CI + EDF methods for nuclear structure

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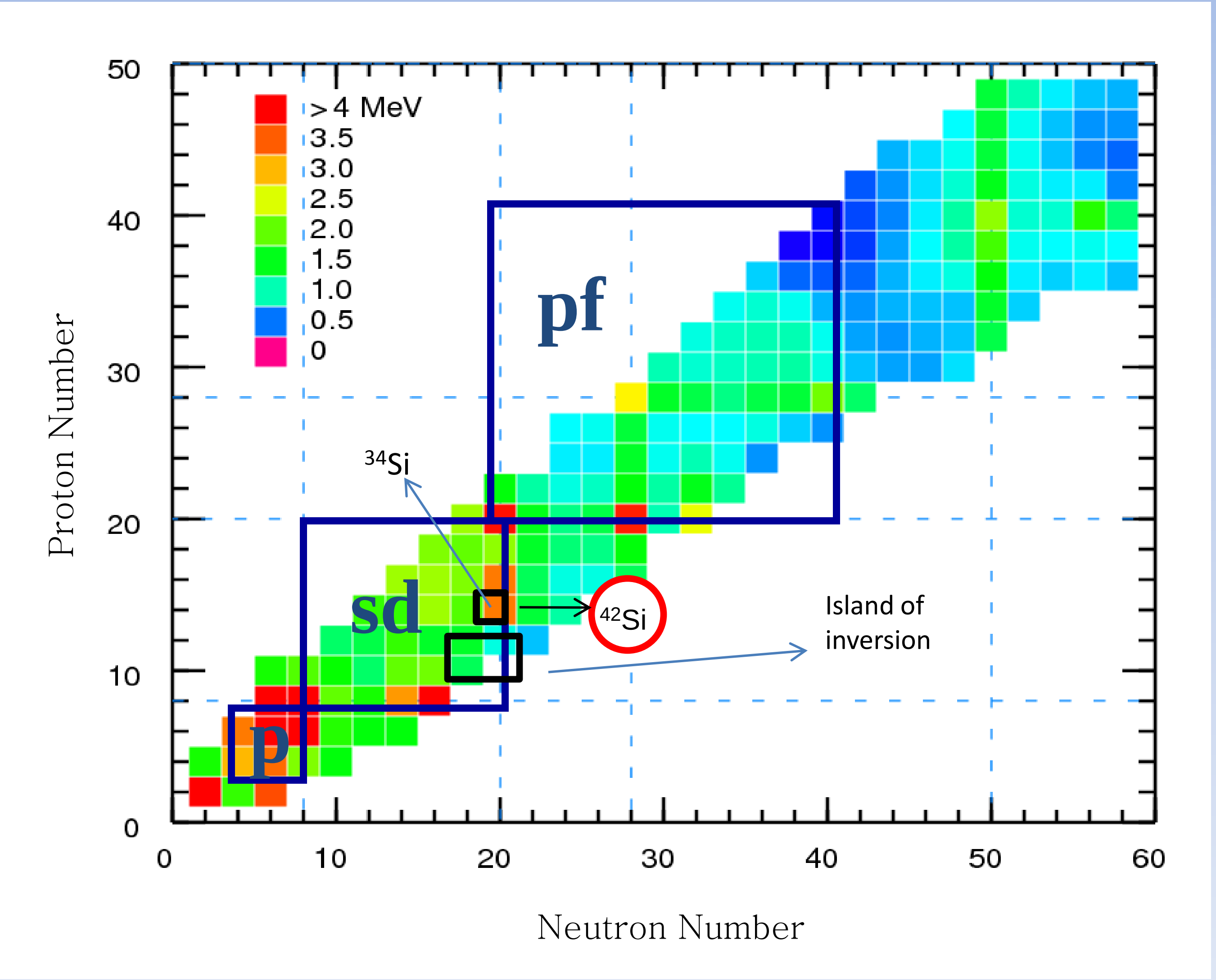
Motivation

- To provide reliable theoretical predictions of nuclear properties for :
  a) nuclei outside of standard model spaces (Ex: ^{42}Si)
  b) nuclei inside standard model spaces that are significantly affected by orbits outside the model space (Ex: island of inversion region)

Regions of Interest

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



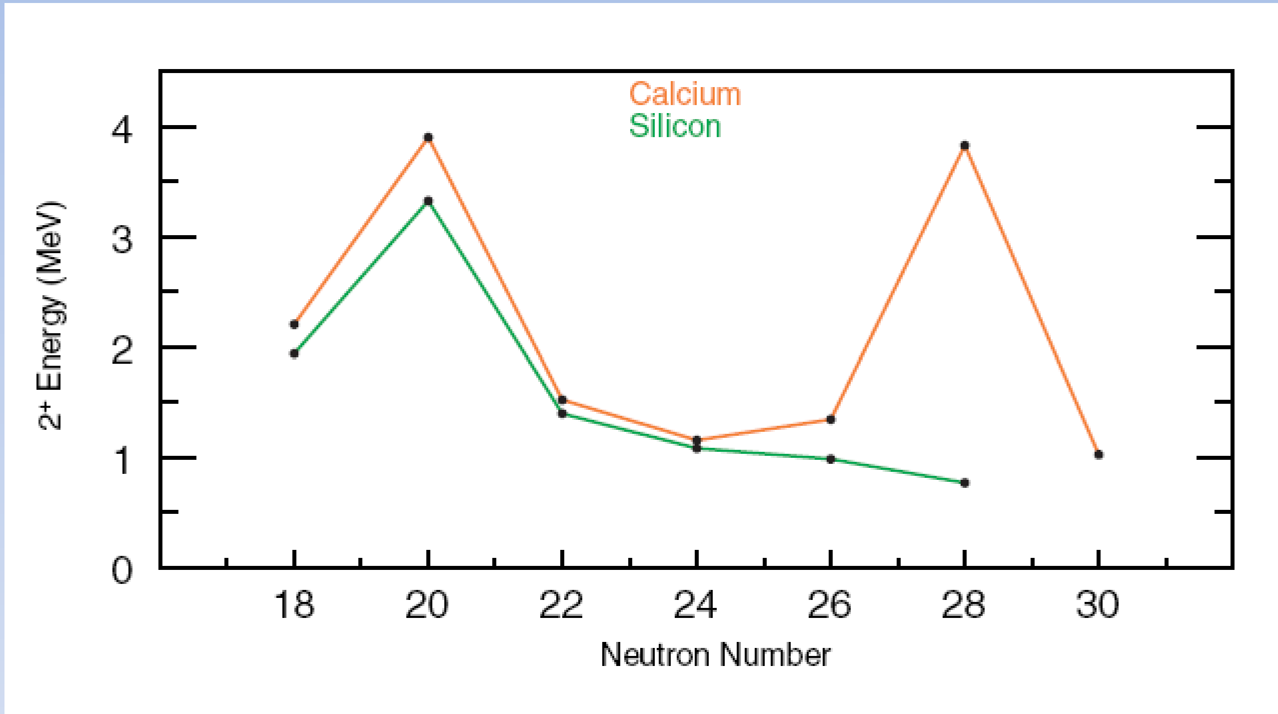
The Case of ^{42}Si

- Very exotic recently observed nucleus
- Interesting due to evolution of N=28 shell structure away from stability
- Outside of standard model spaces
- Simple approximations:

- use model space of sd shell for protons and pf shell for neutrons with USDB interaction for protons and GXPF1 for neutrons

