

Relativistic Wave Equations and Hydrogenic Atoms

B. A. Robson^{1,2} and S. H. Sutanto¹

Received November 2, 1999

The transition probabilities for the components of both the Balmer and Lyman α -lines of hydrogenic atoms are calculated for the nonrelativistic Schrödinger theory, the Dirac theory, and the recently developed eight-component (8-C) formalism. For large Z it is found that all three theories give significantly different results.

1. INTRODUCTION

Recently an eight-component (8-C) relativistic wave equation for spin- $\frac{1}{2}$ particles was proposed (Robson and Staudte, 1996; Staudte, 1996) in an attempt to place particles and antiparticles on a more symmetrical basis than occurs in the Dirac equation. The 8-C equation gives the same bound-state energy eigenvalue spectra for hydrogenic atoms as the Dirac equation but the wavefunctions are different, corresponding to a different Hamiltonian. This difference becomes greater as the nuclear charge Z increases. With a view to ultimately distinguish experimentally between the Dirac equation and the 8-C equation, it is necessary to investigate whether the different wavefunctions lead to different predictions for observable quantities that depend explicitly upon the wavefunctions, e.g., radiative transition probabilities between the hydrogenic atomic bound states. Unfortunately, the 8-C equation differs from the Dirac equation not only in having an enlarged solution space (eight components vs. four components), but also in requiring the use of an indefinite inner product, which complicates a direct comparison between the use of the two relativistic wave equations.

In this paper, the relative transition probabilities for the components of both the Balmer and Lyman α -lines of hydrogenic atoms will be discussed for the Schrödinger (non-relativistic), Dirac, and the 8-C wave equation formalisms.

¹Department of Theoretical Physics, Research School of Physical Sciences and Engineering, The Australian National University, Canberra, ACT 0200, Australia.

²To whom correspondence should be addressed at Department of Theoretical Physics, Research School of Physical Sciences and Engineering, The Australian National University, Canberra, ACT 0200, Australia.

2. SPONTANEOUS EMISSION AND NONRELATIVISTIC SCHRÖDINGER THEORY

The normal decay of an excited atomic state takes place by the spontaneous emission of radiation. This process can be described within the framework of time-dependent perturbation theory and in first order is given by Fermi's "Golden Rule" (Friedrich, 1990)

$$P_{fi} = \frac{2\pi}{\hbar} \langle \phi_f | W | \phi_i \rangle^2 \rho(E_f = E_i). \quad (1)$$

Here P_{fi} is the total probability per unit time for transitions from an initial state ϕ_i to all possible final states ϕ_f , $\rho(E_f)$ is the density of final states and W is the "small perturbation" causing the transition.

In the Schrödinger theory, the perturbing interaction (in the Coulomb gauge) to first order is given by

$$W_s = -\frac{e}{2\mu c} [\mathbf{p} \cdot \mathbf{A} + \mathbf{A} \cdot \mathbf{p}] \quad (2)$$

where \mathbf{p} is the momentum operator associated with the electron, \mathbf{A} is the vector potential operator associated with the electromagnetic field, $e = -|e|$ is the charge on the electron, and μ is the reduced mass of the hydrogenic atom.

The nonrelativistic Hamiltonian for the hydrogenic atom is

$$H_s = \frac{\mathbf{p}^2}{2\mu} - \frac{Ze^2}{r} \quad (3)$$

where $r = |\mathbf{r}|$ (measured in atomic length units), $\mathbf{r} = \mathbf{r}_e - \mathbf{r}_Z$, \mathbf{r}_e and \mathbf{r}_Z being the spatial coordinates of the electron and the nucleus, respectively.

In the Schrödinger theory, spin may be included in the two-component form and the eigenfunctions of the spin-independent Hamiltonian (3) can be written

$$|n, j, l, m_j\rangle = \sum_{m, m_s} R_{nl}(r) Y_{lm}(\Omega) \chi_{\frac{1}{2}m_s} C \left(l \frac{1}{2} j; m m_s m_j \right). \quad (4)$$

Here n , j , l , and m are the usual principal, total angular momentum, orbital angular momentum, and azimuthal quantum numbers, respectively. The spin quantum number, m_s , takes only the two values $+\frac{1}{2}$ and $-\frac{1}{2}$ so that it is convenient to represent the spin wavefunctions $\chi_{\frac{1}{2}m_s}$ in the form

$$\chi_{\frac{1}{2}\frac{1}{2}} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \chi_{\frac{1}{2}-\frac{1}{2}} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \quad (5)$$

The coefficient $C(l\frac{1}{2}j; m m_s m_j)$ is the Clebsch–Gordan coefficient as defined by Rose (1957) and which vanishes unless $m_j = m + m_s$. The radial wavefunction $R_{nl}(r)$ is given by

$$R_{nl}(r) = \frac{1}{(2l+1)!} \left[\frac{(n+l)!}{(n-l-1)!2n} \right]^{\frac{1}{2}} \left(\frac{2Z}{n} \right)^{\frac{1}{2}} \left(\frac{2Zr}{n} \right)^l \times \exp(-Zr/n) F(l+1-n, 2l+2; 2Zr/n) \quad (6)$$

where

$$F(a, b; x) = 1 + \frac{ax}{b} + \frac{a(a+1)x}{b(b+1)2!} + \dots \quad (7)$$

is the confluent hypergeometric function. The eigenenergies are given by the Bohr terms

$$E_n = -\frac{\mu e^4 Z^2}{2\hbar^2 n^2}, \quad n = 1, 2, 3, \dots \quad (8)$$

From (1) and (2) the probability per unit time for an atomic transition from an initial state $|\phi_i\rangle \equiv |njlm_j\rangle$ to a final state $|\phi_f\rangle \equiv |n'j'l'm_{j'}\rangle$ accompanied by the emission of a photon with wave vector \mathbf{k}_λ , angular frequency $\omega_\lambda = c|\mathbf{k}_\lambda|$, and polarization vector $\boldsymbol{\pi}_\lambda$ of unit length is given by

$$P_{fi} = \frac{1}{2\pi\hbar} \frac{e^2\omega_\lambda}{\mu^2 c^3} |\langle n'j'l'm_{j'} | e^{-i\mathbf{k}_\lambda \cdot \mathbf{r}} \boldsymbol{\pi}_\lambda \cdot \mathbf{p} | njlm_j \rangle|^2. \quad (9)$$

