

THIS IS THE relation used by Schrödinger* for calculating certain integrals involving Laguerre polynomials.

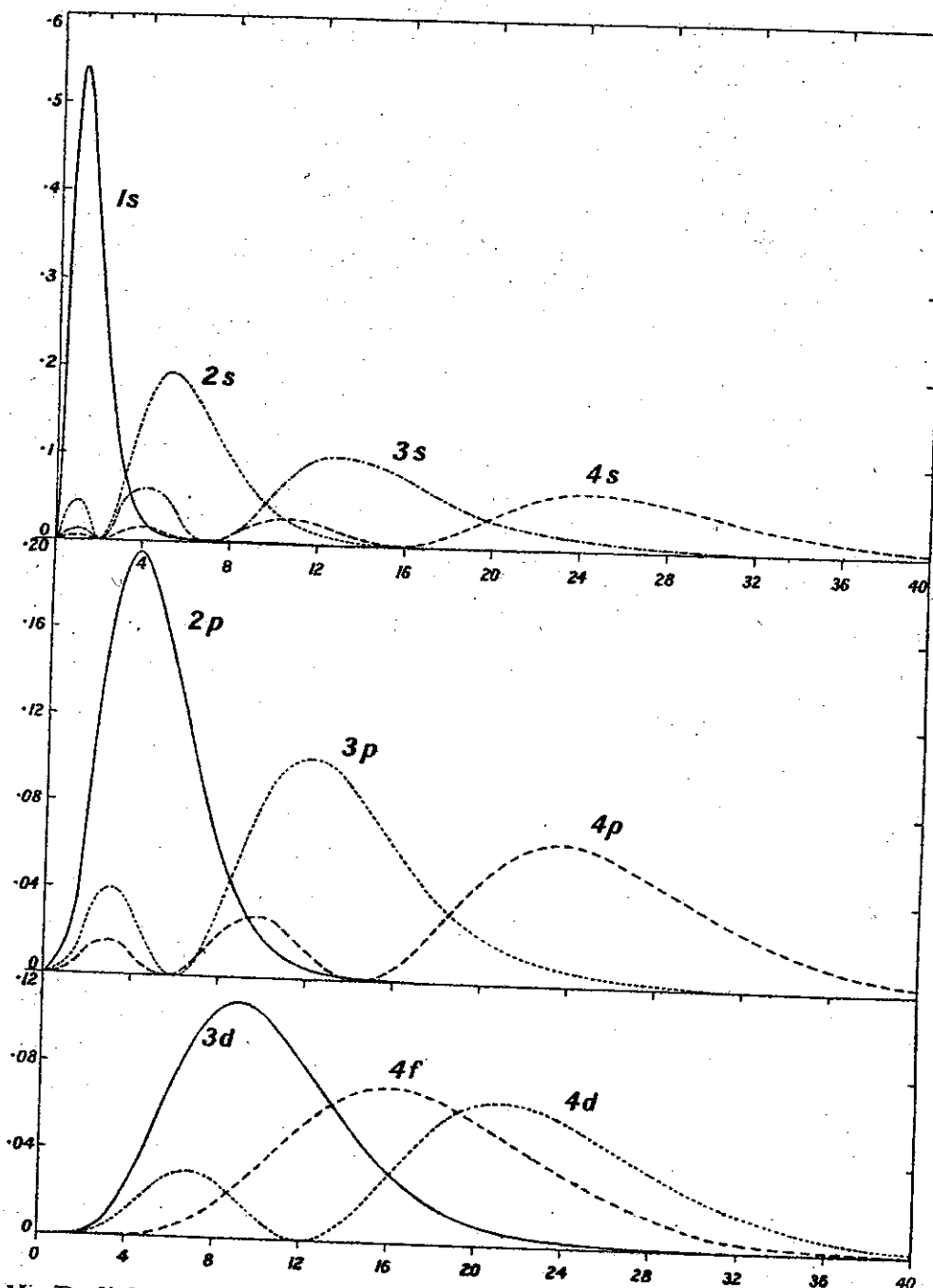


Fig. 15. Radial probability distribution $R^2(nl)$ for several of the lowest levels in hydrogen. (Abscissa is the radius in atomic units.)

