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### THE EINSTEIN A-COEFFICIENT OF SPONTANEOUS EMISSION: A RELATIVISTIC CALCULATION IN THE HEISENBERG REPRESENTATION



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International Atomic Energy Agency and United Nations Educational Scientific and Cultural Organization INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS

#### THE EINSTEIN A-COEFFICIENT OF SPONTANEOUS EMISSION: A RELATIVISTIC CALCULATION IN THE HEISENBERG REPRESENTATION \*

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#### ABSTRACT

We present a simple approach to the relativistic calculation of the rates of spontaneous emission starting from the Heisenberg picture formula for the power radiated by a charged particle undergoing acceleration, and evaluate atomic decay rates using relativistic Dirac-Coulomb wavefunctions. The spin of the electron, embedded in its relativistic wavefunction, is shown to correctly provide the two polarization states of the emitted radiation. We discuss selection rules and calculate the Hydrogen  $2P \rightarrow 1S$  transition rate, among others, to be

 $\Gamma = (6.2650 \pm 0.0007) \times 10^8 s^{-1}$ 

in good agreement with the full field theory calculation as well as with experiment.

MIRAMARE ~ TRIESTE

July 1989

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#### I. INTRODUCTION

The purpose of this paper is to elucidate the origin and mechanism of spontaneous emission and to provide a simple method of calculating more accurate relativistic decay rates than the presently available nonrelativistic ones, for which the literature is  $extensive^{[1,2]}$ .

As is well known, the debate about spontaneous emission has a long history. Different mechanisms and different methods of calculation have been proposed. According to one of the two main pictures, spontaneous emission is due to the fluctuating vacuum of the quantized electromagnetic field<sup>[3]</sup>, while the other attributes it to the radiation reaction force<sup>[4]</sup>. The first idea, taken seriously, gives only half of the Einstein A-coefficient<sup>[5]</sup>. The discussion about the roles of these two mechanisms still goes on<sup>[6]</sup>.

Recently, a relativistic theory of spontaneous emission has been given<sup>[8]</sup> within the framework of the self-energy quantum electrodynamics<sup>[7]</sup>. This approach does not use a second quantized radiation field, but rather the self-field produced by the current distribution  $j_{\mu} = e\bar{\psi}\gamma_{\mu}\psi$  of the electron, and has been successively applied to all other radiative processes<sup>[9]</sup>. In this paper, we implement a different version of this theory, namely that spontaneous emission is simply the radiation emitted by an accelerating charge (which can also, of course, absorb radiation). We use the Larmor formula for the energy emitted by an accelerating relativistic Dirac particle with acceleration  $\mathbf{a} = \dot{\alpha}$ , where  $\alpha(t)$  are the Dirac alpha matrices in the Heisenberg representation.

The relativistic calculation is essential, because the spin of the electron current accounts automatically for the two polarization states of the emitted radiation. This is a solution to the problem of the missing factor of two mentioned above. Aside from the spin degrees of freedom, the relativistic corrections turn out to be small for the H- atom, as

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expected, but might be large for Muonium and other exotic atoms and ions.

In Section II, we derive the decay rate formula. We evaluate the matrix elements in Section III and give a summary, in Section IV, of the selection rules arising from their angular parts. The general results are finally applied to the decay rates of some of the low-lying Hydrogen levels in Section V.

#### II. THEORY

For the time rate at which energy in the form of radiation is emitted by the atomic electron we borrow the classical expression for an electron of charge e undergoing an acceleration<sup>[10]</sup>

$$\frac{dE}{dt} = \frac{e^2}{4\pi} \frac{2}{3e^3} \left\{ \frac{\dot{\mathbf{v}}^2}{1-\beta^2} + \text{terms in } (\mathbf{v}.\dot{\mathbf{v}})\gamma^2 \text{ and } (\mathbf{v}\times\dot{\mathbf{v}})\gamma^2 \right\}$$
(1)

where E is the energy, c is the speed of light,  $\beta = v/c$  and  $\gamma^2 = 1/(1 - \beta^2)$ . In the instantaneous rest frame of the electron, v = 0, we get

$$\frac{dE}{dt} = \frac{e^2}{4\pi} \frac{2}{3} \frac{\dot{\mathbf{v}}}{c^3} \tag{2}$$