Thus the total probability per unit time for an atomic transition from all the initial states with the same n , l to all the final states with the same n' , j' , and l' accompanied by the emission of a photon of arbitrary polarization in any direction is

$$P_T = \sum_{m_{j'}, m_j} \sum_{\lambda} \int P_{fi} d\Omega_k \\ = \frac{2e^2}{\mu^2 c^2 \hbar} \sum_{m_{j'}, m_j} \sum_{\lambda} k_\lambda |\langle n'j'l'm_{j'} | e^{-i\mathbf{k}_\lambda \cdot \mathbf{r}} \boldsymbol{\pi}_\lambda \cdot \mathbf{p} | njlm_j \rangle|^2. \quad (10)$$

Taking the z -axis along \mathbf{k}_λ , i.e., $\mathbf{k}_\lambda = k_\lambda \hat{\mathbf{e}}_z$, the two polarization components $\boldsymbol{\pi}_\lambda$ can be represented by $\boldsymbol{\pi}_\pm = \mp \frac{1}{\sqrt{2}}(\hat{\mathbf{e}}_x \pm i\hat{\mathbf{e}}_y)$. Using the plane wave expansion

in terms of spherical harmonics and spherical Bessel functions

$$e^{-i\mathbf{k}_\lambda \cdot \mathbf{r}} = \sum_L [4\pi(2L + 1)]^{1/2} i^{-L} Y_{L0}(\Omega) j_L(k_\lambda r) \tag{11}$$

we obtain

$$\begin{aligned} & \langle n' j' l' m_{j'} | e^{-i\mathbf{k}_\lambda \cdot \mathbf{r}} \boldsymbol{\pi}_\pm \cdot \mathbf{p} | n j l m_j \rangle \\ &= i \sum_L (2L + 1) i^{-L} \sum_m C\left(l' \frac{1}{2} j'; m + 1 m_j - m m_{j'}\right) C\left(l \frac{1}{2} j; m m_j - m m_j\right) \\ & \times [\langle n' l' || j_L(k_\lambda r) || F_{nl}^{(+)} \rangle C(l' L l \pm 1; 0 0 0) C(l + 1 l l; 0 0 0) \\ & \times C(l + 1 L l'; m \pm 1 0 m \pm 1) C(l l l + 1; m, \pm 1 m \pm 1) \\ & + \langle n' l' || j_L(k_\lambda r) || F_{nl}^{(-)} \rangle C(l' L l - 1; 0 0 0) C(l - 1 l l; 0 0 0) \\ & \times C(l - 1 L l'; m \pm 1 0 m \pm 1) C(l l l - 1; m, \pm 1 m \pm 1)]. \end{aligned} \tag{12}$$

Here the functions $|F_{nl}^{(\pm)}\rangle$ are given by

$$F_{nl}^{(+)}(r) = \left(\frac{d}{dr} - \frac{l}{r}\right) R_{nl}(r) \quad \text{and} \quad F_{nl}^{(-)}(r) = \left(\frac{d}{dr} - \frac{l+1}{r}\right) R_{nl}(r) \tag{13}$$

and we have used (A38) of Bethe and Salpeter (1977). The quantities $\langle n' l' || j_L(k_\lambda r) || F_{nl}^{(\pm)} \rangle$ are radial reduced matrix elements. Using (12) in (10) gives the transition probabilities for the components of the Balmer and Lyman α -lines for various hydrogenic atoms presented in the columns labelled S in Tables I–XII.

Table I. Transition Probabilities (in s^{-1}) for the “Allowed” Components of the Balmer and Lyman α -Lines for $Z = 1$ Hydrogenic Atom for the Schrödinger (S), Dirac (D), and Eight-Component (8-C) Theories

Transition	S	D	8-C
$3D_{5/2} - 2P_{3/2}$	3.881 + 08	3.882 + 08	3.882 + 08
$3D_{3/2} - 2P_{3/2}$	4.312 + 07	4.313 + 07	4.313 + 07
$3D_{3/2} - 2P_{1/2}$	2.156 + 08	2.157 + 08	2.157 + 08
$3P_{3/2} - 2S_{1/2}$	8.984 + 07	8.986 + 07	8.986 + 07
$3P_{1/2} - 2S_{1/2}$	4.492 + 07	4.493 + 07	4.493 + 07
$3S_{1/2} - 2P_{3/2}$	8.422 + 06	8.425 + 06	8.426 + 06
$3S_{1/2} - 2P_{1/2}$	4.211 + 06	4.212 + 06	4.213 + 06
$2P_{3/2} - 1S_{1/2}$	2.507 + 09	2.508 + 09	2.508 + 09
$2P_{1/2} - 1S_{1/2}$	1.254 + 09	1.254 + 09	1.254 + 09

Table II. Transition Probabilities (in s^{-1}) for the “Allowed” Components of the Balmer and Lyman α -Lines for $Z = 18$ Hydrogenic Atom for the Schrödinger (S), Dirac (D), and Eight-Component (8-C) Theories

Transition	S	D	8-C
$3D_{5/2}-2P_{3/2}$	4.069 + 13	4.072 + 13	4.079 + 13
$3D_{3/2}-2P_{3/2}$	4.521 + 12	4.523 + 12	4.501 + 12
$3D_{3/2}-2P_{1/2}$	2.261 + 13	2.280 + 13	2.279 + 13
$3P_{3/2}-2S_{1/2}$	9.419 + 12	9.392 + 12	9.401 + 12
$3P_{1/2}-2S_{1/2}$	4.710 + 12	4.772 + 12	4.803 + 12
$3S_{1/2}-2P_{3/2}$	8.830 + 11	9.263 + 11	9.308 + 11
$3S_{1/2}-2P_{1/2}$	4.415 + 11	4.470 + 11	4.639 + 11
$2P_{3/2}-1S_{1/2}$	2.621 + 14	2.622 + 14	2.645 + 14
$2P_{1/2}-1S_{1/2}$	1.310 + 14	1.319 + 14	1.301 + 14

Table III. Transition Probabilities (in s^{-1}) for the “Allowed” Components of the Balmer and Lyman α -Lines for $Z = 30$ Hydrogenic Atom for the Schrödinger (S), Dirac (D), and Eight-Component (8-C) Theories

