Lecture 13: The Actual Shell Model

- Recalling schematic SM
- Single-particle wavefunctions
- Basis states
- Truncation
- Sketch view of a calculation

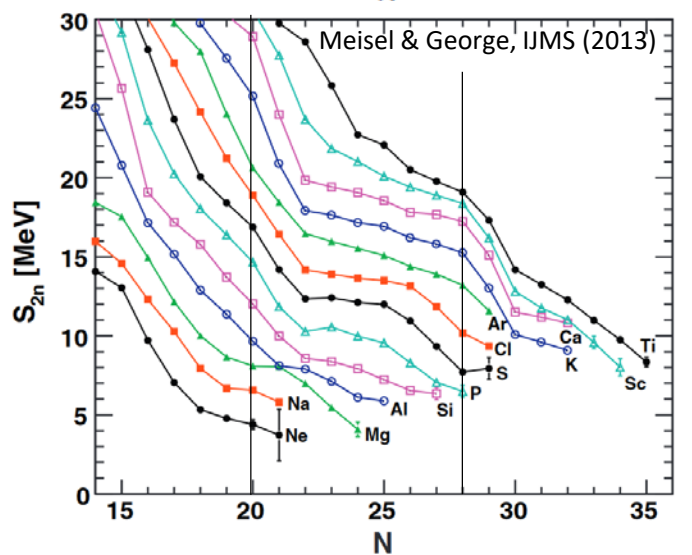# Recall the magic numbers: *2, 8, 20, 28, 50, 82, 126*

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

B.A. Brown, Lecture Notes in Nuclear Structure Physics, 2005.
Adapted from B.A. Brown, C.R. Bronk, & P.E. Hodgson, J. Phys. G (1984)

M.A. Preston, Physics of the Nucleus (1962)

Meisel & George, IJMS (2013)

