

## 5

### Shell structure and magic numbers

#### 5.1 Closed shells in atoms and nuclei

In the 1940s one spoke about ‘magic’ numbers among the nuclei. Such numbers are for the protons and neutrons, respectively

$$Z = 2, 8, 20, 28, 50, 82$$

$$N = 2, 8, 20, 28, 50, 82 \text{ and } 126$$

These series of numbers one now wants to extend to  $Z = 114, 164$  for protons and  $N = 184$  and maybe 228 for neutrons. Nuclei containing the above-listed numbers of neutrons or/and protons are the ones found in figs. 3.8 and 3.9 to be associated with large extra binding energies relative to the predictions of the semi-empirical mass formula. It is natural to associate this extra stability with the filling of nucleon shells. Nuclei with  $N$  or  $Z$  magic are usually called single-closed-shell nuclei, while those with both  $N$  and  $Z$  ‘magic’ are called doubly closed shell nuclei or ‘double-magic’ nuclei. Examples of the latter are  ${}^4_2\text{He}_2$ ,  ${}^{16}_8\text{O}_8$ ,  ${}^{40}_{20}\text{Ca}_{20}$ ,  ${}^{48}_{20}\text{Ca}_{28}$ ,  ${}^{56}_{28}\text{Ni}_{28}$ ,  ${}^{132}_{50}\text{Sn}_{82}$  and  ${}^{208}_{82}\text{Pb}_{126}$ . A nucleus that from theoretical extrapolations is predicted to have similar character is  ${}^{298}_{114}$ , which has  $Z = 114$ ,  $N = 184$ , see chapter 10.

The whole notion of closed shells comes from atomic theory. There the noble gases represent particularly stable and ‘inactive’ electron configurations. The corresponding ‘magic’ numbers in the electron case are

$$Z = 2, 10, 28, 36, 54, 86$$

to which correspond the atoms

$$\text{He, Ne, Ar, Kr, Xe, Rn}$$

It should be well known that the Hamiltonian describing the motion of one particle in a spherical symmetric potential can be separated into the radial

Table 5.1. Closed shells calculated from the pure Coulomb potential.

Shell	$\ell$	States $(n+1)\ell$	Number of electrons	Total	Exp.
1	0	1s	2	2	2
2	0, 1	2s, 1p	2+6	10	10
3	0, 1, 2	3s, 2p, 1d	2+6+10	28	18
4	0, 1, 2, 3	4s, 3p, 2d, 1f	2+6+10+14	60	36
5	0, 1, 2, 3, 4	5s, 4p, 3d, 2f, 1g	2+6+10+14+18	110	54

and angular degrees of freedom. The corresponding quantum numbers are  $n$ , the number of nodes in the radial wave function, the angular momentum  $\ell$  and its projection  $m_\ell$ . As the energy eigenvalues are independent of  $m_\ell$ , one finds subshells of degeneracy  $2(2\ell+1)$  where the two possible spin directions give a factor 2. This degeneracy is partly broken if spin-dependent forces are present (see chapter 6). The subshells of different  $\ell$  quantum numbers are generally denoted by letters, s, p, d, f, g, ... for  $\ell = 0, 1, 2, 3, 4, \dots$

For a Coulomb potential there is an even higher degeneracy as the energy eigenvalues depend only on the  $N = n + \ell + 1$  quantum number.† Thus for ‘hydrogen-like’ atoms with the potential

$$V_C = -\frac{Ze^2}{4\pi\epsilon_0 r}$$

the energy eigenvalues are given as

$$E_N = -\frac{1}{2}mc^2\alpha^2\frac{Z^2}{N^2}$$

where

$$\alpha = \frac{(e^2/4\pi\epsilon_0)}{\hbar c} \simeq \frac{1}{137}$$

is the fine structure constant. With the assumption that, in the many-electron case, the interaction between the different electrons is negligible, it is now straightforward to construct table 5.1. In table 5.1, the first two closed-shell numbers in the next to the last column agree with the empirically known magic numbers of the last column; the other three theoretical numbers are too large. This is mainly due to the fact that the Coulomb potential is smaller than assumed as the inner electrons ‘shield’ the outer electrons from

† We use a notion customary in nuclear physics, with  $n$  being the radial quantum number and  $N$  the principal quantum number.