Transition	S	D	8-C
$3D_{5/2}-2P_{3/2}$	3.133 + 14	3.138 + 14	3.153 + 14
$3D_{3/2}-2P_{3/2}$	3.481 + 13	3.483 + 13	3.435 + 13
$3D_{3/2}-2P_{1/2}$	1.740 + 14	1.782 + 14	1.779 + 14
$3P_{3/2}-2S_{1/2}$	7.252 + 13	7.185 + 13	7.203 + 13
$3P_{1/2}-2S_{1/2}$	3.626 + 13	3.760 + 13	3.831 + 13
$3S_{1/2}-2P_{3/2}$	6.798 + 12	7.748 + 12	7.853 + 12
$3S_{1/2}-2P_{1/2}$	3.399 + 12	3.518 + 12	3.902 + 12
$2P_{3/2}-1S_{1/2}$	2.007 + 15	2.009 + 15	2.058 + 15
$2P_{1/2}-1S_{1/2}$	1.003 + 15	1.021 + 15	9.820 + 14

Table IV. Transition Probabilities (in s^{-1}) for the “Allowed” Components of the Balmer and Lyman α -Lines for $Z = 54$ Hydrogenic Atom for the Schrödinger (S), Dirac (D), and Eight-Component (8-C) Theories

Transition	S	D	8-C
$3D_{5/2}-2P_{3/2}$	3.263 + 15	3.278 + 15	3.329 + 15
$3D_{3/2}-2P_{3/2}$	3.626 + 14	3.629 + 14	3.471 + 14
$3D_{3/2}-2P_{1/2}$	1.813 + 15	1.957 + 15	1.948 + 15
$3P_{3/2}-2S_{1/2}$	7.554 + 14	7.248 + 14	7.295 + 14
$3P_{1/2}-2S_{1/2}$	3.777 + 14	4.268 + 14	4.562 + 14
$3S_{1/2}-2P_{3/2}$	7.081 + 13	1.062 + 14	1.110 + 14
$3S_{1/2}-2P_{1/2}$	3.541 + 13	3.970 + 13	5.614 + 13
$2P_{3/2}-1S_{1/2}$	2.051 + 16	2.053 + 16	2.225 + 16
$2P_{1/2}-1S_{1/2}$	1.026 + 16	1.086 + 16	9.523 + 15

Table V. Transition Probabilities (in s^{-1}) for the “Allowed” Components of the Balmer and Lyman α -Lines for $Z = 74$ Hydrogenic Atom for the Schrödinger (S), Dirac (D), and Eight-Component (8-C) Theories

Transition	S	D	8-C
$3D_{5/2}-2P_{3/2}$	1.140 + 16	1.149 + 16	1.183 + 16
$3D_{3/2}-2P_{3/2}$	1.266 + 15	1.267 + 15	1.165 + 15
$3D_{3/2}-2P_{1/2}$	6.331 + 15	7.299 + 15	7.262 + 15
$3P_{3/2}-2S_{1/2}$	2.638 + 15	2.360 + 15	2.372 + 15
$3P_{1/2}-2S_{1/2}$	1.319 + 15	1.680 + 15	1.943 + 15
$3S_{1/2}-2P_{3/2}$	2.473 + 14	5.085 + 14	5.557 + 14
$3S_{1/2}-2P_{1/2}$	1.236 + 14	1.548 + 14	3.066 + 14
$2P_{3/2}-1S_{1/2}$	6.994 + 16	6.972 + 16	8.153 + 16
$2P_{1/2}-1S_{1/2}$	3.497 + 16	3.891 + 16	3.004 + 16

Table VI. Transition Probabilities (in s^{-1}) for the “Allowed” Components of the Balmer and Lyman α -Lines for $Z = 92$ Hydrogenic Atom for the Schrödinger (S), Dirac (D), and Eight-Component (8-C) Theories

Transition	S	D	8-C
$3D_{5/2}-2P_{3/2}$	2.691 + 16	2.725 + 16	2.852 + 16
$3D_{3/2}-2P_{3/2}$	2.991 + 15	2.992 + 15	2.626 + 15
$3D_{3/2}-2P_{1/2}$	1.495 + 16	1.856 + 16	1.857 + 16
$3P_{3/2}-2S_{1/2}$	6.231 + 15	4.796 + 15	4.721 + 15
$3P_{1/2}-2S_{1/2}$	3.115 + 15	4.658 + 15	6.134 + 15
$3S_{1/2}-2P_{3/2}$	5.839 + 14	1.666 + 15	1.939 + 15
$3S_{1/2}-2P_{1/2}$	2.919 + 14	4.228 + 14	1.316 + 15
$2P_{3/2}-1S_{1/2}$	1.607 + 17	1.580 + 17	2.035 + 17
$2P_{1/2}-1S_{1/2}$	8.036 + 16	9.454 + 16	6.138 + 16

Table VII. Transition Probabilities (in s^{-1}) for the “Forbidden” Components of the Balmer and Lyman α -Lines for $Z = 1$ Hydrogenic Atom for the Schrödinger (S), Dirac (D), and Eight-Component (8-C) Theories

Transition	S	D	8-C
$3D_{5/2}-2P_{1/2}$	1.344 - 04	3.115 - 04	1.019 - 03
$3D_{5/2}-2S_{1/2}$	3.062 + 02	3.063 + 02	3.063 + 02
$3D_{3/2}-2S_{1/2}$	2.041 + 02	2.042 + 02	2.042 + 02
$3P_{3/2}-2P_{3/2}$	4.784 + 01	4.785 + 01	4.785 + 01
$3P_{3/2}-2P_{1/2}$	4.784 + 01	4.785 + 01	4.785 + 01
$3P_{1/2}-2P_{3/2}$	4.784 + 01	4.785 + 01	4.785 + 01
$3P_{1/2}-2P_{1/2}$	1.090 - 10	9.816 - 10	2.727 - 09
$3S_{1/2}-2S_{1/2}$	0.000 + 00	3.756 - 09	3.756 - 09
$2S_{1/2}-1S_{1/2}$	0.000 + 00	4.993 - 06	4.993 - 06

Table VIII. Transition Probabilities (in s^{-1}) for the “Forbidden” Components of the Balmer and Lyman α -Lines for $Z = 18$ Hydrogenic Atom for the Schrödinger (S), Dirac (D), and Eight-Component (8-C) Theories

