

The Einstein A-coefficient of spontaneous emission: a relativistic calculation in the Heisenberg representation

A.O. Barut¹ and Y.I. Salamin²

¹ Physics Department, University of Colorado, Boulder, CO 80309, USA

² Physics Department, Birzeit University, P.O. Box 14 – Birzeit, West Bank of Jordan

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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

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

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

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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 [3], while the other attributes it to the radiation reaction force [4]. The first idea, taken seriously, gives only half of the Einstein A -coefficient [5]. The discussion about the roles of these two mechanisms still goes on [6].

Recently, a relativistic theory of spontaneous emission has been given [8] within the framework of the self-energy quantum electrodynamics [7]. 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 [9]. 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 $a = \dot{\alpha}$, 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 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 Sect. III and give a summary, in Sect. 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 Sect. 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 $\dot{\mathbf{v}}$. For this power, after passing from proper time to ordinary time and after angular integration, we shall adopt the following well-known formula [10]

$$\frac{dE}{dt} = \frac{e^2}{4\pi} \frac{2}{3} \frac{\dot{v}^2}{c^3}. \quad (1)$$

We next turn this into a probability for emission by dividing the expression in (1) by the quantity

$$\Delta E = \int_0^T \frac{dE}{dt} dt \quad (2)$$

which does not necessarily depend upon T , and write

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

Notice that Γ already has the units of s^{-1} .

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 ω is the transition frequency, in the form of radiation. The idea now is to turn (3) into a quantum mechanical expression for the atomic decay rate in two steps [11]: (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 [7, 8]. After this has been done in the system of units where $\hbar = c = 1$, and with the fine structure constant $\alpha = e^2/4\pi$, (3) becomes

$$\Gamma_{n \rightarrow s} = \frac{2}{3} \alpha \frac{|\langle n | \dot{\mathbf{v}} | s \rangle|^2}{\omega} \quad (4)$$

and $\Gamma_{n \rightarrow s}$ 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 (1) is very small. In fact, γ^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

$$\dot{\mathbf{v}} = \frac{d\mathbf{v}}{dt} = i[H, \mathbf{v}] = -[H, [H, \mathbf{r}]]. \quad (5)$$

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

$$\begin{aligned} \langle n | \dot{\mathbf{v}} | s \rangle &= -(E_n - E_s)^2 \mathbf{r}_{ns} \\ &= -\omega^2 \mathbf{r}_{ns} \end{aligned}$$

and hence

$$\Gamma_{n \rightarrow s}(NR) = \frac{2}{3} \alpha \omega^3 |\mathbf{r}_{ns}|^2. \quad (6)$$

Recall that the famous expression for the Einstein A -coefficient of spontaneous emission in the dipole approximation [12] contains a factor of $\frac{4}{3}$ rather than the $\frac{2}{3}$ we have in (6). Customarily, the lost factor of 2 is restored by introducing the familiar concept of polarization by 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 [8]. 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

$$\begin{aligned} \langle s | \dot{\mathbf{v}} | n \rangle &= i \langle s | [H, \alpha] | n \rangle \\ &= i\omega \langle s | \alpha | n \rangle \end{aligned} \quad (7)$$

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 (7) back into (4), we arrive at the simple formula

$$\begin{aligned} \Gamma_{n \rightarrow s} &= \frac{2}{3} \alpha \omega |\langle n | \alpha | s \rangle|^2 \\ &= \frac{2}{3} \alpha \omega |\mathcal{M}_{ns}|^2. \end{aligned} \quad (8)$$

Equation (8) gives the partial decay rate of level n to level s . If one is interested in a calculation of the total decay rate, Γ_n , then one must sum (8) 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 \mathcal{M}_{ns} exactly.

III. The matrix elements

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

$$\begin{aligned} \mathcal{M}_{ns} &= \int d^3x (g_n \Omega_n^\dagger - i f_n \Omega_n^\dagger) \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix} \begin{pmatrix} g_s \Omega_s \\ i f_s \Omega_s \end{pmatrix} \\ &= i \sqrt{(2J_n + 1)(2J_s + 1)} \{R_1 \mathbf{K}_1 - R_2 \mathbf{K}_2\} \end{aligned} \quad (10)$$

where

$$\begin{aligned} R_1 &= \int_0^\infty r^2 dr g_n(r) f_s(r) \\ &= -\sqrt{(1 + \varepsilon_n)(1 - \varepsilon_s)} U_n U_s \{I_1 + I_2 - I_3 - I_4\} \end{aligned} \quad (11a)$$

