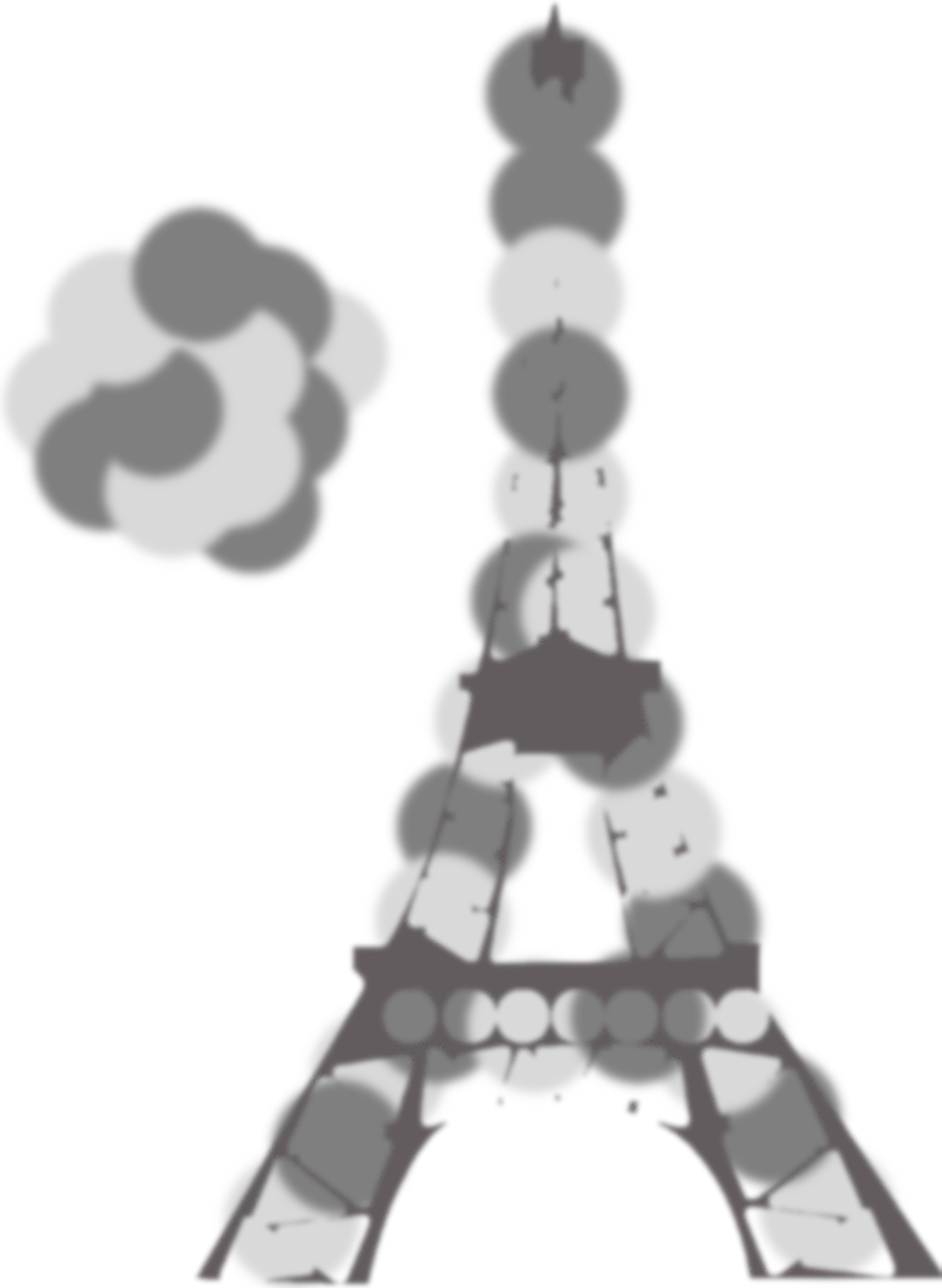
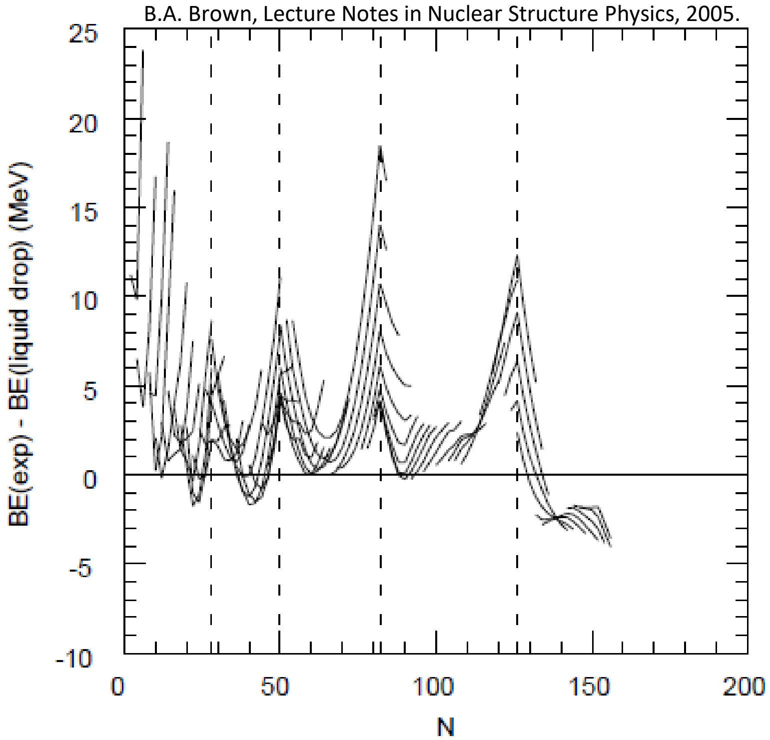
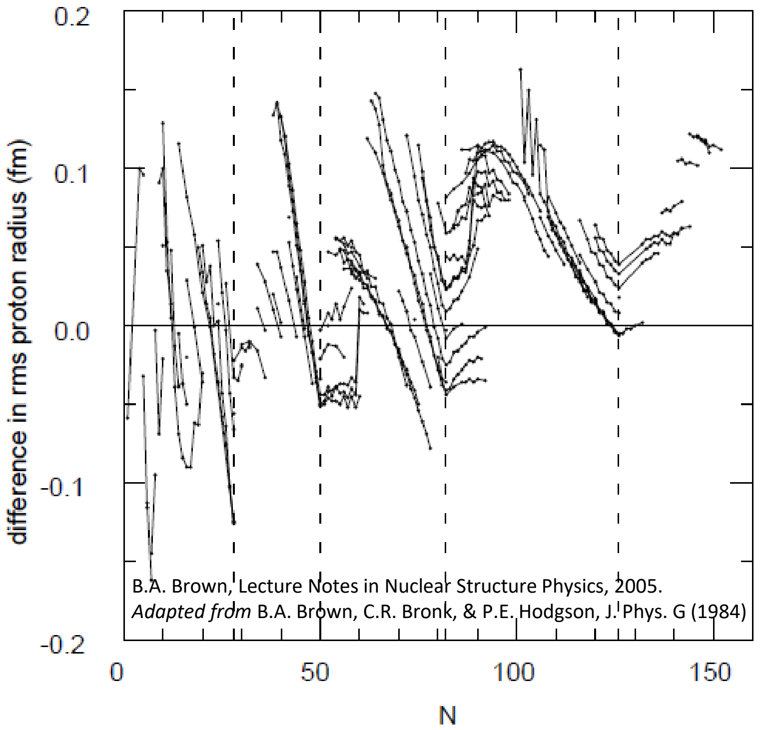
Lecture 3: *Nuclear Structure 1*

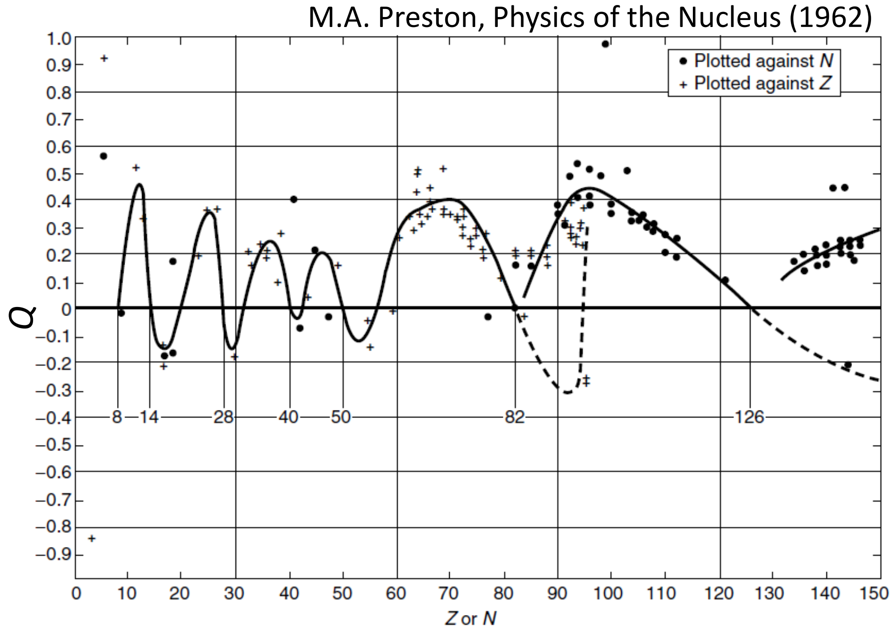
- Why structure?
- The nuclear potential
- Schematic shell model

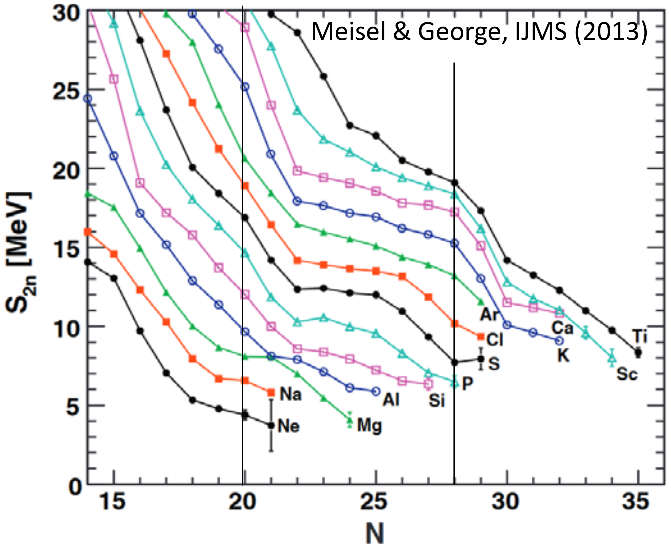


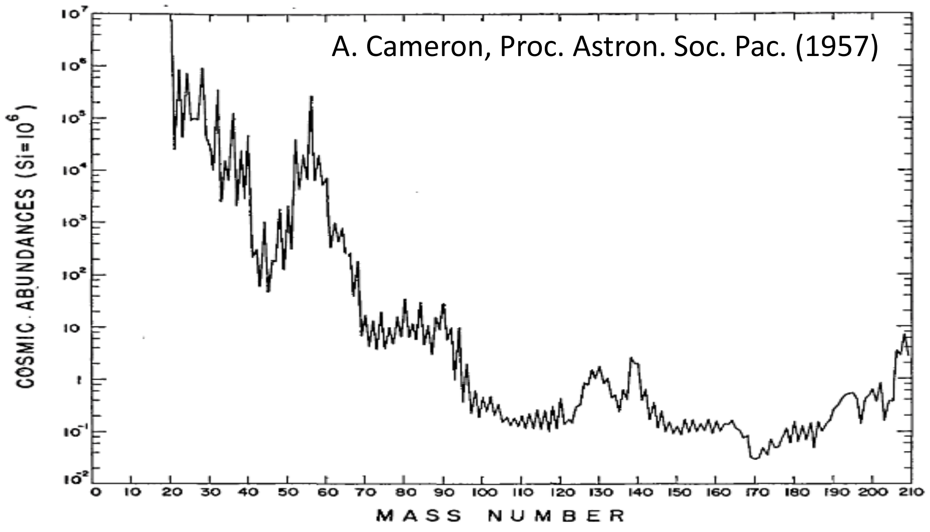
Empirically, several striking trends related to Z,N. *e.g.*