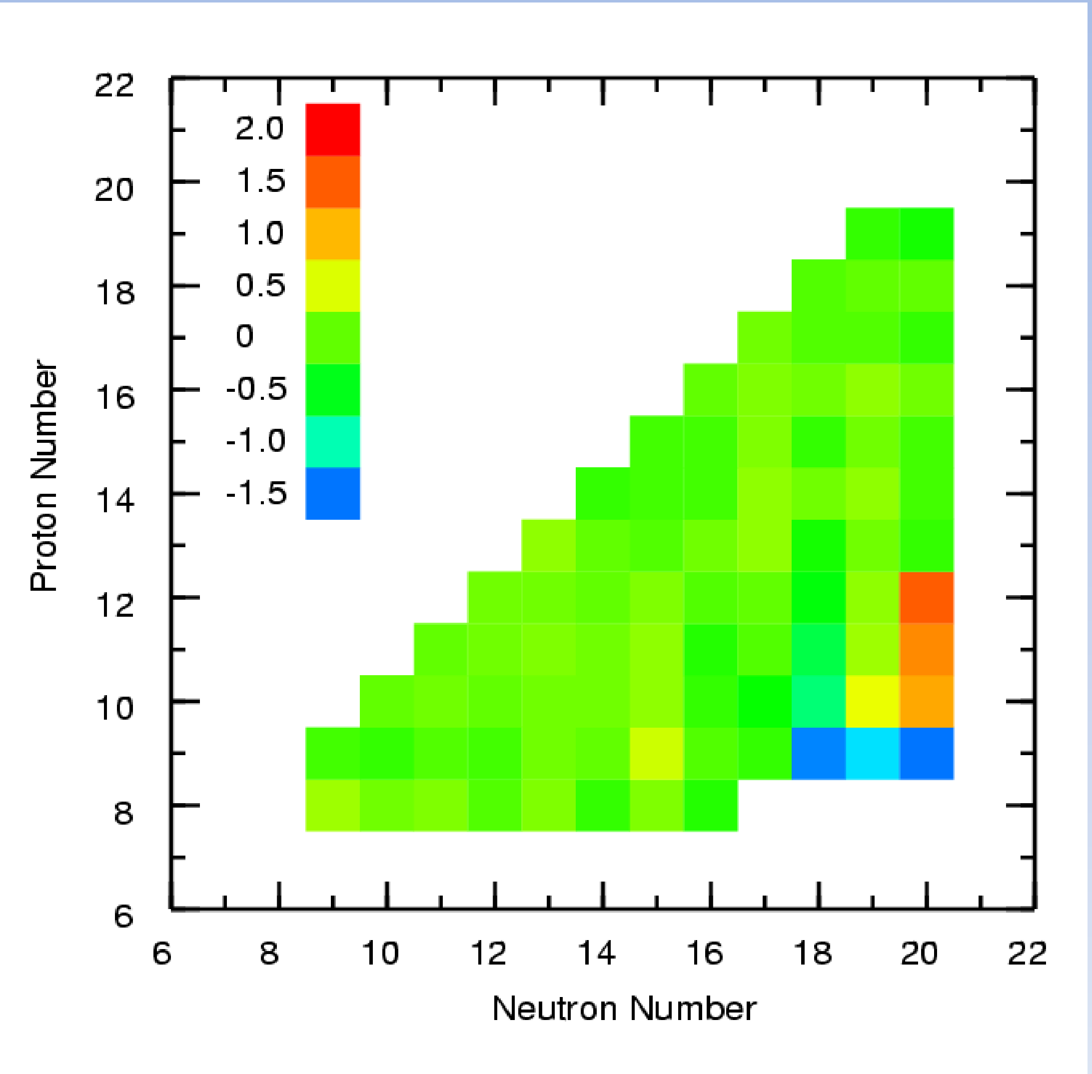
- use spdf model space with truncation

Shell Structure at N=28: Experimental Data



USD Ground State Energies

Legend:
$E_{th} - E_{exp}$
(MeV)

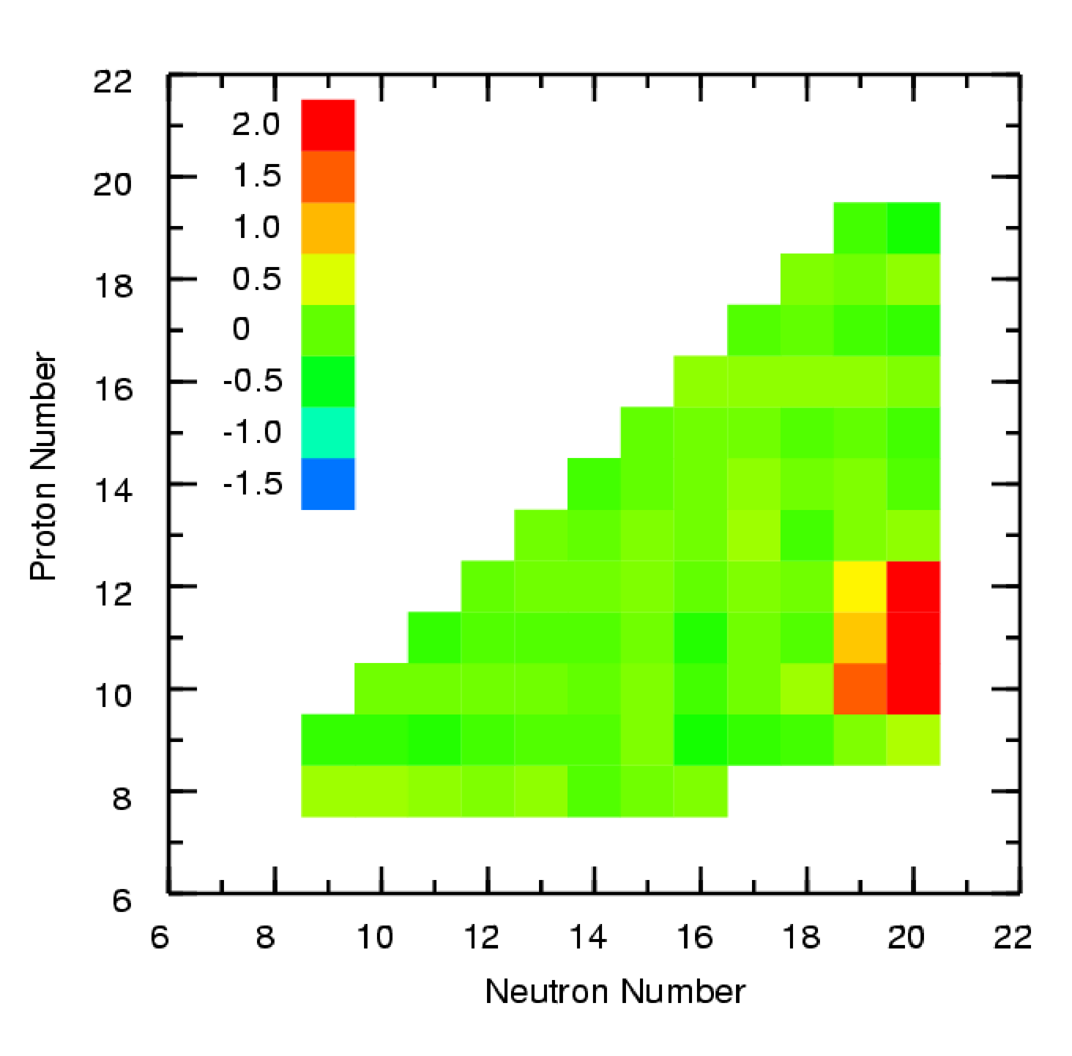


Progress

- USDA/B interactions created in 2006 due in part to experimental interest in exotic nuclei in the sd shell
- 608 energy levels in the fit- more due to experimental progress in 20 years
- Many new levels were far from valley of stability, resulting in better agreement for exotic nuclei

