Calculations in the ^{68}Ni Region

Angelo Signoracci
MSU/NSCL
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Basics of Nuclear Physics

- Nucleus of an atom is made up of protons and neutrons, collectively called nucleons (N)
- Schrodinger Equation: $H \Psi = E \Psi$ (time-independent)
- Force between nucleons is not known analytically
- Two-body forces are not sufficient for accurate calculations
- Approximations must be used to make predictions for energies and other properties of all but the very lightest nuclei

Configuration Interaction (CI)

- Also known as the shell model
- Generally limited to specific regions of the nuclear chart, especially by mass
- Uses a doubly magic nucleus as the core and treats it as the vacuum
- Uses effective single particle energies (SPEs) and two body matrix elements (TBMEs)

CI Pros and Cons

- Pros: Simple wavefunctions
  150 keV rms

- Cons: Limited in excitation energy and mass
  Need effective SPEs and TBMEs for good results

Energy Density Functional (EDF)

- Instead of finding the wavefunction of the nuclear system, energies of states are written as a function of one-body density matrices
- No large matrix diagonalization as in the solution of the Schrodinger equation
- Currently uses empirical interactions, but ultimately microscopic NN and NNN interactions should provide the most meaningful results

EDF Pros and Cons

- Pros: Uses full single particle space
  Single parameterization produces
  results for all nuclei

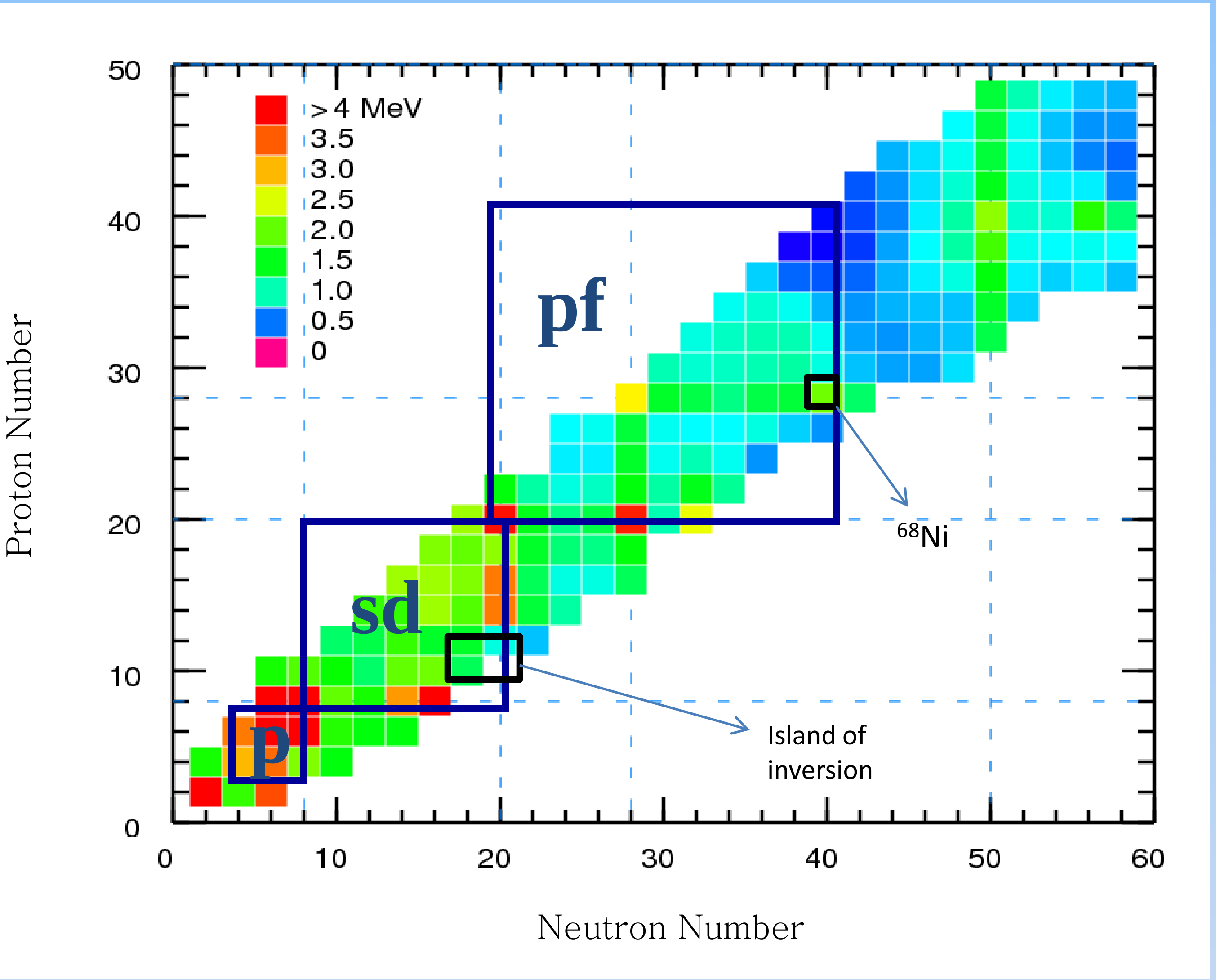
- Cons: Lack of universal parameterization
  600 keV rms
  Missing dynamic correlations
  Limited to certain states

