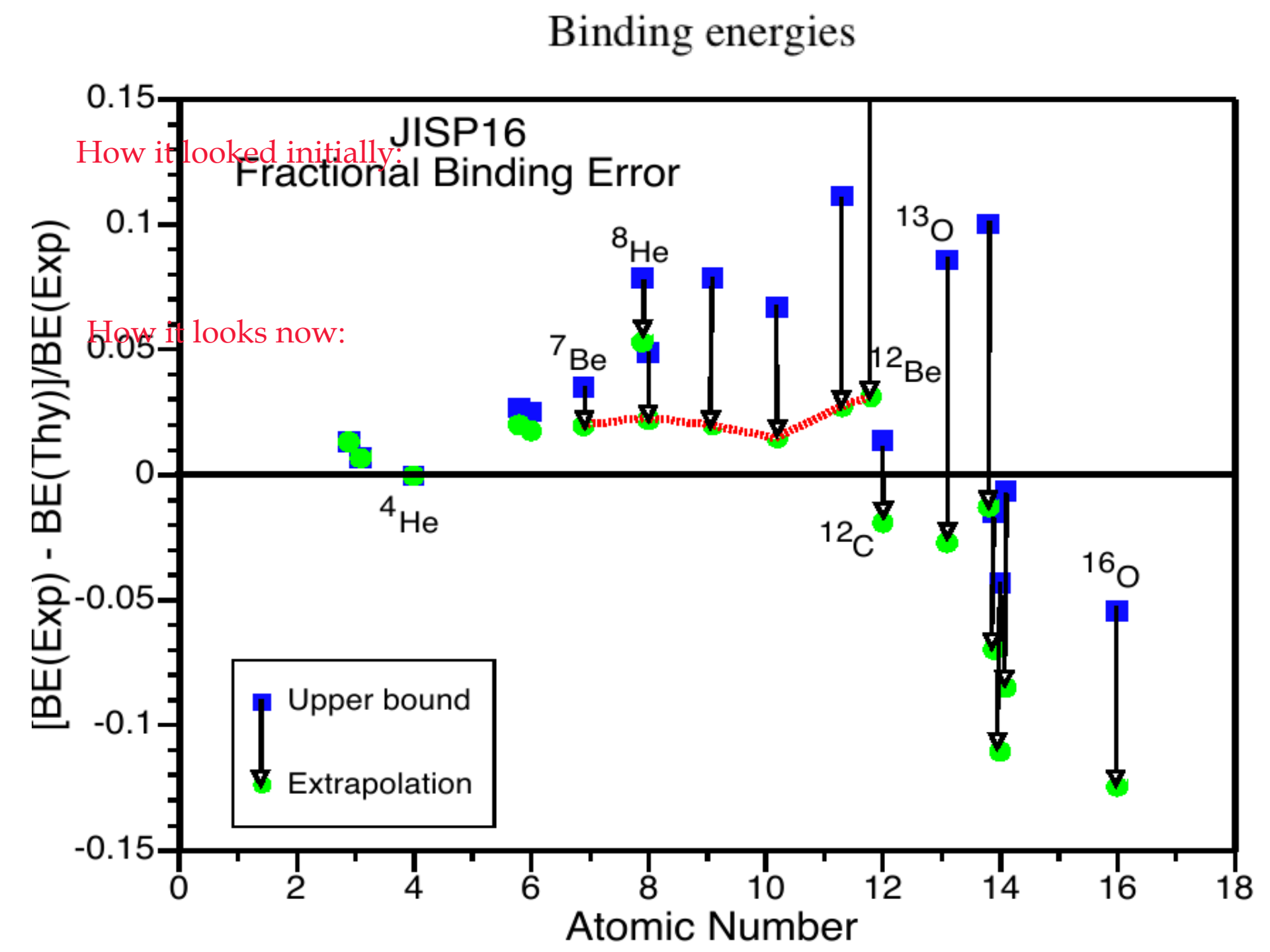
* 1,990,061,078 basis states
* each ħΩ point requires 2 to 3 hours on 7,626 quad-core compute nodes (30,504 processors in total) at the Jaguar supercomputer at ORNL