USDB Ground State Energies

Legend:
$E_{th} - E_{exp}$
(MeV)



B.A.Brown and W.A. Richter, PRC 74, 034315 (2006)

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
- Find uncorrelated SPEs by calculating single particle states relative to the target nucleus

Application to ^{34}Si

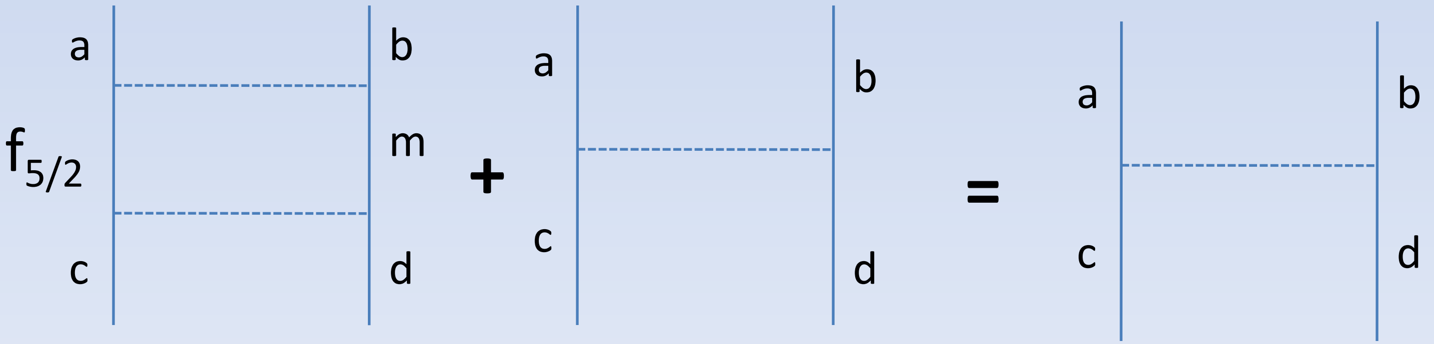
- Best target for calculations in the island of inversion region; also provides starting point for calculations of ^{42}Si
- Model space is sd shell plus pf neutron orbits (10 orbits total)
- “vlowk” similarity transformation used to renormalize the N3LO interaction to third order in perturbation theory up to $8\hbar\omega$
- Harmonic oscillator wavefunctions and SPEs used for renormalization
- Skyrme interaction with a tensor force (skxtb) chosen for Hartree Fock calculations

Method for CI calculation

- 1st iteration: use TBME and HF SPEs as input, truncate space by filling ν-$d_{5/2}$ and not allowing ν-$f_{5/2}$ excitations
- Do not reproduce experimental level schemes, even in 1p/1h states
- Know that different Skyrme interactions result in SPEs that vary by ~ 1 MeV – any specific choice does not produce reliable SPEs for use in CI calculation

Fitting Procedure

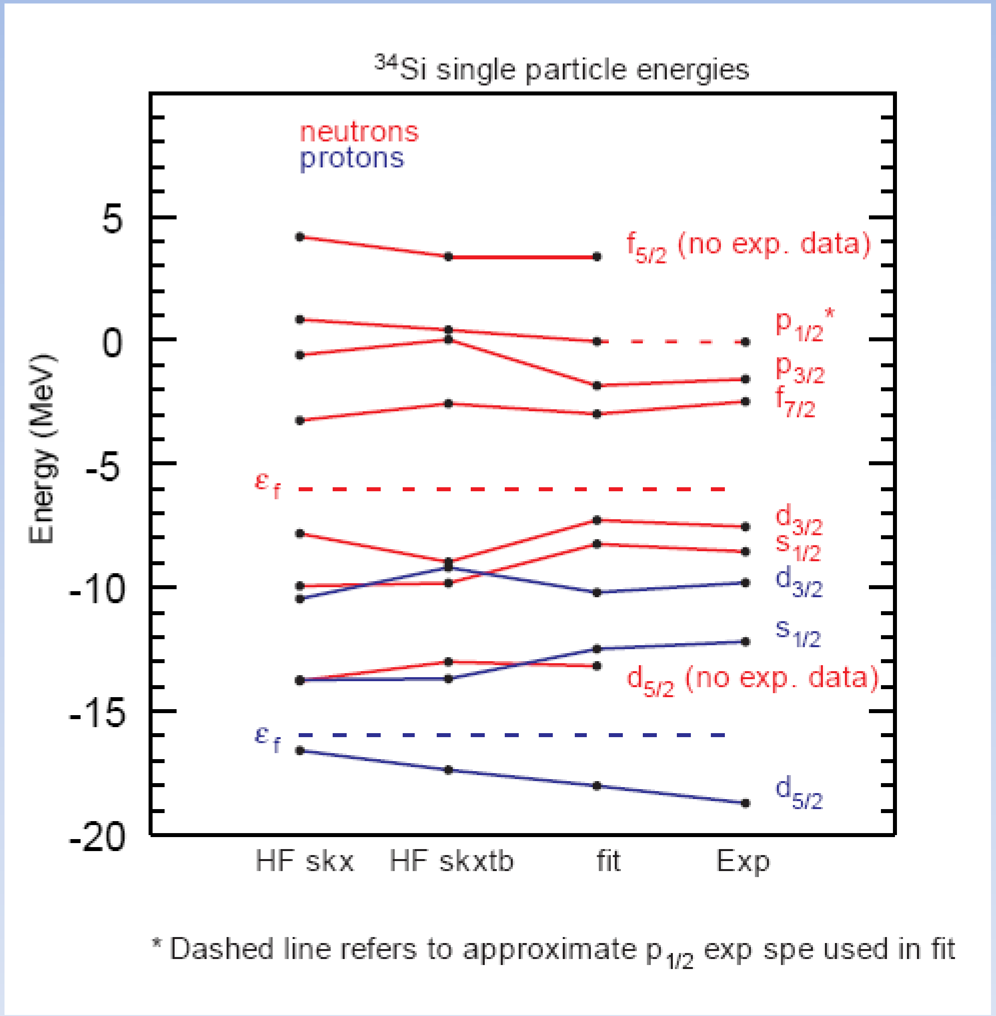
- Treat SPEs as parameters
- Fit to 27 states in $^{32\text{-}36}Si$, ^{33}Al, ^{35}P, $^{31,32}Mg$, ^{36}S
- Use singular value decomposition method to derive best fit SPEs in the highly correlated system
- Account for truncated orbits Ex: $\nu\text{-}f_{5/2}$