Table 5.2. *Approximate closed shells resulting from the Coulomb potential with shielding included.*

Shell	$\ell$	States $(n+1)\ell$	Number of electrons	Total	Exp.
1	0	1s	2	2	2
2	0, 1	2s, 1p	2+6	10	10
3	0, 1	3s, 2p	2+6	18	18
4	0, 1, 2	4s, 3p, 1d	2+6+10	36	36
5	0, 1, 2	5s, 4p, 2d	2+6+10	54	54
6	0, 1, 2, 3	6s, 5p, 3d, 1f	2+6+10+14	86	86
7	0, 1, 2, 3	7s, 6p, 4d, 2f	2+6+10+14	118	?
8	0, 1, 2, 3, 4	8s, 7p, 5d, 3f, 1g	2+6+10+14+18	168	?

the nuclear charge. Far away from the nucleus, the Coulomb potential, owing to electrons in deep orbitals, is much weaker than the formula implies. With the shielding included we obtain table 5.2 (where the degeneracy of the shells is only approximate). In this case one has (with a theory based on a Hartree-Fock calculation, see below) succeeded in reproducing the 'magic' numbers associated with the electron shells. The noble gases are predicted at their proper places in the periodic system. The effect of shielding is the largest for orbitals of high  $\ell$ -values. Thus the 1d orbital is displaced from the third shell down to the fourth shell, 2d and 3d appear near the s and p levels of the fifth and sixth shells, respectively. Similarly the 1f orbital occurs first with the s and p levels of the sixth shell etc.

Of considerable interest is the prediction of a new closed shell at  $Z = 118$ , which latter should be another noble gas (it is barely a gas at room temperature as it has a point of condensation just below room temperature). The electron closed shell  $Z = 118$  happens to be close to the island of stability near  $Z = 114$  predicted for the atomic nucleus. For this reason there is some remote possibility that  $Z = 118$  might be produced. Soon after  $Z = 118$ , a new chemistry should begin with the filling of the first atomic g-shell.

We have so far appealed to qualitative ideas of the inertness of a noble gas. To give a more quantitative measure of the shell structure let us study fig. 5.1 of the atomic ionisation energy of the chemical elements of the periodic table. The ionisation energy is the cost in energy of removing the last (and least bound) electron. According to a theorem from Hartree-Fock theory (Koopman's theorem), the ionisation energy is very near to the

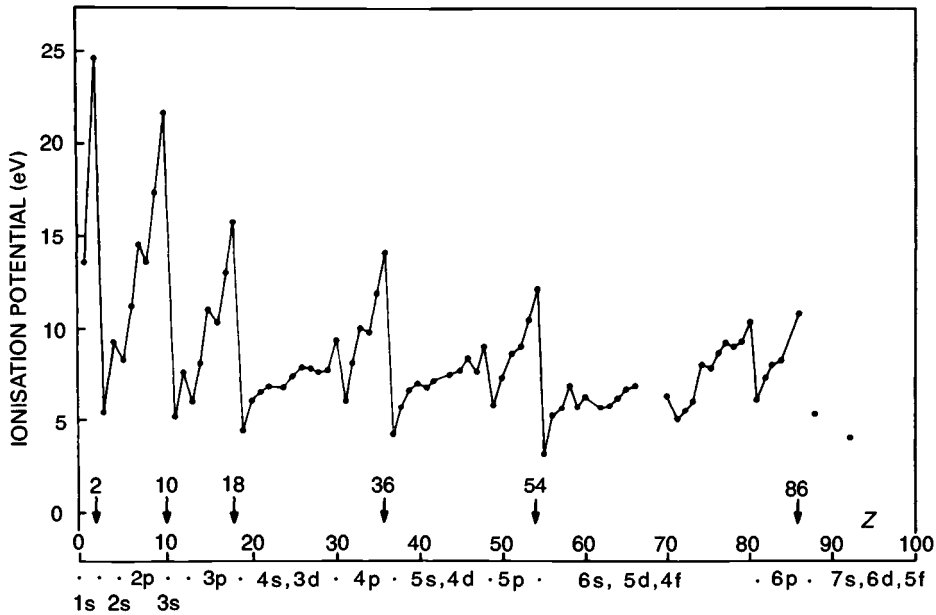


Fig. 5.1. Experimental value of the atomic ionisation potential as a function of  $Z$ , exhibiting the strong effects of closed shells at  $Z = 2, 10, 18, 36, 54$  and  $86$  (from Bohr and Mottelson, 1969).

single-electron energy of the valence electron that is removed when the atom becomes singly ionised.

