N-Body Systems and the Nuclear Shell Model: I

F. Nowacki

Institut Pluridisciplinaire Hubert CURIEN STRASBOURG

UNIVERSITÉ DE STRASBOURG

European Summer University
Strasbourg, June 29^{th}/July 4^{th}-2009

powered by LaTeX

Bibliography

- Basic ideas and concepts in nuclear physics
  an introductory approach
  Heyde K.
  IOP Publishing 1994
- Shell model applications in nuclear spectroscopy
  Brussaard P.J., Glaudemans P.W.M.
  North-Holland 1977
- The nuclear shell model
  Heyde K.
  Springer-Verlag 1994
- The nuclear shell model
  A. Poves and F. Nowacki
  Lecture Notes in Physics **581** (2001) 70ff
- The shell model as a unified view of nuclear structure
  E. Caurier, G. Martinez-Pinedo, F. Nowacki, A. Poves, A. P. Zuker
  Rev. Mod. Phys. 77, 427 (2005)

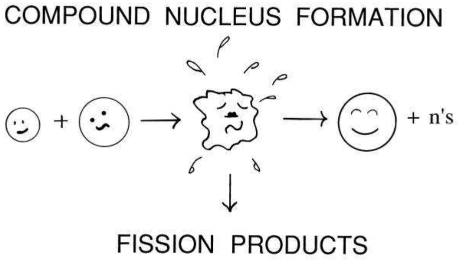
Outline

- Lecture 1: Introduction and basic notions
- Lecture 2: Shell model codes

Basic Notions

First insights on nuclear structure:

- liquid-drop model (Bethe and Bacher, 1936; von Weizsäcker, 1935): drops of charged, incompressible, liquid nuclear matter
- compound nucleus model of nuclear reactions (Bohr, 1936): incident neutron's energy dissipate totally via collisions



Atomic shell structure

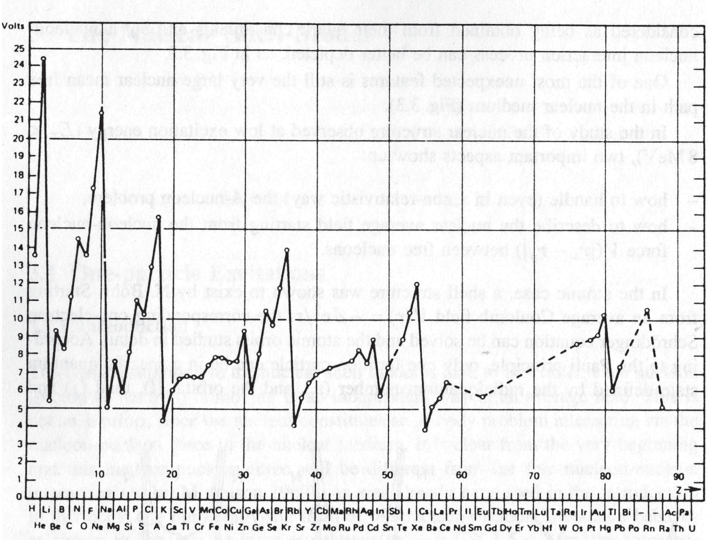


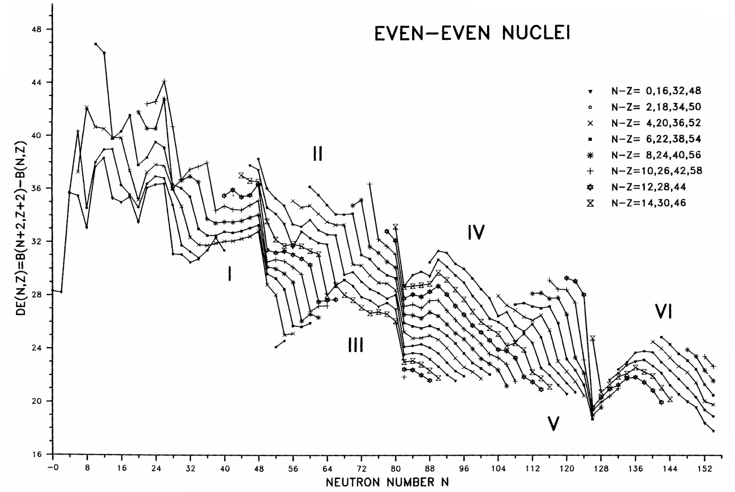
Fig. 3.4. Dependence of the ionization potential of the neutral atom on the atomic number Z [taken from (Herzberg 1944)]