Thesis Project

- Combining CI and EDF methods into a new hybrid method
- Primarily want the overall accuracy of CI with the generality and microscopic description of EDF
- Produce the most accurate theoretical calculations for many nuclei, especially those outside of standard model spaces

Standard Model Spaces

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



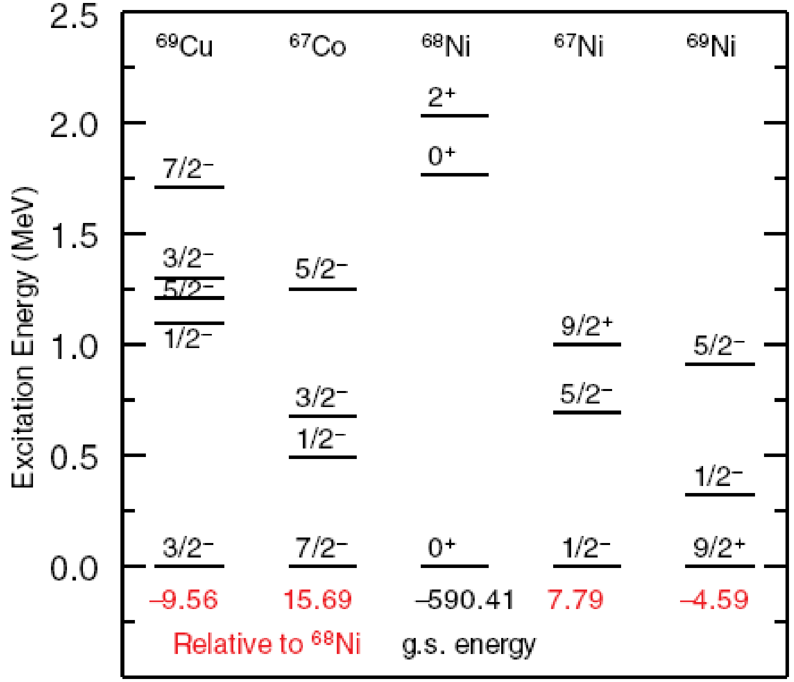
Application of Hybrid Method to ^{68}Ni

- Closed subshell configuration allows method to calculate interaction for ^{68}Ni and nearby nuclei (^{68}Ni region)
- Region is interesting due to possible inverted order in the filling of both neutron and proton orbits
- Calculation is too large for CI, plus region extends outside of pf model space
- EDF doesn’t provide accurate enough predictions for experimentalists, and isn’t able to produce calculations for all low-lying excited states