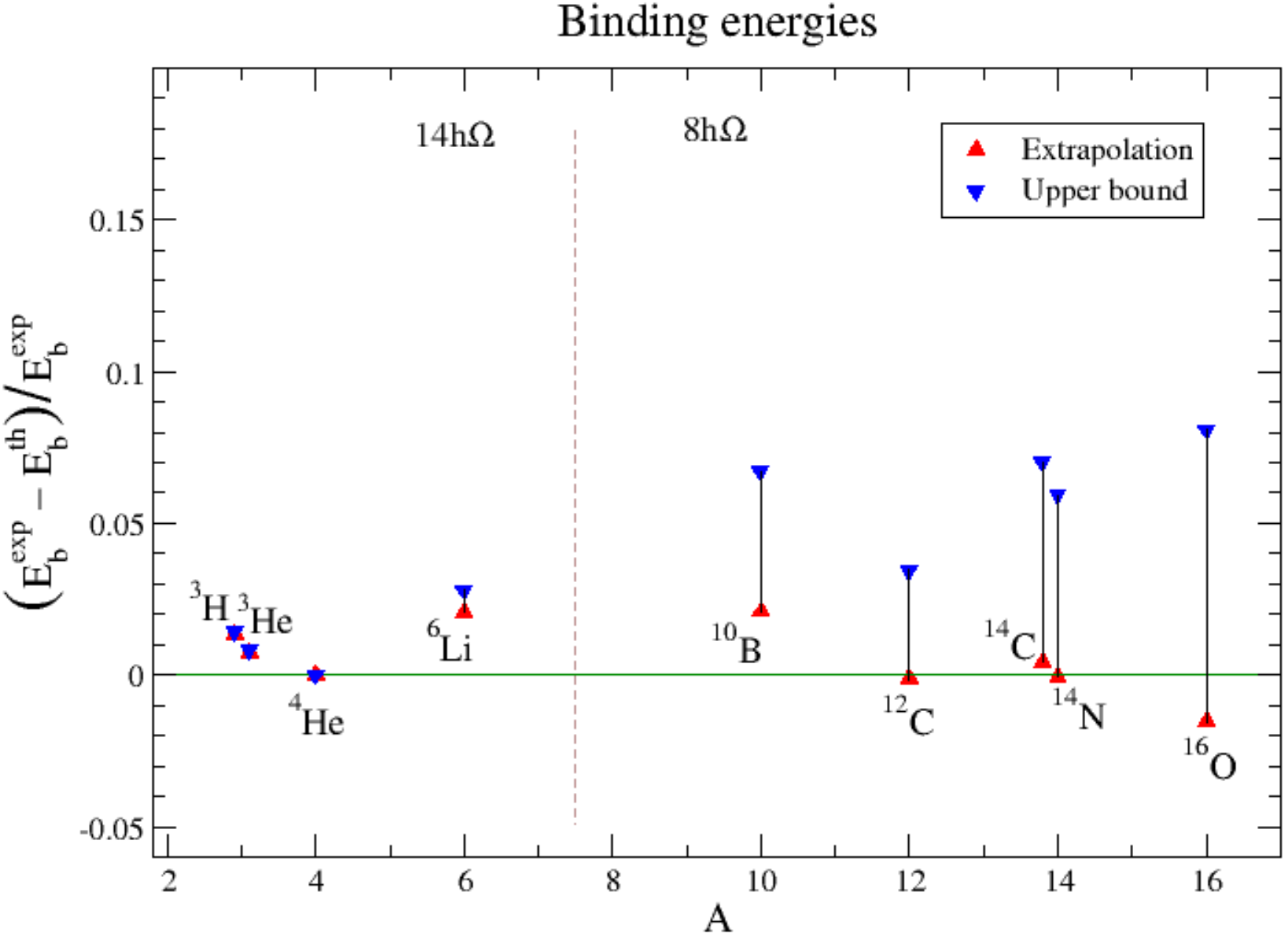
Nucleus	Extrapolation A	Extrapolation B	Experiment
^{13}O	–75.7(2.2)	–77.6(3.0)	–75.556
^{14}B	–84.4(3.2)	–86.6(3.8)	–85.423
^{14}F	–70.9(3.6)	–73.1(3.7)	74.00(0.04)