Basic Notions

Experimental evidences for shell structure in nuclei:

- magic numbers

α lines systematics



Basic Notions

Experimental evidences for shell structure in nuclei:

- magic numbers
- single particle states
- magnetic moments

BUT strong successes of liquid-drop and compound-nucleus models as evidence against collisionless single-particle motion assumed in the shell model

Basic Notions

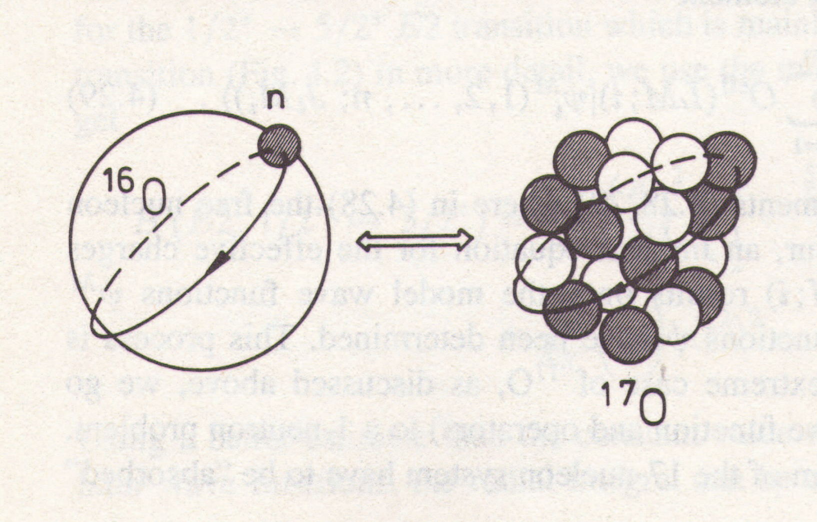
Soon it was realized that for fermions:

- compound-nucleus reactions occur at relatively high excitations energies where many collisions are not Pauli blocked
- at low energy, suppression of collisions by Pauli exclusion

➔ Single Particle Motion can persist

Independant Particle Model

Interaction of a nucleon with ALL the other particles is approximated by a central potential:



Independant Particle Model

Interaction of a nucleon with ALL the other particles is approximated by a central potential. One common potential is the Harmonic Oscillator potential:

$$U(r) = \frac{1}{2} m\omega^2 r^2$$

- m mass of the nucleon,
- $\hbar\omega$ energy quantum of the harmonic oscillator
- r distance between nucleon and origin of coordinate frame

Schrödinger equation for the nucleon in the harmonic oscillator potential:

$$h^{(0)}\phi(r) = \{T(k) + U(r)\}\phi(r) = \epsilon\phi(r)$$

with $h^{(0)} = \dfrac{p^2}{2m} + \dfrac{1}{2} m\omega^2 r^2$

Independant Particle Model

$h^{(0)}$ commutes with $\vec{l}^2$, l_z operators, and the equation is separable in radial and angular coordinates and the eigenfunctions are given as the product function of radial and angular parts:

$$\phi_{nlm}(r) = R_{nl}(r)\ Y_{lm}(\theta, \phi)$$

- $R_{nl}(r)$ solution of radial equation, characterized by n radial quantum number
- l and m being the quantum numbers of the angular momentum and its projection
- $Y_{lm}(\theta, \phi)$ normalized eigenfunction of the orbital momentum operator

