Rev. 2 answers
p. 29 'is wf a Slater determinants?'
on p. 37 'wf is a linear combination of Slater determinants'

Obertelli and Sagawa page 100 give simple argument
for $\boldsymbol{d}$ binding with the tensor force
inputs:
permutation symmetry
and thus which variations of $\vec{\sigma} \cdot \vec{r}$ are favored
outputs:
the binding of the $\boldsymbol{d}$
the sign of its quadrupole moment

p.s. there's a caveat for 1/Nc expansion in updated notes for Lecture 6:
it fails badly for certain $\boldsymbol{K}$ decays to π's, the 'ΔI = 1/2' rule

Independent particle picture; Structure A$\leq$8 + Permutation symmetry; DFT

- **Independent particle approximation**
  Motivation for single-particle motion in mean field
  Harmonic oscillator wavefunctions
  Deformation sans microscopic calculation: Nilsson model

Refs: Wong Ch. 7, Obertelli+Sagawa Ch. 7

- **Structure of light nuclei A$\leq$8:**
  Delineation and ordering of most states with
  Simple rules (no detailed interactions...)+
  Systematic accounting of permutation symmetry with Young diagrams

- **Calculating mean field: Wong 7.3; Obertelli+Sagawa Ch. 3.5,3.6 remains a major challenge**
Describe/sketch Hartree-Fock: based on a variational principle that gets g.s. energy right for a given Hamiltonian
Describe/sketch Energy Density Functionals which are tuned substantially
Goal: some feel for inputs, outputs, successes and challenges of mean field calculations

A.B. will give 2 lectures on from first-principles calculations after the midterm

Independent particles moving in their average field: qualitative support

- **Bohr and Mottleson p. 189:**

Mean free path larger than nucleon spacing $\rightarrow \approx$ validity of Fermi gas model.

Mean free path larger than the nucleus leads to regularities of quantized orbits of individual nucleons

O&S: zero-point energy fluctuation:

$$\Delta E = \frac{(\delta p)^2}{2m} \sim \frac{\hbar^2}{m(\Delta x)^2} \sim \frac{\hbar^2}{m r_c^2}$$

For a molecule, $V \sim \frac{e^2}{a} \sim \hbar^2 m_e a^2$ **with**

$$a_{\mathrm{Bohr}} = \frac{\hbar^2}{m_e e^2}$$

Molecule: $\Delta E/V \sim 1/2000$;

Deuteron: $\Delta E/B_n \sim 100$.

$\rightarrow$ **atoms in molecules are confined and somewhat classical;**

nucleons in nuclei are nearly unbound and can be treated as moving in an average potential

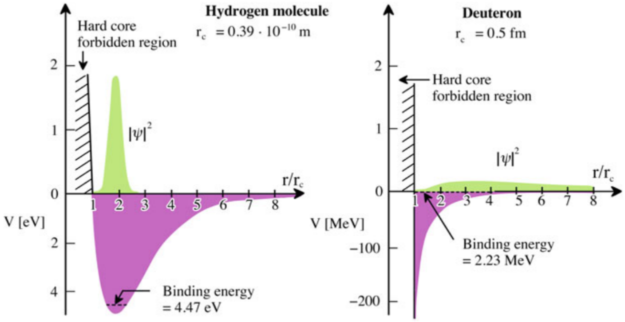


Fig. 7.1 Molecular and nuclear potentials and corresponding wave functions of diatomic molecule

Nuclear observable discontinuities

Like chemistry's electron shell model, near-degeneracy of the single-particle orbits leads to discontinuities in nuclear properties:

Binding energies wrt liquid drop:

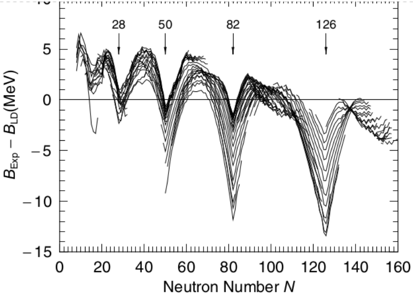


Fig. 5.1 Deviation of experimental masses from theoretical predictions based on the liquid-drop mass formula which does not contain any quantum information on the nuclear shell structure. The deviation is plotted as a function of the neutron number and shows a clear over binding at magic numbers 28, 50, 82 and 126. The modern version of the macroscopic model FRDM2012 is adopted as the liquid-drop binding energy $B_{\rm LD}$ [1]. Courtesy P. Möller

(O&S credit Möller)

Goeppert Mayer's Nobel Lecture: "Failures of the shell model" ☹

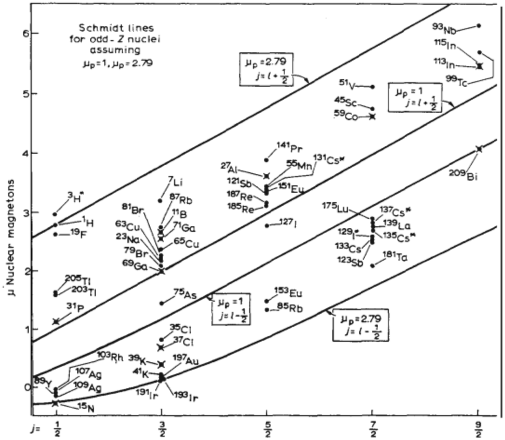


Fig. 8. Magnetic moments of nuclei with odd proton, even neutron number.

$$\frac{\mu_{\rm s.p.}}{\mu_{\rm nm}} = j\left(g_l \pm \frac{g_s - g_l}{2l+1}\right) \text{ for } j = l \pm \frac{1}{2} \qquad \text{W4-53}$$

(Simple expression for odd-N odd-Z couples 2 μ's given J)

Wong: complications away from closed shells:

complex configurations; MEC's; nucleon g_s changing in medium ☹

Prediction even-Z odd-N: $\mu \approx \pm\mu_{\rm neutron}$ →

$$\frac{\mu_{\rm s.p.}}{\mu_{\rm nm}} = j(g_l \pm \frac{g_s - g_l}{2l+1}) \text{ for } j = l \pm \frac{1}{2}$$ W4-53

- $\pi(d_{3/2})$ cancels spin, orbital $\rightarrow \mu_{\rm s.p.}$=0.1245

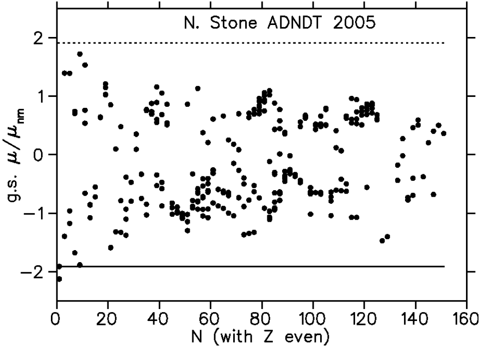
^{35,37,39,41,43,45}K, $J^\pi = 3/2^+$: μ/μ_{nm} = 0.16 to 0.39

^{33,35,37}Cl, $J^\pi = 3/2^+$: μ/μ_{nm} = 0.68 to 0.82

- Since *n* has no electric charge,

g_l=0 for *n*, and single-particle model has a simple prediction for odd-N, even Z: $\mu_{\rm s.p.} \approx \mp\mu_{\rm neutron}$

$|\mu_{\rm oddNevenZ}|$ falls with A, i.e. complexity?
Some restoration near closed shells?:
the N=126 values are from Pb closed shell Z=82.



- Rather than look at these for changes in g_S in the medium, people look at isoscalar combinations of isobaric mirror nuclei.

We looked in detail at μ in A=3, and isoscalar combination of isobaric mirror μ being free of meson exchange currents.
This is related to G-T strength, see β decay later

Harmonic oscillator wf's

The simplest mean-field potentials include:
simple square well potential;
harmonic oscillator approximating this.
1-body hamiltonian:
Wong Eq. 7-11 $h(r) = -\frac{\hbar^2}{2\mu}\nabla^2 + \frac{1}{2}\mu\omega_o^2 r^2$
(r nucleon coordinate, μ **its reduced mass)**
States are degenerate with energy
$\epsilon_N = (N + \frac{3}{2})\hbar\omega_0$ **and allowed orbital angular momenta** $l = N, N-2, \ldots 1$ **or 0, parity** $(-1)^l$

Table 7-1: Harmonic oscillator radial wave functions.