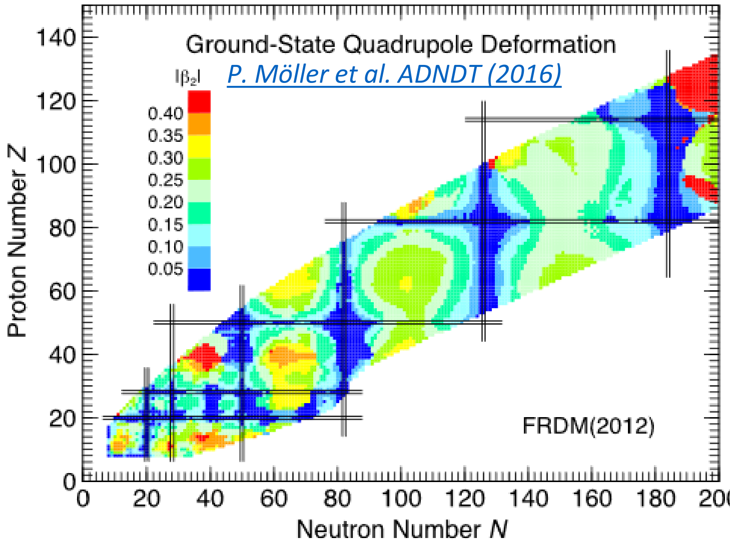








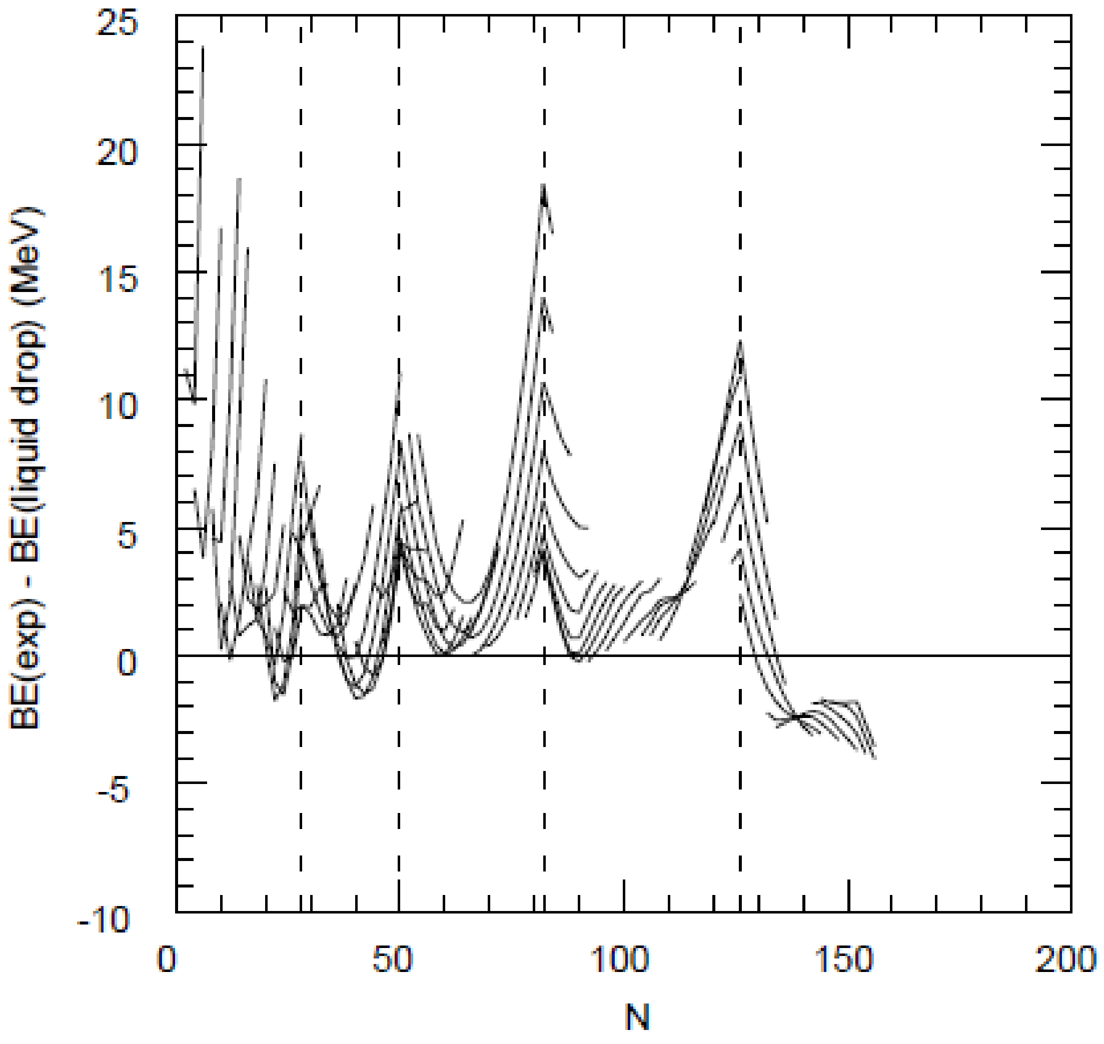


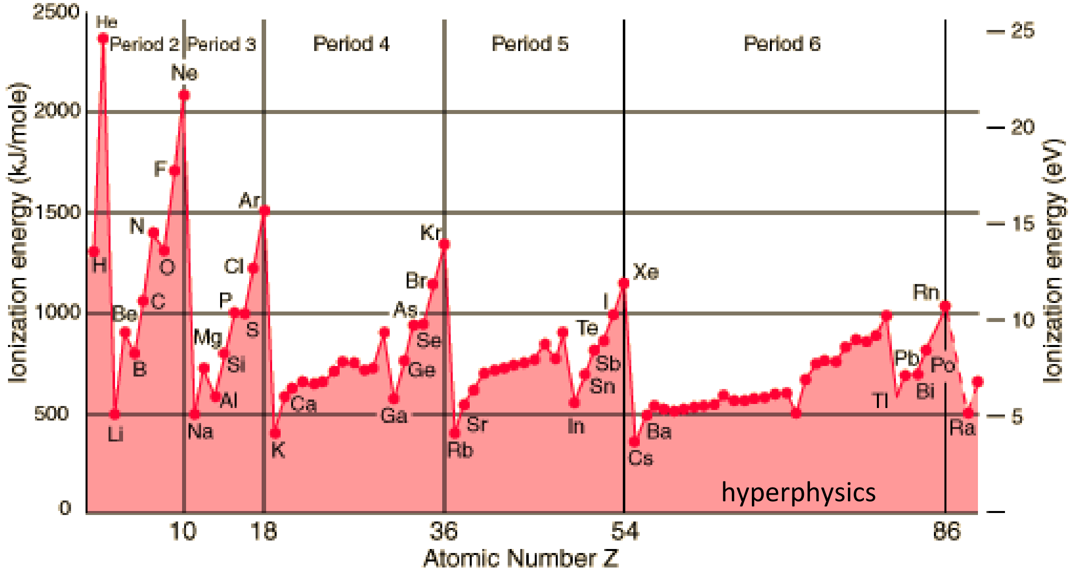


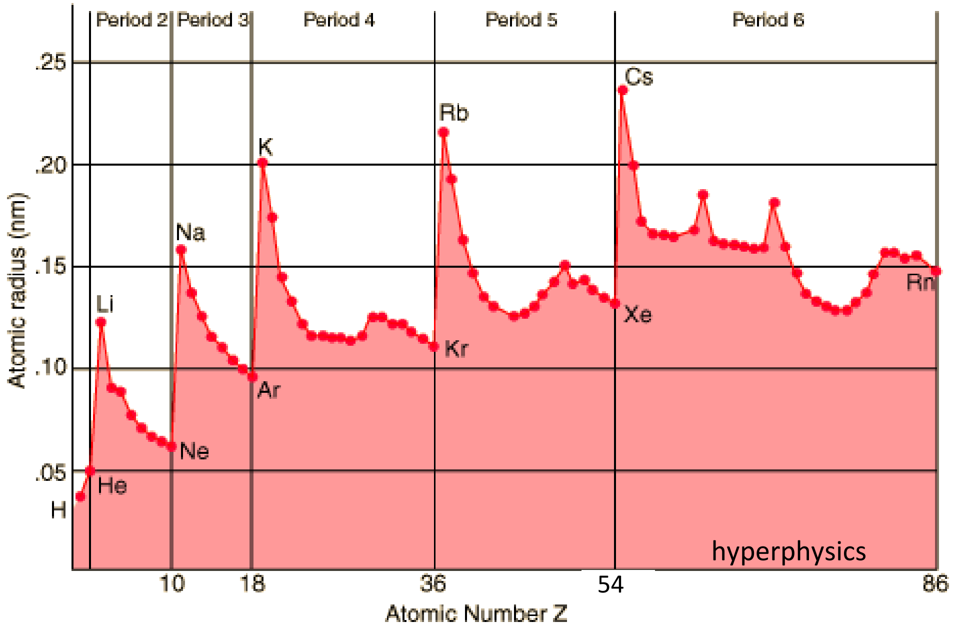
First magic number evidence compilation by M. Göppert-Mayer Phys. Rev. 1948

...reminiscent of atomic structure

B.A. Brown, Lecture Notes in Nuclear Structure Physics, 2005.







Shell Structure

Atomic

- Central potential (Coulomb) generated by nucleus
- Electrons are essentially non-interacting
- Solve the Schrödinger equation for the Coulomb potential and find characteristic (energy levels) shells: *shells at 2, 10, 18, 36, 54, 86*

Nuclear

- No central object
  …but each nucleon is interacted on by the other A-1 nucleons and they're relatively compact together
- Nucleons interact very strongly
  …but if nucleons in nucleus were to scatter, Pauli blocking prevents them from scattering into filled orbitals. Scattering into higher-E orbitals is unlikely. i.e. there is no "weak interaction paradox"
- Can also solve the Schrödinger equation for energy levels (shells) …but obviously must be a different potential: *shells at 2, 8, 20, 28, 50, 82, 126*

…you might be discouraged by points 1 and 2 above, but, remember:
If it's stupid but it works, it isn't stupid.

Calculating eigenstates of the system, a.k.a single particle levels

- The behavior of a quantum-mechanical system is described by the wave function ψ
- For a particle in some potential, we can solve for ψ using the Schrödinger equation,
  - $H\psi = E\psi \quad a.k.a.\ T\psi + V\psi = E\psi \ a.k.a. -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi$ (in cartesian coordinates, $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$)
- The solutions ψ are the eigenfunctions and their eigenvalues are the corresponding energy E
- As a bonus, when ψ can be expressed in terms of spherical harmonics, $\psi = R(r)Y^l{}_m(\theta,\phi)$
  we also get the angular momentum for that particular eigenfunction,
  and parity, since the function is either odd or even

- Mathematical challenges aside, to get any traction we obviously need to assume a potential V
- For a single nucleon in the field of a nucleus,
  - V should approximate the mean-field generated by all other nucleons
  - The solutions will be single-particle levels,
    i.e. discrete states the nucleon can occupy

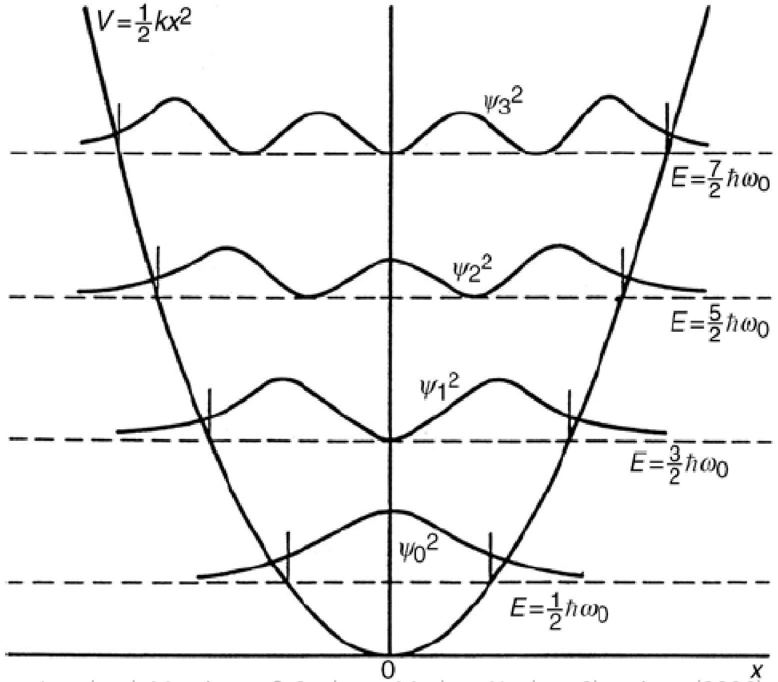
- Since nucleons are indistinguishable, we only need to solve for the single-particle levels for a nucleon and then we can fill those levels (working in terms of increasing E) to generate a model to calculate the properties of our nucleus

First stab at the potential, V: **The Harmonic Oscillator**

- Based on some evidence (and logic) that nuclei aren't perfectly constant in density, Heisenberg (Z. Phys. 1935) posited that a parabolic potential could be assumed, conveniently allowing the adoption of the harmonic oscillator solutions
  (one of the few analytically solved systems!)
- This provides evenly spaced energy levels $n \geq 1$, with $E_n = \left(n - 1 + \frac{1}{2}\right)\hbar\omega$.
- The corresponding angular momenta are $l = n - 1, n - 3, \ldots \geq 0$.
- The number of particles per angular momentum is $2(2l + 1)$ for $2l + 1$ projections & 2 spins
- So, the number of particles per level is:

i.e. only odd or even functions are allowed for each oscillator shell

n	l	# per level	Cumulative
1	0	2(2*0+1) = 2	2
2	1	2(2*1+1) = 6	8
3	0,2	2(2*0+1) = 2 + = 12 2*(2*2+1) = 10	20
4	1,3	2*(2*1+1) = 6 + = 20 2*(2*3+1) = 14	40
5	0,2,4	2*(2*0+1) = 2 + 2*(2*2+1) = 10 = 30 + 2*(2*4+1) = 18	70

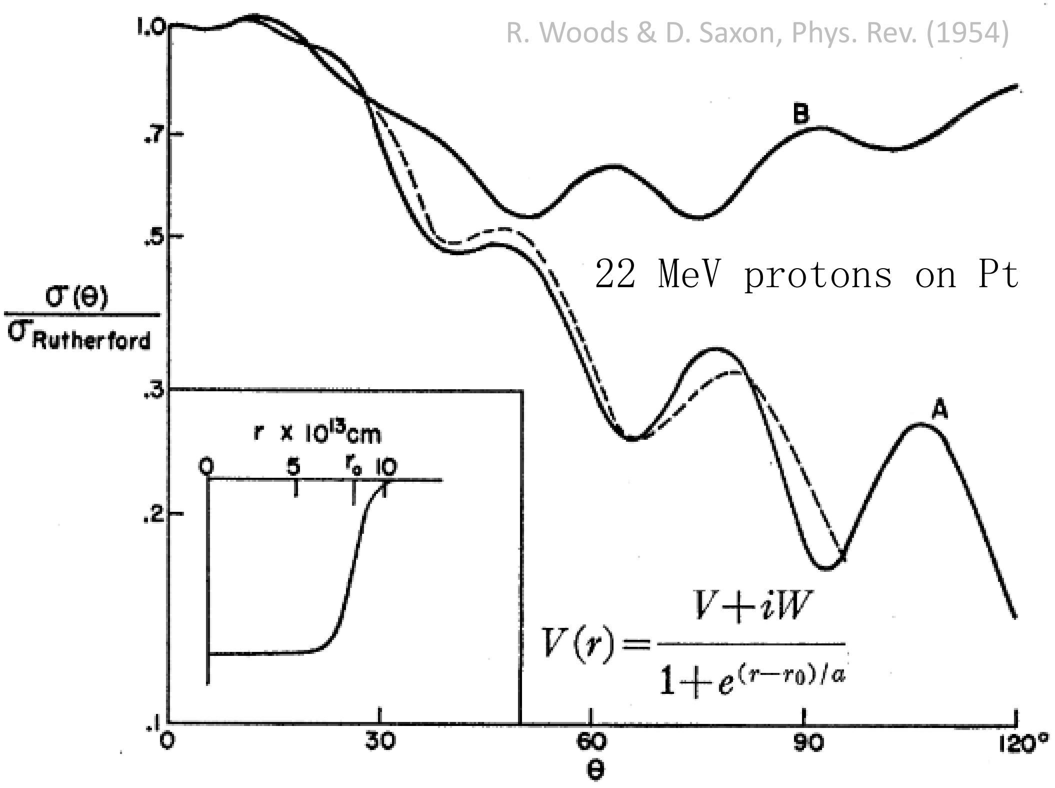


Loveland, Morrissey, & Seaborg, Modern Nuclear Chemistry (2006)

Could the HO potential still be useful for some cases?
…can get the job done for light nuclei (e.g. [H. Guo et al. PRC 2017](#))
…but need to be careful, because can impact results ([B.Kay et al PRL 2017](#))

Move to an empirical potential: **Woods-Saxon**

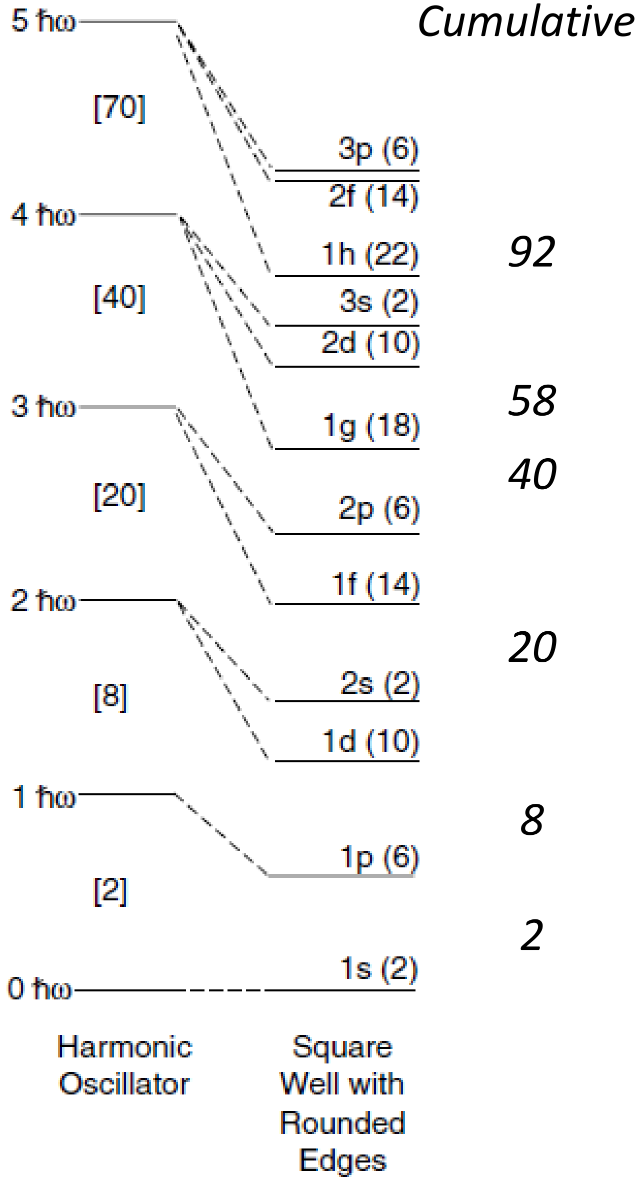
- Since the nuclear interaction is short-range, a natural improvement would be to adopt a central potential mimicking the empirical density distribution
- This is basically a square well with soft edges, as described by the Woods-Saxon potential:



