The Physics of Nuclei
II: Nuclear Structure

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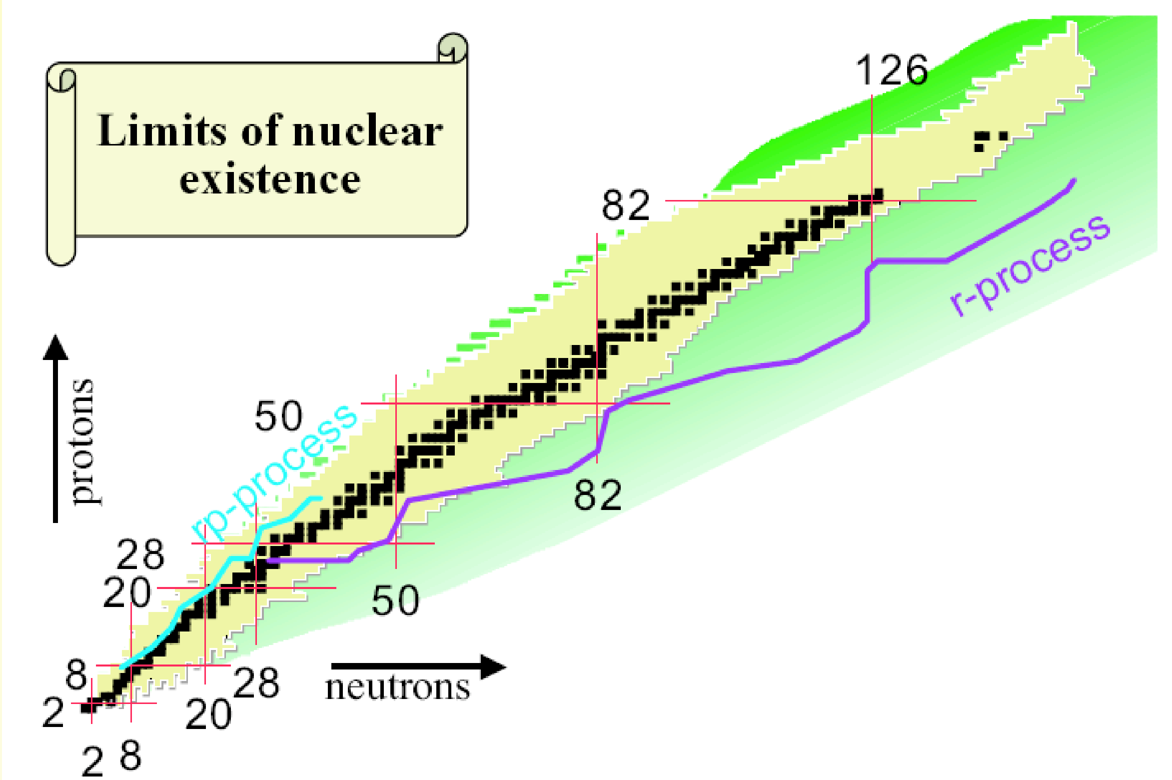
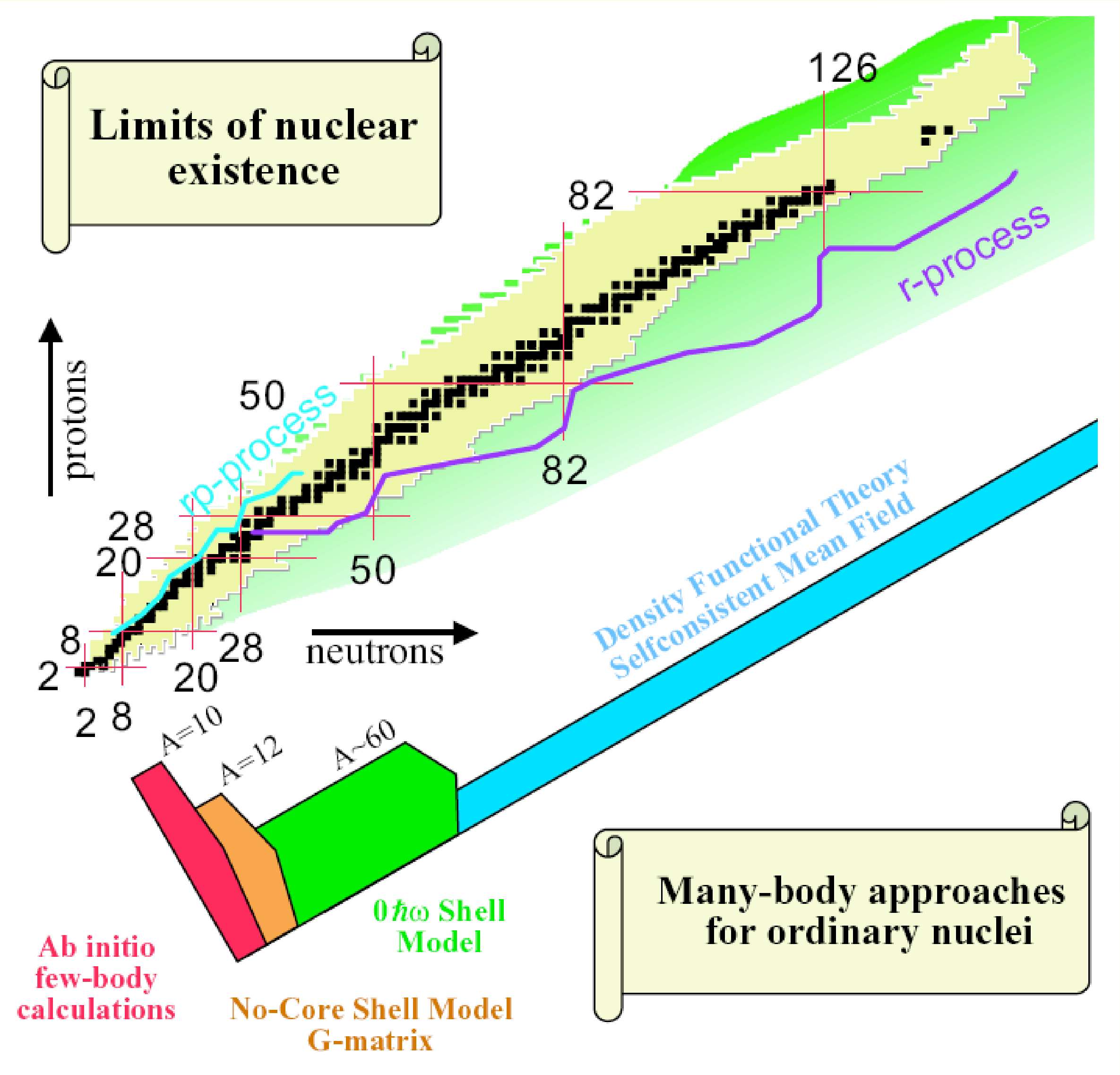
Structure Synopsis

- Heavier Nuclei, so:
- Simpler Structure Theories:
  - Liquid-Drop model
  - Magic Numbers at Shells; Deformation; Pairing
  - Shell Model
  - Hartree-Fock (Mean-field; Energy Density Functional)

Segré Chart of Isotopes



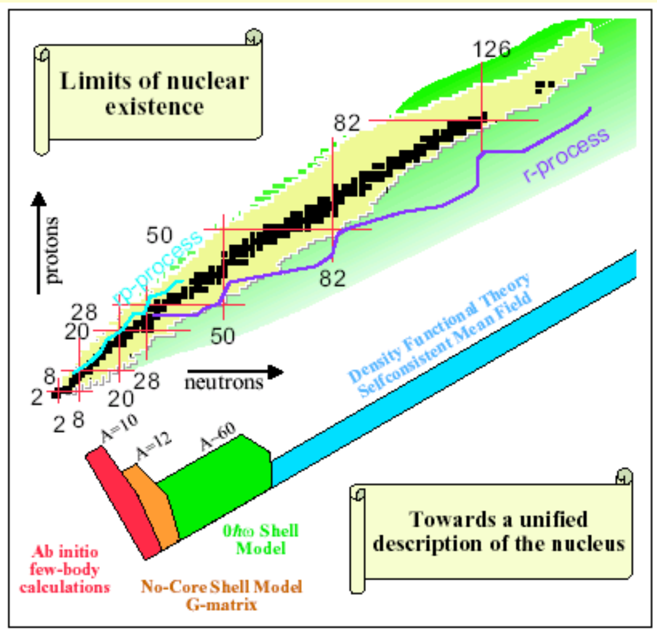
Segré Chart of Isotopes



Nuclei with A≥16

- Start with Liquid-Drop model
  - Parametrise binding energies
  - Look for improvements
    - Magic Numbers for Shells
    - Shell Corrections
    - Deformation
    - Pairing
- Shell Model
- Mean field: Hartree-Fock

Nuclear masses: what nuclei exist?



One goal in theory is to accurately describe the binding energy

$$M(Z,N,A) = Zm_h + Nm_n - BE(Z,N,A)$$

- Let's start with the semi-empirical mass formula, Bethe-Weizsäcker formual, or also the liquid-drop model.

$$BE(Z,N,A) = a_V A - a_{Surf} A^{2/3} - a_{sym}\frac{(Z-N)^2}{A} +$$

$$a_{Coul} Z(Z-1)A^{-1/3} + \Delta_{Pair} + \delta_{Shell}$$

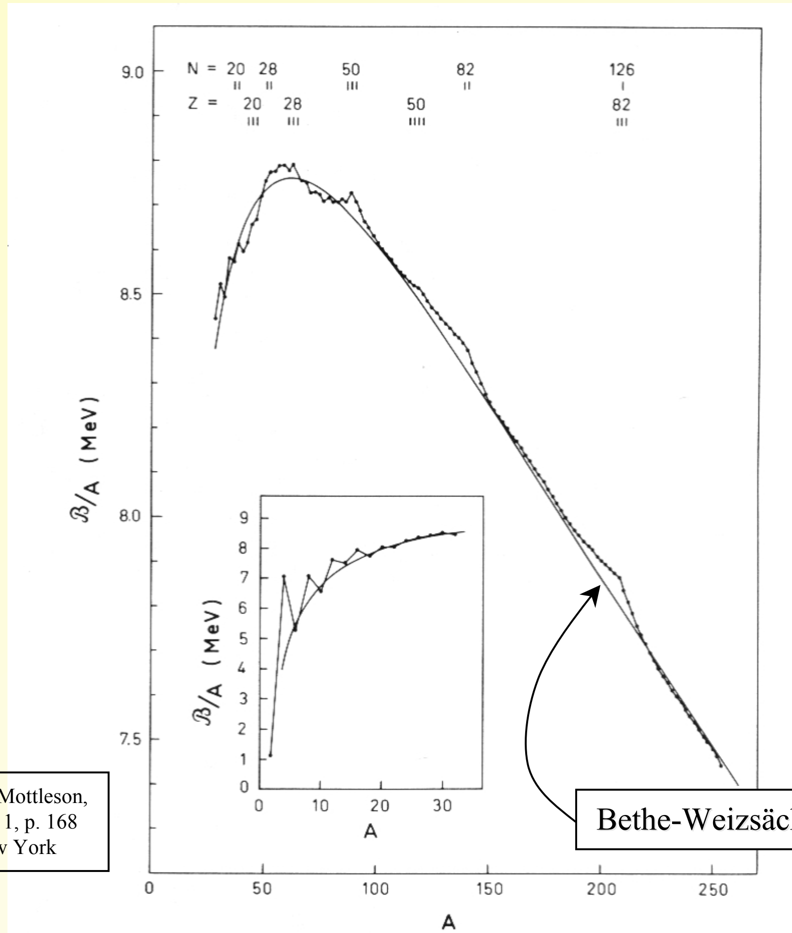
  - There are global Volume, Surface, Symmetry, and Coulomb terms
  - And specific corrections for each nucleus due to pairing and shell structure

$$a_V = 15.85\ \text{MeV}$$
$$a_{Surf} = 18.34\ \text{MeV}$$
$$a_{Symm} = 23.21\ \text{MeV}$$
$$a_{Coul} = 0.71\ \text{MeV}$$

Values for the parameters, A.H. Wapstra and N.B. Gove, Nulc. Data Tables 9, 267 (1971)

Nuclear masses, what nuclei exist?

$$BE(Z,N,A) = a_V A - a_{Surf} A^{2/3} - a_{sym}\frac{(Z-N)^2}{A} + a_{Coul} Z(Z-1)A^{-1/3}$$



Bethe-Weizsäcker formula

From A. Bohr and B.R. Mottleson, *Nuclear Structure*, vol. 1, p. 168 Benjamin, 1969, New York

Liquid-drop isn't too bad! There are notable problems though.