and

$$\begin{aligned} R_2 &= \int_0^\infty r^2 dr f_n(r) g_s(r) \\ &= -\sqrt{(1 - \varepsilon_n)(1 + \varepsilon_s)} U_n U_s \{I_1 - I_2 + I_3 - I_4\} \end{aligned} \quad (11b)$$

with

$$\begin{aligned} I_1 &= \int_0^\infty r^2 A_n(r) A_s(r) dr \\ &= n_r s_r \sum_{p=0}^{n_r-1} \sum_{q=0}^{s_r-1} (-n_r + 1)_p (-s_r + 1)_q \mathcal{H}_{pq} \end{aligned} \quad (12a)$$

$$\begin{aligned} I_2 &= \int_0^\infty r^2 A_n(r) B_s(r) dr \\ &= n_r (N_s - \kappa_s) \sum_{p=0}^{n_r-1} \sum_{q=0}^{s_r} (-n_r + 1)_p (-s_r)_q \mathcal{H}_{pq} \end{aligned} \quad (12b)$$

$$I_3 = \int_0^\infty r^2 B_n(r) A_s(r) dr$$

$$= (N_n - \kappa_n) s_r \sum_{p=0}^{n_r} \sum_{q=0}^{s_r-1} (-n_r)_p (-s_r+1)_q \mathcal{H}_{pq} \quad (12c)$$

$$I_4 = \int_0^\infty r^2 B_n(r) B_s(r) dr$$

$$= (N_n - \kappa_n)(N_s - \kappa_s) \sum_{p=0}^{n_r} \sum_{q=0}^{s_r} (-n_r)_p (-s_r)_q \mathcal{H}_{pq} \quad (12d)$$

and

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

Moreover (see Appendix B)

$$\mathbf{K}_1 = [(2J_n+1)(2J_s+1)]^{-\frac{1}{2}} \int \Omega_n^\dagger \sigma \Omega_s d\phi$$

$$= (-1)^{1-M_n-M_s-l_n-l_s} \{ (a+b) \hat{i} + i(a-b) \hat{j} + (c-d) \hat{k} \} \delta_{l_n l_s}, \quad (14a)$$

and

$$\mathbf{K}_2 = [(2J_n+1)(2J_s+1)]^{-\frac{1}{2}} \int \Omega_n^\dagger \sigma \Omega_s d\phi$$

$$= (-1)^{1-M_n-M_s-l_n-l_s} \{ (A+B) \hat{i} + i(A-B) \hat{j} + (C-D) \hat{k} \} \delta_{l_n l_s} \quad (14b)$$

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

$$a = \begin{pmatrix} l_n & \frac{1}{2} & J_n \\ M_n - \frac{1}{2} & \frac{1}{2} & -M_n \end{pmatrix} \begin{pmatrix} l_s & \frac{1}{2} & J_s \\ M_s + \frac{1}{2} & -\frac{1}{2} & -M_s \end{pmatrix} \quad (15a)$$

$$b = \begin{pmatrix} l_n & \frac{1}{2} & J_n \\ M_n + \frac{1}{2} & -\frac{1}{2} & -M_n \end{pmatrix} \begin{pmatrix} l_s & \frac{1}{2} & J_s \\ M_s - \frac{1}{2} & \frac{1}{2} & -M_s \end{pmatrix} \quad (15b)$$

$$c = \begin{pmatrix} l_n & \frac{1}{2} & J_n \\ M_n - \frac{1}{2} & \frac{1}{2} & -M_n \end{pmatrix} \begin{pmatrix} l_s & \frac{1}{2} & J_s \\ M_s - \frac{1}{2} & \frac{1}{2} & -M_s \end{pmatrix} \quad (15c)$$

$$d = \begin{pmatrix} l_n & \frac{1}{2} & J_n \\ M_n + \frac{1}{2} & -\frac{1}{2} & -M_n \end{pmatrix} \begin{pmatrix} l_s & \frac{1}{2} & J_s \\ M_s + \frac{1}{2} & -\frac{1}{2} & -M_s \end{pmatrix} \quad (15d)$$

Finally, A , B , C and D can readily be written down from the expressions for a , b , c and d , respectively, by letting $l_n \rightarrow l_n$ and $l_s \rightarrow l_s$.

When (14) are put back into (10) and after squaring \mathcal{M}_{ns} and substituting the result in (8), remembering to sum over M_n and M_s , the total decay rate of the n th atomic level becomes

$$\Gamma_n = \frac{2}{3} \alpha \sum_{s(<n)} \frac{(2J_n+1)(2J_s+1)}{2l_n+1} \omega_{ns} \sum_{M_n M_s} \{ R_1^2 [2(a^2+b^2 - cd) + c^2 + d^2] + R_2^2 [2(A^2+B^2-CD) + C^2 + D^2] - 2R_1 R_2 [2(aA+bB) + cC + dD - cD - dC] \}. \quad (16)$$

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

IV. The selection rules

From the Kronecker δ -function in (14), we can immediately write down the following rules:

(i) $\mathbf{K}_1 = 0$ unless $l_n - l_s = 0$.

