Ab inito calculations of Be isotopes with JISP16

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SciDAC project – NUCLEI
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PetaApps award
PIs: Jerry Draayer (LSU), James P Vary (ISU), Ümit V Çatalyürek (OSU), Masha Sosonkina (ODU/AL)

INCITE award – Computational Nuclear Structure
lead PI: James P Vary (ISU)

NERSC CPU time
Given a Hamiltonian operator

\[ \hat{H} = \sum_{i<j} \frac{(\vec{p}_i - \vec{p}_j)^2}{2m_A} + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} + \ldots \]

solve the eigenvalue problem for wave function of \( A \) nucleons

\[ \hat{H} \Psi(r_1, \ldots, r_A) = \lambda \Psi(r_1, \ldots, r_A) \]

- eigenvalues \( \lambda \) discrete (quantized) energy levels
- eigenvectors: \( |\Psi(r_1, \ldots, r_A)|^2 \) probability density for finding nucleons 1, \ldots, \( A \) at \( r_1, \ldots, r_A \)
Self-bound quantum many-body problem, with $3A$ degrees of freedom in coordinate (or momentum) space.

Not only 2-body interactions, but also intrinsic 3-body interactions and possibly $4$- and higher $N$-body interactions.

Strong interactions, with both short-range and long-range pieces.

Uncertainty quantification for calculations needed:
- for comparisons with experiments
- for comparisons between different methods

Sources of numerical uncertainty:
- statistical and round-off errors
- systematical errors inherent to the calculational method:
  - CI methods: finite basis space
  - Monte Carlo methods: sensitivity to the trial wave function
  - Lattice calculations: finite volume and lattice spacing
- uncertainty of the nuclear potential.
Nuclear interaction

Nuclear potential not well-known . . .
though in principle calculable from Quantum Chromo Dynamics

\[ \hat{H} = \hat{T}_{\text{rel}} + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} + \ldots \]

In practice, alphabet of realistic potentials
- Argonne potentials: AV8’, AV18
  - plus Urbana 3NF (UIX)
  - plus Illinois 3NF (IL7)
- Bonn potentials
- Chiral NN interactions
  - plus chiral 3NF, ideally to the same order
- . . .
- JISP16
- . . .
Phenomeological $NN$ interaction: JISP16

J-matrix Inverse Scattering Potential tuned up to $^{16}O$
- Constructed to reproduce $np$ scattering data
- Finite rank separable potential in H.O. representation
- Nonlocal $NN$-only potential
- Use Phase-Equivalent Transformations (PET) to tune off-shell interaction to
  - binding energy of $^3H$ and $^4He$
  - low-lying states of $^6Li$ (JISP6, precursor to JISP16)
  - binding energy of $^{16}O$

Available online at www.sciencedirect.com

Realistic nuclear Hamiltonian: Ab exitu approach

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www.elsevier.com/locate/physletb

J-matrix Inverse Scattering Potentials

- Constructed as matrix in H.O. basis
  - $2n + l \leq 8$ for even partial waves, limited to $J \leq 4$
  - $2n + l \leq 9$ for odd partial waves, limited to $J \leq 4$
  - $\hbar \omega = 40$ MeV
- $\chi^2/$datum of 1.05 for the 1999 $np$ data base (3058 data)
- No charge symmetry breaking
- Use PET to improve
  - deuteron quadrupole moment
  - $^3$H and $^4$He binding energies
  - binding energies low-lying states of $^6$Li: JISP6
  - binding energy of $^{16}$O: JISP16
  - additional tuning, more accurate calculations: JISP16$^{2010}$
    reproduces $^{16}$O within numerical error estimates of 3%
    Shirokov, Kulikov, Maris, Mazur, Mazur, Vary, arXiv:0912.2967
### JISP16 results for few-body systems