Transition	S	D	8-C
$3D_{5/2}-2P_{1/2}$	1.480 + 06	3.524 + 06	1.162 + 07
$3D_{5/2}-2S_{1/2}$	1.040 + 10	1.065 + 10	1.072 + 10
$3D_{3/2}-2S_{1/2}$	6.934 + 09	7.081 + 09	7.110 + 09
$3P_{3/2}-2P_{3/2}$	1.626 + 09	1.626 + 09	1.627 + 09
$3P_{3/2}-2P_{1/2}$	1.626 + 09	1.640 + 09	1.660 + 09
$3P_{1/2}-2P_{3/2}$	1.626 + 09	1.632 + 09	1.634 + 09
$3P_{1/2}-2P_{1/2}$	3.889 + 02	3.603 + 03	1.019 + 04
$3S_{1/2}-2S_{1/2}$	0.000 + 00	1.379 + 04	1.396 + 04
$2S_{1/2}-1S_{1/2}$	0.000 + 00	1.816 + 07	1.839 + 07

Table IX. Transition Probabilities (in s^{-1}) for the “Forbidden” Components of the Balmer and Lyman α -Lines for $Z = 30$ Hydrogenic Atom for the Schrödinger (S), Dirac (D), and Eight-Component (8-C) Theories

Transition	S	D	8-C
$3D_{5/2}-2P_{1/2}$	8.798 + 07	2.199 + 08	7.345 + 08
$3D_{5/2}-2S_{1/2}$	2.224 + 11	2.378 + 11	2.419 + 11
$3D_{3/2}-2S_{1/2}$	1.483 + 11	1.572 + 11	1.591 + 11
$3P_{3/2}-2P_{3/2}$	3.478 + 10	3.480 + 10	3.486 + 10
$3P_{3/2}-2P_{1/2}$	3.478 + 10	3.561 + 10	3.688 + 10
$3P_{1/2}-2P_{3/2}$	3.478 + 10	3.511 + 10	3.534 + 10
$3P_{1/2}-2P_{1/2}$	6.421 + 04	6.268 + 05	1.833 + 06
$3S_{1/2}-2S_{1/2}$	0.000 + 00	2.397 + 06	2.485 + 06
$2S_{1/2}-1S_{1/2}$	0.000 + 00	3.105 + 09	3.217 + 09

Table X. Transition Probabilities (in s^{-1}) for the “Forbidden” Components of the Balmer and Lyman α -Lines for $Z = 54$ Hydrogenic Atom for the Schrödinger (S), Dirac (D), and Eight-Component (8-C) Theories

Transition	S	D	8-C
$3D_{5/2}-2P_{1/2}$	9.638 + 09	2.868 + 10	1.007 + 11
$3D_{5/2}-2S_{1/2}$	7.506 + 12	9.335 + 12	9.903 + 12
$3D_{3/2}-2S_{1/2}$	5.004 + 12	6.079 + 12	6.347 + 12
$3P_{3/2}-2P_{3/2}$	1.176 + 12	1.180 + 12	1.183 + 12
$3P_{3/2}-2P_{1/2}$	1.176 + 12	1.268 + 12	1.439 + 12
$3P_{1/2}-2P_{3/2}$	1.176 + 12	1.205 + 12	1.254 + 12
$3P_{1/2}-2P_{1/2}$	2.279 + 07	2.696 + 08	8.938 + 08
$3S_{1/2}-2S_{1/2}$	0.000 + 00	1.030 + 09	1.167 + 09
$2S_{1/2}-1S_{1/2}$	0.000 + 00	1.255 + 12	1.418 + 12

Table XI. Transition Probabilities (in s^{-1}) for the “Forbidden” Components of the Balmer and Lyman α -Lines for $Z = 74$ Hydrogenic Atom for the Schrödinger (S), Dirac (D), and Eight-Component (8-C) Theories

Transition	S	D	8-C
$3D_{5/2}-2P_{1/2}$	1.190 + 11	4.452 + 11	1.689 + 12
$3D_{5/2}-2S_{1/2}$	4.922 + 13	7.462 + 13	8.420 + 13
$3D_{3/2}-2S_{1/2}$	3.281 + 13	4.795 + 13	5.274 + 13
$3P_{3/2}-2P_{3/2}$	7.731 + 12	7.811 + 12	7.822 + 12
$3P_{3/2}-2P_{1/2}$	7.730 + 12	8.871 + 12	1.176 + 13
$3P_{1/2}-2P_{3/2}$	7.730 + 12	7.957 + 12	9.046 + 12
$3P_{1/2}-2P_{1/2}$	5.283 + 08	8.181 + 09	3.264 + 10
$3S_{1/2}-2S_{1/2}$	0.000 + 00	3.123 + 10	4.040 + 10
$2S_{1/2}-1S_{1/2}$	0.000 + 00	3.489 + 13	4.477 + 13

3. DIRAC THEORY

In the Dirac theory of spontaneous emission, the perturbing interaction (in the Coulomb gauge) to first order is

$$W_D = -e\alpha \cdot \mathbf{A} \quad (14)$$

where

$$\alpha = \begin{pmatrix} \mathbf{0} & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & \mathbf{0} \end{pmatrix} \quad (15)$$

$\boldsymbol{\sigma}$ being the usual Pauli spin vector with components

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (16)$$

Table XII. Transition Probabilities (in s^{-1}) for the “Forbidden” Components of the Balmer and Lyman α -Lines for $Z = 92$ Hydrogenic Atom for the Schrödinger (S), Dirac (D), and Eight-Component (8-C) Theories

Transition	S	D	8-C
$3D_{5/2}-2P_{1/2}$	6.730 + 11	3.338 + 12	1.422 + 13
$3D_{5/2}-2S_{1/2}$	1.797 + 14	3.469 + 14	4.280 + 14
$3D_{3/2}-2S_{1/2}$	1.198 + 14	2.219 + 14	2.655 + 14
$3P_{3/2}-2P_{3/2}$	2.830 + 13	2.900 + 13	2.882 + 13
$3P_{3/2}-2P_{1/2}$	2.829 + 13	3.478 + 13	6.010 + 13
$3P_{1/2}-2P_{3/2}$	2.829 + 13	2.848 + 13	3.895 + 13
$3P_{1/2}-2P_{1/2}$	4.619 + 09	1.029 + 11	5.367 + 11
$3S_{1/2}-2S_{1/2}$	0.000 + 00	3.930 + 11	6.179 + 11
$2S_{1/2}-1S_{1/2}$	0.000 + 00	3.894 + 14	6.005 + 14

