

Overview of bound-state many-body methods

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FRIB-TA Workshop on "From Bound states...to the continuum", June 11, 2018



Welcome to the workshop!



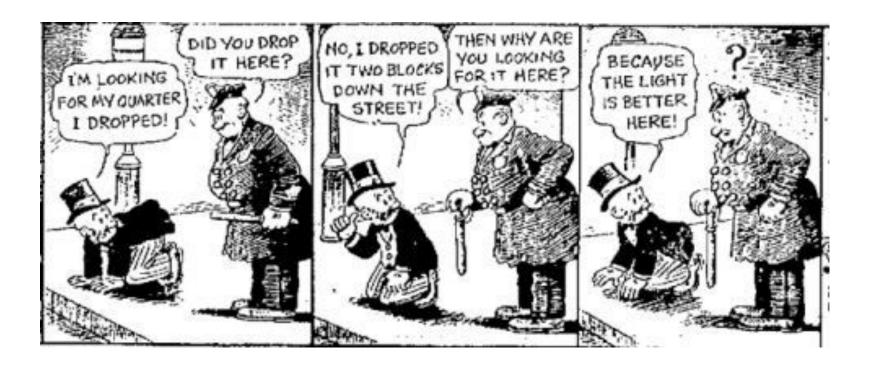
Welcome to the workshop!

Thank you to co-organizers:

(Pierre Descouvemont), **Kristina Launey,** (Dean Lee), Marek Płoszajczak, Sofia Quaglioni, and Jimmy Rotureau

Filomena Nunes for wise advice Gillian Olson for administrative help









Theory





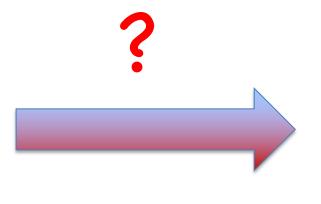
Theory



Experiment









Theory

Experiment









...and what is left in darkness.

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What is



Bound state methods

A 'tasting menu' of methods (may leave some out, sorry!)

- Variational + Green Function Monte Carlo (GFMC)
- Coupled clusters (CC)
- Basis diagonalization ~configuration-interaction no-core shell model (NCSM), beyond mean-field (BMF)
- Energy density functionals (EDF)

Other methods:

- Few body: Faddeev, hyperspherical harmonic (HH)
- Monte Carlo lattice
- Effective-field-theory (EFT)-like
- ...?







- * square integrable wave functions, vanish as $r \rightarrow infinity$
- * straightforward normalization and interpretation of matrix elements
- * many different approaches, can benchmark against each other (GFMC vs CC vs NCSM vs HH)





Ideal framework (for strong correlations) is in relative (Jacobi) coordinates, i.e., HH methods.

Bound state methods



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Bound state methods

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Work in lab frame (single-particle coordinates) makes antisymmetry easier, but



Ideal framework is in relative (Jacobi) coordinates, i.e., HH methods.

Antisymmetry restricts this to about 6 particles

Work in lab frame (single-particle coordinates) makes antisymmetry easier, but

- Center-of-mass motion must be dealt with
- Must work hard to build in correlations





- Tails of wave functions often problematic (should fall off as $\exp(-\kappa E)$, $\kappa^2 \sim \text{separation energy}$
- -> state dependent tails