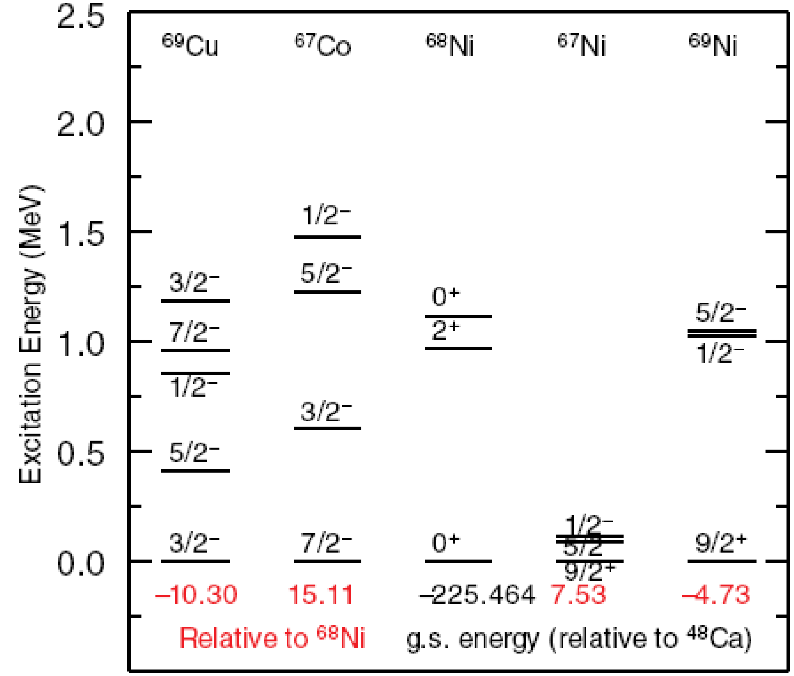
Research at LLNL

- Hybrid method had already been developed but not finalized
- MSU's CI code had to be modified to run on Linux
- Practicum advisor had his own CI code in development
- Large-scale calculations in ^{68}Ni region run on LLNL clusters
- Collaboration led to emphasis on maximizing HPC resources by parallelizing the code with MPI

Comparison of Level Schemes



Experimental level schemes



Theoretical level schemes

Conclusions

- Many improvements have already been made to the method, with more expected in the next year
- Expect better results now, but have possibly already produced the best existent calculations
- Summer experience emphasized the need to optimally parallelize the CI code
- Work currently underway
- Results led to the study of a similar but lighter (i.e. less computationally intensive) region, called the island of inversion
- See poster for more information

Acknowledgements

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- Erich Ormand
- LLNL
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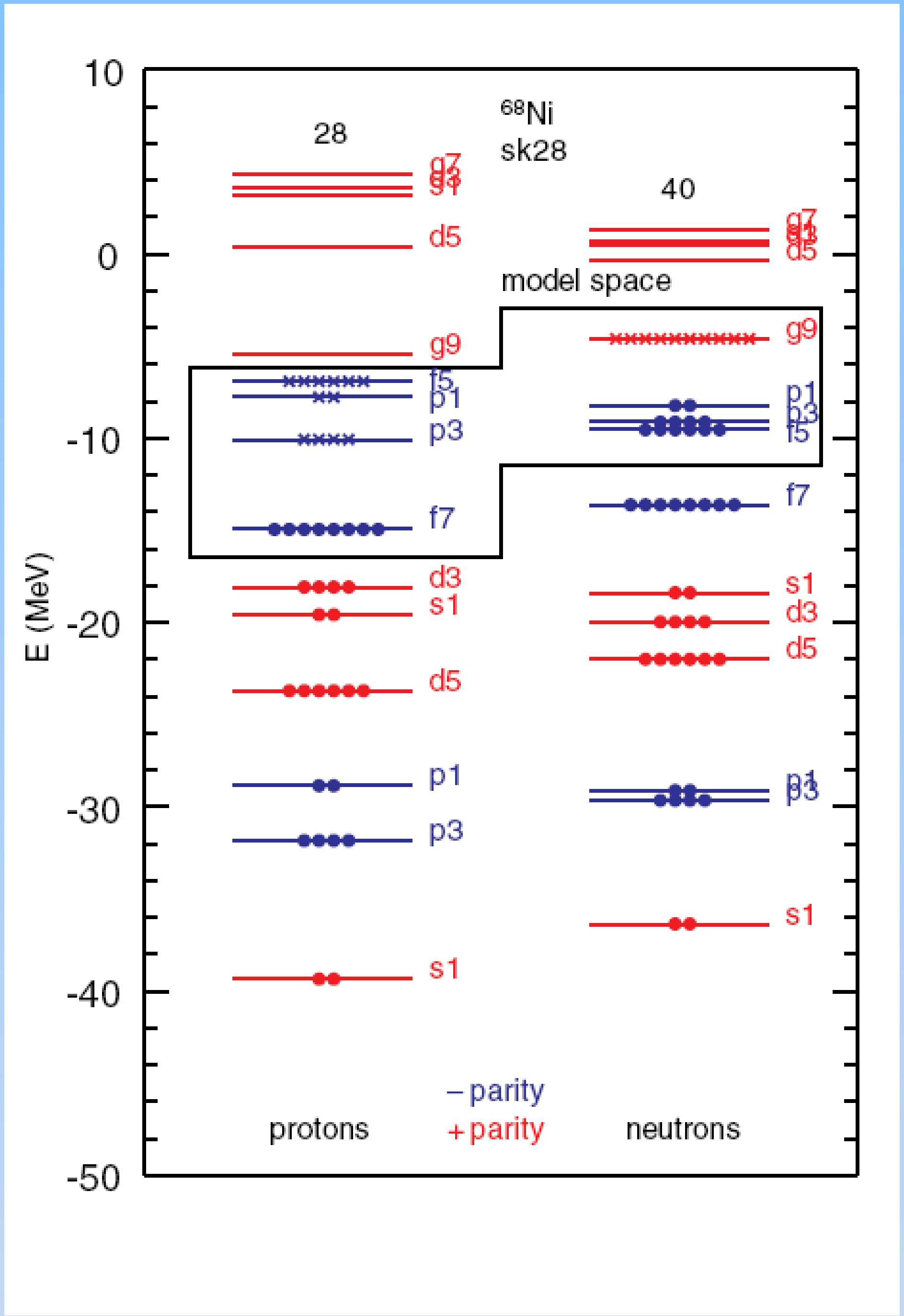

