Shell model formalism

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CEA/Saclay

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Outline

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Statement of the problem

- Interested in solution to the Schrödinger equation

$$H|\Psi\rangle = E|\Psi\rangle$$

$$H = \sum_{l_1 l_2} t_{l_1 l_2} c^\dagger_{l_1} c_{l_2} + \frac{1}{(2!)^2} \sum_{l_1 l_2 l_3 l_4} \bar{v}_{l_1 l_2 l_3 l_4} c^\dagger_{l_1} c^\dagger_{l_2} c_{l_4} c_{l_3} + \frac{1}{(3!)^2} \sum_{l_1 l_2 l_3 l_4 l_5 l_6} \bar{w}_{l_1 l_2 l_3 l_4 l_5 l_6} c^\dagger_{l_1} c^\dagger_{l_2} c^\dagger_{l_3} c_{l_6} c_{l_5} c_{l_4} + \dots$$

- Standard eigenvalue problem, but two issues arise for nuclei
- Mesoscopic system
  - 10s-100s of particles
  - Too many permutations to solve computationally
  - System not large enough to treat statistically
- Nuclear Hamiltonian
  - Nucleons are composite particles (quark/gluon degrees of freedom → QCD)
  - Low-energy nuclear physics is typically insensitive to quark dynamics
  - Chiral effective field theory (χEFT) provides a low-energy effective approach
  - Nuclear interaction depends on renormalization, is not analytic
  - The nuclear Hamiltonian is scale-dependent
- Exact solution impossible- attempt reasonable approximations

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Nuclear Forces

- Interaction between two point-like nucleons?
  - Can determine a two-body interaction from nucleon-nucleon (NN) scattering
  - Can derive a Hamiltonian from χEFT based on QCD order by order
  - Coupling constants are parameters, can be fit to experimental scattering data
- Complications
  - Nucleus with mass A has, in principle, $A-$body Hamiltonian
  - Difficult to implement for structure calculations
  - Even with exact Hamiltonian, calculations are expensive
- Hierarchy in forces ($NN > NNN > NNNN \ldots$)
  - Suggested empirically
  - Confirmed by χEFT
- Limit to three-body forces in nuclear Hamiltonian
- Assume bare microscopic interactions (NN and NNN) are known
  - Underlying approximation to all further results
  - Will not evaluate effect of initial interaction
- Similarities to atomic problem suggest simpler calculational methods

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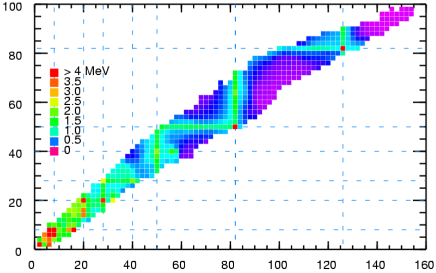
Single particle shell structure

- 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 $E(2+)$[a], low $B(E2)$, BE ...

$\rightarrow$ "magic" numbers

  - Indicative of single particle shell closures (e.g., group 18 noble gases)
  - Collisions within the nucleus are suppressed due to the Pauli principle

$E(2^+)$ as a function of proton (y-axis) and neutron (x-axis) number



[a] Figure courtesy of Alex Brown

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  $\rightarrow$ "magic" numbers

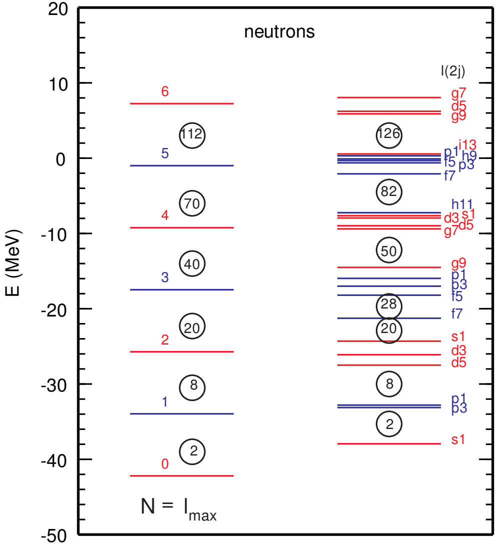
  - Collisions within the nucleus are suppressed due to the Pauli principle
- Nuclear Hamiltonian:

