Using CI and EDF methods for nuclear structure calculations

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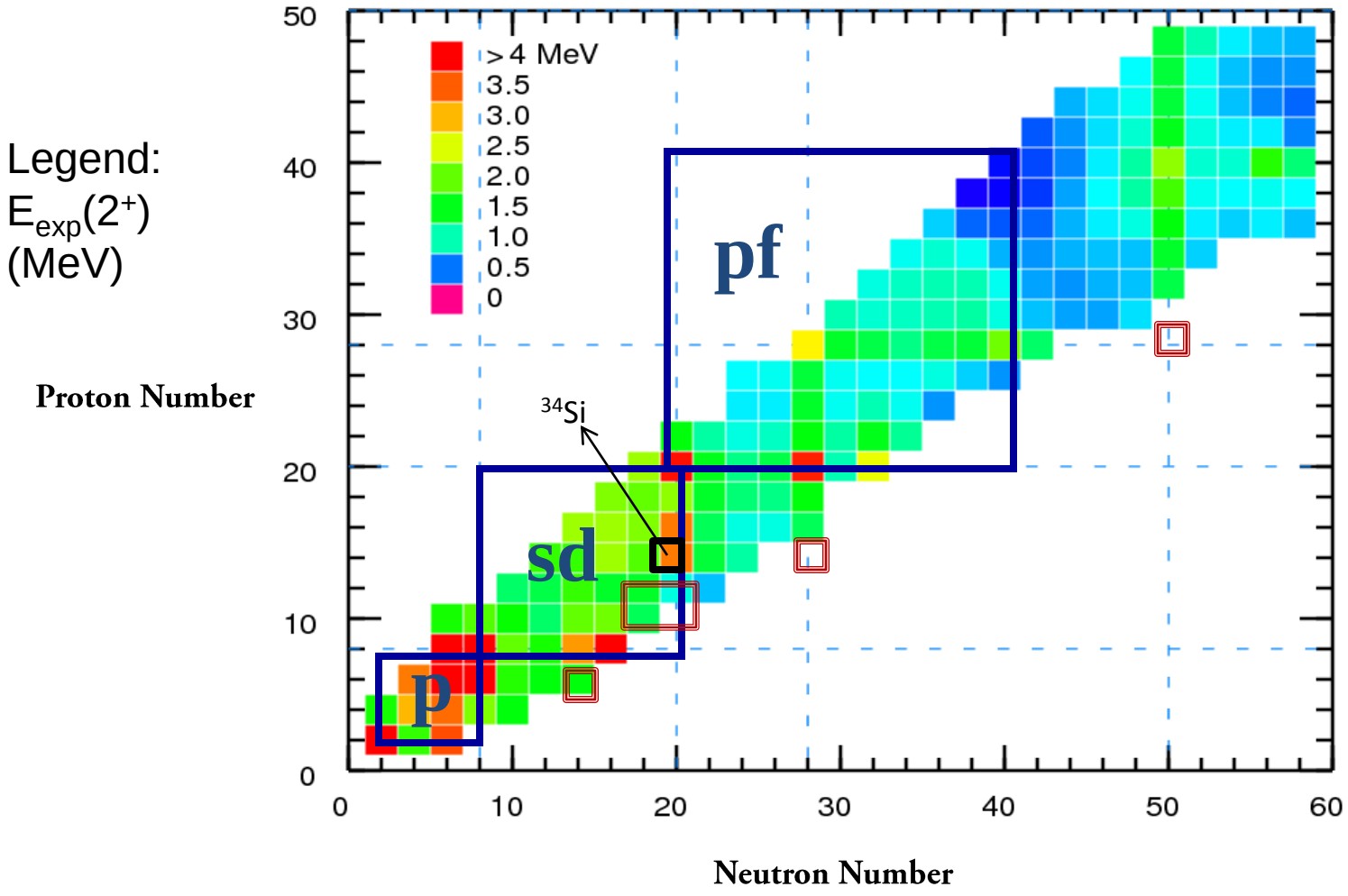
Motivation

- 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)

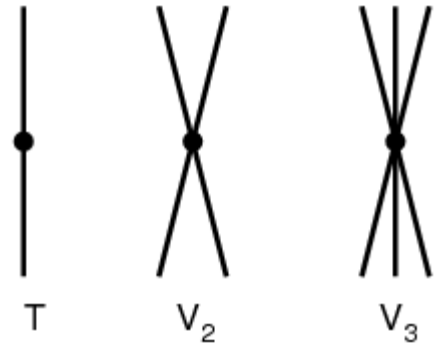
Standard Shell Model Spaces



Method

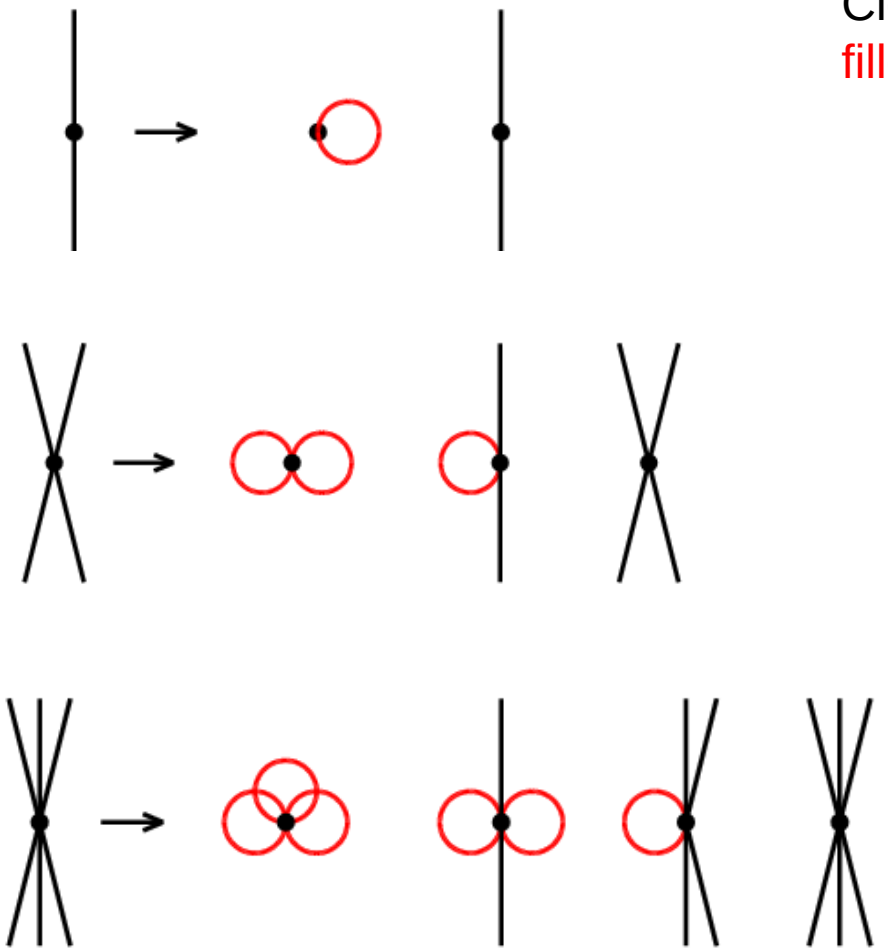
- Combination of Configuration Interaction (CI) and Energy Density Functional (EDF) methods
- Select a target nucleus and model space
- Use Skyrme Hartree Fock to calculate BE, SPE spectra, and radial wavefunctions
- Renormalize NN interaction (N3LO or Argonne V18) using G-matrix inversion or “vlowk” 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