Choice of wave function basis

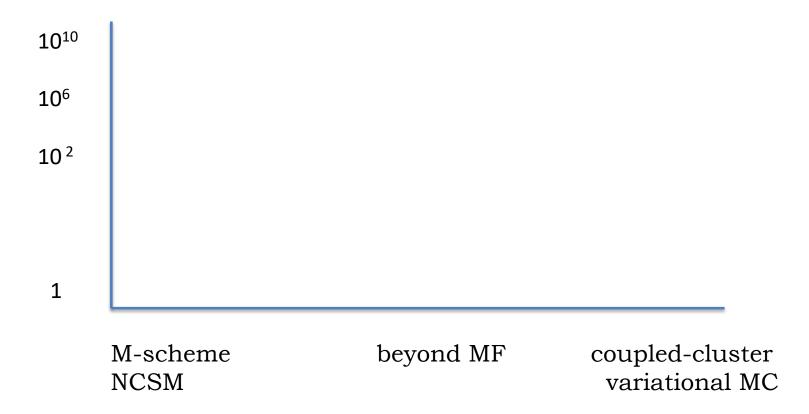


One chooses between a few, complicated states or many simple states

Choice of wave function basis



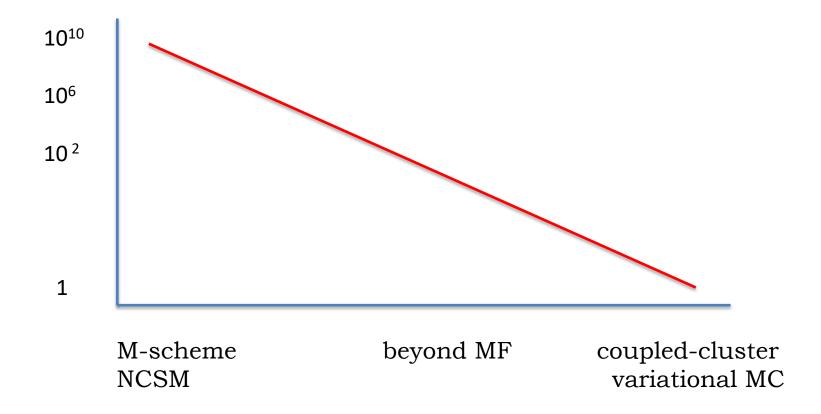
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Correlations



Another set of descriptions are *short-range* vs. *long-range* correlations (e.g., deformation)

Explicit short-range correlations

Long-range correlations

Correlations

Explicit

short-range correlations



Another set of descriptions are *short-range* vs. *long-range* correlations (e.g., deformation)

VMC/
GFMC
CC

NCSM

BMF

Long-range correlations



Most many-body methods for beyond A ~ 6 use single-particle framework, that is,

start from *Slater determinant(s):* antisymmetric products of single particle wave functions

- \rightarrow arises out of
 - (a) mean-field picture
 - (b) power of creation/annihilation operator formalism
 - (c) lack of imagination for anything else



Product wavefunction ("Slater Determinant")

$$\Psi(\vec{r}_1, \vec{r}_2, \vec{r}_3 \dots) = \phi_{n_1}(\vec{r}_1)\phi_{n_2}(\vec{r}_2)\phi_{n_3}(\vec{r}_3)\dots\phi_{n_N}(\vec{r}_N)$$

Each many-body state can be *uniquely* determined by a list of "occupied" single-particle states = "occupation representation"

$$|\alpha\rangle = \hat{a}_{n_1}^+ \hat{a}_{n_2}^+ \hat{a}_{n_3}^+ \dots \hat{a}_{n_N}^+ |0\rangle$$



Variational Monte Carlo (VMC)

| Ψ > = Slater determinant x two-body correlation ("Jastrow-like") functions $f(r_i-r_i)$

→ Large dimensional integrals, evaluated by MC

minimize
$$\frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$



Green Function / Diffusion MC (GFMC)

Starting from VMC wave function $| \Psi >$, evolve in imaginary time

$$\exp(-H\tau) \mid \Psi >$$
.



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"Gold standard" in *ab initio* calculations for light nuclei (A < 16)

Can handle 'hard core' potentials e.g. Argonne V18





Green Function / Diffusion MC (GFMC)

Starting from VMC wave function $| \Psi \rangle$, evolve in imaginary time

Non-local potentials troublesome.

 $\exp(-H\tau) \mid \Psi >$.



3-body handled perturbatively

Need all spin-isospin components, limited to A < 16 (alternate: Auxiliary-field DMC to handle spin-isospin fluctuations)

Excited states difficult

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<u>Coupled clusters.</u> Starting from Slater determinant, apply "cluster" operator and minimize energy:

$$\mid \Psi \rangle = \exp(T) \mid SD \rangle$$
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- Can handle "bare"/hard core interactions up many shells → short range correlations
- Nonlocal interactions no problem
- Polynomial scaling of work (linked diagrams only)



<u>Coupled clusters.</u> Starting from Slater determinant, apply "cluster" operator and minimize energy:

$$\mid \Psi \rangle = \exp(T) \mid SD \rangle$$
.