68Ni
sk28
28
40
model space
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E (MeV)
g7
d5
g9
f5
p1
p3
f7
d3
s1
d5
p1
p3
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g7
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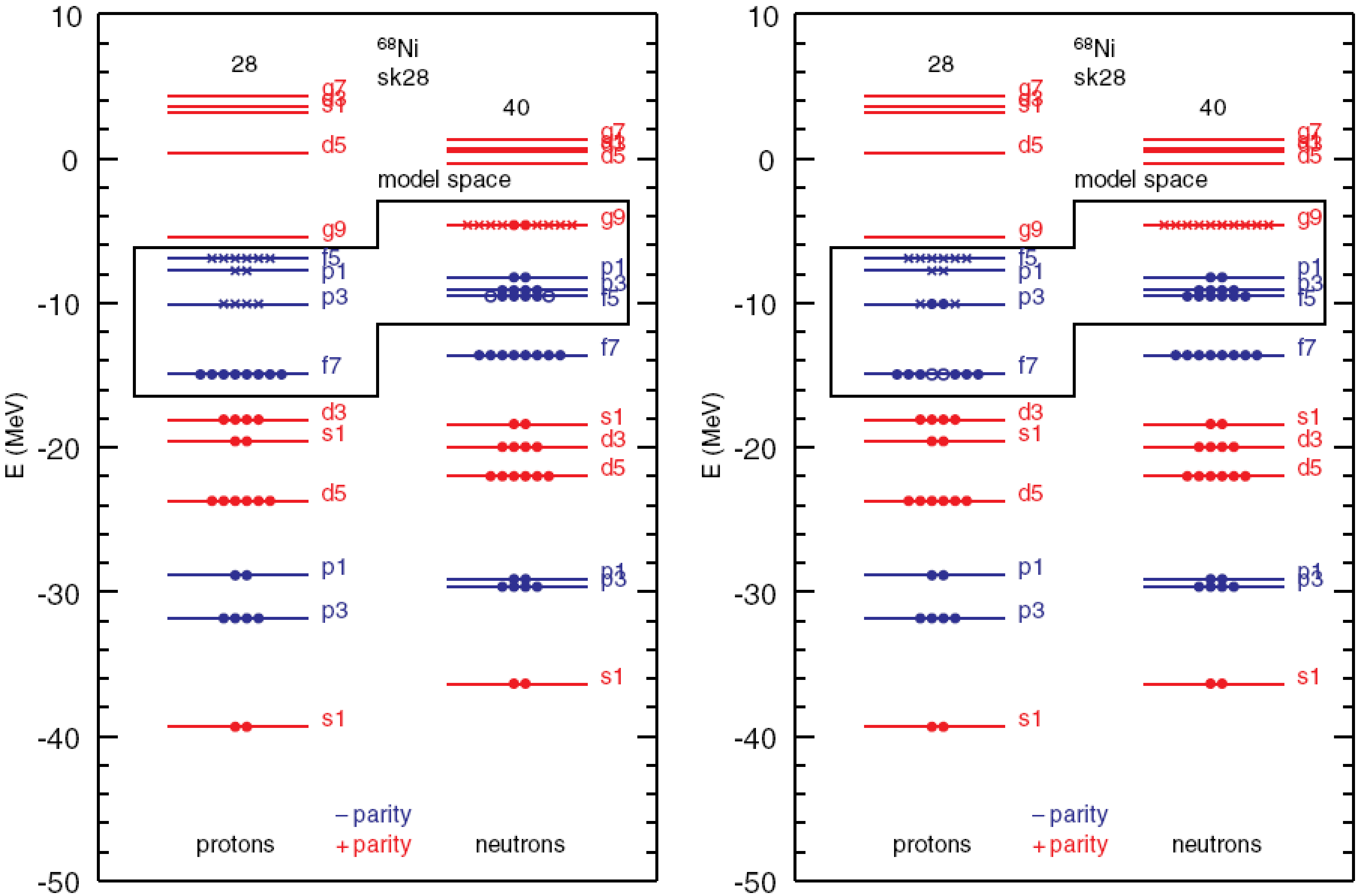
s1
protons
– parity
+ parity
neutrons