$$
\begin{aligned}
H &= T + V \\
&= \sum_{l_1 l_2} t_{l_1 l_2} c_{l_1}^{\dagger} c_{l_2} + \frac{1}{(2!)^2} \sum_{l_1 l_2 l_3 l_4} \bar{v}_{l_1 l_2 l_3 l_4} c_{l_1}^{\dagger} c_{l_2}^{\dagger} c_{l_4} c_{l_3} + \ldots \\
&= [T + V_{mf}] + [V - V_{mf}] \\
&= \quad H_0 \quad + \quad H_1
\end{aligned}
$$

- Analytic solutions to one-body $H_0 = \sum_i \epsilon_i a_i^{\dagger} a_i$ provide typical single particle bases
- A-body (in principle) residual interaction treated approximately

Harmonic oscillator (HO) single particle bases

- Neutron single particle orbits
- Determine $\hbar\omega$ empirically
- For ^{132}Sn, $\hbar\omega \approx 8$ MeV



Outline

Motivation

- Need to simplify the nuclear many-body problem
- Harmonic oscillator potential (with spin-orbit) reproduces magic numbers
- Results in large energy gaps between bunches of single particle orbits
- Fundamental assumptions
  1. Interested in low-energy nuclear properties
  2. Strongly bound single particle orbits are rarely excited $\rightarrow$ core
  3. Properties outside core can be represented by few orbits
- Physical energy scale limited approximately by single particle energy gaps

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Independent particle model

- Simplest approximation: easy to solve, limited applicability
- Find exact solution to basis $H_0|\phi_i\rangle = \epsilon_i|\phi_i\rangle$
- Core of mass A_c with Z_c protons and N_c neutrons (Z_c, N_c closed subshells)
- Single Slater determinant describes wavefunctions

$$|\Phi^{A_c}\rangle \equiv |\phi_1\phi_2 \ldots \phi_{Z_c}\rangle \otimes |\phi_1\phi_2 \ldots \phi_{N_c}\rangle$$

- Energy of core

$$E_c = \sum_{i=1}^{Z_c} \epsilon_i + \sum_{i=1}^{N_c} \epsilon_i$$

- Nuclei with $A_c + 1$ are given by $|\Phi^{A+1}\rangle = a_i^\dagger|\Phi^A\rangle$ with $i = Z_c + 1, N_c + 1$
- Energy relative to core

$$E_{(c+p)} - E_c = \epsilon_{(Z_c+1)} \qquad E_{(c+n)} - E_c = \epsilon_{(N_c+1)}$$

- Slater determinant is tailored to reproduce experimental data
  - Correlations implicitly included $\rightarrow$ experiments measure many-body system
  - Dominant states are reproduced, but fragmentation occurs
  - Distinct from other Slater determinant methods like EDF methods

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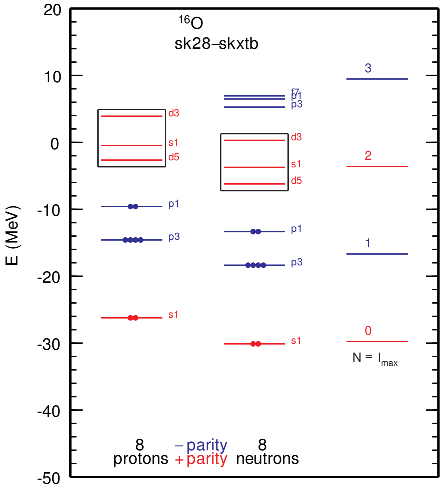
^{16}O in independent particle model



- Single Slater determinant
- $BE(^{17}O) - BE(^{16}O) = 4.14$ MeV
- $BE(^{18}O) - BE(^{16}O) = 12.19$ MeV
- Too simple model already!

