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Current Status of Very-Large-Basis Hamiltonian Diagonalizations for Nuclear Physics

Calvin W. Johnson

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CIPANP, June 1, 2018

An all-too-common view:

An all-too-common view:

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Dark matter, string theory, neutrino physics….

An all-too-common view:

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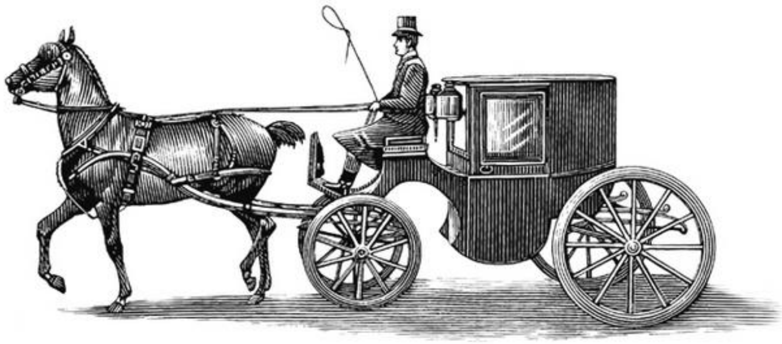

Dark matter, string theory, neutrino physics....

Nuclear structure physics

An all-too-common view:

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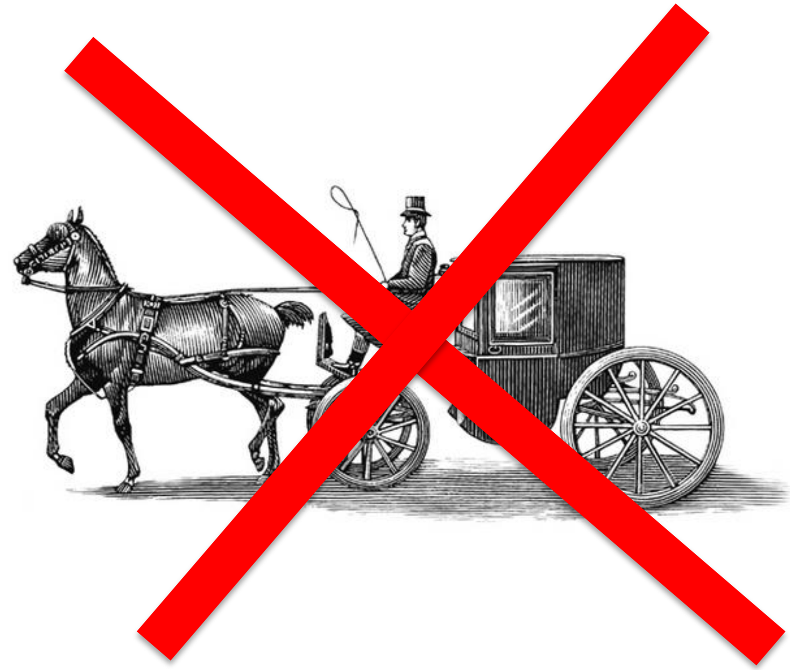

Dark matter, string theory, neutrino physics....

Nuclear structure physics

A better view:

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Dark matter, string theory, neutrino physics....

Nuclear structure physics

A better view:

Modern nuclear structure physics is rigorous, vigorous, and *the launchpoint for many other investigations.*

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To detect dark matter,
one needs **nuclear cross-sections**.
For neutrino physics, **nuclear cross-sections**.
For neutrinoless ββ decay, **need nuclear matrix element**
For parity/time-reversal violation (e.g. EDM),
need nuclear matrix element….

To compute electromagnetic and weak transition rates, we use Fermi's (actually Dirac's) Golden Rule from time-dependent perturbation theory:

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$$R_{i \to f} = \frac{2\pi}{\hbar} \left| \langle f | \hat{O} | i \rangle \right|^2 \frac{dN_f}{dE}$$

Transition probability (strength)

$$\langle f | \hat{O} | i \rangle = \sum_{a,b} \langle a | \hat{O} | b \rangle \langle f | \hat{c}_a^+ \hat{c}_b | i \rangle$$

Many-body matrix element

One-body matrix element

One-body density matrix elements between many-body states

(can also generalize to two-body transition operators)

To get the many-body states, we use the matrix formalism (a.k.a *configuration-interaction)*

$$\hat{\mathbf{H}}|\Psi\rangle = E|\Psi\rangle$$

$$|\Psi\rangle = \sum_{\alpha} c_{\alpha}|\alpha\rangle \qquad H_{\alpha\beta} = \langle\alpha|\hat{\mathbf{H}}|\beta\rangle$$

$$\sum_{\beta} H_{\alpha\beta} c_{\beta} = E c_{\alpha} \quad \text{if} \quad \langle\alpha|\beta\rangle = \delta_{\alpha\beta}$$

Issues:

$$\sum_{\beta} H_{\alpha\beta} c_{\beta} = E c_{\alpha} \qquad |\Psi\rangle = \sum_{\alpha} c_{\alpha} |\alpha\rangle$$

- Origin of Hamiltonian matrix elements

Semi-phenomenological vs. *ab initio*
(fit to *A*-body vs. fit to few-body)

- Representation and selection of basis

(basis "scheme" and model space)

- Computation with Hamiltonian matrix element

Storage vs. construction "on-the-fly"

Modern many-body calculations

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No-core shell model: in harmonic oscillator basis, "all" particles active (up to N_{max} h.o. excitation quanta), with high-precision interaction (e.g. chiral EFT, HOBET, etc.) fit to *few-body* data

