Effective Interactions for Nuclear Structure Calculations

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CEA/Saclay

SPhN seminar, 9 March 2012

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- ESNT Tutorial: 23-27 April, 2012 on shell model techniques
- Registration is full
- Check ESNT website for lecture topics and schedule

Single particle shell structure

- Mean field in the nucleus produced by A nucleons composing it
  - Familiar idea (atoms- low density of electrons and point-like nucleus)
  - Experimental observations: high $E(2+)$, low $B(E2), BE \ldots$

$\rightarrow$ "magic" numbers

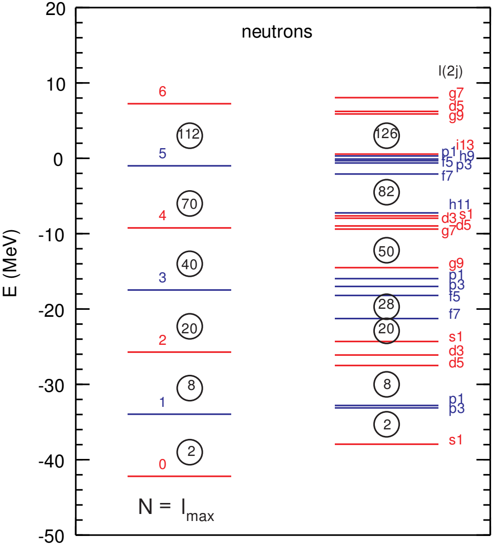
  - Collisions within the nucleus are suppressed due to the Pauli principle
- Nuclear Hamiltonian: $H = T + V = \sum_{i=1}^{A} t(r_i) + \sum_{\substack{j=2 \\ i<j}}^{A} v(\mathbf{r_i}, \mathbf{r_j}) + \ldots$

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

- Analytic solutions to H_0 provide typical single particle bases

Comparison of single particle bases

- Neutron single particle orbits in ^{132}Sn
- Empirically, $\hbar\omega \approx 8$ MeV for ^{132}Sn, ≈ 12 MeV for $A = 30$
- Select few orbits which can reproduce low-lying states of nuclei outside a core
- Reduces problem from A-body to $(A - A_{\text{core}})$-body



Configuration Interaction (CI) theory

- Limited to specific regions of the nuclear chart, mainly by mass
- With typical computing resources, full CI solutions can be accessed up to $A \approx 60$
- Exact solution of the Schrödinger equation within the model space
- Only need an accurate determination of the Hamiltonian in reduced model space
- General Procedure
  - Select a doubly magic nucleus as the core and treat it as vacuum
  - Select a model space outside of the core
  - Interaction composed of single particle energies (SPE) and two-body matrix elements (TBME)
  - Determine SPE from theoretical or "experimental" single particle states
  - Determine TBME from renormalization procedure
  - Can treat SPE and TBME as parameters and fit to experimental data
- Advantages
  - Accuracy ($\approx$ 150 keV rms)
  - Simple wavefunctions
- Disadvantages
  - Limited in excitation energy and mass
  - Empirical SPE and TBME
  - Each model space requires its own interaction

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Energy Density Functional (EDF) methods

- Treats energy as a functional of one body density matrices
- Standard formulations (e.g. Skyrme, Gogny) are empirical
- 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 rms to known binding energies
  - Missing dynamic correlations
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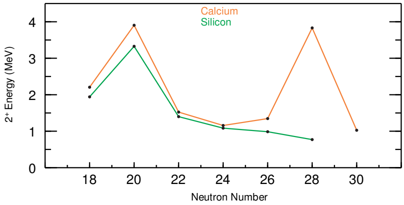
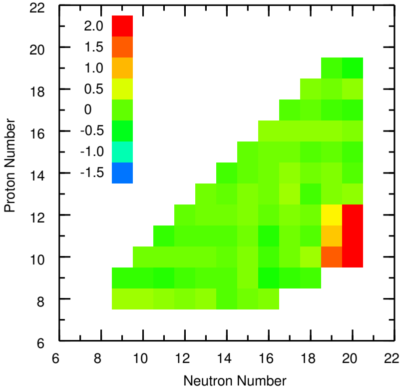
Motivation