Connection to Hartree-Fock (HF)

Schrödinger equation $H|\Psi\rangle = E|\Psi\rangle$

- Independent particle model:
  - Approximate H by $H_0 = T + V_{mf}$
  - Select reasonable V_{mf}
  - Solve $H_0|\phi_i\rangle = \epsilon_i|\phi_i\rangle$
  - $E_0 = \sum_{i=1}^{A} \epsilon_i$ for A nucleons
  - No correlations
  - Only appropriate for closed shells ± 1

- (symmetry-restricted) Hartree-Fock:
  - Approximate $|\Psi\rangle$ by $|\Phi\rangle = \prod_{i=1}^{A} a_i^\dagger|0\rangle$
  - Variational principle (minimizes energy)
  - Determine single particle basis $\{|\phi\rangle\}$
  - Limited correlations
  - Best near closed shells

Shell model

- Independent particle model is not rich enough
- Single-reference Hartree-Fock is better but suffers from same limitations
- Need to include correlations without solving full many-body problem
- Select core with A_c as before (closed subshells)
  - Treat core as vacuum based on large energy gap in single particle orbits
  - Fewer nucleons treated explicitly (valence particles $A_{val} = A - A_c$)
- Limit to "valence orbits" up to another large energy gap
- Reduction in model space (and number of particles)
  - Schrödinger equation can be solved completely
  - Separation into long-range and short-range correlations
  - Long-range correlations are completely included
- Can other effects be included?
  1. Polarization of the core by valence particles
  2. Virtual scattering of valence particles into higher-lying orbits
  3. Full short-range correlations

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Effective interaction

- Incorporate effects from outside of the model space into the Hamiltonian
- Still, cannot account for everything (e.g., short-range correlations)
- Reduction in degrees of freedom = reduction in possibilities
- Production of interactions is extremely important
  - Multiple lectures will focus on various procedures and mindsets
  - Tutorial sessions devoted to derivation and implementation
  - Will proceed currently with a general Hamiltonian

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Effective interaction

- Representation of effective interaction in reduced model space
  1. Single particle energies (SPE): ϵ_i where i refers to valence orbits
  2. Two-body matrix elements (TBME):

$$\langle (ab)_{JT} | V_{ms} | (cd)_{JT} \rangle$$

    - Model space orbits a, b, c, d
    - Angular momentum and isospin J and T, respectively
    - V_{ms} is the effective interaction in the reduced model space
    - Finite number of TBME for a given model space determined by J and T coupling
- V_{ms} distinct from original Hamiltonian
- Lowest order (monopole) of multipole expansion of the interaction

$$\bar{V}_{ab}^{T} = \frac{\sum_J (2J+1)\langle (ab)_{JT} | V_{ms} | (ab)_{JT} \rangle [1 - (-1)^{J+T}\delta_{ab}]}{\sum_J (2J+1)[1 - (-1)^{J+T}\delta_{ab}]}$$