We next turn this into a probability for emission by dividing the expression in equation (2) by the quantity

$$\Delta E = \int_0^T \frac{dE}{dt} dt \tag{3}$$

which does not necessarily depend upon T, and write

$$\Gamma = \frac{dE/dt}{\Delta E} \approx \frac{e^2}{4\pi} \frac{2}{3} \frac{\dot{\mathbf{v}}^2}{c^3 \Delta E}$$
(4).

Notice that  $\Gamma$  already has the units of  $s^{-1}$ .

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In quantum mechanics, the radiation process is described as follows. As the electron makes a transition from a (stationary) excited state n to the ground (or less excited) state s, it emits energy of the magnitude  $\Delta E = \hbar \omega$ , where  $\hbar$  is Planck's constant and  $\omega$  is the transition frequency, in the form of radiation. The idea now is to turn (4) into a quantum mechanical expression for the atomic decay rate in two steps<sup>[11]</sup>: (a) We let  $\Delta E = \hbar \omega$  and (b) We replace the acceleration  $\dot{\mathbf{v}}$  by the matrix element of the acceleration operator between the initial and final states. In other words, we let  $\dot{\mathbf{v}} = \langle s | \dot{\mathbf{v}}_{op} | n \rangle$ . This procedure is further justified by comparing it with the Schrödinger picture calculation<sup>[7,8]</sup>. After this has been done in the system of units where  $\hbar = c = 1$ , and with the fine structure constant  $\alpha = e^2/4\pi$ , equation (4) becomes

$$\Gamma_{n \to s} = \frac{2}{3} \alpha \frac{|\langle n|\dot{\mathbf{v}}|s \rangle|^2}{\omega}$$
(5)

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and  $\Gamma_{n\to s}$  is identified with the decay rate of level *n* to level *s*. In the lab frame, the contribution of all terms beyond the first one in equation (1) is very small. In fact,  $\gamma^2$  differs from unity by a few parts in  $10^{-7}$  for an electron in its first excited state and gets only closer to one for higher states.

Now, from the Heisenberg equations, we have

$$\hat{\mathbf{v}} = \frac{d\mathbf{v}}{dt} = i[H, \mathbf{v}] = -[H, [H, \mathbf{r}]]$$
(6)

We look first at the nonrelativistic limit, where H is the Schrödinger Hamiltonian and r is the position operator of the atomic electron. Therefore

$$< n |\dot{\mathbf{v}}|_{s} > = -(E_n - E_s)^2 \mathbf{r}_{ns}$$
  
 $= -\omega^2 \mathbf{r}_{ns}$ 

and hence

$$\Gamma_{n \to s}(NR) = \frac{2}{3} \alpha \omega^3 |\mathbf{r}_{ns}|^2 \tag{7}$$

$$=i\sqrt{(2J_n+1)(2J_s+1)} \{R_1\mathbf{K}_1 - R_2\mathbf{K}_2\}$$
(10)

Recall that the famous expression for the Einstein A-coefficient of spontaneous emission in the dipole approximation<sup>[12]</sup> contains a factor of  $\frac{4}{3}$  rather than the  $\frac{2}{3}$  we have in equation (7). Customarily, the lost factor of 2 is restored by introducing the familiar concept of polarization for the emitted photon. We shall show, however, that if relativistic Dirac-Coulomb wavefunctions, with their full spin dependence, were used instead of the Schrödinger ones, the final result will numerically agree with experiment, without the need to invoke the polarized photon concept at all<sup>[8]</sup>. The light emitted from the relativistic electron with spin has the two polarizations. On the other hand, in the relativistic case, with  $\mathbf{v} = \alpha$ , where  $\alpha = (\alpha_1, \alpha_2, \alpha_3)$  represent the Dirac alpha matrices, we have