(ii) $\mathbf{K}_2 = 0$ unless $l_n - l_s = 0$.

These follow from $\delta_{l_n l_s}$ and $\delta_{l_n l_s}$, 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)

(1) a and A vanish unless $M_s - M_n = -1$.

(2) b and B vanish unless $M_s - M_n = +1$.

(3) c , 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 Sect. V, rules (i) and (ii) prohibit some transitions from taking place altogether.

V. Examples

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

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

$l_n - l_s = -1$ and $l_n - l_s = +1$ render $\mathbf{K}_1 = \mathbf{K}_2 = 0$ and hence this transition is strictly forbidden.

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

$l_n - l_s = l_n - l_s = 0$ implies that both \mathbf{K}_1 and \mathbf{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

$$\Gamma_{2P_{\frac{3}{2}} \rightarrow 1S_{\frac{1}{2}}} = \frac{1}{2} \left(\frac{2}{3} \right)^3 \alpha \omega \{ R_1^2 + 9R_2^2 + 6R_1 R_2 \} \quad (17)$$

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

$$R_1 = 2^{2\gamma-\frac{1}{2}} \left[\frac{(2\gamma+1)(1+\varepsilon_n)(1-\varepsilon_s)}{N-1} \right]^{\frac{1}{2}} \frac{N^{\gamma+1}(N-3)}{(N+1)^{2\gamma+2}}$$

$$R_2 = \eta R_1$$

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

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

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

$$\Gamma_{2P_{\frac{3}{2}} \rightarrow 1S_{\frac{1}{2}}} \approx \frac{1}{3} \left(\frac{2}{3} \right)^8 m\alpha (Z\alpha)^4. \quad (18)$$

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

$l_n - l_s = 0$ implies that $\mathbf{K}_1 \neq 0$ while $l_s - l_n = -2$

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

$$\Gamma_{2P_{\frac{3}{2}} \rightarrow 1S_{\frac{1}{2}}} = 4\left(\frac{2}{3}\right)^3 \alpha \omega R_1^2 \quad (19)$$

where

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

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

$$\Gamma_{2P_{\frac{3}{2}} \rightarrow 1S_{\frac{1}{2}}} \approx \frac{2}{3}\left(\frac{2}{3}\right)^8 m\alpha(Z\alpha)^4. \quad (20)$$

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

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

It is a common practice to report the total decay rate of the $2P \rightarrow 1S$ transition as the weighted sum $\frac{1}{3}\Gamma_{2P_{\frac{3}{2}} \rightarrow 1S_{\frac{3}{2}}} + \frac{2}{3}\Gamma_{2P_{\frac{1}{2}} \rightarrow 1S_{\frac{1}{2}}}$, where the weights are calculated assuming that all the $2P$ sublevels are equally probable [14]. The weight factors have been included in our main result, (16), for the partial decay rate of a sublevel (see the two paragraphs flanking (16)). Thus, the reader should not be alarmed by the appearance of (21).

The uncertainty reported in (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 [8].

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 [13]. In particular, the inclusion of the spin of the source has rendered the sum over the photon polarization states unnecessary [8].

In its approximate form, (8) gives a number easy to remember, namely $\Gamma_{2P \rightarrow 1S} \approx \left(\frac{2}{3}\right)^8 m\alpha(Z\alpha)^4$, (see (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 due to the neglect of some relativistic terms, for the complete relativistic calculation gives a small nonvanish-

ing rate for this decay which has been calculated for all Z -values in precise agreement with QED [15].

Finally, we think that the calculation of the matrix elements in Sect. 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.

Appendix A: the Dirac-Coulomb wavefunctions

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

$$\psi_n(x) = \begin{pmatrix} g_n(r) & \Omega_n(\hat{r}) \\ i f_n(r) & \Omega_{n'}(\hat{r}) \end{pmatrix}. \quad (A1)$$

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

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

$$f_n(r) = -\sqrt{1-\varepsilon_n} U_n(A_n + B_n) \quad (A3)$$

where

$$U_n = \frac{2(\lambda_n)^{\frac{3}{2}}}{\Gamma(2\gamma_n+1)} \left[\frac{\Gamma(2\gamma_n+n_r+1)}{4N_n(N_n-\kappa_n)n_r!} \right]^{\frac{1}{2}}$$

$$A_n(r) = n_r F(-n_r+1, 2\gamma_n+1; 2\lambda_n r) e^{-\lambda_n r} (2\lambda_n r)^{\gamma_n-1}$$

$$B_n(r) = (N_n - \kappa_n) F(-n_r, 2\gamma_n+1; 2\lambda_n r) e^{-\lambda_n r} (2\lambda_n r)^{\gamma_n-1}$$