- Difficulty in extrapolation from stable isotopes

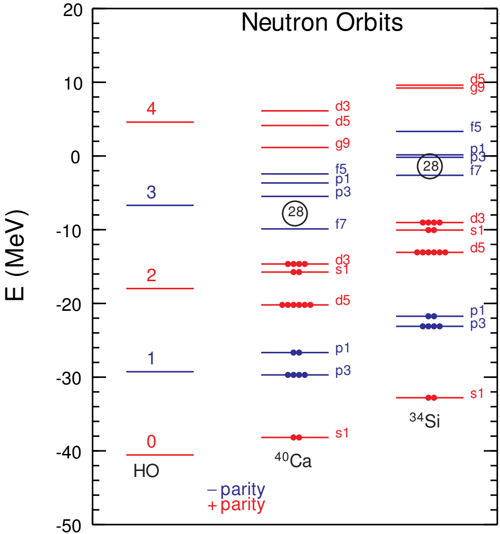


- Standard model spaces do not always account for the proper degrees of freedom



Motivation

- With empirical Skyrme EDF
  - Adequately reproduce ground states of all nuclei
  - Shell structure coincides with magic numbers
  - Shell structure "evolves" away from stability
- Behavior of neutron orbits depends on proton occupation



Motivation

- Away from stability
  - Rare isotope beams provide access to regions without reliable theoretical predictions
  - Standard formulation of CI theory is less practical
  - Renormalization methods could account for behavior of exotic nuclei
  - Loosely bound orbits are often important valence orbitals
- Desire accuracy of CI theory and generality of EDF methods
- Incorporate both into a new theoretical technique
- Focus on producing reliable calculations outside of standard shell model spaces

Procedure

- Choose a model space and target nucleus (not necessarily the core)
- Calculate *BE*, SPE, and wavefunctions of target via Skyrme Hartree-Fock theory
- Convert *NN* interaction to a low momentum interaction using "v_{lowk}"
- Similarity transformation in momentum space with sharp cutoff
- Renormalize two-body matrix elements (TBME)
- Sum over contributions outside the model space (basis-dependent)
  - 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 required for CI calculations
- SPE for the effective interaction from Skyrme Hartree-Fock theory are unreliable
- For "doubly magic" target, 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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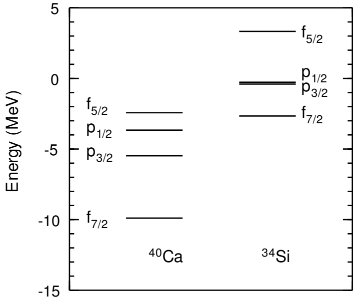
Typical implementation

- Target nucleus must have closed-subshell structure
- Low-energy degrees of freedom expressed in choice of model space
- Skyrme interaction: Skxtb (includes tensor force)
- *NN*-interaction: N3LO interaction derived from χEFT, fit to scattering data
- v_{lowk} cutoff $\Lambda = 2.0$ fm^{-1}
- Second order in perturbation theory up to $6\hbar\omega$ excitations
- Unless specified, SHF basis

Application to *sdpf* model space



Model Space Neutron Orbits in SHF Basis

- Model space: *sd* protons, *pf* neutrons
- Two target nuclei ^{34}Si and ^{40}Ca
- Four interactions total
- New empirical interaction (SDPF-U)
  - Different TBME for $Z \leq 14$ and $Z \geq 15$
  - Reproduces data for exotic isotopes
- Reduced *nn* pairing TBME by 300 keV for $Z \leq 14$
- Amount determined empirically
- Reduction ≈ decrease in core polarization

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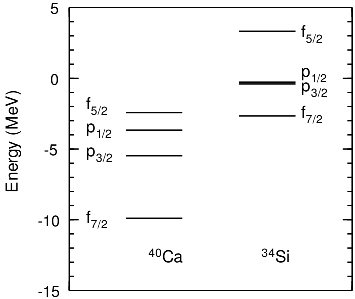

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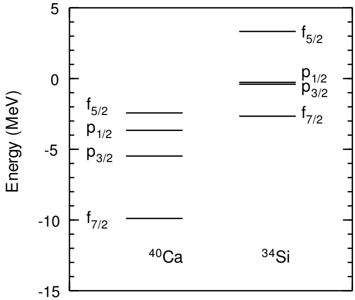

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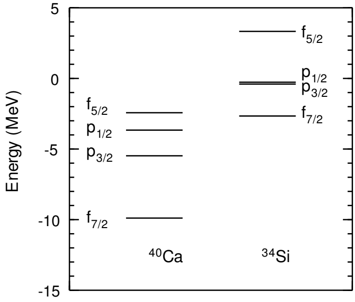

