## Overview of bound-state many-body methods

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## Welcome to the workshop!

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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

## Workshop goals



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## Workshop goals



## Theory

## Workshop goals



Theory

## Experiment

## Workshop goals



Theory


Experiment

## Workshop goals

## What is illuminated....



## Workshop goals

## What is illuminated....


...and what is left in darkness.

## 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
- ....?

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## Bound state methods



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


## Bound state methods



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

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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


## Bound state methods



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


## Choice of wave function basis

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

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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

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Long-range correlations

## Bound state methods - in detail

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

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Product wavefunction ("Slater Determinant")
$\Psi\left(\vec{r}_{1}, \vec{r}_{2}, \vec{r}_{3} \ldots\right)=\phi_{\text {(nI) }}\left(\vec{r}_{1}\right) \phi_{\text {(n) }}\left(\vec{r}_{2}\right) \phi_{\text {(n) }}\left(\vec{r}_{3}\right) \ldots \phi_{\text {®n }}\left(\vec{r}_{N}\right)$
Each many-body state can be uniquely determined by a list of "occupied" single-particle states
= "occupation representation"

$$
|\alpha\rangle=\hat{a}_{n_{1}}^{+} \hat{a}_{n_{2}}^{+} \hat{a}_{n_{3}}^{+} \ldots \hat{a}_{n_{N}}^{+}|0\rangle
$$

## Bound state methods - in detail

## Variational Monte Carlo (VMC)

$\Psi>=$ Slater determinant x two-body correlation ("Jastrow-like") functions $f\left(r_{i}-r_{j}\right)$
$\rightarrow$ Large dimensional integrals, evaluated by MC

$$
\text { minimize } \quad \frac{\langle\Psi| H|\Psi\rangle}{\langle\Psi \mid \Psi\rangle}
$$

## Bound state methods - in detail

## Green Function /Diffusion MC (GFMC)

Starting from VMC wave function| $\Psi>$, evolve in imaginary time
$\exp (-H \tau) \mid \Psi>$.

## Bound state methods - in detail

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

```
exp(-H \tau) | \Psi >.
```



```
"Gold standard" in ab initio calculations
for light nuclei (A < 16)
Can handle 'hard core' potentials
e.g. Argonne V18
```

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## Bound state methods - in detail

## Green Function /Diffusion MC (GFMC)

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

Non-local potentials troublesome.
$\exp (-H \tau) \mid \Psi>$.
3-body handled perturbatively


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

Excited states difficult
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## Bound state methods - in detail

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

$$
|\Psi>=\exp (T)| S D>.
$$

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

$$
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- Can handle "bare"/hard core interactions
 ${ }_{\circ}$ up many shells $\rightarrow$ short range correlations - Nonlocal interactions no problem - Polynomial scaling of work (linked diagrams only)


## Bound state methods - in detail

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

$$
|\Psi>=\exp (T)| S D>.
$$

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


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## Bound state methods - in detail saniligitar

## Basis diagonalization

Expand wave function in (orthonormal) basis

$$
\begin{gathered}
\hat{\mathbf{H}}|\Psi\rangle=E|\Psi\rangle \\
|\Psi\rangle=\sum_{\alpha} c_{\alpha}|\alpha\rangle \quad H_{\alpha \beta}=\langle\alpha| \hat{\mathbf{H}}|\beta\rangle \\
\sum H_{\alpha \beta} c_{\beta}=E c_{\alpha} \quad \text { if } \quad\langle\alpha \mid \beta\rangle=\delta_{\alpha \beta}
\end{gathered}
$$

## Bound state methods - in detail

## 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

## Bound state methods - in detail

## 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) $\rightarrow$ limited number of shells/short range correlations
$\rightarrow$ often prefer "softened" forces for better convergence



## Bound state methods - in detail

## Energy density functionals

Minimize Kohn-Sham density functional $\mathrm{E}(\rho)$
Related: Hartree-Fock (-Bogoliubov), beyond Mean-Field such as RPA, generator coordinate

## Bound state methods - in detail

## Energy density functionals

Minimize Kohn-Sham density functional $\mathrm{E}(\rho)$


- 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


## Bound state methods - in detail

## Energy density functionals

Minimize Kohn-Sham density functional E( $\rho$ )

- 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

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## 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 $p f$ shell with GX1A interaction

No-core shell model: in harmonic oscillator basis, "all" particles active (up to $\mathrm{N}_{\max }$ 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 $\mathrm{N}_{\max }=10 \ldots 22$
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Extend applicability of diagonalization

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## A deep dive into basis diagonalization

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## 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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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), $\operatorname{Sp}(3, R)$, 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.

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

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: ${ }^{12} \mathrm{C} \mathrm{N}_{\max }=8$
scheme basis dim
M $\quad 0.6 \times 10^{9}$
$\mathrm{J}(\mathrm{J}=4) \quad 9 \times 10^{7}$
SU(3) $\quad 9 \times 10^{6}$
(truncated)
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\# of nonzero matrix elements $5 \times 10^{11}$ $3 \times 10^{13}$
$2 \times 10^{12}$

From Dytrych, et al, arXiv:1602.02965
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\# of nonzero matrix elements $5 \times 10^{11} \quad 4 \mathrm{~Tb}$ of memory! $3 \times 10^{13} \quad 240 \mathrm{~Tb}$ of memory!
$2 \times 10^{12} \quad 16 \mathrm{~Tb}$ of memory!