Fitting Procedure II

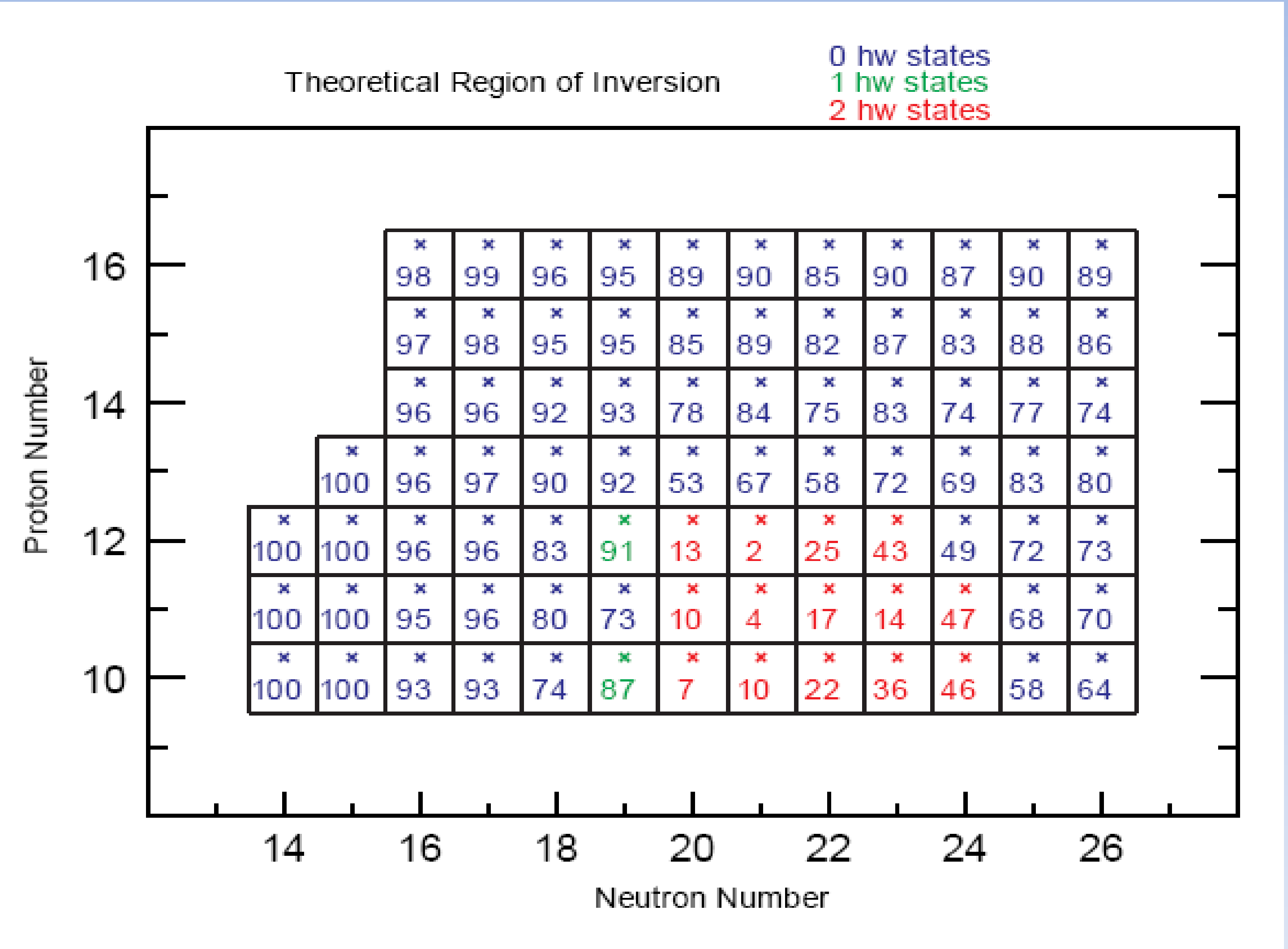
- One extra parameter, an overall normalization of the interaction, also included to improve E_x of 2^+ states in 2p/2h nuclei
- Needed to account for the spread of the wavefunction for loosely bound neutrons -> HO wavefunctions are not sufficient
- Iterative fit run again to find new SPEs
- Rms of 27 levels in the fit: 256 keV
- ^{34}Si Correlation Energy: -1.993MeV
- Interaction then used to calculate nuclei of recent experimental interest in or near the island of inversion

Evolution of SPEs

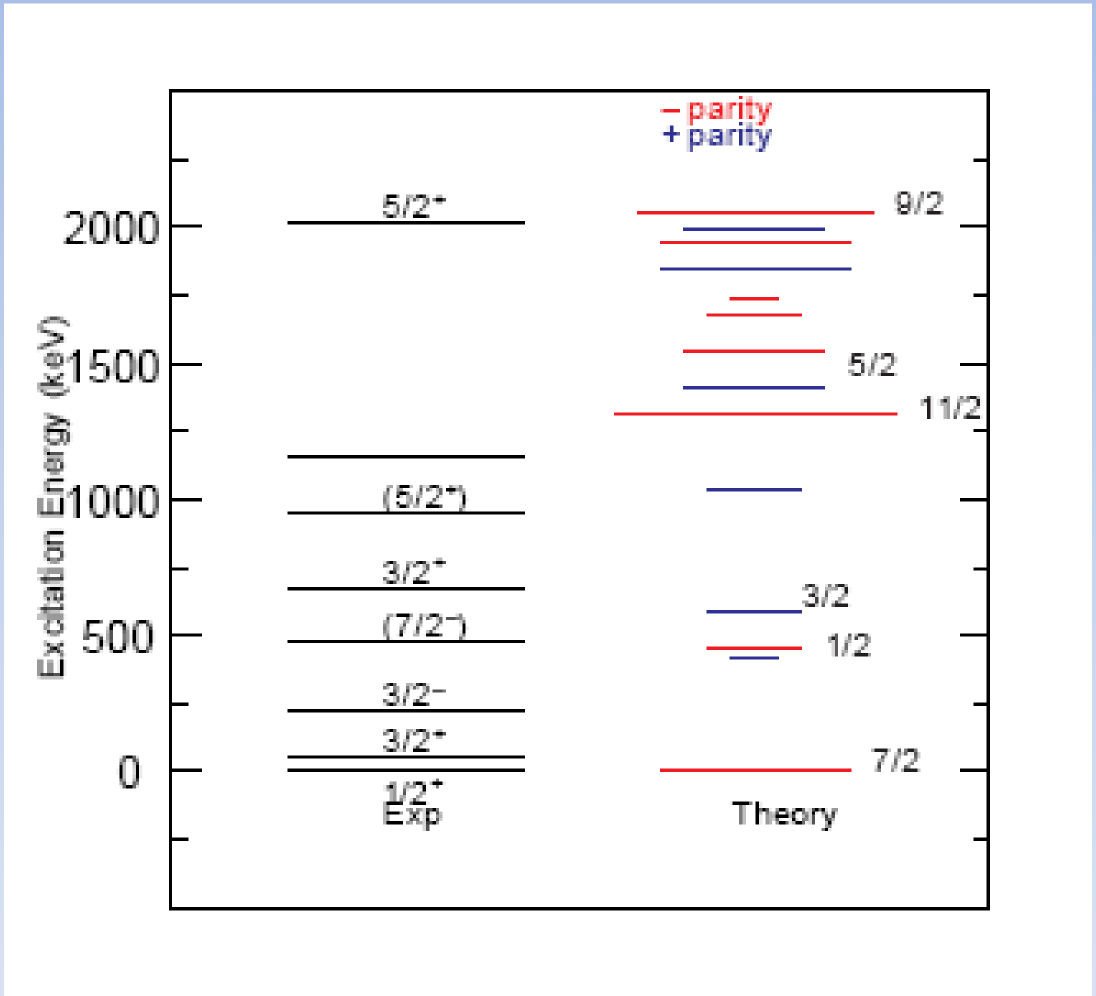


B.A. Brown, PRC 58, 220 (1998)
B.A.Brown et al., PRC 74 061303(R) (2006)