$$< s|\dot{\mathbf{v}}|n > = i < s|[H, \alpha]|n >$$
$$= i\omega < s|\alpha|n >$$
(8)

where H here is the Dirac Hamiltonian of the atomic electron and  $|n\rangle$  and  $|s\rangle$  belong to its set of eigenstates and  $\omega = E_n - E_s$ . Putting (8) back into (5), we arrive at the simple formula

$$\Gamma_{n \to s} = \frac{2}{3} \alpha \omega | \langle n | \alpha | s \rangle |^{2}$$
$$= \frac{2}{3} \alpha \omega |\mathcal{M}_{ns}|^{2}$$
(9)

Equation (9) gives the partial decay rate of level n to level s. If one is interested in a calculation of the total decay rate,  $\Gamma_n$ , then one must sum (9) over all states s, where s < n, as well as over the total magnetic quantum numbers  $M_n$  and  $M_s$ . In the next Section, we evaluate the matrix elements  $M_{ns}$  exactly.

#### **III. THE MATRIX ELEMENTS**

With the help of Appendix A, and with  $\alpha$  in the standard representation,  $\mathcal{M}_{ns}$  becomes

$$\mathcal{M}_{n*} = \int d^3x \left( g_n \Omega_n^{\dagger} - i f_n \Omega_{n'}^{\dagger} \right) \begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix} \begin{pmatrix} g_s \Omega_s \\ i f_s \Omega_{s'} \end{pmatrix}$$
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where

$$R_{1} = \int_{0}^{\infty} r^{2} dr \ g_{n}(r) f_{s}(r)$$
  
=  $-\sqrt{(1 + \epsilon_{n})(1 - \epsilon_{s})} \ U_{n} \ U_{s} \ \{I_{1} + I_{2} - I_{3} - I_{4}\}$  (11a)

and

$$R_{2} = \int_{0}^{\infty} r^{2} dr f_{n}(r) g_{s}(r)$$
  
=  $-\sqrt{(1-\epsilon_{n})(1+\epsilon_{s})} U_{n} U_{s} \{I_{1} - I_{2} + I_{3} - I_{4}\}$  (11b)

with

$$I_{1} = \int_{0}^{\infty} r^{2} A_{n}(r) A_{s}(r) dr = n_{r} s_{r} \sum_{p=0}^{n_{r}-1} \sum_{q=0}^{s_{r}-1} (-n_{r}+1)_{p} (-s_{r}+1)_{q} \mathcal{H}_{pq}$$
(12a)

$$I_{2} = \int_{0}^{\infty} r^{2} A_{n}(r) B_{s}(r) dr = n_{r} (N_{s} - \kappa_{s}) \sum_{p=0}^{n_{r}-1} \sum_{q=0}^{s_{r}} (-n_{r} + 1)_{p} (-s_{r})_{q} \chi_{pq}$$
(12b)

$$I_{3} = \int_{0}^{\infty} r^{2} B_{n}(r) A_{s}(r) dr = (N_{n} - \kappa_{n}) s_{r} \sum_{p=0}^{n_{r}} \sum_{q=0}^{s_{r}-1} (-n_{r})_{p} (-s_{r}+1)_{q} \lambda_{pq}$$
(12c)

$$I_{4} = \int_{0}^{\infty} r^{2} B_{n}(r) B_{s}(r) dr = (N_{n} - \kappa_{n}) (N_{s} - \kappa_{s}) \sum_{p=0}^{n_{r}} \sum_{q=0}^{s_{r}} (-n_{r})_{p} (-s_{r})_{q} \mathcal{X}_{pq}$$
(12d)

and

$$\mathcal{H}_{pq} = (2\lambda_n)^{\gamma_n + p-1} (2\lambda_s)^{\gamma_s + q-1} \frac{\Gamma(\gamma_n + \gamma_s + p + q + 1)}{(2\gamma_n + 1)_p (2\gamma_s + 1)_q p! q! (\lambda_n + \lambda_s)^{\gamma_n + \gamma_s + p + q + 1}}$$
(13)