e.g. *p*-shell nuclides up to N_{max} = 10 … 22

Ab initio/ “No-core shell model”: take to infinite limit

Two parameters: h.o. basis frequency Ω
and model space cutoff N_{max}

Naïve expectation: take N_{max} -> infinity
Converged results independent of Ω

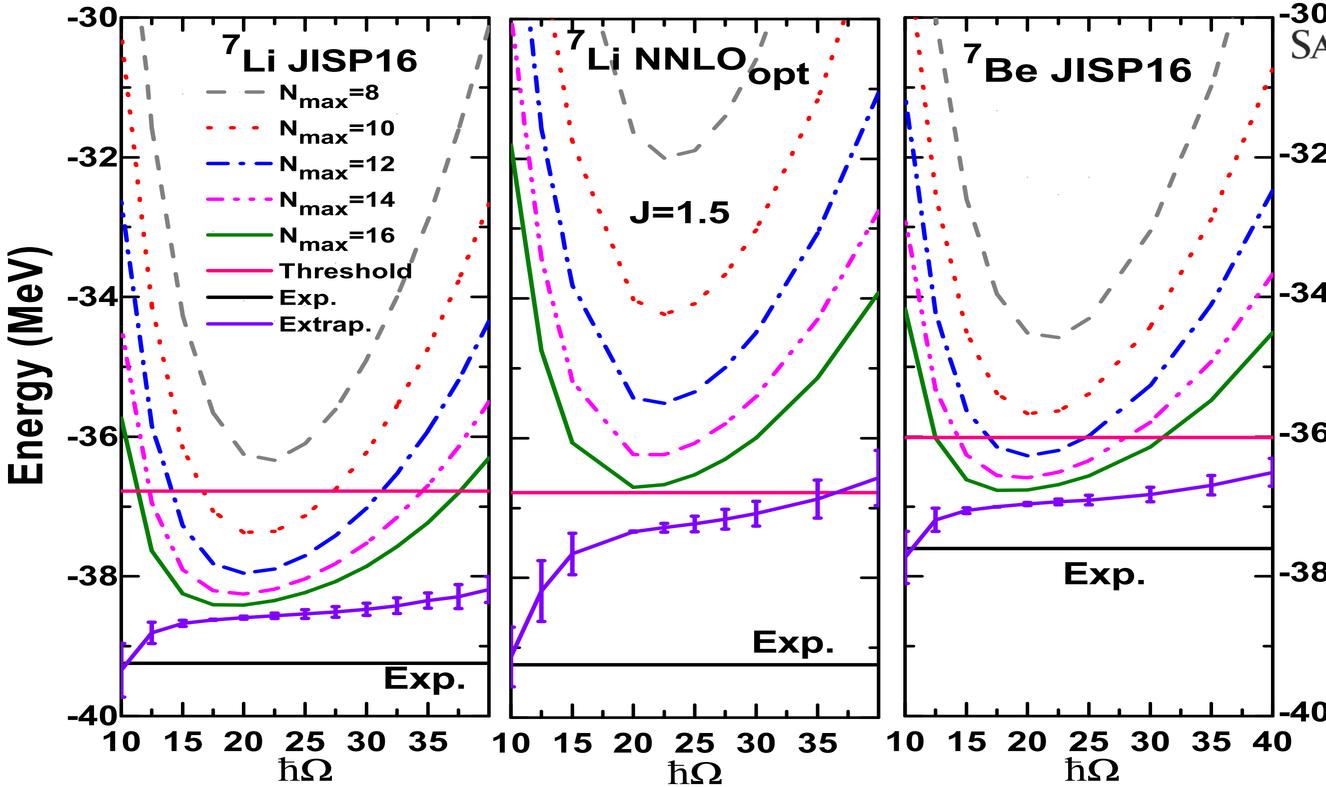

FIG. 1. (Color online) The energy of the ground state (J=$\frac{3}{2}$) for ^{7}Be and ^{7}Li with the JISP16 and NNLO$_{\rm opt}$ interactions as a function of HO energy. In this figure and the following figures, for ^{7}Li and ^{7}Be, the $N_{\rm max}$ value ranges from 8 up to 16. The increment of $N_{\rm max}$ is 2. Extrapolated ground state energies are shown in purple with uncertainties depicted as vertical bars.

From Heng, Vary, Maris: arXiv:1602.00156

Extrapolation via assumed exponential $E(N_{\max}) = E(\infty) + a\exp(-cN_{\max})$

Choice of wave function basis

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One chooses between *a few, complicated states* or *many simple states*

Choice of wave function basis

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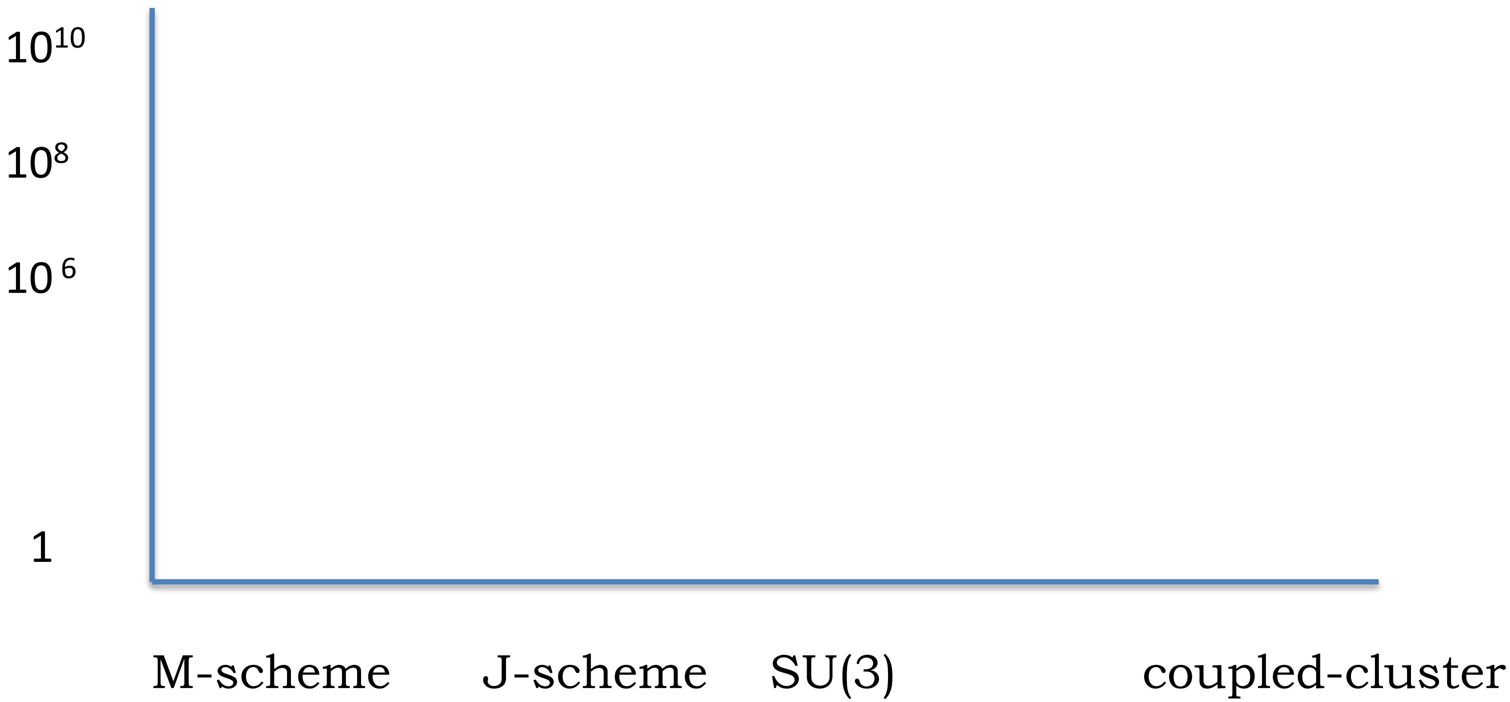