R. Woods & D. Saxon, Phys. Rev. (1954)

- Using the Woods-Saxon is a good idea because of commitment to reality… but we're no wiser as to the origin of the magic numbers

Was this step completely useless? No! It broke the degeneracy in ℓ

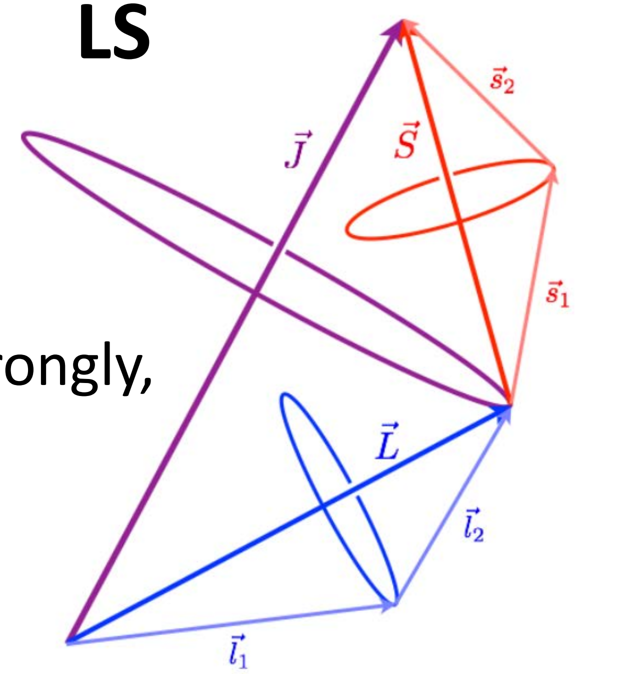


Loveland, Morrissey, & Seaborg, Modern Nuclear Chemistry (2006)

The missing link: **the spin-orbit interaction**

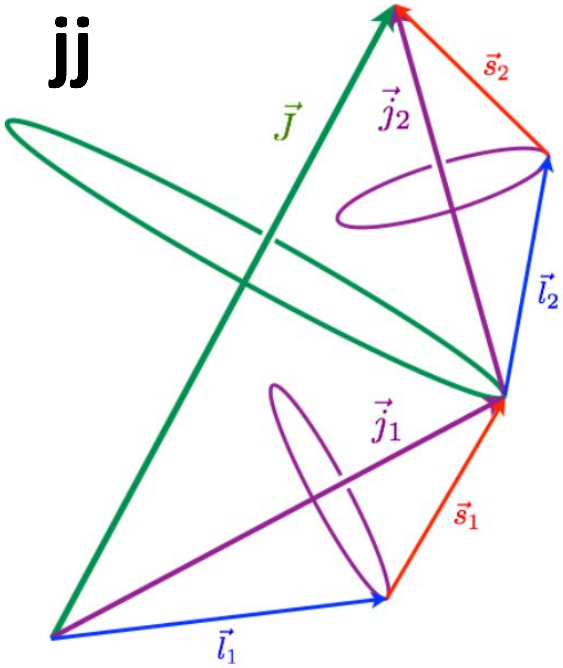
- Due to desperation or genius (or both) Maria Göppert-Mayer
  [Phys. Rev. February 1949] (and nearly simultaneously Haxel, Jensen, & Suess [Phys. Rev. April 1949])
  posited that nucleon spin and orbital angular momentum interacted strongly, making j the good quantum number for a nucleon: $\vec{j} = \vec{l} + \vec{s}$
- Prior to this approach,
  angular momentum was coupled as is typically done for atoms,
  where $\vec{J} = \vec{L} + \vec{S}$, $\vec{L} = \sum_{nucleons} \vec{l}$, and $\vec{S} = \sum_{nucleons} \vec{s}$
  - This is “LS coupling”
- Positing that the spin-orbit interaction is stronger than spin-spin or orbit-orbit means that instead, $\vec{J} = \sum_{nucleons} \vec{j}$ and $\vec{j} = \vec{l} + \vec{s}$
  - This is “jj coupling”

LS



A. Kastberg, Lecture Notes Physique Atomique

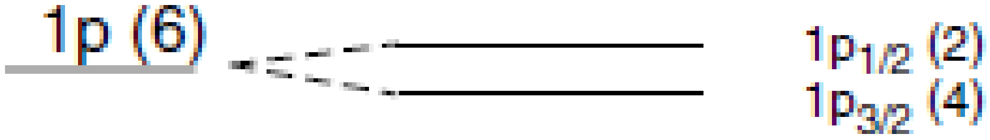
jj



The missing link: **the spin-orbit interaction**

- Now, in considering a valence nucleon, we should calculate its j
- j can only take on values: $|l - s| \leq j \leq |l + s|$ …so for our nucleons, $\left|l - \frac{1}{2}\right| \leq j \leq \left|l + \frac{1}{2}\right|$, i.e. l and s are either aligned ($l + s$) or anti-aligned ($l - s$)
  - For $l = 0$: $j = \frac{1}{2}$; $l = 1$: $j = \frac{1}{2}\, or\, \frac{3}{2}$; $l = 2$: $j = \frac{3}{2}\, or\, \frac{5}{2}$; $l = 3$: $j = \frac{5}{2}\, or\, \frac{7}{2}$ … etc.
- Each j has $2j + 1$ projections (a.k.a. # of protons or neutrons, depending which nucleon we're discussing)
  - i.e. 2 states for $j = \frac{1}{2}$, 4 states for $j = \frac{3}{2}$, 6 states for $j = \frac{5}{2}$, 8 states for $j = \frac{7}{2}$ …etc.
- The spin-orbit interaction means there's a j-dependent part of the nuclear potential, so the levels corresponding to different j for some l will be split in energy.
- For nucleons, cases with aligned l and j are energetically favored, so, for example, $l = 1, j = \frac{3}{2}$ will be lower in energy than $l = 1, j = \frac{1}{2}$

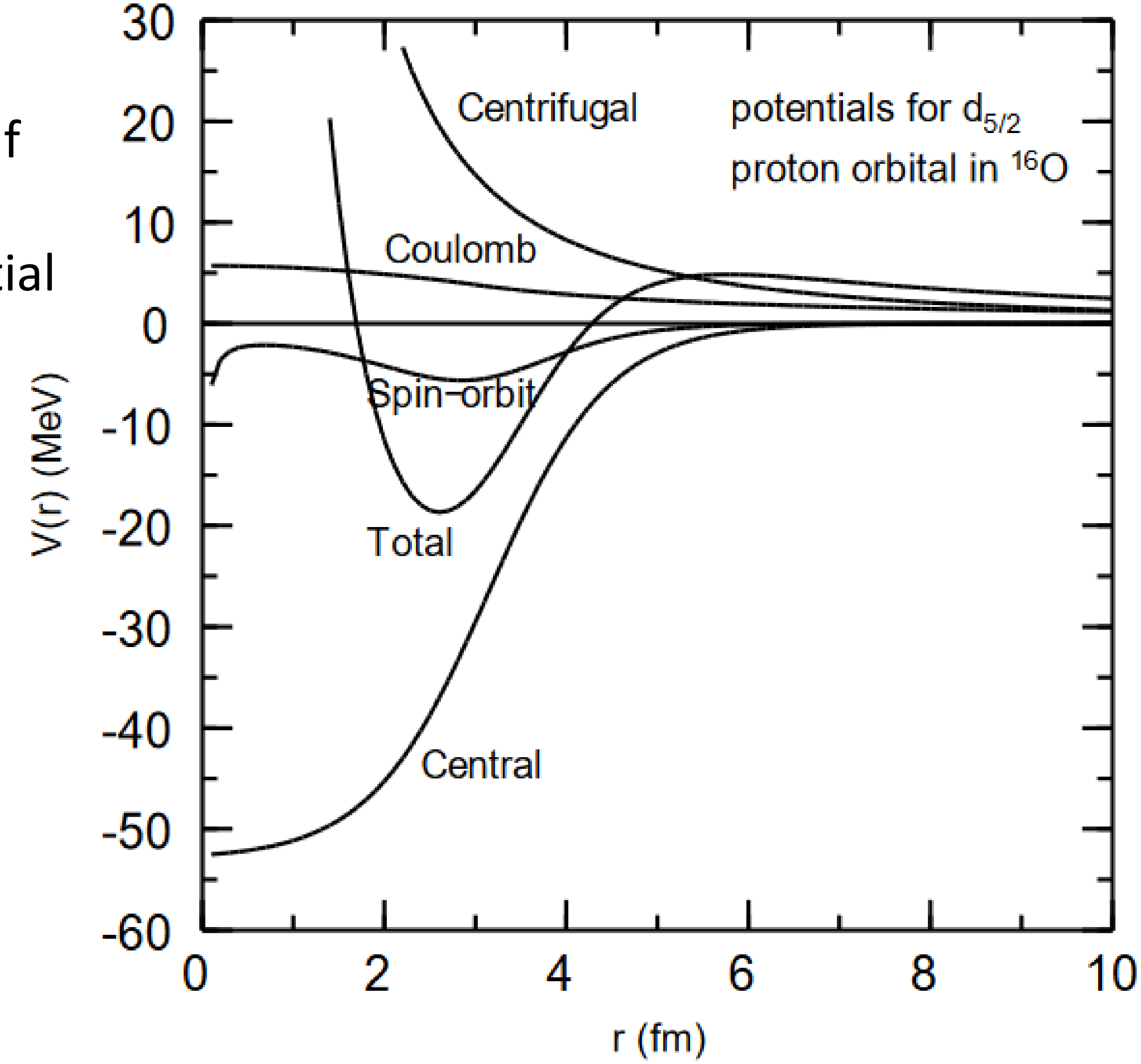
- While we're at it, note the spectroscopic notation:
  - $l = 0, 1, 2, 3, 4, 5, \ldots$ = "s", "p", "d", "f", "g", "h" …



Result: the **nuclear potential**

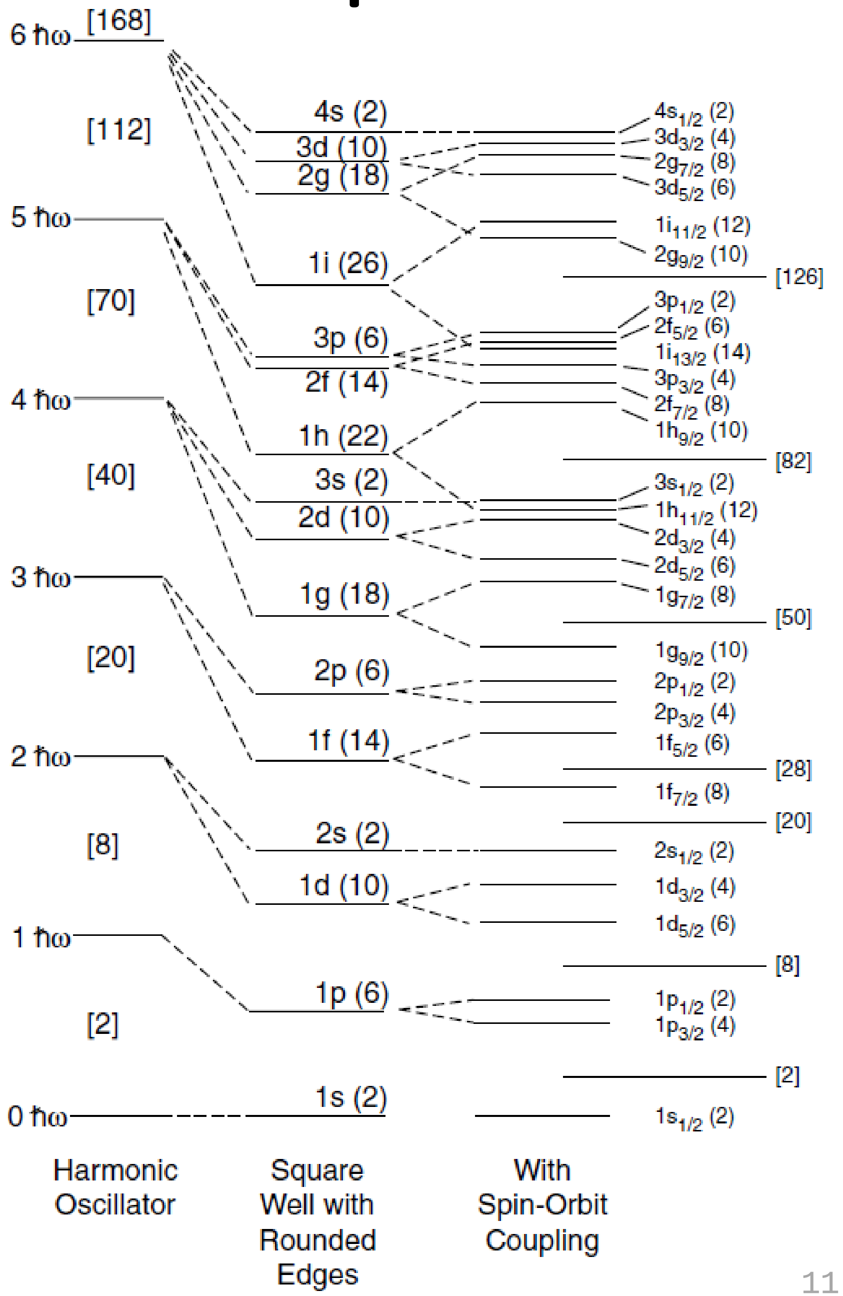
- Nucleons within a nucleus can be treated as if they are
  - **Attracted** by a Woods-Saxon central potential
  - **Repelled** by a Coulomb potential from a charged sphere (if proton)
  - **Attracted *or* Repelled** if l and s are parallel or anti-parallel by the spin-orbit force (Peaks at surface)
  - **Repelled** by a centrifugal barrier (if the nucleon were to exit the nucleus, carrying away angular momentum $l > 0$)

B.A. Brown, Lecture Notes in Nuclear Structure Physics, 2005.