A. Cameron, Proc. Astron. Soc. Pac. (1957)

Ground-State Quadrupole Deformation
P. Möller et al. ADNDT (2016)
FRDM(2012)
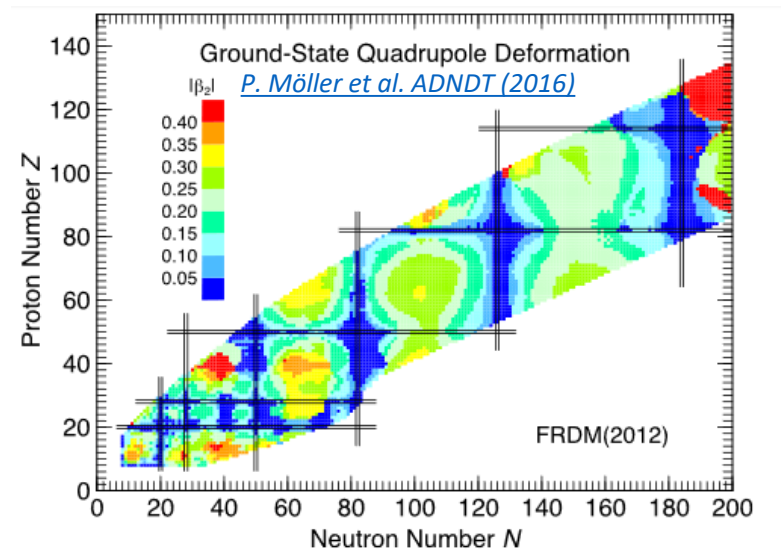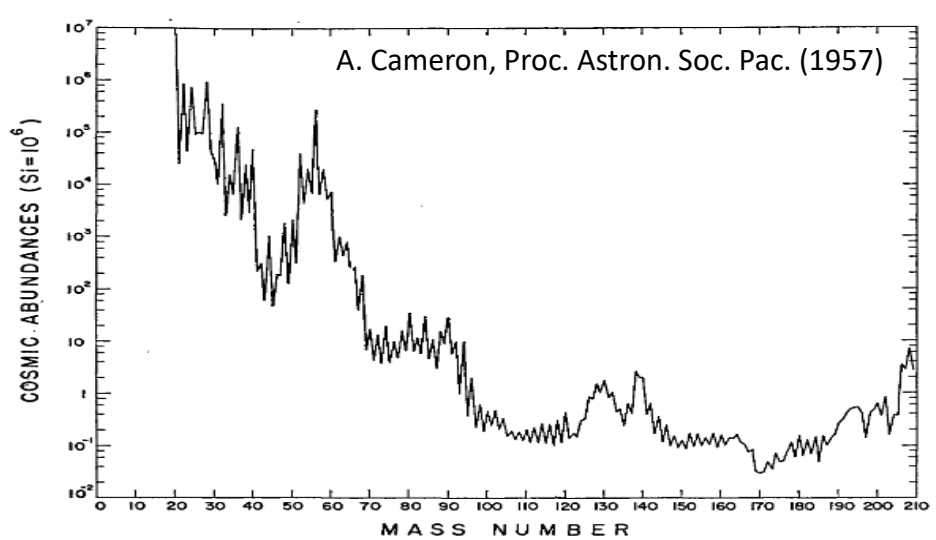