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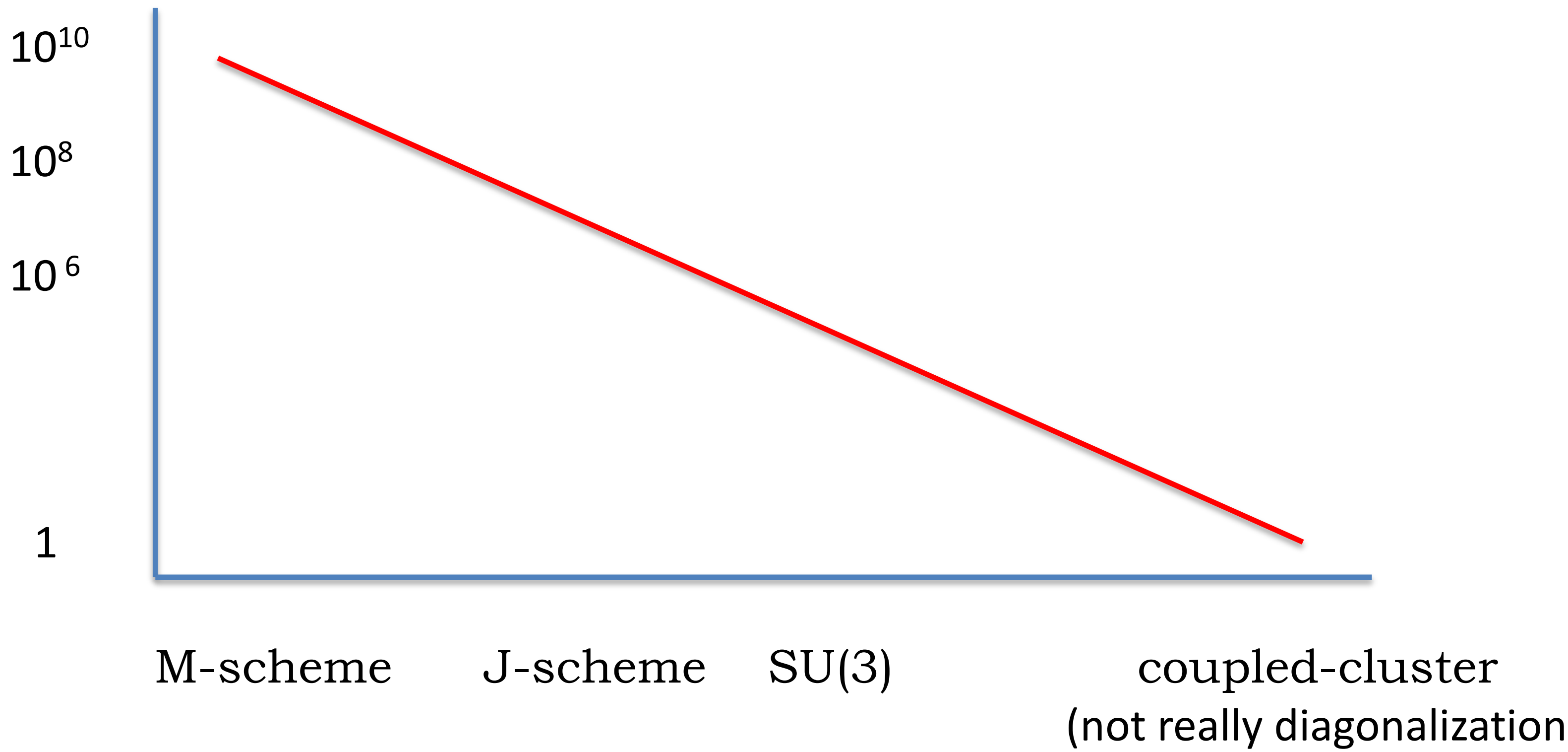

Choice of wave function basis

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One chooses between *a few, complicated states*
or *many simple states*

M-scheme: basis states with fixed total J_z
Simple and easy to construct/work with
Requires large dimension basis

J-scheme: basis states with fixed total J
Enforced rotational symmetry, smaller dimensions
Generally built from *M*-scheme states

Choice of wave function basis

One chooses between *a few, complicated states* or *many simple states*

Symmetry-adapted (SU(3), Sp(3,R), etc):
States from selected group irreps
Enforced symmetries, rotational + translational, smaller dimensions
Often built from *M*-scheme states

It’s also important to know:

Computational burden is *not* primarily the dimension but is the # of nonzero Hamiltonian matrix elements.

$$\sum_{\beta} H_{\alpha\beta} c_{\beta} = E c_{\alpha}$$

J-scheme matrices are smaller but much denser than M-scheme, and "symmetry-adapted" (i.e. SU(3)) matrices are smaller (and denser) still.

example: ^{12}C $N_{max} = 8$

scheme	basis dim
M	0.6×10^9
J (J=4)	9×10^7
SU(3)	9×10^6

(truncated)

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J (J=4)	9×10^7	3×10^{13}
SU(3) (truncated)	9×10^6	2×10^{12}

From Dytrych, et al, arXiv:1602.02965

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scheme	basis dim	# of nonzero matrix elements	
M	0.6×10^9	5×10^{11}	4 Tb of memory!
J (J=4)	9×10^7	3×10^{13}	240 Tb of memory!
SU(3)	9×10^6	2×10^{12}	16 Tb of memory!

(truncated)

From Dytrych, et al, arXiv:1602.02965

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Older codes (e.g., OXBASH) stored nonzero matrix elements on hard drive -> I/O as bottleneck

More recent codes (e.g., MFDn) store nonzero matrix elements in RAM -> requires supercomputer

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Alternate approach: "on-the-fly/factorization" pioneered by ANTOINE code
used by NuShellX, BIGSTICK, KSHELL codes

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Alternate approach: "on-the-fly/factorization"
pioneered by ANTOINE code
used by NuShellX, BIGSTICK, KSHELL codes

"On-the-fly" uses the fact that only two (or three) particles at a time interact; the rest are spectators
-> "loop over spectators"

A description of the "factorization" algorithm:
CWJ, W. Ormand, P. Krastev, Comp. Phys. Comm. **184**, 2761(2013)

J-scheme matrices are smaller but much denser than M-scheme, and "symmetry-adapted" (i.e. SU(3)) matrices are smaller still.

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(truncated)		On-the-fly requires only 43 Gb!	

