Effective Interactions for Nuclear Structure Calculations

Angelo Signoracci

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Basic Quantum Mechanics

$$H\Psi = E\Psi$$

$$H = T + V = \sum_{i=1}^{A} t(r_i) + \sum_{\substack{i,j=1 \\ i<j}}^{A} v(\mathbf{r_i}, \mathbf{r_j}) + \dots$$

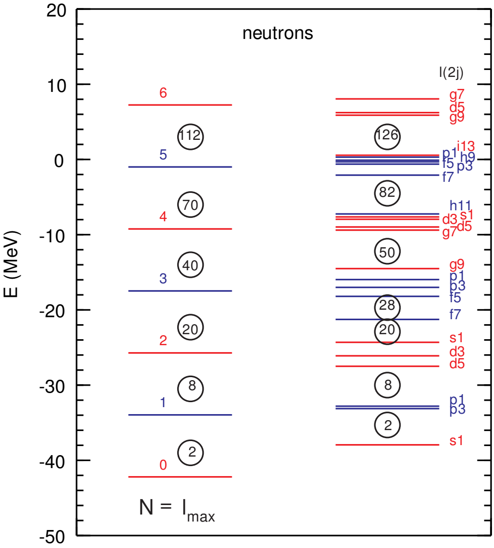
$$H = H_0 + H_1 = [T + V_{mf}] + [V - V_{mf}]$$

$$V_{mf} = \sum_{i=1}^{A} v(\mathbf{r_i})$$

- Schrödinger Equation
- Nuclear Hamiltonian
- H_1 can be treated perturbatively
- Mean field potential

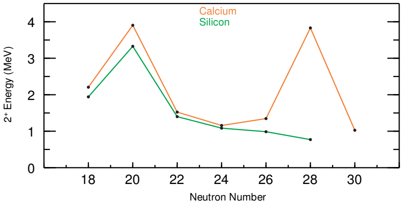
Motivation

- Single particle basis for neutron orbits in ^{132}Sn from a solution to the Schrödinger equation for mean field Hamiltonians
- Empirically, $\hbar\omega$ energy scale is given by the mass ($\approx$ 8 MeV for ^{132}Sn, but $\approx$ 12 MeV for nuclei around $A = 30$)

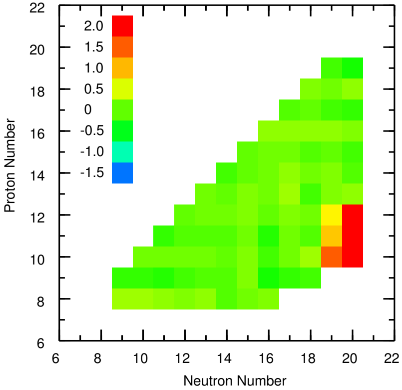


Motivation

- Difficulty in extrapolation from stable isotopes



- Standard model spaces do not always account for the proper degrees of freedom



Motivation

- Away from stability
  - Recent and future experiments with rare isotope beams provide new data in regions without reliable theoretical predictions
  - Standard formulation of Configuration Interaction (CI) theory is less practical
  - Renormalization methods, as generally used in literature, do not account for behavior of exotic nuclei
  - Loosely bound orbits are often important valence orbitals
- Develop a new theoretical technique to combine existing procedures in nuclear theory, inluding CI and Energy Density Functional (EDF) methods, to produce reliable calculations outside of standard shell model spaces
- Desire the accuracy of the CI techniques and the generality of EDF methods

Procedure

- Choose a model space and target nucleus (not necessarily the core)
- Calculate binding energy, single particle energies (SPE), and radial wavefunctions of the target nucleus via Skyrme Hartree-Fock theory
- Convert N^{3}LO interaction (two-body interaction derived from χEFT and fit to *NN* scattering data) to a low momentum interaction using v_{lowk}, a similarity transformation in momentum space with a sharp cutoff of 2.0 fm^{-1}
- Renormalize two-body matrix elements (TBME), summing over contributions outside the model space in two different single-particle bases
  - Harmonic Oscillator (HO): HO wavefunctions and single particle energies
  - Skyrme Hartree-Fock (SHF): SHF wavefunctions and single particle energies
- Output TBME are in the form of an effective interaction for CI calculations
- SPE for the effective interaction from Skyrme Hartree-Fock theory are unreliable
- For target nuclei with "doubly magic" behavior, use experimental one-nucleon separation energies; otherwise, parameterize and fit to available data