- Works best at or near closed shells
- Excited states difficult





Basis diagonalization

Expand wave function in (orthonormal) basis

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

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

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



Basis diagonalization

Expand wave function in (orthonormal) basis

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



- Works well away from closed shells
- Excited states arise naturally
- Can handle wide variety of forces



Basis diagonalization

Expand wave function in (orthonormal) basis

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

- Work grows exponentially (must cancel linked diagrams)→ limited number of shells/short range correlations
- → often prefer "softened" forces for better convergence





Energy density functionals

Minimize Kohn-Sham density functional E(ρ)

Related: Hartree-Fock (-Bogoliubov), beyond Mean-Field such as RPA, generator coordinate



Energy density functionals

Minimize Kohn-Sham density functional E(ρ)



- Broadest application: works throughout the chart of nuclides
- Naturally handles deformation and (if in Bogoliubov-type extension) pairing
- "In principle" exact via Kohn-Sham theorem
- Implicitly includes correlations



Energy density functionals

Minimize Kohn-Sham density functional E(ρ)

- Excited states generally require BMF methods
- BMF methods generally require refit of functional
- Kohn-Sham tells us functional exists, not how to find it



Slouching towards the continuum



An incomplete overview of strategies to connect bound states to scattering states:

- Exact/full treatment: Faddeev/hyperspherical harm.
- Change boundary conditions: complex basis methods (e.g., Gamow basis), also used in GFMC talks by Nazarewicz, Fossez, Xu, Hu, Ploszajczk, Barrett
- Discretize continuum: J-matrix, LIT, Luscher cf. talks by Shirokov, Koenig, Zhang
- Embed BS in continuum: NCSMC, EFT, effective "optical potential" cf. talks by Quaglioni, Elster, Rotureau, Rupak, Idini



A deep dive into basis diagonalization



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 $N_{max} = 10 \dots 22$



"Ab initio medium/heavy nuclei" Semi-Phenomenological: usually for

medium- to heavy-massive, with fixed core,

with well-tuned interaction In-medium

similarity

e.g. sd shell wit renormalization pf shell wit group, etc

cf talk by H. Hergert

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



A deep dive into basis diagonalization

- Easy to understand and flexible
- Works well away from closed shells, easily generates excited states



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Extend applicability of diagonalization





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- Works well away from closed shells, easily generates excited states
- 'Unlinked diagrams' → exponential (not polynomial) growth in work → limited model space

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Extend applicability of diagonalization



A deep dive into basis diagonalization

Some strategies

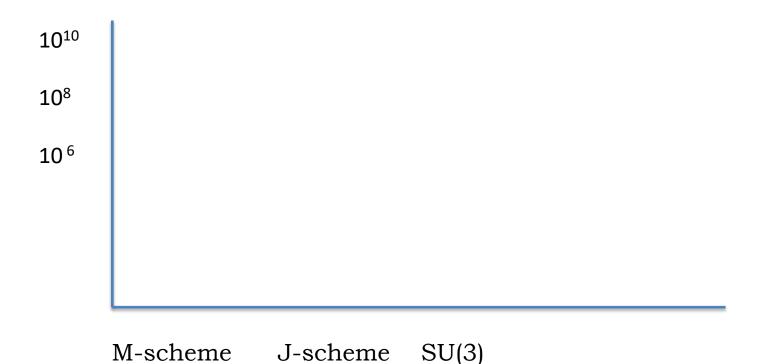
- More efficient representation: Symmetry-adapted (SA) basis, on-the-fly Hamiltonian
- Some basis states are more important that others: SA basis, importance truncated basis, MC shell model
- Use better basis states: natural orbitals, SA basis
- Use better *extrapolation*: IR/UV extrapolation, natural orbitals, machine learning