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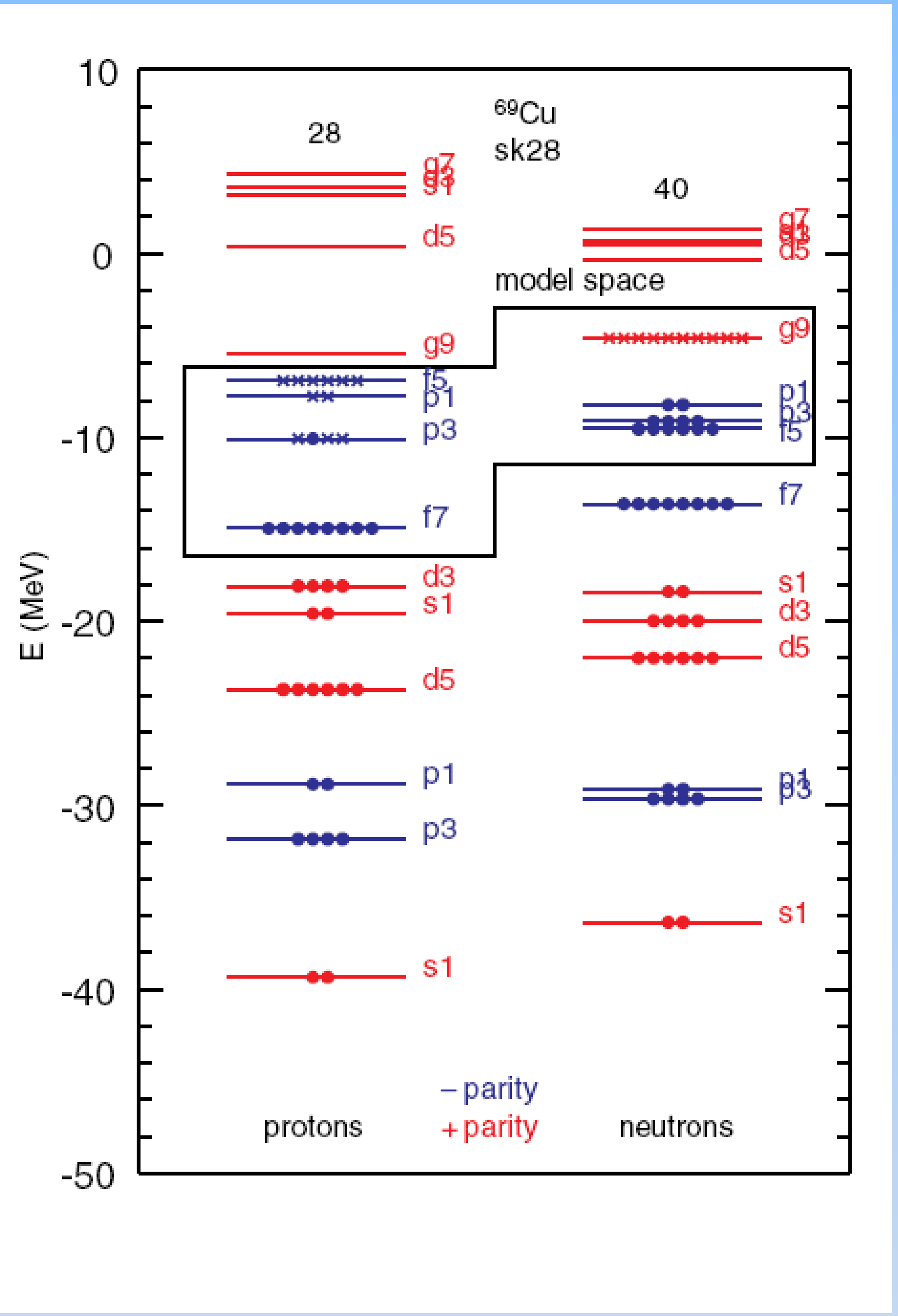