- S.K. Bogner, R.J. Furnstahl, and A. Schwenk, Prog. Part. Nucl. Phys. **65**, 94 (2010)

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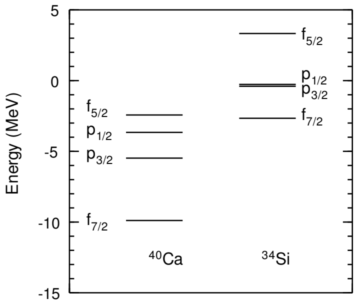
Application to *sdpf* Model Space



Model Space Neutron Orbits in SHF Basis

- Model space is *sd* protons and *pf* neutrons (seven orbits total)
- Two target nuclei ^{34}Si and ^{40}Ca are used in both bases (four interactions total)
- New interaction, SDPF-U, has different TBME for $Z \leq 14$ and $Z \geq 15$ to account for different behavior based on number of protons (i.e. based on how exotic the nucleus is)
- The neutron-neutron pairing elements are reduced by 300 keV for the $Z \leq 14$ interaction to better reproduce data

- Nowacki and Poves, Phys. Rev. C **79** 014310 (2009)

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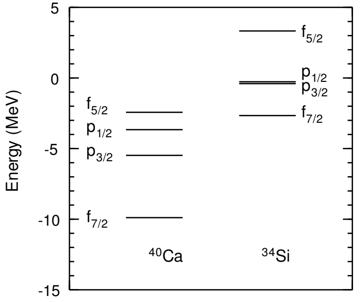

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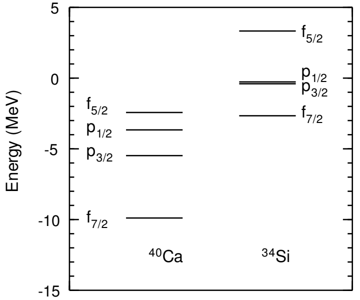

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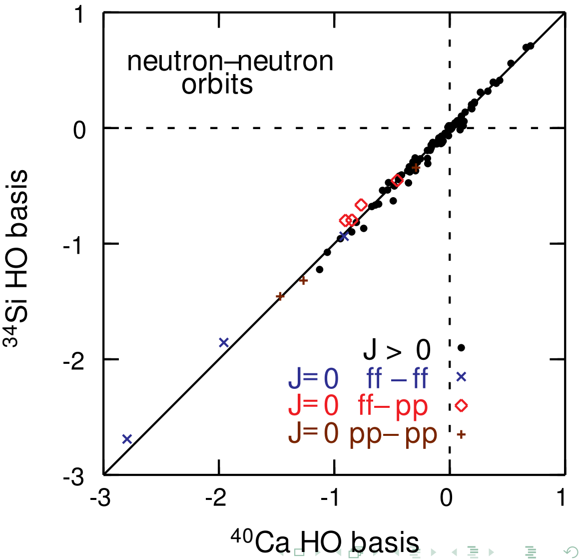
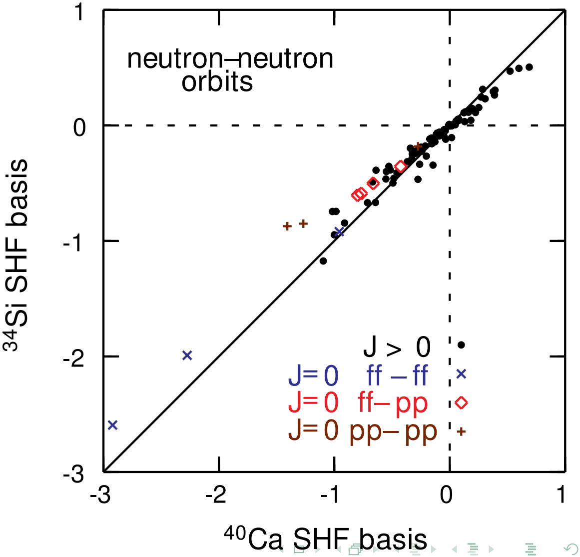
Results for matrix elements in MeV

- Pairing matrix elements are singled out due to their importance in ground state properties of even-even nuclei
- In HO basis, change in nucleus does not affect neutron-neutron pairing matrix elements (diagrams involving excitations of protons are unlinked)