$R_{1s}(r) = 2\left(\frac{\nu^3}{\pi}\right)^{1/4} e^{-\nu r^2/2}$	$R_{1p}(r) = \sqrt{\frac{2^3}{3}}\left(\frac{\nu^5}{\pi}\right)^{1/4} r e^{-\nu r^2/2}$
$R_{1d}(r) = \sqrt{\frac{2^4}{15}}\left(\frac{\nu^7}{\pi}\right)^{1/4} r^2 e^{-\nu r^2/2}$	$R_{2s}(r) = \sqrt{\frac{2^3}{3}}\left(\frac{\nu^3}{\pi}\right)^{1/4} (\frac{3}{2} - \nu r^2)\, e^{-\nu r^2/2}$
$R_{1f}(r) = \sqrt{\frac{2^5}{105}}\left(\frac{\nu^9}{\pi}\right)^{1/4} r^3 e^{-\nu r^2/2}$	$R_{2p}(r) = \sqrt{\frac{2^4}{15}}\left(\frac{\nu^5}{\pi}\right)^{1/4} (\frac{5}{2} - \nu r^2)\, r e^{-\nu r^2/2}$
$R_{1g}(r) = \sqrt{\frac{2^6}{945}}\left(\frac{\nu^{11}}{\pi}\right)^{1/4} r^4 e^{-\nu r^2/2}$	$R_{2d}(r) = \sqrt{\frac{2^5}{105}}\left(\frac{\nu^7}{\pi}\right)^{1/4} (\frac{7}{2} - \nu r^2)\, r^2 e^{-\nu r^2/2}$
$R_{3s}(r) = \sqrt{\frac{2^3}{15}}\left(\frac{\nu^3}{\pi}\right)^{1/4} (\frac{15}{4} - 5\nu r^2 + \nu^2 r^4)\, e^{-\nu r^2/2}$	

Note: As approximate single-particle wave functions for a nucleus, the oscillator parameter, $\nu = m\omega_0/\hbar$, may be taken to be $A^{-1/3}$ femtometers squared.

Harmonic oscillator wavefunctions provide for some operators analytic solutions for computation. A useful basis for computation of many-body systems where 10^N **integrals may be needed to diagonalize a Hamiltonian.**
Woods-Saxon potential $h(r) = \frac{-V_0}{1+e^{(r-R)/a}}$ **with, e.g.,** R**=1.25A**$^{1/3}$**,** a**=0.524 fm has same shells, with better numerical wf's with longer tails**
There is a smooth potential with analytic wf's Ginocchio Ann Phys 159 467 (1985) **which may retain utility** Pittel JPhysG 24 1461 (1998); W. Haxton, private conversation 1994

Spin-orbit term critical to get shells right

$$h(r) = -\frac{\hbar^2}{2\mu}\nabla^2 + \frac{1}{2}\mu\omega_o^2 r^2 + a(A)\vec{s}\cdot\vec{l}$$

$$\epsilon_N = (N + \tfrac{3}{2})\hbar\omega_0 + \tfrac{1}{2}al \quad \text{for } j = l + \tfrac{1}{2},$$
$$-\tfrac{1}{2}a(l+1) \text{ for } j = l - \tfrac{1}{2},$$

Goeppert Mayer and Jensen (1955) Fig. IV.3 $\rightarrow$
The HO shells work up to N=Z=20 or so.

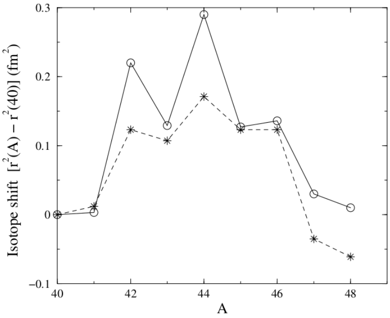
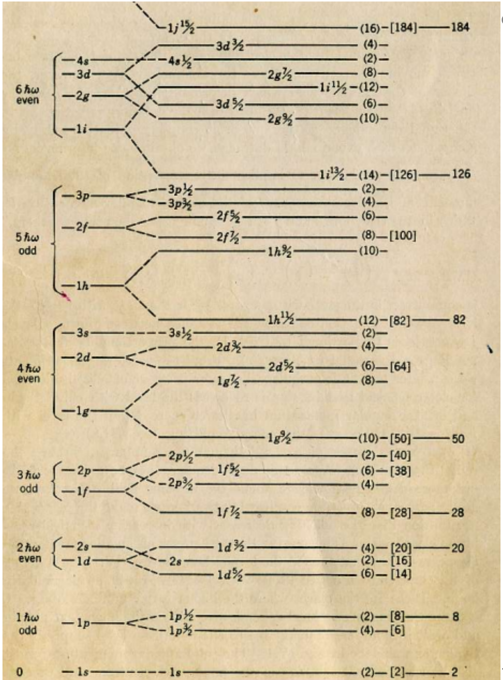


FIG. 2. Isotope shifts in calcium. The experimental data (circles connected by a solid line) and the shell model results,

The $f_{7/2}$ orbital is needed for closed-shell behavior of $^{48}_{20}Ca^{28}$ (and $^{56}_{28}Ni^{28}$). **Caurier PLB 522 240 (2001)**



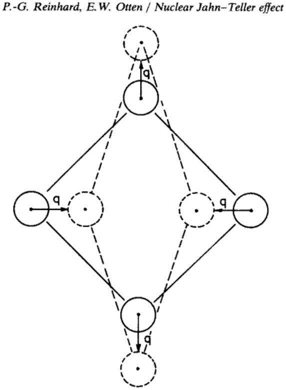
Deformation and symmetry

Jahn-Teller theorem: Jahn, Teller 1937

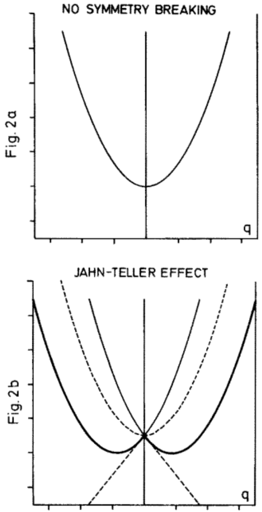
Symmetry-driven degenerate electron states in (“nonlinear”) molecules are not stable: small perturbations will cause an instability toward states with lower degeneracy and less symmetry.
The symmetry is said to be spontaneously broken, by deformation (among other things)

Reinhard, Otten NPA420 173 (1984)

An interaction linear in deformation q removes degeneracy for $q \neq 0$, driving to a less symmetric ground state.



Molecule with $E \propto q^2$, invariant under 90°



“we conclude from this parallelism in molecular and nuclear physics that spontaneous symmetry breaking by the Jahn-Teller effect is a general feature of many-body systems which provides a linear coupling between their microscopic and collective degrees of motion.”

(Other ways to remove the degeneracy produce variations)

Nilsson model

Deformation is complex to calculate microscopically.
Nilsson model describes it:
3D harmonic oscillator with different-size axes, fixed phenomenologically, so with axial symmetry:

$$h = \frac{p^2}{2m} + \frac{1}{2}\mu(\omega_z^2 z^2 + \omega_\perp^2(x^2+y^2)) + \nu_{ll}\hbar\omega_o(\vec{l}^2 - \langle \vec{l}^2\rangle) + \nu_{ls}\hbar\omega_o(\vec{l}\cdot\vec{s})$$

For x,y,z coordinates remember

$$E = (n_x + n_y + n_z + \tfrac{3}{2})\hbar\omega$$

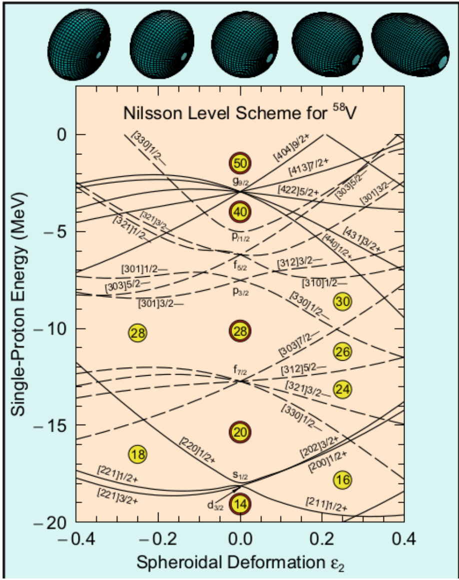
Here, $E = (n_z + \frac{1}{2})\hbar\omega_z + (n_\perp + 1)\hbar\omega_\perp$

so E **changes with deformation** $\rightarrow$

States at large deformation labelled by $[N, n_z, \Lambda]\Omega$ **with**
n_z **the number of quanta along the z-axis,**
Λ **the projection of the orbital angular momentum along the z-axis, and**
Ω **the projection of the total angular momentum along the z-axis**

ψ_{Nilsson} **can be expanded in spherical** ψ_{HO}

classical: Chandrasekhar "Ellipsoidal Figures of Equilibrium"



O&S credit P. Möeller and T. Ichikawa

• Structure of light nuclei:
Systematic accounting of permutation symmetry with Young diagrams

Coupling one to four valence-shell nucleons describes many low-lying $J^\pi; T$ states in light nuclei + dominant L configuration (decays, reactions...)