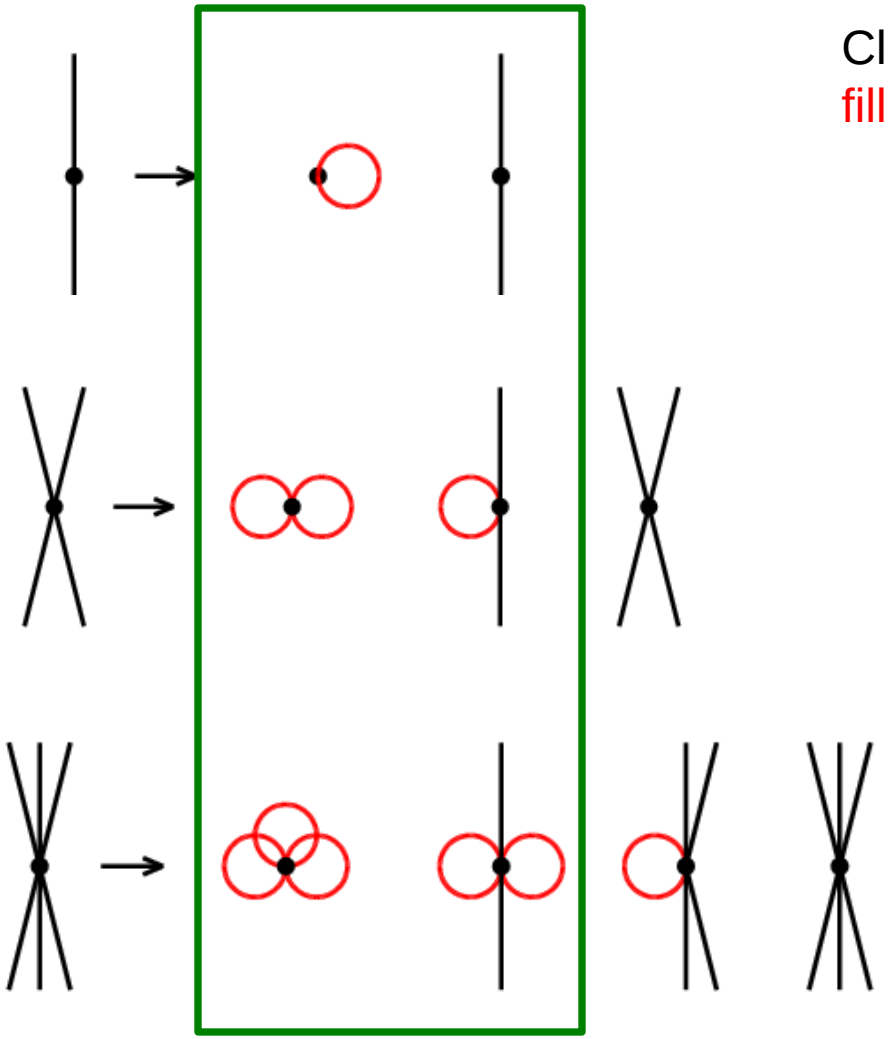
Nuclear Interaction



Closed-shell vacuum

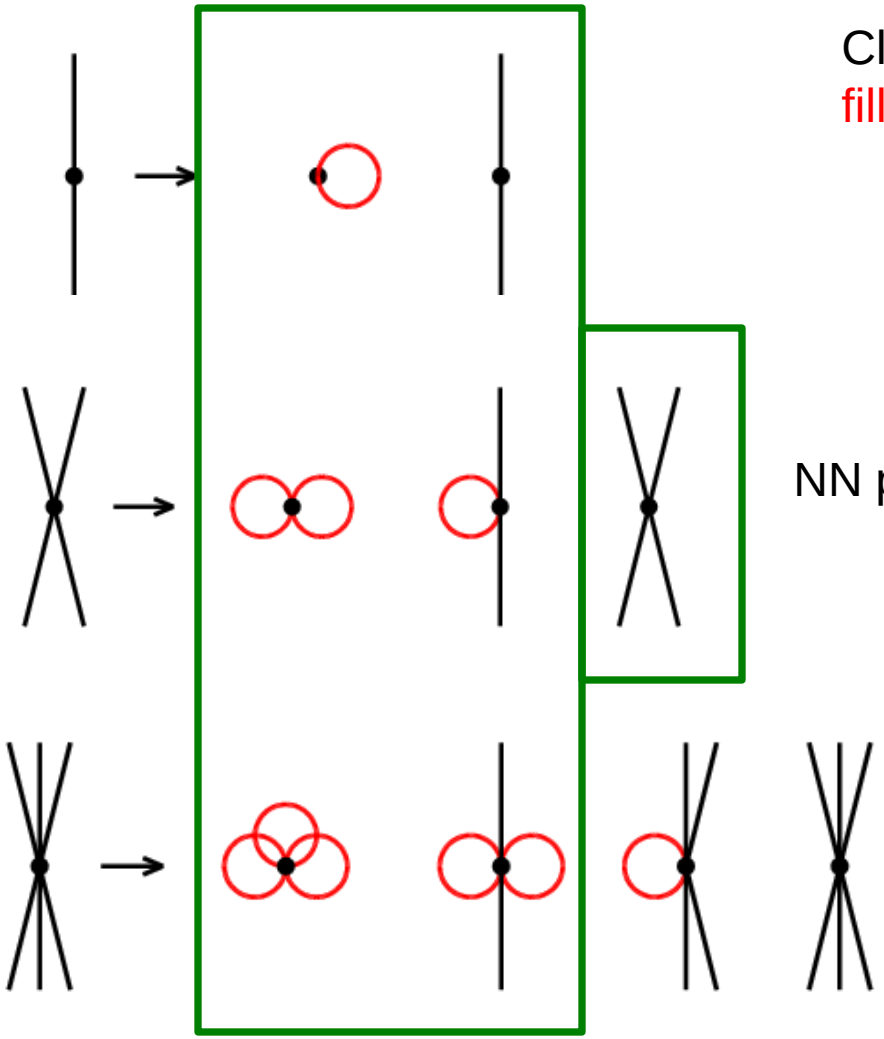
filled orbitals





Closed-shell vacuum
filled orbitals

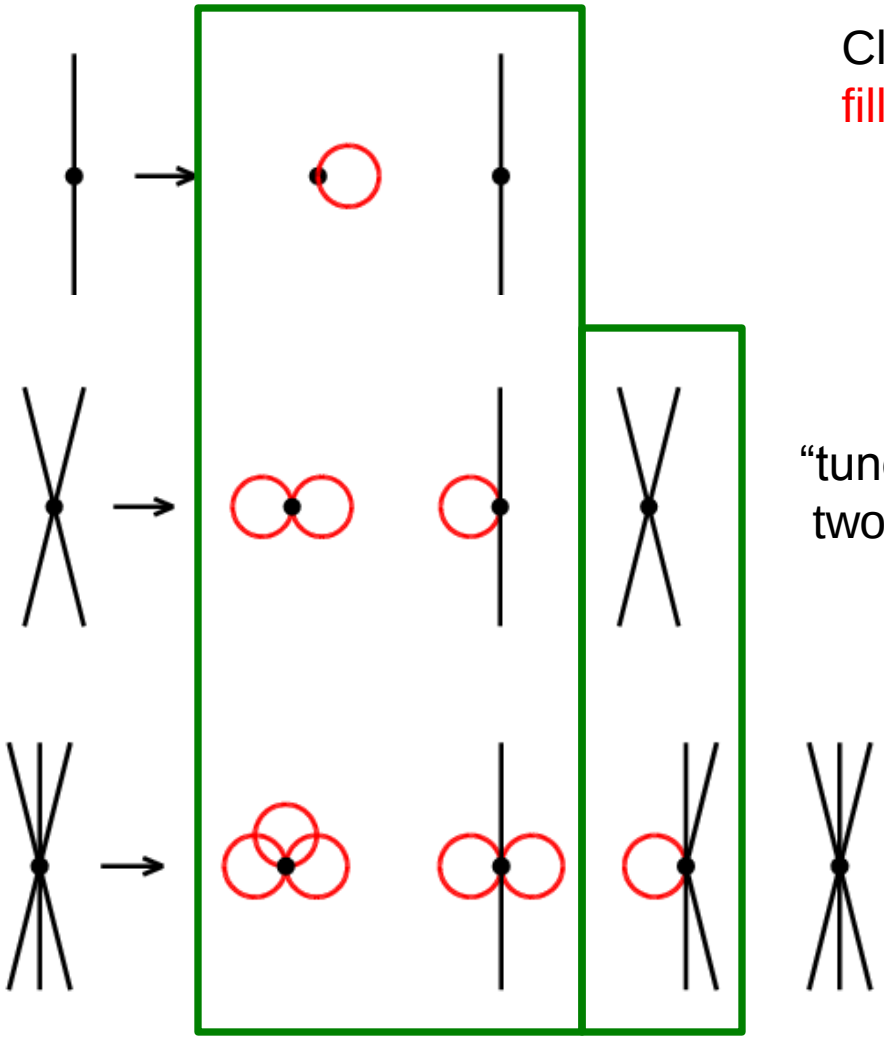
Skyrme
phenomenology



Closed-shell vacuum