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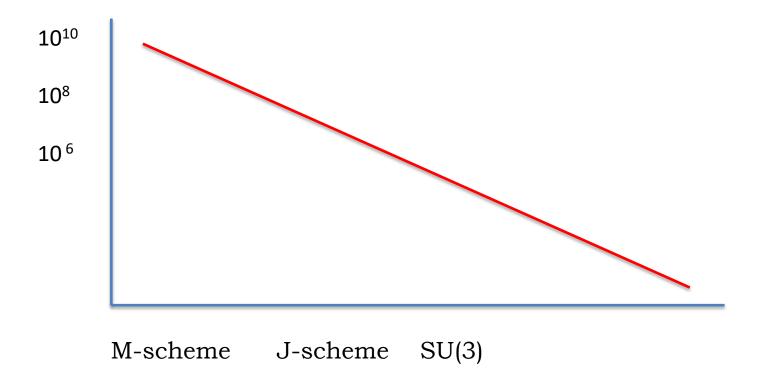


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M-scheme: basis states with fixed total J_z Simple and easy to construct/work with Requires large dimension basis

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



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

See talks by Caprio, Mercenne, Launey,



It's also important to know:

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

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



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

scheme basis dim

M 0.6×10^9

 $J (J=4) 9 \times 10^7$

SU(3) 9 x 10⁶

(truncated)



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

scheme basis dim # of nonzero matrix elements

M 0.6×10^9 5×10^{11}

J (J=4) 9 x 10⁷ 3 x 10¹³

SU(3) 9×10^6 2×10^{12}

(truncated)

From Dytrych, et al, arXiv:1602.02965



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

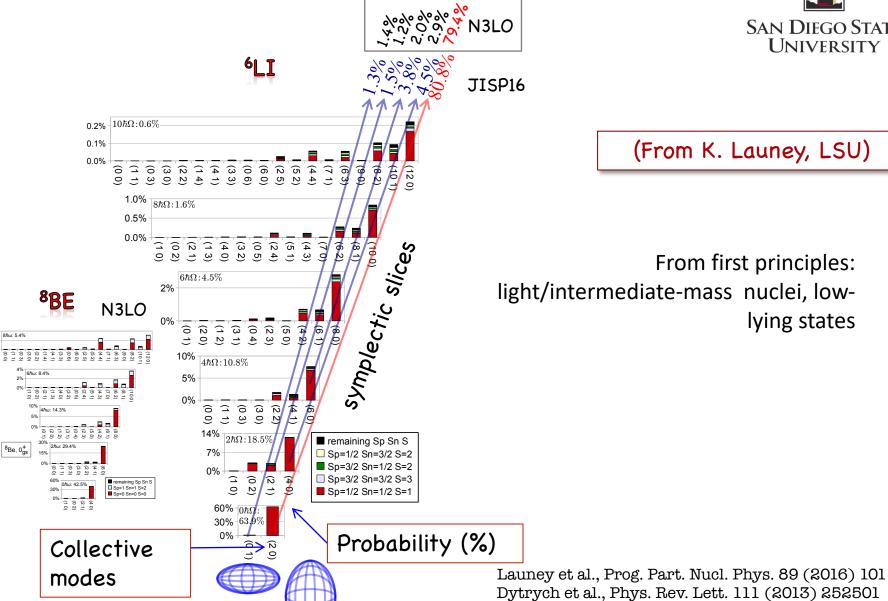
scheme basis dim # of nonzero matrix elements M 0.6×10^9 5×10^{11} 4 Tb of memory! J (J=4) 9×10^7 3×10^{13} 240 Tb of memory! SU(3) 9×10^6 2×10^{12} 16 Tb of memory!

(truncated)

From Dytrych, et al, arXiv:1602.02965

Symplectic Sp(3,R) Symmetry

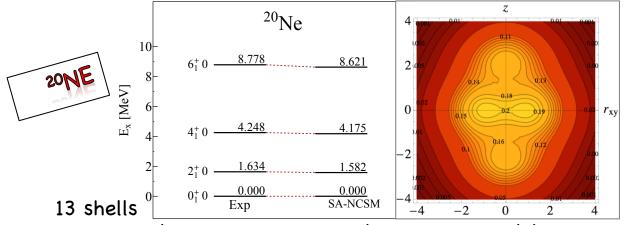




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Collectivity features





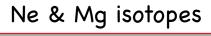
SA-NCSM (selected model space): 50 million SU(3) states

Complete model space: 1000 billion states

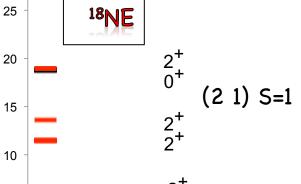
Experiment....... 17.7(18) W.u.