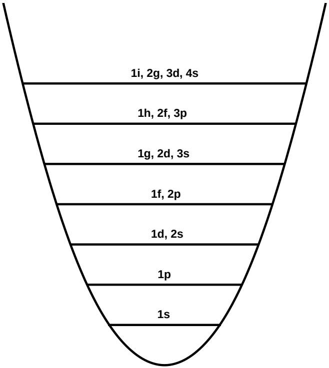
Harmonic Oscillator

In the harmonic oscillator case, the eigenvalues are:

$$\epsilon_{nl}^{(0)} = (N + \frac{3}{2})\hbar\omega = (2(n-1) + l + \frac{3}{2})\hbar\omega$$

- $N = 2(n-1) + l$ total oscillator quanta excited
- $(n-1)$ number of nodes of $R_{nl}(r)$ between $r = 0$ and $r = \infty$
- atomic spectroscopic notation for $l = 0, 1, 2, 3, 4, ...$ as s,p,d,f,g, ...

Independant Particle Model



N	E_N	d_N	$\sum_N d_N$	$n(l)$	parity
0	$\frac{3}{2}\hbar\omega$	2	2	$1s$	+
1	$\frac{5}{2}\hbar\omega$	6	8	$1p$	-
2	$\frac{7}{2}\hbar\omega$	12	20	$1d, 2s$	+
3	$\frac{9}{2}\hbar\omega$	20	40	$1f, 2p$	-
4	$\frac{11}{2}\hbar\omega$	30	70	$1g, 2d, 3s$	+
5	$\frac{13}{2}\hbar\omega$	42	112	$1h, 2f, 3p$	-
6	$\frac{15}{2}\hbar\omega$	56	168	$1i, 2g, 3d, 4s$	+

IPM interpretations

Note on Proposed Schemes for Nuclear Shell Models*

EUGENE FEENBERG AND KENYON C. HAMMACK
Washington University, St. Louis, Missouri

AND

L. W. NORDHEIM
Duke University, Durham, North Carolina

February 23, 1949

THE two papers by the present writers[1,2] on nuclear shell structure, cover very similar ground, such as assignment of orbital configurations on basis of spins and magnetic moments, statistics of isomerism, and the character of β-transitions. Both papers suggest level schemes to account for the empirically found regularities in nuclear structure. The two schemes are, however, not identical, and even a third proposal has been made by Maria G. Mayer,[3] on basis of the data collected in references 1 and 2. It may thus be of value to explain the relations between these papers.

The basis of all the considerations on shell structure is the observation that the level schemes in a simple potential well give a good account of the regularities of nuclear structure for neutron and proton numbers below 20. Such regularities persist also for heavier nuclei, though they do not correlate with the simple well scheme. These facts suggest, however, that a rearrangement of levels may be successful.

TABLE I. Proposed schemes for nuclear shells.

No. of particles in nucleus	8	20	50	82
No. of particles in shell	2+6	12	30	32
Feenberg and Hammack	$(1s)^2(2p)^6$ $(1s)^2(2p)^6$	$(2s)^2(3d)^{10}$ $(3d)^{10}$	$(4f)^{14}(5g)^{18}$	$(6h)^{22}(4d)^{10}$
Nordheim	$(1s)^2(2p)^6$	$(2s)^2(3d)^{10}$	$(4f)^{14}(3p)^6(4d)^{10}$	$(5g)^{18}(5f)^{14}$
Mayer	$(1s)^2(2p)^6$	$(2s)^2(3d)^{10}$	$(4f)^{14}(3p)^6(5g_{9/2})^{10}$	$(5g_{7/2})^8(4d)^{10}(3s)^2(6h_{11/2})^{12}$
Order of levels in potential well	$1s, 2p, 3d, 2s, 4f, 3p, 5g, 4d, 3s, 6h, 5f, 4p, 7i$			

that a rearrangement of levels may be successful.