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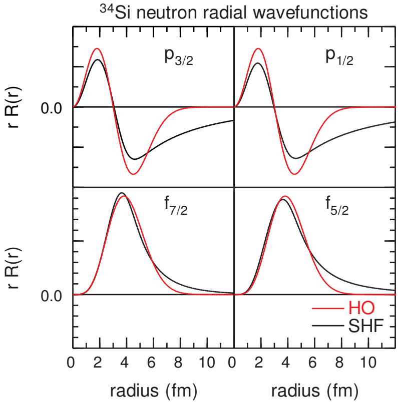
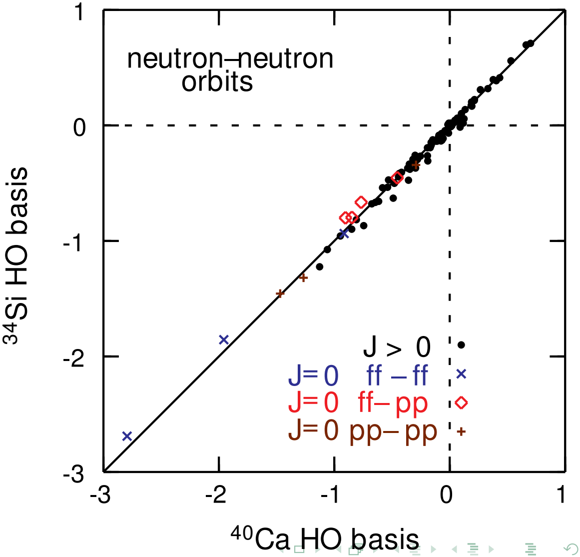
Wavefunction expansions



- 99% of $f_{7/2}$ orbit and 97% of $f_{7/2}$ orbit represented by R_{03}^{HO}
- 80% of $p_{3/2}$ orbit and 78% of $p_{1/2}$ orbit represented by R_{11}^{HO}

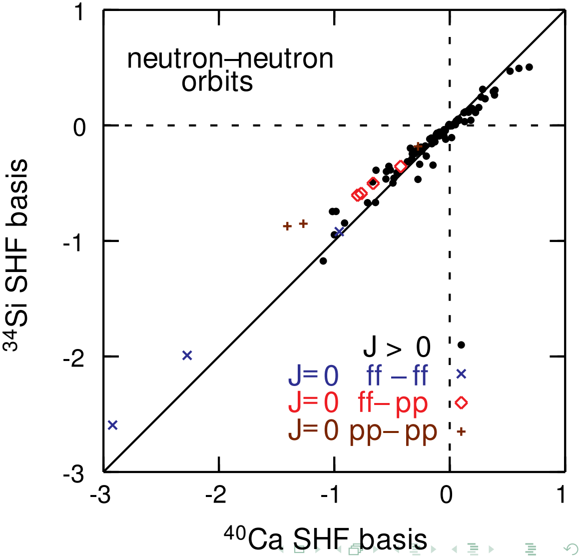
Results for matrix elements in MeV

- Pairing matrix elements singled out
- Important in ground state properties of even-even nuclei
- In HO basis, change in nucleus does not affect *nn* pairing TBME
- Diagrams involving excitations of protons are unlinked



Results for matrix elements in MeV

- Pairing matrix elements singled out
- Important in ground state properties of even-even nuclei
- Pairing matrix elements reduced in SHF basis
- On average, 214 keV reduction for ^{34}Si target relative to ^{40}Ca target
- Microscopic procedure- no parameters tuned



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 *pp*/*pn* TBME are used
- Isolates the effect due to *nn* TBME
- Calculations with NUSHELLX in *sdpf* model space

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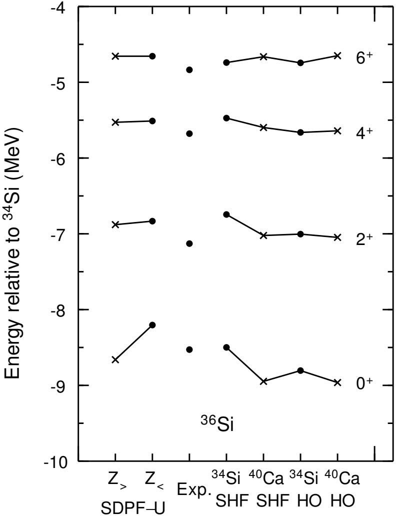
Comparison to experiment and empirical Interactions