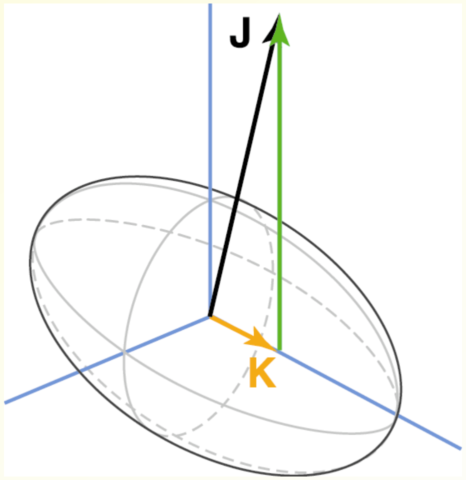
Can we do better and what about the microscopic structure?

Nuclear masses, what nuclei exist?

- How about deformation?
- For each energy term, there are also shape factors dependent on the quadrupole deformation parameters β and γ

$$B_{Surf} \approx 1 + \frac{2}{5}\left(\sqrt{\frac{5}{4\pi}}\beta\right)^2 - \frac{2}{21}\left(\sqrt{\frac{5}{4\pi}}\beta\right)^3 \cos 3\gamma + \ldots$$

$$B_{Coul} \approx 1 - \frac{1}{5}\left(\sqrt{\frac{5}{4\pi}}\beta\right)^2 - \frac{1}{105}\left(\sqrt{\frac{5}{4\pi}}\beta\right)^3 \cos 3\gamma + \ldots$$



$$R(\theta,\varphi) = R_0\left[1 + a_{20}Y_{20}(\theta,\varphi) + a_{22}\left(Y_{22}(\theta,\varphi) + Y_{2-2}(\theta,\varphi)\right)\right]$$

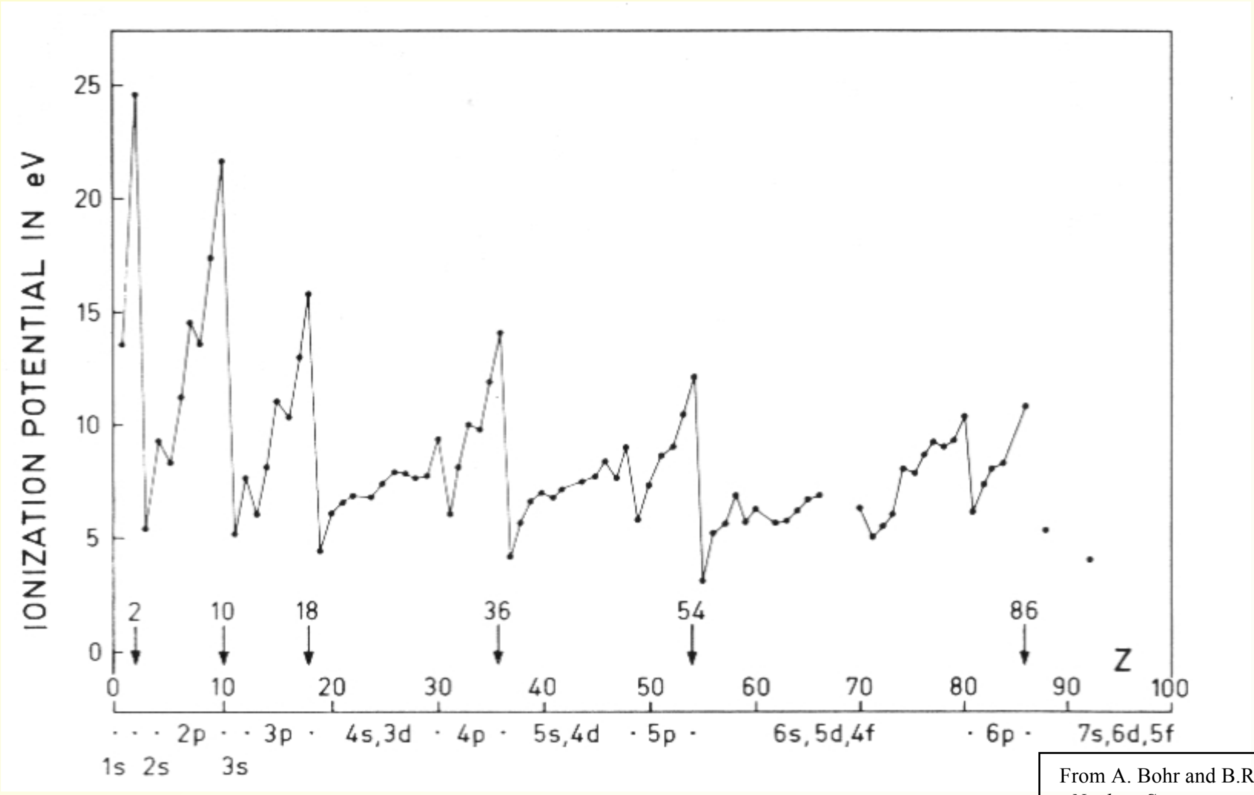
$$a_{20} = \beta\cos\gamma$$

$$a_{22} = \left(\beta/\sqrt{2}\right)\sin\gamma$$

Note that the liquid drop always has a minimum for a spherical shape!
So, where does deformation come from?

Shell structure - evidence in atoms

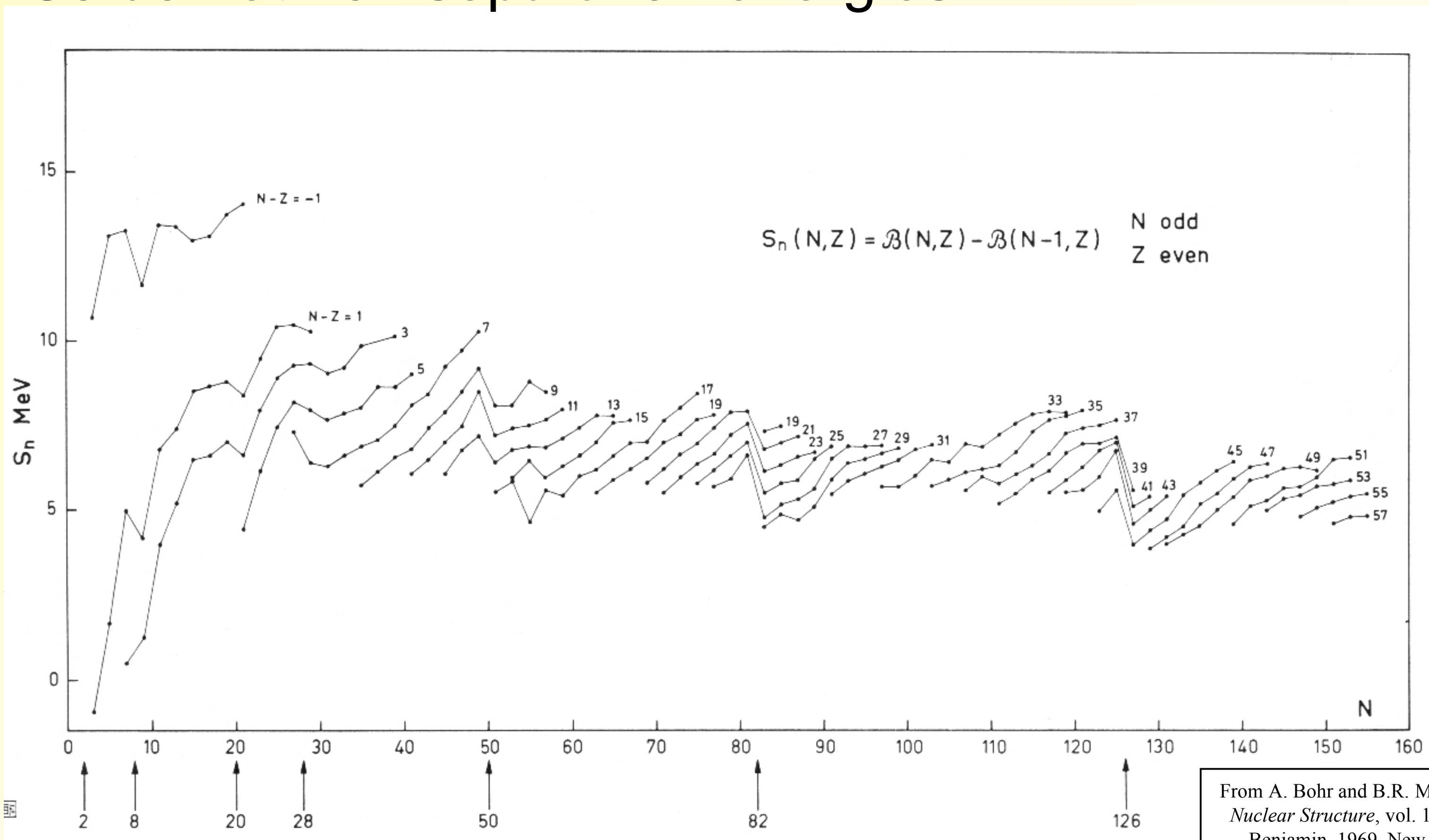
- Atomic ionization potentials show sharp discontinuities at shell boundaries



From A. Bohr and B.R. Mottleson, *Nuclear Structure*, vol. 1, p. 191 Benjamin, 1969, New York