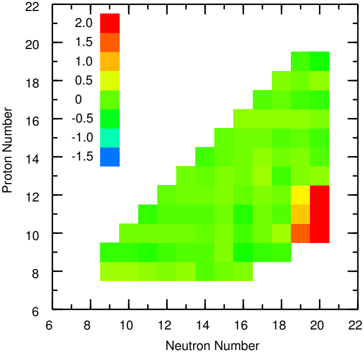
Results for matrix elements in MeV

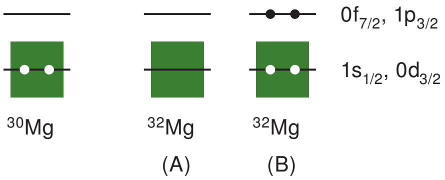
- Pairing matrix elements are singled out due to their importance in ground state properties of even-even nuclei
- Pairing matrix elements exhibit a general trend towards reduction in the SHF basis and are reduced by 214 keV on average for the ^{34}Si target relative to the ^{40}Ca target using a microscopic procedure



Island of Inversion Region

- For exotic isotopes around $Z = 11$, $2p2h$ $(2\hbar\omega)$ configurations are important at $N = 20$
- Nuclei with significant contributions from $2\hbar\omega$ configurations in the ground state have been observed for $N \geq 19$ and $Z \leq 13$
- Experimental boundaries may be outside the reach of current rare isotope facilities





Island of Inversion Region

- Theoretical calculations can predict the properties of unknown exotic isotopes
- Model space composed of *sd* protons and $0d_{3/2}, 1s_{1/2}, 0f_{7/2}, 1p_{3/2}, 1p_{1/2}$ neutrons
- To reproduce low-energy behavior of nuclei throughout the island of inversion region with one interaction, accurate SPE and reasonable treatment of three-body forces are necessary
- Thirteen parameters are included: eight for SPE, four for three-body forces, and one phenomenological overall normalization
- Normalization reduces the strength of the interaction by $\approx 10\%$ to reproduce 2^+ states in even-even nuclei
- 43 states are implemented in an iterative fitting procedure
- rms deviation is 370 keV

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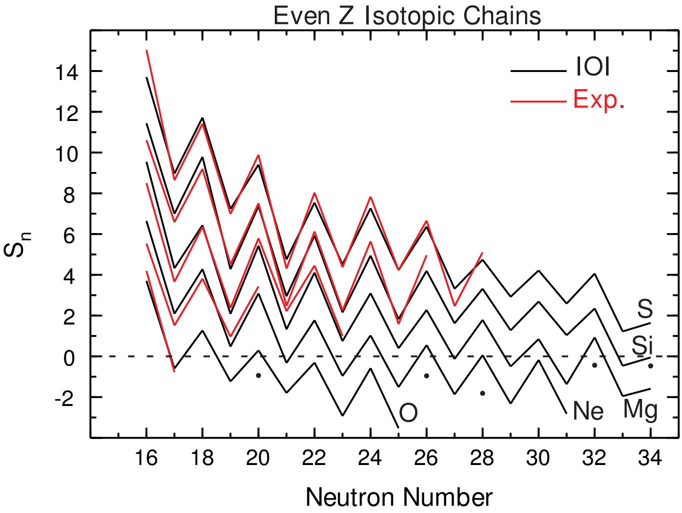
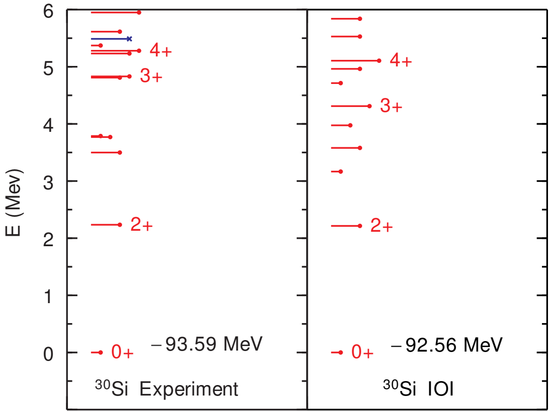
Systematic Trends