- Experimental data not reproduced
- Level density too low for ^{40}Ca target
- ^{36}Si 0^+ changes by 300 keV
- Better agreement after reduction in TBME
- 223 keV rms to the four known states for ^{34}Si SHF
- Inclusion of *NNN* forces necessary for hundred keV accuracy



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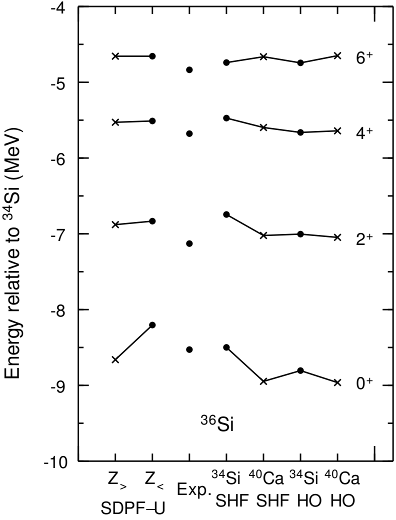

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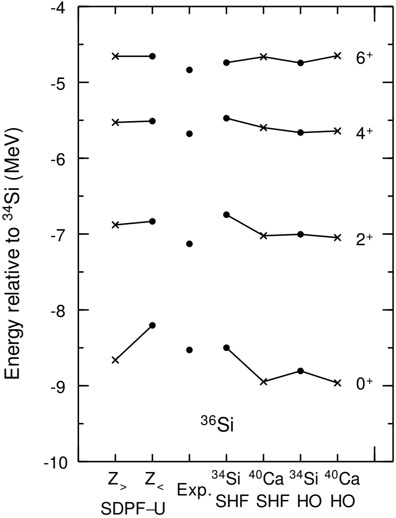

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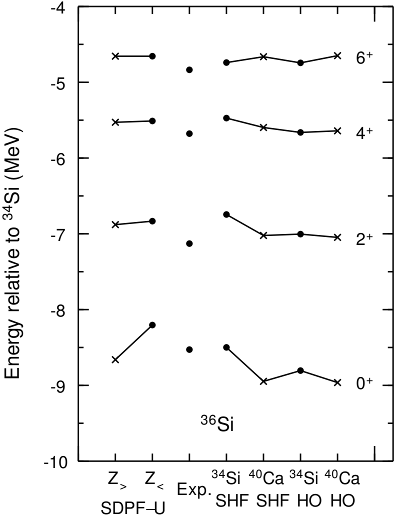
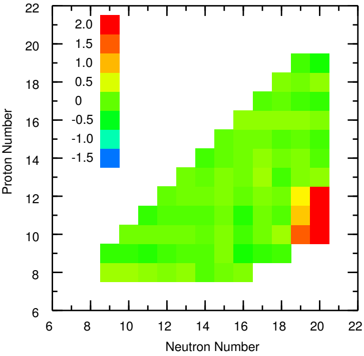
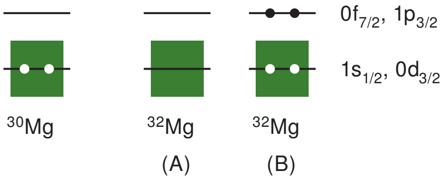


Island of Inversion region

- Exotic isotopes $Z \approx 11, N \approx 20$
- Ground state configurations contain $2p2h$ ($2\hbar\omega$) excitations
- Observed for some nuclei with $N \geq 19$ 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
- Can calculate nuclei throughout island of inversion region with one interaction
- Need accurate SPE and reasonable *NNN* forces to reproduce low-energy behavior
- 13 parameters: 8 SPE, 4 for three-body forces, and overall normalization
- Normalization $\approx 10\%$ reduction to reproduce 2^+ states
- 43 states are implemented in an iterative fitting procedure
- rms deviation is 370 keV