Putting it all together: **“shells” from the nuclear potential**

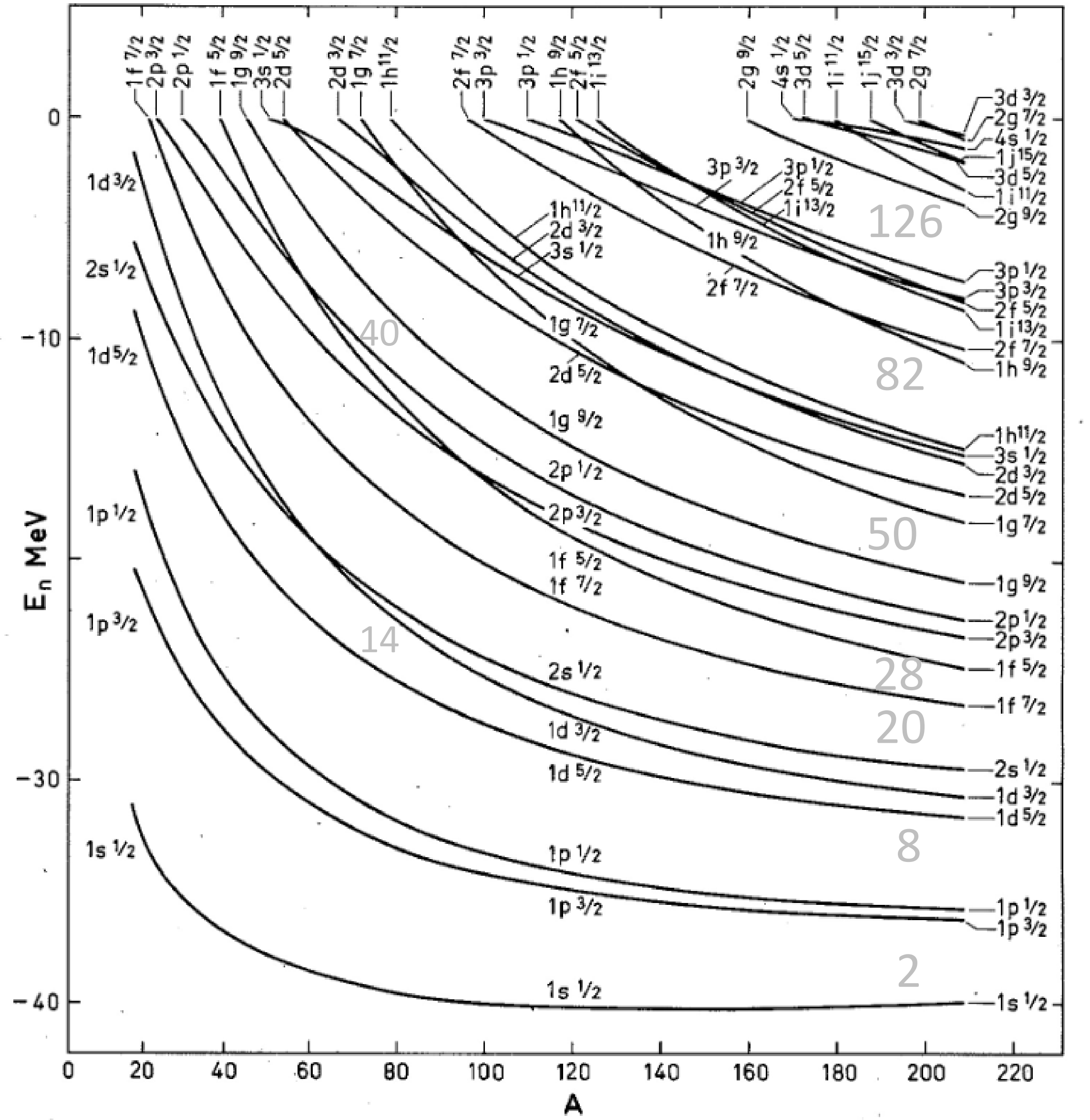
- Considering the nucleus as nucleons interacting in a mean-field potential, generated by the spatial distribution of all other nucleons, and each nucleon having a strong interaction between its orbital & spin angular momentum, properly predicts the magic numbers.
- Note that **neutrons and protons are considered separately**.
- When adding neutrons or protons to a nucleus, the lowest energy state will (generally) consist of filling each orbital as you go upward.
- The regions between the large gaps in nucleon energy are referred to as “shells”.
  - E.g. Between 8 and 20 neutrons (or protons) is the “sd-shell”, between 28 and 40 neutrons (or protons) is the “fp-shell”.
  - More exotic neutron-rich nuclides exist, so typically people are talking about the neutron shell
  - Nucleons can get excited into higher-lying states, so states above the ground-state are relevant in calculations



Loveland, Morrissey, & Seaborg, Modern Nuclear Chemistry (2006)

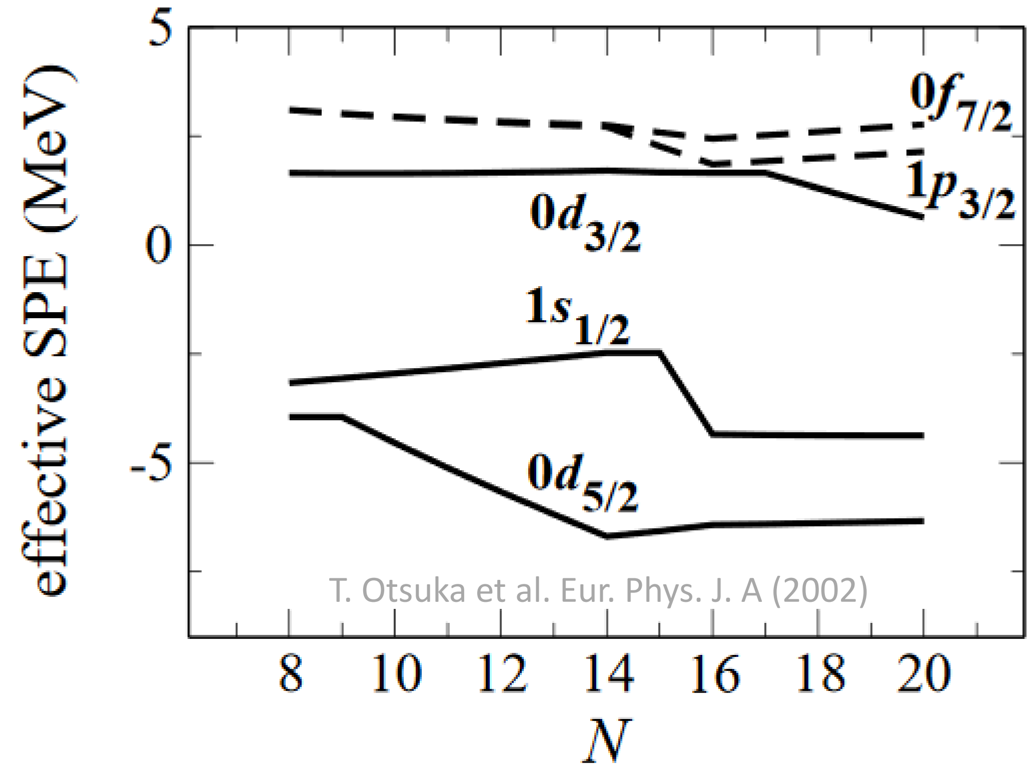
As a heads-up, level ordering doesn't follow a fixed set of rules

For stable, spherical nuclides:



Bohr & Mottelson, Nuclear Structure, Vol. I (1969)

For, e.g, n-rich O isotopes:



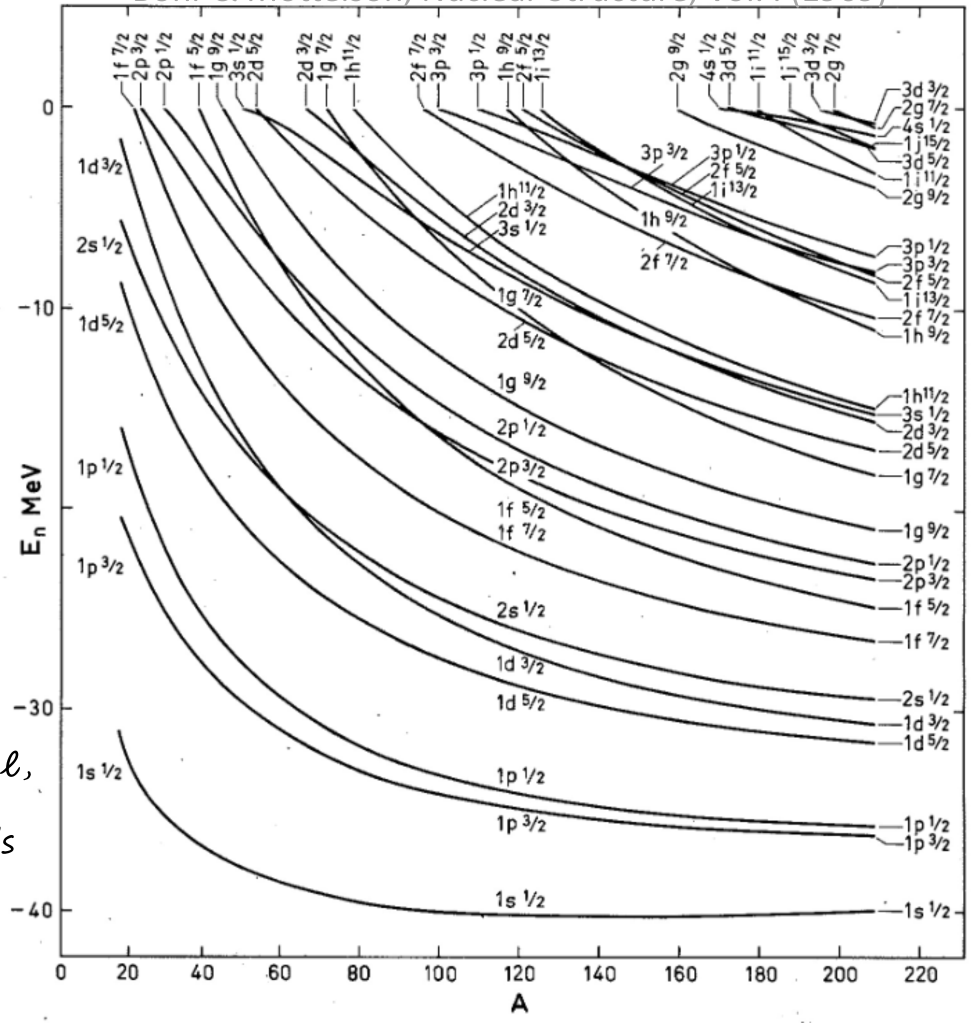
Magic numbers "break down" and new ones can appear for exotic nuclides

Common form for the **nuclear potential**

- $V(r) = V_{central}(r) + V_{spin-orbit}(r)\vec{l}\cdot\vec{s} + V_{Coulomb}(r) + V_{centrifugal}(r)$
  - $V_{central}(r) = V_{ce}\left(\frac{1}{1+\exp\left(\frac{r-R_{ce}}{a_{ce}}\right)}\right)$
    - $V_{ce,protons} = V_0 + \frac{N-Z}{A}V_1$ or $V_{ce,neutrons} = V_0 - \frac{N-Z}{A}V_1$
  - $V_{spin-orbit}(r) = V_{so}\frac{1}{r}\frac{\partial}{\partial r}\left(\frac{1}{1+\exp\left(\frac{r-R_{so}}{a_{so}}\right)}\right)$
  - $V_{Coulomb}(r) = \begin{cases} \frac{Ze^2}{r} & \text{for } r \geq R_c \\ \frac{Ze^2}{R_c}\left(\frac{3}{2} - \frac{r^2}{2R_c^2}\right) & \text{for } r \leq R_c \end{cases}$
  - $V_{centrifugal}(r) = \frac{\hbar^2}{2\mu_{reduced}}\frac{l(l+1)}{r^2}$

This is only relevant when a nucleon is removing/adding orbital angular momentum ℓ, so you would not use it to calculate single particle levels

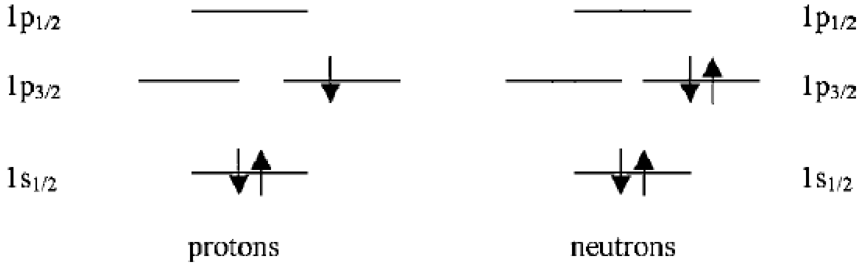
Bohr & Mottelson, Nuclear Structure, Vol. I (1969)



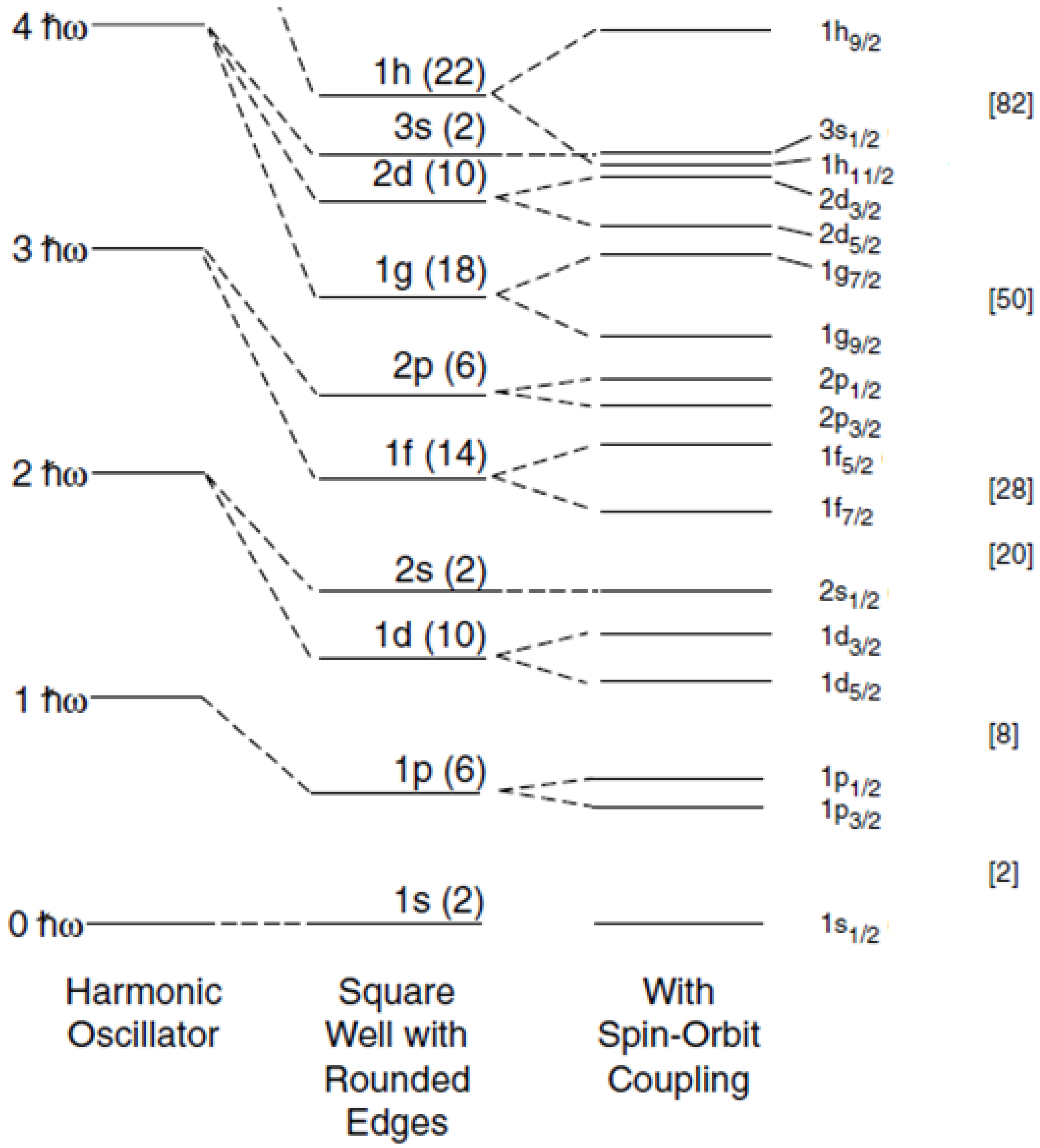
- Typically, $R_{ce} = R_{so} = R_c = r_0 A^{1/3}$
- For $r_0 = 1.27fm, a_{ce} = a_{so} = 0.67fm$, $V_0 = -55MeV, V_1 = -33MeV, V_{so} = -0.44V_{ce}$, get neutron single-particle energies above