Moreover (see Appendix B)

$$\mathbf{K}_{1} = [(2J_{n}+1)(2J_{e}+1)]^{-\frac{1}{2}} \int \Omega_{n}^{\dagger} \sigma \ \Omega_{e'} \ do$$
  
=  $(-1)^{1-M_{n}-M_{e}-\ell_{n}-\ell_{e'}} \{(a+b)\hat{i}+i(a-b)\hat{j}+(c-d)\hat{k}\} \ \delta_{\ell_{n}\ell_{e'}}$  (14a)

$$\mathbf{K}_{2} = [(2J_{n}+1)(2J_{s}+1)]^{-\frac{1}{2}} \int \Omega_{n'}^{\dagger} \sigma \Omega_{s} \, d\sigma$$
$$= (-1)^{1+M_{n}-M_{s}-\ell_{n'}-\ell_{s}} \{(A+B)\hat{i} + i(A-B)\hat{j} + (C-D)\hat{k}\} \, \delta_{\ell_{n'}\ell_{s}} \qquad (14b)$$

where  $do \equiv \sin^2 \theta d\theta d\phi$ , and

$$a = \begin{pmatrix} \ell_n & \frac{1}{2} & J_n \\ M_n - \frac{1}{2} & \frac{1}{2} & -M_n \end{pmatrix} \begin{pmatrix} \ell_s, & \frac{1}{2} & J_s \\ M_s + \frac{1}{2} & -\frac{1}{2} & -M_s \end{pmatrix}$$
(15a)

$$b = \begin{pmatrix} \ell_n & \frac{1}{2} & J_n \\ M_n + \frac{1}{2} & -\frac{1}{2} & -M_n \end{pmatrix} \begin{pmatrix} \ell_{\bullet'} & \frac{1}{2} & J_s \\ M_{\bullet} - \frac{1}{2} & \frac{1}{2} & -M_s \end{pmatrix}$$
(15b)

$$c = \begin{pmatrix} \ell_n & \frac{1}{2} & J_n \\ M_n - \frac{1}{2} & \frac{1}{2} & -M_n \end{pmatrix} \begin{pmatrix} \ell_{s'} & \frac{1}{2} & J_s \\ M_s - \frac{1}{2} & \frac{1}{2} & -M_s \end{pmatrix}$$
(15c)

$$d = \begin{pmatrix} \ell_n & \frac{1}{2} & J_n \\ M_n + \frac{1}{2} & -\frac{1}{2} & -M_n \end{pmatrix} \begin{pmatrix} \ell_{s'} & \frac{1}{2} & J_s \\ M_s + \frac{1}{2} & -\frac{1}{2} & -M_s \end{pmatrix}$$
(15d)

Finally, A, B, C and D can readily be written down from the expressions for a, b, c and d, respectively, by letting  $\ell_n \to \ell_{n'}$  and  $\ell_{s'} \to \ell_s$ .

When equations (14) are put back into (10) and after squaring  $M_{ns}$  and substituting the result in equation (9), remembering to sum over  $M_n$  and  $M_s$ , the total decay rate of the nth atomic level becomes

$$\Gamma_{n} = \frac{2}{3} \alpha \sum_{s \langle \langle n \rangle} \frac{(2J_{n}+1)(2J_{s}+1)}{2\ell_{n}+1} \omega_{ns} \sum_{M_{n}M_{s}} \{R_{1}^{2}[2(a^{2}+b^{2}-cd)+c^{2}+d^{2}] + R_{2}^{2}[2(A^{2}+B^{2}-CD)+C^{2}+D^{2}] - 2R_{1}R_{2}[2(aA+bB)+cC+dD-cD-dC]\}$$
(16)

Notice that in our final result, equation (16), we have divided by the degeneracy  $g_n = 2\ell_n + 1$  of the *n*th level, following general practice. In the next section, we go back to equations (14) and extract selection rules from them.