filled orbitals

NN potential with V_lowk

Skyrme
phenomenology

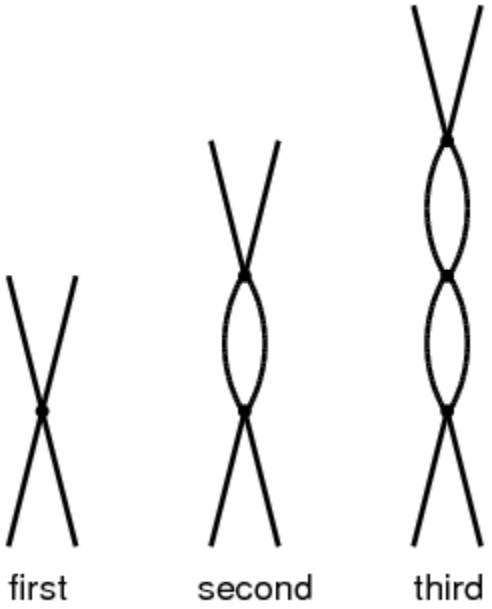


Closed-shell vacuum
filled orbitals

“tuned” valence
two-body matrix elements

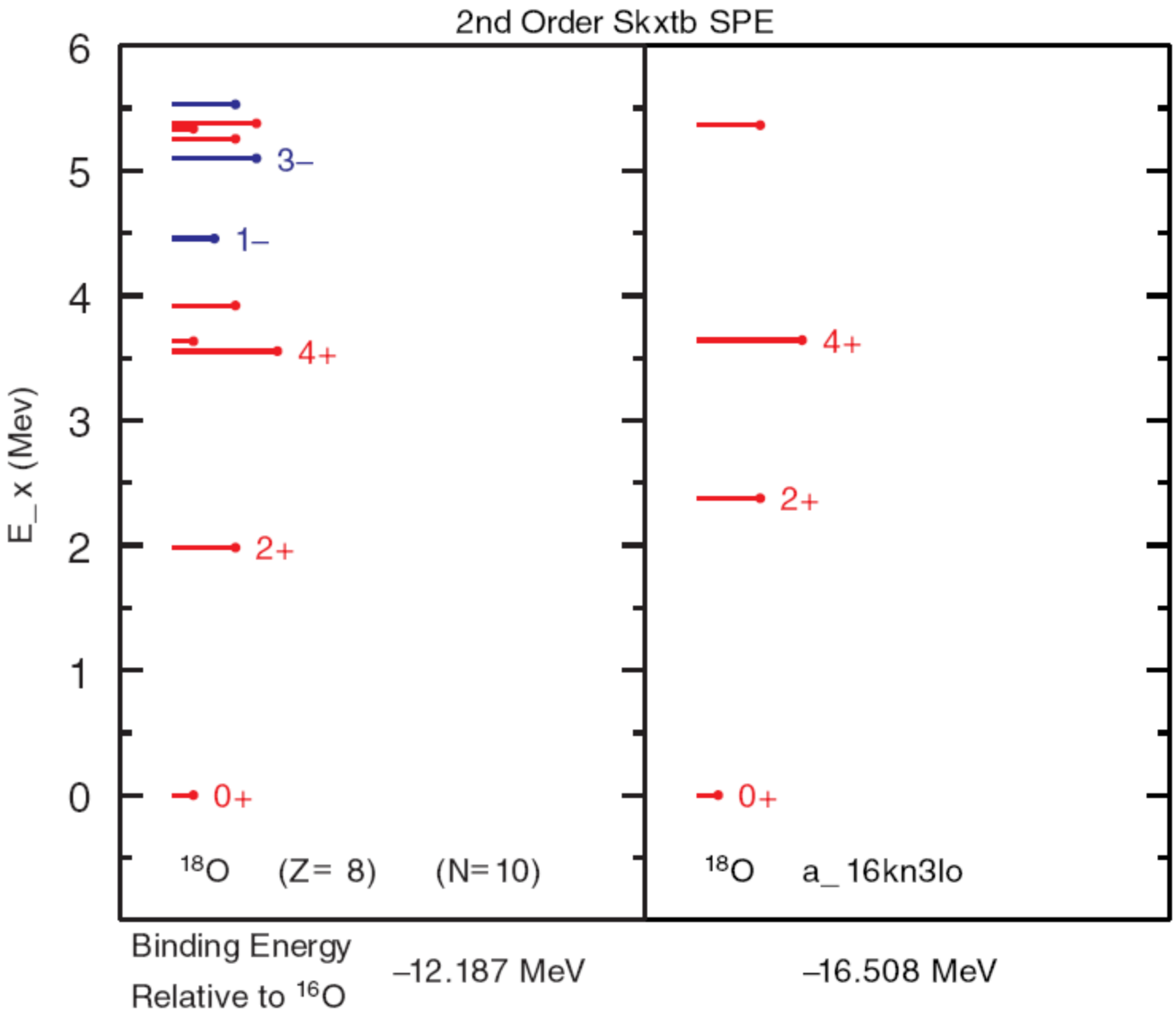
Skyrme
phenomenology