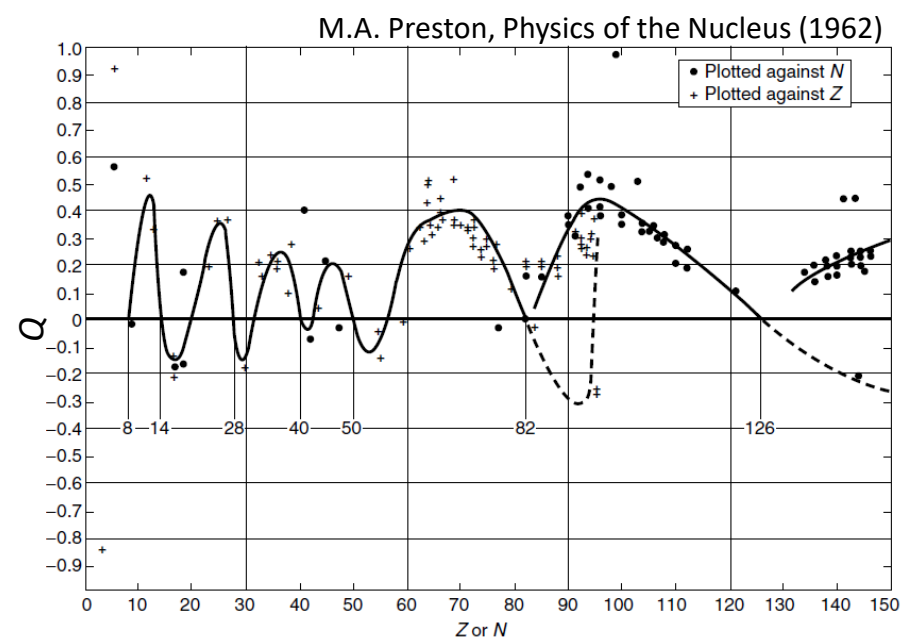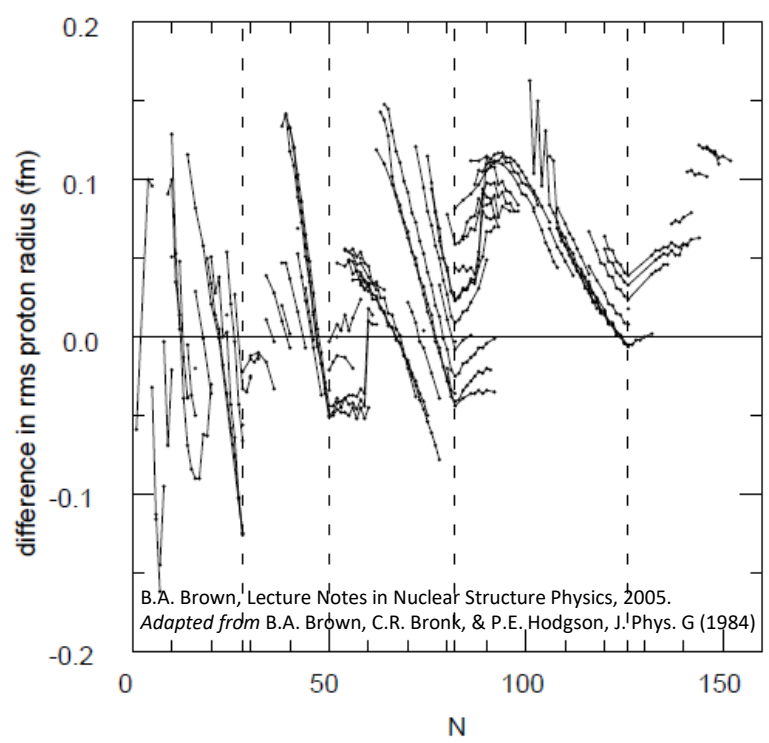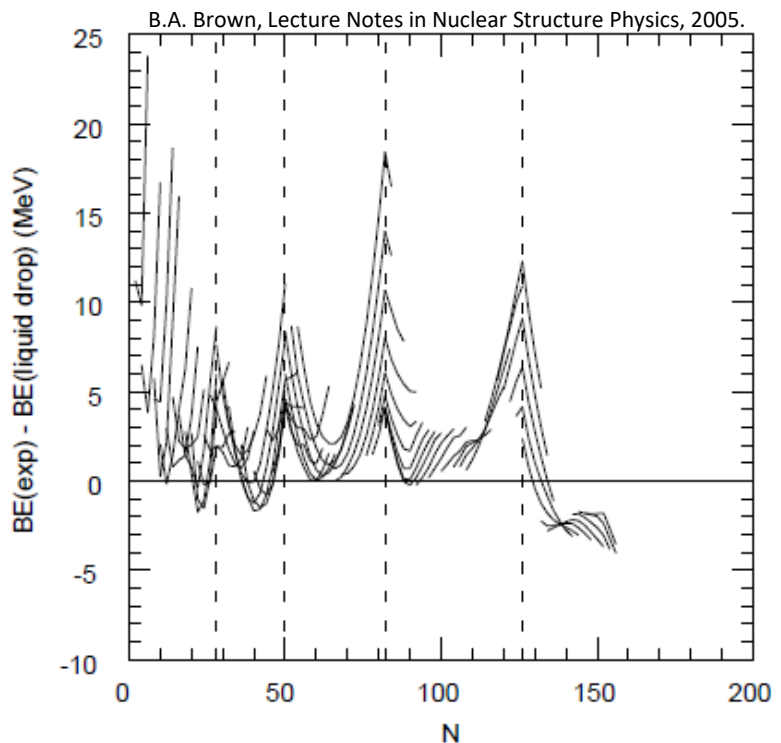
*First magic number evidence compilation
by M. Göppert-Mayer Phys. Rev. 1948*