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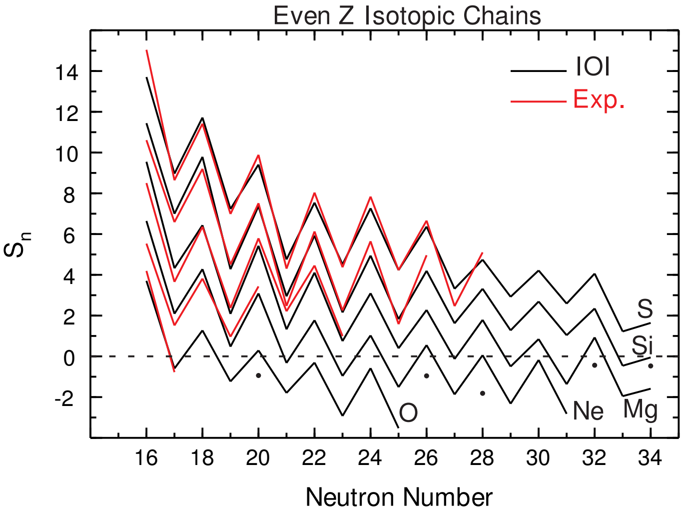

- $S_n(^AZ) = BE(^AZ) - BE(^{A-1}Z)$
- If $S_n > 0$, but $S_{2n}(^AZ) = BE(^AZ) - BE(^{A-2}Z) < 0$, nucleus is unbound

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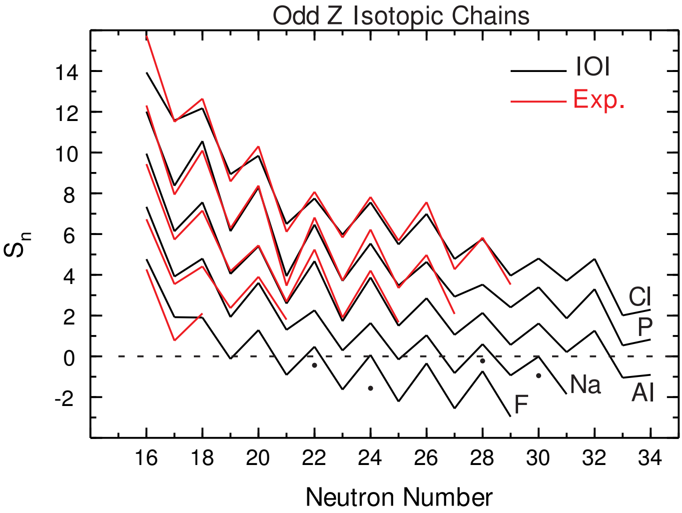

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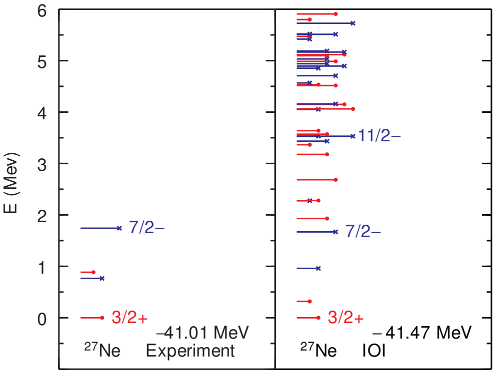
^{26}Ne(d,p)^{27}Ne

- Example of possible calculation
- States in ^{27}Ne populated by transfer



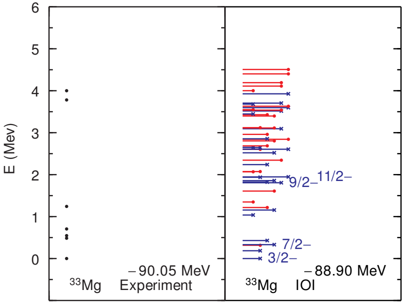
^{26}Ne(d,p)^{27}Ne

- Comparison between spectroscopic factors for states in ^{27}Ne
- Experimental values from Phys. Rev. C **85**, 011302(R) (2012)

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
$7/2^-$	1.74	1.670	0.35(10)	0.46

^{33}Mg β^- decay

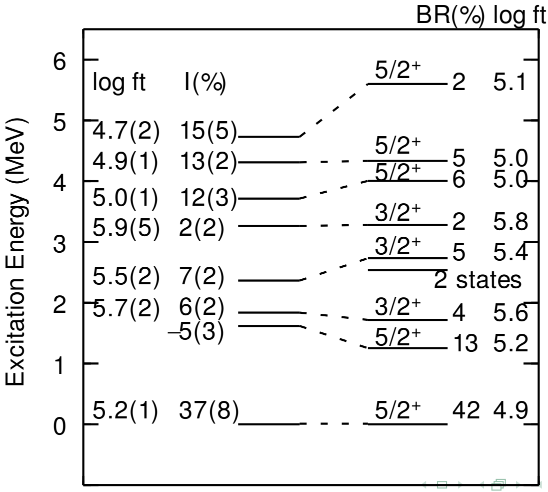
- Ground state of ^{33}Mg $J = 3/2$
- Two recent experiments have led to conflicting parity assignments
- Four theoretical states occur at $E_x \leq 370$ keV
- $3/2^-$ states: $E_x = 0$, $E_x = 186$ keV
- $3/2^+$ state: $E_x = 316$ keV