Region of Inversion from fit to ^{34}Si

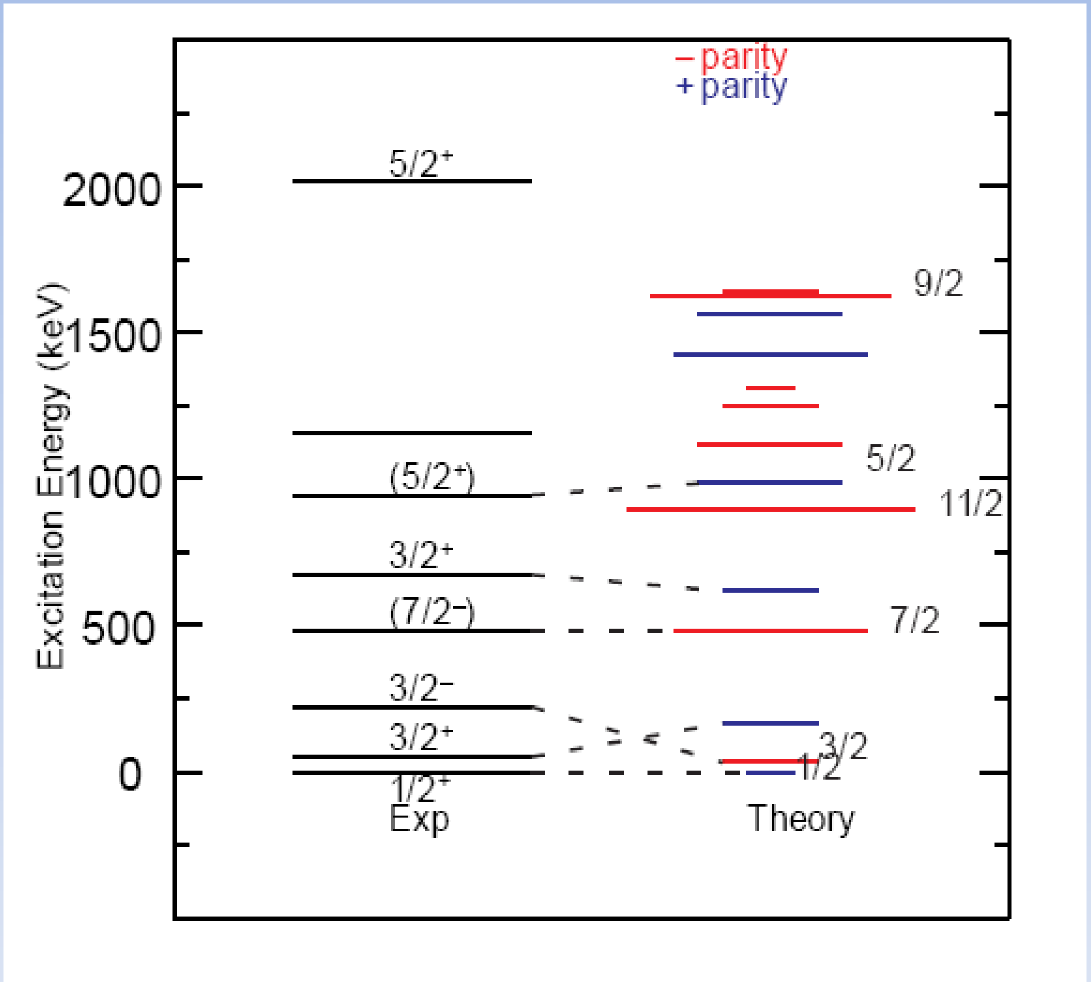


^{31}Mg Level Scheme



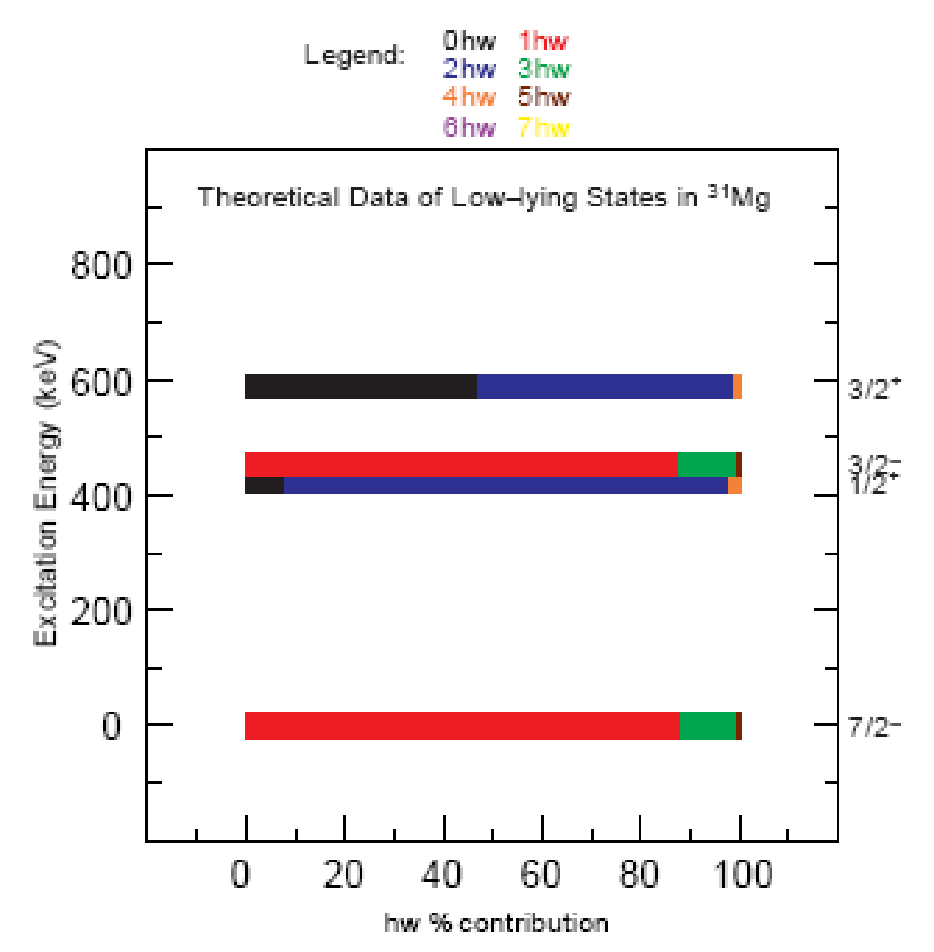
D. Miller et al., PRC 79, 054306 (2009)