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Links to free, open-source many-body codes:

fribtheoryalliance.org

In particular `BIGSTICK`, available from:
github.com/cwjsdsu/BigstickPublick

Manual at arXiv:1801.08432

Despite advances, it is easy to get to model spaces beyond our reach:

N_{max} calculations:

^{12}C $N_{max} = 4$ dim 1 million

^{12}C $N_{max} = 6$ dim 30 million

^{12}C $N_{max} = 8$ dim 500 million

^{12}C $N_{max} = 10$ dim 7.8 billion

^{12}C $N_{max} = 12$ dim 81 billion

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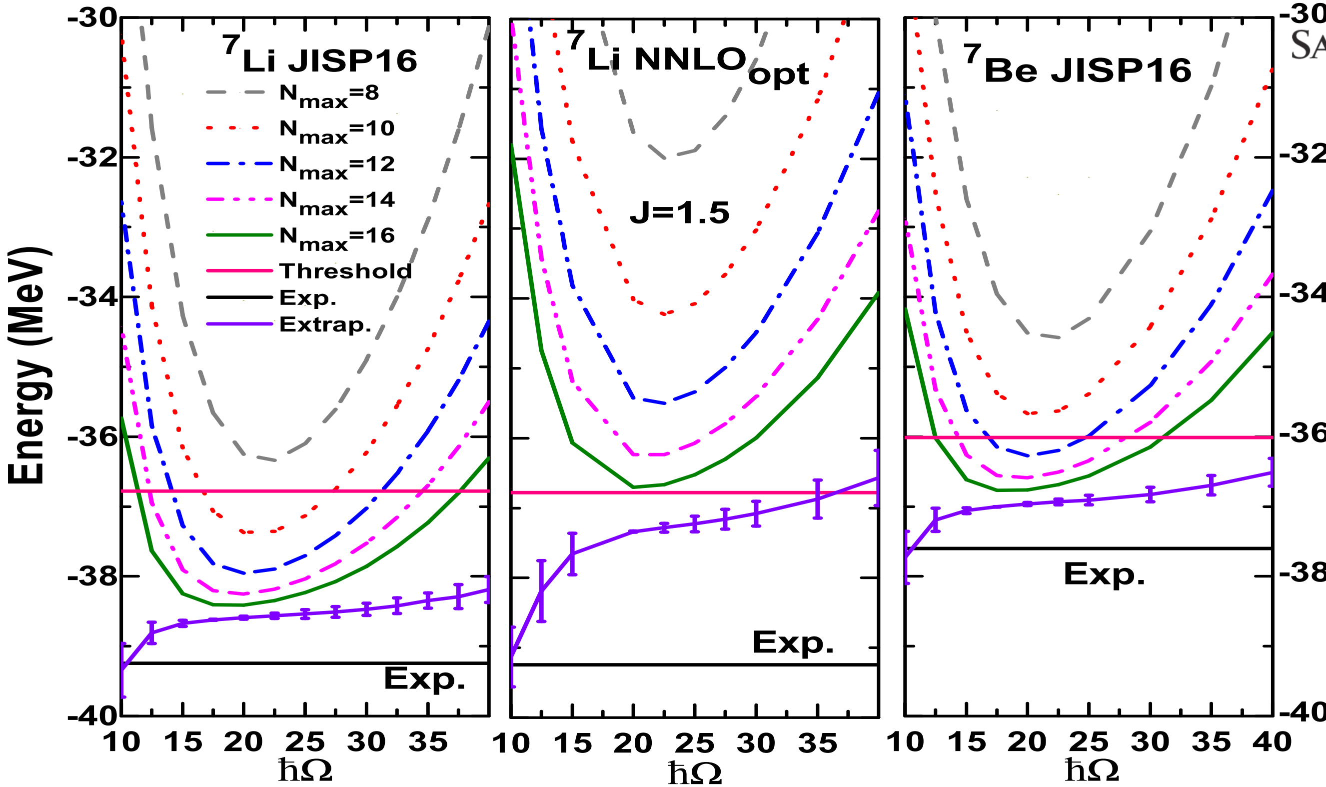
^{12}C $N_{max} = 12$ dim 81 billion

Largest (?) known calculation, ^{6}Li, $N_{max}=22$, 25 billion (Forssen *et al*, arXiv:1712.09951 with `pANTOINE`)



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From Heng, Vary, Maris: arXiv:1602.00156

Extrapolation via assumed exponential $E(N_{\rm max}) = E(\infty) + a\exp(-cN_{\rm max})$

Paths for going forward/upwards:

-- Human learning, part I: Infrared extrapolation

-- Human learning, part II: The right degrees of freedom ("symmetry-adapted bases")

-- Human learning, part III: The right degrees of freedom: natural orbitals

-- Machine learning

Paths for going forward/upwards:

-- Human learning, part I: Infrared extrapolation

Idea: truncation in h.o. space (N_{max}) = "wall"
Extrapolate as "wall" -> infinity (infrared limit)

e.g., S. More *et al* Phys. Rev. C 87, 044326 (2013)

(also need convergence in ultraviolet (UV) limit)