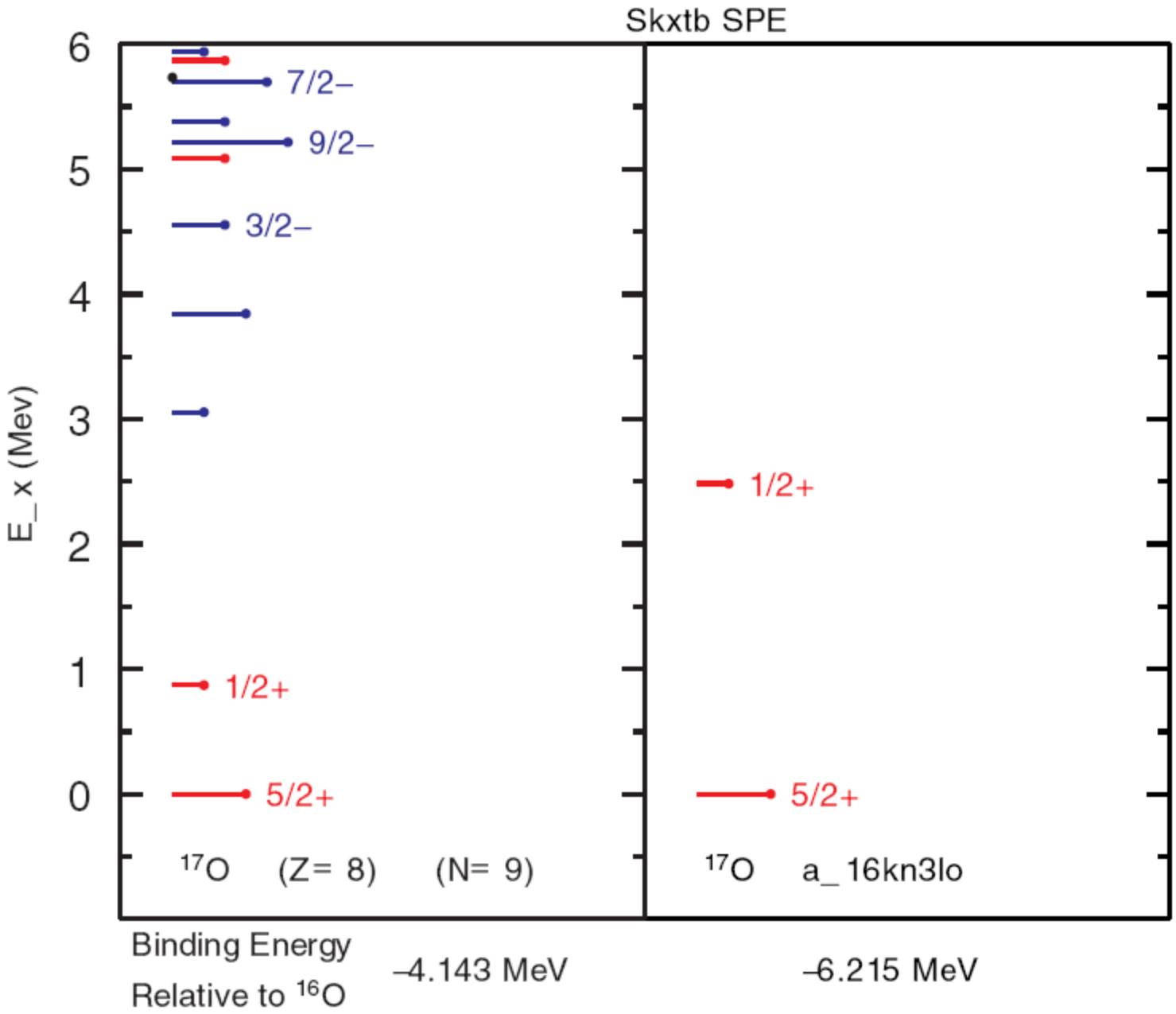
Order of Perturbation Theory

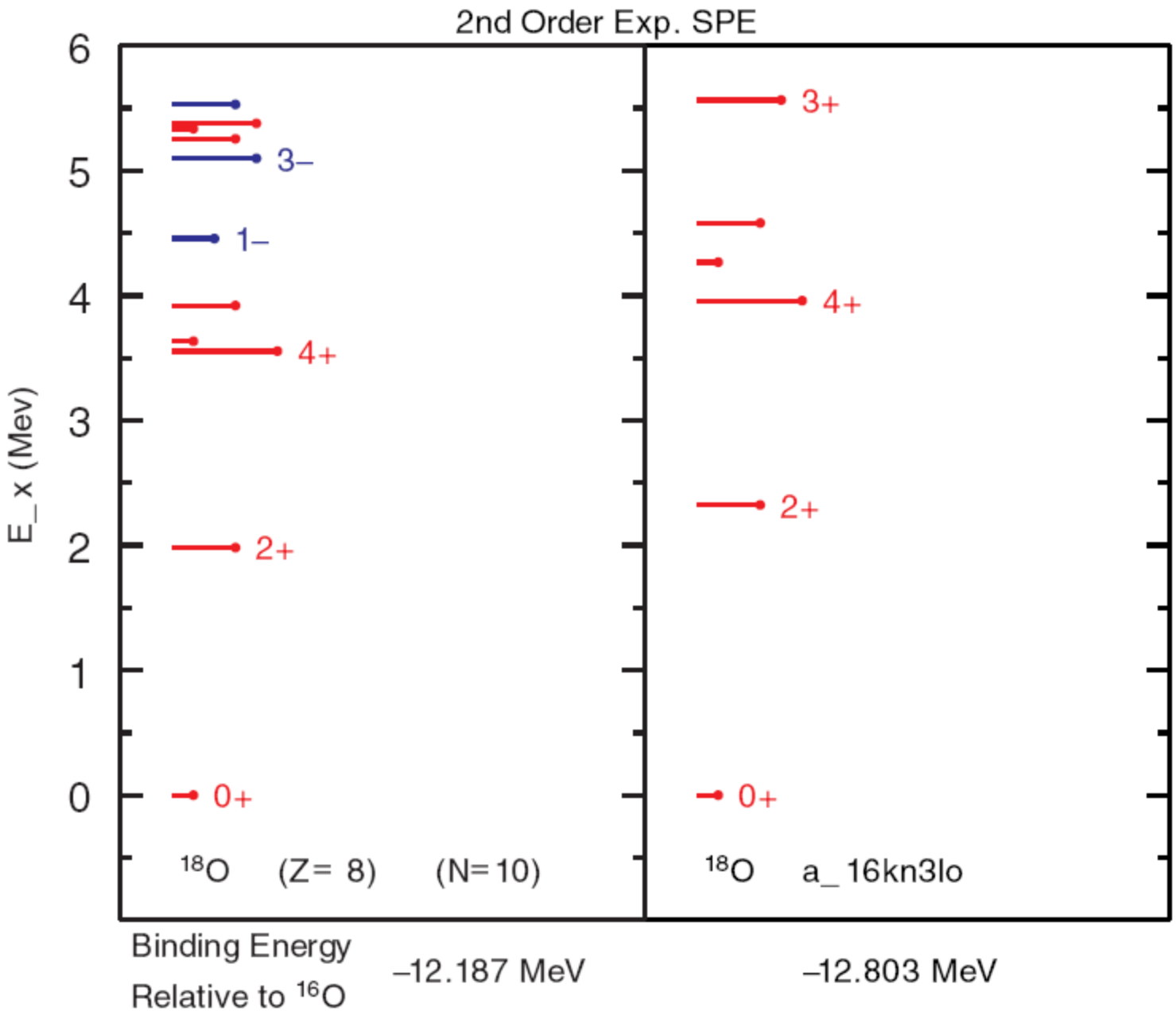


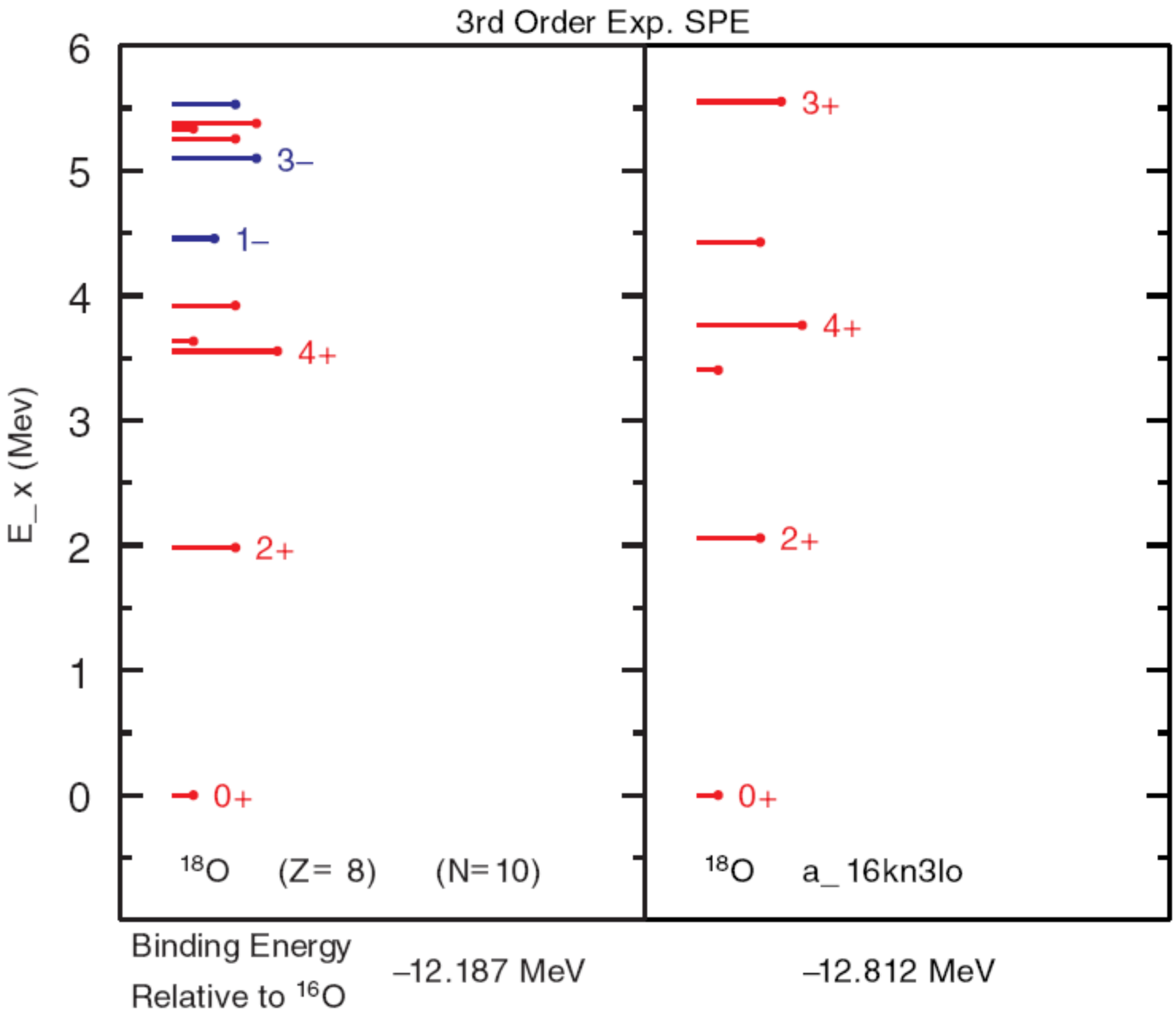
Example of Procedure

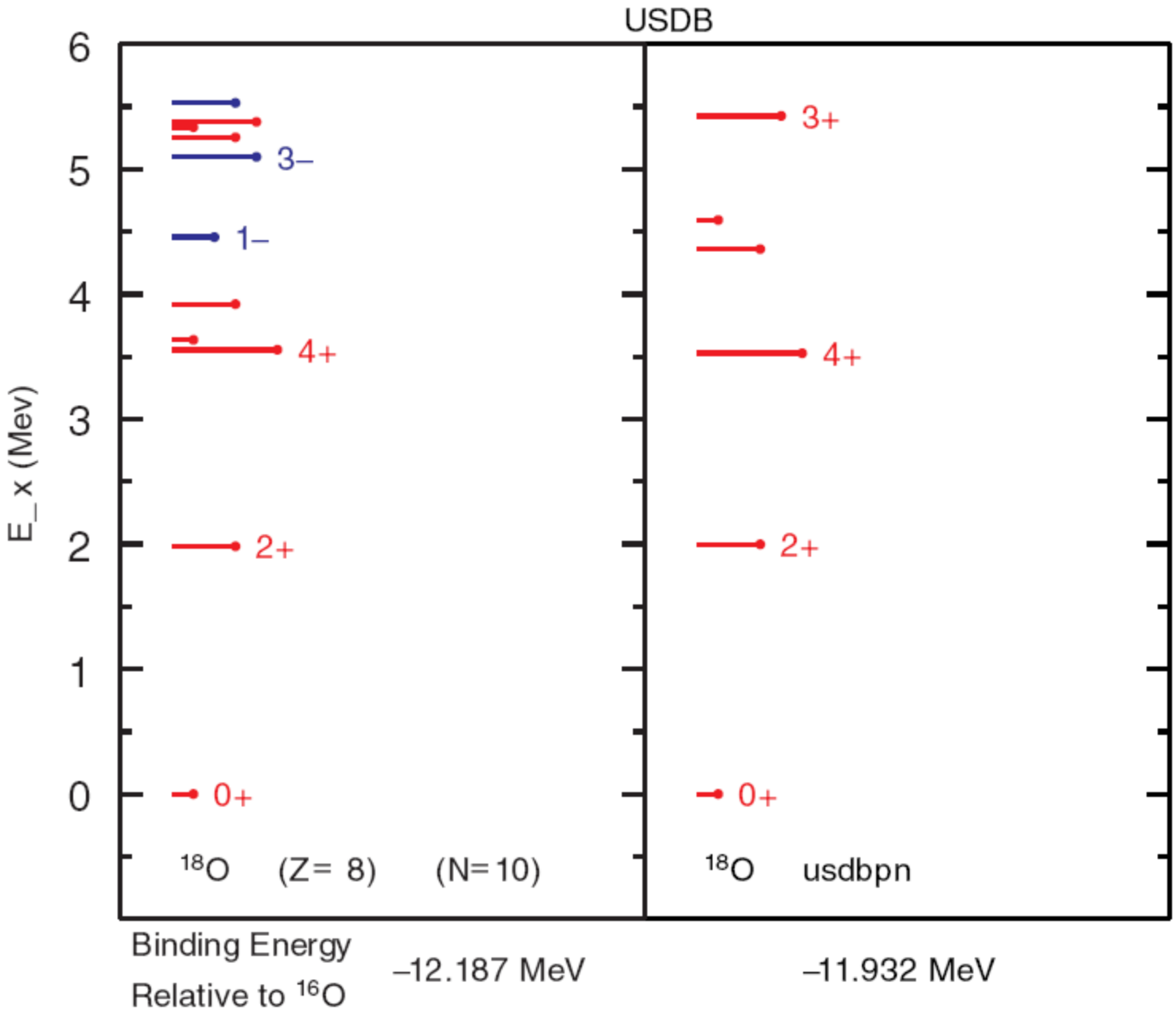
- Start with ^{16}O as a closed core
- Choose sd orbits as model space