- 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

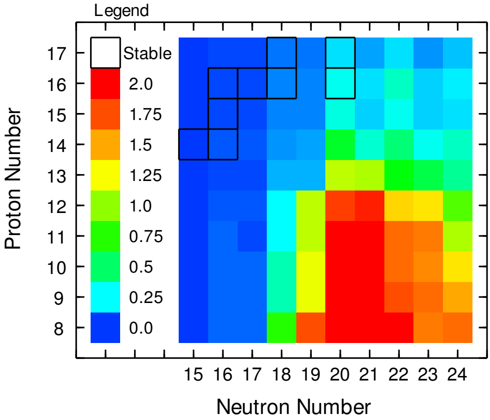


^{33}Mg β^- decay

- 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
- Next step: additional measurements which resolve isomers

Ground State Occupations

- Single configuration has $1\hbar\omega$ excitation if *sd* neutron is promoted into *pf* shell
- At $N = 20$, corresponds to $1p1h$ configuration
- Average $\hbar\omega$ of many-body 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
- Compare to experiment and to empirical SDPF-U interaction
- Provide information on applying renormalization procedure for exotic nuclei

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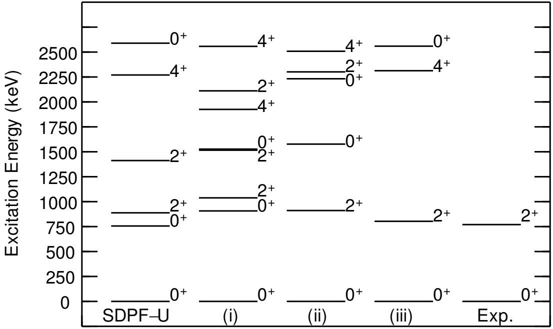
- Level density and behavior very different for three cases
- Theoretical conclusions depend on experimental determination of 4_1^+ and 0_2^+



^{42}Si Level Scheme

Summary of Applications

- Realistic Basis
  - Loosely bound orbits exhibit long tail, reducing TBME involving those orbits
  - Energy of single particle orbits can differ greatly for stable and exotic isotopes
  - HO basis results in stronger interaction and overbinding
  - Shown for two particle case, effect 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
  - *BE* and low-lying states agree with experiment for 100 nuclei
  - All level schemes accessible http://www.nscl.msu.edu/∼brown/resources/island/jpg/island.htm
  - 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
  - Three different applications of the method reproduce the known states in ^{42}Si
  - Predictions of 4_1^+ and 0_2^+ states vary significantly
  - Detection enables an evaluation of techniques to calculate exotic isotopes

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Conclusion and Outlook

- Overall Methodology
  - Microscopic *NN* interaction can be renormalized directly in reduced model space
  - Interactions do not need to be determined empirically
  - Basis and target nucleus used in renormalization are important- choose judiciously
  - Single particle energies from EDF methods are unreliable and need to be improved
- Outlook
  - More calculations outside of standard model spaces (^{68}Ni, ^{20}C, . . .)
  - Addition of three-body forces at the effective two-body level
  - More accurate determination of SPE

- B.A. Brown, A.S., and M. Hjorth-Jensen, Phys. Lett. B **695**, 507 (2011)
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Current Research

- Standard coupled cluster (CC) theory
  - Like CI, another method to approximate the Schrödinger equation in realistic nuclei
  - Exponential ansatz: $|\Psi\rangle = e^{T}|\Phi\rangle$ where T is the cluster operator
  - Physical wavefunction is built through np-nh excitations of HF wavefunction
  - Primarily employed for light and closed-shell nuclei
- Extension to Bogoliubov coupled cluster (BCC) theory
  - For calculations of open-shell nuclei, expansion techniques like CC break down
  - Reference state explicitly breaks symmetry to account for superfluid character
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Additional Information