Filling the shells

- We can construct a nucleus using our “shell model”:
  - A nucleon will go in the lowest-energy level which isn’t already filled, i.e.
    - the largest angular momentum, j
    - for the lowest orbital angular momentum, l
    - for the lowest oscillator shell, n
  - $2j+1$ protons or neutrons are allowed per level
  - Each level is referred to by its nlj
    - n by the # for the oscillator shell (convention either starts with 0 or 1)
    - l by spectroscopic notation (s=0,p=1,d=2,f=3,…)
    - j by the half-integer corresponding to the spin
- For example: ^{7}Li (Z=3, N=4)

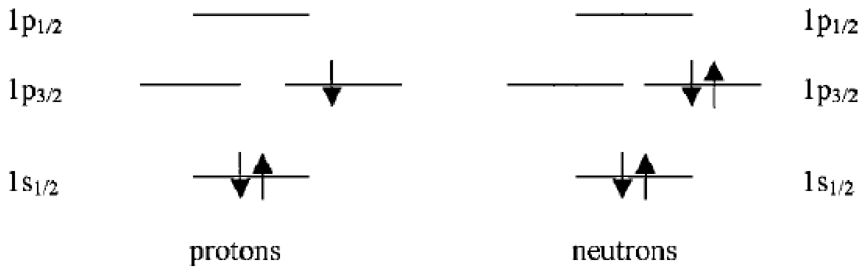


Loveland, Morrissey, & Seaborg, Modern Nuclear Chemistry (2006)



Basic properties from the shell model: J^{π}

- Recall that, from the pairing hypothesis, nucleons pair & cancel spins.
- So, the unpaired nucleons determine the properties of a nucleus.
  Unpaired nucleons sum to determine the spin & multiply to determine the parity
- Revisiting ^{7}Li:

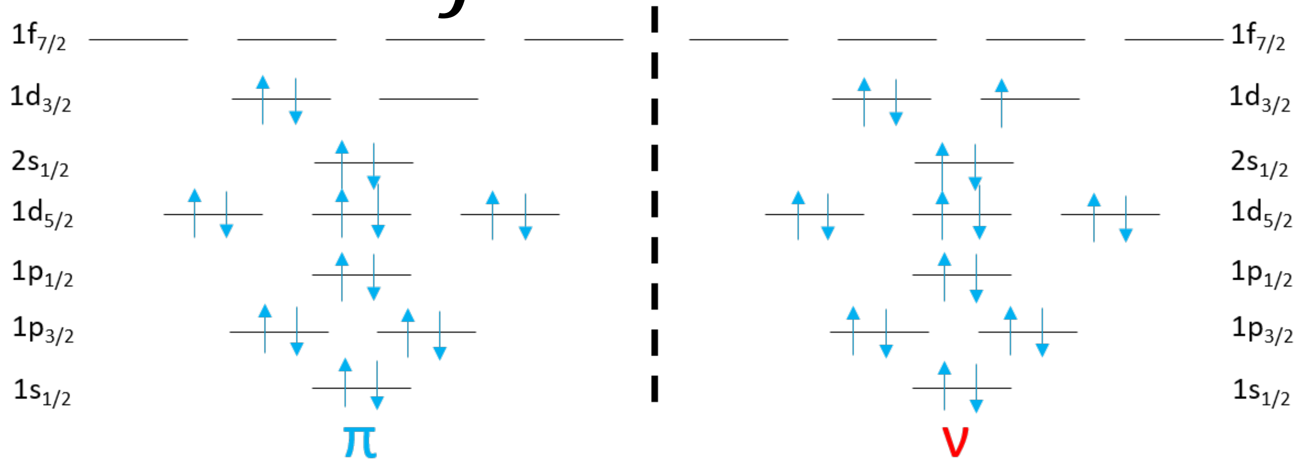


  - The only nucleon without a dance partner is the $1p_{3/2}$ proton; i.e. $J = 3/2,\ \pi = (-1)^1$
    So, the ^{7}Li ground-state should be $J^{\pi} = \frac{3}{2}^{-}$
  - What's the lowest energy excitation possible? (note pairing is strong)
    Moving the $p_{3/2}$ proton up to $p_{1/2}$
  - So, the first excited state of ^{7}Li should be $J^{\pi} = \frac{1}{2}^{-}$
  - Compare to data:

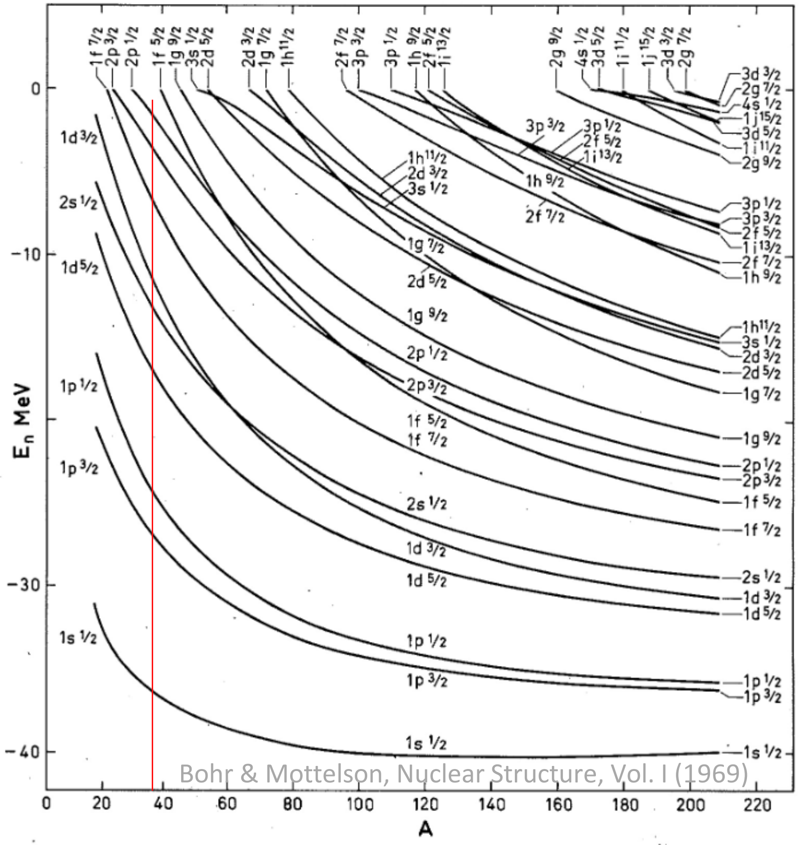
Basic properties from the shell model: J^{π}

- Now that we're feeling fat & sassy, let's try another case: ^{37}**Ar**
- Based on our shell-model, we expect the ground-state to be $3/2^{+}$

  …and it is!

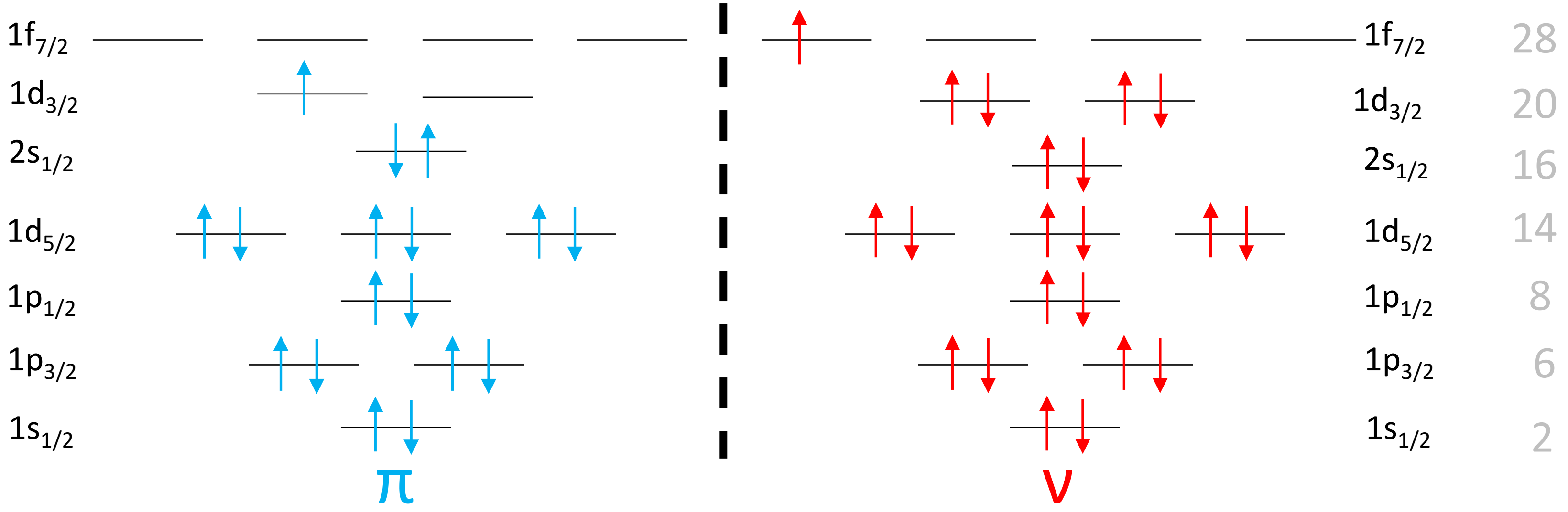


- Now for the first excited state, a logical thought would be the odd $d_{3/2}$ neutron would pop up to the $f_{7/2}$ level, creating a state with $7/2^{-}$
  - …but the first excited state is $1/2^{+}$ (the 2nd x.s. is $7/2^{-}$)
- What happened?
  - We have to keep in mind pairing & energy-costs
  - The $2s_{1/2}$-$1d_{3/2}$ gap is smaller than the $1d_{3/2}$-$1f_{7/2}$ gap (for low A)
  - And, **pairing energy increases with the l of the level**



Basic properties from the shell model: J^{π}

- Looking at a more complicated case, ^{38}Cl (Z=17, N=21)



- 2 valence nucleons: one $d_{3/2}$ proton and one $f_{7/2}$ neutron
- Allowed couplings are $|j_1 - j_2| \leq J \leq |j_1 + j_2|$
- So for this case: $J = 2, 3, 4, 5$
- How do we decide which combination has the lowest energy?

Using the descriptively named: "jj coupling rules for Odd-Odd nuclei" from Brennan & Bernstein (Phys. Rev. 1960)

Basic properties from the shell model: J^{π} for odd-odd

- For Odd-Z, Odd-N nuclides, need a method to determine which jj-coupling is the lowest energy
- An empirically-based set of rules was developed by Brennan & Bernstein (Phys. Rev. 1960)
- They noticed that, when coupling j, $j_1 = l_1 \pm s_1$ and $j_2 = l_2 \pm s_2$,
  - **Rule 1**: If ($j_1 = l_1 + s_1$ and $j_2 = l_2 - s_2$) <u>*or*</u> ($j_1 = l_1 - s_1$ and $j_2 = l_2 + s_2$), then $J = |j_1 - j_2|$
    - e.g. for a $d_{3/2}$ proton $\left(j_p = 2 - \frac{1}{2} = \frac{3}{2}\right)$ and a $f_{7/2}$ neutron $\left(j_n = 3 + \frac{1}{2} = \frac{7}{2}\right)$, $J = \frac{7}{2} - \frac{3}{2} = 2$
      For this case, $\pi = \prod \pi_i = (-1)^2 * (-1)^3 = -$

      Ex: ^{38}Cl
  - **Rule 2**: If ($j_1 = l_1 + s_1$ and $j_2 = l_2 + s_2$) <u>*or*</u> ($j_1 = l_1 - s_1$ and $j_2 = l_2 - s_2$), then $J = |j_1 \pm j_2|$
    - e.g. for a $d_{5/2}$ proton $\left(j_p = 2 + \frac{1}{2} = \frac{5}{2}\right)$ and a $d_{5/2}$ neutron $\left(j_n = 2 + \frac{1}{2} = \frac{5}{2}\right)$, $J = \frac{5}{2} + \frac{5}{2} = 5$
      For this case, $\pi = \prod \pi_i = (-1)^2 * (-1)^2 = +$

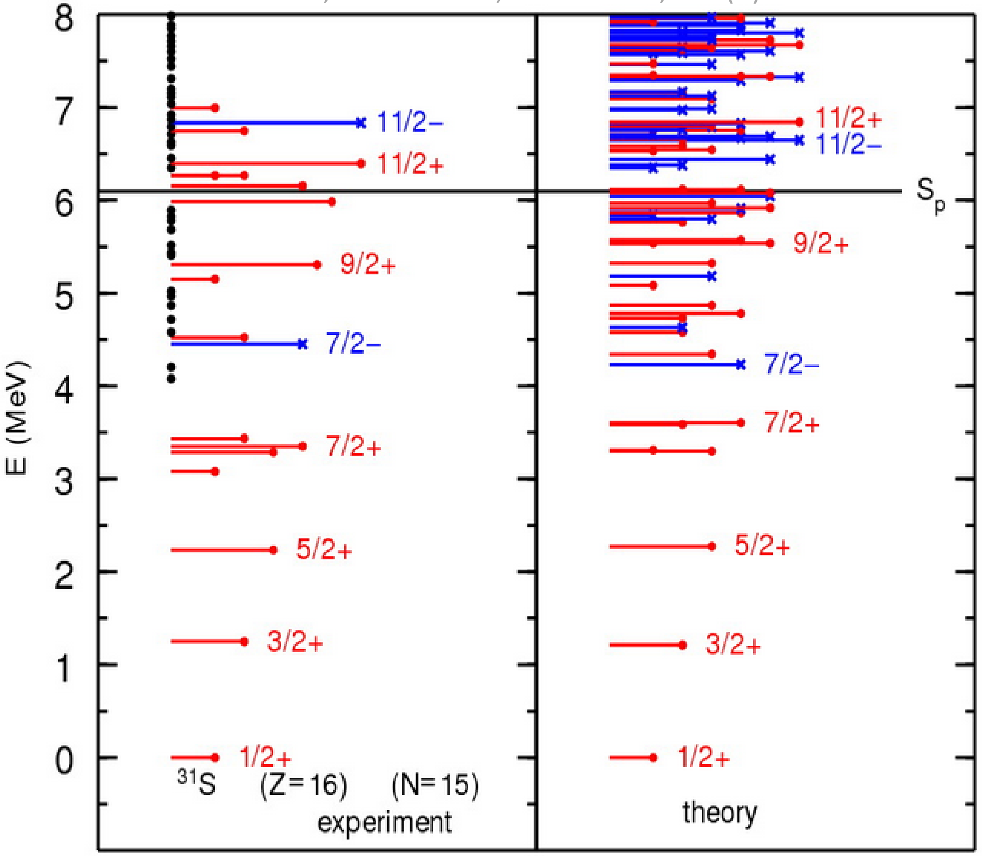
      Ex: ^{26}Al
  - **Rule 3**: If one odd nucleon has been promoted (e.g. to an s-orbital to pair with a nucleon), leaving behind a "hole", and the other odd nucleon stays a particle, then $J = j_1 + j_2 - 1$
    - e.g. for a $d_{3/2}$ proton hole $\left(j_p = \frac{3}{2}\right)$ and a $f_{7/2}$ neutron $\left(j_n = \frac{7}{2}\right)$, $J = \frac{7}{2} + \frac{3}{2} - 1 = 4$
      For this case, $\pi = \prod \pi_i = (-1)^2 * (-1)^3 = -$