- Use Skyrme interaction with a tensor force (skxtb) for Hartree Fock calculations
- Renormalize N3LO interaction with vlowk similarity transformation
- Compare results to experimental data and to phenomenological potentials
- Try to understand discrepancies and establish the best possible method to produce two-body matrix elements

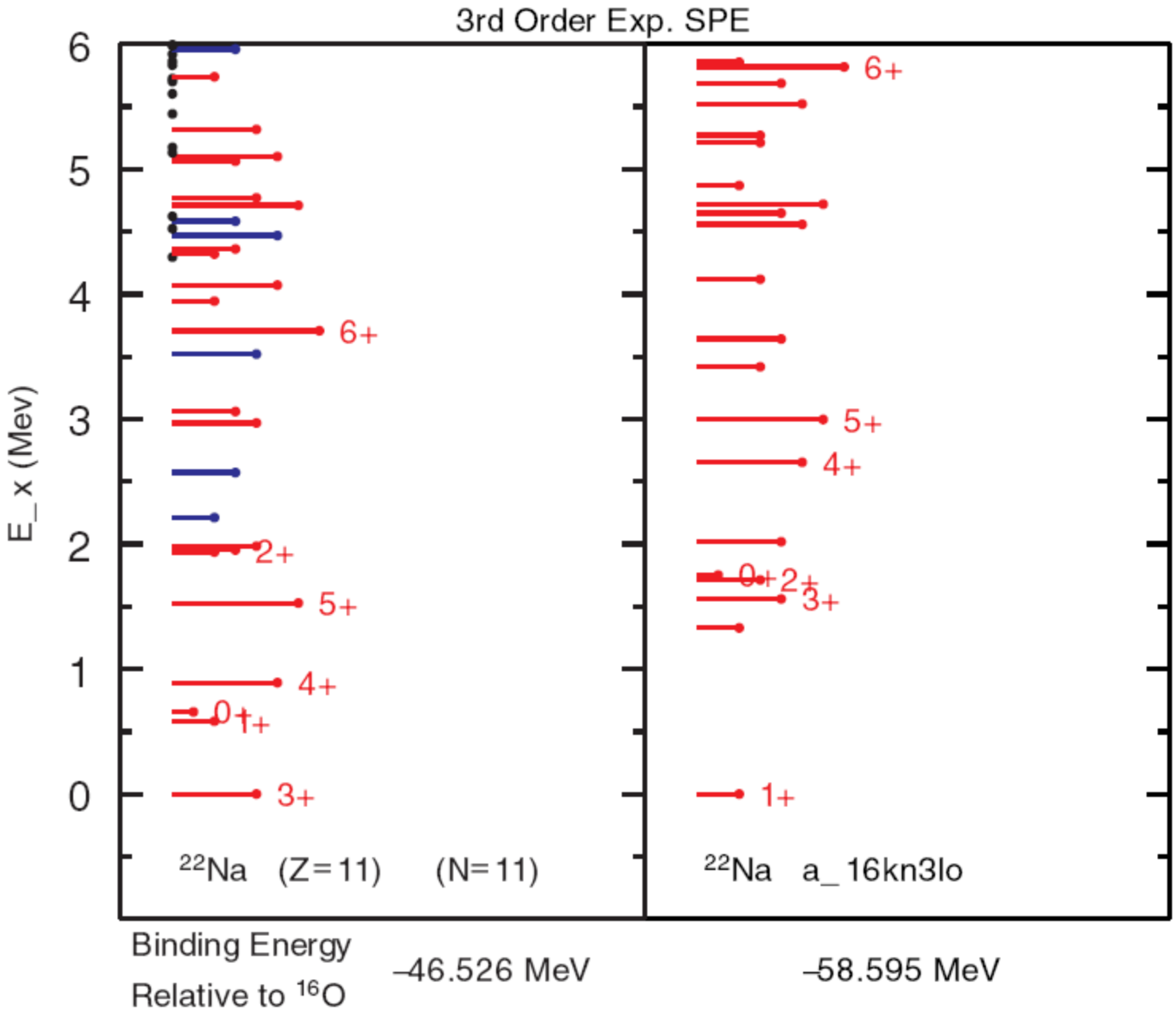

2nd Order Skxtb SPE
E_x (Mev)
6
5
4
3
2
1
0
3–
1–
4+
2+
0+
4+
2+
0+
18O (Z= 8) (N=10)
18O a_16kn3lo
Binding Energy
Relative to 16O
–12.187 MeV
–16.508 MeV