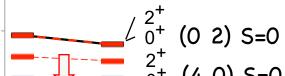
9 shells 1.13 W.u.

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









N2LOopt; 9 shells, $\hbar\omega$ = 15 MeV

Grigor Sargsyan, PhD student, LSU

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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



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)



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

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)		On-the-fly requires only 43 Gb!	

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

TE



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

fribtheoryalliance.org

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

Manual at arXiv:1801.08432



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

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



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

¹²⁸Te: dim 13 million (laptop)

¹²⁷I: dim 1.3 billion (small supercomputer)

¹²⁸Xe: dim 9.3 billion (supercomputer)

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



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



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

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

Modern many-body calculations



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 $N_{max} = 10 \dots 22$



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

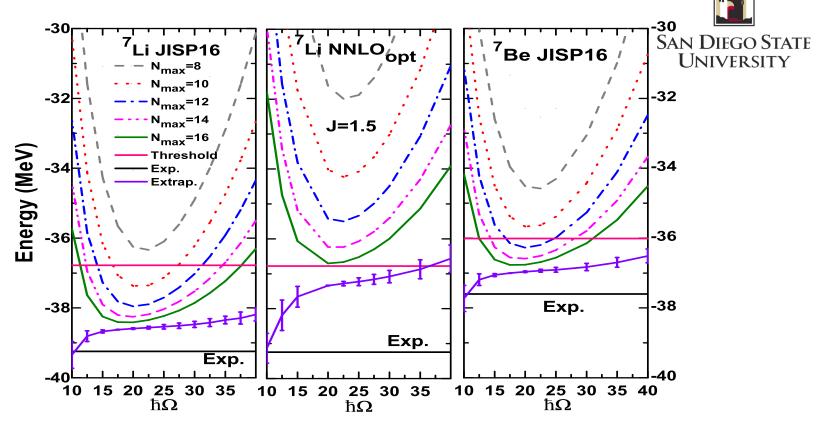


FIG. 1. (Color online) The energy of the ground state $(J=\frac{3}{2})$ for ⁷Be and ⁷Li with the JISP16 and NNLO_{opt} interactions as a function of HO energy. In this figure and the following figures, for ⁷Li and ⁷Be, the N_{max} value ranges from 8 up to 16. The increment of N_{max} is 2. Extrapolated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

From Heng, Vary, Maris: arXiv:1602.00156 Extrapolation via assumed exponential $E(N_{\text{max}}) = E(\infty) + a \exp(-cN_{\text{max}})$



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)



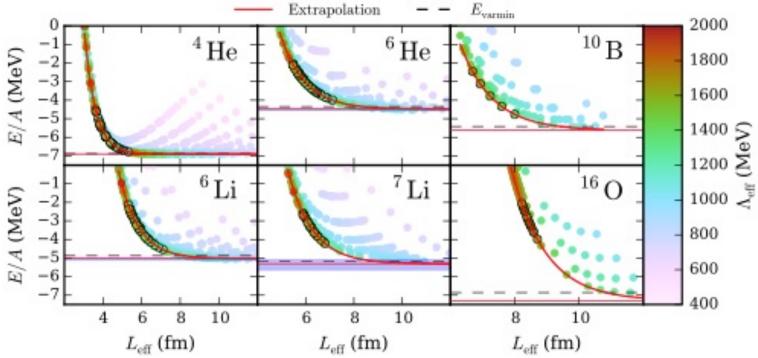


FIG. 4. (Color online) Extrapolations of the binding energy per particle for several p-shell nuclei computed with the NCSM. The color of each circular marker indicates the UV cutoff of that calculation with darker colors corresponding to larger cutoffs. Markers with a black border are included in the 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 III: The right degrees of freedom: **natural orbitals**