TABLE I. Proposed schemes for nuclear shells.

No. of particles in nucleus	8	20	50	82
No. of particles in shell	2+6	12	30	32
Feenberg and Hammack	$(1s)^2(2p)^6$ $(1s)^2(2p)^6$	$(2s)^2(3d)^{10}$ $(3d)^{10}$	$(4f)^{14}(5g)^{18}$	$(6h)^{22}(4d)^{10}$
Nordheim	$(1s)^2(2p)^6$	$(2s)^2(3d)^{10}$	$(4f)^{14}(3p)^6(4d)^{10}$	$(5g)^{18}(5f)^{14}$
Mayer	$(1s)^2(2p)^6$	$(2s)^2(3d)^{10}$	$(4f)^{14}(3p)^6(5g_{9/2})^{10}$	$(5g_{7/2})^8(4d)^{10}(3s)^2(6h_{11/2})^{12}$
Order of levels in potential well	$1s$, $2p$, $3d$, $2s$, $4f$, $3p$, $5g$, $4d$, $3s$, $6h$, $5f$, $4p$, $7i$			

Basic Notions

Empirical construction by M. Goeppert Mayer and H. Jensen of a harmonic oscillator mean field plus a spin-orbit term to reproduce the magic numbers:

Thanks are due to Enrico Fermi for the remark, “Is there any indication of spin-orbit coupling ?” which was the origin of this paper.

Maria Goeppert Mayer
On Closed Shells in Nuclei. II
Physical Review 75, 1969 (1949)

Basic Notions

Empirical construction by M. Goeppert Mayer and H. Jensen of a harmonic oscillator mean field plus a spin-orbit term to reproduce the magic numbers:

$$U(r) = \frac{1}{2}m\omega^2 r^2 + D\vec{l}^2 - C\vec{l}.\vec{s}$$

Such a term does not commute with L_z and s_z but DOES commute with $\vec{j}^2 = (\vec{l} + \vec{s})^2$ and $j_z = l_z + s_z$, $\vec{j}^2$, $\vec{s}^2$:

$$-\vec{l}.\vec{s} = -\frac{1}{2}(\vec{j}^2 - \vec{l}^2 - \vec{s}^2) = -\frac{1}{2}(j(j+1) - l(l+1) - \frac{3}{4})$$

$$= \left.\begin{array}{ll} l+1 & \text{for j=l-}\frac{1}{2} \\ -l & \text{for j=l+}\frac{1}{2} \end{array}\right\}$$

powered by LaTeX

Basic Notions

With spin-orbit coupling, the solutions are:

$$\phi_{nljm}(r,\sigma) \;=\; R_{nl}(r)\,[Y_l(\theta,\phi)\,\chi_{\frac{1}{2}}(\sigma)]_j^m$$

where the orbital and spin wave functions coupling is

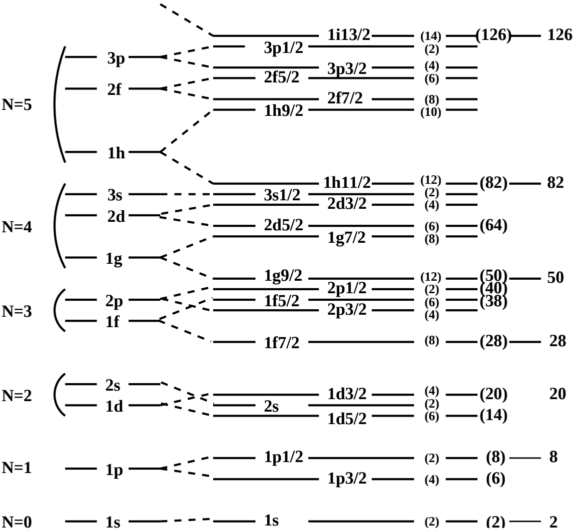
$$\phi_{nljm}(r,\sigma) \;=\; R_{nl}(r)\sum_{m_l,m_s}\langle lm_l \quad \frac{1}{2}m_s|jm\rangle Y_l^{m_l}(\theta,\phi)\chi_{\frac{1}{2}}^{m_s}(\sigma)$$