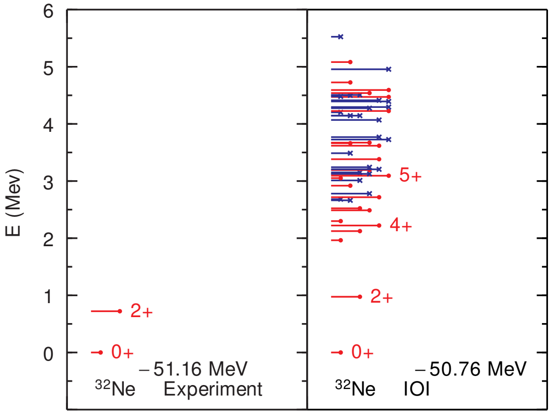
- $S_n(^{A}Z) = BE(^{A}Z) - BE(^{A-1}Z)$
- If $S_n > 0$, but $S_{2n}(^{A}Z) = BE(^{A}Z) - BE(^{A-2}Z) < 0$, nucleus is unbound

Representative Nuclei



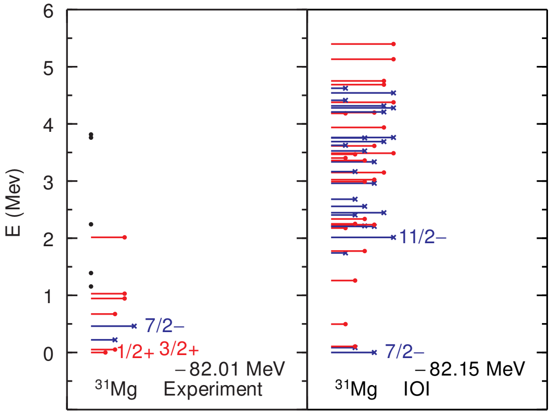
- Towards stability by the removal of four neutrons

Representative Nuclei



- Into the island of inversion ($\approx$ 20% of the wavefunction in standard configuration)
- Comparison to data is often difficult because few states are known

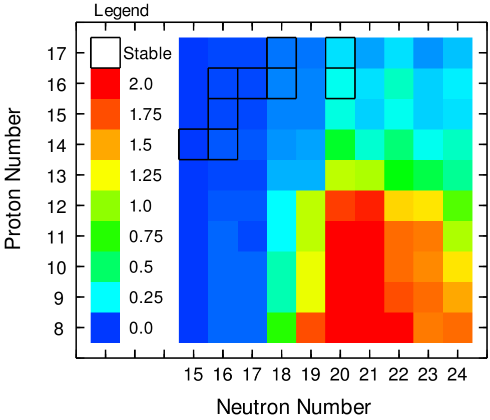
Representative Nuclei



- Includes data from D. Miller et al., Phys. Rev. C **79**, 054306 (2009)
- Lowest four experimental states were included in the fit

Ground State Occupations

- A single configuration has a $1\hbar\omega$ excitation if an *sd* neutron is promoted into the *pf* shell ($1p1h$ at $N = 20$)
- Many-body states are linear combinations of many configurations $\rightarrow$ average $\hbar\omega$ of the ground state is plotted
- Island of inversion represented by red, orange, and yellow boxes



Application to ^{42}Si

- Three different interactions were produced for calculations of ^{42}Si:
  - (i) the interaction from the island of inversion region
  - (ii) same as (i), but with SPE "evolved" to reproduce behavior at ^{42}Si
  - (iii) new interaction in the *sdpf* model space with ^{42}Si as the target
- Comparison to experiment and to the empirical SDPF-U interaction provides information on the extension of effective interactions away from the target and best method to apply the renormalization procedure

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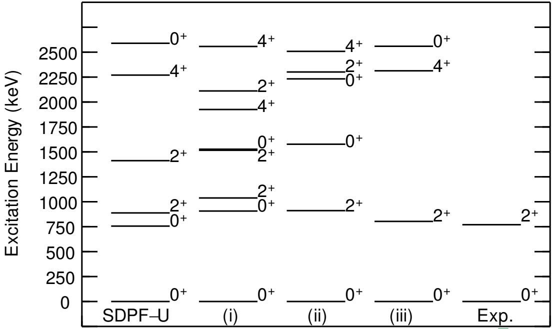
  - (iii) new interaction in the *sdpf* model space with ^{42}Si as the target
- Level density and behavior very different for three cases
- Experimental determination of 4_1^+ and especially 0_2^+ very important for theoretical conclusions