Model Spaces

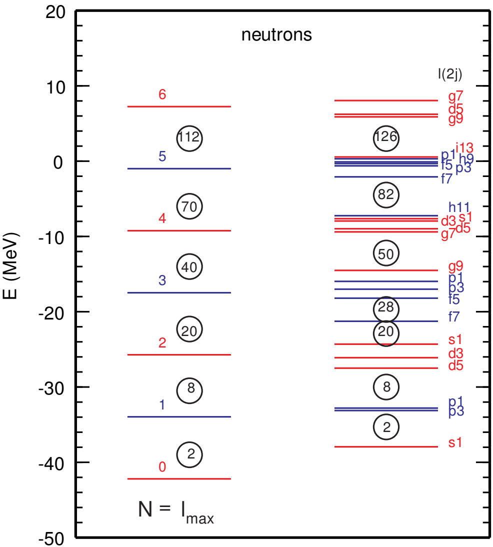
Common model spaces

Oscillator shells

- $N = 0, 1, 2, 3 \rightarrow s, p, sd, pf$

Beyond *pf* shell

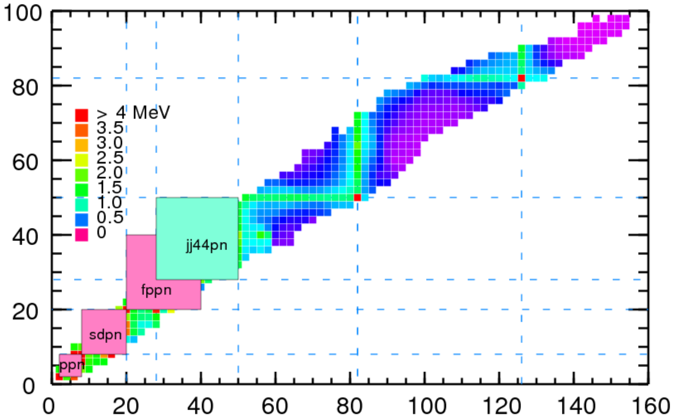
- include $j_>$ orbit of next shell
- $j_>$ refers to $j = \ell_{max} + \frac{1}{2}$
- $j_<$ refers to $j = \ell_{max} - \frac{1}{2}$



Model Spaces

- Most common model spaces (courtesy of Alex Brown)

$E(2^+)$ as a function of proton (y-axis) and neutron (x-axis) number



Model Spaces

- Inclusion of $j_>$ orbit (courtesy of Alex Brown)

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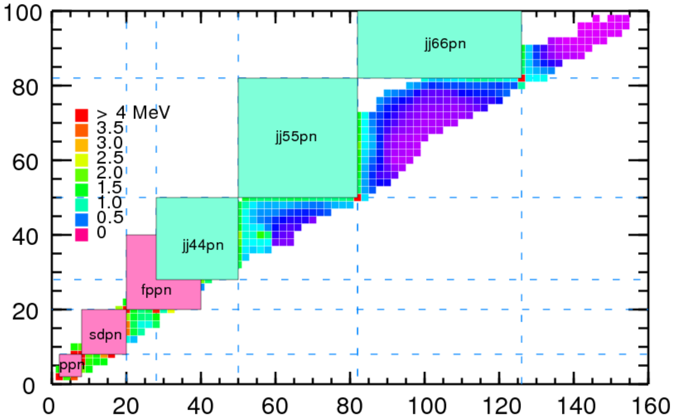

Model Spaces

- Extension to heavier nuclei with $N > Z$ (courtesy of Alex Brown)
- Based on stable magic numbers → island of inversion region?

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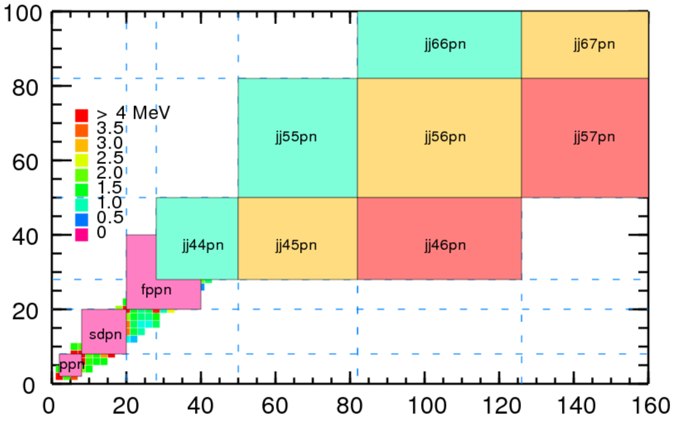

Summary

- Cannot solve full Schrödinger equation beyond lightest nuclei
- Search for approximate techniques
- Because nuclei display shell structure via “magic” numbers
  - Break Hamiltonian into mean field and residual interaction
  - Solve mean field Hamiltonian for single particle basis
  - Utilize large energy gaps in basis to isolate few valence orbits
  - Treat core of model space as vacuum
  - Solve Schrödinger equation exactly in reduced model space
- Typically called shell model in nuclear physics
- Falls under more general category of configuration interaction (CI) theory