the corresponding energies being

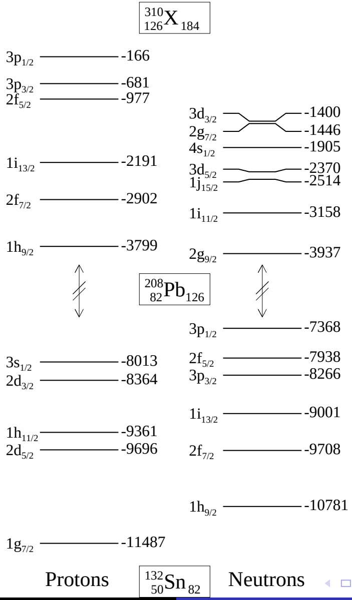
$$\epsilon_{nljm} = \hbar\omega\left[N+\frac{3}{2}+Dl(l+1)+C\left\{\begin{array}{ll} l+1 & j=l-\frac{1}{2} \\ -l & j=l+\frac{1}{2}\end{array}\right\}\right]$$

with $N = 2(n-1)+l$

Basic Notions



Single Particle Levels around ^{208}Pb



Evidence for IP shell model

Z	isotope	observed	shell model orbit
3	^{9}Li	$3/2^-$	$0p_{\frac{3}{2}}$
5	^{13}B	$3/2^-$	$0p_{\frac{3}{2}}$
7	^{17}N	$1/2^-$	$0p_{\frac{1}{2}}$
9	^{21}F	$5/2^+$	$0d_{\frac{5}{2}}$
11	^{25}Na	$5/2^-$	$0d_{\frac{5}{2}}$
13	^{29}Al	$5/2^+$	$1s_{\frac{1}{2}}$
15	^{33}P	$1/2^+$	$0d_{\frac{3}{2}}$
17	^{37}Cl	$3/2^+$	$0d_{\frac{3}{2}}$
19	^{41}K	$3/2^+$	$0d_{\frac{3}{2}}$
21	^{45}Sc	$7/2^-$	$0f_{\frac{7}{2}}$
23	^{49}V	$7/2^-$	$0f_{\frac{7}{2}}$
25	^{45}Mn	$7/2^-$	$0f_{\frac{7}{2}}$
27	^{57}Co	$7/2^-$	$0f_{\frac{7}{2}}$
29	^{61}Cu	$3/2^-$	$1p_{\frac{3}{2}}$
31	^{65}Ga	$3/2^-$	$1p_{\frac{3}{2}}$
33	^{69}As	$5/2^-$	$0f_{\frac{5}{2}}$
35	^{73}Br	$1/2^-$	$0f_{\frac{5}{2}}$

Ground state J^π of $N = Z + 3$ nuclei:

$$\left.\begin{array}{r} j \text{ in } \phi_{nljm_j} \longrightarrow J \\ l \text{ in } \phi_{nljm_j} \longrightarrow (-)^l = \pi \end{array}\right\} \longrightarrow J^\pi$$

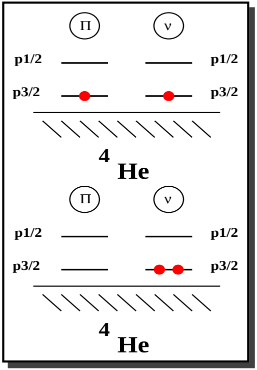
^{6}Li spectrum

two particles system $(j_1 j_2)^{J,T}$:

$(p_{\frac{3}{2}} p_{\frac{3}{2}})^{J=1,3 \quad T=0}$, $(p_{\frac{3}{2}} p_{\frac{3}{2}})^{J=0,2 \quad T=1}$