Also

$$F(-n, b; z) = \sum_{m=0}^n \frac{(-n)_m}{(b)_m} \frac{z^m}{m!}; (b)_m = \frac{\Gamma(b+1)}{\Gamma(b)}; (b)_0 \equiv 1$$

and where

$$\lambda_n = \frac{Z\alpha m}{N_n}, N_n = [n^2 - 2n_r(|\kappa_n| - \gamma_n)]^{\frac{1}{2}}$$

$$E_n^2 = -\lambda_n^2 + m^2, \gamma_n = [\kappa_n^2 - (Z\alpha)^2]^{\frac{1}{2}}$$

$$n_r = n - |\kappa_n|, \varepsilon_n = \frac{E_n}{m}$$

$$\kappa_n = \begin{cases} -(l_n+1), & \text{if } J_n = l_n + \frac{1}{2}; \\ l_n, & \text{if } J_n = l_n - \frac{1}{2}. \end{cases}$$

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

$$\Omega_n = (-1)^{\frac{1}{2}-l_n-M_n} \sqrt{2J_n+1} \sum_{m_n \mu_n} \begin{pmatrix} l_n & \frac{1}{2} & J_n \\ m_n & \mu_n & -M_n \end{pmatrix} |l_n m_n\rangle \chi_{\mu_n} \quad (A3)$$

$\Omega_{n'}$ is obtainable from Ω_n by letting $l_n \rightarrow l_{n'}$ and $m_n \rightarrow m_{n'}$ and χ_{μ_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

$$\begin{aligned} K_{1x} &= [(2J_n + 1)(2J_s + 1)]^{-\frac{1}{2}} \int \Omega_n^\dagger \sigma_x \Omega_{s'} d\omega \\ &= (-1)^{1-l_n-l_{s'}-M_n-M_s} \sum_{m_n m_{s'}} \sum_{\mu_n \mu_{s'}} \begin{pmatrix} l_n & \frac{1}{2} & J_n \\ m_n & \mu_n & -M_n \end{pmatrix} \\ &\quad \cdot \begin{pmatrix} l_{s'} & \frac{1}{2} & J_s \\ m_{s'} & \mu_{s'} & -M_{s'} \end{pmatrix} \\ &\quad \cdot \langle l_n m_n | l_{s'} m_{s'} \rangle \chi_{\mu_n}^\dagger \sigma_x \chi_{\mu_{s'}} \end{aligned} \quad (\text{B1})$$

Using $\langle l_n m_n | l_{s'} m_{s'} \rangle = \delta_{l_n l_{s'}} \delta_{m_n m_{s'}}$ and $\chi_{\mu_n}^\dagger \sigma_x \chi_{\mu_{s'}} = \delta_{\mu_n, -\mu_{s'}}$, K_{1x} becomes

$$\begin{aligned} K_{1x} &= (-1)^{1-l_n-l_{s'}-M_n-M_s} \sum_{m_n \mu_n} \begin{pmatrix} l_n & \frac{1}{2} & J_n \\ m_n & \mu_n & -M_n \end{pmatrix} \\ &\quad \cdot \begin{pmatrix} l_{s'} & \frac{1}{2} & J_s \\ m_n & -\mu_n & -M_{s'} \end{pmatrix} \delta_{l_n l_{s'}}. \end{aligned} \quad (\text{B2})$$

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

$$m_n = M_n - \mu_n = M_{s'} + \mu_{s'}. \quad (\text{B3})$$

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

$$K_{1x} = (-1)^{1-l_n-l_{s'}-M_n-M_s} \{a+b\} \delta_{l_n l_{s'}}. \quad (\text{B4})$$

Equation (B3), on the other hand, gives the conditions for the nonvanishing of a and b when μ_n is set equal to $+\frac{1}{2}$ and $-\frac{1}{2}$, respectively. K_{1y} and K_{1z} can be derived

in a similar fashion, the only difference being that

$$\chi_{\mu_n}^\dagger \sigma_y \chi_{\mu_{s'}} = (-1)^{1-\mu_n} \delta_{\mu_n, -\mu_{s'}} \quad (\text{B5})$$

and

$$\chi_{\mu_n}^\dagger \sigma_z \chi_{\mu_{s'}} = (-1)^{\frac{1}{2}-\mu_n} \delta_{\mu_n, \mu_{s'}} \quad (\text{B6})$$

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