#### IV. THE SELECTION RULES

From the Kronecker  $\delta$ - function in equations (14), we can immediately write down the following rules:

(i)  $\mathbf{K}_1 = 0$  unless  $\ell_n - \ell_{s'} = 0$ .

(ii)  $\mathbf{K}_2 = 0$  unless  $\ell_{n'} - \ell_s = 0$ .

These follow from  $\delta_{\ell_n \ell_{s'}}$  and  $\delta_{\ell_n \ell_{s'}}$ , respectively. On the other hand,  $\delta_{m_n m_{s'}}$  and  $\delta_{m_{n'} m_{s'}}$  impose the following conditions upon the various components of  $\mathbf{K}_1$  and  $\mathbf{K}_2$  (see equation B3 in Appendix B)

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- (1) a and A vanish unless  $M_s M_n = -1$ .
- (2) b and B vanish unless  $M_{\bullet} M_n = +1$ .
- (3) e, C, d and D vanish unless  $M_s M_n = 0$ .

As usual, in a specific calculation, attention paid to these rules will prove to be timesaving. As we shall have occasion to encounter in section  $\mathbf{V}$ , rules (i) and (ii) prohibit some transitions from taking place altogether.

#### V. EXAMPLES

We now apply equation (16) to the following transitions in Hydrogen:

(1) The  $2S \rightarrow 1S$  transition:

 $\ell_n - \ell_{s'} = -1$  and  $\ell_{n'} - \ell_s = +1$  render  $K_1 = K_2 = 0$  and hence this transition is strictly forbidden.

(2) The  $2P_{\frac{1}{4}} \rightarrow 1S_{\frac{1}{4}}$  transition:

 $\ell_n - \ell_{s'} = \ell_{n'} - \ell_s = 0$  imples that both  $K_1$  and  $K_2$  are nonzero. Furthermore, equations (15) together with the rules (1) through (3), yield (summation over  $M_n$  and  $M_s$  is implied)

$$a^{2} = b^{2} = \frac{1}{36}, c^{2} = d^{2} = \frac{5}{36}, cd = \frac{1}{9}, A^{2} = B^{2} = C^{2} = D^{2} = \frac{1}{4},$$
  
 $CD = 0, aA = bB = -\frac{1}{12}, cC = dD = \frac{1}{12}, cD = dC = \frac{1}{6}.$ 

Thus

$$\Gamma_{2P_{\frac{1}{2}} \to 1S_{\frac{1}{2}}} = \frac{1}{2} (\frac{2}{3})^3 \alpha \ \omega \ \{R_1^2 + 9R_2^2 + 6R_1R_2\}$$
(17)

On the other hand, equations (11) and (12) yield

$$R_{1} = 2^{2\gamma - \frac{1}{2}} \left[ \frac{(2\gamma + 1)(1 + \epsilon_{n})(1 - \epsilon_{s})}{N - 1} \right]^{\frac{1}{2}} \frac{N^{\gamma + 1}(N - 3)}{(N + 1)^{2\gamma + 2}}$$

$$R_{2} = \eta R_{1}$$

$$\eta = \left[ \frac{(1 - \epsilon_{n})(1 + \epsilon_{s})}{(1 + \epsilon_{n})(1 - \epsilon_{s})} \right]^{\frac{1}{2}} \frac{(N^{2} - N + 2)}{N(N - 3)}$$

where  $\gamma = \sqrt{1 - (Z\alpha)^2}$ ,  $N = \sqrt{2\gamma + 2}$ ,  $\epsilon_n = \sqrt{1 - (Z\alpha/N)^2}$ ,  $\epsilon_s = \gamma$  and  $\omega = m(\epsilon_n - \epsilon_s)$  and m is the electron's reduced mass in the atom.