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## Symplectic Sp(3,R) Symmetry



## Collectivity features


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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)
$J$-scheme matrices are smaller but much denser than M-scheme, and "symmetry-adapted" (i.e. SU(3)) matrices are smaller still.
example: ${ }^{12} \mathrm{C} \mathrm{N}_{\text {max }}=8$
scheme basis dim \# of nonzero matrix elements

| M | $0.6 \times 10^{9}$ |
| :--- | ---: |
| $J(J=4)$ | $9 \times 10^{7}$ |
| $S U(3)$ | $9 \times 10^{6}$ |

(truncated) $5 \times 10^{11} \quad 4 \mathrm{~Tb}$ of memory! $3 \times 10^{13} \quad 240 \mathrm{~Tb}$ of memory!
$2 \times 10^{12} \quad 16 \mathrm{~Tb}$ of memory!
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

Links to free, open-source many-body codes:
fribtheoryalliance.org

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

Manual at arXiv:1801.08432

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Despite advances, it is easy to get to model spaďés ${ }^{\text {ERSITY }}$ beyond our reach:
sd shell: max dimension 93,000. Can be done in a few minutes on a laptop.
$p f$ shell: ${ }^{48} \mathrm{Cr}$, dim 2 million, $\sim 10$ minutes on laptop ${ }^{52} \mathrm{Fe}$, $\operatorname{dim} 110$ million, a few hours on modest workstation ${ }^{56} \mathrm{Ni}$, dim 1 billion, 1 day on advanced workstation ${ }^{60} \mathrm{Zn}$, dim 2 billion, < 1 hour on supercomputer

Despite advances, it is easy to get to model spadee serity beyond our reach:
shells between 50 and $82\left(0 g_{7 / 2} 2\right.$ s $\left.1 \mathrm{~d} 0 h_{11 / 2}\right)$
${ }^{128} \mathrm{Te}$ : dim 13 million (laptop)
${ }^{127}$ I: dim 1.3 billion (small supercomputer)
${ }^{128} \mathrm{Xe}$ : dim 9.3 billion (supercomputer)
${ }^{129} \mathrm{Cs}$ : dim 50 billion (haven't tried!)

Despite advances, it is easy to get to model spaCe $S^{\text {FRSITY }}$ beyond our reach:
$\mathrm{N}_{\text {max }}$ calculations:
${ }^{12} \mathrm{C}_{\mathrm{N}_{\text {max }}}=4$ dim 1 million
${ }^{12} C N_{\text {max }}=6$ dim 30 million
${ }^{12} \mathrm{C}^{2} \mathrm{~N}_{\max }=8$ dim 500 million
${ }^{12} \mathrm{C} \mathrm{N}_{\max }=10 \operatorname{dim} 7.8$ billion
${ }^{12} \mathrm{C} \mathrm{N}_{\text {max }}=12$ dim 81 billion

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${ }^{12} \mathrm{C} \mathrm{N}_{\max }=12$ dim 81 billion

Largest (?) known calculation, ${ }^{6}$ Li, $\mathrm{N}_{\text {max }}=22$, 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 $\mathrm{N}_{\text {max }}$ 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 $\mathrm{N}_{\max }=10 \ldots 22$

Ab initio/ "No-core shell model": take to infinite limit
Two parameters: h.o. basis frequency $\Omega$ and model space cutoff $\mathrm{N}_{\max }$

Naïve expectation: take $\mathrm{N}_{\text {max }}$-> infinity Converged results independent of $\Omega$


FIG. 1. (Color online) The energy of the ground state ( $\mathrm{J}=\frac{3}{2}$ ) for ${ }^{7} \mathrm{Be}$ and ${ }^{7} \mathrm{Li}$ with the JISP16 and NNLO opt interactions as a function of HO energy. In this figure and the following figures, for ${ }^{7} \mathrm{Li}$ and ${ }^{7} \mathrm{Be}$, the $N_{\text {max }}$ 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 $E\left(N_{\max }\right)=E(\infty)+a \exp \left(-c N_{\max }\right)$

Idea: truncation in h.o. space $\left(\mathrm{N}_{\max }\right)=$ "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)


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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 horiwontal red (gray) line marks the value of $E_{\infty}$ with uncertainty estimates indicated as blue (gray) bands. The dashed black line marks the variational minimum $E_{\text {varmin }}$ 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


# From <br> Constantinou et al, 

arXiv:1605.04976

FIG. 4: Infrared basis extrapolations for the ${ }^{6} \mathrm{He}$ 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.
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Harmonic Oscillator


From R. Roth, talk at TRIUMF, Feb 2018

Harmonic Oscillator
Natural Orbitals


From R. Roth, talk at TRIUMF, Feb 2018

## Paths for going forward/upwards:

## -- Machine learning

## -- Machine learning

## From Negoita et al, arXiv:1803.03215 <br> 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
$N_{\max }=12,14,16$, and 18. The lowest horizontal line corresponds to the ANN nearly converged result at $N_{\text {max }}=70$.

## -- 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 $N_{\max }=12,14,16$, and 18 . The highest curve corresponds to the ANN nearly converged result at $N_{\max }=90$.

## Diagonalization and the continuum:

Strategies:

- 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... what else do we get?
- 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?

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## Workshop goals



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Theory


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