^{14}F spectrum

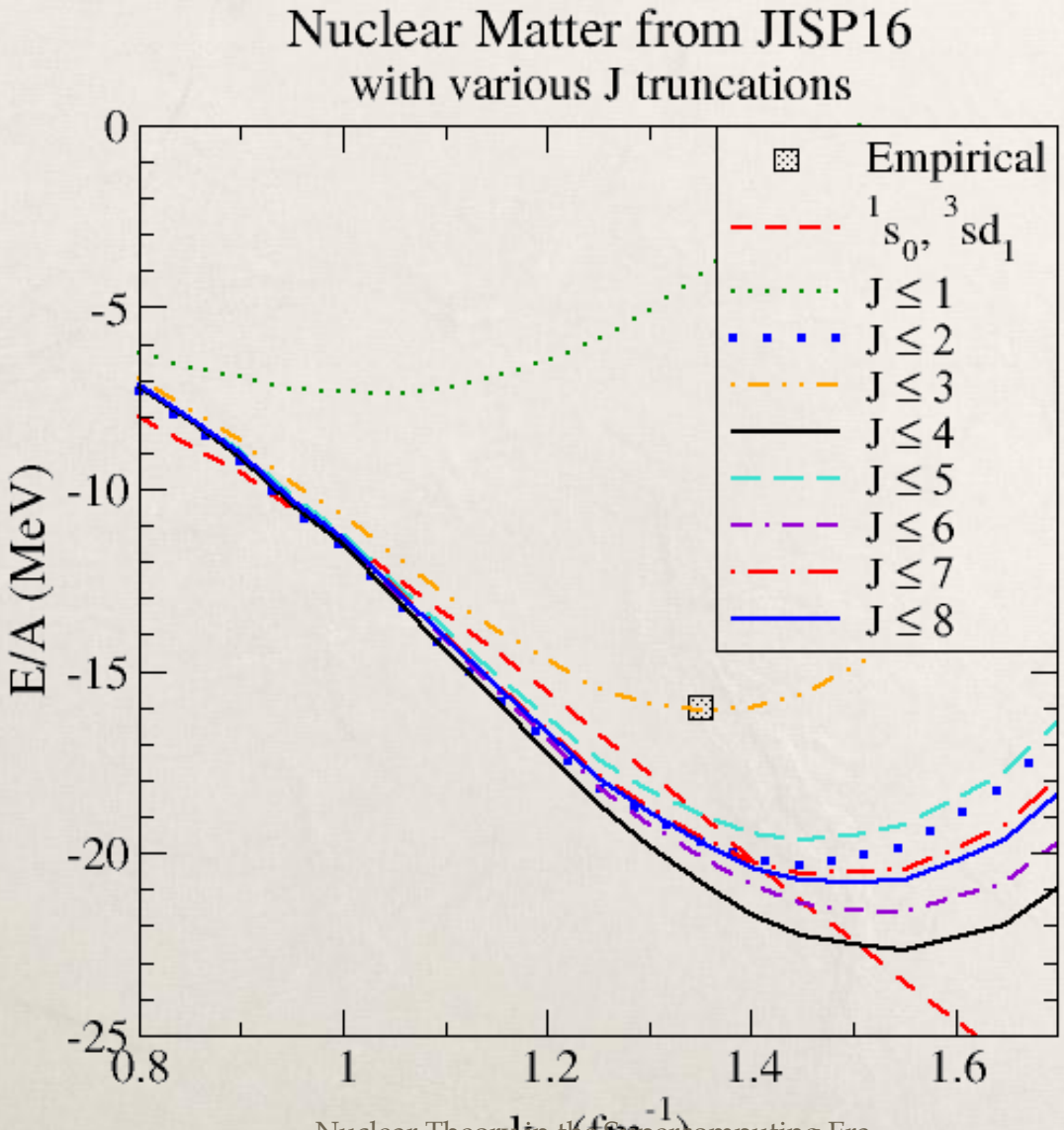


* Deficiency of JISP16 revealed by NCFC extrapolations


Binding energies
JISP16
Fractional Binding Error
How it looked initially:
How it looks now:
[BE(Exp) - BE(Thy)]/BE(Exp)
Atomic Number
Upper bound
Extrapolation
4He
7Be
8He
12Be
12C
13O
16O
0.15
0.1
0.05
0
-0.05
-0.1
-0.15
0
2
4
6
8
10
12
14
16
18

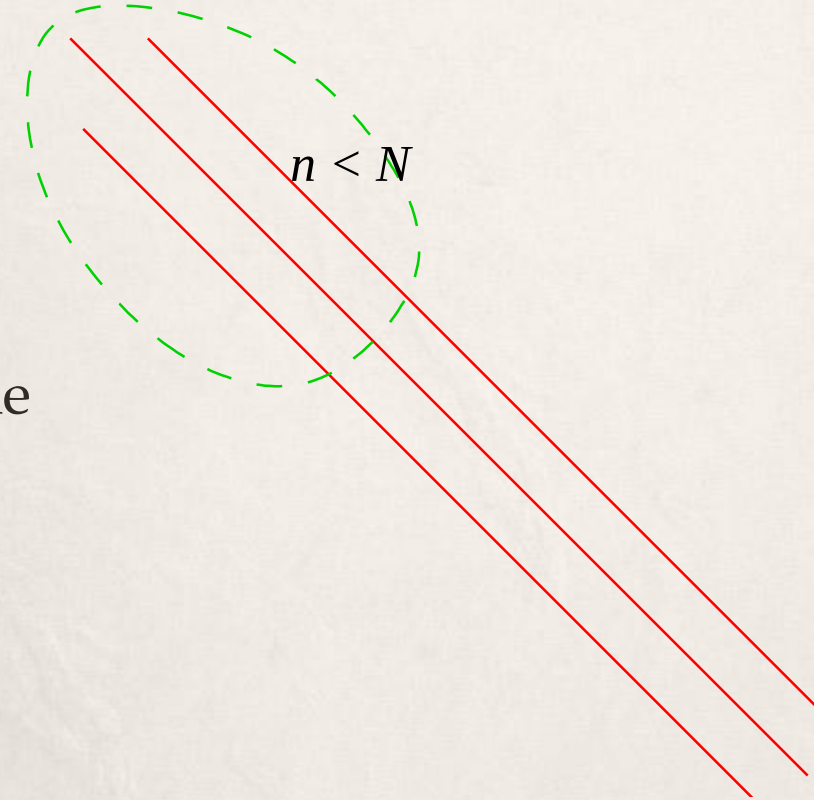

Binding energies
14hΩ
8hΩ
Extrapolation
Upper bound
$\left(E_b^{exp} - E_b^{th}\right)/E_b^{exp}$
0.15
0.1
0.05
0
-0.05
2
4
6
8
10
12
14
16
A
^{3}H
^{3}He
^{4}He
^{6}Li
^{10}B
^{12}C
^{14}C
^{14}N
^{16}O

Nuclear matter with JISP16



What is next?