see talk by Fasano

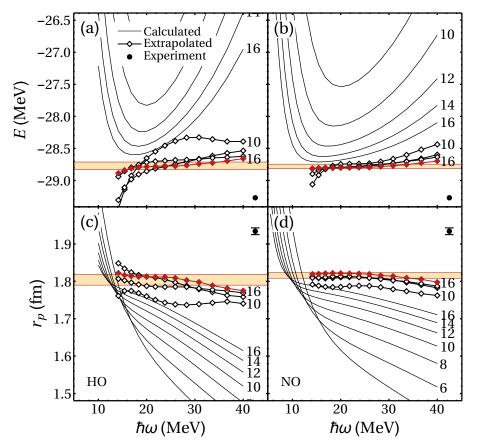


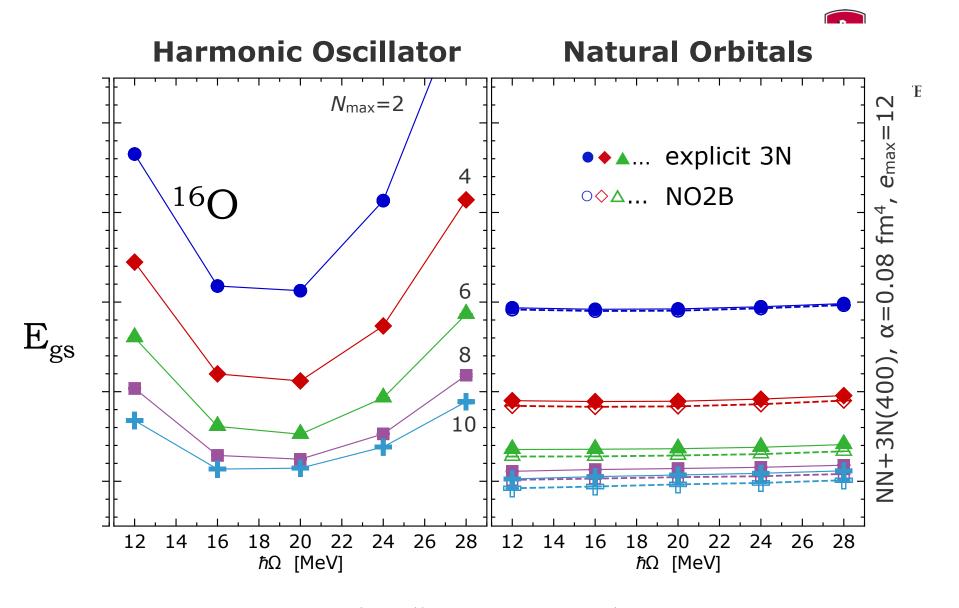
FIG. 4: Infrared basis extrapolations for the 6 He ground state energy (top) and point proton radius (bottom), based on calculations in the harmonic oscillator basis (left) and natural orbital basis (right). The extrapolations (diamonds) are shown along with the underlying calculated results (plain lines)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



