

Using [3.47] we see that [3.50] becomes

$$|N_{nl}|^2 \left(\frac{na_\mu}{2Z} \right)^3 \int_0^\infty e^{-\rho} \rho^{2l} [L_{n+l}^{2l+1}(\rho)]^2 \rho^2 d\rho = 1 \quad [3.51]$$

It is shown in Appendix 3 that the integral over ρ can be evaluated by using the generating function [3.45]. The result is (see [A3.26])

$$\int_0^\infty e^{-\rho} \rho^{2l} [L_{n+l}^{2l+1}(\rho)]^2 \rho^2 d\rho = \frac{2n[(n+l)!]^3}{(n-l-1)!} \quad [3.52]$$

so that the normalised radial functions for the bound states of one-electron atoms may be written as [2]

$$R_{nl}(r) = - \left\{ \left(\frac{2Z}{na_\mu} \right)^3 \frac{(n-l-1)!}{2n[(n+l)!]^3} \right\}^{1/2} e^{-\rho/2} \rho^l L_{n+l}^{2l+1}(\rho) \quad [3.53]$$

$$\rho = \frac{2Z}{na_\mu} r, \quad a_\mu = \frac{4\pi\epsilon_0\hbar^2}{\mu e^2}$$

As an illustration of the above formulae, we shall consider the case of an 'infinitely heavy' nucleus, so that a_μ reduces to $a_0 = 4\pi\epsilon_0\hbar^2/me^2$, the first Bohr radius. The first few radial eigenfunctions are then given explicitly by

$$\begin{aligned} R_{10}(r) &= 2(Z/a_0)^{3/2} \exp(-Zr/a_0) \\ R_{20}(r) &= 2(Z/2a_0)^{3/2} (1 - Zr/2a_0) \exp(-Zr/2a_0) \\ R_{21}(r) &= \frac{1}{\sqrt{3}} (Z/2a_0)^{3/2} (Zr/a_0) \exp(-Zr/2a_0) \\ R_{30}(r) &= 2(Z/3a_0)^{3/2} (1 - 2Zr/3a_0 + 2Z^2r^2/27a_0^2) \exp(-Zr/3a_0) \\ R_{31}(r) &= \frac{4\sqrt{2}}{9} (Z/3a_0)^{3/2} (1 - Zr/6a_0)(Zr/a_0) \exp(-Zr/3a_0) \\ R_{32}(r) &= \frac{4}{27\sqrt{10}} (Z/3a_0)^{3/2} (Zr/a_0)^2 \exp(-Zr/3a_0) \end{aligned} \quad [3.54]$$

In order to express these functions in atomic units (a.u.) one just sets $a_0 = 1$ in [3.54]. To take into account the reduced mass effect, we should replace a_0 by $a_\mu = a_0(m/\mu)$.

Using the radial wave functions [3.53] together with the explicit expressions of the spherical harmonics given in Table 2.1, we display in Table 3.1 the complete normalised bound state hydrogenic eigenfunctions $\psi_{nlm}(r, \theta, \phi)$ for the first three shells (i.e. the K, L and M shells corresponding respectively to the values $n = 1, 2$ and 3 of the principal quantum number) for the case of an

[2] In writing [3.53] we have used the fact that the radial eigenfunctions $R_{nl}(r)$ may be taken to be real without loss of generality.

Table 3.1 The complete normalised hydrogenic wave functions corresponding to the first three shells, for an 'infinitely heavy' nucleus. The quantity $a_0 = 4\pi\epsilon_0\hbar^2/me^2$ is the first Bohr radius. In order to take into account the reduced mass effect one should replace a_0 by $a_\mu = a_0(m/\mu)$

Shell	Quantum numbers $n \quad l \quad m$	Spectroscopic notation	Wave function $\psi_{nlm}(r, \theta, \phi)$
K	1 0 0	1s	$\frac{1}{\sqrt{\pi}} (Z/a_0)^{3/2} \exp(-Zr/a_0)$
	2 0 0	2s	$\frac{1}{2\sqrt{2\pi}} (Z/a_0)^{3/2} (1 - Zr/2a_0) \exp(-Zr/2a_0)$
	2 1 0	2p ₀	$\frac{1}{4\sqrt{2\pi}} (Z/a_0)^{3/2} (Zr/a_0) \exp(-Zr/2a_0) \cos \theta$
	2 1 ±1	2p _{±1}	$\mp \frac{1}{8\sqrt{\pi}} (Z/a_0)^{3/2} (Zr/a_0) \exp(-Zr/2a_0) \sin \theta \exp(\pm i\phi)$
L	3 0 0	3s	$\frac{1}{3\sqrt{3\pi}} (Z/a_0)^{3/2} (1 - 2Zr/3a_0 + 2Z^2r^2/27a_0^2) \exp(-Zr/3a_0)$
	3 1 0	3p ₀	$\frac{2\sqrt{2}}{27\sqrt{\pi}} (Z/a_0)^{3/2} (1 - Zr/6a_0)(Zr/a_0) \exp(-Zr/3a_0) \cos \theta$
	3 1 ±1	3p _{±1}	$\mp \frac{2}{27\sqrt{\pi}} (Z/a_0)^{3/2} (1 - Zr/6a_0)(Zr/a_0) \exp(-Zr/3a_0) \sin \theta \exp(\pm i\phi)$
	3 2 0	3d ₀	$\frac{1}{81\sqrt{6\pi}} (Z/a_0)^{3/2} (Z^2r^2/a_0^2) \exp(-Zr/3a_0) (3 \cos^2 \theta - 1)$
	3 2 ±1	3d _{±1}	$\mp \frac{1}{81\sqrt{\pi}} (Z/a_0)^{3/2} (Z^2r^2/a_0^2) \exp(-Zr/3a_0) \sin \theta \cos \theta \exp(\pm i\phi)$
	3 2 ±2	3d _{±2}	$\frac{1}{162\sqrt{\pi}} (Z/a_0)^{3/2} (Z^2r^2/a_0^2) \exp(-Zr/3a_0) \sin^2 \theta \exp(\pm 2i\phi)$