$(p_{\frac{3}{2}} p_{\frac{1}{2}})^{J=1,2, \ T=0}$, $(p_{\frac{3}{2}} p_{\frac{1}{2}})^{J=1,2, \ T=1}$

$(p_{\frac{1}{2}} p_{\frac{1}{2}})^{J=1 \ T=0}$, $(p_{\frac{1}{2}} p_{\frac{1}{2}})^{J=0 \ T=1}$



powered by LaTeX

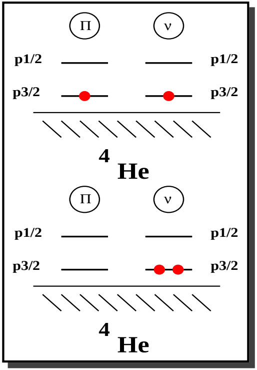
^{6}Li spectrum

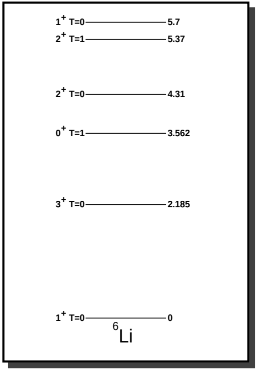
two particles system $(j_1 j_2)^{J,T}$:

$(p_{\frac{3}{2}}p_{\frac{3}{2}})^{J=1,3 \quad T=0}$, $(p_{\frac{3}{2}}p_{\frac{3}{2}})^{J=0,2 \quad T=1}$

$(p_{\frac{3}{2}}p_{\frac{1}{2}})^{J=1,2,\ T=0}$, $(p_{\frac{3}{2}}p_{\frac{1}{2}})^{J=1,2,\ T=1}$

$(p_{\frac{1}{2}}p_{\frac{1}{2}})^{J=1\ T=0}$, $(p_{\frac{1}{2}}p_{\frac{1}{2}})^{J=0\ T=1}$





Single Particle in potential:

$$h^{(0)}\phi_a(r) = \{T(k) + U(r)\}\phi_a(r) = \epsilon_a\phi_a(r)$$

System of A independant particles:

$$\mathcal{H}^{(0)} = \sum_{k=1}^{A}\{T(k) + U(r(k))\}$$

The eigenfunctions of $\mathcal{H}^{(0)}$ are

$$\Phi_{a_1 a_2 \ldots a_A}(1, 2, \ldots, A) = \prod_{k=1}^{A}\phi_{a_k}(r(k))$$

with the eigenvalues $E^{(0)} = \sum_{k=1}^{A}\epsilon_{a_k}$.

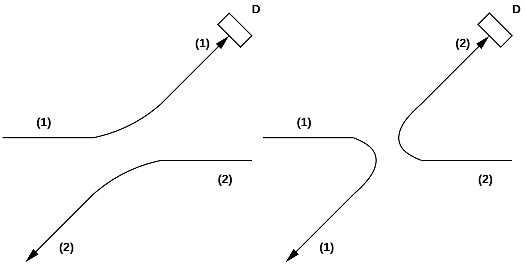
System of identical particles

For a system of identical particles, one needs to take into account that the particles are indistinguishable

➡ total wave function is (anti)symmetric
with exchange of two particles

System of identical particles

- in quantum mechanics, particle exchange degeneracy:



there exist two possible distinct final states (orthogonal) but associated to a single physical state (no possible measurement to distinguish them)

powered by LaTeX

System of identical particles

- symmetrisation postulate

For a system of identical particles, only some (N-body) eigenfunctions describe physical states: they are antisymmetric (with respect to permutations of particles) for fermions and symmetric for bosons

If $|u\rangle$ is a physical ket, $\{\mathrm{P}_\alpha|u\rangle\}$ is also a physical ket