The Dirac Hamiltonian for the hydrogenic atom

$$H_D = c\boldsymbol{\alpha} \cdot \mathbf{p} + \beta\mu c^2 - \frac{Ze^2}{r} \tag{17}$$

with

$$\beta = \begin{pmatrix} \mathbf{1}_2 & \mathbf{0} \\ \mathbf{0} & -\mathbf{1}_2 \end{pmatrix}. \tag{18}$$

The eigenfunctions of the Hamiltonian (17) can be written

$$|njlm_j\rangle = \sum_{m_s} \left[\begin{matrix} g(r)C(l\frac{1}{2}j; mm_s m_j)Y_{lm}(\Omega)\chi_{\frac{1}{2}m_s} \\ if(r)C(\bar{l}\frac{1}{2}j; mm_s m_j)Y_{\bar{l}m}(\Omega)\chi_{\frac{1}{2}m_s} \end{matrix} \right] \tag{19}$$

where $\bar{l} = l \pm 1$ for $j = l \pm \frac{1}{2}$ and the radial functions are (Bethe and Salpeter, 1977)

$$\begin{aligned} g(r) = & -\frac{[\Gamma(2\gamma + \tilde{n} + 1)^{\frac{1}{2}}]}{\Gamma(2\gamma + 1)(\tilde{n}!)^{\frac{1}{2}}} \left[\frac{(1 + \epsilon)}{4N(N - \kappa)} \right]^{\frac{1}{2}} \left(\frac{2Z}{N} \right)^{\frac{3}{2}} \left(\frac{2Zr}{N} \right)^{\gamma-1} \\ & \times \exp(-Zr/N) [-\tilde{n}F(1 - \tilde{n}, 2\gamma + 1; 2Zr/N) \\ & + (N - \kappa)F(-\tilde{n}, 2\gamma + 1; 2Zr/N)] \end{aligned} \tag{20}$$

and

$$\begin{aligned} f(r) = & -\frac{[\Gamma(2\gamma + \tilde{n} + 1)^{\frac{1}{2}}]}{\Gamma(2\gamma + 1)(\tilde{n}!)^{\frac{1}{2}}} \left[\frac{(1 - \epsilon)}{4N(N - \kappa)} \right]^{\frac{1}{2}} \left(\frac{2Z}{N} \right)^{\frac{3}{2}} \left(\frac{2Zr}{N} \right)^{\gamma-1} \\ & \times \exp(-Zr/N) [\tilde{n}F(1 - \tilde{n}, 2\gamma + 1; 2Zr/N) \\ & + (N - \kappa)F(-\tilde{n}, 2\gamma + 1; 2Zr/N)]. \end{aligned} \tag{21}$$

Here

$$\begin{aligned} \kappa = & -(l + 1) && \text{for } j = l + \frac{1}{2} \\ = & +l && \text{for } j = l - \frac{1}{2} \end{aligned} \tag{22}$$

$$\gamma = [\kappa^2 - \alpha^2 Z^2]^{\frac{1}{2}} \quad \text{with } \alpha = e^2/\hbar c. \tag{23}$$

$$\tilde{n} = n - |\kappa| \tag{24}$$

$$\epsilon = \left[1 + \frac{\alpha^2 Z^2}{(\tilde{n} + \gamma)^2} \right]^{-\frac{1}{2}} \tag{25}$$

and

$$N = [n^2 - 2\tilde{n}(|k| - \gamma)]^{\frac{1}{2}}. \tag{26}$$

Corresponding to (9) we have

$$P_{fi} = \frac{1}{2\pi\hbar} \frac{e^2\omega_\lambda}{c} |\langle n' j' l' m_{j'} | e^{-i\mathbf{k}_\lambda \cdot \mathbf{r}} \boldsymbol{\pi}_\lambda \cdot \boldsymbol{\alpha} | n j l m_j \rangle|^2. \tag{27}$$

Using spherical components of $\boldsymbol{\alpha}$:

$$\alpha_0 = \alpha_z, \quad \alpha_\pm = \mp \frac{1}{\sqrt{2}}(\alpha_x \pm i\alpha_y) \tag{28}$$

and the plane-wave expansion (11) one obtains

$$\begin{aligned} & \langle n' j' l' m_{j'} | e^{-i\mathbf{k}_\lambda \cdot \mathbf{r}} \alpha_\pm | n j l m_j \rangle \\ &= \mp i\sqrt{2} \sum_L i^{-L} (2L+1) \left[\langle g' \| j_L(k_\lambda r) \| f \rangle C\left(l' \frac{1}{2} j'; m_j \pm \frac{1}{2}, \pm \frac{1}{2} m_j \pm 1\right) \right. \\ & \quad \times C\left(\bar{l}' \frac{1}{2} j'; m_j \pm \frac{1}{2}, \mp \frac{1}{2} m_j\right) C\left(\bar{l}' L l'; m_j \pm \frac{1}{2} 0 m_j \pm \frac{1}{2}\right) C(l' L \bar{l}'; 0 0 0) \\ & \quad - \langle f' \| j_L(k_\lambda r) \| g \rangle C\left(\bar{l}' \frac{1}{2} j'; m_j \pm \frac{1}{2}, \pm \frac{1}{2} m_j \pm 1\right) \\ & \quad \left. \times C\left(l \frac{1}{2} j; m_j \pm \frac{1}{2}, \mp \frac{1}{2} m_j\right) C\left(l L \bar{l}'; m_j \pm \frac{1}{2} 0 m_j \pm \frac{1}{2}\right) C(\bar{l}' L l; 0 0 0) \right] \tag{29} \end{aligned}$$

where $\alpha_\pm \equiv \boldsymbol{\pi}_\pm \cdot \boldsymbol{\alpha}$. Using (29) in the relation corresponding to (10):

$$P_T = \frac{2e^2}{\hbar} \sum_{m_{j'}, m_j} \sum_{\lambda} k_\lambda |\langle n' j' l' m_{j'} | e^{-i\mathbf{k}_\lambda \cdot \mathbf{r}} \boldsymbol{\pi}_\lambda \cdot \boldsymbol{\alpha} | n j l m_j \rangle|^2 \tag{30}$$

gives the transition probabilities for the components of the Balmer and Lyman α -lines for various hydrogenic atoms presented in the columns labelled D in Tables I–XII.