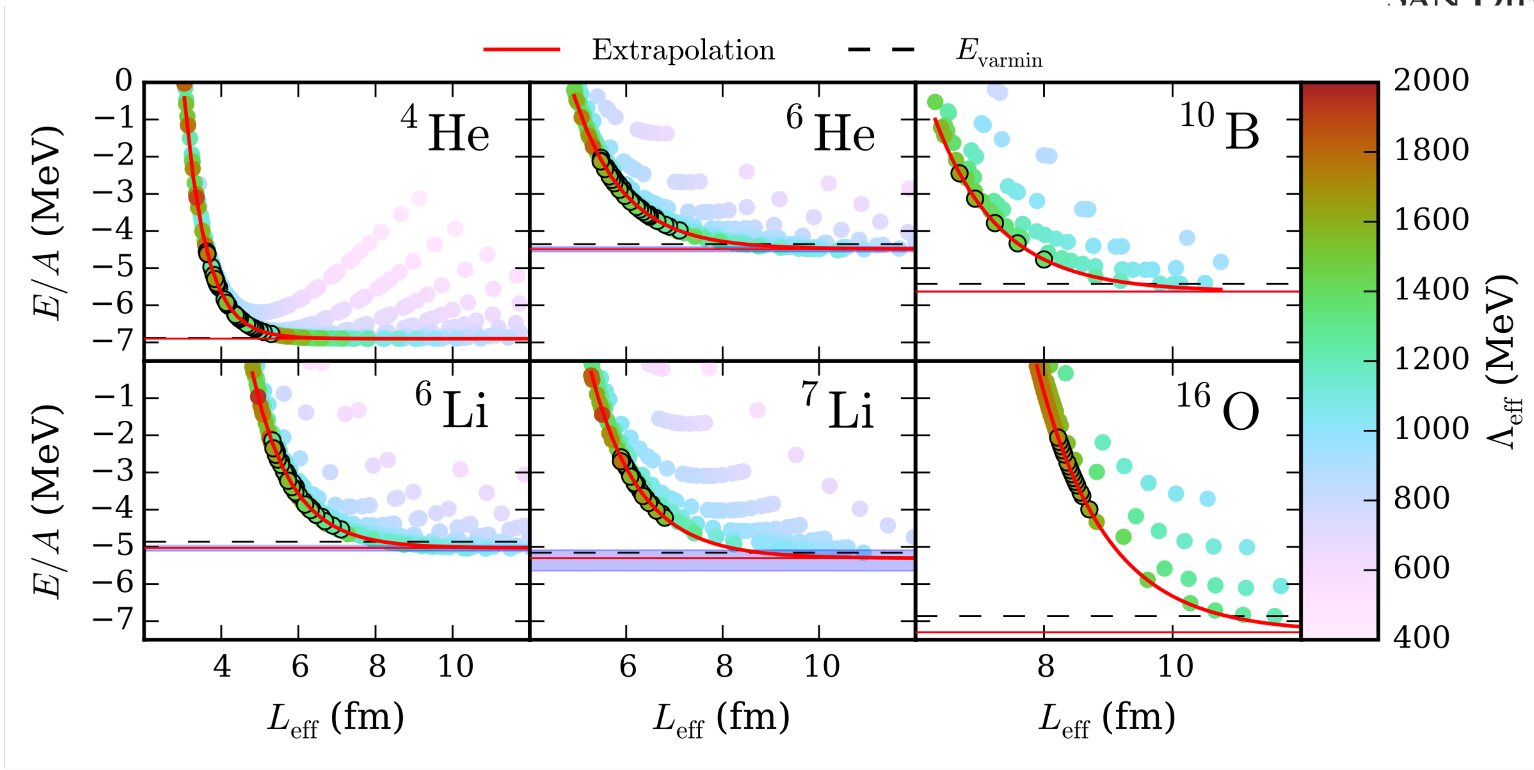


FIG. 4. (Color online) Extrapolations of the binding energy per particle for several p-shell nuclei computed with the NCSM. The color of each circular marker indicates the UV cutoff of that calculation with darker colors corresponding to larger cutoffs. Markers with a black border are included in the extrapolation. The solid red (gray) curve shows the exponential fit (16), and the horizontal red (gray) line marks the value of E_∞ with uncertainty estimates indicated as blue (gray) bands. The dashed black line marks the variational minimum E_{varmin} for the largest model space included in the fit.

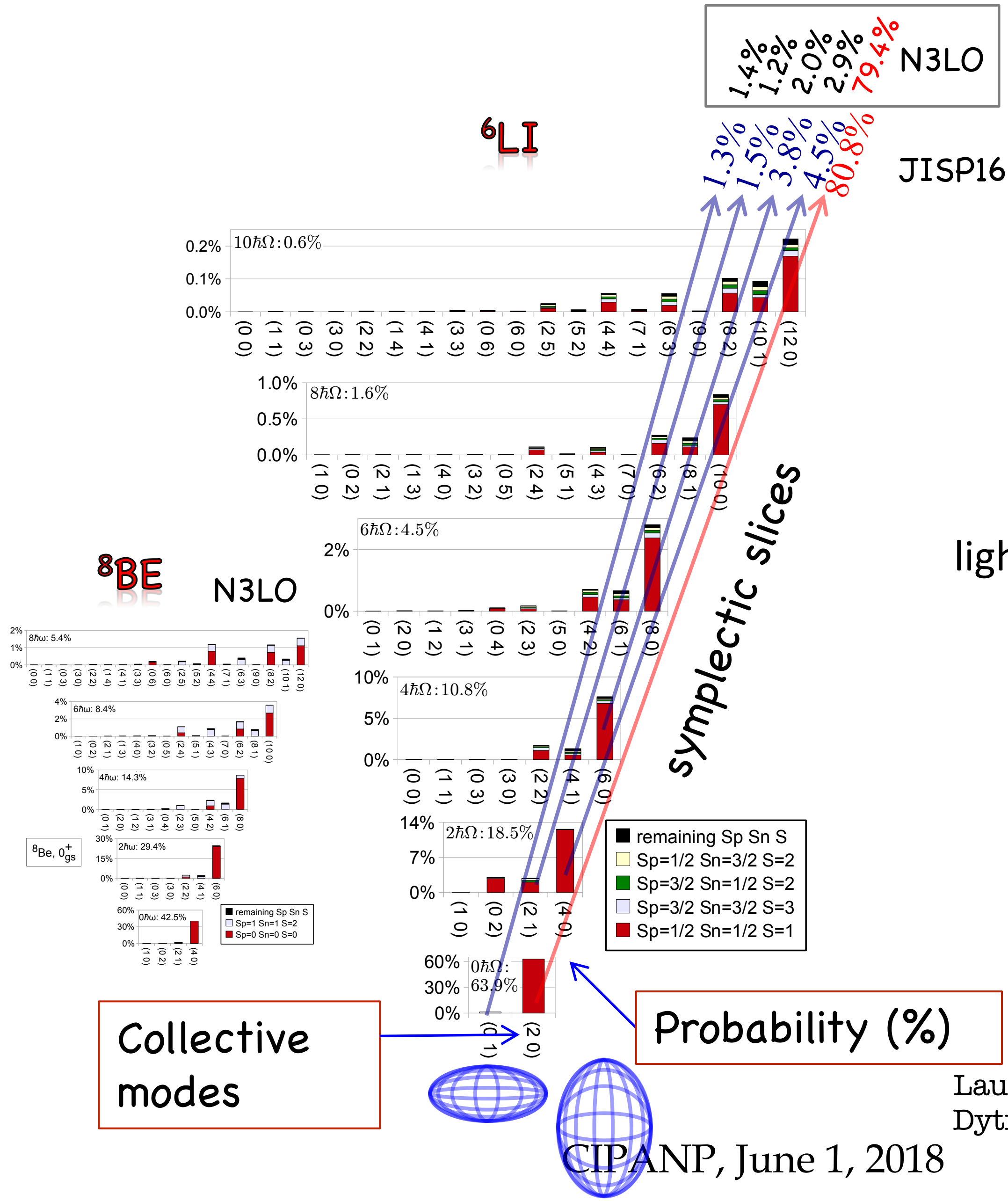
From Wendt *et al*, Phys. Rev. C 91, 061301 (2015)

Paths for going forward/upwards:

-- Human learning, part II: The right degrees of freedom, **“symmetry-adapted bases”**

Symplectic Sp(3,R) Symmetry

(From K. Launey, LSU)



From first principles: light/intermediate-mass nuclei, low-lying states

Launey et al., Prog. Part. Nucl. Phys. 89 (2016) 101
Dytrych et al., Phys. Rev. Lett. 111 (2013) 252501

Collectivity features

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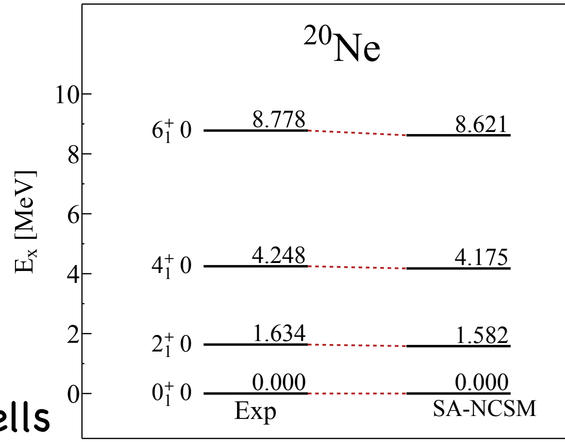
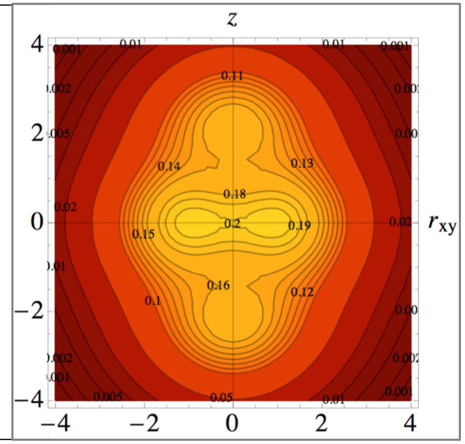
20NE