For fermions, the physical kets are those obtained by antisymmetrization :

$$\mathrm{A}|u\rangle \text{ avec } \mathrm{A}=\frac{1}{N!}\sum_{\alpha}\epsilon_\alpha \mathrm{P}_\alpha$$

System of identical particles

- example with two particles:

$|u\rangle = \phi_a(1)\phi_b(2)$ and $\mathcal{E}_u = \{\phi_a(1)\phi_b(2),\ \phi_a(2)\phi_b(1)\}$

$$A|u\rangle = \tfrac{1}{2}(\phi_a(1)\phi_b(2) - \phi_a(2)\phi_b(1))$$

Pauli principle: if $\phi_a = \phi_b$, $A|u\rangle = 0$

- example with three particles:

$|u\rangle = \phi_a(1)\phi_b(2)\phi_c(3)$ and

$$\begin{aligned}
\mathcal{E}_u &= \{\phi_a(1)\phi_b(2)\phi_c(3), \phi_a(2)\phi_b(3)\phi_c(1), \phi_a(2)\phi_b(1)\phi_c(3),\\
&\quad \phi_a(3)\phi_b(1)\phi_c(2), \phi_a(3)\phi_b(2)\phi_c(1), \phi_a(1)\phi_b(3)\phi_c(2)\}\\
A|u\rangle &= \tfrac{1}{6}\ (\ \phi_a(1)\phi_b(2)\phi_c(3) + \phi_a(2)\phi_b(3)\phi_c(1) + \phi_a(3)\phi_b(1)\phi_c(2)\\
&\quad -\phi_a(2)\phi_b(1)\phi_c(3) - \phi_a(3)\phi_b(2)\phi_c(1) - \phi_a(1)\phi_b(3)\phi_c(2))
\end{aligned}$$

System of identical particles

- two particles case:

$$\Phi_{ab}(1,2) = \sqrt{\frac{1}{2}}\{\phi_a(1)\phi_b(2) - \phi_a(2)\phi_b(1)\} = \sqrt{\frac{1}{2}}\begin{vmatrix} \phi_a(1) & \phi_a(2) \\ \phi_b(1) & \phi_b(2) \end{vmatrix}$$

i. e. a Slater Determinant

- three particles case:

$$\Phi_{abc}(1,2,3) = \sqrt{\frac{1}{6}}\begin{vmatrix} \phi_a(1) & \phi_a(2) & \phi_a(3) \\ \phi_b(1) & \phi_b(2) & \phi_b(3) \\ \phi_c(1) & \phi_c(2) & \phi_c(3) \end{vmatrix}$$

developped with the Sarrus rule

$$\begin{aligned}\Phi_{abc}(1,2,3) = \sqrt{\tfrac{1}{6}} \quad & \{\phi_a(1)\phi_b(2)\phi_c(3) + \phi_a(3)\phi_b(1)\phi_c(2) + \phi_a(2)\phi_b(3)\phi_c(1) \\ & -\phi_a(3)\phi_b(2)\phi_c(1) - \phi_a(2)\phi_b(1)\phi_c(3) - \phi_a(1)\phi_b(3)\phi_c(2)\}\end{aligned}$$

System of identical particles

A particles case:

$$\Phi_{a_{\alpha 1} a_{\alpha 2} \ldots a_{\alpha A}}(1,2,\ldots,A) = \sqrt{\frac{1}{A!}} \begin{vmatrix} \phi_{a_{\alpha 1}}(r(1)) & \phi_{a_{\alpha 1}}(r(2)) & \ldots & \phi_{a_{\alpha 1}}(r(A)) \\ \phi_{a_{\alpha 2}}(r(1)) & \phi_{a_{\alpha 2}}(r(2)) & \ldots & \phi_{a_{\alpha 2}}(r(A)) \\ \vdots & \vdots & \vdots & \vdots \\ \phi_{a_{\alpha A}}(r(1)) & \phi_{a_{\alpha A}}(r(2)) & \ldots & \phi_{a_{\alpha A}}(r(A)) \end{vmatrix}$$