• Simple guidelines on configurations with lowest energy then reproduce lowest level order

Strong interaction, because it's short range and attractive, favors symmetric and lowest L

For a given L, spin-orbit $\vec{L} \cdot \vec{S}$ favors largest J

Demonstrative examples, not proofs. Some naive states will be ruled out. Few explicit (anti)symmeterized $\psi' s$: instead arguments for their existence.
A=6,5,4,7,8 'Conspiracy' against $(S; T) = (3/2, 3/2)$

Refs. Bohr and Mottleson Appendix 1C; (EGA UW Phys562); PDG;
de-Shalit and Talmi, Nuclear Shell Theory (Dover) Ch. 32 "The Group Theoretical...";
Frank Close "Intro to Quarks and Partons" for more general Young techniques

Young Tableaux: systematic delineation of permutation symmetry.

No formal proofs here: just rules

Example

$$\begin{array}{|c|c|}\hline 1 & 2 \\ \hline 3 \\ \cline{1-1}\end{array}$$

Diagram of permutations of *n* objects

In each box is a label for the state: here just the 1st, 2nd, 3rd object; labels are in arbitrary order, but must keep that order

Rows are symmetric under permutation: this example is symmetric for first 2 objects

Columns antisymmetric under permutation

Labels can't decrease going $\rightarrow$ in any row

Labels can't decrease going $\downarrow$ in any column

Can't have same labels in any 2 elements (boxes) in any column (but can duplicate in rows)

Young Tableaux example: A=3 system

$\psi_{\text{space}}\psi_{\text{spin}}\psi_{\text{isospin}}$ **must be antisymmetric**

ψ_{space}

Consider states where all 3 nucleons have L=0

No sublevels: must be symmetric, i.e.

$\psi_S(1)\psi_S(2) - \psi_S(2)\psi_S(1) = 0$

1	2	3

ψ_{spin}

We had mixed symmetry

1	2
3	

ψ_{isospin}

We had mixed symmetry

1	3
2	

We've laid these functions out previously– we're just using these diagrams as tools to account for possibilities of number of states with various total quantum numbers and properties

or consider $\psi_{\text{isospin}}\psi_{\text{spin}}$ together for one example (it's ok– we're just changing our labels without explicitly writing it...) and writing the antisymmetric diagram filled with 3 out of 4 states:

1
2
3

Can we have S=3/2 T=1/2?

(Remember Δ(1232) S=3/2 t=3/2 is symmetric)

Evaluate by considering A=3 as a 'hole' in the A=4 system $\rightarrow$

A=3 allowed spin, isospin

$$\begin{array}{|c|}\hline 1 \\ \hline 2 \\ \hline 3 \\ \hline \end{array}$$

S=? T=?

Consider A=4

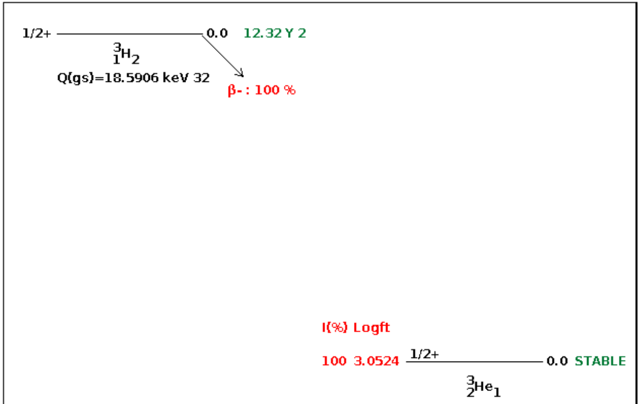
$$\begin{array}{|c|}\hline 1 \\ \hline 2 \\ \hline 3 \\ \hline 4 \\ \hline \end{array}$$

4 is the maximum number of particles to be put into 4 states. Closed shell. Totally antisymmetric. S=0, T=0.

Then

$$\begin{array}{|c|}\hline 1 \\ \hline 2 \\ \hline 3 \\ \hline \end{array} \quad = \quad \begin{array}{|c|}\hline 1 \\ \hline 2 \\ \hline 3 \\ \hline 4 \\ \hline \end{array} \quad - \quad \begin{array}{|c|}\hline \\ \hline \end{array}$$

S=?, T=? S=0, T=0 $S = \frac{1}{2}$, $T = \frac{1}{2}$



$(S, T) = (\frac{1}{2}, \frac{1}{2})$ only, no $(\frac{3}{2}, \frac{3}{2})$

These are the only A=3 bound states.

There are no experimentally known unbound resonances.

There are theoretical possibilities for unbound resonances in the 3 proton and 3 neutron systems.

One antisymmetric wf in S, T i.e. spin, isospin for 4 nucleons

One reason we're considering S, T together here: there is no simple product wf $\psi_S \psi_T$ antisymmetric for 4 nucleons. They must be built from mixed symmetry in S and mixed symmetry in T.

L. Cohen Nucl Phys 20 690 (1960) contructs three $L = 0$ functions with appropriate antisymmetry, building the S, T i.e. spin,isospin parts from mixed permutation symmetry terms similar to H&M. One is a Slater determinant for 4 particle wf's a, b, c, d in slots numbered i=1,4, which is completely antisymmetric under particle exchange:

$$\begin{vmatrix} \phi_a(1) & \phi_a(2) & \phi_a(3) & \phi_a(4) \\ \phi_b(1) & \phi_b(2) & \phi_b(3) & \phi_b(4) \\ \phi_c(1) & \phi_c(2) & \phi_c(3) & \phi_c(4) \\ \phi_d(1) & \phi_d(2) & \phi_d(3) & \phi_d(4) \end{vmatrix}$$

defining $\phi_a = |p\uparrow\rangle$, $\phi_b = |p\downarrow\rangle$, $\phi_a = |n\uparrow\rangle$, $\phi_a = |n\downarrow\rangle$ one gets 24 similar terms, e.g. 1st term symmetric in 3 and 4: $\phi_a(1)\phi_b(2) * (\phi_c(3)\phi_d(4) - \phi_c(4)\phi_d(3))$= $p\uparrow p\downarrow (n\uparrow n\downarrow - n\downarrow n\uparrow)$

The next natural term in the determinant is symmetric in 2 and 4,
$-\phi_a(1)\phi_b(3)(\phi_c(2)\phi_d(4) - \phi_c(4)\phi_d(2))$ = $-p\uparrow n\uparrow p\downarrow n\downarrow + p\uparrow n\downarrow p\downarrow n\uparrow$

This is likely the ugliest possible way to write it out, but I don't think any two terms can be combined.

To show this is actually $S = 0$ and $T = 0$ requires Cohen's formalism.

JB can 'derive' the ^{3}He wf we've used from a Slater determinant, but has to fix n pointing up, which presumes the answer that p is always paired

Note tables of Δ that include t have no S=3/2, t=1/2, π=+ resonance.