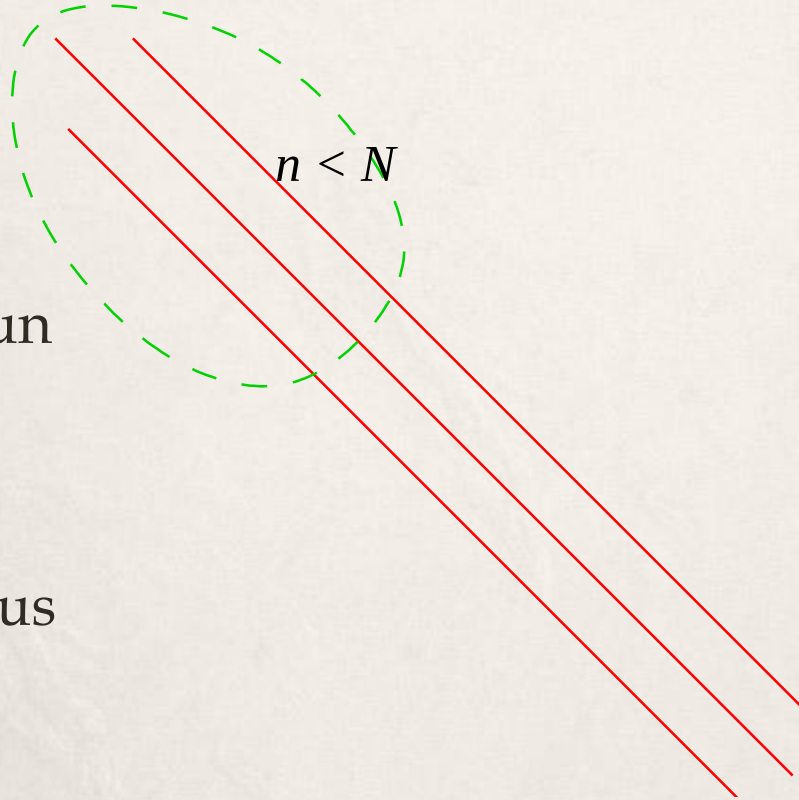
Possible many-body *ab initio* applications



n-A scattering: if A wave function is obtained with $N_{max} = 0$, everything looks like a conventional Lanczos SM run in the A+1 system with a specific pivot vector. The SM Lanczos basis is extended analytically to involve states with large quanta. Interpretation of the results is different.

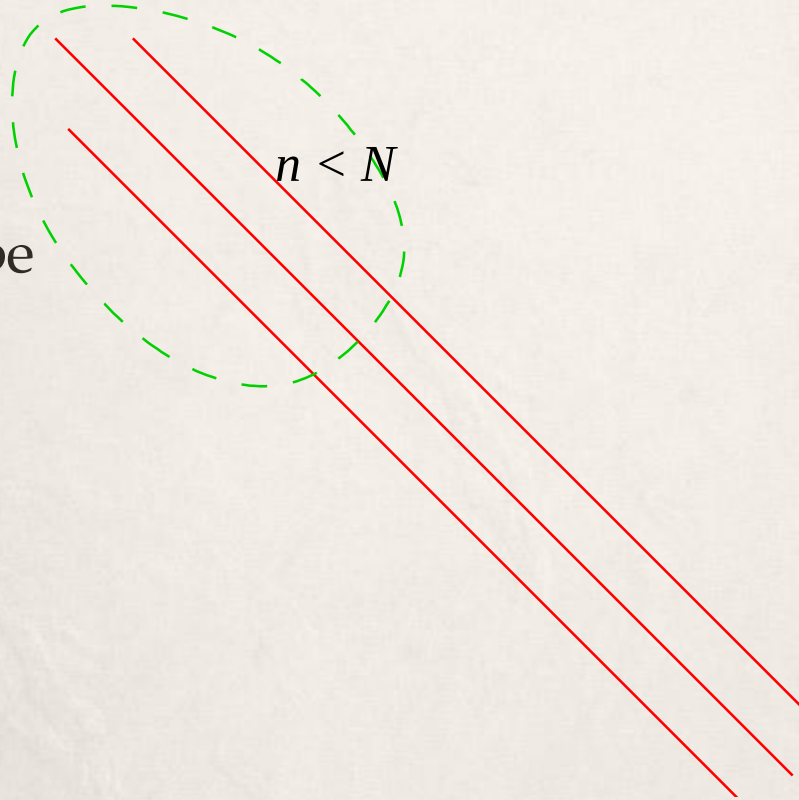
$a_n = \cos\delta s_n + \sin\delta c_n$, $n \geq N$.

