

Since the number of elements in the PSE is a physical reality and beyond discussion, by comparison of Fig. 5 with Fig. 1 we conclude that in fact pairs of rows rather than single rows (as in the case of the H-atom) form complete shells and that the degeneracy of a PSE-shell is twice that of a hydrogen shell. In order to lift this additional degeneracy, analogue to the postulation of a spin $s = \pm 1/2$ in the non relativistic treatment of the hydrogen atom, we postulate for the PSE in addition a quasi spin property described by a quantum number $c = \pm 1/2$. Similar to the total angular momentum quantum number $j = l + s = l \pm 1/2$ a total radial quantum number q may be defined as

$$q = \bar{n}_r + c = \bar{n}_r \pm 1/2 = q_{\pm},$$

where the states q_+ correspond to the upper and the states q_- to the lower half of a double shell.

Every element of the PSE is thus defined by a set of five quantum numbers $(\bar{n}_r, c; l, m, s)$. The boxes of the PSE (Fig. 1) are obtained by generating the set (Fig. 5 b):

$$\{(\bar{n}_r, l)\} = \left\{(\nu, \bar{N} - \nu)\right\}_{\substack{\nu=0, 1, 2, \dots, \bar{N}, \\ \bar{N}=0, 1, 2, \dots, d(=3)}} \quad (16a)$$

where \bar{N} is used as a short notation for $(N-2)/2$. The multiplicity $4(2l+1)$ of each box, produced by

$$c = \pm 1/2, \quad -l \leq m \leq +l, \quad s = \pm 1/2 \quad (16b)$$

gives then the $4(2l+1)$ chemical elements of the box.

If we define a principal quantum number \bar{n} such that it is of the same form as the conventional principal quantum number n ,

$$\bar{n} = \bar{n}_r + l + 1 \quad (17)$$

the states (\bar{n}, l) of a double shell in the PSE look the same as the states of a shell in the H-atom (Fig.

5 c). The order of filling, however, is opposite in the two cases.

It may be mentioned that a substitution $2l = \hat{l}$ which would reduce Eq. (13 b) to the form of Eq. (12), is not possible since the degeneracy of a state \hat{l} would be different from $2(2\hat{l}+1)$ as required by a row of the PSE. Physically, l is uniquely defined by the rotational symmetry of the problem and cannot be reinterpreted.

With respect to the nomenclature it would be of some advantage not to introduce a principal quantum number at all, but rather use the maximum angular momentum \hat{l} of the shell instead. If one designates further the radial quantum number not by n_r but by l' , one has simply for every shell

$$l + l' = \hat{l} = \text{const.}$$

The energies depend on $(\hat{l}+1)$ and for $\hat{l}=0$ one has a zero point energy as in the case of the harmonic oscillator.

4.3. Wave Functions

The coefficients in the dimensionless radial wave functions, Eq. (4), depend on κ as given in Table 1; in physical space, however, the radial functions are independent on κ and can be written as

$$R_{\kappa, n^*, l}(r) = A_0 e^{-k_0 r/n^*} \left(\frac{k_0 r}{\kappa n^*}\right)^l L_{\frac{1}{2}n^*+1}^{2l+1} \left(\frac{2 k_0 r}{n^*}\right) \quad (18)$$

where A_0 is a normalization factor, $L_{\frac{1}{2}n^*+1}^{2l+1}$ are associated Laguerre polynomials, $k_0 = 2 \mu Z e^2/\hbar^2$ and n^* assumes by Eq. (8) only even integers, $n^* = 2, 4, 6, \dots$. Since the factor κ^{-l} can be absorbed into the normalization constant, the radial functions are — apart from their different labelling — identical to those given in the literature⁵ for the hydrogen atom.

The complete wave function for the Coulomb problem should allow for the duplicity of the shells

κ	$l=3$	$l=2$	$l=1$	$l=0$	\hat{l}	
1	1, 0, 0, 0	1, -1/3, 0, 0 1, 0, 0, 0	1, -1, 1/5, 0 1, -1/2, 0, 0 1, 0, 0, 0	1, -3, 2, -1/3 1, -2, 2/3, 0 1, -1, 0, 0 1, 0, 0, 0	3 2 1 0	
	1/2	1, 0, 0, 0	1, -1/6, 0, 0 1, 0, 0, 0	1, -1/2, 1/20, 0 1, -1/4, 0, 0 1, 0, 0, 0	1, -3/2, 1/2, -1/24 1, -1, 1/6, 0 1, -1/2, 0, 0 1, 0, 0, 0	3 2 1 0

Table 1. The coefficients a_0, a_1, a_2, a_3 of the dimensionless radial functions, Eq. (4), for $\kappa=1$ and $\kappa=1/2$.