Wilson 'The Excited States of the Proton' Comments Nucl. Part. Phys 1 (1967) 128

TABLE OF RESONANCES[a]

Notation	Mass (MeV)	Spin	Parity	Isotopic spin	Width (MeV)
N_α	939	1/2	+	1/2	Stable
	1688	5/2	+	1/2	110
N_γ	1518	3/2	−	1/2	105
	2190	7/2	−	1/2	200
	2650	(11/2)	−	1/2	300
	3030	(15/2)	(−)	1/2	400
	1400	1/2	+	1/2	200
	1570	1/2	−	1/2	130
	1670	5/2	−	1/2	140
	1700	1/2	−	1/2	240
Δ_δ	1236	3/2	+	3/2	120
	1920	7/2	+	3/2	200
	2420	(11/2)	+	3/2	275
	2850	(15/2)	(+)	3/2	300
	3230	(19/2)	(+)	3/2	440
	1670	1/2	−	3/2	180
	2080				40
	2190				40

The goal of an M-scheme table is to assign permutation symmetry to each possible value of L. Here is how to make one (easier with a blackboard or a pencil):

• Write all the possible combinations of *m*'s that add up to a given *M*, with all allowed symmetries under permutation following the Young diagram rules.
(When I line them up in a nice table? I'm ignoring the actual work:)

• Grouping them by permutation symmetry, assign them to an *L*. (There is likely a formal proof that all configurations for a given L must have the same permutation symmetry– it seems plausible.) Handy tricks:
(Ignore negative *M*– these are obvious from nonnegative *M* and don't add info.)

First consider "the stretched state is always symmetric" and assign the max ℓ symmetric configuration to *L* = max *M*. Find the rest of the *M*'s needed, with same symmetry, to account for that max *L*. (Then I line them up in the nice table– traditionally one just crosses them off on a blackboard).

Continue to gather all the *M*'s one needs for each *L*, all with given permutation symmetry. The rest usually shake down from there.
One gets an orphan single M=0 state that one assigns to L=0.

This is just a plausibility argument. There is likely a formal proof that this procedure gives you the correct permutation symmetry for each L.

Young Tableaux example: 'm-scheme' Consider 2 P-shell particles, each with ℓ=1

(Answer is obvious for 2 particles (A=6, 5), but we'll need this for A=7)

- **Label state boxes with $m = \ell_3$**

(Our arbitrary ordinal box labels end up kinda backwards in the simplest way to do it: $m = \ell$ is the 'first' label, $m = \ell - 1$ the 'second', $m = \ell - 2$ the 'third'...)

- **Consider all configurations possible for each $M = L_3$ (nonnegative for brevity)**
- **Account completely for these configurations with values of L, all M from same permutation symmetry configuration**

$M = 2$	$\begin{array}{\|c\|c\|}\hline 1 & 1 \\ \hline\end{array}$	$\begin{array}{\|c\|}\hline \cancel{1} \\ \hline \cancel{1} \\ \hline\end{array}$	
$M = 1$	$\begin{array}{\|c\|c\|}\hline 1 & 0 \\ \hline\end{array}$ $\begin{array}{\|c\|c\|}\hline \cancel{0} & \cancel{1} \\ \hline\end{array}$	$\begin{array}{\|c\|}\hline 1 \\ \hline 0 \\ \hline\end{array}$	
$M = 0$	$\begin{array}{\|c\|c\|}\hline 1 & -1 \\ \hline\end{array}$ $\begin{array}{\|c\|c\|}\hline \cancel{-1} & \cancel{1} \\ \hline\end{array}$	$\begin{array}{\|c\|}\hline 1 \\ \hline -1 \\ \hline\end{array}$	$\begin{array}{\|c\|c\|}\hline 0 & 0 \\ \hline\end{array}$ $\begin{array}{\|c\|}\hline \cancel{0} \\ \hline \cancel{0} \\ \hline\end{array}$
	L=2	L=1	L=0

Summary:

- **L=2, L=0 with symmetric configurations**

We'll be assuming symmetric configurations have lower energy

- **L=1 has an antisymmetric configuration.**

Note that π given by $(-1)^{\ell_1} \times (-1)^{\ell_2}$ so we don't get $\pi = -$ states with 2 p-shell nucleons

We'll need this 'm-scheme' for 3 particles for A=7

Energy Levels of Neutral Oxygen (O I)

Configuration	Term	J	Level(cm^{-1})	Ref.
$2s^2 2p^4$	^{3}P	2	0.000	MG93
		1	158.265	MG93
		0	226.977	MG93
$2s^2 2p^4$	^{1}D	2	15867.862	MG93
$2s^2 2p^4$	^{1}S	0	33792.583	MG93
$2s^2 2p^3(^4S^\circ)3s$	$^5S^\circ$	2	73768.200	MG93
$2s^2 2p^3(^4S^\circ)3s$	$^3S^\circ$	1	76794.978	MG93
$2s^2 2p^3(^4S^\circ)3p$	^{5}P	1	86625.757	MG93
		2	86627.778	MG93
		3	86631.454	MG93
$2s^2 2p^3(^4S^\circ)3p$	^{3}P	2	88631.146	MG93
		1	88630.587	MG93
		0	88631.303	MG93
$2s^2 2p^3(^4S^\circ)4s$	$^5S^\circ$	2	95476.728	MG93
$2s^2 2p^3(^4S^\circ)4s$	$^3S^\circ$	1	96225.049	MG93
$2s^2 2p^3(^4S^\circ)3d$	$^5D^\circ$	4	97420.630	MG93
		3	97420.716	MG93
		2	97420.839	MG93

Parity from orbitals. (Not total L)

$$\pi = \prod_{i=1}^{\text{unpaired}} (-1)^{\ell_i}$$

$\leftarrow$ example from atomic physics

- First ^3P has total orbital angular momentum $L = 1$ (odd), while π is from four p orbitals $(-1)^1(-1)^1(-1)^1(-1)^1 = +1$.
- Similarly, this $^5S^o$ has $L = 0$ but three p orbitals and one s, so π= -1 (thus the o label used in atomic physics)
- while same L=0 ^1S has even number of p orbitals so has π=+1

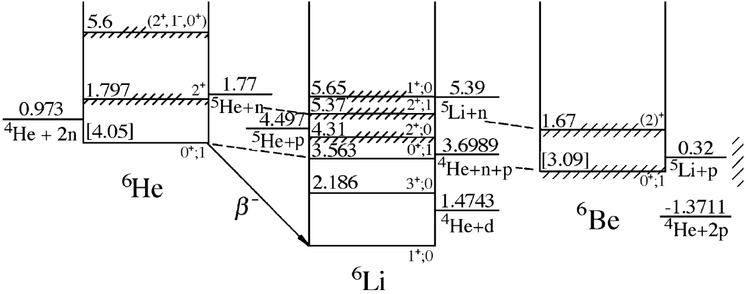
A=6 from two 1p nucleons; assume 1s shell is filled, $S = T = 0$, passive

2 particles in the 1p shell. Identify quantum numbers of partitions, couple them:

ψ_{space} $\boxed{p \mid p}$ **L=0, 2, not 1**

Yes, $\vec{1} + \vec{1}$ can be 1, but we just showed this was antisymmetric under exchange

So $\psi_{\text{spin}}\psi_{\text{isospin}}$ must be antisymmetric. For 2 particles exactly as in *d*: (S;T) = (1;0) or (0;1)



With permutation symmetry under control, couple these possibilities to $\vec{J} = \vec{L} + \vec{S}$:

$J^\pi; T$	$^{2S+1}S_J$
From L=0 "*d*-like":	
$1^+; 0$	$^3S_1$
$0^+; 1$	$^1S_1$
From L=2:	
$1^+, 2^+, 3^+; 0$	$^3D_{1,2,3}$
$2^+; 1$	$^1D_2$

For given space symmetry, lowest L tends to lie lowest

Highest *J* has lowest energy (spin-orbit $\vec{L} \cdot \vec{S}$)

All states accounted for ☺

There are $\pi = -$ (unbound) states at much higher excitation ? $\rightarrow$

$\pi = -$ states?

We found

ψ_{space} $\psi_{\text{spin-iso}}$

p
p

(S;T)= (0;0) or (1;1)

$\Rightarrow \pi = +$ for L=1.