The global phase is determined by the order of the indices: α_1,α_2, ...α_A with $\alpha_i \equiv \{n_i l_i j_i m_i\}$

Occupation number formalism to simplify such expressions:

$$\Phi_{a_{\alpha 1} a_{\alpha 2} \ldots a_{\alpha A}}(1,2,\ldots,A) = a^{\dagger}_{a_{\alpha 1}} \ldots a^{\dagger}_{a_{\alpha A}} |0\rangle$$

only occupation numbers of the single particle orbits are necessary (no labelling of the particles)

Second quantization

- Creation and annihilation operators:

$a_i^\dagger \; |0\rangle = |i\rangle \qquad a_i \; |i\rangle = |0\rangle \qquad$ vacuum $|0\rangle$ such $a_i \; |0\rangle = 0$

For fermions, antisymmetry ensured by anti-commutation rules:

$$\{a_i^\dagger, a_j^\dagger\} = \{a_i, a_j\} = 0$$
$$\{a_i^\dagger, a_j\} = \delta_{i,j}$$

- One body operators:

$$O^{(1)} = \sum_{i=1}^{A} O(r(i)),$$

whose matrix elements are $\langle i|O|j\rangle = \int \; \phi_i^*(r) O \phi_j(r) dr$

will write in second quantization as

$$\hat{O} = \sum_{i,j} \langle i|o|j\rangle a_i^\dagger a_j$$

ex: $\tilde{n} = \sum_i \tilde{n}_i = \sum_i a_i^\dagger a_i$

Second quantization

- Two body operators:

  $$O^{(2)} = \sum_{1=j<k}^{A} O(r(i), r(j)),$$

  whose matrix elements are $\langle ij|O|kl\rangle =$

  $$\int \phi_i^*(r(1))\phi_j^*(r(2))(1-P_{12})O\phi_k(r(1))\phi_l(r(2))dr(1)dr(2)$$

  will write in second quantization as

  $$\hat{O} = \frac{1}{4}\sum_{i,j,k,l}\langle ij|O|kl\rangle a_i^\dagger a_j^\dagger a_l a_k$$

  ex: $\mathcal{H}$, $\beta\beta$ operator

Hartree Fock

Link between nucleon-nucleon effective interaction and mean-field : Hartree-Fock approximation

$$\mathcal{H} = \sum_{i=1}^{A} t_i + \frac{1}{2} \sum_{\substack{i \neq j \\ j=1}}^{A} v_{ij}$$

two body term replaced by a one body potential (mean field) $\mathcal{U}$

$$\mathcal{H}^{(0)} = \sum_{i=1}^{A} t_i + \mathcal{U}_i$$

Hartree Fock

$\mathcal{H}^{(0)}$ eigenfunctions are:

$$\Psi_{a_1 a_2 \ldots a_A}(1,2,\ldots,A) = det(\prod_{k=1}^{A} \phi_{a_k}(r(k)))$$
$$= \prod_{k=1}^{A} a_k^{\dagger}|0\rangle$$

$\phi_{a_k}(r(k))$ obtained by minimisation of the total energy

$$E = \frac{\langle\Psi|\mathcal{H}|\Psi\rangle}{\langle\Psi|\Psi\rangle}$$

- masses, radii, charge density distribution ...
- magic numbers, single particle energies, individual wave functions ...

see P.H. Heenen lectures on Friday

Correlations in nuclei

- for the description of nuclei, mean field is only the starting point

To be continued ...

Correlations in nuclei

- for the description of nuclei, mean field is only the starting point
- the two body residual interaction (correlations) is reponsable for the detailled structure of nuclei

To be continued ...

Correlations in nuclei

- for the description of nuclei, mean field is only the starting point
- the two body residual interaction (correlations) is reponsable for the detailled structure of nuclei
- in particular, correlations can induce coherent phenomena i. e. **collectivity**

To be continued ...