Summary of Applications

- Realistic Basis
  - Loosely bound orbits exhibit long tail behavior, reducing the strength of TBME involving those orbits
  - Energy of single particle orbits can differ greatly for stable and exotic isotopes
  - HO basis leads to a stronger interaction that results in overbinding even in the two particle case, an effect which gets magnified as more particles are added
  - A realistic basis is essential for an accurate description of the effective interaction for exotic nuclei as determined by the renormalization of an *NN* interaction
- Island of Inversion Region
  - One hundred nuclei were calculated, with binding energies and low-lying states in good agreement with available experimental data including the 370 keV rms deviation (all comparisons accessible)
  - Neutron dripline and boundaries of island of inversion have been determined
  - Isotopes in the island of inversion region extend beyond those observed to date
- ^{42}Si
  - Level schemes with three different applications of the method reproduce the known states in ^{42}Si
  - Predictions of the 4_1^+ and 0_2^+ states vary significantly
  - Detection will enable the evaluation of different techniques to calculate exotic isotopes

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Conclusion and Outlook

- Overall Methodology
  - The microscopic N^3LO interaction can be renormalized into an effective interaction in the nuclear medium using v_{lowk} and many-body perturbative techniques with a realistic single particle basis determined from Skyrme Hartree-Fock theory
  - This effective interaction can be directly used as the input to a CI calculation, with single particle energies taken from Skyrme Hartree-Fock
  - Interactions do not need to be determined empirically
  - Single particle energies from EDF methods are unreliable and need to be improved
  - Basis and target nucleus used in renormalization are important and must be chosen judiciously
- Outlook
  - More calculations outside of standard model spaces (^{68}Ni, ^{20}C, ...)
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Acknowledgements

- Guidance Committee: Alex Brown (advisor), Carlo Piermarocchi, Jon Pumplin, Michael Thoennessen, Vladimir Zelevinsky
- Morten Hjorth-Jensen
- DOE NNSA SSGF program

Additional Information

Configuration Interaction (CI) Theory

- Limited to specific regions of the nuclear chart, mainly by mass
- General Procedure:
  - Select a doubly magic nucleus as the core and treat it as vacuum
  - Select a model space outside of the core
  - Determine single particle energies (SPE) from experimental single particle states
  - Determine two body matrix elements (TBME) from renormalization procedure
  - Can treat SPE and TBME as parameters and fit them to best reproduce data
  - TBME of the form $\langle (ab)J|V|(cd)J\rangle$ where V is the interaction and a,b,c,d refer to orbits in the model space
- Advantages
  - Accuracy ($\approx$ 150 keV rms)
  - Simple wavefunctions
- Disadvantages
  - Limited in excitation energy and mass
  - Need effective SPE and TBME for good results
  - Different parameters for each model space; need to perform fit for each region of interest

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  - Different parameters for each model space; need to perform fit for each region of interest

Energy Density Functional (EDF) Methods

- Treats energy as a functional of one body density matrices, i.e. $E[\rho] = \int d\mathbf{r}\mathcal{E}[\rho(\mathbf{r})]$
- Standard formulations (e.g. Skyrme, Gogny) are empirical, but ultimately should connect to underlying *NN* and *NNN* interactions
- Advantages
    - Utilizes full single particle space
    - Single parameterization produces results for all nuclei
    - Relative ease of calculations for ground states
- Disadvantages
    - Lack of universal parameterization
    - 600 keV - 1.2 MeV rms deviation to ground state masses
    - Missing dynamic correlations in current functionals
    - Limited to certain states

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SHF Basis

- Typical harmonic oscillator basis $\Psi_{nlm_l}(\vec{r}) = R^{HO}_{nl}(\mathrm{r})\ Y_{lm_l}(\theta,\phi)$ is implemented easily
  - Realistic bases come in many forms, but the Skyrme Hartree-Fock basis is chosen
  - Since it does not have a clean analytic expression, the radial wavefunctions are implemented via an expansion of the HO basis

$$\psi^{SHF}_{nlj}(\vec{r}) = \sum_n a_n R^{HO}_{nl}(r)[Y_l(\theta,\phi)\otimes\chi_s]_j$$

- a_n^2 gives the percentage of a HO basis radial wavefunction in the SHF basis solution
- SHF can only be solved for bound orbits
- Approximations can be done for orbits unbound by a few MeV, but the HO basis is used for more unbound orbits
- Gram-Schmidt process is used to ensure orthonormality of basis
- Single Particle Energies
  - Divergences can occur in the renormalization procedure due to energy denominators for model space orbits with small energy differences
  - Orbits inside the model space are set to identical valence energies in order to prevent divergences