Shell structure - neutron separation energies

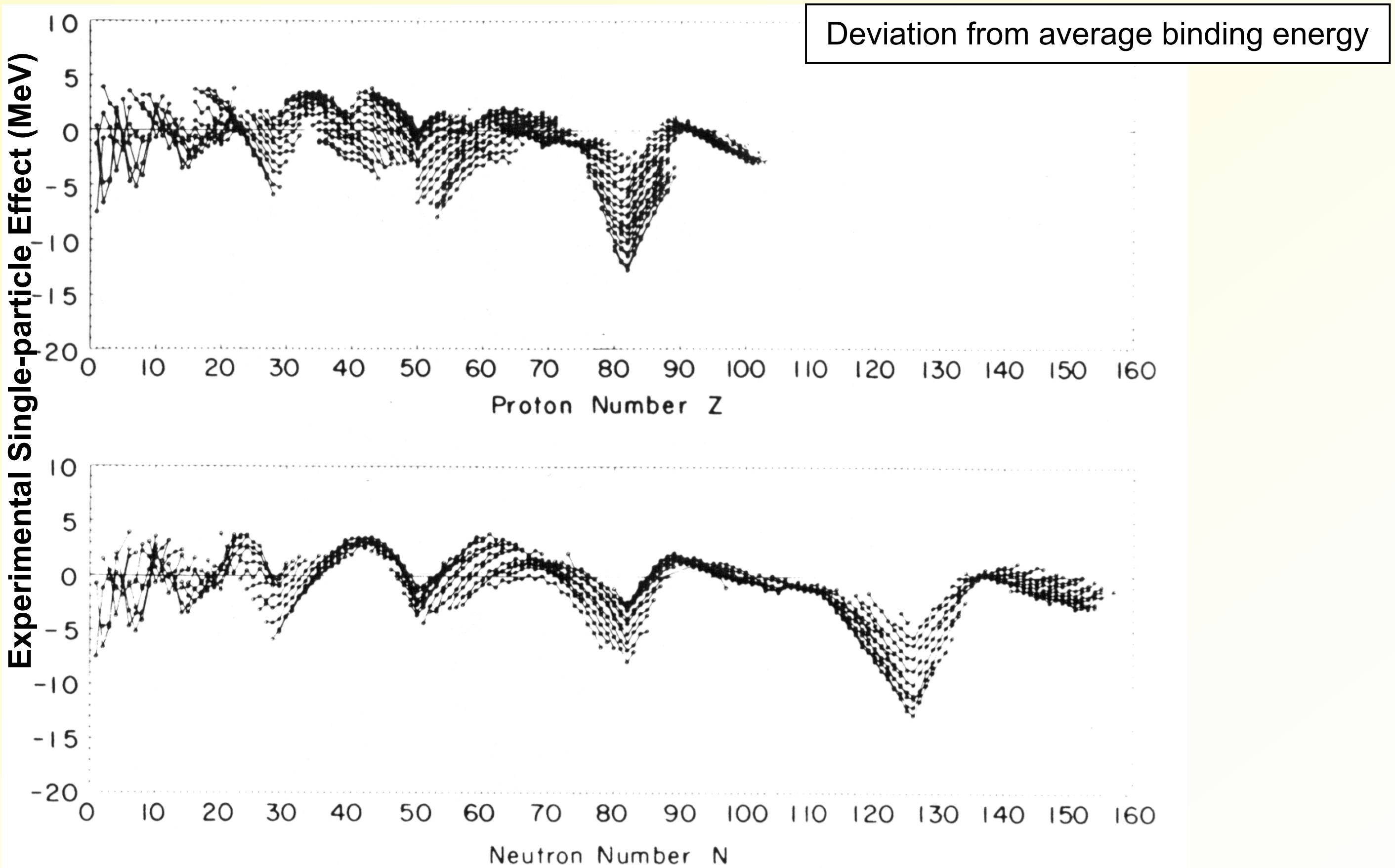
- So do neutron separation energies



From A. Bohr and B.R. Mottleson, *Nuclear Structure*, vol. 1, p. 193 Benjamin, 1969, New York

More evidence of shell structure

- Binding energies show preferred magic numbers
  - 2, 8, 20, 28, 50, 82, and 126

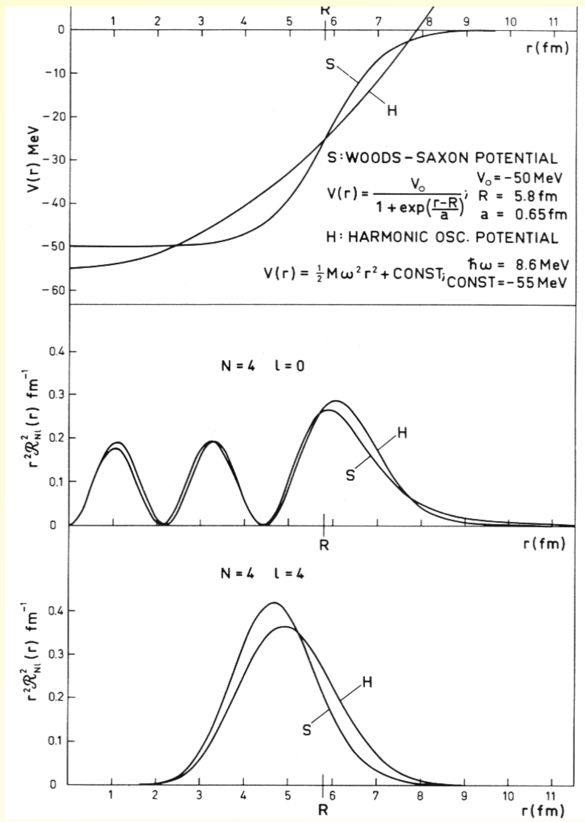


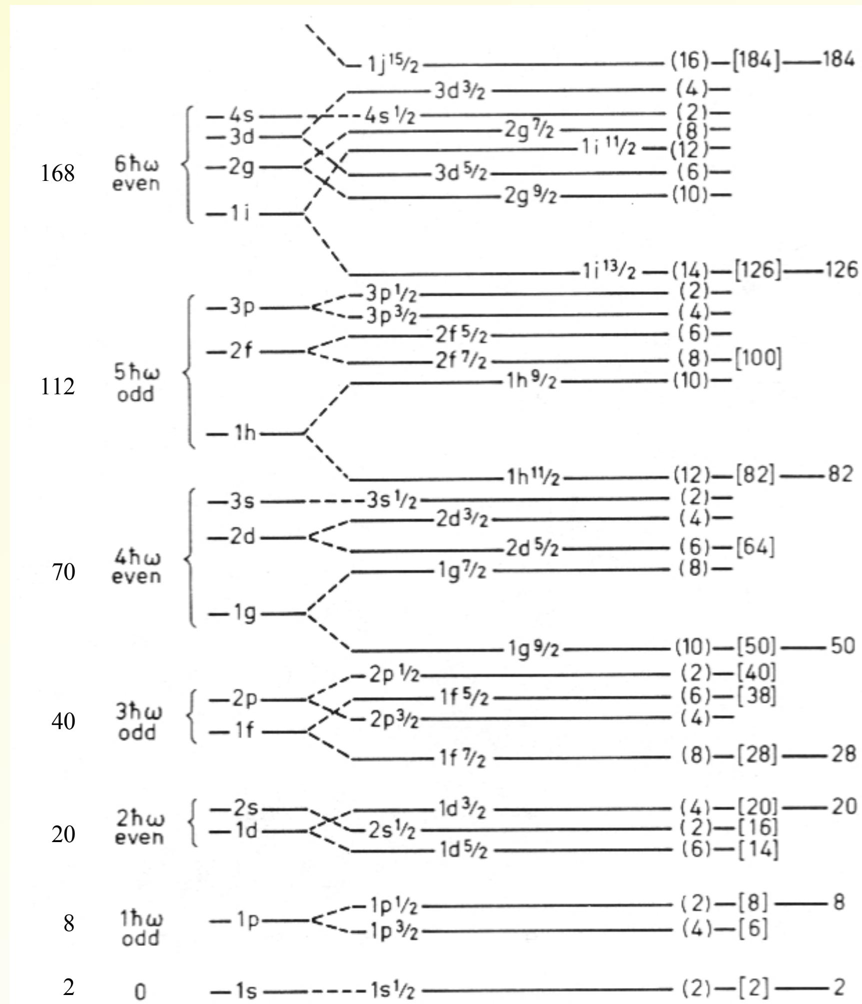
From W.D. Myers and W.J. Swiatecki, Nucl. Phys. **81**, 1 (1966)

Origin of the shell model

- Goeppert-Mayer and Haxel, Jensen, and Suess proposed the independent-particle shell model to explain the magic numbers

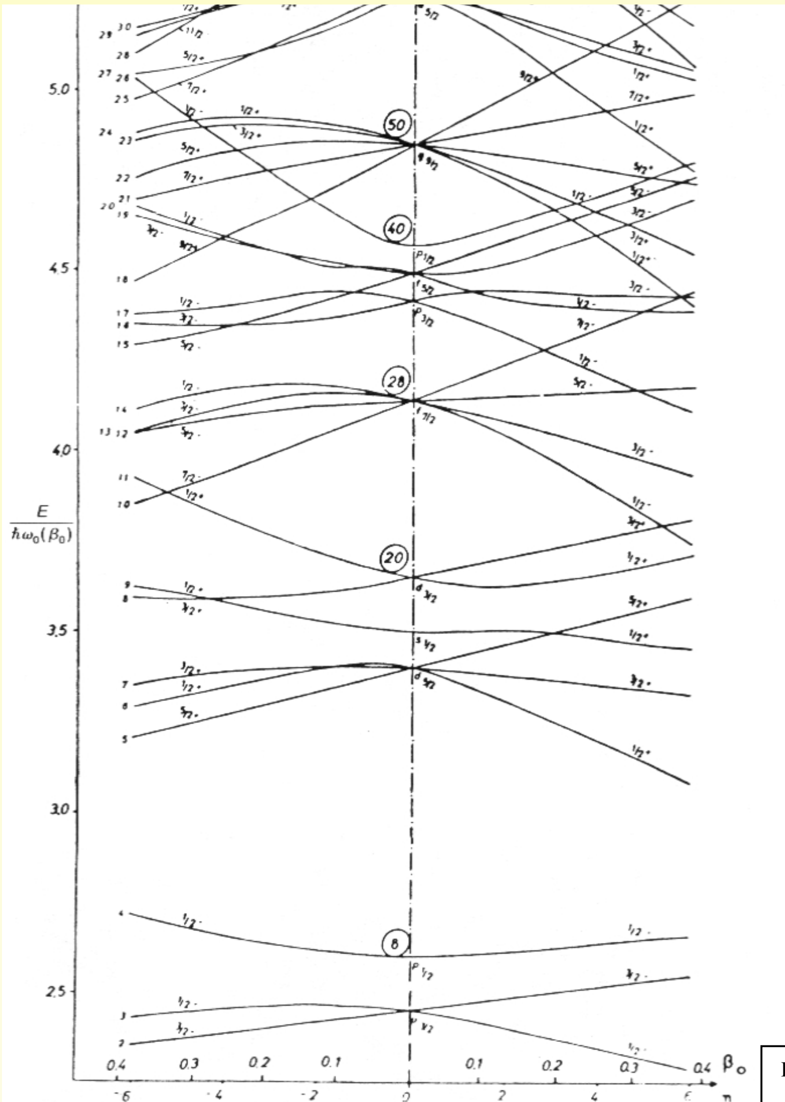
Harmonic oscillator with spin-orbit is a reasonable approximation to the nuclear mean field





M.G. Mayer and J.H.D. Jensen, *Elementary Theory of Nuclear Shell Structure*,p. 58, Wiley, New York, 1955

Nilsson Hamiltonian - Poor man's Hartree-Fock



Oblate, γ=60˚

Prolate, γ=0˚

From J.M. Eisenberg and W. Greiner, *Nuclear Models*, p 542, North Holland, Amsterdam, 1987