#### Deuteron properties

<table>
<thead>
<tr>
<th></th>
<th>E (MeV)</th>
<th>( r_p ) (fm)</th>
<th>( Q ) (e fm(^2))</th>
<th>( A_s ) (fm(^{-1/2}))</th>
<th>( A_d/A_s )</th>
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</thead>
<tbody>
<tr>
<td>expt.</td>
<td>-2.224575</td>
<td>1.971(6)</td>
<td>0.2859(3)</td>
<td>0.8846(9)</td>
<td>0.0256(4)</td>
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<tr>
<td>JISP16</td>
<td>-2.224575</td>
<td>1.964</td>
<td>0.2886</td>
<td>0.8629</td>
<td>0.0252</td>
</tr>
<tr>
<td>AV18</td>
<td>-2.224575</td>
<td>1.967</td>
<td>0.270</td>
<td>0.8850</td>
<td>0.0250</td>
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</tbody>
</table>

Selected \( A = 3 \) and \( 4 \) results

<table>
<thead>
<tr>
<th></th>
<th>( E_b(\text{^3H}) )</th>
<th>( \mu(\text{^3H}) )</th>
<th>( \mu(\text{^3He}) )</th>
<th>( E_b(\text{^4He}) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>expt.</td>
<td>8.482</td>
<td>2.979</td>
<td>-2.128</td>
<td>28.296</td>
</tr>
<tr>
<td>JISP16</td>
<td>8.369(2)</td>
<td>2.667</td>
<td>-1.819</td>
<td>28.299</td>
</tr>
<tr>
<td>AV18</td>
<td>7.61(1)</td>
<td></td>
<td></td>
<td>24.07(4)</td>
</tr>
<tr>
<td>AV18+IL2</td>
<td>8.43(1)</td>
<td>2.568(1)</td>
<td>-1.762(1)</td>
<td>28.37(3)</td>
</tr>
</tbody>
</table>

Many-Body systems

Configuration Interaction methods

- Expand wave function in basis states $|\Psi\rangle = \sum a_i |\Phi_i\rangle$

- Express Hamiltonian in basis $\langle \Phi_j | \hat{H} | \Phi_i \rangle = H_{ij}$

- Diagonalize Hamiltonian matrix $H_{ij}$

- Complete basis $\rightarrow$ exact result

  - caveat: complete basis is infinite dimensional

- In practice

  - truncate basis

  - study behavior of observables as function of truncation

- Computational challenge

  - construct large $(10^{10} \times 10^{10})$ sparse symmetric real matrix $H_{ij}$

  - use Lanczos algorithm
to obtain lowest eigenvalues & eigenvectors
**Basis space expansion**

- Expand wave function in basis states $|\Psi\rangle = \sum a_i |\Phi_i\rangle$
- Many-Body basis states $|\Phi_i\rangle$ Slater Determinants of Single-Particle states $|\phi\rangle$

$$\Phi_i(r_1, \ldots, r_A) = \frac{1}{\sqrt{(A!)}} \begin{vmatrix} \phi_{i1}(r_1) & \phi_{i2}(r_1) & \ldots & \phi_{iA}(r_1) \\ \phi_{i1}(r_2) & \phi_{i2}(r_2) & \ldots & \phi_{iA}(r_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_{i1}(r_A) & \phi_{i2}(r_A) & \ldots & \phi_{iA}(r_A) \end{vmatrix}$$

- Single-Particle basis states
  - eigenstates of $\hat{L}^2$, $\hat{S}^2$, $\hat{J}^2$, and $\hat{J}_z$
  - labelled by quantum numbers $|n, l, s, j, m\rangle$
  - radial wavefunctions
    - Harmonic Oscillator
    - Wood–Saxon basis
      (Negoita, PhD thesis 2010)
    - Coulomb–Sturmian
      (Caprio, Maris, Vary, PRC86, 034312 (2012))
    - Berggren
    - Rotureau, last week
    - ...
**Truncation scheme**

- $M$-scheme: Many-Body basis states eigenstates of $\hat{J}_z$

\[ \hat{J}_z |\Phi_i\rangle = M |\Phi_i\rangle = \sum_{k=1}^{A} m_{ik} |\Phi_i\rangle \]

- single run gives spectrum
- alternatives: $LS$ scheme, Coupled-$J$ scheme, Symplectic basis, ...