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Shell structure is a problem of quantum mechanics

- 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,
    - $H\psi = E\psi$ 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

# Magic numbers (a.k.a. shells) appear from single particle levels calculated with a 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.
- 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

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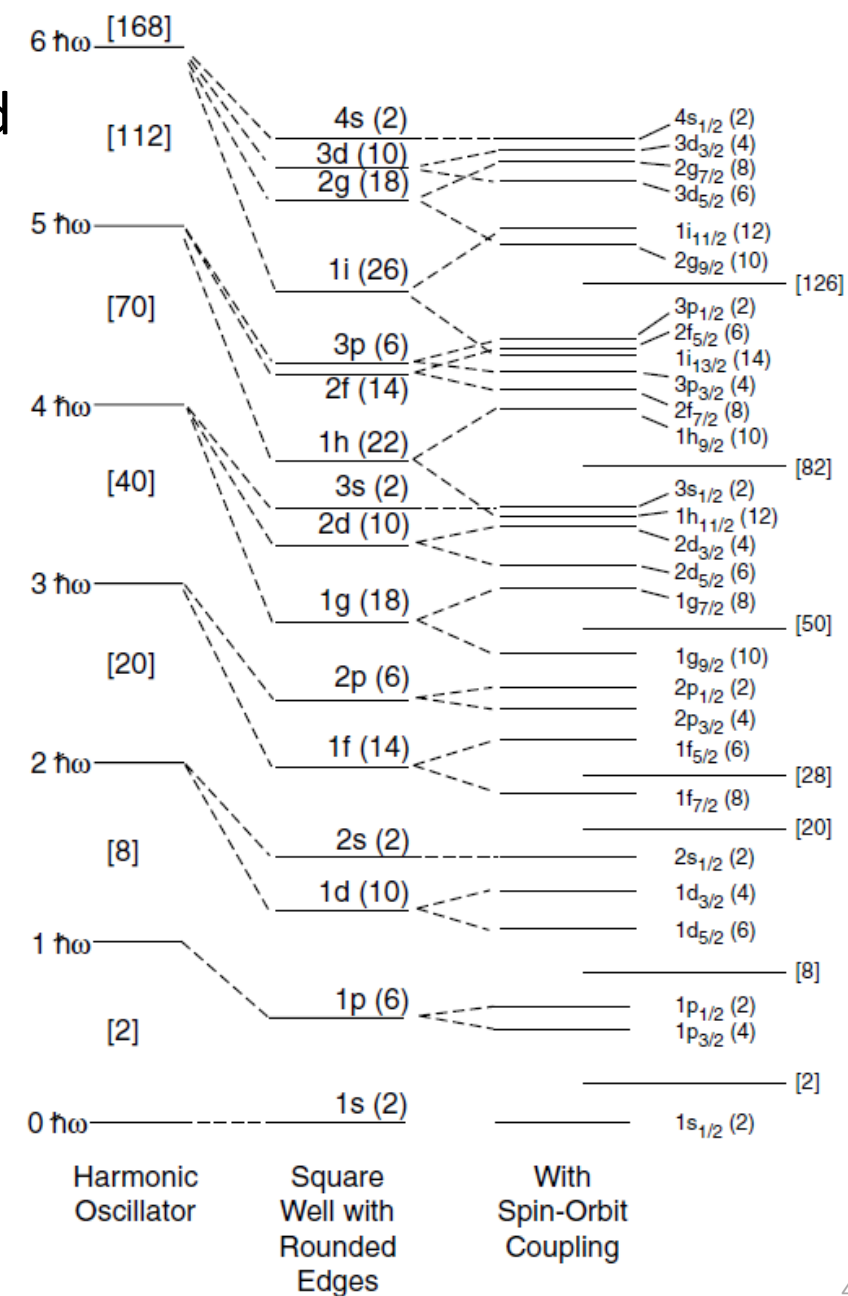
Filling single particle levels results in a nuclear state