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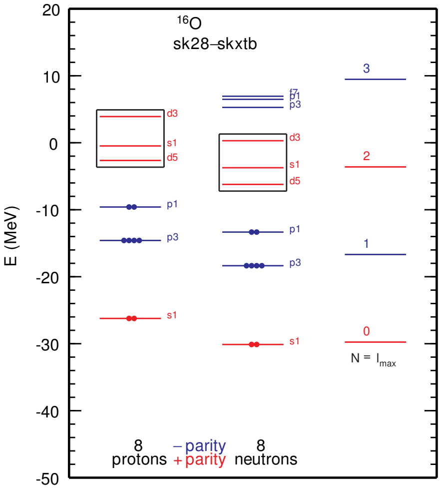
Opening remarks

- Hamiltonian operating only in the reduced model space is required
- For now, given empirically by USDB interaction[1]
- SPE and TBME parameterized (66 parameters in all)
- Fit to experimental energies in *sd* shell
  - Iterative procedure of CI calculations for states accessible in the model space
  - See Lecture VII for details
- Use *sd* shell as example, same principles apply throughout nuclear chart

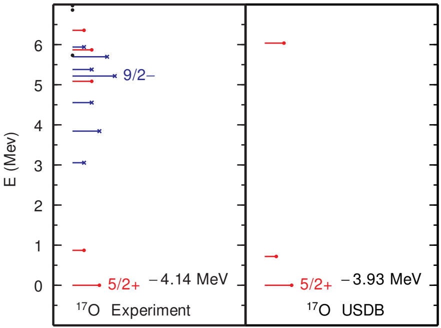
[1] B.A. Brown and W.A. Richter, Phys. Rev. C **74**, 034315 (2006)

^{16}O as core



- *sd* model space outlined
- Separation from *p* and *pf* shells
- $N = 0, 1$ oscillator shells filled
- $|^{16}\text{O}\rangle \equiv |0\rangle$
- $E(^{16}\text{O}) = 0$

Simplest system- ^{17}O



- One valence neutron
- Three orbits to occupy
- $\binom{12}{1} = 3$ possibilities to add nucleons
- Three possible states[a]

[a] See Lecture II for counting procedure

- Experiment displays richer behavior
  1. Intruder states (only positive-parity many-body states from *sd* orbits)
  2. Fragmentation of single particle strength due to correlations
- Calculated $BE_{USDB}(^{17}\text{O}) = 3.93$ MeV, whereas $BE_{exp}(^{17}\text{O}) = 131.76$ MeV
- USDB selects ^{16}O as vacuum with $E = 0$ MeV
- $BE_{exp}(^{17}\text{O}) - BE_{exp}(^{16}\text{O}) = 4.14$ MeV

Spectroscopic factors

- Basis-independent, but not observable
- Spectroscopic probability matrices

$$S_{\mu}^{+pq} \equiv \langle \Psi_0^A | a_p | \Psi_{\mu}^{A+1} \rangle \langle \Psi_{\mu}^{A+1} | a_q^{\dagger} | \Psi_0^A \rangle$$

and

$$S_{\nu}^{-pq} \equiv \langle \Psi_0^A | a_q^{\dagger} | \Psi_{\nu}^{A-1} \rangle \langle \Psi_{\nu}^{A-1} | a_p | \Psi_0^A \rangle$$

- Spectroscopic factors (SF) found from tracing spectroscopic probability matrices
- In reduced model space, recover typical "definitions"

$$SF_{\mu}^{+} \equiv |\langle \Psi_{\mu}^{A+1} | a_q^{\dagger} | \Psi_0^A \rangle|^2$$

and

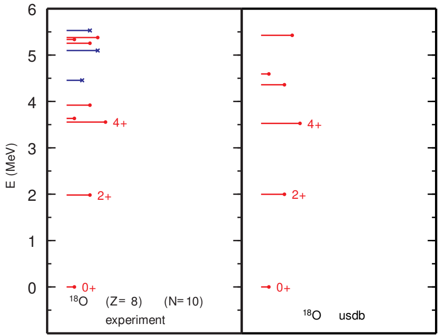
$$SF_{\nu}^{-} \equiv |\langle \Psi_{\nu}^{A-1} | a_p | \Psi_0^A \rangle|^2$$

Spectroscopic factors

- For ^{17}O in *sd* shell, each state carries full spectroscopic strength
  - Only one valence particle
- "Experimental" SF
  - $SF = 0.81$ for $\frac{5}{2}^+$ ground state of ^{17}O [a]
  - $SF = 0.67$ for $\frac{3}{2}^+$ "single particle peak" at 5.09 MeV[b]
  - $SF = 0.06$ for $\frac{3}{2}^+$ state at 5.87 MeV[c]
- Problematic for calculations? Is ^{16}O a good enough core?