From next shell?

p	s

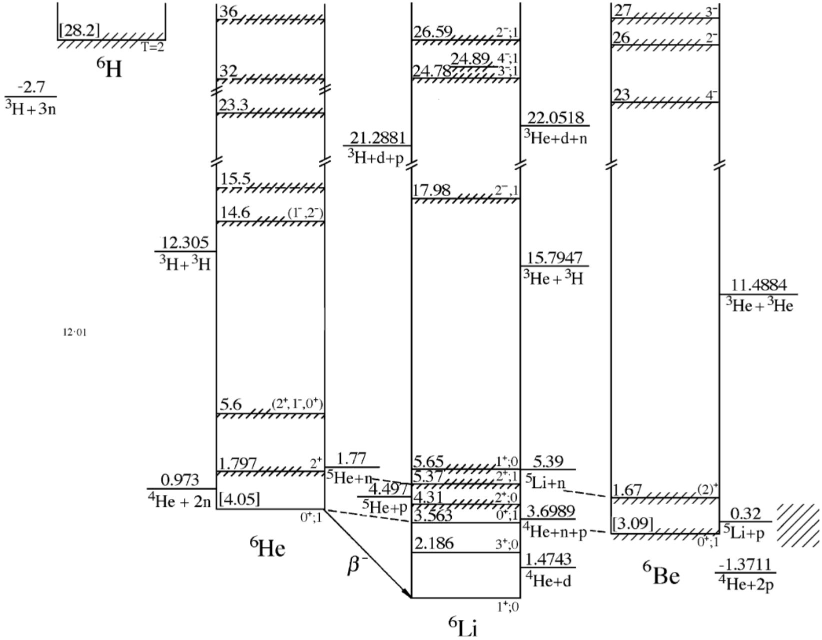
predicts J^π; T

$2^-;0$ $1^-;0$ $0^-;0$ $1^-;1$

none seen

To get 4^-, 3^-, maybe?

s	s	s
p	p	p



Tilley *et al.* **Nuclear Physics A 708 (2002) 3**

A=4: only 1 bound state

ψ_{space}

s	s	s	s

L=0

$\psi_{\text{spin}}\psi_{\text{isospin}}$

S=0, T=0

^{4}He: $J^\pi; T = 0^+; 0$

Excited states?

ψ_{space}

Since we can symmeterize anything, consider

s	s	s	p

The center of mass is moving, and this is spurious.
Abstractly:
in many bases $r\phi_s \propto \phi_p$
i.e. $\vec{r}$ $\boxed{s\,|\,s\,|\,s\,|\,s} \rightarrow \boxed{s\,|\,s\,|\,s\,|\,p}$
A serious technical issue in many shell-model and other calculations

So instead we consider

ψ_{space}

s	s	s
p		

$\rightarrow$

A=4 excited states

ψ_{space}

s	s	s
p		

L=1

$\pi = -$

$\psi_{\text{spin-isosp}}$

(S,T)=
(?,?)

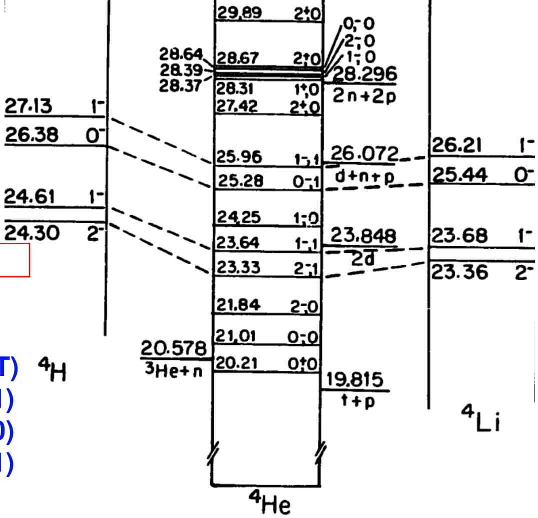
$(\frac{1}{2}, \frac{1}{2})$
(one hole)

$\otimes$ $(\frac{1}{2}, \frac{1}{2})$

= (1,1) (1,0) (0,1) (0,0)

= (0, 0) $\oplus$

$\Rightarrow$ (S;T)
(1;1)
(1;0)
(0;1)



$T = 1 \;\; {}^3P_{0,1,2}, {}^1P_1 \quad J^\pi = 0^-, 1^-, 1^-, 2^-$ ☺ exactly these are there

$T = 0 \;\; {}^3P_{0,1,2} \quad J^\pi = 0^-, 1^-, 2^-$ ☺ exactly these are there

The first 0^+, $T = 0$ state does not fit ☹: similar states exist in ^{8}Be, ^{12}C, ^{16}O, ^{40}Ca, considered 'intruder' α states from a higher (or lower, excited) shell.
Higher-lying $\pi = +$ states are ... two p particles?

A=5: no bound states

Can't have for space:

1	2	3	4	5

because would need for spin $\times$ isospin:

1
2
3
4
5

yet we only have 2 spin $\times$ 2 isospin = 4 possibilities

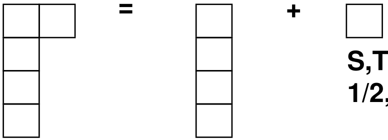
Instead we have:

space:

s	*s*	*s*	*s*
p			

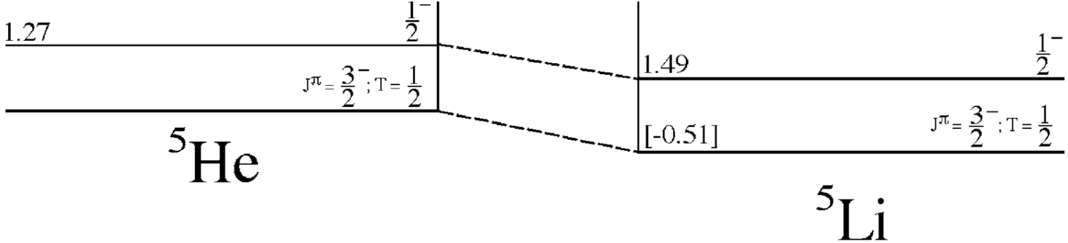
L=1 (finally, a $\pi = -$ state)

spin-isospin:



S,T= 1/2,1/2 **S,T= 0,0** **S,T= 1/2,1/2**

With antisymmeterization known ok, we can couple these possibilities:
$\vec{J} = \vec{L} + \vec{S}$ so $J^\pi; T = 1/2^-; 1/2$ and $3/2^-; 1/2$ with $^{2S+1}L_J$= $^2P_{3/2}$, $^2P_{1/2}$, and higher J lower E
Consistent with shell model, with fewer assumptions. Excited states $\rightarrow$



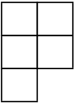
A=5 excited states

ψ_{space}

s	s	s
p	p	

L=0, 2 $\pi = +$

$\psi_{\text{spin-isospin}}$ to 'balance'



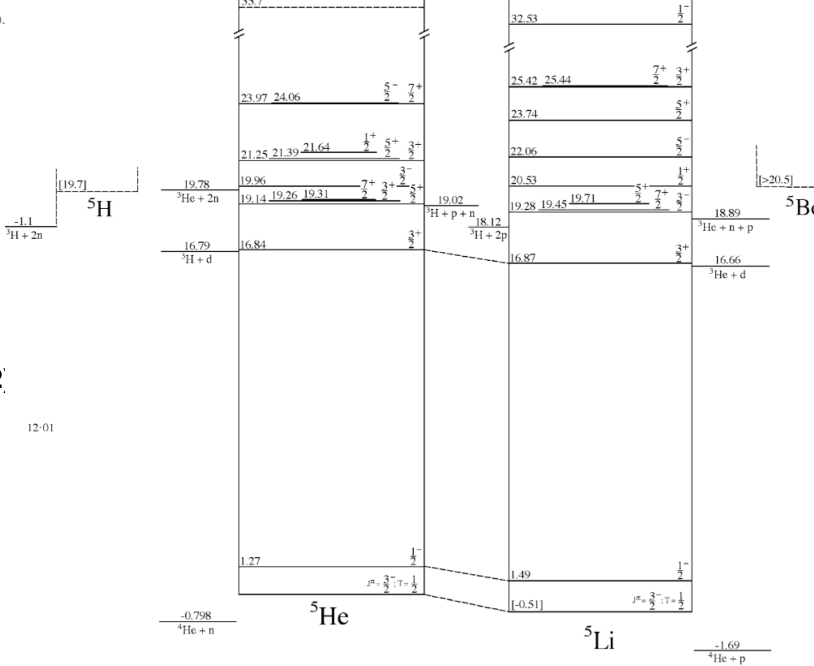
~~$(S;T) = (3/2;3/2)$~~ is fully stretched and symmetric

(S;T)=(3/2;1/2),(1/2;3/2),(1/2;1/2)

$J^\pi = 3/2^+, 1/2^+, 5/2^+, 7/2^+$ ☺

The $5/2^-$ ☹ is maybe 3 p-shell particles?