SHF basis

- Harmonic oscillator basis implemented easily
  - $\psi^{HO}_{nlm_l}(\vec{r}) = R^{HO}_{nl}(r) Y_{lm_l}(\theta, \phi)$
  - Typically implemented in nuclear structure calculations
- Skyrme Hartree-Fock basis is chosen for realistic basis
  - Does not have a clean analytic expression
  - Radial wavefunctions implemented via an expansion of the HO basis

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

  - In practice, expansion is limited to n_{max}
- Percentage of HO basis radial wavefunction given by a_n^2
- SHF can only be solved for bound orbits
- Orbits unbound by few MeV solved approximately
- HO basis used for more unbound orbits
- Gram-Schmidt process is used to ensure orthonormality of basis
- Single Particle Energies
  - Renormalization procedure sums over diagrams with energy denominators
  - Divergences can occur for model space orbits with small energy differences
  - Identical valence energies for model space orbits to prevent divergences

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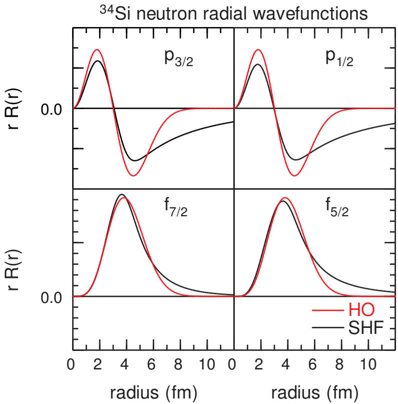
Wavefunction expansions

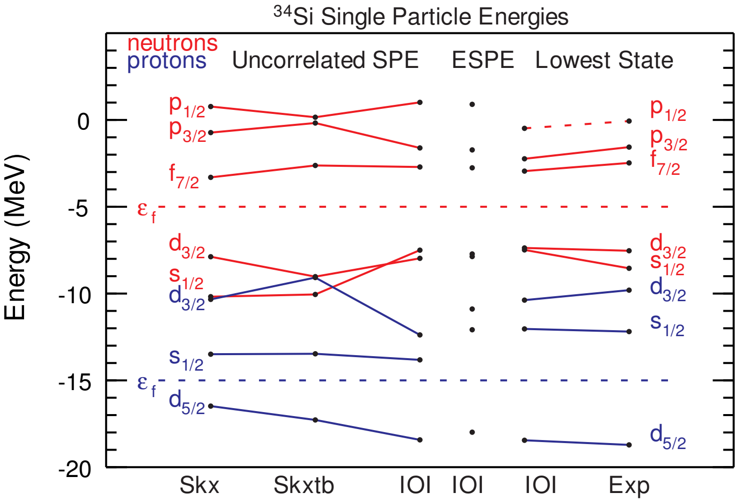
- Renormalization cutoff at 6 $\hbar\omega$
  - Sets $n_{max} = 4$ for $p_{3/2}, p_{1/2}$ orbits and $n_{max} = 3$ for $f_{7/2}, f_{5/2}$ orbits
  - Only 1% and 3% of $f_{7/2}$ and $f_{5/2}$ strength missing due to cutoff
  - Significant strength missing for $p_{3/2}$ and $p_{1/2}$ (16% and 18%)
- Calculation to $n_{max} = 6$ for all four orbits
  - Possible to first order in perturbation theory
  - Missing strength for $f_{7/2}, f_{5/2}, p_{3/2}, p_{1/2}$: 0%,0%,2%,3%
  - a_n coefficients then renormalized so that $\sum_{n=0}^{n_{max}} a_n^2 = 1$
  - Expansion accounts for "long-tail" behavior of p orbits due to loose binding

Wavefunction expansions



- 99% of $f_{7/2}$ orbit and 97% of $f_{7/2}$ orbit represented by R_{03}^{HO}
- 80% of $p_{3/2}$ orbit and 78% of $p_{1/2}$ orbit represented by R_{11}^{HO}

Systematic Trends



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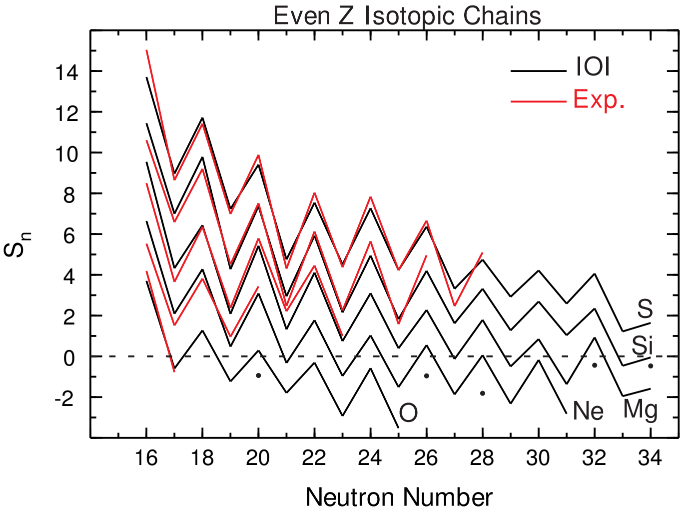