- To construct a nucleus from the schematic 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 largest 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)
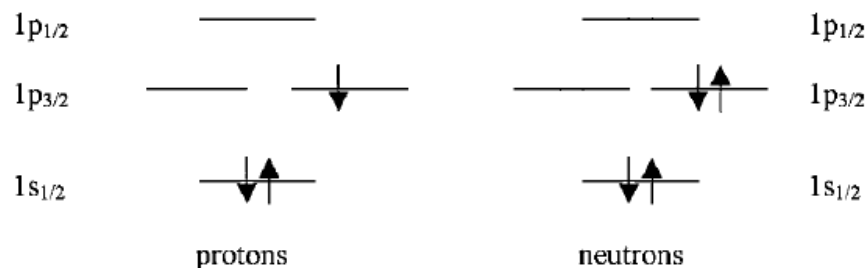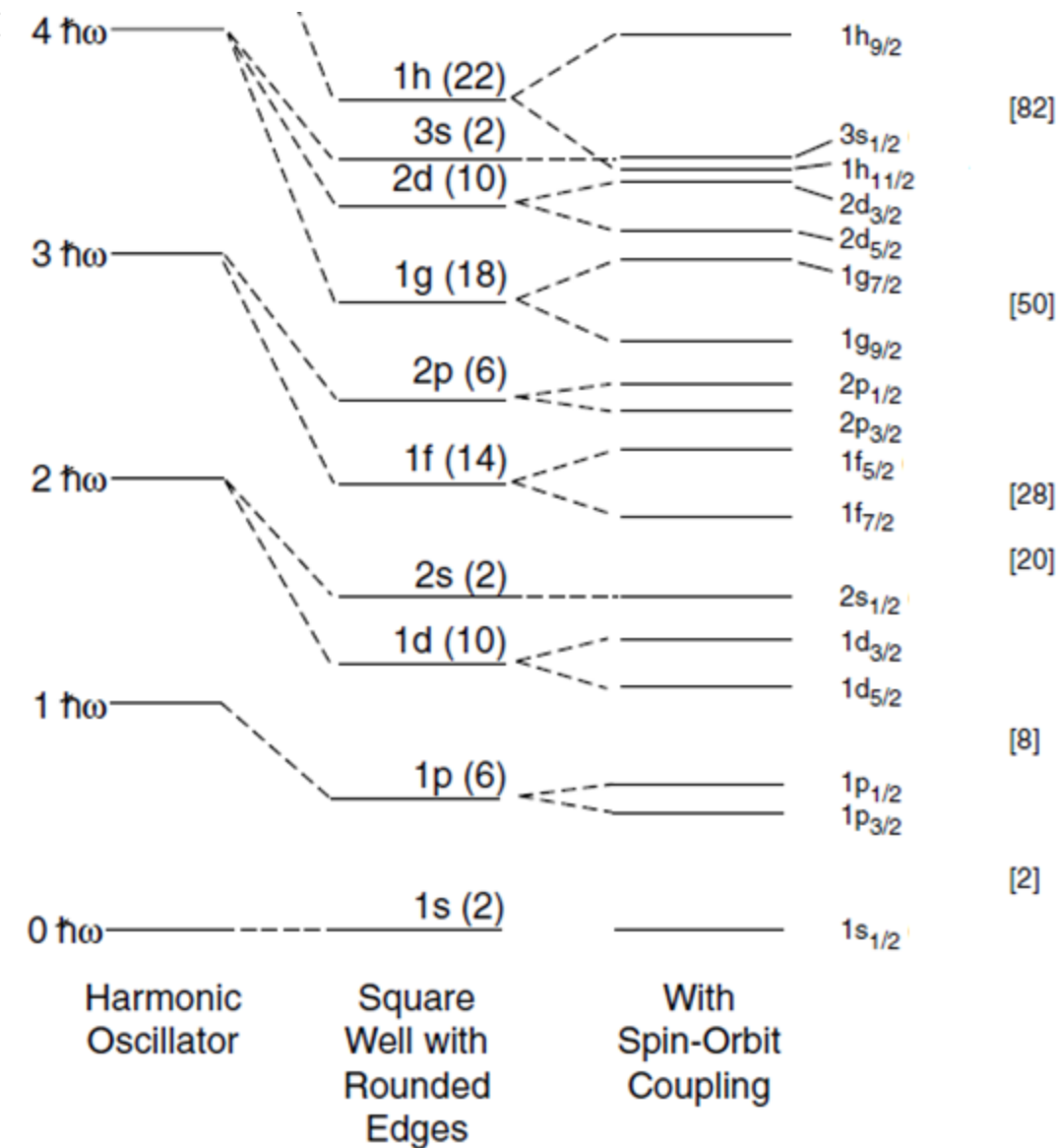
Wait a second! How is this *actually* done?

1. Solve the Schrödinger equation for some potential to get the eigenstates.
   These single-particle states will be combined to construct a many-body wavefunction

2. The many-body wavefunction is constructed by "creating" or "annihilating" nucleons to fill (or be removed from) single-particle states
   [and moved from or into other states, since the total number of particles is conserved]

3. The ground state is found by creating particles to fill single-particle levels up to the Fermi level. Excited states are found by perturbing the ground-state wavefunction by creating and/or annihilating some number of particles.

4. The energy associated with a given "configuration" (a.k.a. wavefunction with a particular number of particles and/or holes created) is solved for the configuration's wavefunction and the adopted Hamiltonian using a bit of fancy footwork.
   [the spin & parity would be calculated just as we did for the schematic shell model]

5. Typically all of this has to be done for a limited set of single-particle states, since the dimensionality blows-up rapidly

Constructing the basis: Solving for single-particle states

- To calculate single-particle states, we need a Hamiltonian: $H = T + V = \sum_i^A t_i + \sum_i^A v_i$

- t_i are just the kinetic energies, $\vec{p}_i^2/2m_i$, and for the potential terms, we will stick to two-body forces, $\sum_{ij}^A v(x_i, x_j)$

- Writing down a potential with some strength depending on two separate positions is difficult and so instead a central potential is used.