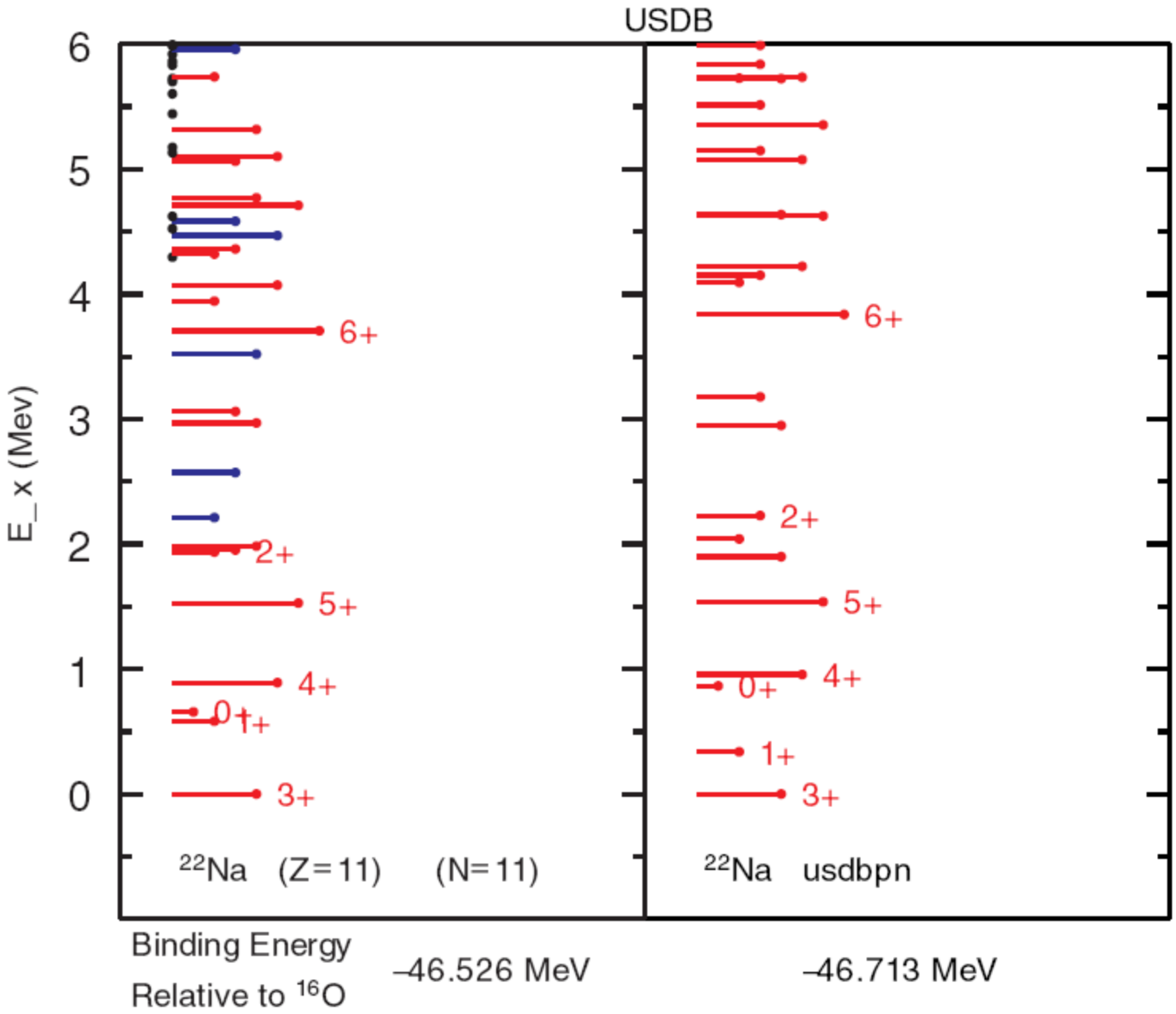

Skxtb SPE
E_x (Mev)
6
5
4
3
2
1
0
7/2–
9/2–
3/2–
1/2+
5/2+
1/2+
5/2+
17O (Z= 8) (N= 9)
17O a_16kn3lo
Binding Energy
Relative to 16O
–4.143 MeV
–6.215 MeV


2nd Order Exp. SPE
E_x (Mev)
6
5
4
3
2
1
0
3–
1–
4+
2+
0+
3+
4+
2+
0+
18O (Z= 8) (N=10)
18O a_16kn3lo
Binding Energy
Relative to 16O
–12.187 MeV
–12.803 MeV