Anisotropic harmonic oscillator

$$\frac{p^2}{2m}+\frac{m}{2}\left(\omega_x^2x^2+\omega_y^2y^2+\omega_z^2z^2\right)-2\hbar\omega_0\kappa\vec{\ell}\cdot\vec{s}-\hbar\omega_0\kappa\mu\vec{\ell}^2$$

$$\hbar\omega_0=41A^{1/3}\ \mathrm{MeV}$$

$$\omega_x=\omega_0 e^{\sqrt{\frac{5}{4\pi}}\beta\cos(\gamma+2\pi/3)}$$

$$\omega_y=\omega_0 e^{\sqrt{\frac{5}{4\pi}}\beta\cos(\gamma-2\pi/3)}$$

$$\omega_z=\omega_0 e^{\sqrt{\frac{5}{4\pi}}\beta\cos\gamma}$$

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Nuclear masses
Shell corrections to the liquid drop

- Shell correction
  - In general, the liquid drop does a good job on the bulk properties
    - The oscillator doesn't!
  - But we need to put in corrections due to shell structure
    - Strutinsky averaging; difference between the energy of the discrete spectrum and the averaged, smoothed spectrum

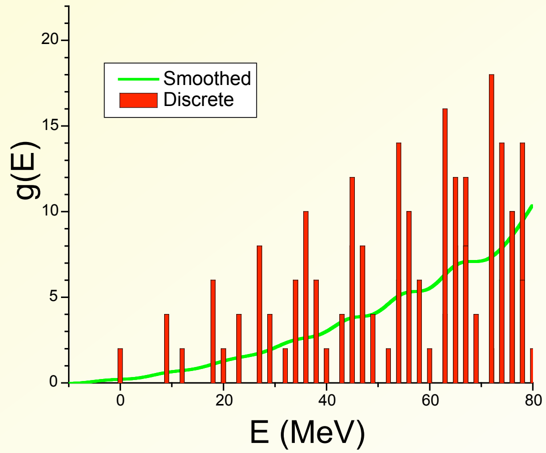
Discrete spectrum

$$g(\varepsilon) = \sum_i \delta(\varepsilon - \varepsilon_i)$$

$$N = \int_{-\infty}^{\varepsilon_F} g(\varepsilon) d\varepsilon$$

$$E_{Discrete} = \int_{-\infty}^{\varepsilon_F} \varepsilon g(\varepsilon) d\varepsilon$$

Mean-field single-particle spectrum



Smoothed spectrum

$$\tilde{g}(\varepsilon) = \sum_i f\left(\frac{\varepsilon - \varepsilon_i}{\gamma}\right)\delta(\varepsilon - \varepsilon_i)$$

$$N = \int_{-\infty}^{\tilde{\varepsilon}_F} \tilde{g}(\varepsilon) d\varepsilon$$

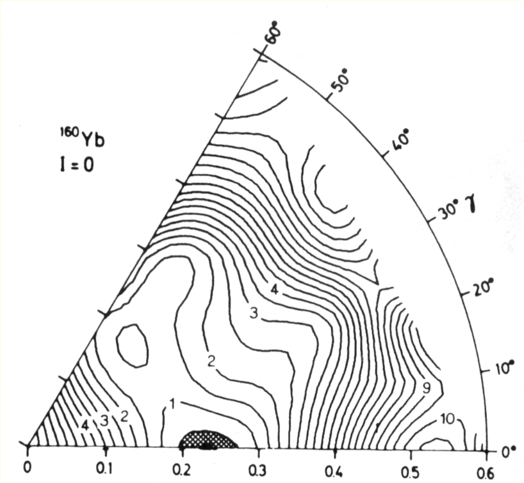
$f(x) = L(x) e^{-(\varepsilon-\varepsilon_i)^2/\gamma^2} / 2\sqrt{\pi}\,\gamma$
is a modified Gaussian
$\gamma \approx \hbar\Omega$

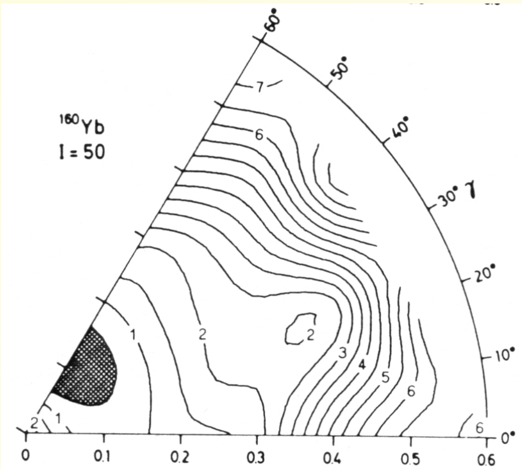
$$E_{\text{Strutinsky}} = \int_{-\infty}^{\tilde{\varepsilon}_F} \varepsilon \tilde{g}(\varepsilon) d\varepsilon$$

$$\delta_{Shell} = E_{Discrete} - E_{Strutinsky}$$

Nilsson-Strutinsky and deformation

- Energy surfaces as a function of deformation





From C.G. Andersson,et al., Nucl. Phys. **A268**, 205 (1976)

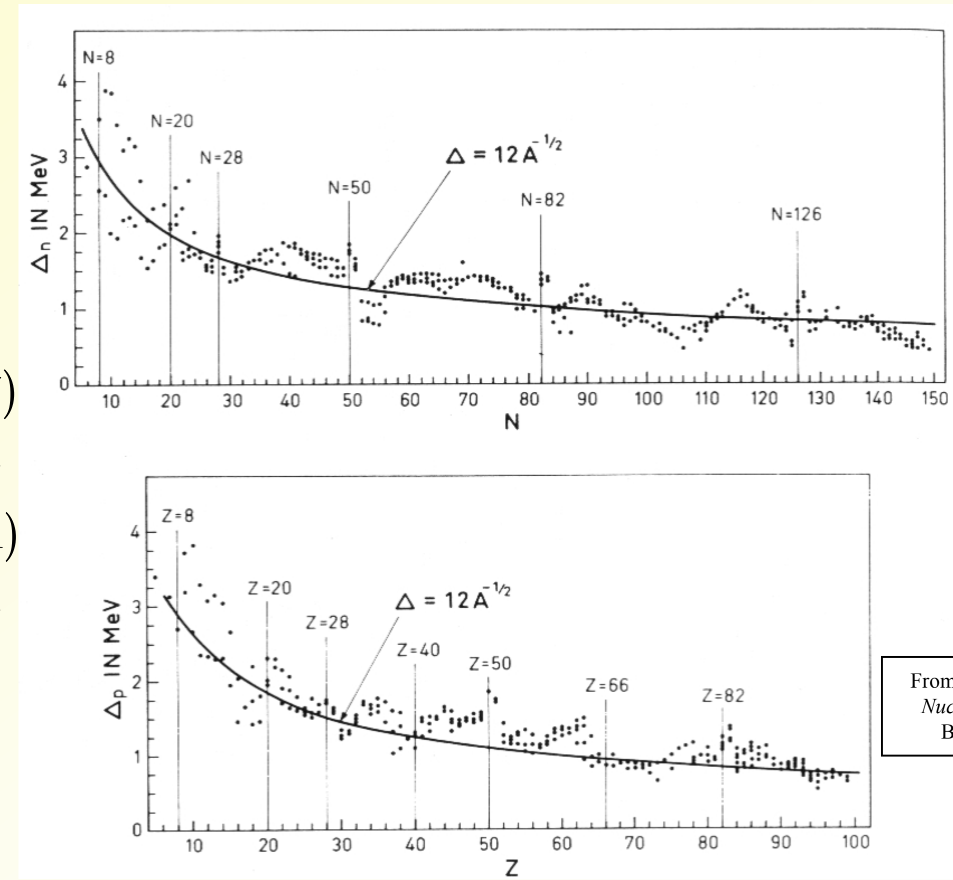
Nilsson-Strutinsky is a mean-field type approach that allows for a comprehensive study of nuclear deformation under rotation and at high temperature

Nuclear masses
Pairing corrections to the liquid drop

- Pairing: $$\Delta_{Pair}(Z,N,A) \approx -(+)12A^{-1/2};\quad \text{even - even(odd - odd)}$$
$$= 0;\quad \text{odd - even(even - odd)}$$

$$\Delta_n = \tfrac{1}{4}\{BE(N-2,Z) - 3BE(N-1,Z) + 3BE(N,Z) - BE(N+1,Z)\}$$

$$\Delta_p = \tfrac{1}{4}\{BE(N,Z-2) - 3BE(N,Z-1) + 3BE(N,Z) - BE(N,Z+1)\}$$



From A. Bohr and B.R. Mottleson, *Nuclear Structure*, vol. 1, p. 170 Benjamin, 1969, New York

The Shell Model

- More microscopic theory
  - Include all nucleons
  - Fully antisymmetrised wave functions
  - Include all correlations in a ‘shell’.
  - Harmonic Oscillator basis states.
- Effective Hamiltonian
  - Still needed!
  - Find or fit potential matrix elements,

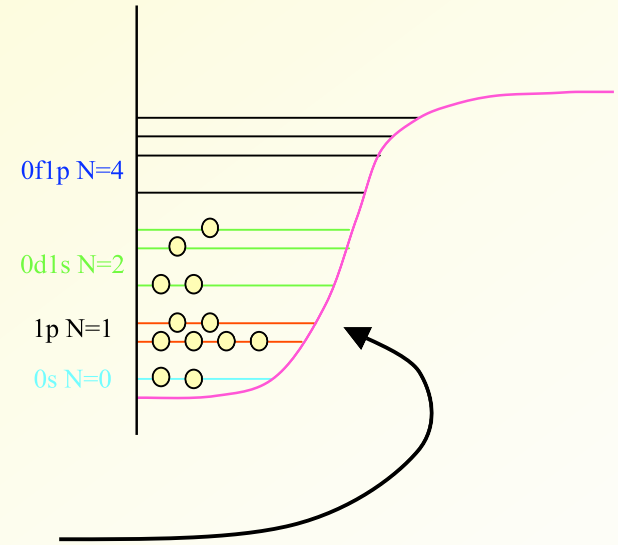
Many-body Hamiltonian

- Start with the many-body Hamiltonian

$$H = \sum_i \frac{\vec{p}_i^{\,2}}{2m} + \sum_{i<j} V_{NN}\left(\vec{r}_i - \vec{r}_j\right)$$

- Introduce a mean-field U to yield basis

$$H = \sum_i \left(\frac{\vec{p}_i^{\,2}}{2m} + U\left(r_i\right)\right) + \sum_{i<j} \underbrace{V_{NN}\left(\vec{r}_i - \vec{r}_j\right) - \sum_i U\left(r_i\right)}_{\text{Residual interaction}}$$



- The mean field determines the shell structure
- In effect, nuclear-structure calculations rely on perturbation theory

The success of any nuclear structure calculation depends on the choice of the mean-field basis and the residual interaction!

