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## Non-Markovian treatment of the spontaneous $2P_{1/2} \rightarrow 1S_{1/2}$ transition in the Dirac hydrogen atom

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**Abstract.** For the first time to the author's knowledge, a rigorous mathematical treatment of the spontaneous  $2P_{1/2} \rightarrow 1S_{1/2}$  transition, going beyond the usual Markov approximation, is presented in the case of the Dirac hydrogen atom. The relevant transition matrix elements of the Dirac Hamiltonian are calculated without the dipole approximation. Further, a non-Markovian equation of motion for the non-decay probability of the unstable  $2P_{1/2}$  state is derived, by using a self-consistent projection-operator method recently developed by the present author. By a rigorous analytical treatment of the non-Markovian equation, deviations from exponential decay for asymptotic times are obtained. Moreover, by careful error estimations deviations from exponential decay for finite times with definite validity range are also calculated. Finally, for the radiative lineshape a new quasi-Lorentzian distribution is obtained.

### 1. Introduction

The non-Markovian behaviour in the case of the spontaneous emission from a non-relativistic hydrogenic atom has recently been examined in great detail (see [1, 2] and the references quoted therein). (Hereafter reference [2] will be referred to as I.) Similar calculations in the case of the Dirac hydrogen atom seem to be lacking in the literature. As was shown elsewhere (in the non-relativistic case) [1], in order to be able to carry out such a calculation, the retardation effects are to be taken into account (no kind of dipole approximation leading to incorrect asymptotic results is permitted), and a self-consistent projection-operator method (SCPOM) [3] has to be applied.

In the present paper we study the non-Markovian (non-exponential) decay for the  $2P_{1/2} \rightarrow 1S_{1/2}$  transition in the case of a Dirac hydrogenic atom (some preliminary results were presented in [4]). The first step in our treatment is the cumbersome, but absolutely necessary, calculation of the transition matrix elements for the  $2P_{1/2} \rightarrow 1S_{1/2}$  transition (without making the dipole approximation). After this, the second step is the derivation of a closed non-Markovian equation of motion for the probability amplitude for finding the atom in the initial state  $2P_{1/2}$  and the radiation field in the vacuum field. This is achieved by applying an SCPOM, developed in [3], to the Dirac equation. The third step consists in applying the method of the Laplace transform and its inverse to the non-Markovian equation. This yields analytic results for the *deviations from exponential decay* which are valid for *asymptotic* and *finite times*. It should be emphasized that all the results presented in the present paper possess definite validity ranges based on careful error estimations, which are absolutely necessary in a rigorous mathematical treatment.

Finally, a new expression for the frequency spectrum of the spontaneously emitted radiation showing a quasi-Lorentzian shape is calculated.

The paper is organized as follows. In section 2 the Dirac Hamiltonian for interaction between the hydrogenic atom and the radiation field is presented. In section 3, by using an SCPOM, a non-Markovian equation of motion for the non-decay probability amplitude of the unstable state is derived. Moreover, the corresponding matrix elements of the transition  $2P_{1/2} \rightarrow 1S_{1/2}$  are used without applying the dipole approximation. In section 4, the non-Markovian equation of section 3 is treated analytically. Deviations from exponential decay being valid for asymptotic and finite times are calculated. In section 5 a quasi-Lorentzian expression for the radiative lineshape is obtained. In section 6 all results obtained are extensively discussed and compared with the previous work in this field. Finally, in appendix A analytic results for the transition matrix elements in the Dirac hydrogen atom are derived, and in appendix B an integral appearing in section 4 is evaluated exactly.

## 2. The Dirac interaction Hamiltonian

By using the second quantization for electrons and photons, the relativistic Dirac Hamiltonian  $-\epsilon\alpha \cdot A$  for the interaction between the atom and the radiation field takes the following form:

$$H(t) = \sum_{s,s',\beta,\lambda} \int_0^\infty dk a_{\beta,\lambda}(k) c_s^+ c_{s'} H_{\beta,\lambda}^{s,s'}(k) \exp[i(\omega_{ss'} - \omega)t] + \text{HC} \quad (2.1)$$

in the interaction picture. The transition matrix elements are given by

$$H_{\beta,\lambda}^{s,s'}(k) = e \int d^3r A_{\beta,\lambda}(k, \mathbf{r}) u_s^+(\mathbf{r}) \alpha u_{s'}(\mathbf{r}) \quad (2.2)$$