The corresponding quantity in the nuclear case is the neutron separation energy or the proton separation energy, respectively. Similarly to the ionisation energy in the electron case, the neutron separation energy is the minimum energy it costs to remove one neutron from a nucleus. This latter quantity is plotted in fig. 5.2 as a function of neutron number  $N$ . In particular the  $N = 82$  and  $N = 126$  shells are clearly visible. The effects of shells are, however, somewhat less pronounced in the nucleon case than in the electron case.

To sum up the philosophy implicit in the foregoing discussion, the following note should be made. In the atomic case the sudden discontinuities in certain atomic properties over the periodic table can be understood as effects of quantal states in an atomic potential varying smoothly with  $Z$ . In the nuclear case the analogous discontinuities in masses and separation energies can again be understood from quantal shells in a nuclear potential. We just have to find the potential.

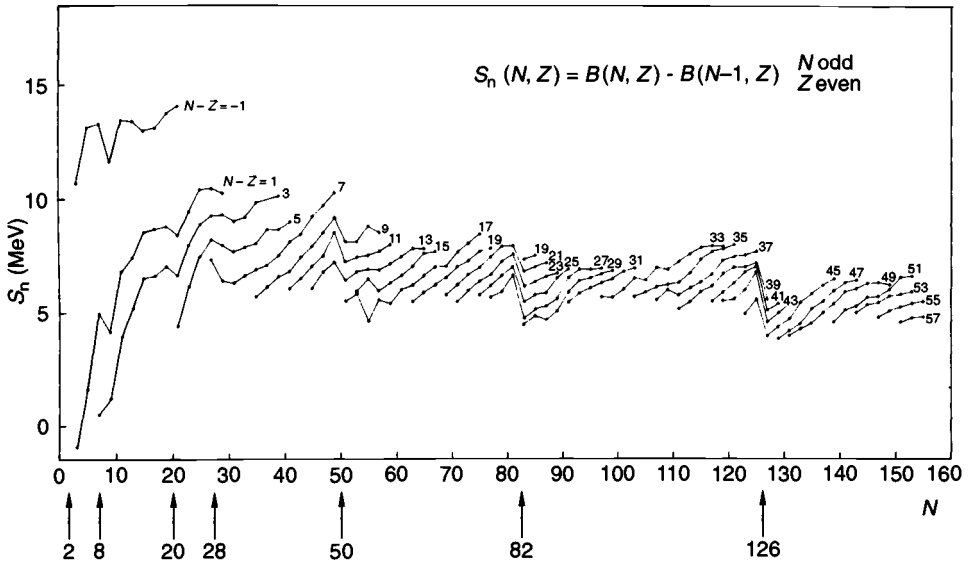


Fig. 5.2. Neutron separation energies for even- $Z$ , odd- $N$  elements as a function of neutron number  $N$ . Note the sudden drop in separation energies in passing the closed neutron shells at  $N = 50, 82$  and  $126$  (from Bohr and Mottelson, 1969).

## 5.2 The atomic and nuclear one-body potentials

In the atomic case it is very apparent that the concept of a one-body potential in which the electrons move is a very successful concept. This is so in spite of the fact that many electrons are involved in addition to the central nuclear charge, assumed to rule alone according to the most elementary considerations. The more refined concept of a screened central nuclear charge is a further improvement, enough to account for the closed shells.

A few words may be needed to clarify further the concept of a one-body potential. This implies that one particle at a time can be considered present in a static potential whose only coordinates are those of the one particle in question, as position  $\mathbf{r}$ , momentum  $\mathbf{p}$  and spin  $s$ . Formally, such a one-body potential is obtained from the self-consistent field method proposed by Hartree (1928). For the atom the Hartree or Hartree-Fock (Fock, 1930) method is well established. For nucleons the procedure is highly similar though complicated by the fact of the immense complication of the basic two-body nuclear interaction.