      Ex: ^{40}K

**These don't always work…but when they don't, this can tell you something:*
Either there's more than a single-particle level interaction going on,
or your particle(s)/hole(s) don't occupy the levels we naïvely assumed.
(e.g. S. Liddick et al. Phys. Rev. C 2004)

Shell-model is pretty good at predicting J^{π} (among other things)

B. Brown, W.A. Richter, & C. Wrede, PRC(R) 2014



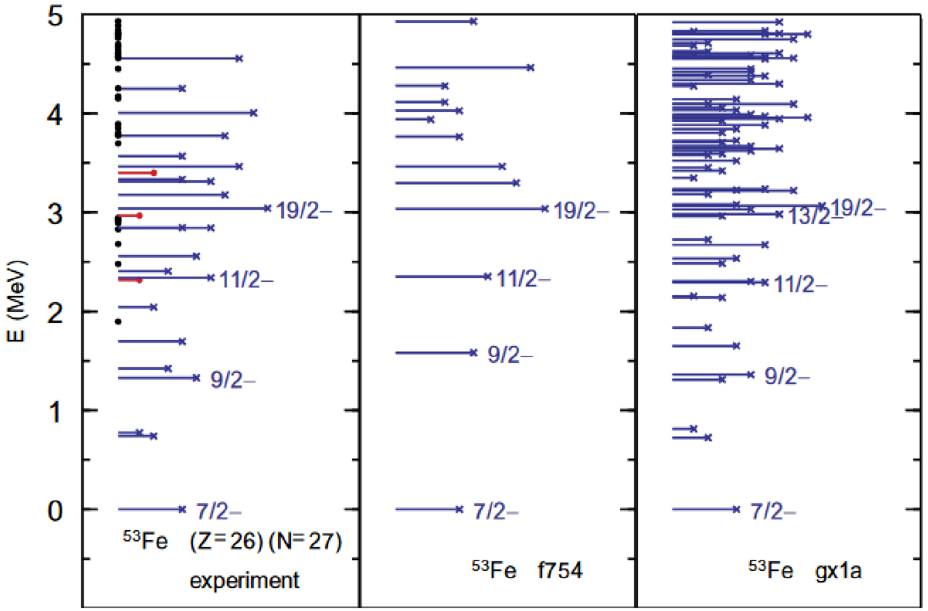
…some major challenges are

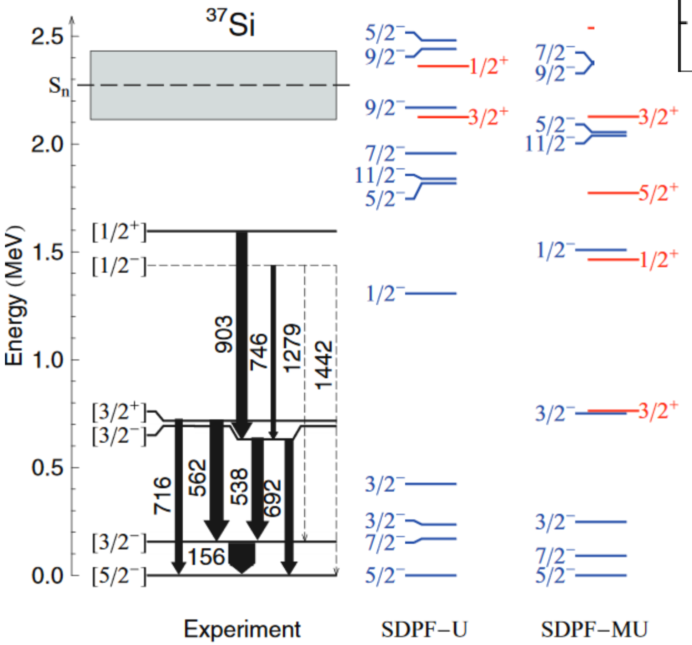
including all the
relevant levels
in the calculation

and

choosing
a good
interaction
between
nucleons

B. Brown & W. Rae, Nuc. Dat. Sheets (2014)

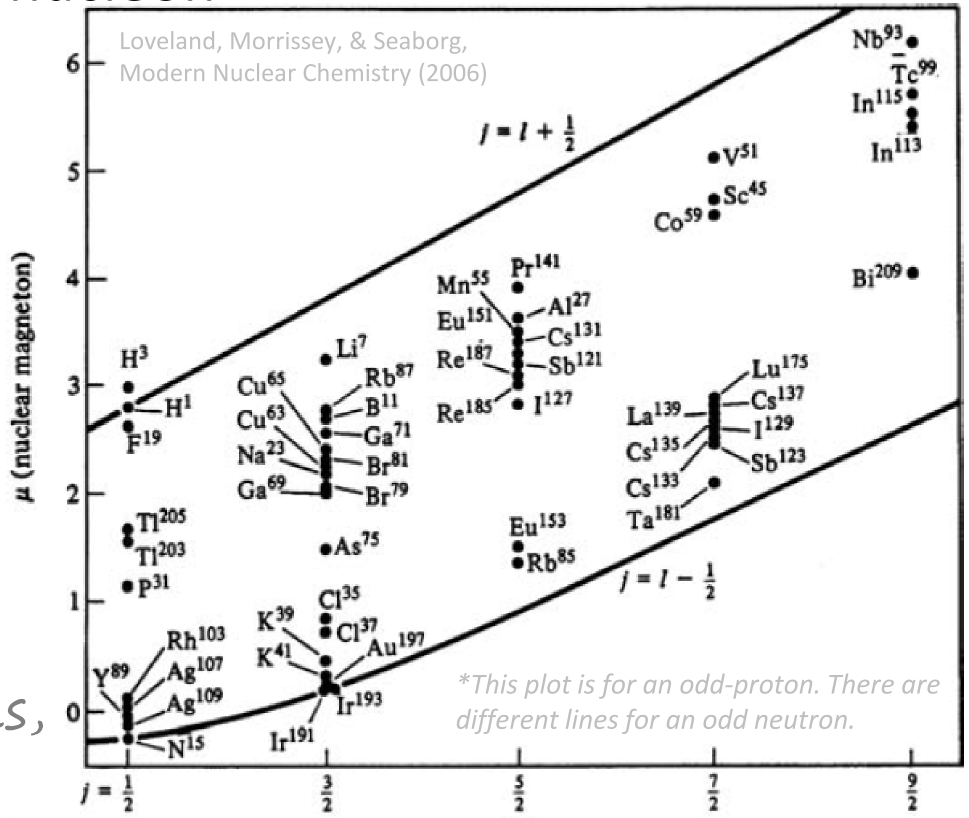




S.R. Stroberg et al. Phys Rev. C (2014)

What else are J^{π} predictions good for? Magnetic dipole moments

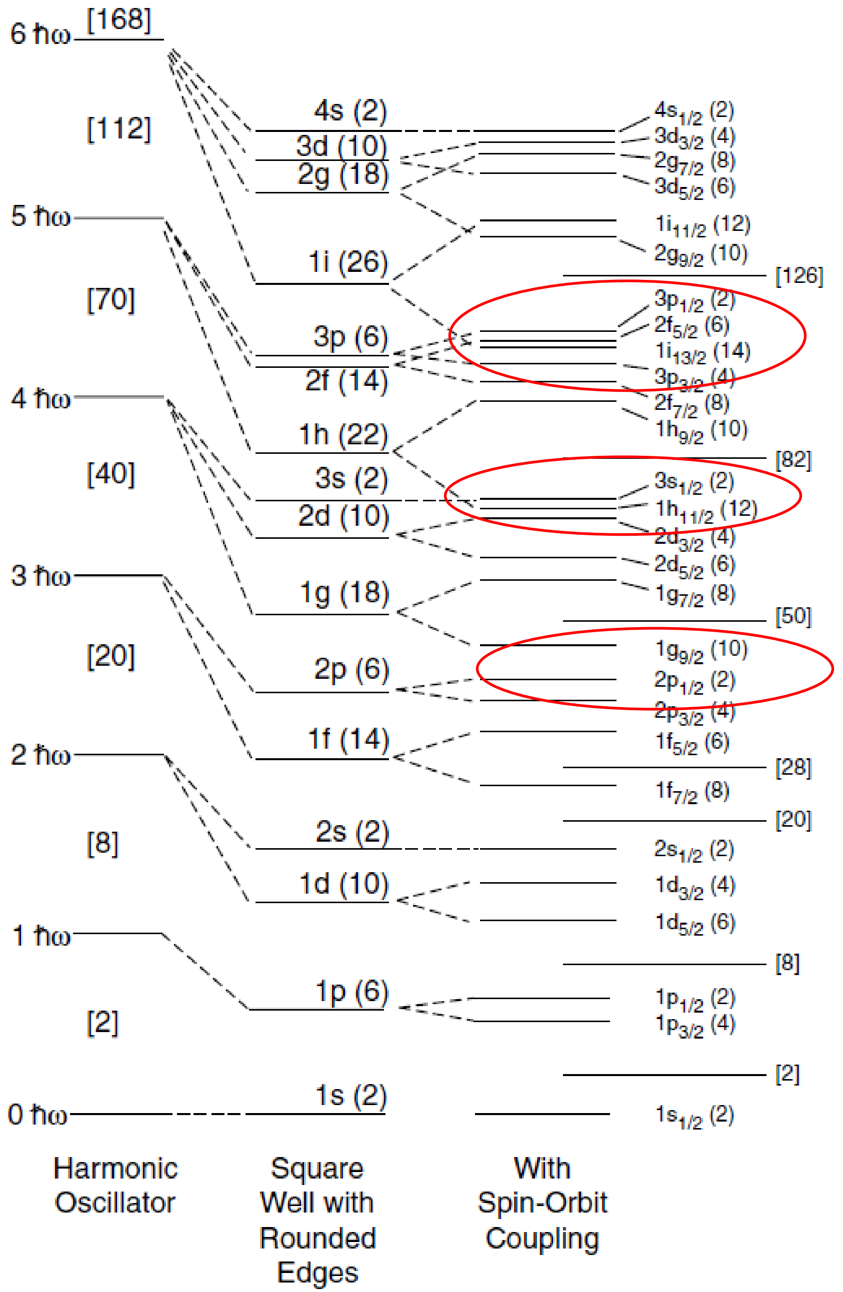
- Recall that for a single particle, the magnetic dipole moment is: $\mu = j g_j \mu_N$
- After some fancy footwork, it can be shown that the Landé g-factor can be expressed as:
  - $g_j = \left(\frac{j(j+1)+l(l+1)-s(s+1)}{2j(j+1)}\right) g_l + \left(\frac{j(j+1)-l(l+1)+s(s+1)}{2j(j+1)}\right) g_s$
- Since spins cancel for paired nucleons, we might expect the magnetic dipole moment of a nucleus with 1-unpaired nucleon to be determined by that nucleon
  Expected values of μ are therefore:
  - $\mu = j g_j = l g_l + \frac{1}{2} g_s$ for $j = l + \frac{1}{2}$
  - $\mu = j g_j = j\left(1 + \frac{1}{2l+1}\right) g_l - j\left(\frac{1}{2l+1}\right) g_s$ for $j = l - \frac{1}{2}$
  - Protons: $g_l = 1, g_s = 5.6$, Neutrons: $g_l = 0, g_s = -3.8$
  - These boundaries are the "Schmidt lines"
    (Th. Schmidt, Z.Phys. (1937))
    and nearly all measured g_j fall between these



As with excited state J^{π}'s, deviation between experiment & shell model predictions tell us something interesting is going on. E.g. mixing between single-particle occupations, polarization of the core, corrections to meson-exchange mediating the nuclear force [(G. Neyens, Rep. Prog. Phys. (2003)](), *J. Booten et al. Phys.Rev.C (1991))*

What else are J^{π} predictions good for? **Isomers** (long-lived x.s.)

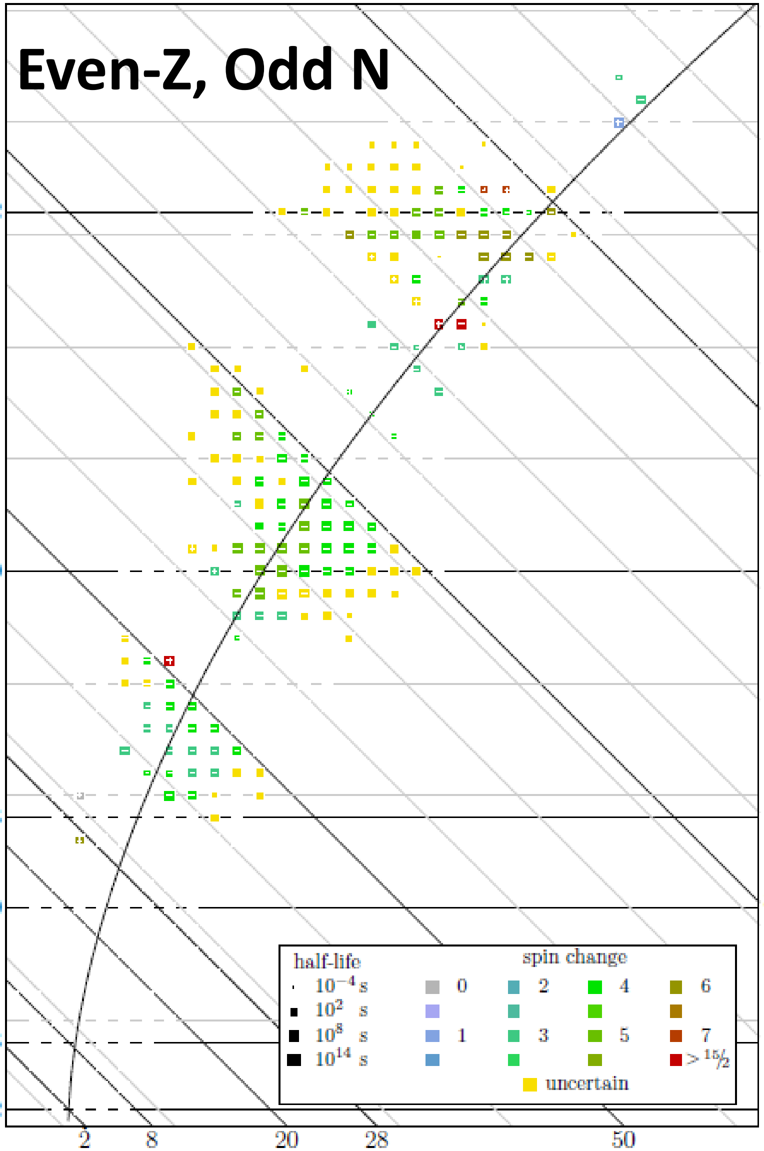
- Most excited states decay via γ-emission in a matter of femto-seconds, but some stick around for many nanoseconds, milliseconds, seconds, or even universe lifetimes.
- These are meta-stable states, a.k.a. isomers
- The reason is γ-emission is suppressed, since it would require large angular momentum transfer
- So, where do we expect low-lying high-j excited states?
  - Where a large Δj exists between neighboring levels (thanks to the spin-orbit interaction) that are near the last single particle orbit.
    - Namely, below magic #'s 50, 82, 126
    - For these cases, we expect a parity change
  - Where multiple j are possible for the ground-state (but one is favored by the Brennan-Bernstein rules) and high-j single-particle levels are involved
    - Namely, odd-odd nuclei
    - For these cases, we don't expect a parity change