The 16.8 MeV $^4S_{3/2}$ $J^\pi = 3/2^+$ decays mostly to d not α which needs final state L=2



low-lying A=7 will have

ψ_{space}

symmetric

p	p	p

$\Rightarrow$

$\psi_{\text{spin-isosp}}$

$(S; T) = (\frac{1}{2}; \frac{1}{2})$

What L's allowed? 'm-scheme'

labels by $m = L_3$

$\leftarrow$ rows don't decrease m

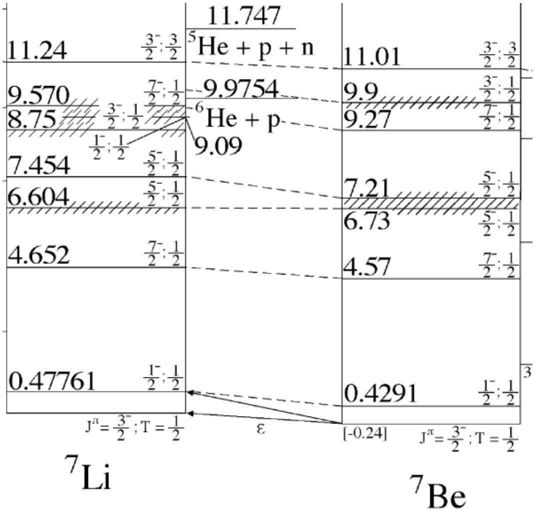
M=3	1	1	1
M=2	1	1	0
M=1	1	0	0
M=0	0	0	0

$\uparrow$ L=3

+

1	1	-1
1	0	-1

$\uparrow$ L=1



Lowest L lies lowest

For given L, highest J is lowest $^2P_{3/2}$, $^2P_{1/2}$, $^2F_{7/2}$ $^2F_{5/2}$

L=1,3 fully account for m's: No $L = 0, 2$, No $T = 3/2$. Need mixed symmetry partitions for $T = 3/2$, or for $\pi = +$ of which none are known.

A=8 low-lying states

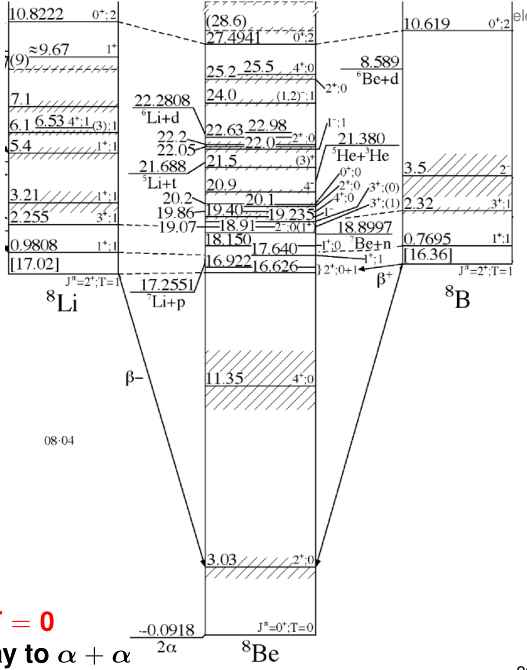
Assume inert 1s core of 4 nucleons

ψ_{space} symmetric	$\psi_{\text{spin-isosp}}$ antisymmetric
p p p p $\Rightarrow$	(single column of 4 boxes)

$M=4$	1 1 1 1	S=0,T=0		
$M=3$	1 1 1 0			
$M=2$	1 1 0 0	1 1 1 -1		
$M=1$	1 0 0 0	1 1 0 -1		
$M=0$	0 0 0 0	1 0 0 -1	1 1 -1 -1	
	L=4	L=2	L=0	

$S=0 \Rightarrow J=L$: ${}^1S_0$, ${}^1D_2$, ${}^1G_4$: 0^+, 2^+, 4^+, all $T=0$

All ^{8}Be unbound to decay to $\alpha+\alpha$



A=8 higher-lying states:

Assume inert core of four 1s nucleons

ψ_{space}

p	p	p
p		

$\Rightarrow$

Should be able to make $L = 1, 2, 3$

$\psi_{\text{spin}-\text{isosp}}$

$(S, T) = (1, 1), (1, 0), (0, 1)$

(All $\pi = +$, 4 p-shell particles)

Lowest-energy expected states:

$^3P_{0,1,2}$ $T = 1$

$^3P_{0,1,2}$ $T = 0$

$^1P_0$ $T = 1$

with highest J lowest E

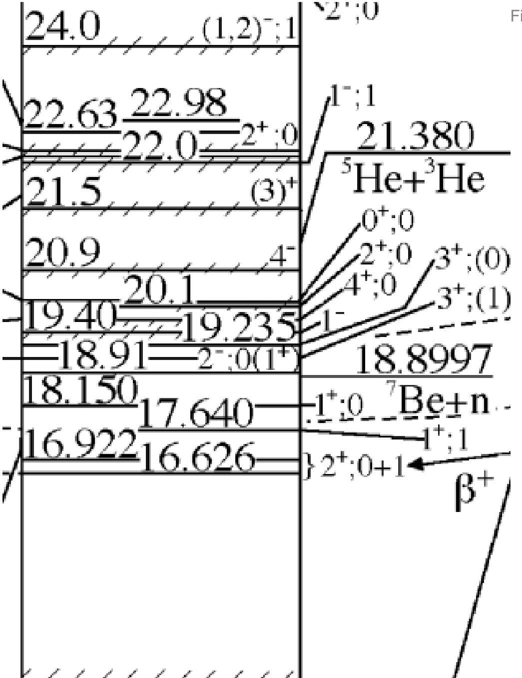
Then:

$^3D_{1,2,3}$ $T = 1$

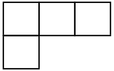
$^3D_{1,2,3}$ $T = 0$

$^1D_2$ $T = 1$

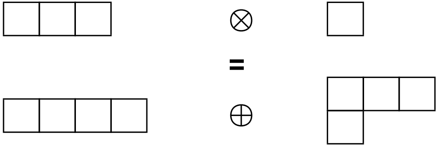
20.1 MeV 0^+; $T = 0$ has 2 possible mixed-symmetry configurations, or is partly the g.s. 2α-like configuration



Observations ^{8}Be 2^{+} T=0,1



$\leftarrow$ These configurations look like ^{7}Be+n and ^{7}Li+p $\rightarrow$



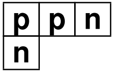
In terms of isospin, we can decompose

$$|^{7}\mathrm{Be}+n\rangle = \frac{|10\rangle+|00\rangle}{\sqrt{2}}$$

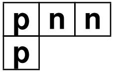
$$|^{7}\mathrm{Li}+p\rangle = \frac{|10\rangle-|00\rangle}{\sqrt{2}}$$

They would decay into these channels, except it's (slightly) energy forbidden

Can investigate by $^{7}\mathrm{Li}(d,n)^{8}\mathrm{Be}$ and (nowadays) $^{7}\mathrm{Be}(d,p)^{8}\mathrm{Be}$



$\leftarrow$ $p's$ are symmetric so closer together, Coulomb energy higher than $\rightarrow$



So the 16.92 MeV state looks more like $^{7}\mathrm{Be}+n$

Nuclear mean field model The mean field is an approximation in which each particle of a system composed of A nucleons moves in an external field (*mean field*) generated by the remaining $A - 1$ nucleons. In the HF theory, the mean field is constructed self-consistently through NN interactions. The fundamental assumption of the HF theory is an anti-symmetrized product of independent particle wave functions for A-body wave function, the so-called Slater determinant

$$\Psi_{\rm HF}(\mathbf{r_1}, \mathbf{r_2}, \cdots, \mathbf{r_A}) = \mathcal{A}\{\phi_1\phi_2\cdots\phi_A\}, \tag{3.1}$$

where $\mathcal{A}$ is the anti-symmetrization operator and ϕ_i is a single-particle wave function. The single-particle wave function $\phi_i(\mathbf{r})$ is determined by an application of variational principle. The variational principle states that the energy expectation value of the Hamiltonian is stational for a small variation of a single-particle wave function $\phi_i(\mathbf{r})$

$$\delta\langle\Psi_{\rm HF}|H|\Psi_{\rm HF}\rangle = \langle\delta\Psi_{\rm HF}|H|\Psi_{\rm HF}\rangle = 0. \tag{3.2}$$

Our A=3 configuration can be written as a Slater determinant. JB surmises we're only entangling 2 degrees of freedom, *S*, *T*.
Our premise was that almost all ground states had $\psi_{\rm space}$ symmetric, and clearly then one can write $\psi_{S,T}$ as Slater determinant.
JB surmises that our mixed symmetry space/spin/isospin terms may not be Slater determinants. Such configurations entangle three degrees of freedom.