Single-particle wave functions

- With the mean-field, we have the basis for building many-body states
- This starts with the single-particle, radial wave functions, defined by the radial quantum number n, orbital angular momentum l, and z-projection m

$$\varphi_{nlm}(\vec{\mathrm{r}}) = R_{nl}(r) Y_{lm}(\hat{\mathrm{r}})$$

  – Now include the spin wave function: $\chi^{S}_{\frac{1}{2}s_z}$

- Two choices, jj-coupling or ls-coupling
  – Ls-coupling

$$\varphi_{nlms_z}(\vec{\mathrm{r}}) = \varphi_{nlms_z}(\vec{\mathrm{r}})\chi^{S}_{\frac{1}{2}s_z} = R_{nl}(r) Y_{lm}(\widehat{\mathrm{r}})\chi^{S}_{\frac{1}{2}s_z}$$

  – jj-coupling is very convenient when we have a spin-orbit ($l \cdot s$) force

$$\varphi_{nljj_z}(\vec{\mathrm{r}}) = R_{nl}(r)\left[Y_l(\hat{\mathrm{r}}) \otimes \chi^{S}_{\frac{1}{2}}\right]^{jj_z}$$

$$\left[Y_l(\hat{\mathrm{r}}) \otimes \chi^{S}_{\frac{1}{2}}\right]^{jj_z} = \sum_{ms_z} \left(lm \tfrac{1}{2} s_z \mid jj_z\right) Y_{lm}(\hat{\mathrm{r}})\chi^{S}_{\frac{1}{2}s_z}$$

Multiple-particle wave functions

- Total angular momentum, and isospin; $\chi^{T}_{\frac{1}{2}s_z}$
- Anti-symmetrized, two particle, jj-coupled wave function

$$\psi^{j_1 j_2}_{JMTT_z} = \left\{ \left[\varphi_{n_1 l_1 j_1}(\vec{r}_1) \otimes \varphi_{n_2 l_2 j_2}(\vec{r}_2) \right]^{JM} + (-1)^{j_1 + j_2 + J + T} \left[\varphi_{n_2 l_2 j_2}(\vec{r}_1) \otimes \varphi_{n_1 l_1 j_1}(\vec{r}_2) \right]^{JM} \right\}$$
$$\left[\chi^{T}_{\frac{1}{2}}(1) \otimes \chi^{T}_{\frac{1}{2}}(2) \right]^{TT_z} \Big/ \sqrt{2(1+\delta_{12})}$$

  - Note $J+T$=odd if the particles occupy the same orbits
- Anti-symmetrized, two particle, LS-coupled wave function

$$\psi^{LS}_{JMTT_z} = \left\{ \left(\left[\varphi_{n_1 l_1}(\vec{r}_1) \otimes \varphi_{n_2 l_2}(\vec{r}_2) \right]^{L} - (-1)^{l_1 + l_2 + L + S + T} \left[\varphi_{n_2 l_2}(\vec{r}_1) \otimes \varphi_{n_1 l_1}(\vec{r}_2) \right]^{L} \right) \otimes \left[\chi^{S}_{\frac{1}{2}}(1) \otimes \chi^{S}_{\frac{1}{2}}(2) \right]^{S} \right\}^{JM}$$
$$\left[\chi^{T}_{\frac{1}{2}}(1) \otimes \chi^{T}_{\frac{1}{2}}(2) \right]^{TT_z} \Big/ \sqrt{2(1+\delta_{12})}$$

Two-particle wave functions

- Of course, the two pictures describe the same physics, so there is a way to connect them
  - Recoupling coefficients $(\hat{j} = \sqrt{2j+1})$

$$\psi^{j_1 j_2}_{JMTT_z} = \sum_{LS} \hat{j}_1 \hat{j}_1 \hat{L} \hat{S} \begin{Bmatrix} l_1 & \frac{1}{2} & j_1 \\ l_2 & \frac{1}{2} & j_2 \\ L & S & J \end{Bmatrix} \psi^{LS}_{JMTT_z}$$

- Note that the wave functions have been defined in terms of $\vec{r}_1$ and $\vec{r}_2$, but often we need them in terms of the relative coordinate $r = |\vec{r}_1 - \vec{r}_2|$
  - We can do this in two ways
    - Transform the operator

$$V(\ldots) = \sum \frac{(-1)^l F_l(r_1, r_2)}{\ldots} [\ldots]^{00}$$

Quadrupole, l=2, component is large and very important

$$F_l(r_1, r_2) = \frac{2l+1}{2} \int_0 P_l(\cos\theta) V(|\vec{r}_1 - \vec{r}_2|) \sin\theta_{12} d\theta_{12}$$

Two-particle wave functions in relative coordinate

- Use Harmonic-oscillator wave functions and decompose in terms of the relative and center-of-mass coordinates, i.e.,

$$r = \left|\vec{r}_1 - \vec{r}_2\right|; \qquad R = \left|\vec{r}_1 + \vec{r}_2\right|/2$$

- Harmonic oscillator wave functions are a very good approximation to the single-particle wave functions
- We have the useful transformation

$$\left[\phi_{n_1 l_1}(\vec{r}_1) \otimes \phi_{n_1 l_1}(\vec{r}_1)\right]^{L'M'} = \sum_{nlNL} M(nlNL; n_1 l_1 n_2 l_2)\left[\phi_{nl}(\vec{r}) \otimes \phi_{NL}(\vec{R})\right]^{L'M'}$$

  - $2n_1+l_2+2n_2+l_2=2n+l+2N+L$
  - Where the $M(nlNL;n_1l_1n_2l_2)$ is known as the Moshinksy bracket
  - Note this is where we use the jj to LS coupling transformation
  - For some detailed applications look in *Theory of the Nuclear Shell Model*, R.D. Lawson, (Clarendon Press, Oxford, 1980)

Many-particle wave function

- To add more particles, we just continue along the same lines
- To build states with good angular momentum, we can bootstrap up from the two-particle case, being careful to denote the distinct states
  - This method uses Coefficients of Fractional Parentage (CFP)

$$\left| j^N \alpha JM \right\rangle = \sum_{\alpha' J'} \left[j^{N-1} \alpha' J' j J \middle| \right\} j^N \alpha J \Big] \left[\left| j^{N-1} \alpha' J' \right\rangle \otimes \left| j \right\rangle \right]^{JM}$$

- Or we can make a many-body Slater determinant that has only a specified J_z and T_z and project J and T

$$\Phi(1,2,\ldots,A) = \frac{1}{\sqrt{A!}} \begin{vmatrix} \phi_{n_i l_i j_i j_{z_i}}(\mathbf{r}_1) & \phi_{n_i l_i j_i j_{z_i}}(\mathbf{r}_2) & \cdots & \phi_{n_i l_i j_i j_{z_i}}(\mathbf{r}_A) \\ \phi_{n_j l_j j_j j_{z_j}}(\mathbf{r}_1) & \phi_{n_j l_j j_j j_{z_j}}(\mathbf{r}_2) & & \phi_{n_j l_j j_j j_{z_j}}(\mathbf{r}_A) \\ & \vdots & \ddots & \vdots \\ \phi_{n_l l_l j_l j_{z_l}}(\mathbf{r}_1) & \phi_{n_l l_l j_l j_{z_l}}(\mathbf{r}_2) & \cdots & \phi_{n_l l_l j_l j_{z_l}}(\mathbf{r}_A) \end{vmatrix}$$

In general Slater determinants are more convenient

Second Quantization

- Second quantization is one of the most useful representations in many-body theory
- Creation and annihilation operators
  - Denote $|0\rangle$ as the state with no particles (the vacuum)
  - a_i^+ creates a particle in state *i;* $\quad a_i^+|0\rangle = |i\rangle, \quad a_i^+|i\rangle = 0$
  - a_i annihilates a particle in state *i;* $\quad a_i|i\rangle = |0\rangle; \quad a_i|0\rangle = 0$
  - Anti-commutation relations:

$$\{a_i^+, a_j^+\} = \{a_i, a_j\} = 0$$

$$\{a_i, a_j^+\} = \{a_j^+, a_i\} = \delta_{ij}$$

- Many-body Slater determinant

$$\Phi = \frac{1}{\sqrt{A!}} \begin{vmatrix} \phi_i(\mathbf{r}_1) & \phi_i(\mathbf{r}_2) & \dots & \phi_i(\mathbf{r}_A) \\ \phi_j(\mathbf{r}_1) & \phi_j(\mathbf{r}_2) & & \phi_j(\mathbf{r}_A) \\ & \vdots & \ddots & \vdots \\ \phi_l(\mathbf{r}_1) & \phi_l(\mathbf{r}_2) & \dots & \phi_l(\mathbf{r}_A) \end{vmatrix} = \underbrace{a_l^+ \dots a_j^+ a_i^+}_{l > \dots > j > i} |0\rangle$$

Second Quantization

- Operators in second-quantization formalism
  - Take any one-body operator O, say quadrupole E2 transition operator $er^2Y_{2\mu}$, the operator is represented as:

$$O = \sum_{ij} \langle j|O|i\rangle a_j^+ a_i$$

  where $\langle j|O|i\rangle$ is the single-particle matrix element of the operator O

  - The same formalism exists for any n-body operator, e.g., for the NN-interaction

$$V = \frac{1}{4}\sum_{ijkl} \langle ij|V|kl\rangle_A a_i^+ a_j^+ a_l a_k = \sum_{i<j,k<l} \langle ij|V|kl\rangle_A a_i^+ a_j^+ a_l a_k$$

$$\langle ij|V|kl\rangle_A = \langle ij|V|kl\rangle - \langle ij|V|lk\rangle$$

    - Here, I've written the two-body matrix element with an implicit assumption that it is anti-symmetrized, i.e.,

$$\rho(r) = \sum_i |\varphi_i(r)|^2 a_i^+ a_i$$

Second Quantization

- Matrix elements for Slater determinants (all *aceklm* different)

$$\langle acekl | a_c^+ a_m | aeklm \rangle = \langle 0 | a_l a_k a_e a_c a_a a_c^+ a_m a_m^+ a_l^+ a_k^+ a_e^+ a_a^+ | 0 \rangle$$

$$= \langle 0 | a_l a_k a_e a_c a_a a_c^+ a_l^+ a_k^+ a_e^+ a_a^+ | 0 \rangle = \langle acekl | a_c^+ | aekl \rangle$$

$$= -\langle 0 | a_l a_k a_e a_c a_a a_l^+ a_k^+ a_e^+ a_c^+ a_a^+ | 0 \rangle = -\langle acekl | acekl \rangle$$

$$= -1$$

Second quantization makes the computation of expectation values for the many-body system simpler

Second Quantization

- Angular momentum tensors
  - Creation operators rotate as tensors of rank j
  - Not so for annihilation operators

$$\tilde{a}_{jm} = (-1)^{j+j_z} a_{j-m}$$

- Anti-symmetrized, two-body state

$$\left| j_a j_b : JM, TT_z \right\rangle = -\frac{1}{\sqrt{1+\delta_{ab}}} \left[a^+_{j_a \frac{1}{2}} \otimes a^+_{j_b \frac{1}{2}} \right]^{JM}_{TT_z} \left| 0 \right\rangle$$

Shell-model mean field

- One place to start for the mean field is the harmonic oscillator
  - Specifically, we add the center-of-mass potential

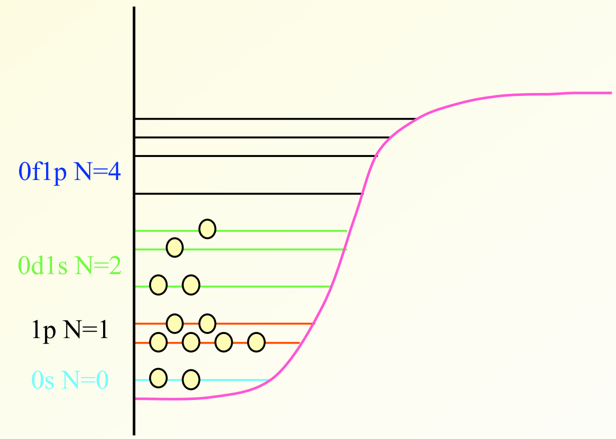
$$H_{CM} = \frac{1}{2} A m \Omega^2 \vec{R}^2 = \sum_i \frac{1}{2} m \Omega \vec{r}_i^{\,2} - \sum_{i<j} \frac{m\Omega^2}{2A} \left(\vec{r}_i - \vec{r}_j \right)^2$$