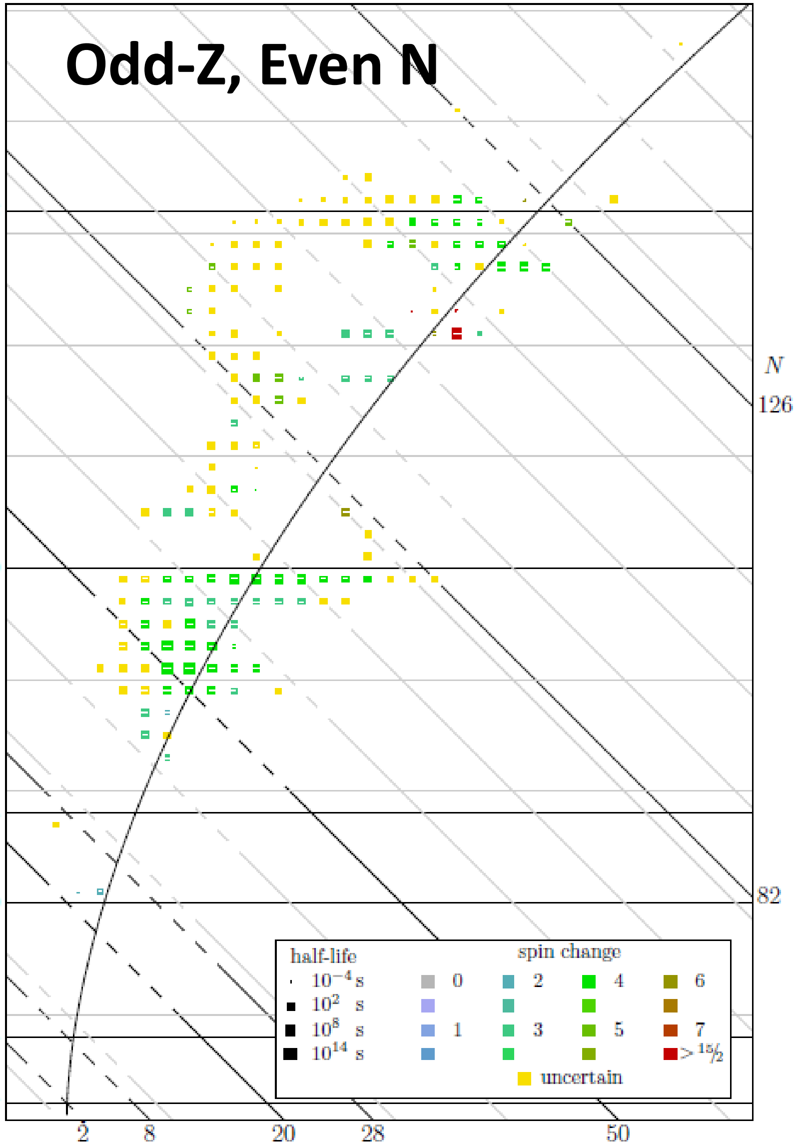


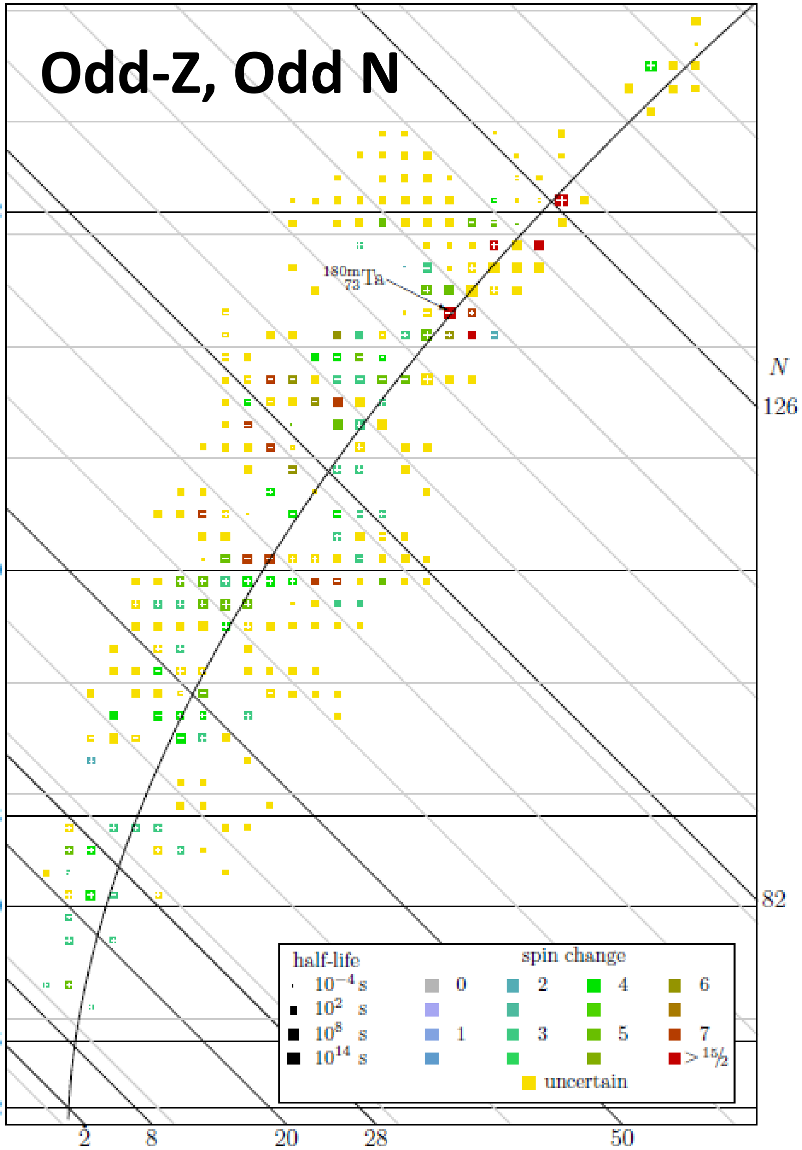
Loveland, Morrissey, & Seaborg, Modern Nuclear Chemistry (2006)

Isomers on the Nuclear Chart

L. van Dommelen, Quantum Mechanics for Engineers (2012)





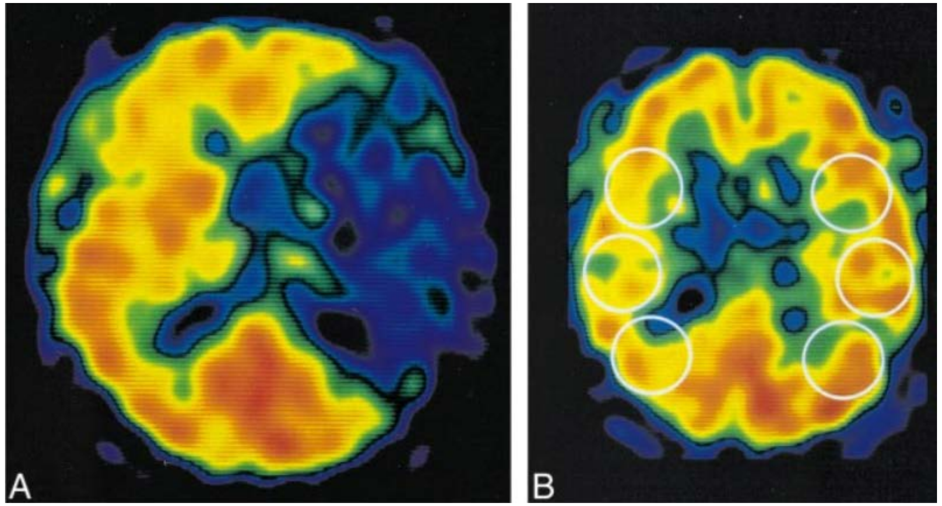


Special cases exist (mostly for higher-A nuclides) where even-even nuclei have isomers
(e.g. M. Müller-Veggian et al., Z.Phys.A (1979))

Impact of Isomers (selected examples)

Medical Imaging

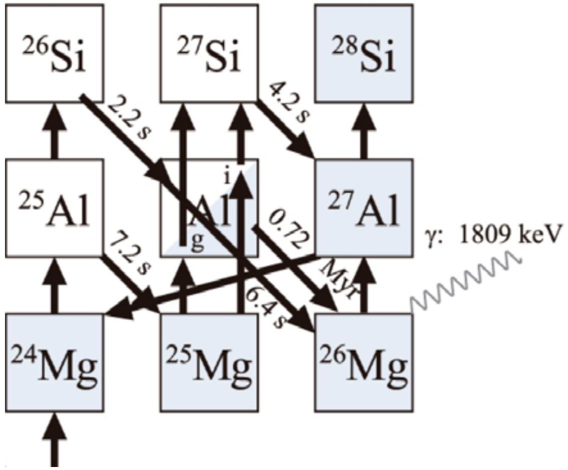
e.g. mapping blood flow in the brain with SPECT using ^{99m}Tc

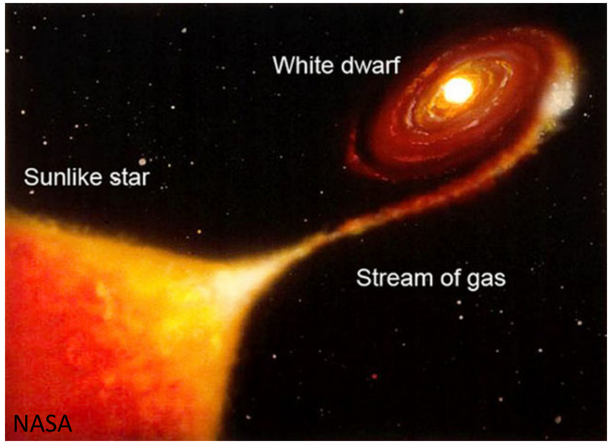


K. Ogasawara et al. American Journal of Neuroradiology (2001)

Nuclear Astrophysics

e.g. ^{26m}Al complicating nova nucleosynthesis calculations





J. José, Stellar Explosions (2015), G. Misch et al. ApJS (2021)

Nuclear Energy Storage

Controlled energy storage and release using isomers and lasers was a hot topic for a while

…but it turns out to be really difficult.

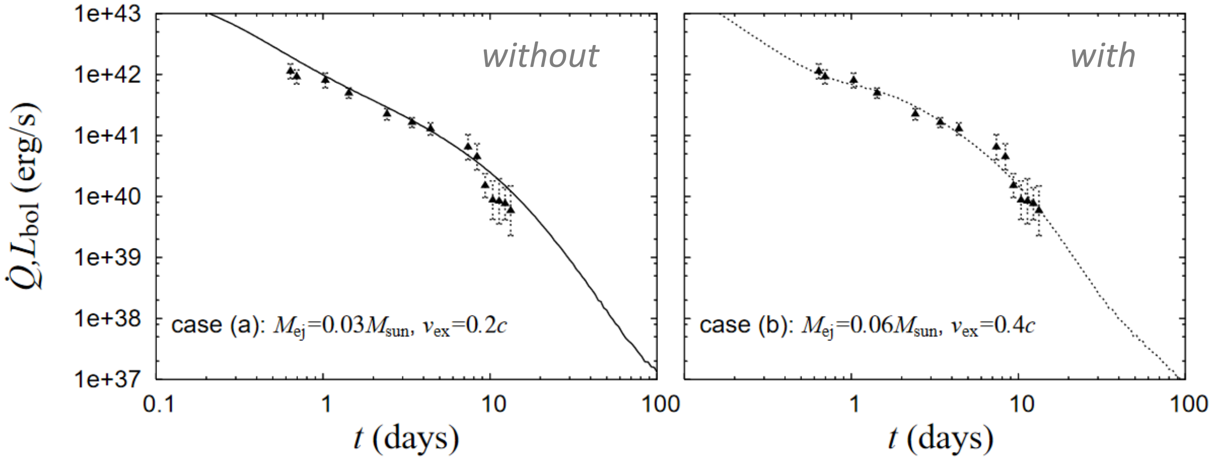
P. Walker & J. Carrol, Physics Today (2005)

Recent theoretical work has found a possible avenue using dielectric cavities.

E. Tkalya PRL (2018)

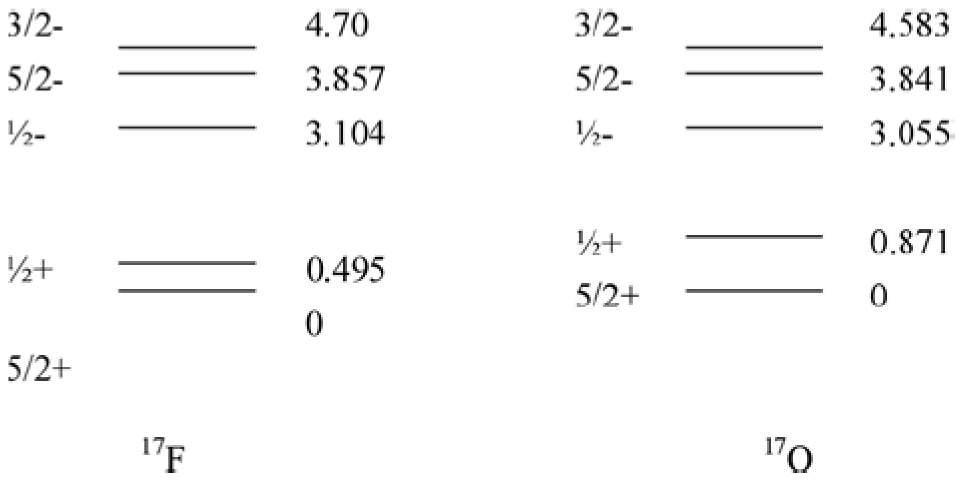
e.g. modifying NS merger ejecta conditions inferred from kilanova light curves

Fujimoto & Hashimoto MNRASL (2020)

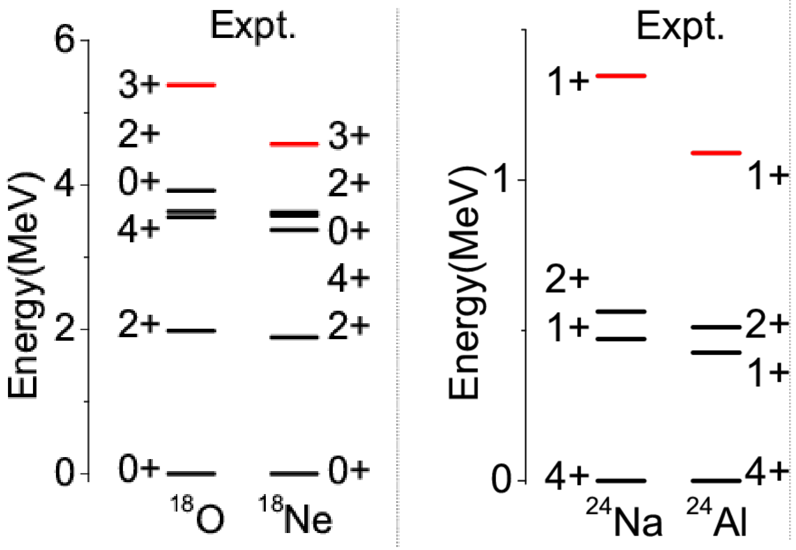


What else are J^{π} predictions good for? Mirror Nuclei

- Note that our methods to determine J^{π} didn't depend on whether we were working with protons or neutrons
- If we interchange N for Z, we will get the same answer
- Such pairs are called "mirror nuclei"
- When we examine the levels for mirror nuclei, correcting for the different Coulomb energy, we see a remarkable similarity
- E.g.