Taking  $\gamma \approx 1$ , gives  $N \approx 2$ ,  $\epsilon_n \approx 1 - \frac{(Z\alpha)^2}{8}$ ,  $\epsilon_s \approx 1 - \frac{(Z\alpha)^2}{2}$ ,  $\eta \approx -1$  and  $\omega \approx \frac{3}{8}m\alpha^2$ , we get

$$\Gamma_{2P_{\frac{1}{2}} \to 1S_{\frac{1}{2}}} \approx \frac{1}{3} (\frac{2}{3})^8 m \alpha (Z\alpha)^4 \tag{18}$$

(3) The  $2P_{\frac{1}{2}} \rightarrow 1S_{\frac{1}{2}}$  transition:

 $\ell_n - \ell_{s'} = 0$  implies that  $\mathbf{K}_1 \neq 0$  while  $\ell_s - \ell_{n'} = -2$  renders  $\mathbf{K}_2 = 0$ . Moreover,  $a^2 = b^2 = \frac{1}{9}$ ,  $c^2 = d^2 = \frac{1}{18}$  and  $cd = -\frac{1}{18}$ . Thus

$$\Gamma_{2P_{\frac{1}{2}} \to 1S_{\frac{1}{2}}} = 4(\frac{2}{3})^3 \ \alpha \omega \ R_1^2 \tag{19}$$

where

$$R_1 = \left[\frac{(1+\epsilon_n)(1-\epsilon_n)}{\Gamma(2\gamma_n+1)\Gamma(2\gamma_n+1)}\right]^{\frac{1}{2}} \frac{2^{\gamma_n+2\gamma_n+\frac{1}{2}}}{3^{\gamma_n+\gamma_n+1}} \Gamma(\gamma_n+\gamma_n+1)$$

and where  $\gamma_n = \sqrt{4 - (Z\alpha)^2}$ ,  $\gamma_s = \sqrt{1 - (Z\alpha)^2}$ ,  $\epsilon_n = \frac{\gamma_n}{2}$ ,  $\epsilon_s = \gamma_s$ , and  $\omega = m(\epsilon_n - \epsilon_s)$ . Here, too, if we take  $\gamma_n \approx 2$ , and  $\gamma_s \approx 1$ , then  $\epsilon_n \approx 1 - \frac{(Z\alpha)^2}{8}$  and  $\epsilon_s \approx 1 - \frac{(Z\alpha)^2}{2}$ , and we get

$$\Gamma_{2F_{\frac{1}{2}} \to 1S_{\frac{1}{2}}} \approx \frac{2}{3} (\frac{2}{3})^{8} m \alpha \ (Z\alpha)^{4}$$
<sup>(20)</sup>

A more careful calculation, however, using the exact expressions (17) and (19), gives

$$\Gamma_{2P \to 1S} = \Gamma_{2P_{\frac{1}{2}} \to 1S_{\frac{1}{2}}} + \Gamma_{2P_{\frac{3}{2}} \to 1S_{\frac{1}{2}}} = (6.2650 \pm 0.0007) \times 10^8 s^{-1}$$
(21)

It is a common practice to report the total decay rate of the  $2P \rightarrow 1S$  transition as the weighted sum  $\frac{1}{3}\Gamma_{2P_{\frac{1}{2}}\rightarrow 1S_{\frac{1}{2}}} + \frac{2}{3}\Gamma_{2P_{\frac{1}{2}}\rightarrow 1S_{\frac{1}{2}}}$ , where the weights are calculated assuming that all the 2P sublevels are equally probable<sup>[13]</sup>. The weight factors have been included in our main result, equation (16), for the partial decay rate of a sublevel (see the two paragraphs flanking equation (16)). Thus, the reader should not be alarmed by the appearance of equation (21).

The uncertainty reported in equation (21) has been calculated from the expression

$$\Delta \Gamma = \frac{\partial \Gamma}{\partial \omega} \, \delta \omega$$

for an uncertainty  $\delta \omega$  in the transition frequency that is of the order of magnitude of the hyperfine splitting  $m\alpha^4$ . This result agrees extremely well with experiment as well as with all preexisting theoretical calculations<sup>[8]</sup>.