[a] J. Lee, M.B. Tsang, and W.G. Lynch, Phys. Rev. C **75**, 064320 (2007)
[b] M. Yasue et al., Phys. Rev. C **46**, 1242 (1992)
[c] M. Yasue et al., Phys. Rev. C **46**, 1242 (1992)

Next simplest system- ^{18}O

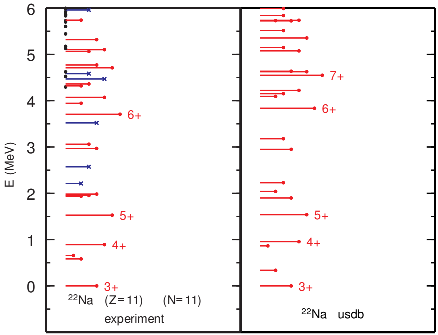


- Two valence neutrons
- Three orbits to occupy
- $\binom{12}{2} = 66$ possibilites to add nucleons
- Only 14 possible states[a]

[a] See Lecture II for counting procedure

- Experiment displays richer behavior, including negative-parity intruder states
- Calculated $BE_{USDB}(^{18}\text{O}) = 11.93$ MeV, whereas $BE_{exp}(^{18}\text{O}) = 139.81$ MeV
- $BE_{exp}(^{18}\text{O}) - BE_{exp}(^{16}\text{O}) = 12.19$ MeV

More complicated- ^{22}Na



- Odd-odd nucleus
- Three neutrons, three protons
- $\binom{12}{3}^2$=48400 possibilities
- 3266 possible states[a]

[a] See Lecture II for counting procedure

- USDB interaction is isospin-symmetric (no Coulomb force!)
- $E_{USDB}(^{22}\text{Na}) = -58.44$ MeV
- $E_{USDB}(^{22}\text{Na}) = -46.71$ MeV (Coulomb corrected)
- $BE_{exp}(^{22}\text{Na}) - BE_{exp}(^{16}\text{O}) = 46.53$ MeV

Comparison to data

- All *sd* nuclei have such level schemes available[2]
- Overall, root-mean-square (rms) deviation of $\approx$ 170 keV to low-energy states
- Only considering states accessible in the model space
- USDB has been used in hundreds of calculations
- Only energies thus far, but good agreement for other nuclear properties
  - To be discussed in more detail later
- Slater determinant of $N = 0, 1$ HO orbits not accurate description of ^{16}O
  - Seen from Hartree-Fock or realistic calculation (e.g., coupled cluster)
  - Correlations contribute multiple MeV to ground state
  - Excited states exist- experimentally $E(0_2^+) = 6.05$ MeV
  - Single particle strength fragmented in ^{17}O[3]
- Still reproduce results in *sd* shell well!
- Long-range correlations cause low-energy behavior in *sd* shell nuclei

[2] http://www.nscl.msu.edu/∼brown/resources/resources.html

[3] T. Duguet and G. Hagen, Phys. Rev. C **85**, 034330 (2012)

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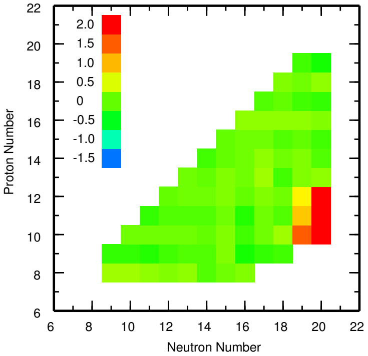
Problems remain

- Even with correct interaction, can fail to reproduce low-energy states

$$BE_{exp}(Z,N) - BE_{th}(Z,N)$$



- Wrong degrees of freedom (missing necessary valence orbits)
- Invalidates assumption that shell gap excludes *pf* orbits
- Referred to as the island of inversion region