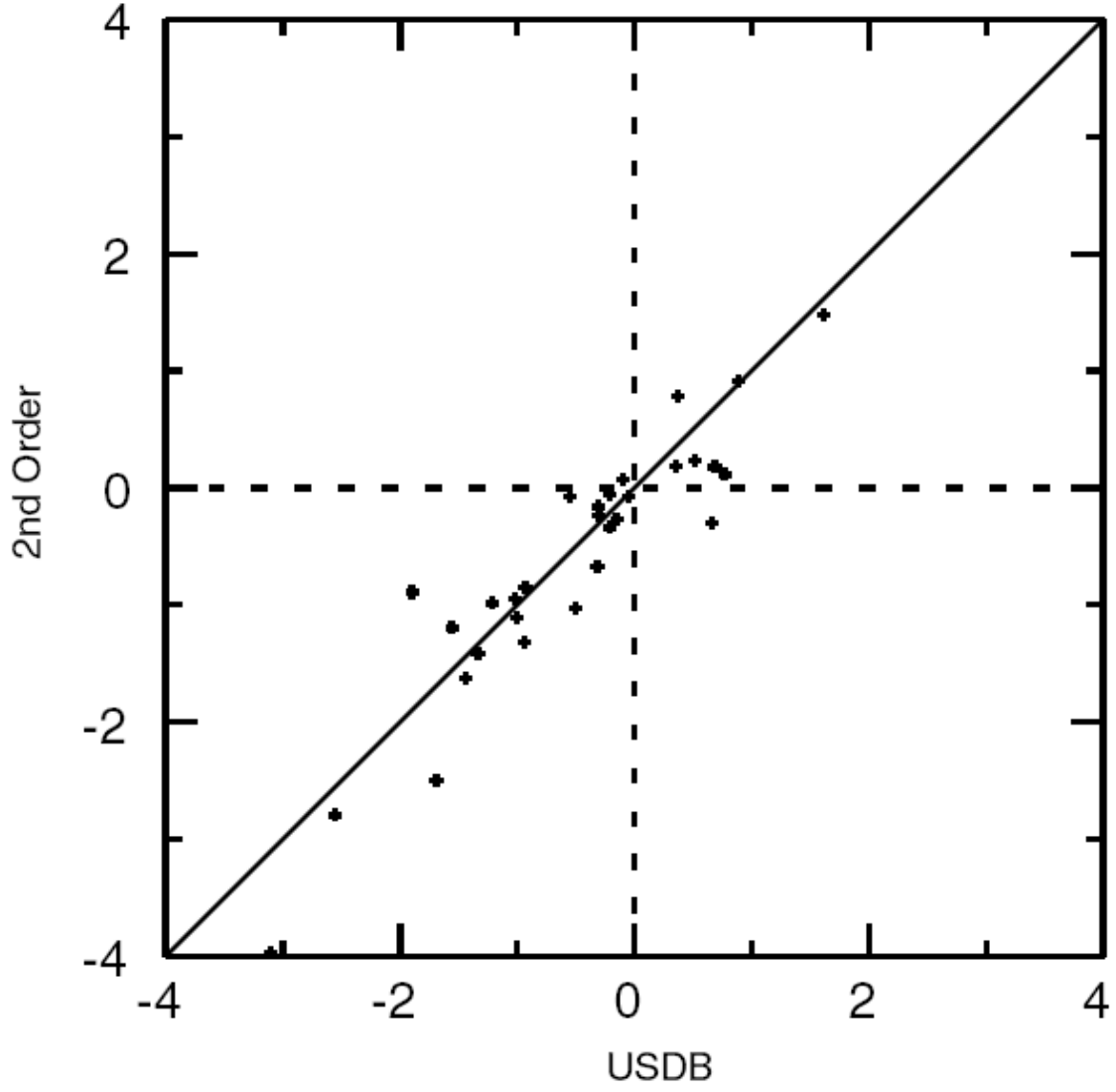

3rd Order Exp. SPE
E_x (Mev)
6
5
4
3
2
1
0
3–
1–
4+
2+
0+
3+
4+
2+
0+
18O (Z= 8) (N=10)
18O a_16kn3lo
Binding Energy
Relative to 16O
–12.187 MeV
–12.812 MeV


USDB
6
5
4
3
2
1
0
E_x (Mev)
3–
1–
4+
2+
0+
3+
4+
2+
0+
18O (Z= 8) (N=10)
18O usdbpn
Binding Energy
Relative to 16O
–12.187 MeV
–11.932 MeV


3rd Order Exp. SPE
E_x (Mev)
6
5
4
3
2
1
0
6+
2+
5+
4+
0+
1+
3+
^{22}Na (Z=11) (N=11)
6+
5+
4+
0+
2+
3+
1+
^{22}Na a_16kn3lo
Binding Energy
Relative to ^{16}O
–46.526 MeV
–58.595 MeV


USDB
E_x (Mev)
6
5
4
3
2
1
0
6+
2+
5+
4+
0+
1+
3+
22Na (Z=11) (N=11)
22Na usdbpn
Binding Energy
Relative to 16O
–46.526 MeV
–46.713 MeV

Comparison of nn orbits

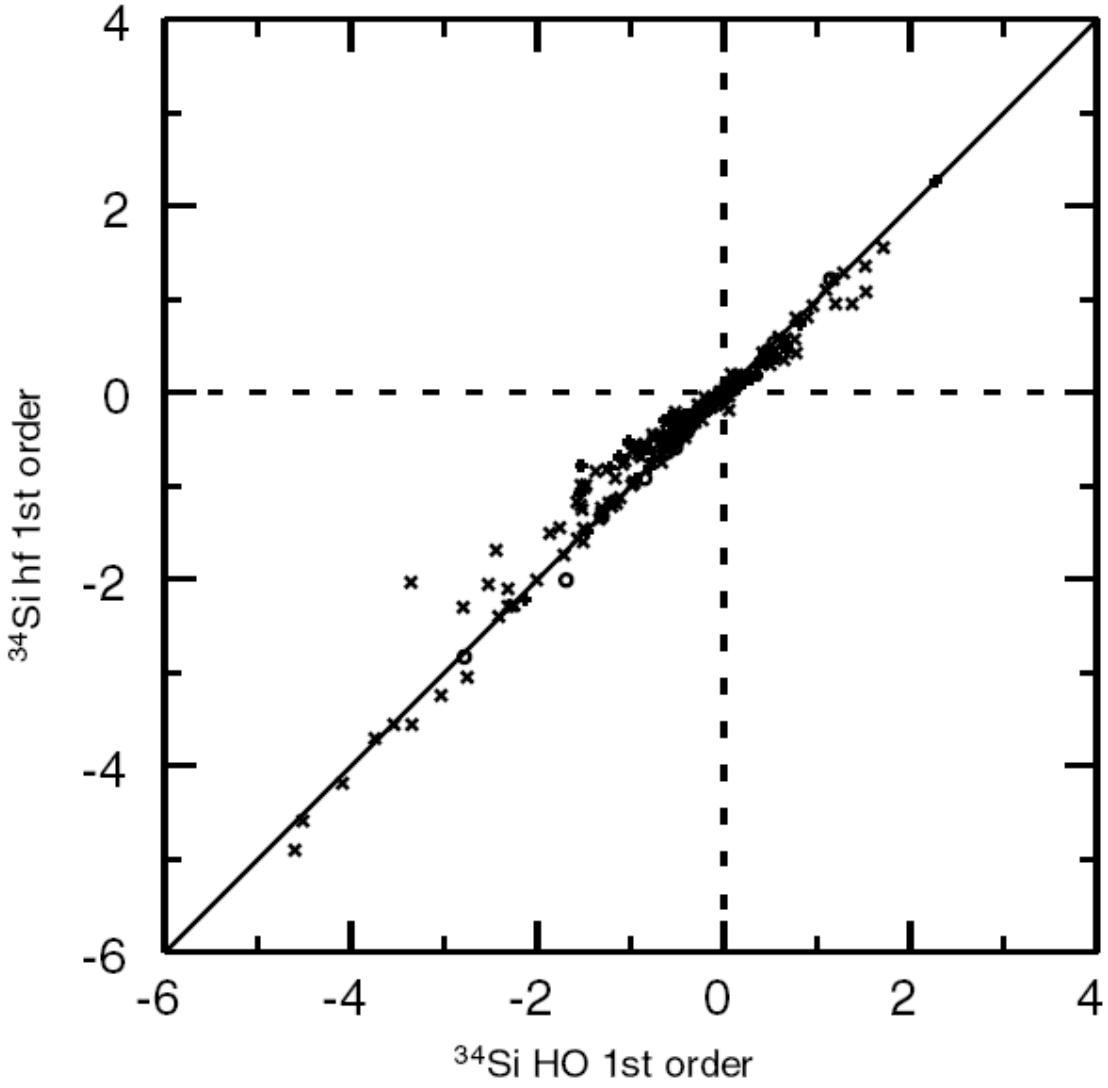


Application to ^{34}Si

- 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 vlowk 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


4
2
0
-2
-4
-6
-6
-4
-2
0
2
4
34Si hf 1st order
34Si HO 1st order

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

Acknowledgements

- Alex Brown
- Morten Hjorth-Jensen
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Renormalization Procedure