  - I.e. rather than actually use the nucleon-nucleon interaction to calculate the self-binding of the nucleons (sort of the volume component of the liquid drop), we approximate self-binding with, e.g., a Woods-Saxon

  - The disadvantage is that the sum of single-particle energies isn't the binding energy, so shell model won't give us binding energies

  - The advantage is that we can actually solve the problem and get useful results, e.g. relative binding energies, excited state energies, wavefunctions for different nuclear states (and therefore wavefunction overlaps between states)

Removal of center-of-mass motion

- Before we get carried away and solve the Schrödinger equation for single-particle energies with the adopted Hamiltonian, we need to correct for an important issue first

- The calculated energy includes some intrinsic component, which we care about, as well as a center-of-mass component, which absolutely does not matter

- Therefore, in the kinetic energy term, we need to replace total kinetic energy $T = \sum_i^A \vec{p}_i^2/2m_i$ with the momentum variance to get the intrinsic KE, $T_{int} = \frac{1}{2m}\sum_i^A\left(\left(\vec{p}_i^2 - \left(\sum_i^A \vec{p}_i^2\right)\right)^2\right)$

- So what we're really solving is $H_{int}\Psi_{int} = E_{int}\Psi_{int}$

Including spin-orbit

- We know from the schematic shell-model that we need to break the degeneracy in energy that states of a given nl have and, from Maria Goeppert Mayer, that spin-orbit is the way to do it

- $V = V_{central} + V_{spin-orbit} = \dfrac{V_0}{1+\exp((\vec{r}-\vec{R})/a)} + \varphi(\vec{r})\vec{l}\cdot\vec{s}$

- Expanding the second term, $\varphi(\vec{r})\vec{l}\cdot\vec{s} = \frac{1}{2}\varphi(\vec{r})\left(\vec{j}^2 - \vec{l}^2 - \vec{s}^2\right)$

- When we finally solve for the energy of a single-particle level, we can compare the solution with and without spin orbit forces to get $\varepsilon_{nlj} = \varepsilon_{nlj}^{(0)} + \Delta\varepsilon_{nlj}$, where an astute quantum mechanic would see $\Delta\varepsilon_{nlj} = \dfrac{Const.}{2}\left(j(j+1) - l(l+1) - s(s+1)\right)$

- Since we have fermions, $s = \frac{1}{2}$ and $j = l \pm \frac{1}{2}$, so

  - $\Delta\varepsilon_{nl(j=l-\frac{1}{2})} = \dfrac{Const.}{2}l$ $\qquad\qquad \Delta\varepsilon_{nl(j=l+\frac{1}{2})} = -\dfrac{Const.}{2}(l+1),$
    where calculating the constant is the radial integral of $\varphi(\vec{r})$ and is essentially empirical

Finally getting on with it & solving for ε_{nlj}

- While $H\Psi = E\Psi$ is cute, it's shorthand for a generally painful differential equation

- The radial equation reads,

$$-\frac{\hbar^2}{2m}\left(\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr} - \frac{l(l+1)}{r^2}\right)R(r) + V(r)R(r) = ER(r)$$

- Actually solving this equation is a problem of mathematics, which you can get into on your own time if you want!
  - The Harmonic Oscillator problem can be solved analytically, and so you can find several presentations for that problem [E.g. in Lecture Notes (M. Jorth Jensen)]
  - A fortran program to calculate single-particle energies for Woods-Saxon potential with parameters of your choosing is WSPOT.for, which can be obtained from Alex Brown (MSU), or by Googling

Creating a many-body wave function

- A many-body wavefunction (i.e. a wavefunction describing many nucleons at once [a.k.a. a nucleus]) is constructed by taking the product of many single-particle wave functions
$$\Psi(a,b,c,\cdots,d) = \varphi_a(1)\varphi_b(2)\varphi_c(3)\cdots$$

- But, any old product won't work. The wavefunction for fermions must be antisymmetric, meaning the wavefunction is mirrored if it is reflected on an axis