4. EIGHT-COMPONENT THEORY

The 8-C equation for a hydrogenic atom in the presence of an external electromagnetic field is, in the Weyl representation, given (Robson and Staudte, 1996) by

$$\left(i\hbar \frac{\partial}{\partial t} \mathbf{1}_8 \right) \Psi_{FV1/2} = H_{FV1/2} \Psi_{FV1/2} \tag{31}$$

where

$$H_{\text{FV}1/2} = \begin{pmatrix} H_\xi & \mathbf{0} \\ \mathbf{0} & H_\eta \end{pmatrix} \quad (32)$$

and

$$\begin{aligned} H_\xi &= (\tau_3 + i\tau_2) \otimes \left(\frac{\hbar^2}{2\mu} \left[-\mathbf{D}^2 \mathbf{1}_2 + \frac{ie}{\hbar c} \boldsymbol{\sigma} \cdot (\mathbf{E} + i\mathbf{B}) \right] \right) \\ &\quad + \tau_3 \otimes (\mu c^2 \mathbf{1}_2) + eA_0 \mathbf{1}_4 \end{aligned} \quad (33)$$

$$\begin{aligned} H_\eta &= (\tau_3 + i\tau_2) \otimes \left(\frac{\hbar^2}{2\mu} \left[-\mathbf{D}^2 \mathbf{1}_2 - \frac{ie}{\hbar c} \boldsymbol{\sigma} \cdot (\mathbf{E} - i\mathbf{B}) \right] \right) \\ &\quad + \tau_3 \otimes (\mu c^2 \mathbf{1}_2) + eA_0 \mathbf{1}_4 \end{aligned} \quad (34)$$

where τ_i are the standard Pauli matrices, \otimes is the Kronecker (direct) product, \mathbf{E} and \mathbf{B} are the electromagnetic field intensities, and $\mathbf{D} = \partial + (ie/\hbar c) \mathbf{A}$ is the usual minimal coupling. Thus in the absence of an external electromagnetic field, the 8-C Hamiltonian for a hydrogenic atom is (setting $A_0 = -Ze/r$)

$$H_8 = \frac{\mathbf{p}^2}{2\mu} X - \frac{iZe^2\hbar}{2\mu cr^3} \boldsymbol{\Sigma} \cdot \mathbf{r} + \mu c^2 Y - \frac{Ze^2}{r} \mathbf{1}_8 \quad (35)$$

where $X = [\mathbf{1}_2 \otimes (\tau_3 + i\tau_2) \otimes \mathbf{1}_2]$, $\boldsymbol{\Sigma} = [\tau_3 \otimes (\tau_3 + i\tau_2) \otimes \boldsymbol{\sigma}]$, and $Y = [\mathbf{1}_2 \otimes \tau_3 \otimes \mathbf{1}_2]$.

It should be noted that in this we have assumed the decoupled form of the 8-C theory so that the inner product is given (Staudte, 1996) by

$$\langle \Psi | \Psi \rangle = \int \Psi^\dagger(x) \tau_5 \Psi(x) d^3x \quad (36)$$

where $\tau_5 = \tau_1 \otimes \tau_3 \otimes \mathbf{1}_2$.

Choosing the Coulomb gauge i.e., $\mathbf{E} = -(1/c)\partial\mathbf{A}/\partial t$, $\mathbf{B} = \nabla \times \mathbf{A}$ for the external field in (33) and (34) gives the perturbing interaction to first order for spontaneous emission as the sum of three terms:

$$W_8 = W_8^{(1)} + W_8^{(2)} + W_8^{(3)} \quad (37)$$

where

$$W_8^{(1)} = -\frac{e}{2\mu c} [\mathbf{p} \cdot \mathbf{A} + \mathbf{A} \cdot \mathbf{p}] X \quad (38)$$

$$W_8^{(2)} = -\frac{ie\hbar}{2\mu c^2} \left[\tau_3 \otimes (\tau_3 + i\tau_2) \otimes \boldsymbol{\sigma} \cdot \frac{\partial}{\partial t} \mathbf{A} \right] \quad (39)$$

$$W_8^{(3)} = -\frac{e\hbar}{2\mu c} [\mathbf{1}_2 \otimes (\tau_3 + i\tau_2) \otimes \boldsymbol{\sigma} \cdot \nabla \times \mathbf{A}]. \tag{40}$$

The eigenfunctions of the Hamiltonian (35) $|njlm_j\rangle$ can be written as (Robson and Staudte, 1996)

$$\sum_{m, m_s} \begin{bmatrix} \bar{g}(r) \{ C(l\frac{1}{2}j; mm_s m_j) Y_{lm}(\Omega) + i\bar{\kappa} C(\bar{l}\frac{1}{2}j; mm_s m_j) Y_{\bar{l}m}(\Omega) \} \chi_{\frac{1}{2}m_s} \\ \bar{f}(r) \{ C(l\frac{1}{2}j; mm_s m_j) Y_{lm}(\Omega) + i\bar{\kappa} C(\bar{l}\frac{1}{2}j; mm_s m_j) Y_{\bar{l}m}(\Omega) \} \chi_{\frac{1}{2}m_s} \\ \bar{g}(r) \{ C(l\frac{1}{2}j; mm_s m_j) Y_{lm}(\Omega) - i\bar{\kappa} C(\bar{l}\frac{1}{2}j; mm_s m_j) Y_{\bar{l}m}(\Omega) \} \chi_{\frac{1}{2}m_s} \\ \bar{f}(r) \{ C(l\frac{1}{2}j; mm_s m_j) Y_{lm}(\Omega) - i\bar{\kappa} C(\bar{l}\frac{1}{2}j; mm_s m_j) Y_{\bar{l}m}(\Omega) \} \chi_{\frac{1}{2}m_s} \end{bmatrix} \tag{41}$$

where $\bar{l} = l \pm 1$ for $j = l \pm \frac{1}{2}$ and the radial functions are given by