We claimed these matched up with excited states, so to get the HF g.s. they are less important, but *L* is not a good quantum number so they can be part of g.s. ψ, too.

See final page 37 for qualifications

See R. Santra and M. Obermeyer, "A 1st encounter with the H-F self-consistent-field method," Amer Jour Phys 89 426 (2021)
Ring and Schuck "The Nuclear Many-Body Problem" works full examples, including Lipkin, Meshkov, and Glick NP 62 188 (1965) useful exactly solvable nuclear model.
Zelevinsky and Volya "Physics of Atomic Nuclei" Wiley 2017 is $0 with UBC library. Full theory formalism and great insight.
Wong 7.3 shows details deriving HF equations
JB's handwritten notes from S. Koonin's lectures, Phys 98b has a little more detail $\longrightarrow$

Moshinsky "How Good is the H-F Approximation?" Amer Jour Phys 36 52 (1968)

2 particles in common HO potential + interacting with HO force, is solvable exactly.
HF equations are also solvable analytically in 1 iteration.

$$H = \tfrac{1}{2}\,[p_1{}^2 + r_1{}^2] + \tfrac{1}{2}\,[p_2{}^2 + r_2{}^2] + \varkappa\,[1/\sqrt{2}\,(\mathbf{r}_1 - \mathbf{r}_2)]^2$$

The exact solution:

$$\psi = \pi^{-3/2}\,(2\varkappa + 1)^{3/8}\,e^{-\frac{1}{2}R^2}e^{-\frac{1}{2}(2\kappa+1)^{1/2}r^2}$$

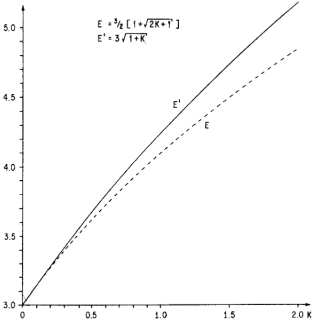
The single-particle wf's:

$$\phi_i(r_i) \propto e^{-\frac{1}{2}\sqrt{\kappa+1}r_i^2}$$

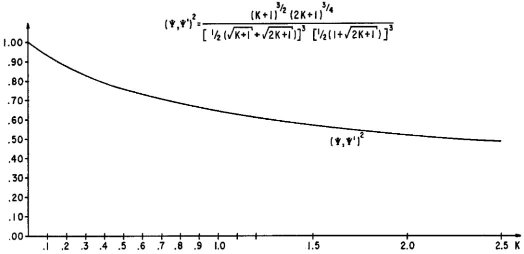
The HF solution:

$$= \pi^{-3/2}\,(\varkappa + 1)^{3/4}\,e^{-\frac{1}{2}(\kappa+1)^{1/2}(r^2+R^2)}$$

The resulting ground state energy is correct to $\sim$ 3.5% at κ=1:



The overlap between g.s. wf and HF wf is relatively poor:



Even though the wf ansatz isn't perfect, g.s. energy is given well because it's the result of a variational method.
The wf ansatz is important for convergence, but the HF method says little about the accuracy of the resulting wf, even in this simple toy system

Skyrme 1956 and Gogny 1975 forces
Optimized for H-F calculation simplicity
O&S Eq. 3.38 Parameters fit to binding energies, radii, and nuclear matter saturation properties

Contact S-wave

momentum-dependent S-wave

momentum-dependent P wave

spin-orbit

$$
\begin{aligned}
V(\mathbf{r}_1, \mathbf{r}_2) = {} & t_0(1 + x_0 P_\sigma)\delta(\mathbf{r}_1 - \mathbf{r}_2) \\
& + t_1(1 + x_1 P_\sigma)\frac{1}{2}[\delta(\mathbf{r}_1 - \mathbf{r}_2)\mathbf{k}^2 + \mathbf{k}'^2\delta(\mathbf{r}_1 - \mathbf{r}_2)] \\
& + t_2(1 + x_2 P_\sigma)\mathbf{k}' \cdot \delta(\mathbf{r}_1 - \mathbf{r}_2)\mathbf{k} \\
& + i W_0(\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2)\mathbf{k}' \times \delta(\mathbf{r}_1 - \mathbf{r}_2)\mathbf{k},
\end{aligned}
$$

Skyrme adds a contact 3-body term (approximating the Δ excitation one) that has the same effect in HF as a 2-body $\rho(r)$-dependent contact term.

Gogny included finite-range forces

$$
\begin{aligned}
V(\mathbf{r}_1, \mathbf{r}_2) = {} & \textstyle\sum_{i=1,2} e^{-(\mathbf{r}_1-\mathbf{r}_2)^2/\mu_i^2}(W_i + B_i P_\sigma - H_i P_\tau - M_i P_\sigma P_\tau) \\
& + i W_0(\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2)\mathbf{k}' \times \delta(\mathbf{r}_1 - \mathbf{r}_2)\mathbf{k} \\
& + t_3(1 + P_\sigma)\rho^{1/3}((\mathbf{r}_1 + \mathbf{r}_2)/2)\delta(\mathbf{r}_1 - \mathbf{r}_2),
\end{aligned}
$$

Resulting H-F equations from O&S:

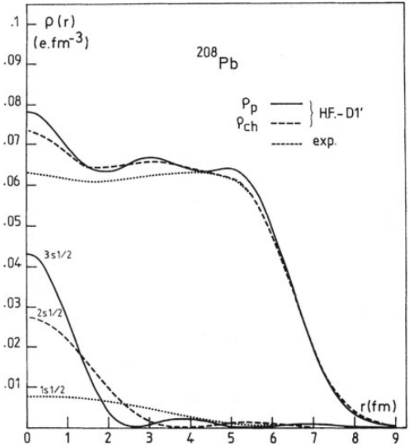
$$\frac{\delta}{\delta\phi_i}(E - \sum_i \varepsilon_i \int |\phi_i(\mathbf{r}_i)|^2 d\mathbf{r}_i) = 0, \tag{3.47}$$

where ε_i is the single-particle energy. We thus obtain the HF equation,

$$-\frac{\hbar^2}{2m}\nabla^2\phi_i(\mathbf{r}_i) + v_i^{\mathrm{HF}}(\mathbf{r_i})\phi_i(\mathbf{r}_i) = \varepsilon_i\phi_i(\mathbf{r}_i), \tag{3.48}$$

where the two-body part of the mean field potential v_i^{HF} is expressed as

$$v_i^{HF}(\mathbf{r_i}) = \sum_j \int d\mathbf{r_j}\langle ij|\widetilde{V}(\mathbf{r_i}, \mathbf{r_j})|ij\rangle + \sum_{j,k} \int d\mathbf{r_j} \int d\mathbf{r_k}\langle ijk|\widetilde{V}(\mathbf{r_i}, \mathbf{r_j}, \mathbf{r_k})|ijk\rangle. \tag{3.49}$$



"$\tilde{V}$ contains both the direct and exchange terms."

These get solved iteratively:
Compute from the ϕ_i's the mean field ν_i^{HF},
solve the Schroedinger-like equation for ϕ_i,
repeat until it converges.

Wong Fig. 7-4 has a similar result.

Outcomes: binding energies, ground-state densities, self-consistent mean fields.

Outcomes do not necessarily include good wf's.