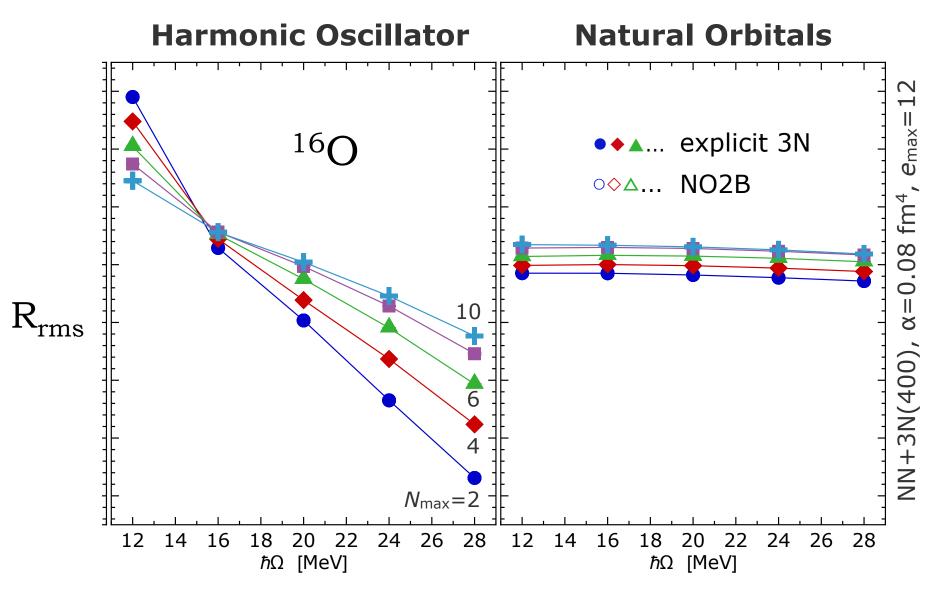
From Constantinou *et al*,

arXiv:1605.04976

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From R. Roth, talk at TRIUMF, Feb 2018



From R. Roth, talk at TRIUMF, Feb 2018



Paths for going forward/upwards:

-- Machine learning



-- Machine learning From Negoita *et al*, arXiv:1803.03215 Extrapolation via Artificial Neural Net (ANN)

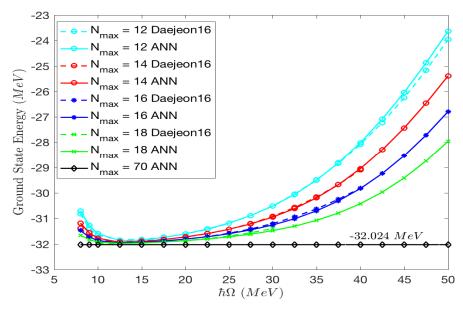


Figure 7. Comparison of the NCSM calculated and the corresponding ANN predicted gs energy values of $^6\mathrm{Li}$ as a function of $\hbar\Omega$ at $N_{\mathrm{max}}=12,14,16,$ and 18. The lowest horizontal line corresponds to the ANN nearly converged result at $N_{\mathrm{max}}=70.$



-- Machine learning

From Negoita et al, arXiv:1803.03215

Extrapolation via Artificial Neural Net (ANN)

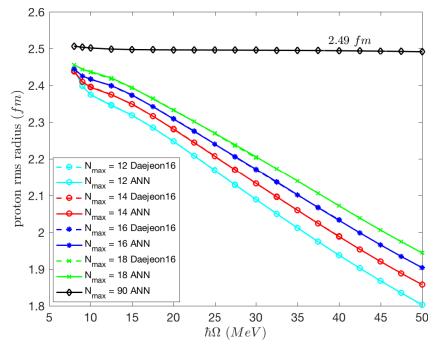


Figure 9. Comparison of the NCSM calculated and the corresponding ANN predicted gs point proton rms radius values of $^6\mathrm{Li}$ as a function of $\hbar\Omega$ for $N_{\mathrm{max}}=12,14,16,$ and 18. The highest curve corresponds to the ANN nearly converged result at $N_{\mathrm{max}}=90.$

Diagonalization and the continuum:



Strategies:

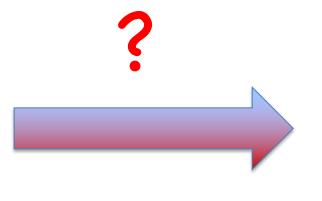
what else do we get?

- Change boundary conditions: complex basis methods
 (e.g., Gamow basis)
 talks by Nazarewicz, Fossez, Xu, Hu, Ploszajczk, Barrett
 Straightforward extension of BS framework; get widths of resonances...
- Discretize continuum: J-matrix. cf. talk by Shirokov Arises "naturally" in SM framework ... so far best with single channel
- Embed BS in continuum: NCSMC, effective "optical potential" cf. talks by Quaglioni, Elster, Rotureau Most "direct" connection to scattering/reaction expts (?) How to extend reach?



Workshop goals







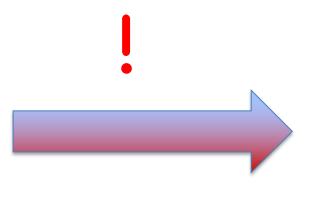
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Workshop goals







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