$$\begin{aligned} \bar{g}(r) &= \frac{|\Lambda|^2 [\Gamma(2\bar{\gamma} + \tilde{n}' + 1)]^{\frac{1}{2}}}{\Gamma(2\bar{\gamma} + 2) [Z(\tilde{n}' - 1)!]^{\frac{1}{2}}} \{2|\Lambda|r\}^{\bar{\gamma}} \{1 + \epsilon + \alpha^2 Z/r\} \\ &\times \frac{\exp(-|\Lambda|r)}{\{2(1 - \bar{\kappa}^2)\}^{\frac{1}{2}}} F(1 - \tilde{n}', 2\bar{\gamma} + 2; 2|\Lambda|r) \end{aligned} \tag{42}$$

$$\begin{aligned} \bar{f}(r) &= \frac{|\Lambda|^2 [\Gamma(2\bar{\gamma} + \tilde{n}' + 1)]^{\frac{1}{2}}}{\Gamma(2\bar{\gamma} + 2) [Z(\tilde{n}' - 1)!]^{\frac{1}{2}}} \{2|\Lambda|r\}^{\bar{\gamma}} \{1 - \epsilon - \alpha^2 Z/r\} \\ &\times \frac{\exp(-|\Lambda|r)}{\{2(1 - \bar{\kappa}^2)\}^{\frac{1}{2}}} F(1 - \tilde{n}', 2\bar{\gamma} + 2; 2|\Lambda|r) \end{aligned} \tag{43}$$

Here

$$\begin{aligned} \bar{\gamma} &= \gamma - 1 \quad \text{for } j = l + \frac{1}{2} \\ &= \gamma \quad \text{for } j = l - \frac{1}{2} \end{aligned} \tag{44}$$

$$Z\alpha\bar{\kappa} = \kappa \pm \gamma \quad \text{for } j = l \pm \frac{1}{2} \tag{45}$$

$$\tilde{n}' + \bar{\gamma} = \tilde{n} + \gamma \tag{46}$$

and

$$|\Lambda| = Z/N. \tag{47}$$

In the eight-component theory, corresponding to (9) we have

$$P_{\bar{n}} = \frac{1}{2\pi\hbar} \frac{e^2 k_\lambda}{\mu^2 c^2} |M_1^\lambda + M_2^\lambda + M_3^\lambda|^2 \tag{48}$$

where

$$M_1^\lambda = \langle n' j' l' m_{j'} | \tau_5 e^{-i\mathbf{k}_\lambda \cdot \mathbf{r}} \boldsymbol{\pi}_\lambda \cdot \mathbf{p} X | n j l m_j \rangle \quad (49)$$

$$M_2^\lambda = -\frac{\hbar k_\lambda}{2} \langle n' j' l' m_{j'} | \tau_5 e^{-i\mathbf{k}_\lambda \cdot \mathbf{r}} \boldsymbol{\pi}_\lambda \cdot \boldsymbol{\Sigma} | n j l m_j \rangle \quad (50)$$

$$M_3^\lambda = -\frac{\hbar k_\lambda}{2} \langle n' j' l' m_{j'} | \tau_5 e^{-i\mathbf{k}_\lambda \cdot \mathbf{r}} \boldsymbol{\pi}_\lambda \cdot \boldsymbol{\Sigma}' | n j l m_j \rangle \quad (51)$$

are the matrix elements corresponding to $W_8^{(1)}$, $W_8^{(2)}$, and $W_8^{(3)}$, respectively, and

$$\boldsymbol{\Sigma}' = \mathbf{1}_2 \otimes (\tau_3 + i\tau_2) \otimes \boldsymbol{\sigma}. \quad (52)$$

Using the plane wave expansion (11) and the polarization components $\boldsymbol{\pi}_\pm$, one obtains

$$\begin{aligned} M_1^{(\pm)} = & 2i \sum_L (2L+1) i^{-L} \sum_{m_s} \left[C\left(l' \frac{1}{2} j'; m_j - m_s \pm 1 m_s m_j \pm 1\right) \right. \\ & \times C\left(l \frac{1}{2} j; m_j - m_s m_s m_j\right) \\ & \times \{ \langle \bar{g}' + \bar{f}' \| j_L(k_\lambda r) \| F_{njl}^{(+)} \rangle C(l+1Ll'; m_j - m_s \pm 10m_j - m_s \pm 1) \\ & \times C(l' Ll + 1; 000) C(l1l + 1; m_j - m_s, \pm 1m_j - m_s \pm 1) \\ & \times C(l+11l; 000) \\ & + \langle \bar{g}' + \bar{f}' \| j_L(k_\lambda r) \| F_{njl}^{(-)} \rangle C(l-1Ll'; m_j - m_s \pm 10m_j - m_s \pm 1) \\ & \times C(l' Ll - 1; 000) C(l1l - 1; m_j - m_s, \pm 1m_j - m_s \pm 1) \\ & \times C(l-11l; 000) \} \\ & - \bar{\kappa}' \bar{\kappa} C\left(\bar{l}' \frac{1}{2} j'; m_j - m_s \pm 1 m_s m_j \pm 1\right) C\left(\bar{l} \frac{1}{2} j; m_j - m_s m_s m_j\right) \\ & \times \{ \langle \bar{g}' + \bar{f}' \| j_L(k_\lambda r) \| F_{njl}^{(+)} \rangle C(\bar{l} + 1L\bar{l}'; m_j - m_s \pm 10m_j - m_s \pm 1) \\ & \times C(\bar{l}' L\bar{l} + 1; 000) C(\bar{l}1\bar{l} + 1; m_j - m_s, \pm 1m_j - m_s \pm 1) \\ & \times C(\bar{l} + 11\bar{l} 000) \\ & + \langle \bar{g}' + \bar{f}' \| j_L(k_\lambda r) \| F_{njl}^{(-)} \rangle C(\bar{l} - 1L\bar{l}'; m_j - m_s \pm 10m_j - m_s \pm 1) \\ & \times C(\bar{l}' L\bar{l} - 1; 000) C(\bar{l}1\bar{l} - 1; m_j - m_s, \pm 1m_j - m_s \pm 1) \\ & \times C(\bar{l} - 11\bar{l}; 000) \} \left. \right] \quad (53) \end{aligned}$$