The total energy density of the Skyrme Hamiltonian for N=Z

$$E = \sum_{i=1}^{A} < i|\frac{p_i^2}{2m}|i > + \frac{1}{2}\sum_{i,j}^{A} < ij|\widetilde{V}(\mathbf{r}_i, \mathbf{r}_j)|ij > + \frac{1}{6}\sum_{i,j,k}^{A} < ijk|\widetilde{V}(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k)|ijk >$$

$$h(\mathbf{r}) = \frac{\hbar^2}{2m}\tau^2 + A\rho^2 + B\rho^3 + C\rho\tau + D(\nabla\rho)^2 + E\rho\nabla\cdot\mathbf{J} + F\mathbf{J}^2$$

where τ and $\mathbf{J}$ are the kinetic density and the spin-orbit density, respectively.

$$\tau(\mathbf{r}) = \sum_i |\nabla^2\phi_i(\mathbf{r})|^2$$

$$\mathbf{J}(\mathbf{r}) = -i\sum_i \phi_i^*(\mathbf{r})\cdot(\nabla\phi_i(\mathbf{r})\times\boldsymbol{\sigma}) .$$

$h(r)$ is our energy density functional, an analytic function of the Skyrme parameters ☺
(motivating Skyrme interactions?)

For $N \neq Z$ use $\rho_\tau = (\rho_n - \rho_p)$

O&S version of related Kohn-Sham eqs. vary ρ and U_{eff}, not ϕ

$$\left\{-\frac{\hbar^2}{2m}\nabla^2 + U_{\text{eff}}\right\}\phi_i(\mathbf{r}) = \varepsilon_i\phi_i(\mathbf{r}), \tag{3.34}$$

i.e., the density obtained $\rho(\mathbf{r}) = \sum_i |\phi_i(\mathbf{r})|^2$ is the exact density. The energy density function is given by

$$E_{\text{KS}}[\rho,\tau] = \int d\mathbf{r}\left\{\frac{\hbar^2}{2m}\tau(\mathbf{r}) + \rho(\mathbf{r})v(\mathbf{r})\right\} + E_{\text{H}}[\rho(\mathbf{r})] + E_{\text{xc}}[\rho(\mathbf{r})], \tag{3.35}$$

where τ is the kinetic energy density. The effective single-particle potential is obtained by the functional derivative of $E_{\text{KS}} - T$ with respect to the density,

$$U_{\text{eff}} = \frac{\delta}{\delta\rho}E_{\text{H}}[\rho] + \frac{\delta}{\delta\rho}E_{\text{xc}}[\rho] + v(\mathbf{r}). \tag{3.36}$$

Kohn-Sham method

(1) determine the functional forms of $E_{\text{H}}[\rho]$ and $E_{\text{xc}}[\rho]$ at one's best,
(2) obtain an initial guess for the density $\rho_{n=0}$ ("n" is the number of iteration),
(3) calculate the effective potential U_{eff} in Eq.(3.36) with $\rho = \rho_n$,
(4) solve the Schrödinger equation (3.34) with the effective potential U_{eff} in Eq.(3.36) and obtain $\phi_i(\mathbf{r})$,
(5) calculate the density $\rho_{n+1}(\mathbf{r})$ for the next trial with the single-particle wave functions $\phi_i(\mathbf{r})$ obtained in step 4,
(6) go back to step (3) and repeat the circle steps (3)–(5) replacing ρ_n by ρ_{n+1} until convergence is achieved.

typical Energy Density Functional approach fits parameters in $h(r)$ directly to E_{binding} and, since it's natural to do, $\langle r^2\rangle$ over many nuclei.

some results of these mean field methods

Brückner-HF uses modern N-N interactions like the ones we've used before today. There are issues integrating over the hard-core repulsion.

Skyrme, Gogny, RMF are all fits to same observables

Table 3.5 Binding energies and rms charge radii of closed-shell nuclei. The BHF stands for Brückner-HF calculations with the Reid soft core potential. Skyrme and Gogny are HF results of effective interactions SIII and D1, respectively, while RMF is relativistic mean field (Hartree) calculations with NL1 interaction

Nuclei		BHF	Skyrme	Gogny	RMF	Exp.
$^{16}_{8}$O	E/A	−3.91	−7.96	−7.80	−7.95	−7.98
	r_c	2.50	2.69	2.74	2.78	2.73
$^{40}_{20}$Ca	E/A	−3.88	−8.54	−8.45	−8.56	−8.55
	r_c	3.04	3.48	3.44	3.50	3.49
$^{90}_{40}$Zr	E/A	—	−8.70	−8.66	−8.74	−8.71
	r_c	—	4.32	4.23	4.28	4.25
$^{208}_{82}$Pb	E/A	−2.52	−7.87	−7.86	−7.85	−7.87
	r_c	4.51	5.57	5.44	5.51	5.50

Additional approaches to EDF's include: getting some terms from microscopic derivation of nuclear matter, then adding phenomenology including surface gradient term (+Coulomb, spin-orbit, pairing) part of the Coulomb is fit to Nolen-Schiffer anomaly of isobaric mirror masses which produces better fits than Skyrme or Gogny with fewer parameters Fayans JETP Lett. 68, 169 (1998)**;**

basing EDF's on better NN interactions and many-body techniques Marino PRC 104 024315 (2021)

• For excited states:

Tamm-Dankoff and Random Phase Approximation... consider excited states of one or two particles above the HF g.s., with interactions between the particles.

Variations on Mean Field approaches:

• Relativistic mean field version (Walecka). Adds fields for nucleons and selected mesons.
(A version with HF exchange term $\leftrightarrow$ includes π)
This gets spin-orbit coupling from relativistic effects, a major success.
Used for dense matter and neutron stars Yang, Piekarewicz AnnRevNuclPartSci 70 21 (2020)

• Covariant density functional theory approaches include relativistic Brückner HF and a good NN interaction like Bonn

S. Shen, H. Liang, WH Long, J. Meng, P. Ring, Prog Part Nuc Phys 109 103713 (2019)
(with wf ansatz from Dirac-Woods-Saxon basis P. Ring EPJ Web of Conferences 178, 02001 (2018)**)**

• Attempts to use more realistic forces from chiral EFT to derive Energy Density Functionals Salvioni J. Phys. G. 47 085107 (2020)
There may be issues with whether chiral EFT should work at the energies needed.

• Attempts to derive Energy Density Functionals from 1st principles and EFT's

Duguet EPJA 59 12 (2023), Furnstahl arXiv:1906.00833.

Summary and unresolved questions

- **Light nuclei: J^π; T and energy order of levels for low-A can be accounted for by:**
  antisymmeterizing space-spin-isospin under exchange;
  Spatially symmetric configurations have lower E (consequence of NN interaction);
  Treating S; T together $\psi_{\text{spin}-\text{isosp}}$ ("Wigner SU(4)");
  higher J for same L lower in energy.

This approach is broken by spin-orbit coupling– does not work well at high-A
(One could account for most states by jj coupling of single particles, but this won't tell you which spin-isospin combinations are allowed.)

- **Hartree-Fock and Kohn-Sham generate self-consistent mean fields by iteration, minimizing g.s. energy by varying ψ's (HF) or the mean field directly (KS)**
  Variational principle $\rightarrow$ naturally accurate g.s. energies, but not necessarily ψ's
  Energy density functionals through Kohn-Sham allow introduction of terms into the mean field, which still needs self-consistency with ψ's– though the parameters are fit to global E_{B} and $\langle r^2 \rangle$, this is much more than the semi-empirical mass guess

- **Are nuclear ψ's always given by the ansatz, by products of single-particle wf's in a Slater determinant? (E.g. one α g.s. is symmetric in space with all antisymmetry in S;T.)**
  Some approaches use "Hartree," ignore "Fock" (RMF extension includes exchange.)
  Is the hard-core NN repulsion still a difficulty for the HF integrals?

Addendum concerning p. 29

C. Robin PRC 103 034325 (2020) "Entanglement rearrangement in self-consistent nuclear structure calculations":

The eigenstates of nuclei can be written as linear combinations of Slater determinants of nucleon wf's

JB notes: the space-symmetric g.s.'s of A=3 and A=4 with antisymmetric $\psi_{S,T}$ can be written as a single Slater determinant. These would have the lowest possible "entanglement entropy," a metric defined in this paper.

To support these statements, it would be nice to write a mixed symmetry space with mixed symmetry spin-isospin wf as an explicit linear combination of more than 1 Slater determinant, but this is beyond JB's ken.

The question remains of what one can say about wf's in self-consistent mean field theories derived from variational principles that minimize the energy. One operational difficulty to get good wf's comes from solving the Schroedinger-like equation with a mean field that is sensitive to interactions and things like sums of squares and exchanges of the wf's, but not all details.