13 shells

SA-NCSM (selected model space): 50 million SU(3) states

Complete model space: 1000 billion states

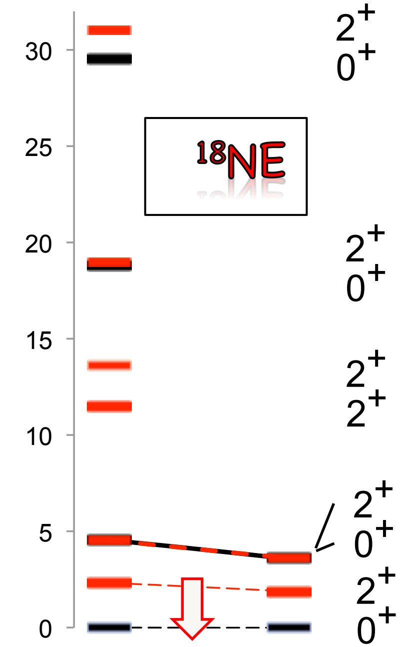
Ne & Mg isotopes

^{18}Ne, B(E2: $2^+ \to 0^+$)

Experiment……… 17.7(18) W.u.

9 shells …………… 1.13 W.u.

33 shells ………….. 13.0(7) W.u.
(no effective charges)



N2LOopt; 9 shells, ħω = 15 MeV

Grigor Sargsyan, PhD student, LSU

CIPANP, June 1, 2018

Paths for going forward/upwards:

-- Human learning, part III: The right degrees of freedom: **natural orbitals**

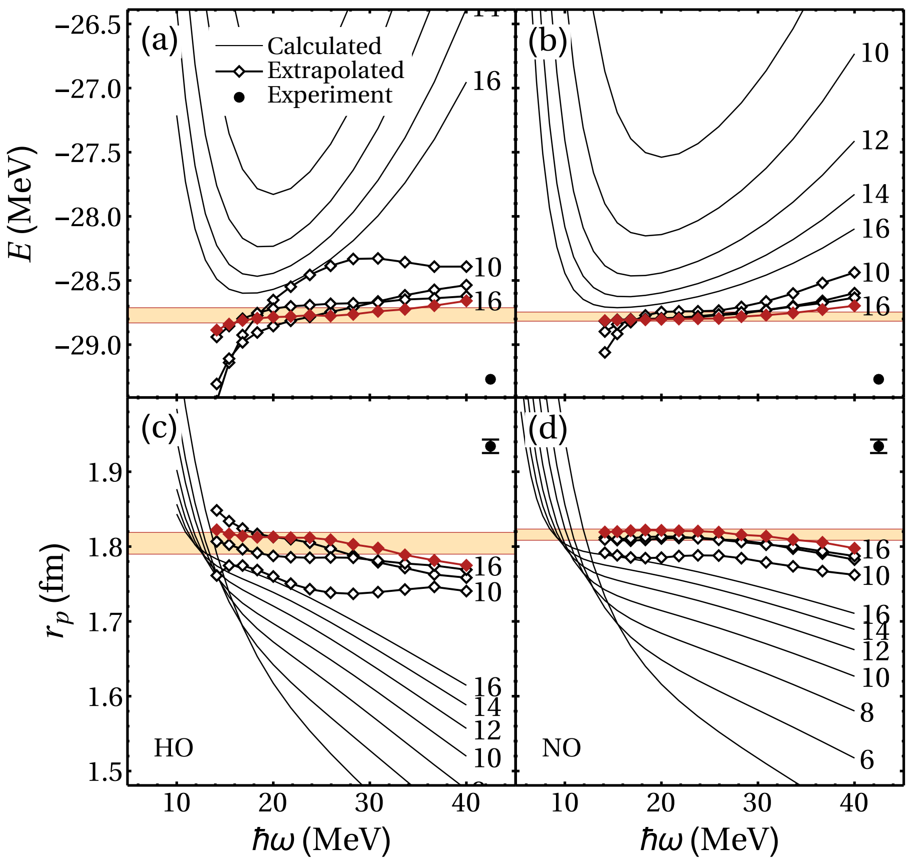
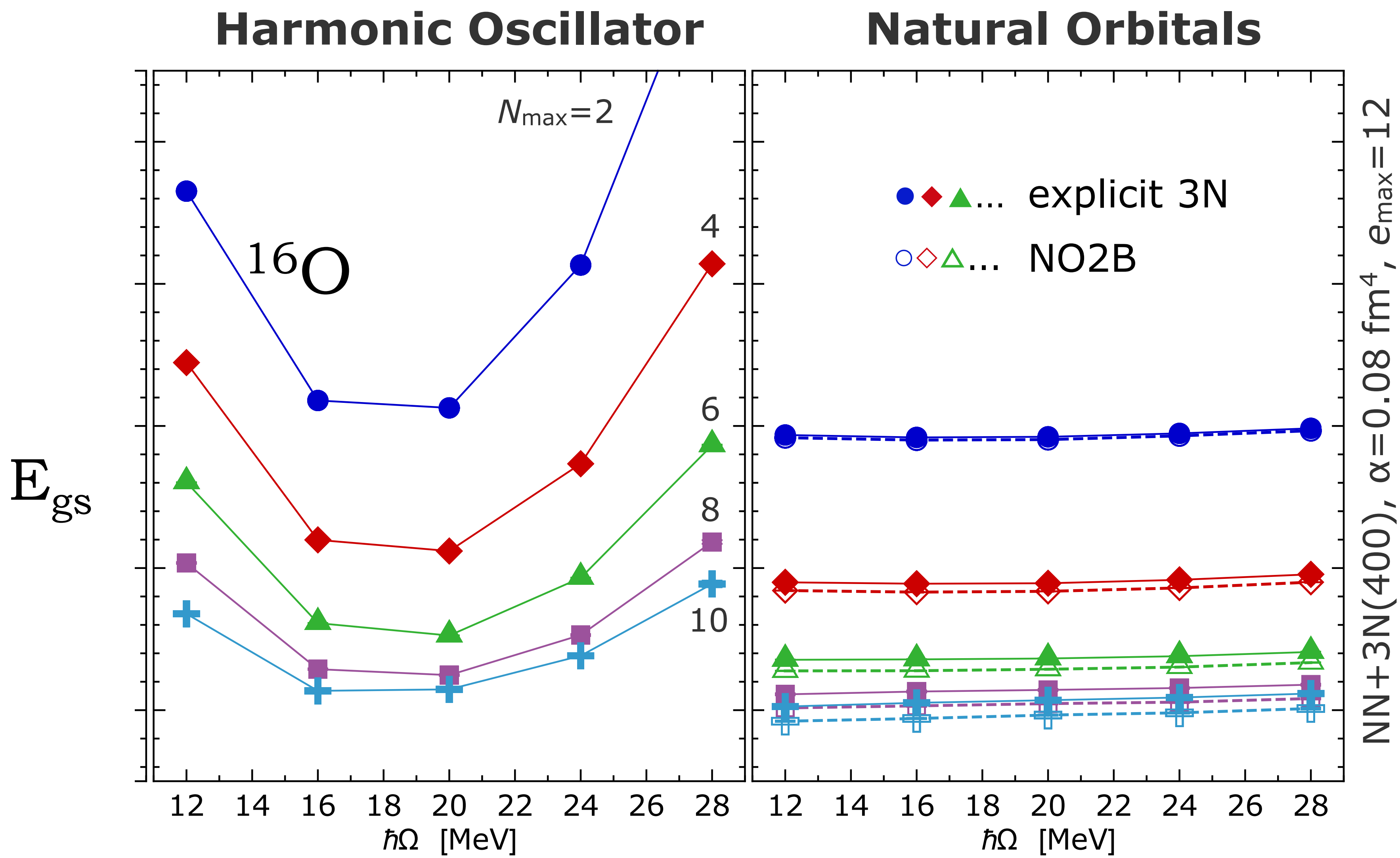