^{31}Mg Modified* Level Scheme

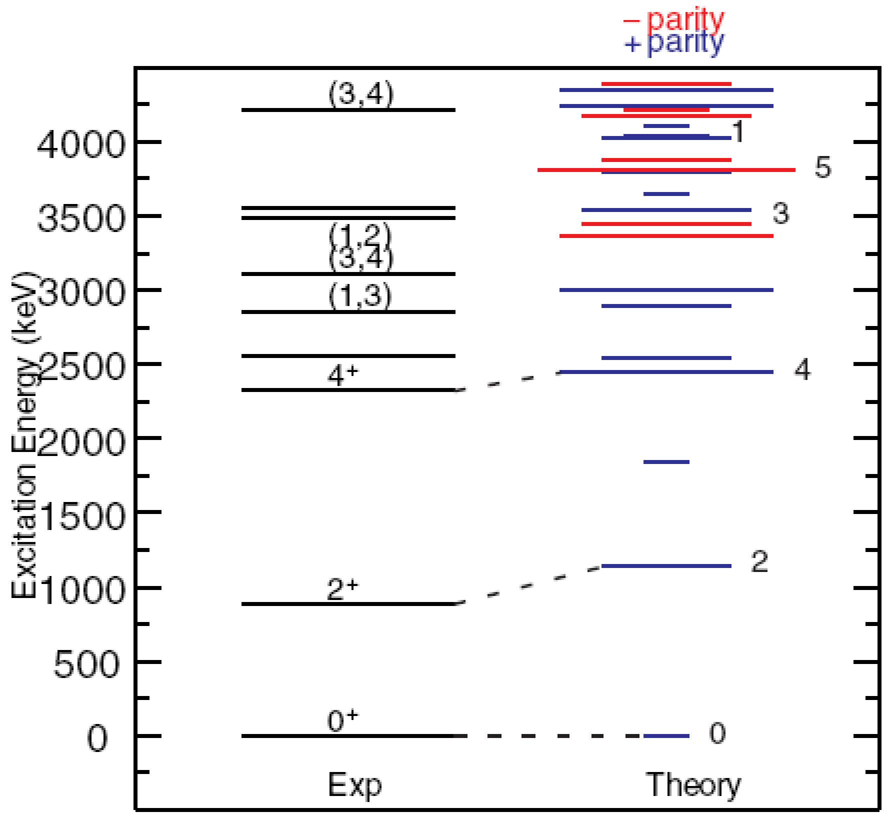


* Energy of lowest $7/2^-$ state increased by 900 keV

Breakdown of ^{31}Mg States



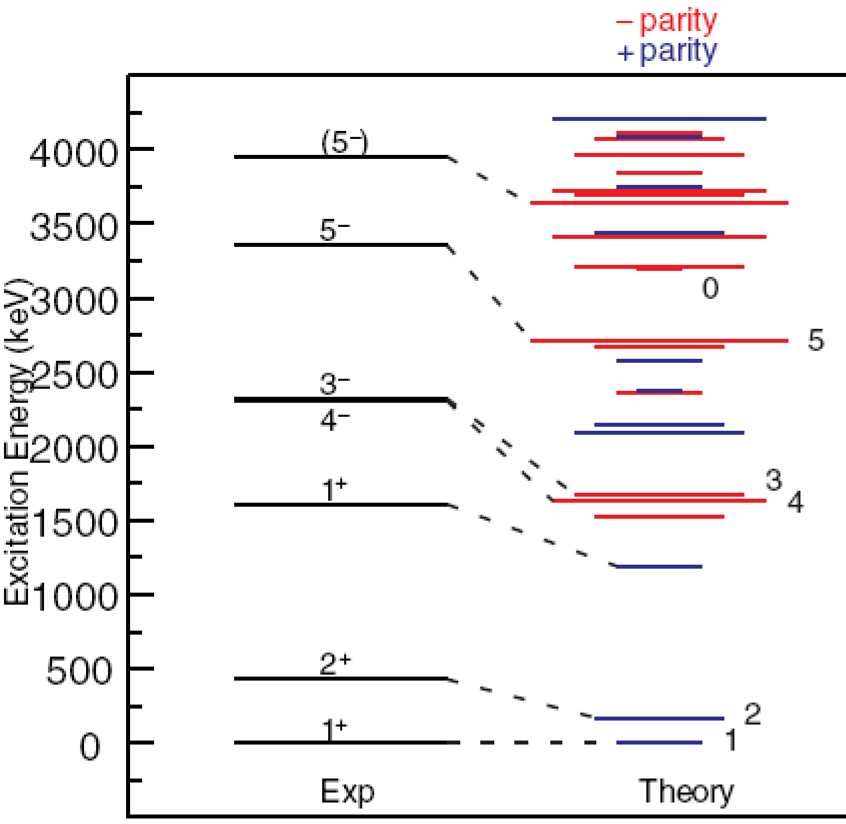
^{32}Mg Level Scheme



^{32}Mg Level Scheme

S. Takeuchi et al., PRC 79, 054319 (2009)

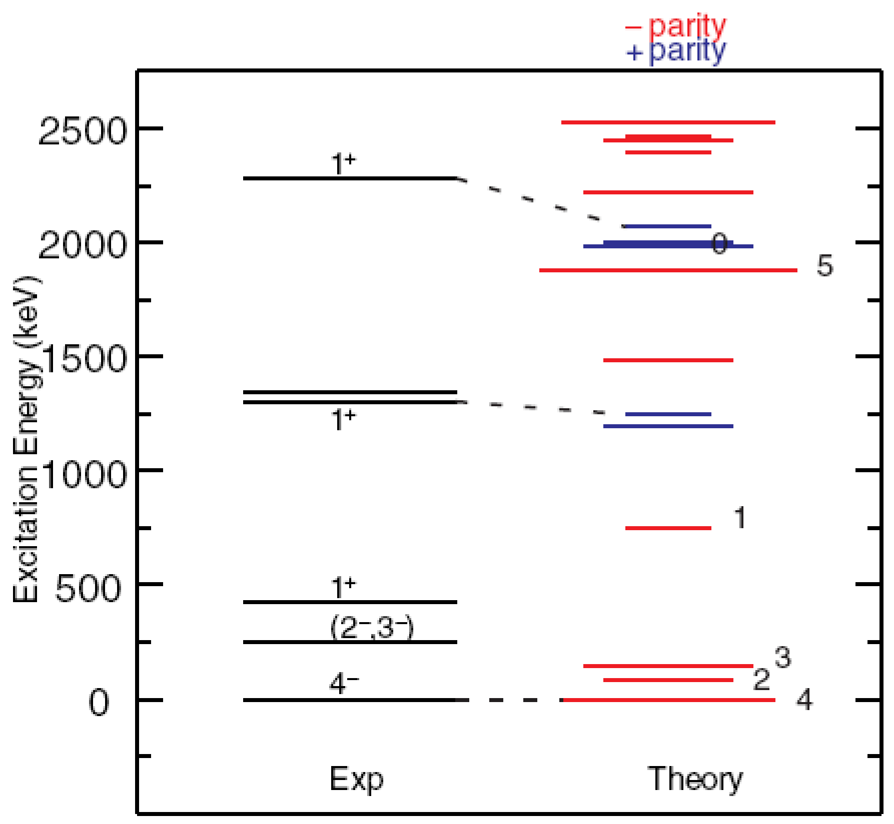
^{34}P Level Scheme



^{34}P Level Scheme

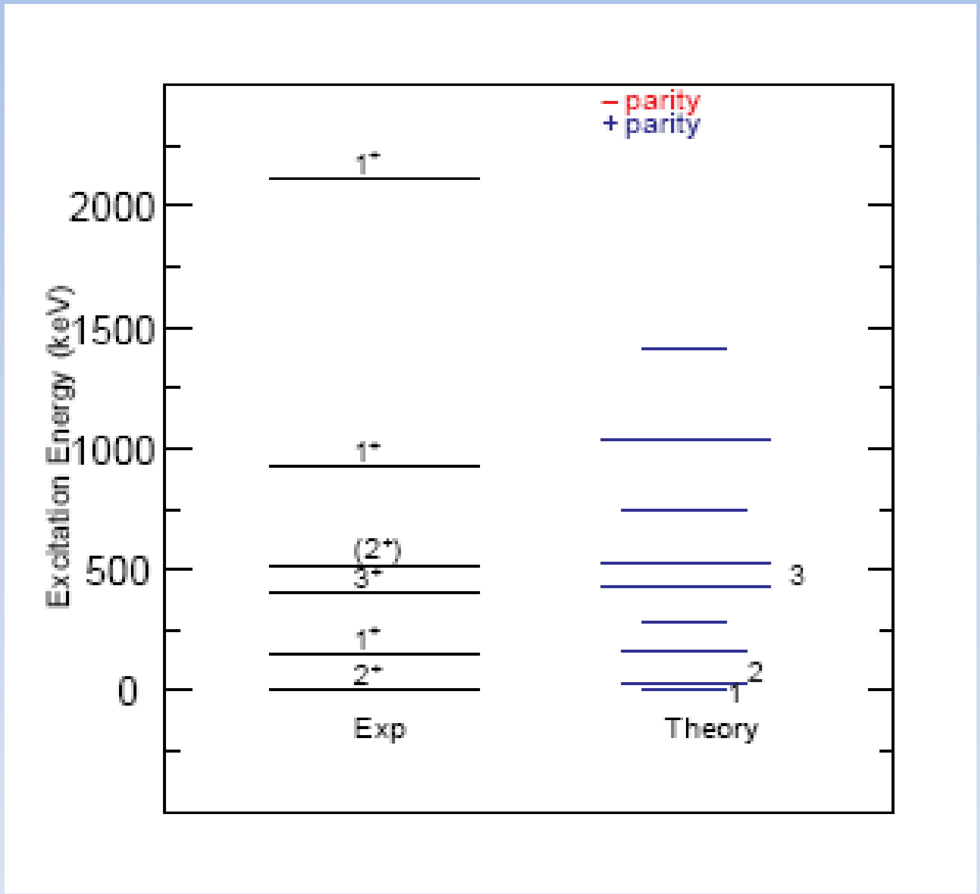
P.C. Bender et al., unpublished

^{36}P Level Scheme