  - The Good:
    - Provides a convenient basis to build the many-body Slater determinants
    - Does not affect the intrinsic motion
    - Exact separation between intrinsic and center-of-mass motion
  - The Bad:
    - Radial behavior is not right for large r
    - Provides a confining potential, so all states are effectively bound

Low-lying structure – The interacting Shell Model

- The interacting shell model is one of the most powerful tools available too us to describe the low-lying structure of light nuclei
- We start at the usual place:

$$H = \sum_i \left(\frac{\vec{p}_i^{\,2}}{2m} + U(r_i) \right) + \sum_{i<j} V_{NN}(\vec{r}_i - \vec{r}_j) - \sum_i U(r_i)$$



- Construct many-body states $|\phi_i\rangle$ so that

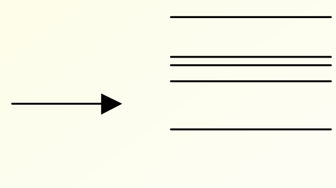
$$\Psi_i = \sum_n C_{in} \phi_n$$

$$\phi = \frac{1}{\sqrt{A!}} \begin{vmatrix} \phi_i(\mathbf{r}_1) & \phi_i(\mathbf{r}_2) & \dots & \phi_i(\mathbf{r}_A) \\ \phi_j(\mathbf{r}_1) & \phi_j(\mathbf{r}_2) & & \phi_j(\mathbf{r}_A) \\ & \vdots & \ddots & \vdots \\ \phi_l(\mathbf{r}_1) & \phi_l(\mathbf{r}_2) & \dots & \phi_l(\mathbf{r}_A) \end{vmatrix}$$

$$= a_l^+ \dots a_j^+ a_i^+ |0\rangle$$

- Calculate Hamiltonian matrix $H_{ij} = \langle \phi_j | H | \phi_i \rangle$
  - Diagonalize to obtain eigenvalues

$$\begin{pmatrix} H_{11} & H_{12} & \cdots & H_{1N} \\ H_{21} & H_{22} & & \\ \vdots & & \ddots & \\ H_{N1} & & \dots & H_{NN} \end{pmatrix}$$



We want an accurate description of low-lying states

Shell model applications

- The practical Shell Model
  1. Choose a model space to be used for a range of nuclei
     - E.g., the 0d and 1s orbits (sd-shell) for ^{16}O to ^{40}Ca or the 0f and 1p orbits for ^{40}Ca to ^{120}Nd
  2. We start from the premise that the effective interaction exists
  3. We use effective interaction theory to make a first approximation (G-matrix)
  4. Then tune specific matrix elements to reproduce known experimental levels
  5. With this empirical interaction, then extrapolate to all nuclei within the chosen model space
  6. Note that radial wave functions are explicitly not included, so we add them in later

The empirical shell model works well!
But be careful to know the limitations!

Simple application of the shell model

- A=18, two-particle problem with ^{16}O core
  - Two protons: ^{18}Ne (T=1)
  - One Proton and one neutron: ^{18}F (T=0 and T=1)
  - Two neutrons: ^{18}O (T=1)

Example: ^{18}O

Question # 1?

- How many states for each J_z? How many states of each J?
  - There are 14 states with J_z=0
    - N(J=0)=3
    - N(J=1)=2
    - N(J=2)=5
    - N(J=3)=2
    - N(J=4)=2

Simple application of the shell model, cont.

Example:

Question #2

- **What are the energies of the three 0^+ states in ^{18}O?**
  - **Use the Universal SD-shell interaction (Wildenthal)**

$$\varepsilon_{0d_{5/2}} = -3.94780$$
$$\varepsilon_{1s_{1/2}} = -3.16354$$
$$\varepsilon_{0d_{3/2}} = 1.64658$$

Measured relative to ^{16}O core
Note $0d_{3/2}$ is unbound

$$\langle 0d_{5/2}0d_{5/2}; J=0, T=1 | V | 0d_{5/2}0d_{5/2}; J=0, T=1 \rangle = -2.8197$$
$$\langle 0d_{5/2}0d_{5/2}; J=0, T=1 | V | 0d_{3/2}0d_{3/2}; J=0, T=1 \rangle = -3.1856$$
$$\langle 0d_{5/2}0d_{5/2}; J=0, T=1 | V | 1s_{1/2}1s_{1/2}; J=0, T=1 \rangle = -1.0835$$
$$\langle 1s_{1/2}1s_{1/2}; J=0, T=1 | V | 1s_{1/2}1s_{1/2}; J=0, T=1 \rangle = -2.1246$$
$$\langle 1s_{1/2}1s_{1/2}; J=0, T=1 | V | 0d_{3/2}0d_{3/2}; J=0, T=1 \rangle = -1.3247$$
$$\langle 0d_{3/2}0d_{3/2}; J=0, T=1 | V | 0d_{3/2}0d_{3/2}; J=0, T=1 \rangle = -2.1845$$

Simple application of the shell model, cont.

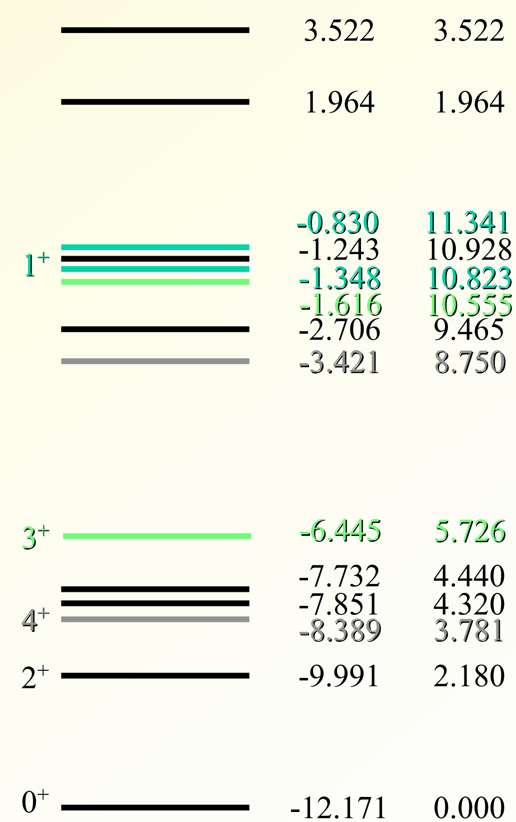
Example:

Finding the eigenvalues

- Set up the Hamiltonian matrix
  - We can use all 14 J_z=0 states, and we'll recover all 14 J-states
  - But for this example, we'll use the two-particle J=0 states

$$\begin{array}{ccc} |(0d_{5/2})^2\rangle_{J=0} & |(1s_{1/2})^2\rangle_{J=0} & |(0d_{3/2})^2\rangle_{J=0} \end{array}$$

$$\mathbf{H} = \begin{pmatrix} -10.7153 & -1.0835 & -3.1856 \\ -1.0835 & -8.4517 & -1.3247 \\ -3.1856 & -1.3247 & 1.1087 \end{pmatrix} \longrightarrow$$



What about heavier nuclei?

- Above A ~ 60 or so the number of configurations just gets to be too large ~ 10^{10}!
- Here, we need to think of more approximate methods
- The easiest place to start is the mean-field of Hartree-Fock
  - But, once again we have the problem of the interaction
    - Repulsive core causes us no end of grief!!
    - So still need effective interactions!
    - At some point use fitted effective interactions like the Skyrme force

Hartree-Fock

- There are many choices for the mean field, and Hartree-Fock is one optimal choice
- We want to find the best single Slater determinant Φ_0 so that

$$\frac{\langle \Phi_0 | H | \Phi_0 \rangle}{\langle \Phi_0 | \Phi_0 \rangle} = \text{minimum} \qquad \langle \delta\Phi_0 | H | \Phi_0 \rangle + \langle \Phi_0 | H | \delta\Phi_0 \rangle = 0$$

$$\Phi_0 = \prod_{i=1}^{A} a_i^+ |0\rangle$$

- Thouless' theorem
  - Any other Slater determinant Φ not orthogonal to Φ_0 may be written as

$$\Phi = \exp\left[\sum_{mi} C_{mi} a_m^+ a_i\right] |\Phi_0\rangle$$

  - Where i is a state occupied in Φ_0 and m is unoccupied
  - Then

$$|\delta\Phi_0\rangle = \sum_{im} C_{mi} a_m^+ a_i |\Phi_0\rangle \qquad \text{and} \quad \langle \Phi_0 | \delta\Phi_0 \rangle = \sum_{im} C_{mi} \langle \Phi_0 | a_m^+ a_i | \Phi_0 \rangle = 0$$

Hartree-Fock

$$H = \sum_i \frac{p_i^2}{m} + \frac{1}{2}\sum_{ij} V\left(\left|\mathbf{r}_i - \mathbf{r}_j\right|\right) = T + \frac{1}{2}\sum_{ij} V_{ij}$$

- Let i,j,k,l denote occupied states and m,n,o,p unoccupied states
- After substituting back we get

$$\langle m|T|i\rangle + \sum_j^{occupied} \langle jm|V|ji\rangle_A = 0$$

- This leads directly to the Hartree-Fock single-particle Hamiltonian h with matrix elements between any two states α and β

$$\langle \alpha|h|\beta\rangle = \langle \alpha|T|\beta\rangle + \sum_j^{occupied} \langle j\alpha|V|j\beta\rangle_A$$

$$= \langle \alpha|T|\beta\rangle + \langle \alpha|U|\beta\rangle$$

Hartree-Fock

- We now have a mechanism for defining a mean-field
  - It does depend on the occupied states
  - Also the matrix elements with unoccupied states are zero, so the first order 1p-1h corrections do not contribute

$$\langle m|T|i\rangle + \sum_{j}^{occupied}\langle jm|V|ji\rangle_A = \langle m|h|i\rangle = 0$$

- We obtain an eigenvalue equation (more on this later)

$$h|i\rangle = \varepsilon_i|i\rangle$$

$$E = \langle\Phi_0|H|\Phi_0\rangle = \sum_i\langle i|T|i\rangle + \frac{1}{2}\sum_{ij}\langle ij|V|ij\rangle_A = \frac{1}{2}\sum_i\left[\langle i|T|i\rangle + \varepsilon_i\right]$$

- Energies of A+1 and A-1 nuclei relative to A

$$E_{A+1} - E_A = \varepsilon_m \qquad E_{A-1} - E_A = -\varepsilon_i$$

Hartree-Fock – Eigenvalue equation

- Two ways to approach the eigenvalue problem
  - Coordinate space where we solve a Schrödinger-like equation
  - Expand in terms of a basis, e.g., harmonic-oscillator wave function
- Expansion
  - Denote basis states by Greek letters, e.g., α

$$|i\rangle = \sum_{\alpha} C_{i\alpha} |\alpha\rangle$$

$$\sum_{\alpha} C_{i\alpha}^{*} C_{j\alpha} = \delta_{ij} \qquad \sum_{i} C_{i\alpha}^{*} C_{i\beta} = \delta_{\alpha\beta}$$

  - From the variational principle, we obtain the eigenvalue equation

$$\sum_{\beta} \left[\langle\alpha|T|\beta\rangle + \sum_{j}^{occupied} \langle\alpha j|V|\beta j\rangle_A \right] C_{i\beta} = \varepsilon_i C_{i\alpha}$$

or

$$\sum_{\beta} \langle\alpha|h|\beta\rangle C_{i\beta} = \varepsilon_i C_{i\alpha}$$