Loveland, Morrissey, & Seaborg, Modern Nuclear Chemistry (2006)

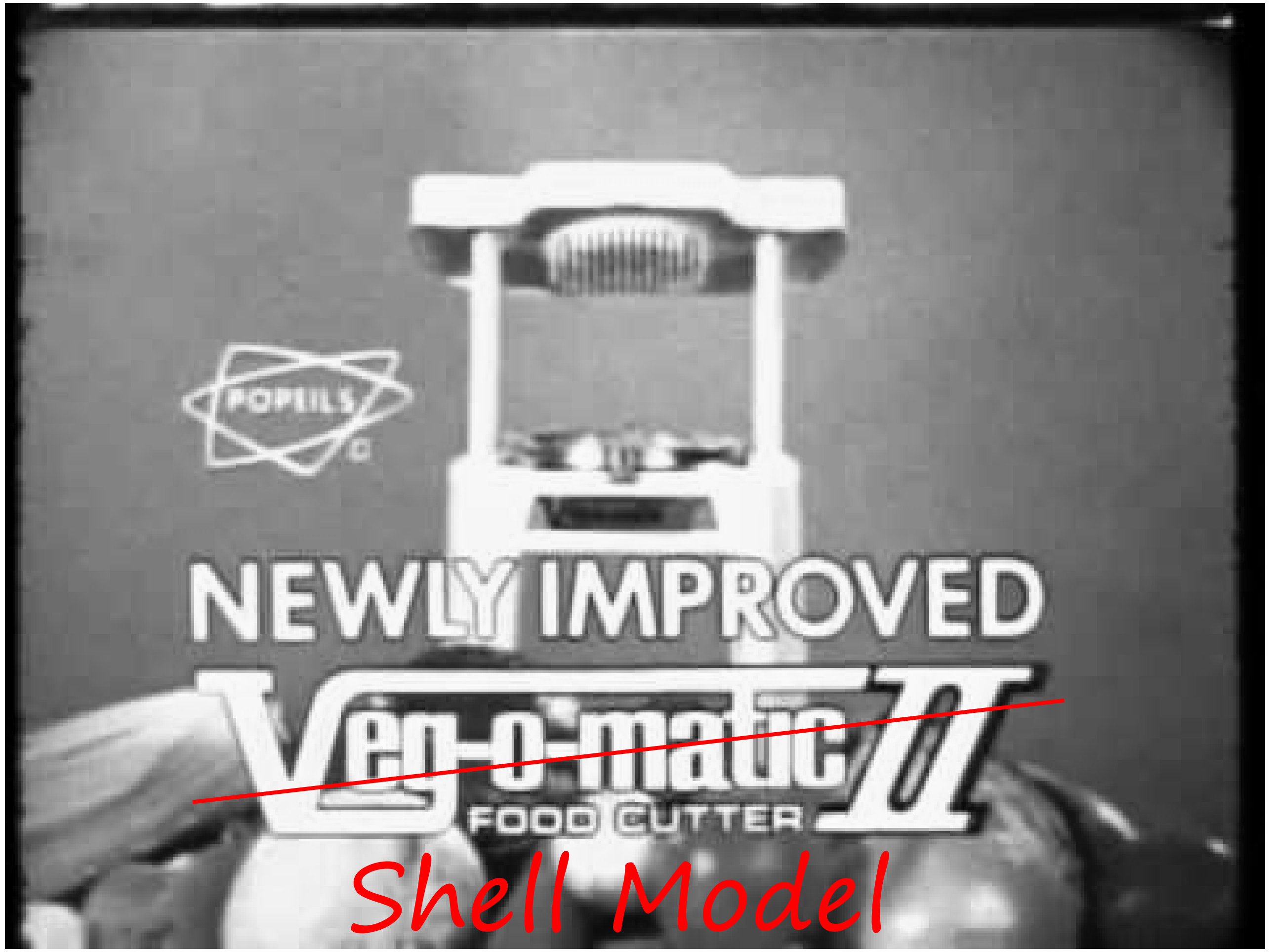


C. Yuan et al., Phys. Rev. C (2014)

- Such mirror symmetry is evidence for charge-independence of the nuclear force and a justification for the concept of isospin

It's also handy when you need estimates for a nucleus you can't access when you can access its mirror (e.g. C.Akers et al. PRC 2016)

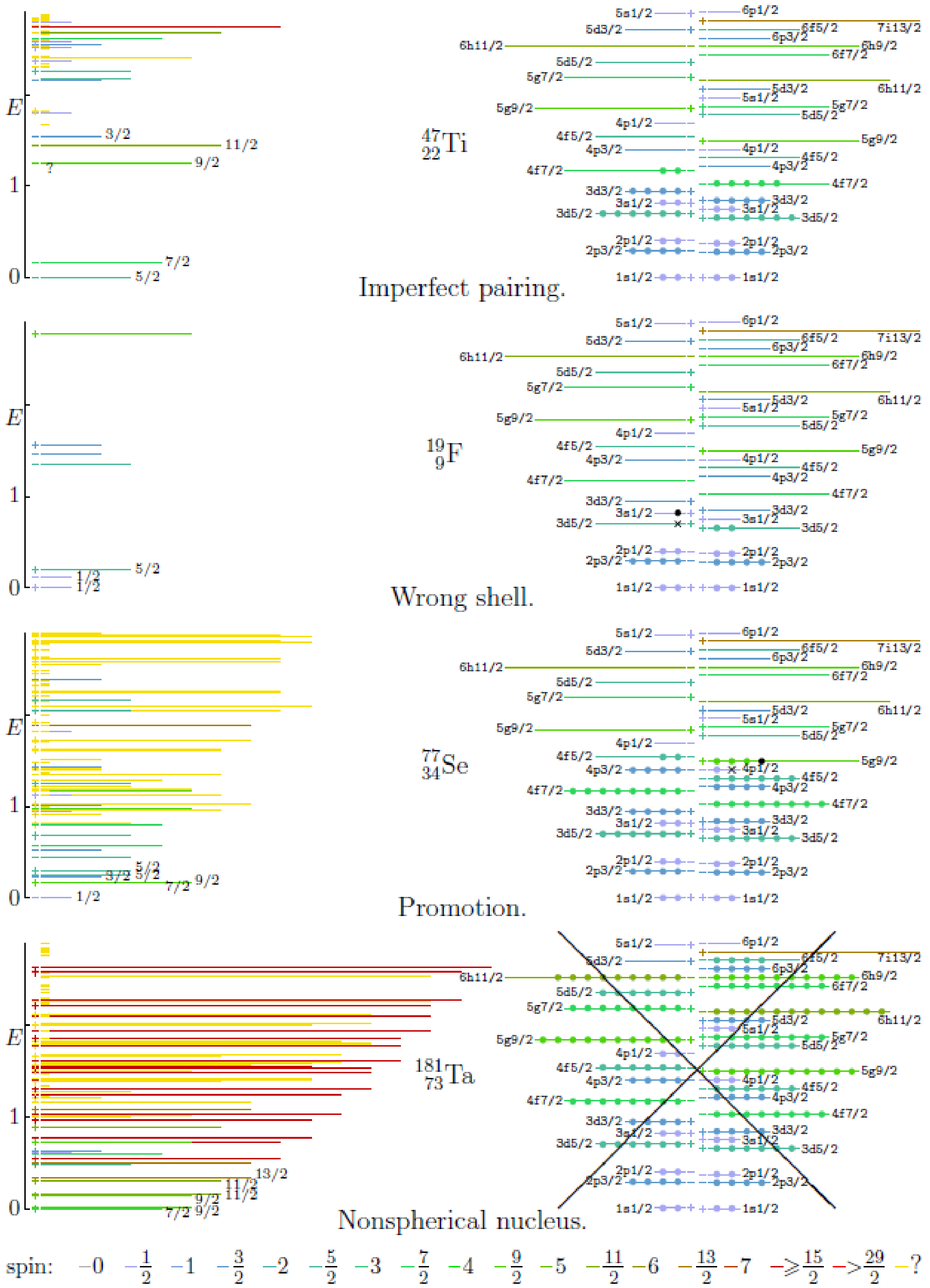
The Shell Model:
It slices, it dices, it makes julienne fries!
What can't it do!?



Shell Model Limitations:

L. van Dommelen, Quantum Mechanics for Engineers (2012)

- You’ll often find the shell model description isn’t as good as you would hope
- The detailed reasons for failures are varied, however, they mostly indicate the basic premise of the calculation is incorrect
- Shell Model calculations (generally speaking) assume
    - Minimally-interacting nucleons (i.e. mostly independent, except pairing)
    - Spherical inert cores of nucleons
- Solutions to these problems are:
    - Modify the shell-model calculation to get the added level of realism
    - Use a different model

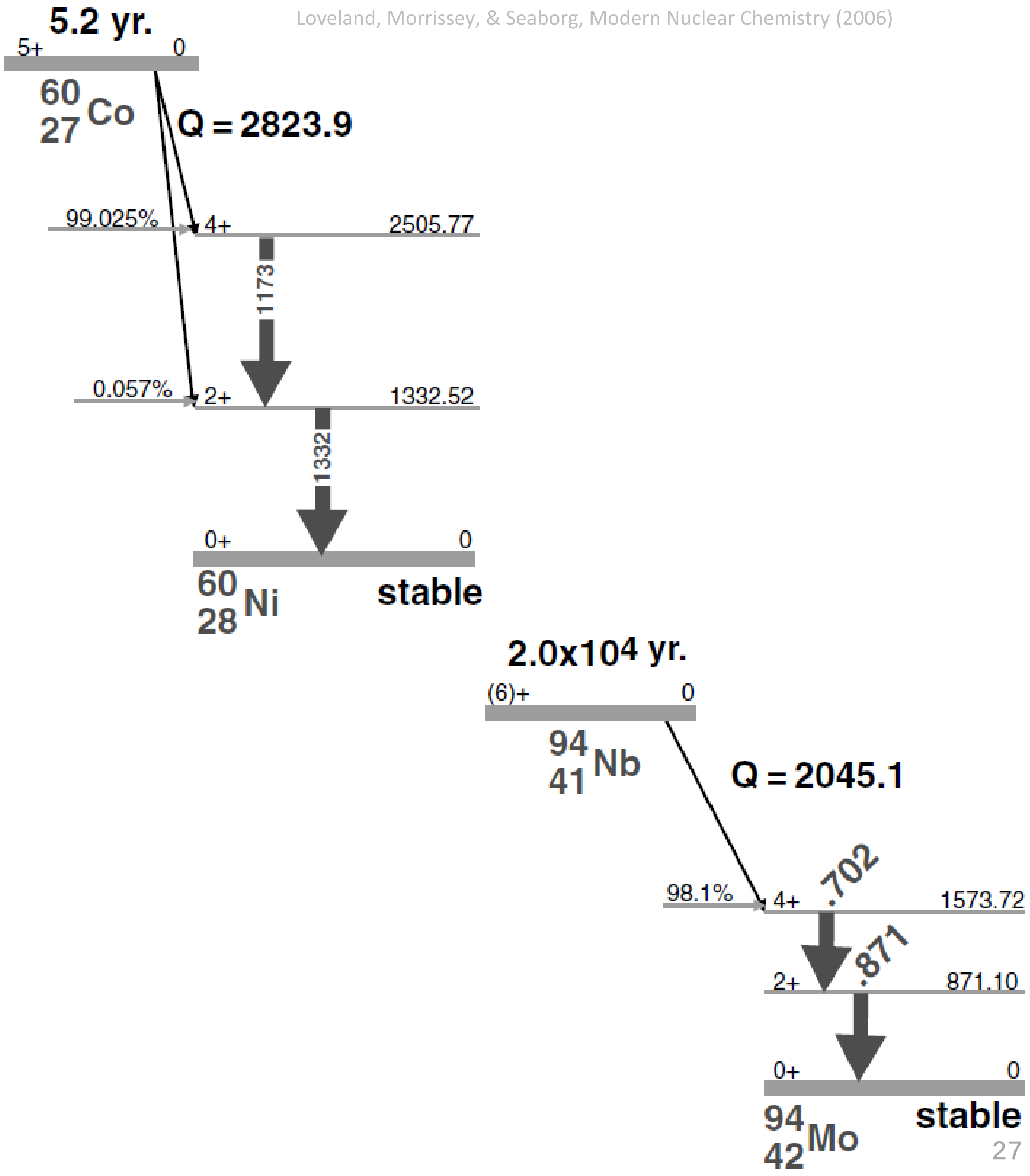


Shell Model Limitations:

Loveland, Morrissey, & Seaborg, Modern Nuclear Chemistry (2006)

- For example, nuclei have series of states that are spaced in energy and linked via transitions that can be described by a collective rotation/vibration of the nucleus.
- The rotational bands of even-even nuclei link the ground state to 2+,4+,6+,8+, etc., excited states

- Another example is the inability to predict nuclear masses.
- Shell model potentials must be adjusted to reproduce the ground-state binding energy
- Some other approach, such as a collective model (e.g. the liquid drop model) is needed instead



How do I do actual shell-model calculations?

- Open-source codes include:
  - NuShellX: http://www.garsington.eclipse.co.uk/, which has a slightly more user-friendly version, NuShellX@MSU, coupled to ENSDF nuclear data, that has a tutorial here
  - BigStick: https://github.com/cwjsdsu/BigstickPublick
  - Many others curated by the FRIB Theory Alliance: https://fribtheoryalliance.org/content/Resources/codes.php

- If you're a DIYer, Morton Hjorth-Jensen developed a how-to guide

Further Reading

- Chapter 6, Appendix E: Modern Nuclear Chemistry (Loveland, Morrissey, Seaborg)
- Chapters 7: Nuclear & Particle Physics (B.R. Martin)
- Chapters 6-8: Lecture Notes in Nuclear Structure Physics (B.A. Brown)
- Chapter 14, Section 12: Quantum Mechanics for Engineers (L. van Dommelen)
- Chapter 1, Section 6: Nuclear Physics of Stars (C. Iliadis)
- Chapter 11: The Atomic Nucleus (R. Evans)