#### VI. DISCUSSION AND CONCLUSIONS

Once more, we have demonstrated, by a simple explicit calculation, that an aspect of the quantized nature of radiation is merely a reflection of the quantized nature of its source, the bound electron<sup>[14]</sup>. In particular, the inclusion of the spin of the source has rendered the sum over the photon polarization states unnecessary<sup>[7]</sup>.

In its approximate form, equation (8) gives a number easy to remember, namely  $\Gamma_{2P\to 1S} \approx (\frac{2}{3})^8 \ m\alpha \ (Z\alpha)^4$ , (see equations (18) and (20) and compare with the rate of positronium decay  $\Gamma_{2\gamma} = \frac{1}{2}m\alpha^5$ ). In the present calculation,, the  $2S \rightarrow 1S$  transition is strictly forbidden by the selection rules. This is maybe due to the neglect of some relativistic terms, for the complete relativistic calculation gives a small nonvanishing rate for this decay |7|.

Finally, we think that the calculation of the matrix elements in Section III and Appendix B will be useful in other atomic calculations involving the use of Dirac-Coulomb wavefunctions, whenever analytic closed form expressions are sought.

#### Acknowledgments

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#### APPENDIX A: THE DIRAC-COULOMB WAVEFUNCTIONS

With the desire to make this paper self-contained, we quote below from reference [8], Appendix B, the Dirac-Coulomb wavefunctions of the discrete part of the spectrum. We write the wavefunction of the *n*th level as

$$\psi_n(\mathbf{x}) = \begin{pmatrix} g_n(r) \ \Omega_n(\hat{r}) \\ if_n(r) \ \Omega_{n'}(\hat{r}) \end{pmatrix}$$
(A1)

In (A1), n and n' stand collectively for all the good quantum numbers of the states. In other words,  $n \equiv (n, J_n, \ell_n, M_n)$  and  $n' \equiv (n, J_n, \ell_{n'}, M_n)$ , where  $\ell_{n'} = 2J_n - \ell_n = \ell_n \pm 1$ . The radial parts in equation (A1) are given by

$$g_n(r) = \sqrt{1 + \epsilon_n} \ U_n \ (A_n - B_n) \tag{A2}$$

$$f_n(\tau) = -\sqrt{1 - \epsilon_n} U_n \left( A_n + B_n \right) \tag{A3}$$

where

$$U_n = \frac{2(\lambda_n)^3}{\Gamma(2\gamma_n+1)} \left[ \frac{\Gamma(2\gamma_n+n_r+1)}{4N_n(N_n-\kappa_n)n_r!} \right]^{\frac{1}{2}}$$
$$A_n(r) = n_r \left[ F(-n_r+1, 2\gamma_n+1; 2\lambda_n r) e^{-\lambda_n r} (2\lambda_n r)^{\gamma_n-1} \right]$$
$$B_n(r) = (N_n - \kappa_n) \left[ F(-n_r, 2\gamma_n+1; 2\lambda_n r) e^{-\lambda_n r} (2\lambda_n r)^{\gamma_n-1} \right]$$

Also

$$F(-n,b;z) = \sum_{m=0}^{n} \frac{(-n)_{m}}{(b)_{m}} \frac{z^{m}}{m!}; \quad (b)_{m} = \frac{\Gamma(b+1)}{\Gamma(b)}; \quad (b)_{0} \equiv 1$$

and where

$$\begin{split} \lambda_n &= \frac{Z\alpha m}{N_n}, \quad N_n = [n^2 - 2n_r(|\kappa_n| - \gamma_n)]^{\frac{1}{2}} \\ E_n^2 &= -\lambda_n^2 + m^2, \quad \gamma_n = [\kappa_n^2 - (Z\alpha)^2]^{\frac{1}{2}} \\ n_r &= n - |\kappa_n|, \quad \epsilon_n = \frac{E_n}{m} \\ \kappa_n &= \begin{cases} -(\ell_n + 1), & \text{if } J_n = \ell_n + \frac{1}{2}; \\ \ell_n, & \text{if } J_n = \ell_n - \frac{1}{2}. \end{cases} \end{split}$$