- $N_{\text{max}}$ truncation: Many-Body basis states satisfy

\[ \sum_{k=1}^{A} \left( 2n_{ik} + l_{ik} \right) \leq N_0 + N_{\text{max}} \]

- exact factorization of Center-of-Mass motion
- alternatives: No-Core Monte-Carlo Shell Model, Importance Truncation, FCI (truncation on single-particle basis only), ...
**Intermezzo: FCI vs. Nmax truncation**

- **$N_{\text{max}}$ truncation**
  - exact factorization of Center-of-Mass motion
  - converges much more rapidly than FCI truncation with basis space dimension

- Infinite basis space limit: No-Core Full Configuration (NCFC)
Intermezzo: *Center-of-Mass excitations*

- Use single-particle coordinates, not relative (Jacobi) coordinates
- straightforward to extend to many particles
- have to separate Center-of-Mass motion from internal motion

Center-of-Mass wave function **factorizes** for
H.O. basis functions in combination with $N_{\text{max}}$ truncation

\[
|\Psi_{\text{total}}\rangle = |\phi_1\rangle \otimes \ldots \otimes |\phi_A\rangle = |\Phi_{\text{Center-of-Mass}}\rangle \otimes |\Psi_{\text{int}}\rangle
\]

where

\[
\hat{H}_{\text{rel}} |\Psi_{j, \text{int}}\rangle = E_j |\Psi_{j, \text{int}}\rangle
\]

- Add Lagrange multiplier to Hamiltonian (Lawson term)

\[
\hat{H}_{\text{rel}} \rightarrow \hat{H}_{\text{rel}} + \Lambda_{CM} \left( \hat{H}_{CM}^{H.O.} - \frac{3}{2} \left( \sum_i m_i \right) \omega \right)
\]

with $\hat{H}_{\text{rel}} = T_{\text{rel}} + V_{\text{rel}}$ the relative Hamiltonian

- separates CM excitations from CM ground state $|\Phi_{CM}\rangle$
**Configuration Interaction Methods**

- Expand wave function in basis states: \( |\Psi\rangle = \sum a_i |\psi_i\rangle \)
- Express Hamiltonian in basis: \( \langle \psi_j | \hat{H} | \psi_i \rangle = H_{ij} \)
- Diagonalize Hamiltonian matrix \( H_{ij} \)
- **Variational**: for any finite truncation of the basis space, eigenvalue is an upper bound for the ground state energy
- Smooth approach to asymptotic value with increasing basis space: No-Core Full Configuration calculation
- **Convergence**: independence of \( N_{\text{max}} \) and H.O. basis \( \hbar \omega \)
- different methods (NCFC, CC, GFMC, . . .) using the same interaction should give same results within (statistical plus systematic) numerical uncertainties

![Graph showing ground state energy vs basis space \( \hbar \omega \)](attachment:image.png)

- Different curves for various values of \( N_{\text{max}} \) (2, 4, 6, 8, 10, 12, 14, 16, expt.)
- Ground state energy in MeV for \( ^4\text{He} \) as a function of basis space \( \hbar \omega \) [MeV]
No-Core CI calculations – main challenge

- Increase of basis space dimension with increasing $A$ and $N_{\text{max}}$
- More relevant measure for computational needs
  - number of nonzero matrix elements
**Accelerating convergence – renormalization techniques**

**Challenge:** achieve numerical convergence for no-core Full Configuration calculations using finite model space calculations

- Renormalize interaction $\rightarrow$ effective interaction $V_{\text{eff}}$
  - can improve quality of results in small model spaces

**Caveats**

- induces many-body forces
  - induced 3-body forces are often neglected
  - induced 4-, 5-, ..., $A$-body forces are always neglected

- variational principle applicable to renormalized Hamiltonian not to original (bare) Hamiltonian
  - often complicates extrapolation to asymptotic values
  - need to renormalize operators as well

**Commonly used renormalization procedures**

- Lee–Suzuki effective interaction
- Similarity Renormalization Group
  - (in particular in combination with chiral interactions)
Ground state energy of $^{16}$O expected to be between variational upper bound without renormalization and lower bound (?) from Lee–Suzuki renormalized interaction

Used in tuning of JISP16

Convergence Lee–Suzuki renormalization not monotonic

Lee–Suzuki result for ground state energy not a lower bound

JISP16 overbinds $^{16}$O by 10% to 15%

Extrapolating to complete basis

Challenge: achieve numerical convergence for no-core Full Configuration calculations using finite model space calculations