- $S_n(^AZ) = BE(^AZ) - BE(^{A-1}Z)$
- If $S_n > 0$, but $S_{2n}(^AZ) = BE(^AZ) - BE(^{A-2}Z) < 0$, nucleus is unbound

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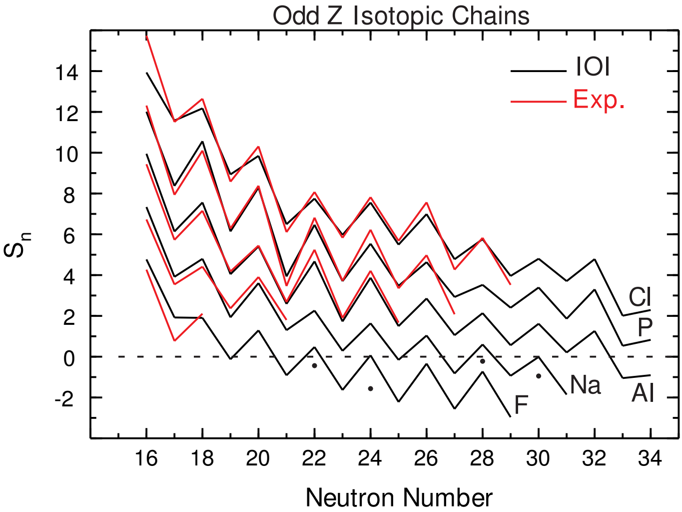

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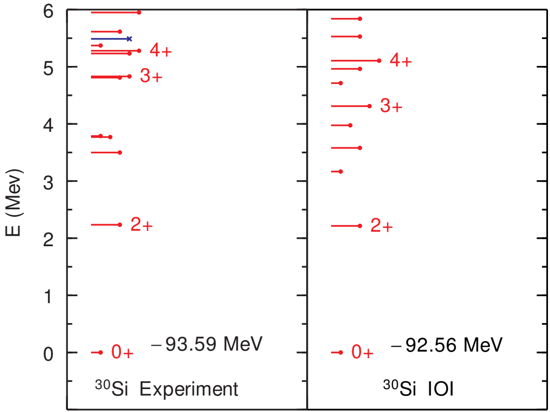
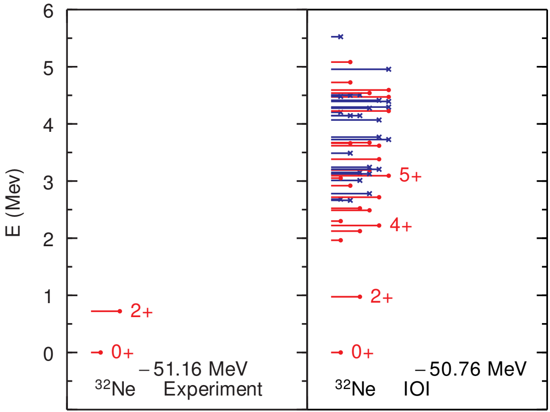
Representative Nuclei



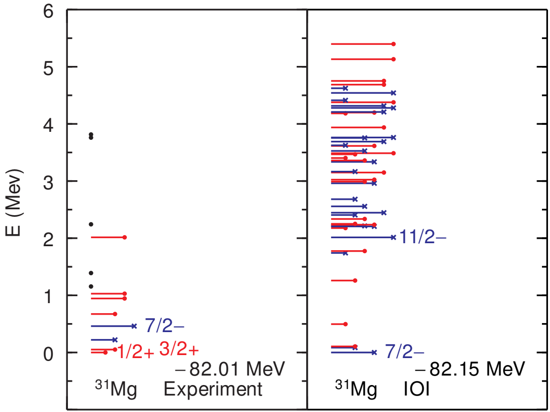
- Towards stability by the removal of four neutrons

Representative Nuclei



- Into the island of inversion (≈ 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