Hartree-Fock – Solving the eigenvalue equation

- As I have written the eigenvalue equation, it doesn't look to useful because we need to know what states are occupied
- We use three steps
  1. Make an initial guess of the occupied states & the expansion coefficients $C_{i\alpha}$
     - For example the lowest Harmonic-oscillator states, or a Woods-Saxon and $C_{i\alpha}=\delta_{i\alpha}$
  2. With this ansatz, set up the eigenvalue equations and solve them
  3. Use the eigenstates $|i\rangle$ from step 2 to make the Slater determinant Φ_0, go back to step 2 until the coefficients $C_{i\alpha}$ are unchanged

The Hartree-Fock equations are solved self-consistently

Hartree-Fock – Coordinate space

- Here, we denote the single-particle wave functions as $\phi_i(\mathrm{r})$

$$-\frac{\hbar^2}{2m}\nabla_1^2\phi_i(\mathbf{r}_1)+\underbrace{\left(\sum_j^{occupied}\int \phi_j^*(\mathbf{r}_2)V(|\mathbf{r}_1-\mathbf{r}_2|)\phi_j(\mathbf{r}_2)d^3r_2\right)}_{\text{Direct or Hartree term: } U_H}\phi_i(\mathbf{r}_1)-\underbrace{\sum_j^{occupied}\int \phi_j^*(\mathbf{r}_2)V(|\mathbf{r}_1-\mathbf{r}_2|)\phi_j(\mathbf{r}_1)\phi_i(\mathbf{r}_2)d^3r_2}_{\text{Exchange or Fock term: } U_F}=\varepsilon_i\phi_i(\mathbf{r}_1)$$

- These equations are solved the same way as the matrix eigenvalue problem before
  1. Make a guess for the wave functions $\phi_i(\mathrm{r})$ and Slater determinant Φ_0
  2. Solve the Hartree-Fock differential equation to obtain new states $\phi_i(\mathrm{r})$
  3. With these go back to step 2 and repeat until $\phi_i(\mathrm{r})$ are unchanged

Again the Hartree-Fock equations are solved self-consistently

Hartree-Fock

Hard homework problem:

- M. Moshinsky, Am. J. Phys. 36, 52 (1968). Erratum, Am. J. Phys. 36, 763 (1968).
- Two identical spin-1/2 particles in a spin singlet interact via the Hamiltonian

$$H = \tfrac{1}{2}\left(p_1^2 + r_1^2\right) + \tfrac{1}{2}\left(p_2^2 + r_2^2\right) + \chi\left[\tfrac{1}{\sqrt{2}}\left(\vec{r}_1 - \vec{r}_2\right)^2\right]$$

- Use the coordinates $\vec{r} = \left(\vec{r}_1 - \vec{r}_2\right)/\sqrt{2}$ and $\vec{R} = \left(\vec{r}_1 + \vec{r}_2\right)/\sqrt{2}$ to show the exact energy and wave function are

$$E = \tfrac{3}{2}\hbar\left(1 + \sqrt{2\chi + 1}\right)$$

$$\Psi(r,R) = \frac{1}{(\pi\hbar)^{3/4}} \exp\left(-R^2/2\hbar\right)\left(\frac{\sqrt{2\chi+1}}{\pi\hbar}\right)^{3/4} \exp\left(-\frac{\sqrt{2\chi+1}}{2\hbar} r^2\right)$$

- Note that since the spin wave function (S=0) is anti-symmetric, the spatial wave function is symmetric

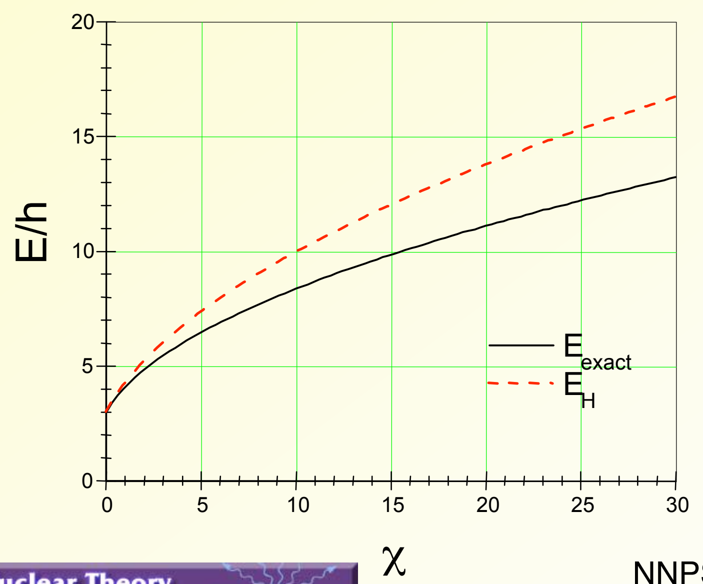
Hartree-Fock

Hard homework problem:

- The Hartree-Fock solution for the spatial part is the same as the Hartree solution for the S-state. Show the Hartree energy and radial wave function are:

$$E_H = 3\hbar\sqrt{\chi+1}$$

$$\Psi(r_1,r_2) = \left(\frac{\sqrt{\chi+1}}{\pi\hbar}\right)^{3/2} \exp\left(-\frac{\sqrt{\chi+1}}{2\hbar} r_1^2\right)\exp\left(-\frac{\sqrt{\chi+1}}{2\hbar} r_2^2\right)$$



Hartree-Fock with the Skyrme interaction

- In general, there are serious problems trying to apply Hartree-Fock with realistic NN-interactions (for one the saturation of nuclear matter is incorrect)
- Use an effective interaction, in particular a force proposed by Skyrme

$$v_{12} = t_0(1 + x_0 P_\sigma)\delta(\vec{r}_1 - \vec{r}_2) + \frac{1}{2} t_1 (1 + x_1 P_\sigma)\left[\delta(\vec{r}_1 - \vec{r}_2)\frac{1}{2i}\left(\vec{\nabla}_1^2 - \vec{\nabla}_2^2\right) + \frac{1}{2i}\left(\overleftarrow{\nabla}_1^2 - \overleftarrow{\nabla}_2^2\right)\delta(\vec{r}_1 - \vec{r}_2)\right] +$$
$$t_2(1 + x_2 P_\sigma)\frac{1}{2i}\left(\overleftarrow{\nabla}_1 - \overleftarrow{\nabla}_2\right)\cdot\delta(\vec{r}_1 - \vec{r}_2)\frac{1}{2i}\left(\vec{\nabla}_1 - \vec{\nabla}_2\right) + W_0(\vec{\sigma}_1 + \vec{\sigma}_2)\cdot\frac{1}{2i}\left(\overleftarrow{\nabla}_1 - \overleftarrow{\nabla}_2\right)\times\delta(\vec{r}_1 - \vec{r}_2)\frac{1}{2i}\left(\vec{\nabla}_1 - \vec{\nabla}_2\right) +$$
$$t_3\delta(\vec{r}_1 - \vec{r}_2)\delta(\vec{r}_2 - \vec{r}_3)$$

  - P_σ is the spin-exchange operator
- The three-nucleon interaction is actually a density dependent two-body, so replace with a more general form, where α determines the incompressibility of nuclear matter

$$\frac{1}{6} t_3 (1 + x_3 P_\sigma)\delta(\vec{r}_1 - \vec{r}_2)\rho^\alpha\left((\vec{r}_1 + \vec{r}_2)/2\right)$$

Hartree-Fock with the Skyrme interaction

- One of the first references: D. Vautherin and D.M. Brink, PRC 5, 626 (1972)
- Solve a Schrödinger-like equation

$$\left[-\vec{\nabla}\cdot\frac{\hbar^2}{2m^*_{\tau_z}(\vec{\mathrm{r}})}\vec{\nabla}+U_{\tau_z}(\vec{\mathrm{r}})-i\vec{W}_{\tau_z}(\vec{\mathrm{r}})\cdot\left(\vec{\nabla}\times\vec{\sigma}\right)\right]\phi^i_{\tau_z}(\vec{\mathrm{r}})=\varepsilon_i\phi^i_{\tau_z}(\vec{\mathrm{r}})$$

τ_z labels protons or neutrons

  - Note the effective mass m^*

$$\frac{\hbar^2}{2m^*_{\tau_z}(\vec{\mathrm{r}})}=\frac{\hbar^2}{2m}+\frac{1}{4}(t_1+t_2)\rho(\vec{\mathrm{r}})+\frac{1}{8}(t_2-t_1)\rho_{\tau_z}(\vec{\mathrm{r}})$$

  - Typically, $m^* < m$, although it doesn't have to, and is determined by the parameters t_1 and t_2
    - The effective mass influences the spacing of the single-particle states
    - The bias in the past was for $m^*/m \sim 0.7$ because of earlier calculations with realistic interactions

Hartree-Fock calculations

- The nice thing about the Skyrme interaction is that it leads to a computationally tractable problem
  - Spherical (one-dimension)
  - Deformed
    - Axial symmetry (two-dimensions)
    - No symmetries (full three-dimensional)
- There are also many different choices for the Skyrme parameters
  - They all do some things right, and some things wrong, and to a large degree it depends on what you want to do with them
  - Some of the leading (or modern) choices are:
    - M^*, M. Bartel *et al.*, NPA386, 79 (1982)
    - SkP [includes pairing], J. Dobaczewski and H. Flocard, NPA422, 103 (1984)
    - SkX, B.A. Brown, W.A. Richter, and R. Lindsay, PLB483, 49 (2000)
    - Apologies to those not mentioned!
  - There is also a finite-range potential based on Gaussians due to D. Gogny, D1S, J. Dechargé and D. Gogny, PRC21, 1568 (1980).
- Take a look at J. Dobaczewski *et al.*, PRC53, 2809 (1996) for a nice study near the neutron drip-line and the effects of unbound states

Nuclear structure

- Remember what our goal is:
  - To obtain a quantitative description of all nuclei within a microscopic frame work
  - Namely, to solve the many-body Hamiltonian:

$$H = \sum_i \frac{\vec{p}_i^{\,2}}{2m} + \sum_{i<j} V_{NN}\left(\vec{r}_i - \vec{r}_j\right) \longrightarrow H = \sum_i \left(\frac{\vec{p}_i^{\,2}}{2m} + U(r_i)\right) + \underbrace{\sum_{i<j} V_{NN}\left(\vec{r}_i - \vec{r}_j\right) - \sum_i U(r_i)}_{\text{Residual interaction}}$$