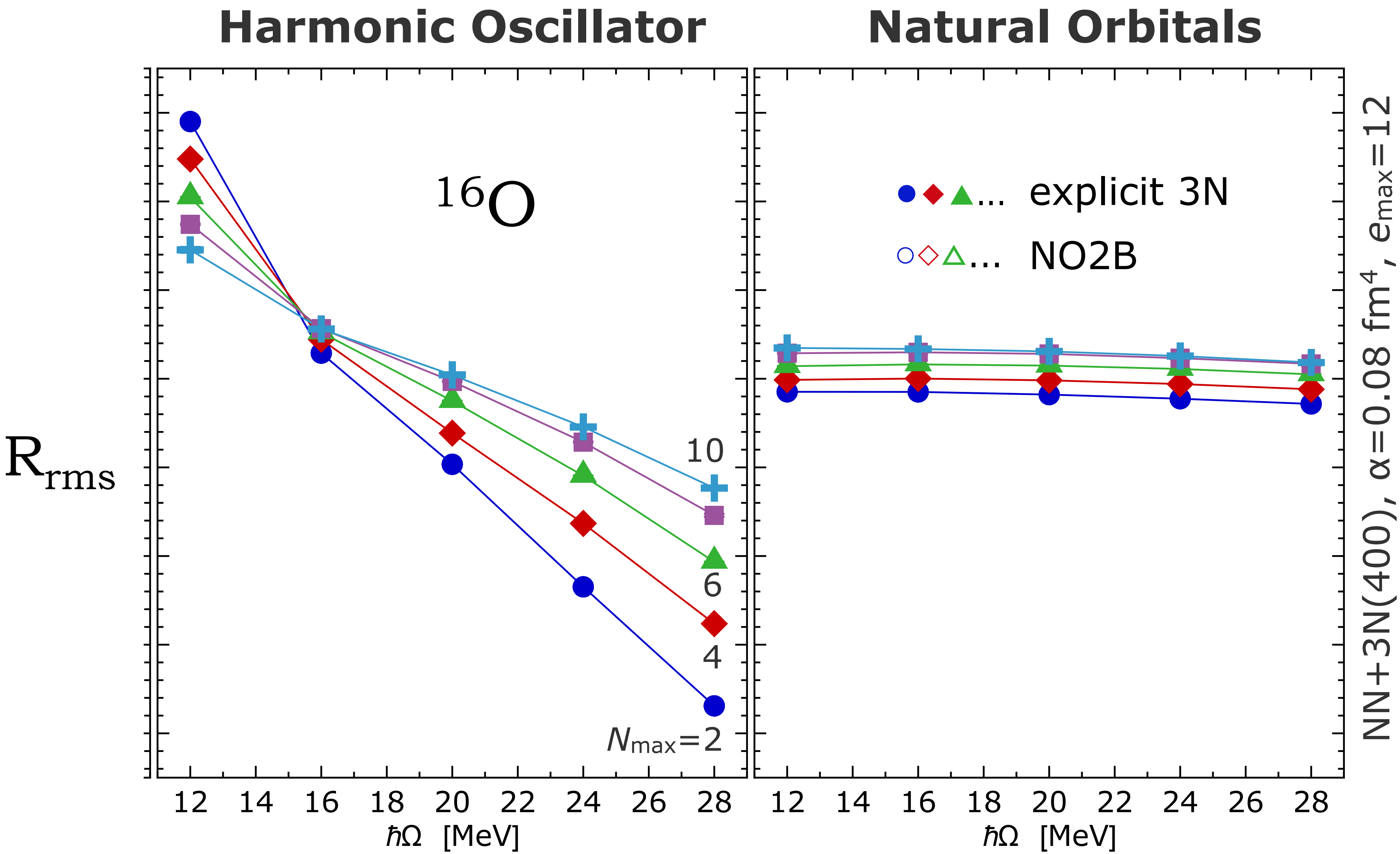
FIG. 4: Infrared basis extrapolations for the ^{6}He ground state energy (top) and point proton radius (bottom), based on calculations in the harmonic oscillator basis (left) and natural orbital basis (right). The extrapolations (diamonds) are shown along with the underlying calculated results (plain lines) as functions of $\hbar\omega$ at fixed $N_{\max}$ (as indicated). Experimental values (circles) are shown with uncertainties. The shaded bands reflect the mean values and standard deviations of the extrapolated results, at the highest $N_{\max}$, over the $\hbar\omega$ range considered.