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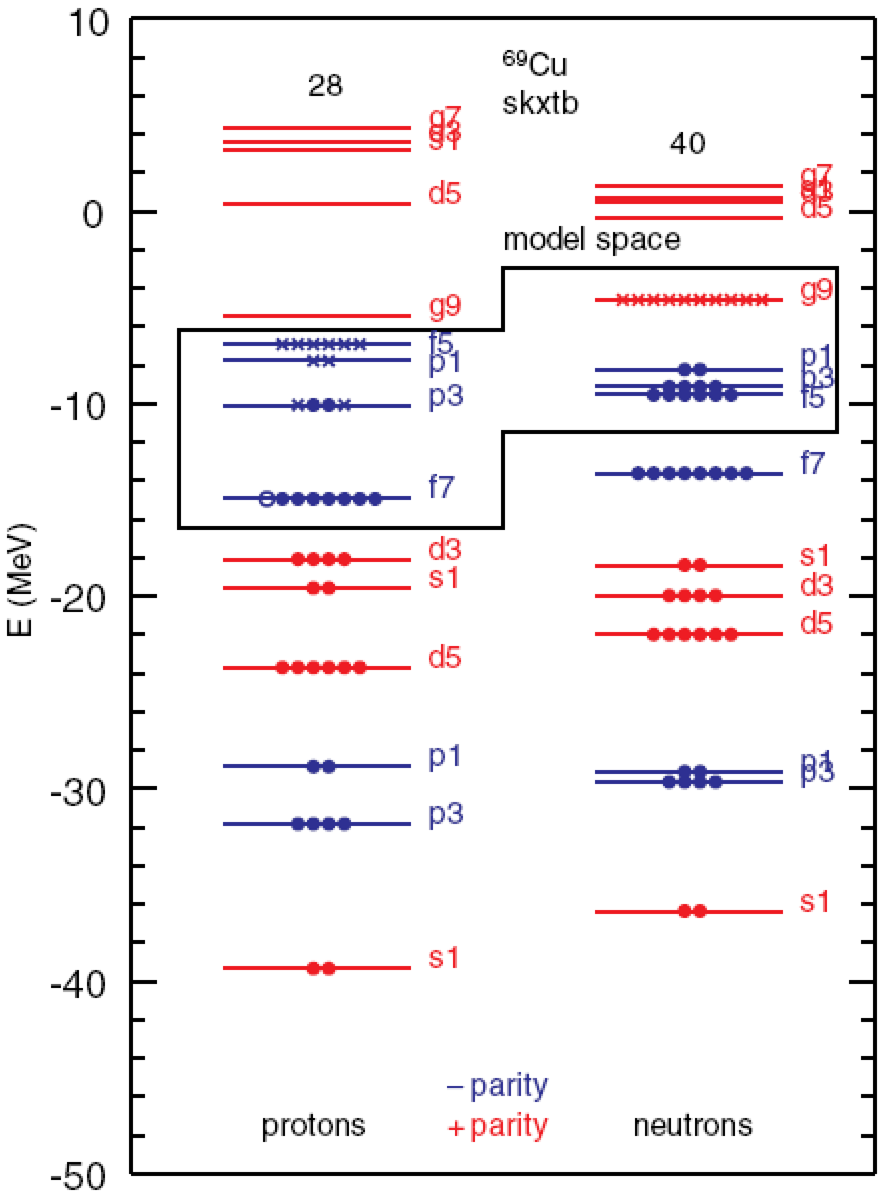