- The way to assure this is with a Slater determinant
$$\Psi(a,b,c,\cdots,d) = \frac{1}{\sqrt{A!}}\det\begin{bmatrix} \varphi_a(1) & \cdots & \varphi_a(A) \\ \vdots & \ddots & \vdots \\ \varphi_N(1) & \cdots & \varphi_N(A) \end{bmatrix}$$
  where a, b, etc. are single particle states and 1,2, etc. are nucleons

- So for 2 particles, $\Psi = \frac{1}{\sqrt{2}}\begin{vmatrix} \varphi_a(1) & \varphi_a(2) \\ \varphi_b(1) & \varphi_b(2) \end{vmatrix} = \frac{1}{\sqrt{2}}[\varphi_a(1)\varphi_b(2) - \varphi_b(1)\varphi_a(2)]$

- Note that if any two rows or columns are the same, their contribution to the determinant vanishes
  - I.e. two particles can't occupy the same state (identical rows) or place (identical columns), enforcing the Pauli principle

Creating a many-body wave function

- The slater determinant we just constructed is the many-body wavefunction for a single combination of single particle states. In principle we could have had a different set of single-particle states occupied (e.g. from an excitation) and therefore had a different wavefunction

- Each slater determinant is one state in a basis of states, which are all orthonormal (basically, perpendicular in multiple dimensions and with unit length).
  - For example, in a spherical basis, each state would correspond to one n, l, m_l
  - Bringing spin-orbit coupling in the picture, one state is specified by n, l, j, m_j

- Writing each Slater determinant as ψ_i, a many-body wavefunction would be described by some combination of these, $\Psi = \sum_i c_i \psi_i$

- Occupying each single-particle state up to the Fermi level provides the ground-state ψ_0, where $c_0 \equiv 1$

- Ψ and the associated E are found by solving the matrix equation $\sum_{ij} \langle \psi_j | H | \psi_i \rangle c_a = E c_b$

- Solving such a matrix is a mathematical feat.
  To do this, you want to diagonalize the matrix and apparently one such technique is the Hartree-Fock method. *Feel free to read about it and teach the rest of us!*

Exponential growth & the need for truncation

- You may have realized a problem looming on the horizon of this method of solving the many-body wavefunction. There is a lot of ways to arrange N nucleons among n single-particle states

- The number of Slater determinants which can be constructed is $\frac{n!}{(n-N)!N!}$

- Recall that the number of single particle states encompassing a harmonic oscillator shell n_r is $2(2l+1)$ states (two spin-1/2 particles for $2l+1$ angular momentum projections) for $l = n_r - 1, n_r - 3, \ldots \geq 0$

- So, including states through the pf shell (i.e. through $n_r = 4$, if we start counting at 1) is 40 states

- For this case, considering the 8 neutrons of ^{16}O results in $\sim 10^9$ Slater determinants

- Multiplying this by the number of proton Slater determinants results in 10^{18}
  (For context, ~10^{17} seconds have elapsed since the Big Bang)

- Tricks exist for solving eigenvalues for large matrices, but the best methods available at the moment are limited to dimensionalities of $\sim 10^{10}$ ([Lecture Notes (M. Jorth Jensen)](#))

- As such, choices need to be made as to which single-particle levels can be left out without doing too much damage to the calculation results, which is known as truncation.

Putting it all together

- To perform a shell model calculation, one must:
    1. Calculate single-particle states by
        a) Choose a nuclear potential…. typically a Woods-Saxon
        b) Choose a basis …. typically states defined by quantum numbers n, l, j, m_j
    2. Construct a many-body basis
        a) Choose the states to include (i.e. truncation) (a.k.a. valence space) …typically a core is "frozen" and a cut-off is chosen based on single-particle energies or the number of allowed particle-hole excitations
        b) A matrix of all possible Slater determinant combinations (sandwiching the Hamiltonian) is constructed
    3. Solve the matrix equation for the eigenfunctions and eigenvalues, resulting in discrete state wavefunctions and energies
    4. Take things a step further by then calculating wavefunction overlaps, which you'll recall are essential ingredients in calculating transition rates (e.g. for β and γ decay)

Further Reading

- Lecture Notes in Nuclear Structure Physics (B.A. Brown)
- Chapter 4: Nuclear Structure from a Simple Perspective (R. Casten)
- "How To Develop A Shell Model Code", MSU PHY981 Lecture Notes (M. Jorth Jensen)