From Constantinou *et al*,

arXiv:1605.04976



From R. Roth, talk at TRIUMF, Feb 2018



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Paths for going forward/upwards:

-- Machine learning

-- Machine learning

From Negoita *et al*, arXiv:1803.03215

Extrapolation via Artificial Neural Net (ANN)

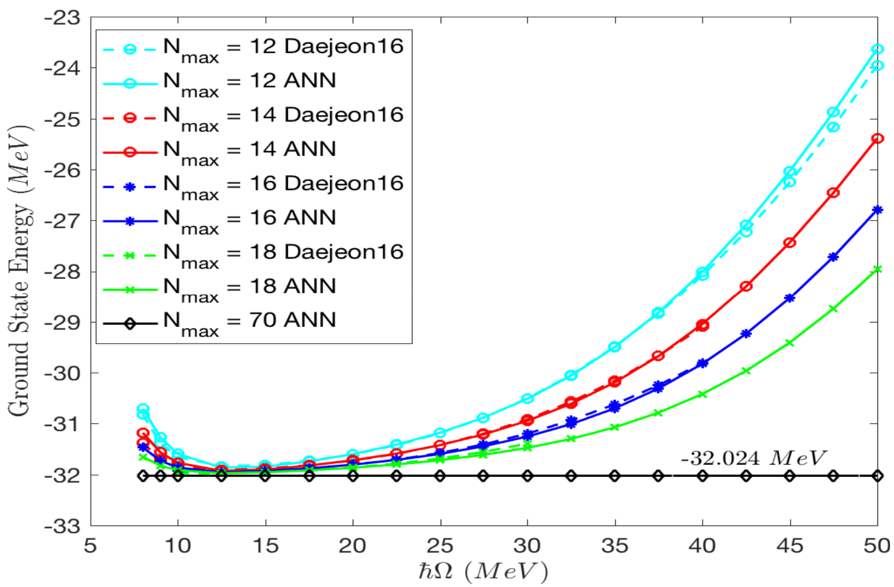

Figure 7. Comparison of the NCSM calculated and the corresponding ANN predicted gs energy values of ^{6}Li as a function of $\hbar\Omega$ at $N_{\max} = 12, 14, 16$, and 18. The lowest horizontal line corresponds to the ANN nearly converged result at $N_{\max} = 70$.

-- Machine learning

From Negoita *et al*, arXiv:1803.03215

Extrapolation via Artificial Neural Net (ANN)

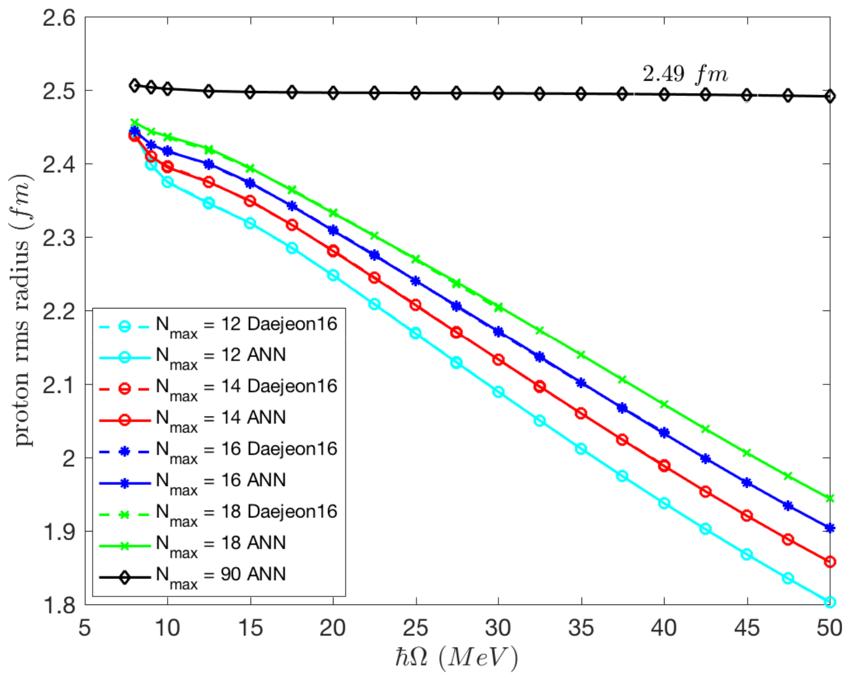

Figure 9. Comparison of the NCSM calculated and the corresponding ANN predicted gs point proton rms radius values of ^{6}Li as a function of $\hbar\Omega$ for $N_{\rm max} = 12, 14, 16$, and 18. The highest curve corresponds to the ANN nearly converged result at $N_{\rm max} = 90$.

Summary:

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Modern nuclear structure physics is **modern** and a vigorous, rigorous discipline, **necessary** for many other fields (astrophysics, tests of fundamental symmetries, etc.)

One approach is **diagonalization of the Hamiltonian in a basis.** Modern techniques and computers can handle up to ~ 25 billion basis states (though that is is not the primarily measure of computational burden) and there are many promising techniques for extending the reach and accuracy of *ab initio* calculations

Additional slides

Modern many-body calculations

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Semi-Phenomenological: usually for medium- to heavy-mass nuclei, with fixed core, with well-tuned (to *A-body* spectra) interaction

e.g. *sd* shell with USDB interaction
pf shell with GX1A interaction

No-core shell model: in harmonic oscillator basis, "all" particles active (up to N_{max} h.o. excitation quanta), with high-precision interaction (e.g. chiral EFT, HOBET, etc.) fit to *few-body* data

e.g. *p*-shell nuclides up to N_{max} = 10 … 22

Modern many-body calculations

"*Ab initio* medium/heavy nuclei"

~~Semi-Phenomenological~~: usually for medium- to heavy-mas[...]lei, with fixed core, with well-tuned [...] interaction

In-medium similarity renormalization group, etc

e.g. *sd* shell wi[...]

pf shell wi[...]

No-core shell model: in harmonic oscillator basis, "all" particles active (up to N_{max} h.o. excitation quanta), with high-precision interaction (e.g. chiral EFT, HOBET, etc.) fit to few-body data

e.g. *p*-shell nuclides up to N_{max} = 10 to 22

Despite advances, it is easy to get to model spaces beyond our reach:

sd shell: max dimension 93,000. *Can be done in a few minutes on a laptop.*

pf shell: ^{48}Cr, dim 2 million, ~10 minutes on laptop
^{52}Fe, dim 110 million, a few hours on modest workstation
^{56}Ni, dim 1 billion, 1 day on advanced workstation
^{60}Zn, dim 2 billion, < 1 hour on supercomputer

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Despite advances, it is easy to get to model spaces beyond our reach:

shells between 50 and 82 ($0g_{7/2}$ 2s1d $0h_{11/2}$)

^{128}Te: dim 13 million (laptop)

^{127}I: dim 1.3 billion (small supercomputer)

^{128}Xe: dim 9.3 billion (supercomputer)

^{129}Cs: dim 50 billion (haven't tried!)

SOME SHELL-MODEL CODES

Matrix storage:
Oak Ridge-Rochester (small matrices)
Glasgow-Los Alamos (M-scheme, stored on disk; introduced Lanczos)
OXBASH /Oxford-MSU (J-scheme, stored on disk)
MFDn/ Iowa State (M-scheme, stored in RAM)
MCSM/ Tokyo (J-scheme from selected states)
Importance Truncation SM/Darmstadt (M-scheme from selected states)
Sym Adapted SM / LSU, Notre Dame (J-scheme + symplectic)

Factorization:
ANTOINE Strasbourg (M-scheme; originator of factorization)
NATHAN Strasbourg (J-scheme)
EICODE (J-scheme)
NuShell/NuShellX (J-scheme)
MSHELL64 / KSHELL Tokyo (M-scheme)
BIGSTICK/ SDSU-Livermore