Around the atom there are really only electrons. In the nucleus the question can in principle be raised of whether it is really a good approximation to talk about neutrons and protons. We shall briefly come back to these problems

in chapter 13. Let us, however, assume that neutrons and protons are enough and that we can assume that the two-body interaction derived from neutron–proton and proton–proton scattering can be used unmodified in the nucleus.

Let us first consider the electron case. The total wave function can be written as a product wave function

$$\psi = \prod_i \phi_i$$

where the one-electron wave functions are given by  $\phi_i$ . We now consider the potential seen by electron  $i$  under the influence of the nucleus and the remaining  $Z - 1$  electrons placed statically in the nucleus:

$$V_i = -\frac{Ze^2}{4\pi\epsilon_0 r_i} + \sum_{j \neq i} \frac{1}{4\pi\epsilon_0} \int \phi_j^* \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} \phi_j d^3r_j$$

leading to the one-particle Schrödinger equation

$$\left( -\frac{\hbar^2}{2m} \nabla_i^2 + V_i \right) \phi_i = e_i \phi_i$$

with the energy eigenvalues  $e_i$ .

Many wave functions and energy levels are obtained and in each level we may place one particle in accordance with the Pauli principle. These  $\phi_j$  are then used to determine new  $\phi_j$  functions or new densities  $\rho_j = \phi_j^* \phi_j$ . One problem then is how to obtain the initial  $\phi_j$  or  $\rho_j$  terms. The answer is that one may ‘guess’ initial  $\phi_j$  or alternatively initial potentials. The solutions can then be iterated.

In the nuclear case, there is no central potential and furthermore, the two-particle interaction is not fully determined. Still, it turns out to be feasible to use a similar approach with a mean-field potential

$$V_i = \sum_j \langle \phi_j | V_{ij} | \phi_j \rangle$$

where the two-particle interactions  $V_{ij}$  in the general case not only depend on distance but also on e.g. momentum and spin. As in the electron case, if the wave function is properly symmetrised, the product of  $\phi_i$  is replaced by a determinant and the expressions above are somewhat generalised (Hartree–Fock method).

Another problem is that the empirical nucleon–nucleon two-body interaction corresponds to an infinite repulsion at very small distances. This leads to convergence problems. To overcome the latter, elaborate technical schemes