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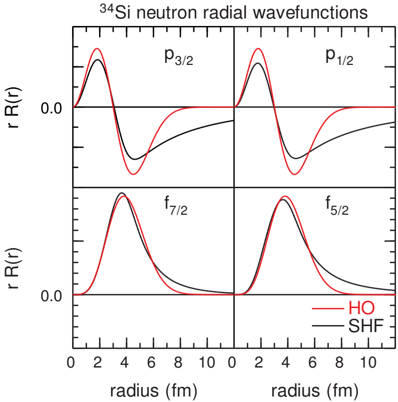
Wavefunction Expansions

- In practice, the expansion over n has to be limited to some n_{max}
- Renormalization cutoff of 6 $\hbar\omega$ gives $n_{max} = 4$ for the $p_{3/2}$ and $p_{1/2}$ orbits and $n_{max} = 3$ for the $f_{7/2}$ and $f_{5/2}$ orbits
- 99% and 97% of the $f_{7/2}$ and $f_{5/2}$ orbits are accounted for in this expansion, but only 84% and 82% of the $p_{3/2}$ and $p_{1/2}$ strength

Wavefunction Expansions

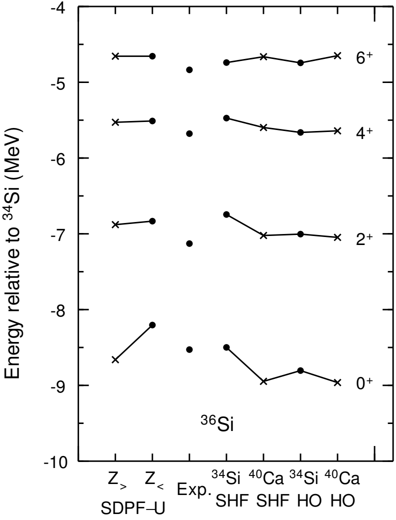


Calculations for ^{36}Si

- Simplest system outside of ^{34}Si core that depends on TBME
- Neutron-rich isotope with well-known level scheme
- For consistency, SDPF-U SPE and proton-proton and proton-neutron TBME are used
- Calculations with NUSHELLX in *sdpf* model space

Comparison to Experiment and to Empirical Interactions

- No result reproduces current experimental data very well; level density too low for ^{40}Ca target
- ^{36}Si 0^+ changes by over 300 keV depending on the target nucleus; good agreement with experiment after reduction in TBME
- 223 keV rms for ^{34}Si SHF to the four known states
- Inclusion of *NNN* forces, at least at effective two-body level, is necessary for accuracy at the hundred keV scale



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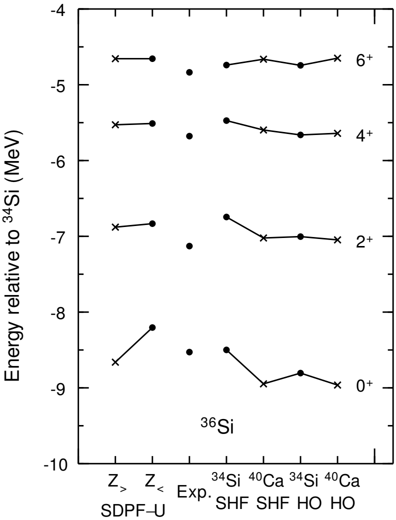

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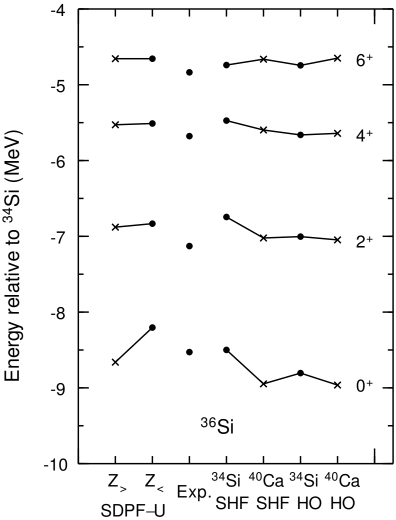