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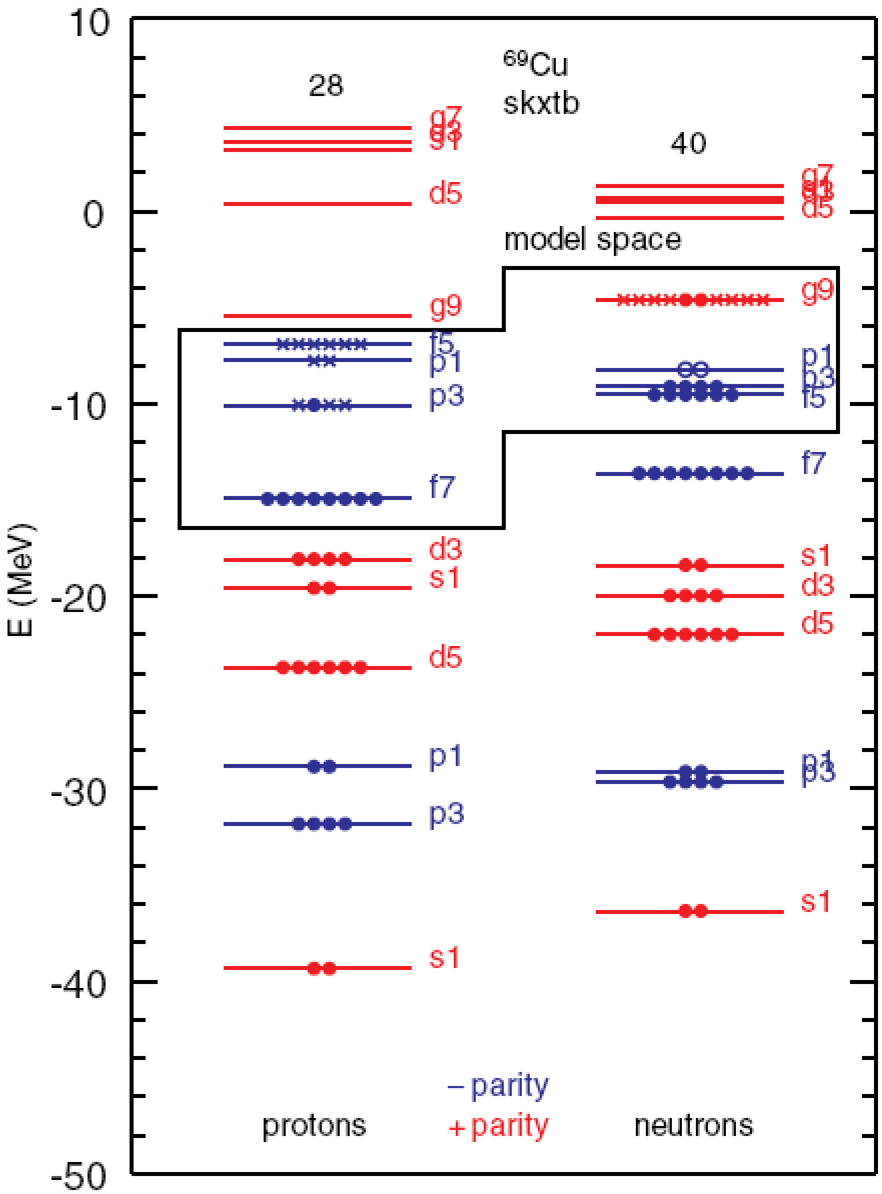

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