Possible many-body *ab initio* applications



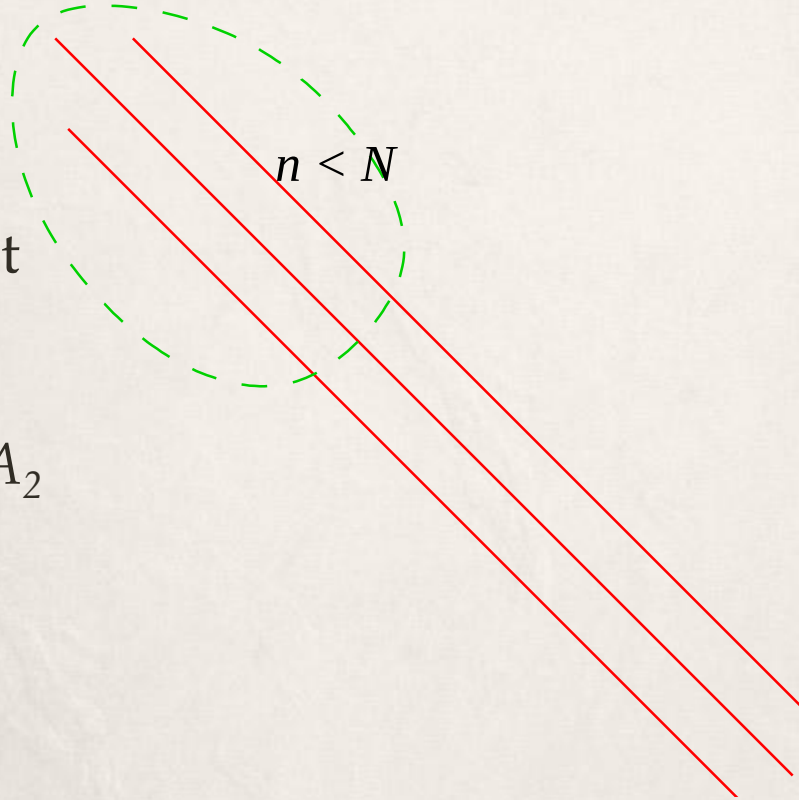
n-A scattering: if A wave function is obtained with $N_{max} > 0$, the Lanczos SM run in the A+1 system become more complicated and involves few additional vectors added to the A+1 system model space. All the rest looks like in the previous case.

Possible many-body *ab initio* applications



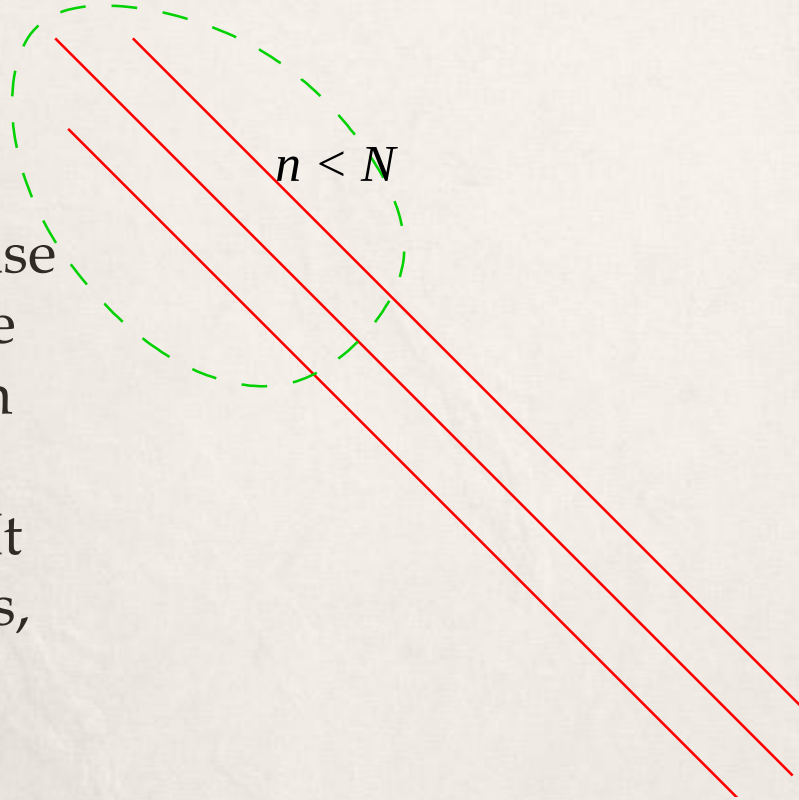
p-A scattering: Coulomb interaction can be included in the approach. This requires adding additional channel states in the Lanczos SM run in the A+1 system – the number of such states is below 100.

Possible many-body *ab initio* applications



$A_1 + A_2$ scattering: looks like that the most complicated problem now is transformation from the $A_1 + A_2$ cluster structure to the SM structure of the $A_1 + A_2$ system.