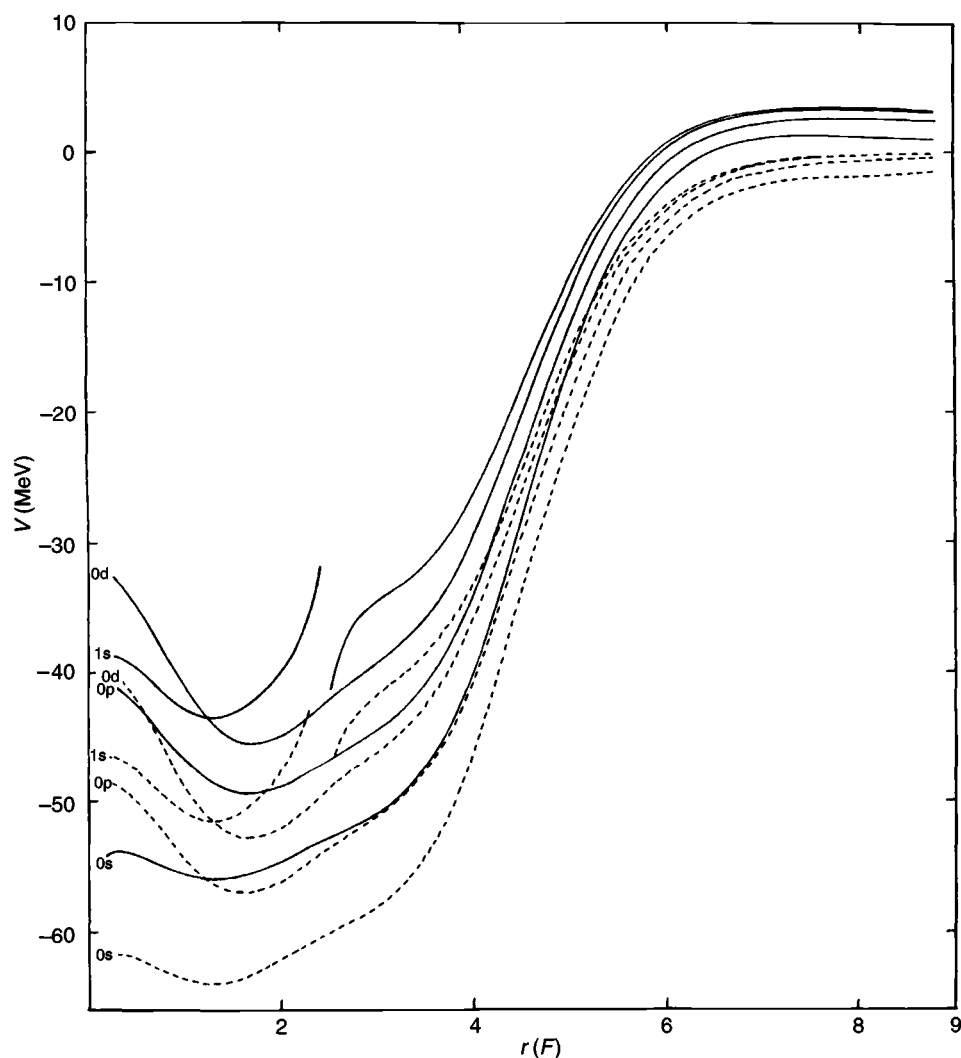


Fig. 5.3. Effective single-proton (solid lines) and single-neutron (dashed lines) potentials for  $^{40}\text{Ca}$  obtained in Hartree-Fock calculations based on the so-called Skyrme interaction. Note that to each orbital corresponds a slightly different potential shape. All these potentials show a radial dependence similar to that of the Woods-Saxon potential (from J.W. Negele, *Phys. Rev.* C1 (1970) 1260).

have been devised by K. Brueckner and his coworkers (1958). Thanks to this development one is therefore presently capable of rather 'realistic' Hartree and Hartree-Fock calculations in nuclear physics.

Based on a more or less 'realistic' nucleon-nucleon interaction, it has been possible to obtain Hartree-Fock one-body potentials for large series of

nuclei as exemplified in fig. 5.3 for  $^{40}\text{Ca}$ . Note that there is one potential for each state. The fact that the Coulomb interaction modifies the orbitals of the protons relative to those of the neutrons leads to a nuclear potential for the protons different from that of the neutrons. The one-body potential can thus at least roughly be derived from the two-body interaction. As a general observation one may note that the potential depth is about 50 MeV in the case illustrated and the radius approximately the same as the matter radius.

We will follow the path taken historically, however. Thus we shall assume a parameter form of a purely empirical potential. The parameters are subsequently determined to fit data as well as possible. This procedure is outlined in the following chapter.

### Exercises

- 5.1 Consider a three-dimensional anisotropic harmonic oscillator potential

$$V = \frac{M\omega_x^2}{2}x^2 + \frac{M\omega_y^2}{2}y^2 + \frac{M\omega_z^2}{2}z^2$$

The corresponding Hamiltonian is separable into the  $x$ -,  $y$ - and  $z$ -directions and the energy eigenvalues are easily obtained as

$$E = \hbar\omega_x \left( n_x + \frac{1}{2} \right) + \hbar\omega_y \left( n_y + \frac{1}{2} \right) + \hbar\omega_z \left( n_z + \frac{1}{2} \right)$$

- (a) In the case of spherical symmetry ( $\omega_x = \omega_y = \omega_z$ ) a large degeneracy is obtained. Calculate the lowest ‘magic’ numbers. Are there any  $\ell$ -shells that are degenerate?
- (b) Another case of large degeneracy is  $\omega_x = \omega_y = 2\omega_z$ . Calculate the ‘magic’ numbers also in this case (the fission isomeric states as well as the superdeformed high-spin states (chapter 12) have a deformation approximately corresponding to this frequency ratio).