Using CI and EDF methods for nuclear structure calculations

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Motivation

• To determine an interaction for shell model calculations in a particular region of interest from a microscopic NN-interaction

• To provide reliable theoretical predictions of nuclear properties for:
  a) nuclei outside of standard model spaces
     (Ex: $^{20}$C, $^{42}$Si, $^{78}$Ni)
  b) nuclei inside standard model spaces that are significantly affected by orbits outside the model space (Ex: island of inversion region)
Standard Shell Model Spaces

Legend:
$E_{\text{exp}}(2^+)$ (MeV)

Proton Number

Neutron Number
Method

• Combination of Configuration Interaction (CI) and Energy Density Functional (EDF) methods
• Select a target nucleus and model space
• Use Skyrme Hartree Fock to calculate BE, SPE spectra, and radial wavefunctions
• Renormalize NN interaction (N3LO or Argonne V18) using G-matrix inversion or “vlowk” similarity transformation with a sharp cutoff in momentum space
• Convert low-k interaction into TBME for a CI calculation
• Find “correlation energy” from difference between CI result and closed-configuration CI result
Nuclear Interaction

\[ T \quad V_2 \quad V_3 \]
Closed-shell vacuum
filled orbitals
Closed-shell vacuum filled orbitals

Skyrme phenomenology
Closed-shell vacuum filled orbitals

NN potential with $V_{\text{lowk}}$

Skyrme phenomenology
Closed-shell vacuum filled orbitals

“tuned” valence two-body matrix elements

Skyrme phenomenology
Order of Perturbation Theory

first  second  third
Example of Procedure

• Start with $^{16}\text{O}$ as a closed core
• Choose sd orbits as model space
• Use Skyrme interaction with a tensor force (skxtb) for Hartree Fock calculations
• Renormalize N3LO interaction with vlowk similarity transformation
• Compare results to experimental data and to phenomenological potentials
• Try to understand discrepancies and establish the best possible method to produce two-body matrix elements
The graph shows the energy levels of the excited states of $^{22}\text{Na}$ and $^{22}\text{Na}$ usdbpn, with $Z=11$ and $N=11$. The energy levels are plotted against binding energy relative to $^{16}\text{O}$, with the following binding energies:

- $^{22}\text{Na}$: $-46.526$ MeV
- $^{22}\text{Na}$ usdbpn: $-46.713$ MeV
Comparison of nn orbits
Application to $^{34}$Si

- Best target for calculations in the island of inversion region; also can provide a starting point for calculations of $^{42}$Si
- Model space:
  - protons: $d_{5/2}, d_{3/2}, s_{1/2}$
  - neutrons: $d_{3/2}, s_{1/2}, f_{7/2}, p_{3/2}, p_{1/2}$
- N3LO interaction with $v_{lowk}$ renormalization up to second order in perturbation theory and up to $4\hbar\omega$
- Harmonic oscillator wavefunctions and SPEs used for renormalization
- SkxTB used for Hartree Fock calculations
- Fit to experimental data to determine appropriate single particle energies
Conclusions

• New hybrid method combines EDF and CI methods to produce reliable estimates of nuclear properties in a greater region of the nuclear chart than standard shell model spaces

• Method itself is general (can get interaction for any model space for any closed-subshell nucleus), although application is still limited by mass due to the use of CI calculations in the final step of the procedure

• Improvements are still possible (e.g. using more realistic wavefunctions) and will be implemented soon, hopefully providing more accurate results
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Renormalization Procedure