In order to normalize the radial functions we need the result

$$\int_0^{\infty} \rho^{2l+2} e^{-\rho} [L_{n+l}^{2l+1}(\rho)]^2 d\rho = \frac{2n[(n+l)!]^3}{(n-l-1)!}, \quad (17)$$

which is readily obtained from the generating function or from Eckart's

* SCHRÖDINGER, Ann. der Phys. 80, 485 (1926).

formula. Therefore the final formula for the normalized radial function $R(nl)$ is

$$R(nl) = \sqrt{\frac{Z(n-l-1)!}{n^2 a [(n+l)!]^3}} e^{-\rho/2} \rho^{l+1} L_{n+l}^{2l+1}(\rho), \quad \rho = \frac{2Zr}{na} \quad (18)$$

which is normalized in the sense $\int_0^\infty R^2(nl) dr = 1$. Several of these functions are given explicitly in Table 1⁵. The probability of finding the electron in dr at r is $R^2(nl) dr$; this distribution function is plotted in Fig. 1⁵ for some of the lowest states.

TABLE 1⁵. Normalized radial eigenfunctions for $Z=1$.*

$$\begin{aligned} R(1s) &= -2re^{-r} & R(3p) &= -\frac{8}{27\sqrt{6}} r^2 e^{-\frac{1}{3}r} (1 - \frac{1}{3}r) \\ R(2s) &= -\frac{1}{\sqrt{2}} re^{-\frac{1}{2}r} (1 - \frac{1}{2}r) & R(4p) &= -\frac{1}{16} \sqrt{\frac{3}{5}} r^3 e^{-\frac{1}{4}r} (1 - \frac{1}{4}r + \frac{1}{80}r^2) \\ R(3s) &= -\frac{2}{3\sqrt{3}} re^{-\frac{1}{3}r} (1 - \frac{2}{3}r + \frac{2}{27}r^2) & R(3d) &= -\frac{4}{81\sqrt{30}} r^3 e^{-\frac{1}{3}r} \\ R(4s) &= -\frac{1}{16} re^{-\frac{1}{4}r} (1 - \frac{3}{4}r + \frac{1}{8}r^2 - \frac{1}{192}r^3) & R(4d) &= -\frac{1}{64\sqrt{5}} r^3 e^{-\frac{1}{2}r} (1 - \frac{1}{2}r) \\ R(2p) &= -\frac{1}{2\sqrt{6}} r^2 e^{-\frac{1}{2}r} & R(4f) &= -\frac{1}{768\sqrt{35}} r^4 e^{-\frac{1}{4}r} \end{aligned}$$

The average values of various powers of r for the hydrogenic wave functions are given in Table 2⁵. †

TABLE 2⁵.

k	$a^{-k} \int_0^\infty r^k R^2(nl) dr$
1	$\frac{1}{2Z} [3n^2 - l(l+1)]$
2	$\frac{n^2}{2Z^2} [5n^2 + 1 - 3l(l+1)]$
3	$\frac{n^2}{8Z^3} [35n^2(n^2 - 1) - 30n^2(l+2)(l-1) + 3(l+2)(l+1)l(l-1)]$
4	$\frac{n^4}{8Z^4} [63n^4 - 35n^2(2l^2 + 2l - 3) + 5l(l+1)(3l^2 + 3l - 10) + 12]$
-1	$\frac{Z}{n^2}$
-2	$\frac{Z^2}{n^2(l + \frac{1}{2})}$
-3	$\frac{Z^3}{n^3(l+1)(l + \frac{1}{2})l}$
-4	$\frac{Z^4 \frac{1}{2} [3n^2 - l(l+1)]}{n^5(l + \frac{3}{2})(l+1)(l + \frac{1}{2})l(l - \frac{1}{2})}$

* In this table r is measured in atomic units. The general eigenfunctions for any Z and arbitrary length unit are obtained by multiplying the functions of this table by $\sqrt{Z/a}$ and replacing r by Zr/a .

† The average values of r^{-5} and r^{-6} may be found in VAN VLECK, Proc. Roy. Soc. A143, 679 (1934).