^{36}P Level Scheme

Due to Discussion: ^{30}Na

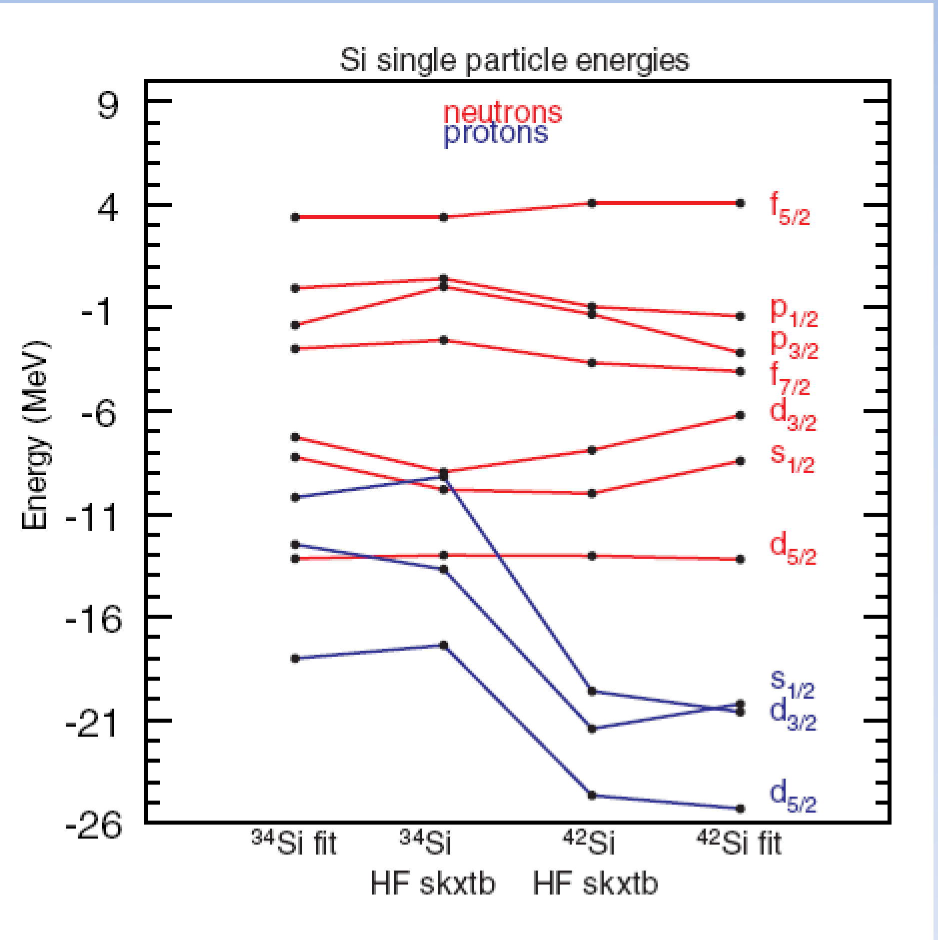


Application to ^{42}Si

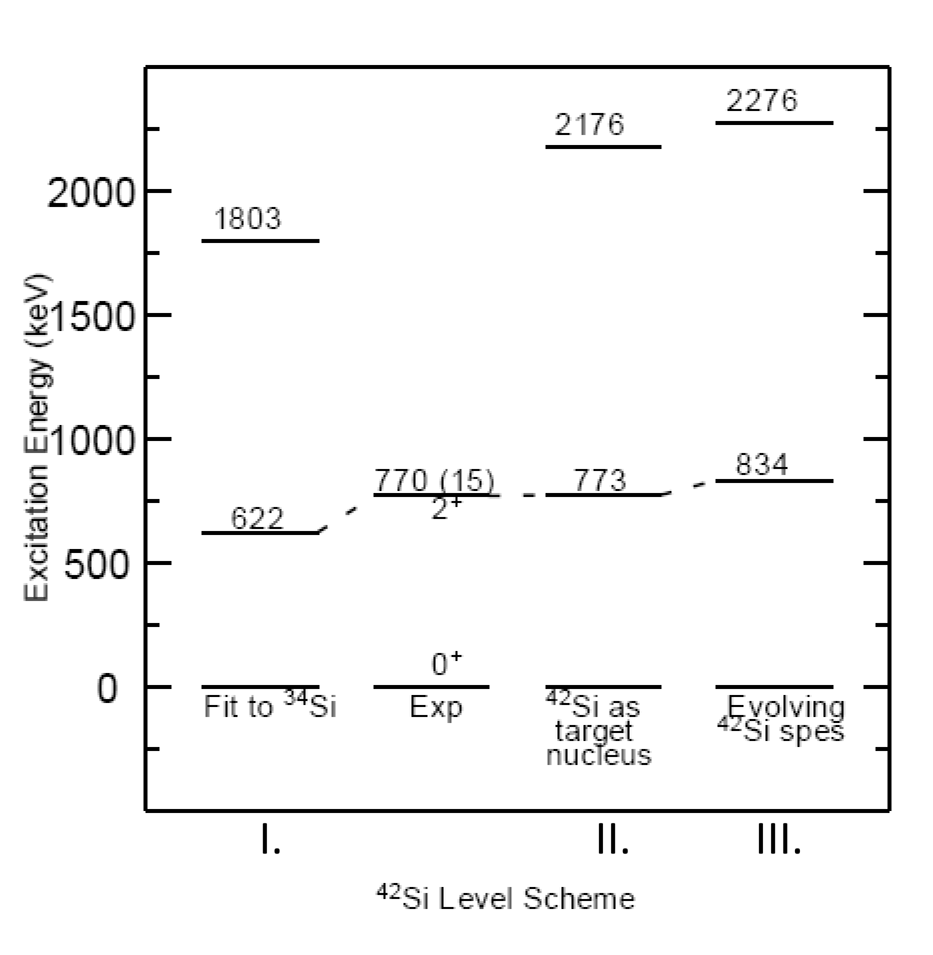
- Three approaches:
- I. Calculation using fit to ^{34}Si
- II. Calculation using ^{42}Si as target nucleus with the same model space used for ^{34}Si, reproducing HF spes
- III. Same as II., except that the spes are modified such that spes satisfy
  $^{34}Si(fit)-^{34}Si(HF) = ^{42}Si(fit)-^{42}Si(HF)$