Perturbation Theory

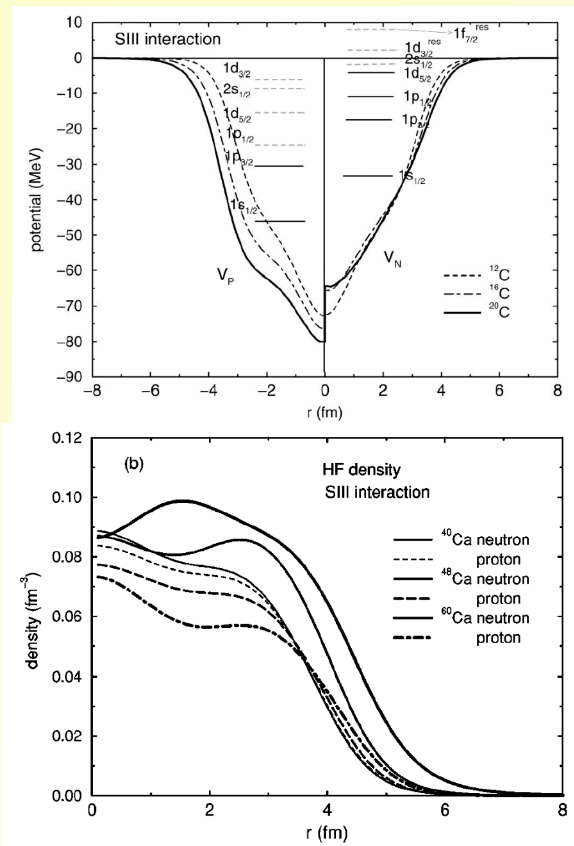
Nuclear structure

- Hartree-Fock is the optimal choice for the mean-field potential *U(r)*!
  - The Skyrme interaction is an “effective” interaction that permits a wide range of studies, e.g., masses, halo-nuclei, etc.
  - Traditionally the Skyrme parameters are fitted to binding energies of doubly magic nuclei, rms charge-radii, the incompressibility, and a few spin-orbit splittings
- One goal would be to calculate masses for all nuclei
  - By fixing the Skyrme force to known nuclei, maybe we can get 500 keV accuracy that CAN be extrapolated into the unknown region
    - This will require some input about neutron densities – parity-violating electron scattering can determine $\langle r^2 \rangle_p - \langle r^2 \rangle_n$.
  - This could have an important impact

Hartree-Fock calculations

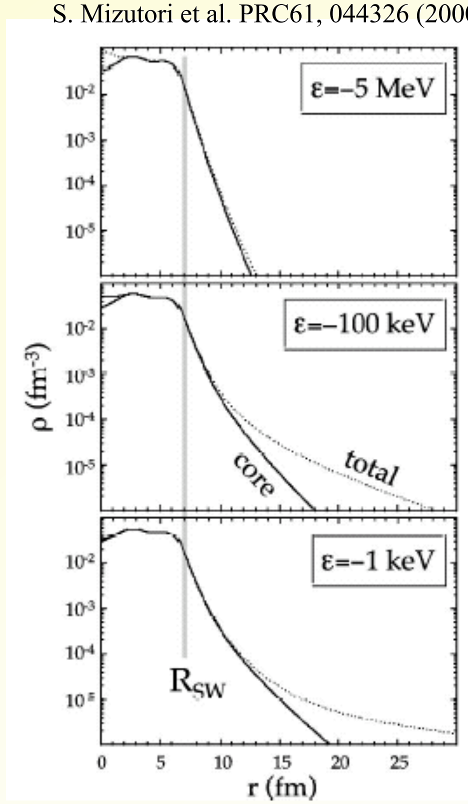
- Permits a study of a wide-range of nuclei, in particular, those far from stability and with exotic properties, halo nuclei

H. Sagawa, PRC65, 064314 (2002)



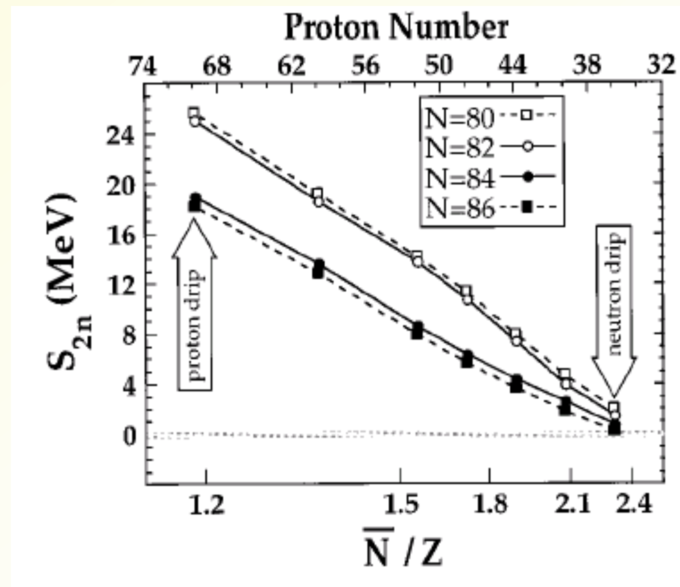
The tail of the radial density depends on the separation energy

S. Mizutori et al. PRC61, 044326 (2000)



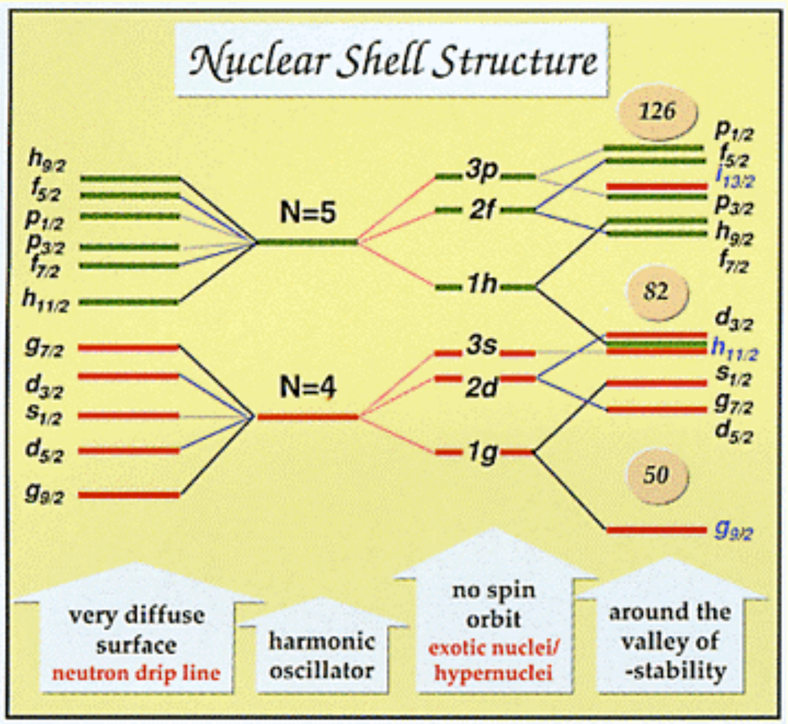
Drip-line studies

J. Dobaczewski *et al.*, PRC53, 2809 (1996)



What can Hartree-Fock calculations tell us about shell structure?

- Shell structure
  - Because of the self-consistency, the shell structure can change from nucleus to nucleus



J. Dobaczewski *et al.*, PRC53, 2809 (1996)

As we add neutrons, traditional shell closures are changed, and may even disappear!

This is <u>THE</u> challenge in trying to predict the structure of nuclei at the drip lines!

Beyond mean field

- Hartee-Fock is a good starting approximation
  - There are no particle-hole corrections to the HF ground state

$$\langle m|T|i\rangle + \sum_{j}^{occupied} \langle jm|V|ji\rangle_A = \langle m|h|i\rangle = 0$$

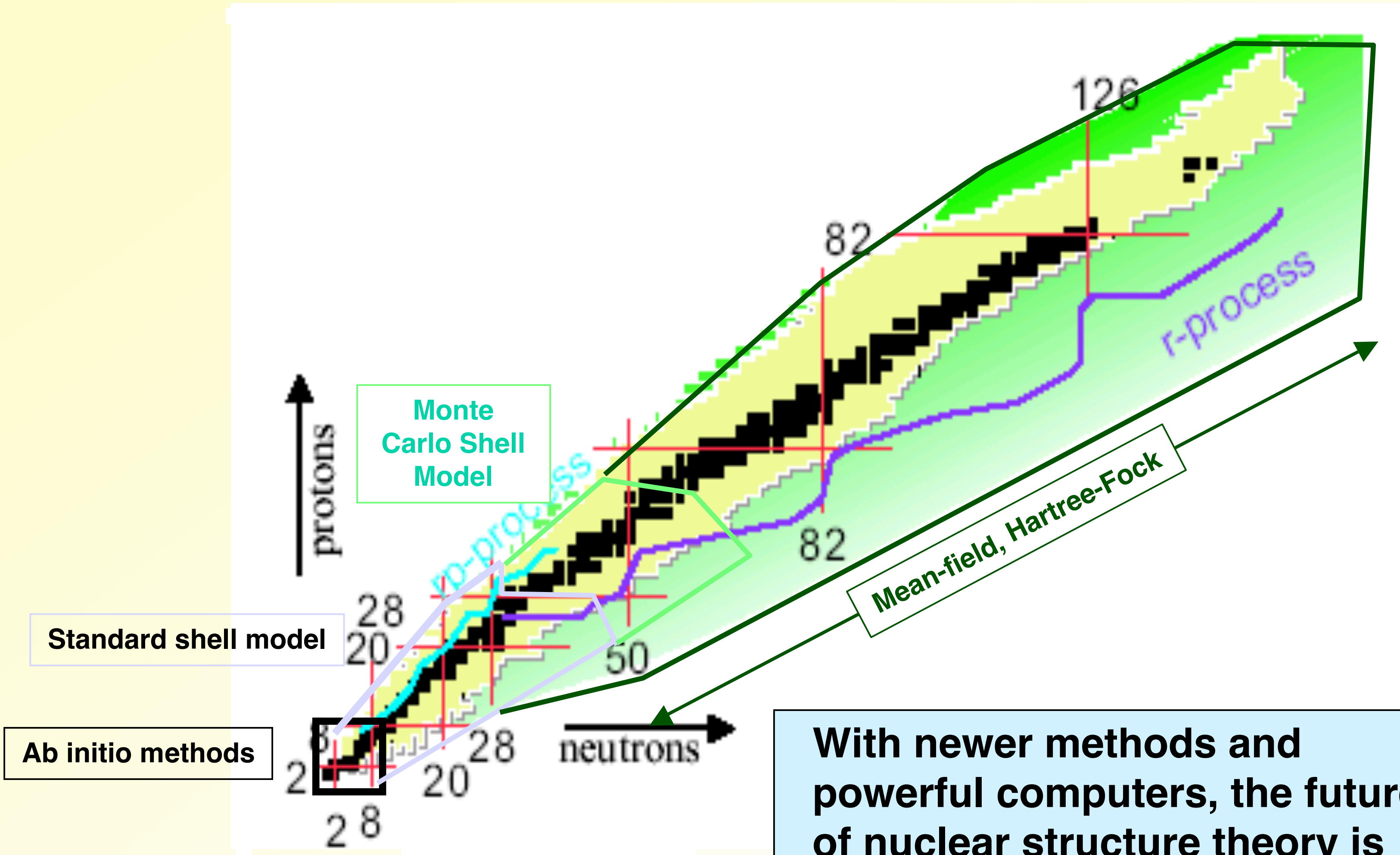
  - The first correction is

$$\frac{1}{4}\sum_{ijmn} \frac{\langle ij|V|mn\rangle_A \langle mn|V|ij\rangle_A}{\varepsilon_i + \varepsilon_j - \varepsilon_m - \varepsilon_n}$$

- However, this doesn't make a lot of sense for Skyrme potentials
  - They are fit to closed-shell nuclei, so they effectively have all these higher-order corrections in them!
- We can try to estimate the excitation spectrum of one-particle-one-hole states – Giant resonances
  - Tamm-Dancoff approximation (TDA)
  - Random-Phase approximation (RPA)

You should look these up!
A Shell Model Description of Light Nuclei, I.S. Towner
The Nuclear Many-Body Problem, Ring & Schuck

Nuclear structure in the future



With newer methods and powerful computers, the future of nuclear structure theory is bright!