$$\begin{aligned}
M_2^{(\pm)} &= \pm \hbar k_\lambda \sqrt{2i} \sum_L (2L+1) i^{-L} \langle \bar{g}' + \bar{f}' \| j_L(k_\lambda r) \| \bar{g} + \bar{f} \rangle \\
&\times \left[\bar{\kappa}' C \left(\bar{l}' \frac{1}{2} j'; m_j \pm \frac{1}{2}, \pm \frac{1}{2} m_j \pm 1 \right) C \left(l \frac{1}{2} j; m_j \pm \frac{1}{2}, \mp \frac{1}{2} m_j \right) \right. \\
&\times C \left(l L \bar{l}'; m_j \pm \frac{1}{2} 0 m_j \pm \frac{1}{2} \right) C(\bar{l}' L l; 0 0 0) \\
&+ \bar{\kappa} C \left(l' \frac{1}{2} j'; m_j \pm \frac{1}{2}, \pm \frac{1}{2} m_j \pm 1 \right) C \left(\bar{l} \frac{1}{2} j; m_j \pm \frac{1}{2}, \mp \frac{1}{2} m_j \right) \\
&\left. \times C \left(\bar{l} L l'; m_j \pm \frac{1}{2} 0 m_j \pm \frac{1}{2} \right) C(l' L \bar{l}; 0 0 0) \right] \quad (54)
\end{aligned}$$

$$\begin{aligned}
M_3^{(\pm)} &= \pm \hbar k_\lambda \sqrt{2} \sum_L (2L+1) i^{-L} \langle \bar{g}' + \bar{f}' \| j_L(k_\lambda r) \| \bar{g} + \bar{f} \rangle \\
&\times \left[C \left(l' \frac{1}{2} j'; m_j \pm \frac{1}{2}, \pm \frac{1}{2} m_j \pm 1 \right) C \left(l \frac{1}{2} j; m_j \pm \frac{1}{2}, \mp \frac{1}{2} m_j \right) \right. \\
&\times C \left(l L l'; m_j \pm \frac{1}{2} 0 m_j \pm \frac{1}{2} \right) C(l' L l; 0 0 0) \\
&- \bar{\kappa}' \bar{\kappa} C \left(\bar{l}' \frac{1}{2} j'; m_j \pm \frac{1}{2}, \pm \frac{1}{2} m_j \pm 1 \right) C \left(\bar{l} \frac{1}{2} j; m_j \pm \frac{1}{2}, \mp \frac{1}{2} m_j \right) \\
&\left. \times C \left(\bar{l} L \bar{l}'; m_j \pm \frac{1}{2} 0 m_j \pm \frac{1}{2} \right) C(\bar{l}' L \bar{l}; 0 0 0) \right]. \quad (55)
\end{aligned}$$

Using (53), (54), and (55) in the relation corresponding to (10):

$$P_T = \frac{2e^2}{\hbar \mu^2 c^2} \sum_{m_j', m_j} \sum_\lambda k_\lambda |M_1^\lambda + M_2^\lambda + M_3^\lambda|^2 \quad (56)$$

gives the transition probabilities for the components of the Balmer and Lyman α -lines for various hydrogenic atoms presented in the columns labelled 8-C in Tables I–XII.

5. COMPARISON OF RESULTS AND CONCLUSION

Tables I–VI show the transition probabilities (in s^{-1}) for the “allowed” components of the Balmer and Lyman α -lines for various hydrogenic atoms ($Z = 1, 18, 30, 54, 74,$ and 92). Tables VII–XII show the corresponding transition probabilities for the “forbidden” components, i.e., those components which are not allowed in the usual dipole approximation (Friedrich, 1990). The columns labelled S show

the results given by the nonrelativistic Schrödinger theory (Eq. (10)). The results for the “allowed” components for hydrogen agree with those of Condon and Shortley (1935). The columns labelled D give the predictions of the Dirac theory (Eq. (30)). These are in close agreement with those of Pal’chikov (1998) and differ considerably from the Schrödinger results for large Z . The columns labelled 8-C show the results for the eight-component theory (Eq. (56)). As for the Dirac theory, the predictions of the 8-C theory for low Z are approximately the same as the Schrödinger predictions. However, for larger values of Z , it is seen that the results differ significantly from both the Schrödinger and Dirac results. These results indicate for the first time that the Dirac and 8-C theories are not identical in all their predictions.

The calculated differences between the two relativistic formalisms imply that in special circumstances it may be possible to determine by observation which theory is valid. However, at the present time, it is impossible to measure directly the transition probabilities for the components of the Balmer and Lyman α -lines for high Z hydrogenic atoms since the lifetimes of the excited states are too short so that the “allowed” transitions are prompt. On the other hand, the “forbidden” transitions are masked by “allowed” transitions, except for the $3D_{5/2}$ to $2P_{1/2}$ or $2S_{1/2}$ transitions. These “forbidden” transitions may eventually be measurable for intermediate Z values ($Z \simeq 50$) where the transition probabilities are $\simeq 6 \times 10^{12} \text{ s}^{-1}$. However for $Z = 50$, the differences between the Dirac and 8-C theories are only $\simeq 5\%$ for the dominant mode $3D_{5/2}$ to $2S_{1/2}$.

REFERENCES

- Bethe, H. A. and Salpeter, E. E. (1977). *Quantum Mechanics of One and Two Electron Atoms*, Plenum, New York.
- Condon, E. U. and Shortley, G. H. (1935). *The Theory of Atomic Spectra*, Cambridge University Press, Cambridge, p. 134.
- Friedrich, H. (1990). *Theoretical Atomic Physics*, Springer, Berlin, Heidelberg.
- Pal’chikov, V. G. (1998). Relativistic transition probabilities and oscillator strengths in hydrogen-like atoms, *Physica Scripta* **57**, 581.
- Robson, B. A. and Staudte, D. S. (1996). An eight-component relativistic wave equation for spin-1/2 particles I, *Journal of Physics A: Mathematical and General* **29**, 157.
- Rose, M. E. (1957). *Elementary Theory of Angular Momentum*, Wiley, New York.
- Staudte, D. S. (1996). An eight-component relativistic wave equation for spin-1/2 particles II, *Journal of Physics A: Mathematical and General* **29**, 169.