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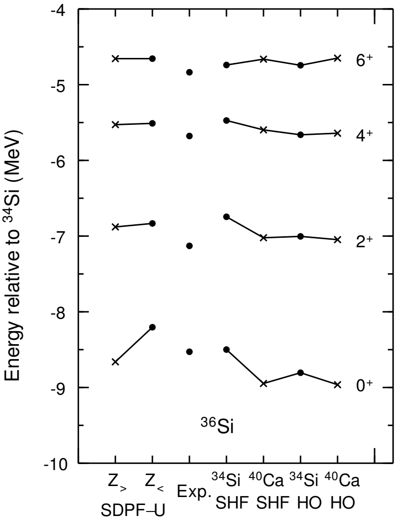
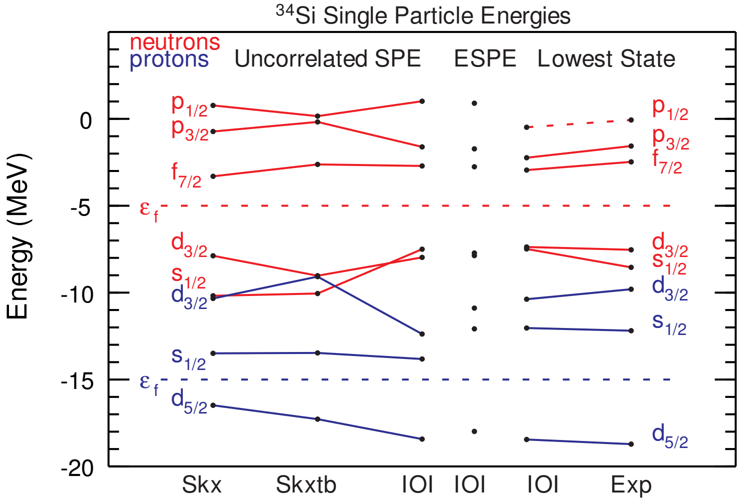


Systematic Trends



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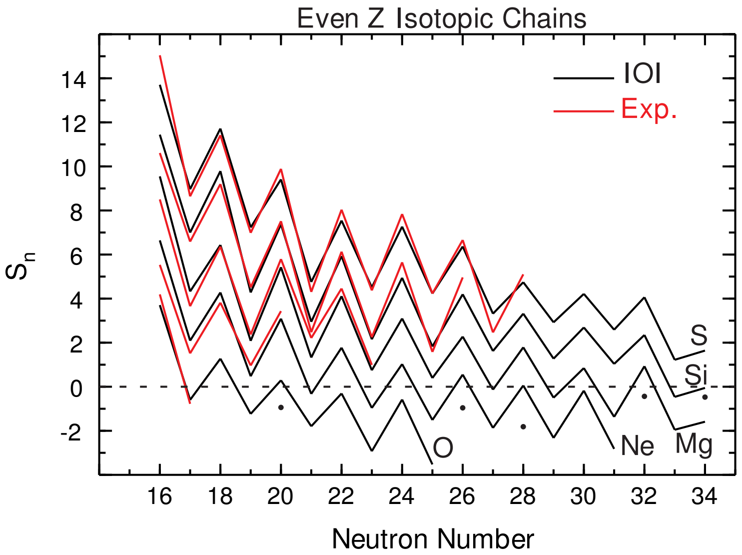

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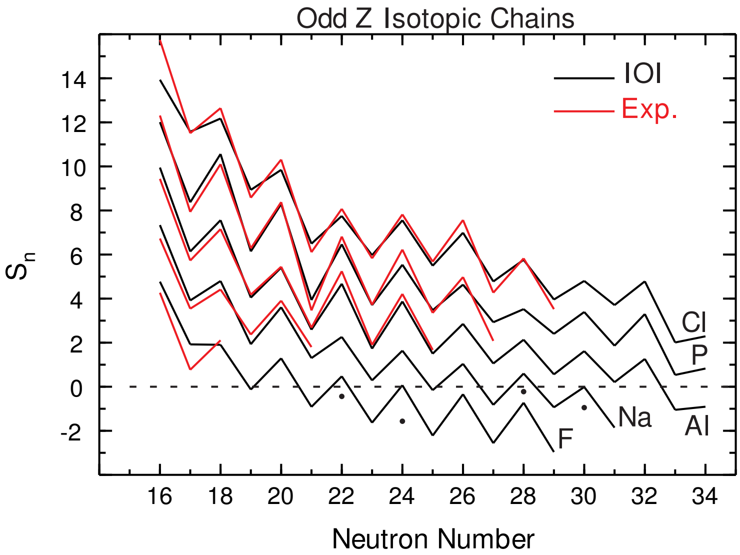
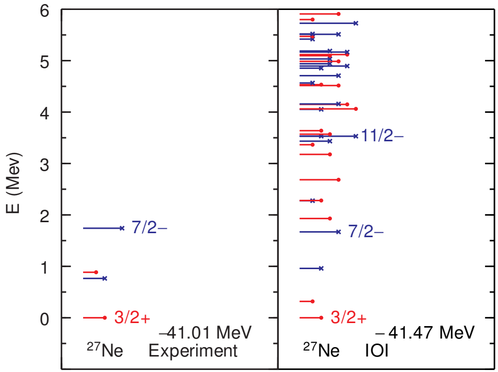