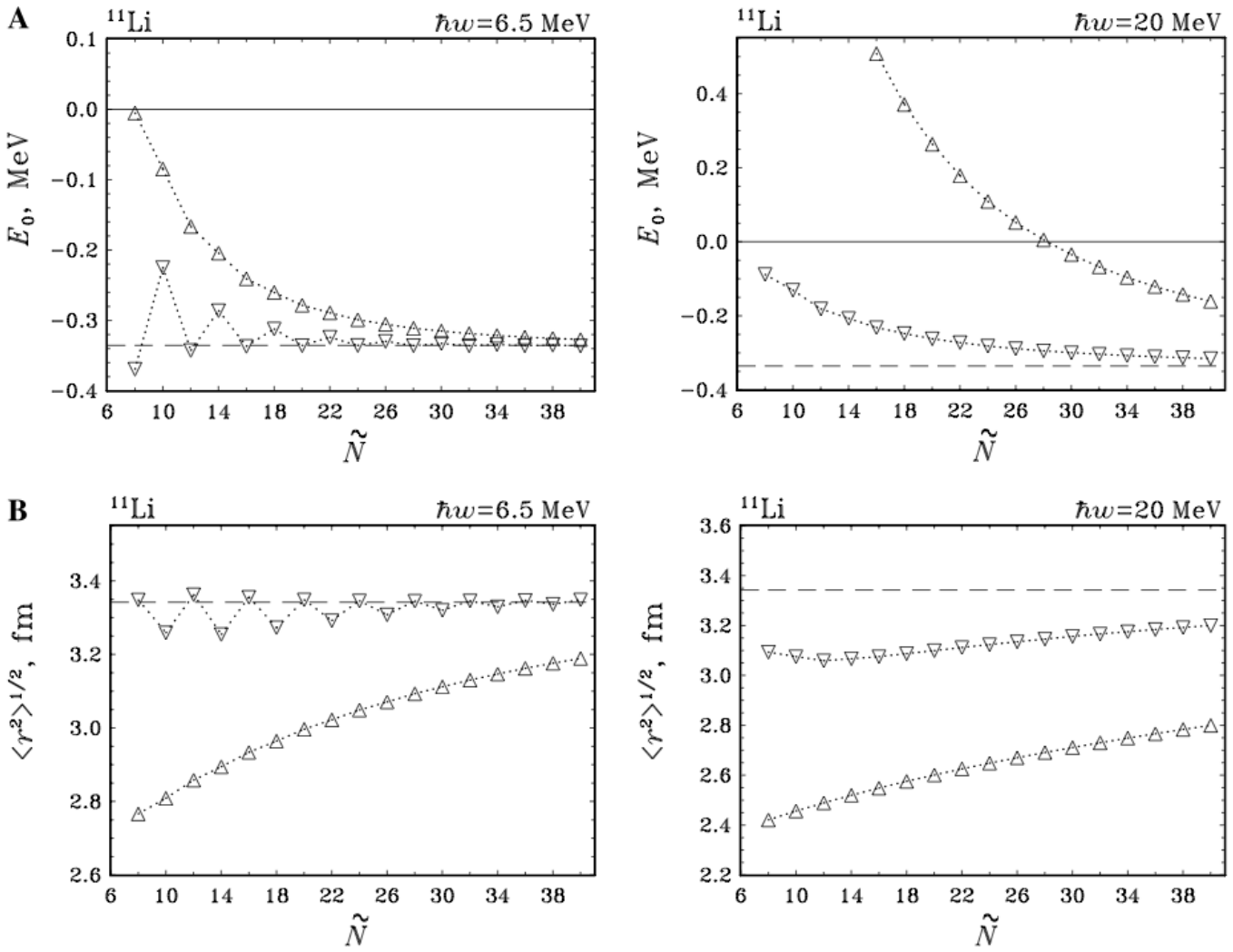
Possible many-body *ab initio* applications



Bound states: the TRR solutions a_n decrease with n when $n > N$ at $E < 0$. Extending the SM Lanczos basis by oscillator states with $n > N$ is equivalent to calculating binding energies as the respective S-matrix pole. It improves the variational binding energies, rms radii, etc.

How does it work and does it work at all?

Bound state:
^{11}Li in a cluster model
Note rms radius



Convergence

* Poor convergence to get reasonable results for phase shifts in available model spaces in systems with $A > 4$.

Hungarian smoothing

* J. Revai, M. Sotona, J. Žofka, J. Phys. G 11, 745 (1985).
* The $N \times N$ potential energy matrix $V_{ij},\ i,j = 1,2,...,N$ is replaced by

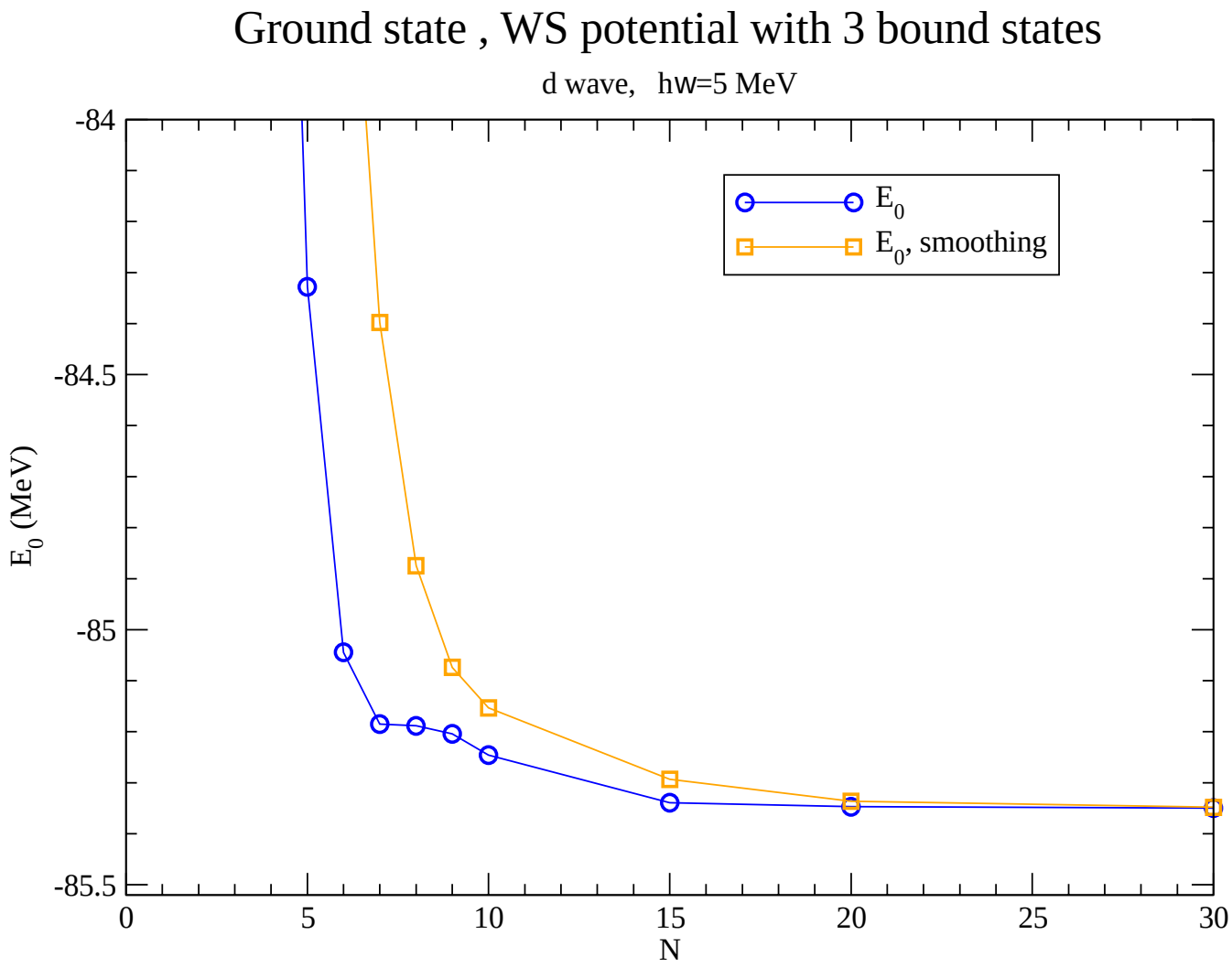
$$\tilde{V}_{ij} = \sigma_i^N V_{ij} \sigma_j^N ,$$