And finally, the angular parts of the wavefunctions are given by

$$\Omega_n = (-1)^{\frac{1}{2} - \ell_n - M_n} \sqrt{2J_n + 1} \sum_{m_n \mu_n} \begin{pmatrix} \ell_n & \frac{1}{2} & J_n \\ m_n & \mu_n & -M_n \end{pmatrix} |\ell_n m_n > \chi_{\mu_n}$$
(A4)

 $m_n 
ightarrow m_{n'}$  and  $\chi_{\mu n}$  is a two-component Pauli spinor.

#### APPENDIX B:THE ANGULAR MATRIX ELEMENTS

In component form, we write

$$\mathbf{K}_1 = (K_{1x}, K_{1y}, K_{1z})$$

where, for example

$$K_{1x} = [(2J_n + 1)(2J_s + 1)]^{-\frac{1}{2}} \int \Omega_n^{\dagger} \sigma_x \,\Omega_{s'} do$$
  
=  $(-1)^{1-\ell_n - \ell_{s'} - M_n - M_s} \sum_{m_n m_{s'} \,\mu_n \mu_s} \left( \begin{array}{cc} \ell_n & \frac{1}{2} & J_n \\ m_n & \mu_n & -M_n \end{array} \right) \left( \begin{array}{cc} \ell_{s'} & \frac{1}{2} & J_s \\ m_{s'} & \mu_s & -M_s \end{array} \right)$   
  $\times < \ell_n m_n |\ell_{s'} m_{s'} > \chi_{\mu_n}^{\dagger} \sigma_x \,\chi_{\mu_s}$  (B1)

Using  $< \ell_n m_n | \ell_s \cdot m_{s'} > = \delta_{\ell_n \ell_s} \cdot \delta_{m_n m_{s'}}$  and  $\chi_{\mu n}^{\dagger} \sigma_x \chi_{\mu s} = \delta_{\mu_n, -\mu_s}, K_{1x}$  becomes

$$K_{1,s} = (-1)^{1-\ell_n - \ell_{s'} - M_n - M_s} \sum_{m_n \mu_n} \begin{pmatrix} \ell_n & \frac{1}{2} & J_n \\ m_n & \mu_n & -M_n \end{pmatrix} \begin{pmatrix} \ell_{s'} & \frac{1}{2} & J_s \\ m_n & -\mu_n & -M_s \end{pmatrix} \delta_{\ell_n \ell_{s'}}$$
(B2)

We get rid of the sum over  $m_n$  by invoking the property of a 3j-symbol, whereby the sum of the entries in its second row should vanish. As a byproduct, we also get

$$m_n = M_n - \mu_n = M_s + \mu_n \tag{B3}$$

When, finally, the summation over  $\mu_n = \pm \frac{1}{2}$  is carried out explicitly, equation (B2) becomes

$$K_{1x} = (-1)^{1-\ell_n - \ell_{p'} - M_n - M_r} \{a + b\} \ \delta_{\ell_n \ell_{p'}}$$
(B4)

Equation (B3), on the other hand, gives the conditions for the nonvanishing of a and b when  $\mu_n$  is set equal to  $+\frac{i}{2}$  and  $-\frac{i}{2}$ , respectively.  $K_{1y}$  and  $K_{1z}$  can be derived in a similar fashion, the only difference being that

$$\chi_{\mu n}^{\dagger} \sigma_y \chi_{\mu s} = (-1)^{1-\mu_s} \, \delta_{\mu_n, -\mu_s} \tag{B5}$$

and

$$\chi_{\mu n}^{\dagger} \sigma_{z} \chi_{\mu s} = (-1)^{\frac{1}{2} - \mu_{n}} \, \delta_{\mu_{n}, \mu_{s}} \tag{B6}$$

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