"evolving" spes based on behavior for a more stable isotope where experimental data exists

Evolution of SPEs in Si



^{42}Si Level Schemes

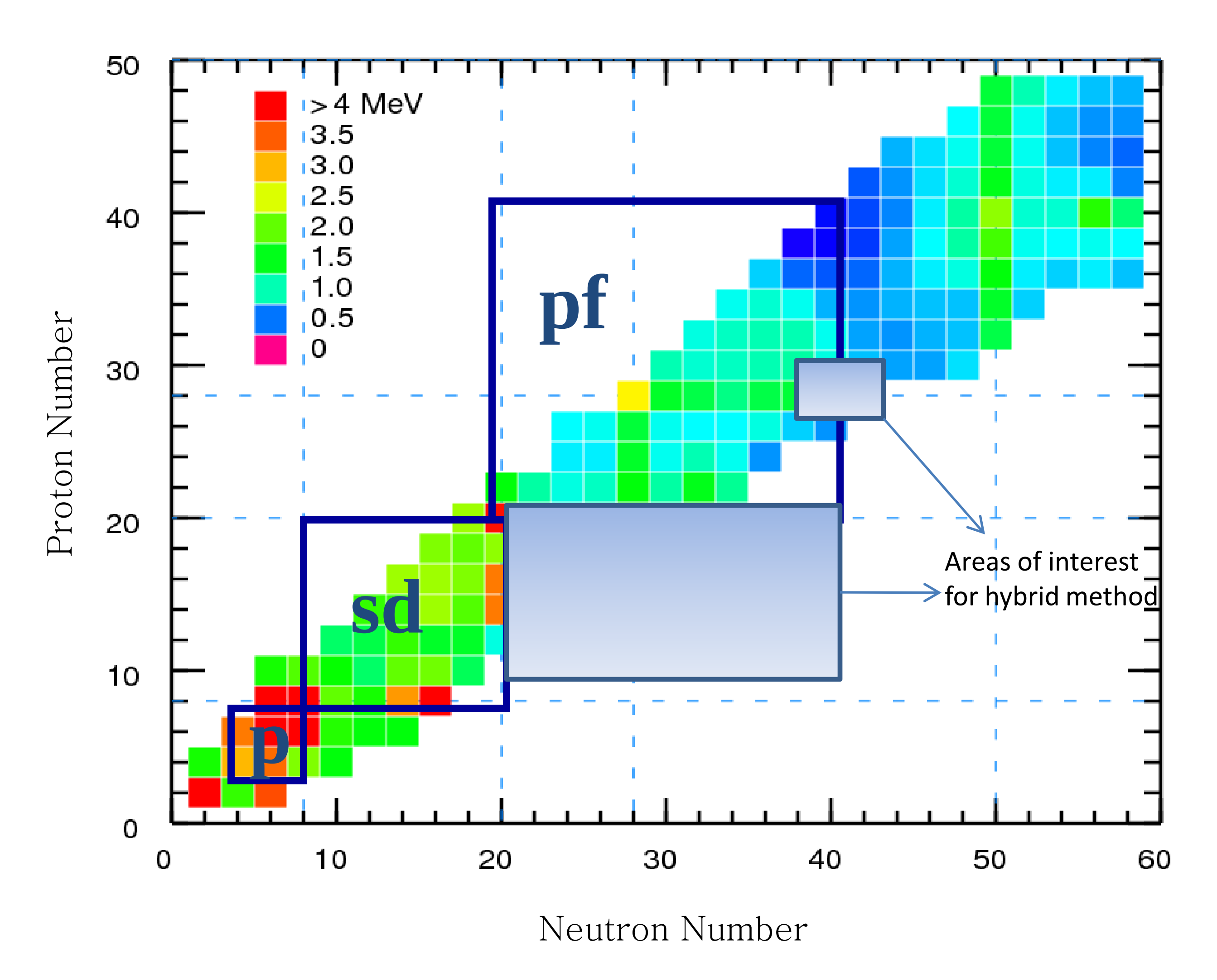


Conclusions

- 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
- Other possible applications: ^{68}Ni region, neutron-rich isotopes with $Z \leq 20$

Other Regions of Interest for Hybrid Method

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



Acknowledgements

- Alex Brown
- Morten Hjorth-Jensen
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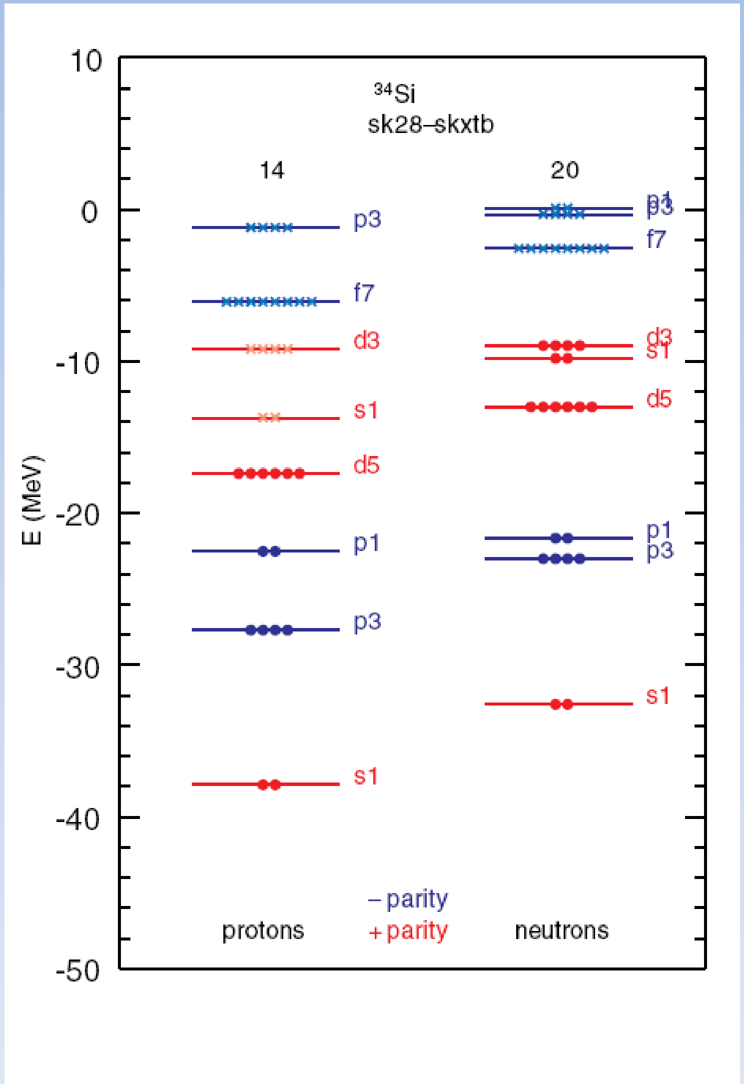
HF SPEs



^{34}Si
sk28–skxtb
14
20
p3
f7
d3
s1
d5
p1
p3
s1
p1
p3
f7
d3
s1
d5
p1
p3
s1
E (MeV)
10
0
-10
-20
-30
-40
-50
– parity
+ parity
protons
neutrons

Renormalization Procedure