- Perform a series of calculations with increasing $N_{\text{max}}$ truncation
- Extrapolate to infinite model space → exact results
- Empirical: binding energy exponential in $N_{\text{max}}$

$$E_{\text{binding}}^N = E_{\text{binding}}^\infty + a_1 \exp(-a_2 N_{\text{max}})$$

- use 3 or 4 consecutive $N_{\text{max}}$ values to determine $E_{\text{binding}}^\infty$
- use $\hbar \omega$ and $N_{\text{max}}$ dependence to estimate numerical error bars


Recent studies of IR and UV behavior
- exponentials in $\sqrt{\hbar \omega/N}$ and $\sqrt{\hbar \omega N}$
  Coon et al, arXiv:1205.3230;
  Furnstahl, Hagen, Papen PRC86, 031301(R) (2012)


Extrapolating to complete basis – in practice

- Perform a series of calculations with increasing $N_{\text{max}}$ truncation
- Use empirical exponential in $N_{\text{max}}$:

$$E_{\text{binding}}^N = E_{\text{binding}}^\infty + a_1 \exp(-a_2 N_{\text{max}})$$

- H.O. basis up to $N_{\text{max}} = 16$: $E_b = -31.49(3)$ MeV
  Cockrell, Maris, Vary, PRC86 034325 (2012)

- Hyperspherical harmonics up to $K_{\text{max}} = 14$: $E_b = -31.46(5)$ MeV
  Vaintraub, Barnea, Gazit, PRC79 065501 (2009)
Accelerating convergence – Coulomb-Sturmian basis

- Asymptotic behavior
  - H.O. basis $\exp(-a\,r^2)$
  - Coulomb–Sturmian basis $\exp(-c\,r)$

- Disadvantage
  - no exact factorization of Center-of-Mass motion
  - in practice, approximate factorization
  - can use Lagrange multiplier to remove spurious state

Caprio, Maris, Vary, PRC86, 034312 (2012)
Coulomb-Sturmian – binding energies

- at $N_{\text{max}} = 4$ further from convergence than H.O. basis
- extrapolate to the same results as H.O. basis
- dashed line: extrapolated result from $N_{\text{max}} = 16$ calculations in H.O. basis

Cockrell, Maris, Vary, PRC86 034325 (2012)
Coulomb-Sturmian – radius

Caprio, Maris, Vary, PRC86, 034312 (2012)

- Exponential extrapolation does not work for radii in H.O. basis
- Exponential extrapolation seems to work for radii in C.S. basis
- Best estimate based on $N_{\text{max}} = 16$ H.O. calculations: 2.3 fm
  Cockrell, Maris, Vary, PRC86 034325 (2012)
- Experimental point-proton radius: 2.45 fm
Ground state energy Be-isotopes with JISP16

Be isotopes with $N_{\text{max}}$:
- $N_{\text{max}} = 14$
- $N_{\text{max}} = 12$
- $N_{\text{max}} = 10$
- $N_{\text{max}} = 8$

Total number of nucleons $A$ vs. ground state energy [MeV]

- Variational bound
- NCFC w. JISP16
- Experiment
Binding energy converges monotonically, with optimal H.O. frequency around $\hbar \omega = 20$ MeV to 25 MeV

Ground state about 0.7 MeV underbound with JISP16

Proton point radius does not converge monotonically

Coulomb–Sturmian basis likely to improve convergence
7Be – Proton density

- Translationally-invariant density – center-of-mass motion taken out
  w. Cockrell, PhD thesis 2012

Slow build up of asymptotic tail of wavefunction

Proton density appears to converge more rapidly at $\hbar \omega = 12.5$ MeV than at 20 MeV because long-range part of wavefunction is better represented with smaller H.O. parameter
Calculation one-body observables: $\langle i | \mathcal{O} | j \rangle \sim \int \mathcal{O}(r) r^2 \rho_{ij}(r) \, dr$