$^{26}Ne(d,p)^{27}Ne$

- Reaction mechanisms can also be calculated with the IOI interaction
- For example, states populated in ^{27}Ne through a transfer reaction



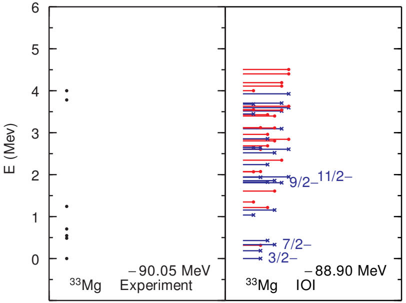
^{26}Ne(d,p)^{27}Ne

- Comparison between experimental and theoretical spectroscopic factors for states in ^{27}Ne
- Experimental values from doctoral thesis of S.M. Brown (University of Surrey, 2010)

J^{π}	$E_{Exp.}$	E_{IOI}	$C^2S_{Exp.}$	C^2S_{IOI}
$3/2^+$	0.000	0.000	0.42(22)	0.58
$3/2^-$	0.765	0.960	0.64(33)	0.63
$1/2^+$	0.885	0.318	0.17(14)	0.41
$7/2^-$	1.714	1.670	0.35(10)	0.46

^{33}Mg β^- decay

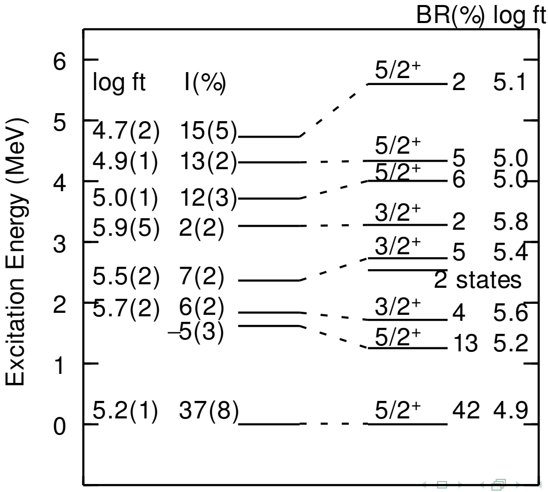
- Ground state J^π of ^{33}Mg is debated: $3/2^+$ or $3/2^-$
- Four theoretical states with $E_x \leq 370$ keV
- Two $3/2^-$ states (g.s. and $E_x = 186$ keV)
- $3/2^+$ state at 316 keV



- V. Tripathi et al., Phys. Rev. Lett. **101**, 142504 (2008)
- D.T. Yordanov et al., Phys. Rev. Lett. **99**, 212501 (2007)

^{33}Mg β^- decay

- Transitions from theoretical $3/2^+$ agree with experiment
- γ decay (not pictured) used to match transitions



^{33}Mg β^- decay

- Decay from the $3/2^+$ state in ^{33}Mg matches experimental transitions
- Half-life is 49 ms in comparison to 89(1) ms, but is ≈ 0.5 s for $3/2^-$ states
- However: measured magnetic moment is -0.75 μ_N, $3/2^+$ state is 0.88 μ_N
- Excited $3/2^-$ state is in reasonable agreement with experiment at -0.82 μ_N
- No state reproduces both the β decay and magnetic moment
- Possible isomer $\rightarrow$ for small energy differences, γ decay is suppressed
- Estimate for upper limit on half-life comes from theoretical β decay
- Additional measurements would be interesting, especially if the setup could resolve isomers