$$\sigma_i^N = \frac{1 - \exp\left\{-[\alpha(i-N-1)/(N+1)]^2\right\}}{1 - \exp(-\alpha^2)}.$$

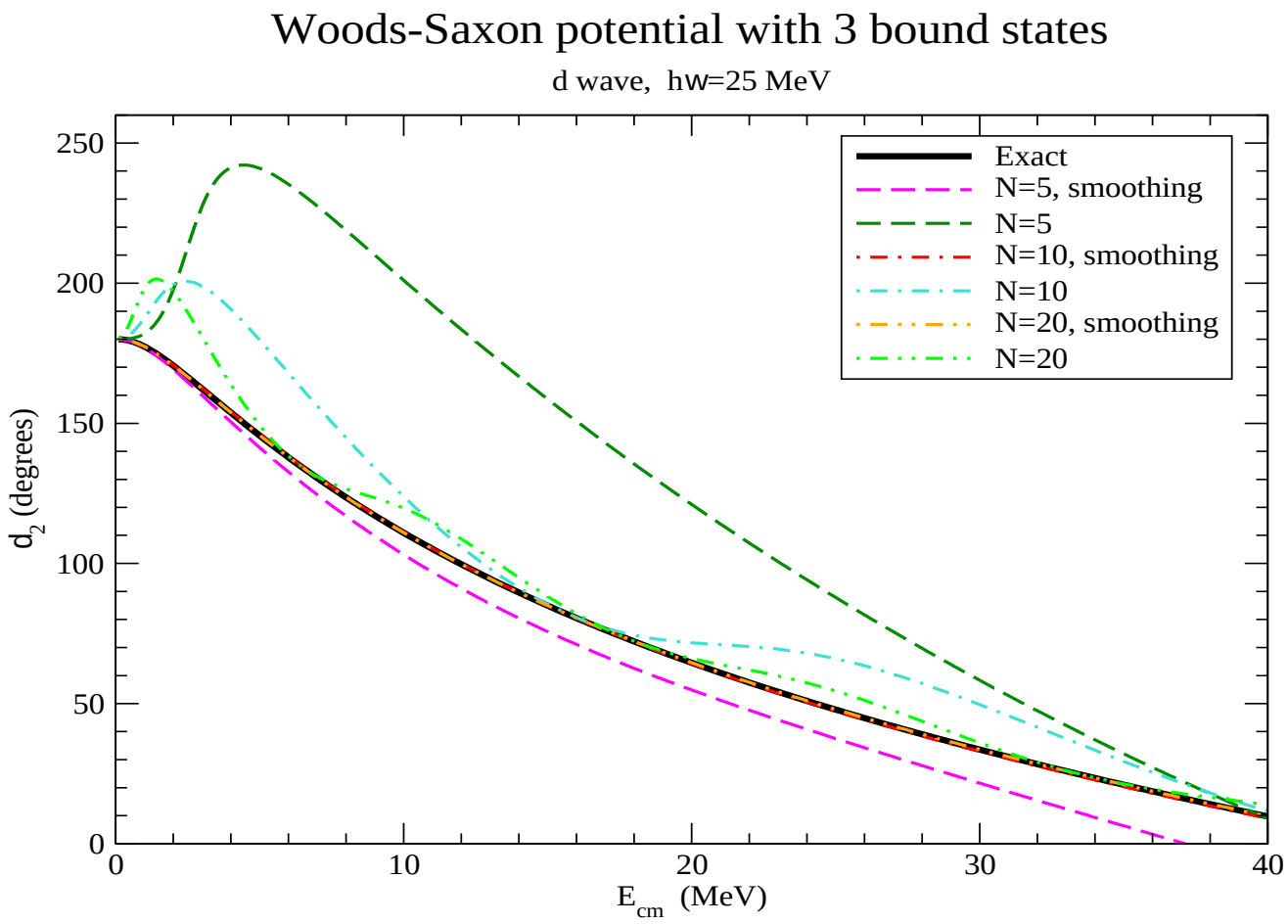
* This is some kind of effective interaction that makes convergence of various observables smoother.
* The properties of such effective interaction were not studied in many-nucleon systems