RMS radius: $\mathcal{O}(r) = r^2$

Slow convergence of RMS radius due to slow build up of asymptotic tail

Ground state RMS radius in agreement with data
7Be – Quadrupole moment

Ground state quadrupole moment in agreement with data

Optimal basis space around $\hbar \omega = 10$ MeV to 12 MeV

Similar slow convergence for E2 transitions
Excitation energy of narrow states converge rapidly agree with experiments

Broad resonances depend $\hbar \omega$

Magnetic moments well converged

2-body currents needed for agreement with data (meson-exchange currents)
E2 observables suggest rotational structure for $\frac{3}{2}$, $\frac{1}{2}$, $\frac{7}{2}$, $\frac{5}{2}$ states

\[
Q(J) = \frac{3}{4} - \frac{J(J + 1)}{(J + 1)(2J + 3)} Q_0
\]

\[
B(E2; i \rightarrow f) = \frac{5}{16\pi} Q_0^2 \left( \left| \begin{array}{c} J_i, \frac{1}{2}; 2, 0 \end{array} \right| J_f, \frac{1}{2} \right)^2
\]
7Be – Structure of \((\frac{5}{2}^-, \frac{1}{2})_1\) (broad) and \((\frac{5}{2}^-, \frac{1}{2})_2\) (narrow) states

Translationally-invariant nucleon densities

Proton density

Neutron density

Cockrell, PhD thesis 2012
**9Be – Ground state properties**

- Convergence pattern natural and unnatural parity looks similar
- Ground state about $1.0 \pm 0.2$ MeV underbound with JISP16
- Lowest unnatural parity state underbound by about $2.7 \pm 0.8$ MeV
  - need next basis space for unnatural parity
  - need improved interaction?
Unnatural parity states systematically underbound by about 1 MeV to 2 MeV compared to lowest natural parity states

interaction JISP16 not good enough?

difference in convergence of pos. and neg. parity states?
Excitation energy $\frac{5}{2}^-$ at 3 MeV well converged (narrow)

Excitation energy $\frac{7}{2}^-$ reasonably converged

Excitation energies broad neg. parity not well converged

Excitation energies pos. parity well converged
Rotational energy for states with axial symmetry \( E(J) \propto J(J + 1) \)

Quadrupole moments for rotational band

\[
Q(J) = \frac{3K^2 - J(J + 1)}{(J + 1)(2J + 3)} Q_0
\]

Quadrupole moments not converged, but ratio of quadrupole moments agree with rotational band structure
\[ 9\text{Be} - \text{Structure: Density } \left( \frac{3}{2}^-, \frac{1}{2}^+ \right) \text{ ground state} \]

Proton and neutron densities, and their difference.

Translationally-invariant proton and neutron densities
Chase Cockrell, PhD thesis, 2012

Emergence of \( \alpha \) clustering?
Rotational bands odd Be isotopes in preparation, w. M. Caprio

Quadrupole moments not converged, but ratio of quadrupole moments agree with rotational band structure
Rotational bands odd Be isotopes in preparation, w. M. Caprio

Also for the unnatural parity states

Quadrupole moments not converged, but ratio of quadrupole moments agree with rotational band structure
Rotational bands even Be isotopes in preparation, w. M. Caprio

$B(E2)$ transitions Be isotopes \textit{in preparation, w. M. Caprio}

![Graph showing $B(E2)$ values for different isotopes of Be](image)

- Rotor prediction
  - $\Delta J = 1$: dashed
  - $\Delta J = 2$: solid

- Ratio's $B(E2)/Q^2$ in agreement with rotational structure as well

Conclusions

- **No-core Configuration Interaction** nuclear structure calculations
  - Binding energy, spectrum
  - $\langle r^2 \rangle$, $\mu$, $Q$, transitions, wfns, one-body densities

- Main challenge: construction and diagonalization of extremely large ($D > 1$ billion) sparse matrices

- Need realistic basis function to improve convergence $\langle r^2 \rangle$, $Q$

- **JISP16**
  - Nonlocal phenomenological 2-body interaction
  - Good description of a range of light nuclei
  - Rapid convergence for binding energies
  - Emergence of rotational bands and clustering in Be-isotopes

- Would not have been possible without collaboration with applied mathematicians and computer scientists
  Aktulga, Yang, Ng (LBNL); Çatalyürek, Saule (OSU); Sosonkina (ODU/AL)