The quantities occurring in 7⁴⁵ are thus completely expressed in terms of the integrals over the radial eigenfunctions.

The calculations may be exemplified by a detailed consideration of the line strengths in the fine structure of H_α, the ensemble of the $n = 3 \rightarrow n = 2$

TABLE 3⁵. Values of $\left[\int_0^\infty r R(n l) R(n' l-1) dr \right]^2$ in atomic units for $n' \neq n$.

$n l$	$n' l-1$	
np	$1s$	$2^8 n^7 (n-1)^{2n-5} (n+1)^{-2n-5}$
	$2s$	$2^{17} n^7 (n^2-1)(n-2)^{2n-6} (n+2)^{-2n-6}$
	$3s$	$2^{23} n^7 (n^2-1)(n-3)^{2n-8} (7n^2-27)^2 (n+3)^{-2n-8}$
	$4s$	$2^{26} 3^{-2} n^7 (n^2-1)(n-4)^{2n-10} (23n^4-288n^2+768)^2 (n+4)^{-2n-10}$
	$5s$	$2^{28} 3^{-2} 5 n^7 (n^2-1)(n-5)^{2n-12} (91n^6-2545n^4+20625n^2-46875)^2 (n+5)^{-2n-12}$
nd	$2p$	$2^{10} 3^{-1} n^9 (n^2-1)(n-2)^{2n-7} (n+2)^{-2n-7}$
	$3p$	$2^{11} 3^2 n^9 (n^2-1)(n^2-4)(n-3)^{2n-8} (n+3)^{-2n-8}$
	$4p$	$2^{30} 3^{-15} n^9 (n^2-1)(n^2-4)(n-4)^{2n-10} (9n^2-80)^2 (n+4)^{-2n-10}$
	$5p$	$2^{11} 3^{-3} 5 n^9 (n^2-1)(n^2-4)(n-5)^{2n-12} (67n^4-1650n^2+9375)^2 (n+5)^{-2n-12}$
nf	$3d$	$2^{13} 3^5 5^{-1} n^{11} (n^2-1)(n^2-4)(n-3)^{2n-9} (n+3)^{-2n-9}$
	$4d$	$2^{23} 3^{-2} 5^{-1} n^{11} (n^2-1)(n^2-4)(n^2-9)(n-4)^{2n-10} (n+4)^{-2n-10}$
	$5d$	$2^{13} 3^{-2} 5^{11} 7^{-1} n^{11} (n^2-1)(n^2-4)(n^2-9)(n-5)^{2n-12} (11n^2-175)^2 (n+5)^{-2n-12}$

TABLE 4⁵. Values of $\left[\int_0^\infty r R(n l) R(n' l-1) dr \right]^2$ in atomic units.

	$2p$	$3p$	$4p$	$5p$	$6p$	$7p$	$8p$
$1s$	1.66	0.267	0.093	0.044	0.024	0.015	0.010
$2s$	27.0	9.4	1.64	0.60	0.29	0.17	0.10
$3s$	0.9	162	29.9	5.1	1.9	0.9	0.5
$4s$	0.15	6.0	540	72.6	11.9	5.7	2.1
$5s$	0.052	0.9	21.2	1125	134	41.4	21.8
$6s$	0.025	0.33	2.9		2835		
$7s$	0.014	0.16	1.4			5292	
$8s$	0.009	0.09	0.8				9072

	$3d$	$4d$	$5d$	$6d$	$7d$	$8d$
$2p$	22.52	2.92	0.95	0.44	0.242	0.149
$3p$	101.2	57.2	8.8	3.0	1.44	0.82
$4p$	1.7	432	121.9	19.3	7.7	3.2
$5p$	0.23	9.1	1181.25	203	36	12.3
$6p$	0.08	1.3		2592		
$7p$	0.03	0.5			4961.25	
$8p$	0.02	0.2				8640

	$4f$	$5f$	$6f$	$7f$	$8f$
$3d$	104.6	11.0	3.2	1.4	0.8
$4d$	252.0	197.8	26.9	8.6	3.9
$5d$	2.75	900			
$6d$	0.32		2187		
$7d$	0.08			4410	
$8d$	0.04				7920