Hungarian smoothing

$\alpha = 5$

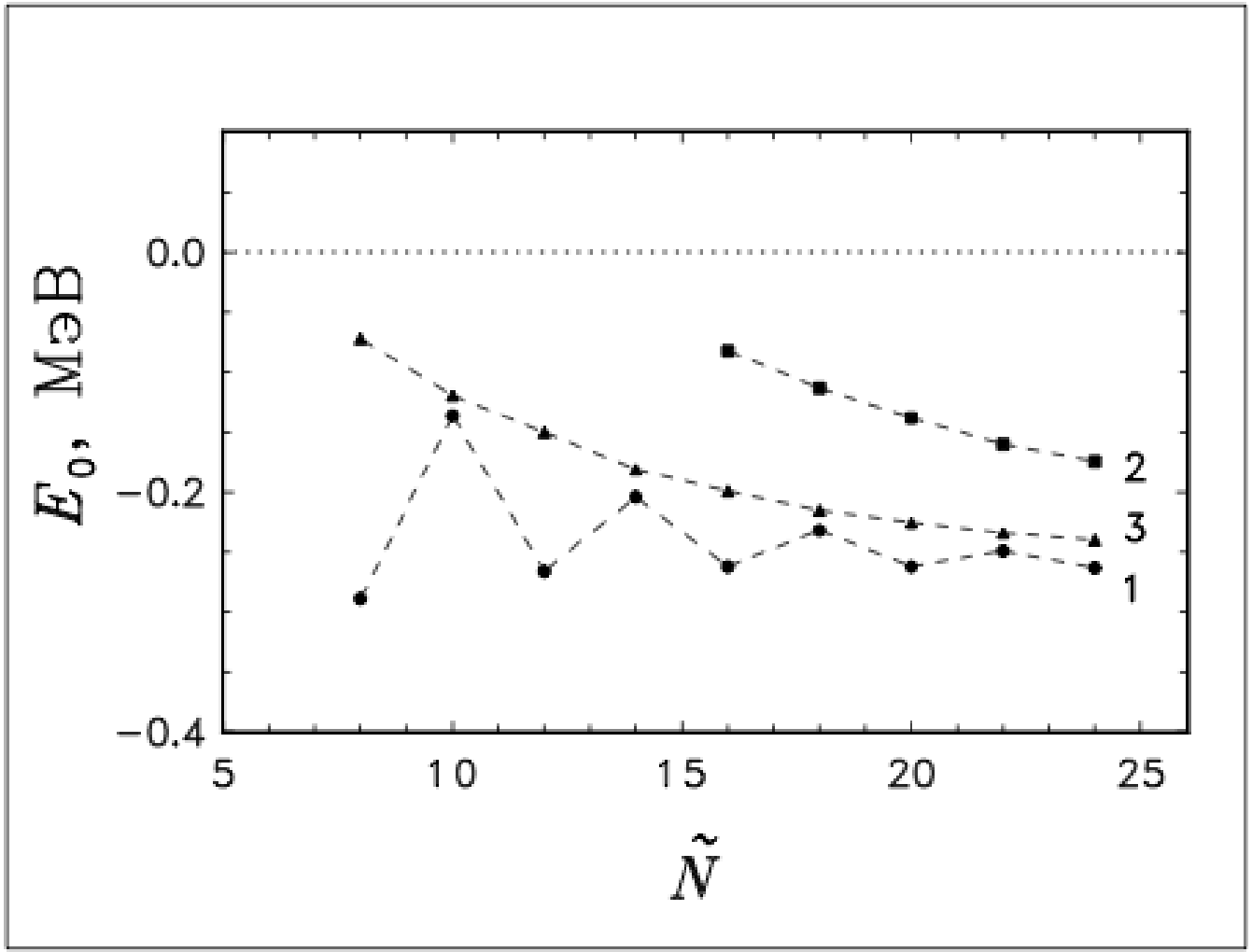


Hungarian smoothing



$\alpha = 5$

Hungarian smoothing



$\alpha = 5$

Conclusions

* I've tried to formulate scattering theory in a way that it looks very like a conventional shell model, no-core shell model. That means that it can be more or less easily implemented in *ab initio* nuclear structure models.

* I've recalled an idea of Hungarian smoothing, a simple effective interaction that smooths convergence of various observables and simplifies extrapolations. Probably, it would be interesting to study it in many-body applications in more detail.

* JISP16 is a reasonable *NN* interaction describing a wide range of data. Further development of improved releases of JISP interaction is under way.

* Knowing phase shifts one can get eigenstates to be obtained in *ab initio* NCSM with given $N_{\max}$ and $\hbar\Omega$.

Conclusions

Thank you!