where we expanded the vector potential in terms of electric multipoles  $A_\beta^e(k, \mathbf{r})$  and magnetic multipoles  $A_\beta^m(k, \mathbf{r})$ ,  $\beta = (J, M)$  ( $J$  and  $M$  are the angular momentum and magnetic quantum numbers, respectively) [5]:

$$A(\mathbf{r}) = - \sum_{\beta,\lambda} \int_0^\infty dk a_{\beta,\lambda}(k) A_{\beta,\lambda}(k, \mathbf{r}) + \text{HC} \quad (2.3)$$

with

$$A_{\beta,\lambda}(k, \mathbf{r}) = (2\hbar ck)^{1/2} i^J [i\lambda A_\beta^e(k, \mathbf{r}) + A_\beta^m(k, \mathbf{r})] \quad (2.4)$$

$$A_{JM}^e(k, \mathbf{r}) = - \sqrt{\frac{J}{2J+1}} j_{J+1}(kr) Y_{J,J+1,M}(\Omega) + \sqrt{\frac{J+1}{2J+1}} j_{J-1}(kr) Y_{J,J-1,M}(\Omega) \quad (2.5)$$

$$A_{JM}^m(k, \mathbf{r}) = j_J(kr) Y_{J,J,M}(\Omega). \quad (2.6)$$

Here  $j_J(kr)$  are the spherical Bessel functions and  $Y_{J,L,M}(\Omega)$ ,  $\Omega = \vartheta, \varphi$  are the spherical vector harmonics given in the spherical basis-vector system [6]:

$$Y_{J,L,M} = \begin{pmatrix} Y_{J,L,M}^{(+)} \\ Y_{J,L,M}^{(0)} \\ Y_{J,L,M}^{(-)} \end{pmatrix} = \sum_{q=-1}^1 e_q Y_{L,M-q} \langle L, 1, M-q, q | J, M \rangle \quad (2.7)$$

$$e_{\pm 1} = \mp \frac{1}{\sqrt{2}} (e_x \pm i e_y) \quad e_0 = e_z \quad (2.8)$$

where the corresponding Clebsch-Gordan coefficients can be found in [5], and the spherical harmonics are defined by

$$Y_{l,m}(\Omega) = (-1)^m \left[ \frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!} \right]^{1/2} e^{im\varphi} P_l^m(\cos \vartheta) \tag{2.9}$$

with  $P_l^m(\cos \vartheta)$  as the associated Legendre polynomials. (Here, unlike Bethe and Salpeter [7], we used the conventional definition of  $Y_{l,m}(\Omega)$ .)

In our notation (cf (2.1)-(2.3))  $c_s^+$ ,  $c_s$  are the fermion creation and annihilation operators for an electron in state  $s$ ,  $a_{\beta,\lambda}^+(k)$ ,  $a_{\beta,\lambda}(k)$  are the boson creation and annihilation operators for a photon with frequency  $\omega = kc$ , helicity  $\lambda$  and  $\beta = (J, M)$ . Furthermore,  $\omega_{ss'} = (E_s - E_{s'})/\hbar$  are the atomic transition frequencies and  $\alpha$  is the Dirac operator [7, 8]

$$\alpha = \begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix} \tag{2.10}$$

with  $\sigma$  as the Pauli spin operators and  $u_s(\mathbf{r})$  are the Dirac eigenfunctions corresponding to the energy eigenvalues  $E_s$  of an electron in a Coulomb potential (see appendix A).

### 3. Non-Markovian equation of motion for the $2P_{1/2} \rightarrow 1S_{1/2}$ transition

The relativistic Schrödinger (Dirac) equation in the interaction picture reads as

$$\frac{d|\Psi(t)\rangle}{dt} = -\frac{i}{\hbar} H(t)|\Psi(t)\rangle \tag{3.1}$$

where, since we are interested in the decay of the bound state  $2P_{1/2}$  of an electron in a hydrogen atom, we choose the special initial condition

$$|\Psi(0)\rangle = |1(\varepsilon)\rangle_A \otimes |V\rangle_R \tag{3.2}$$

with

$$|1(\varepsilon)\rangle_A = |n=2, l=1, j=\frac{1}{2}, m=(\varepsilon)\frac{1}{2}\rangle, \varepsilon = (+, -) \tag{3.3}$$

as the initial state of the electron in the atom, and  $|V\rangle_R$  as the vacuum state (no photons) of the radiation field.

In order to derive a non-Markovian equation of motion for the decay of the state  $|\Psi(0)\rangle$ , we apply the SCPOM developed in [3] to the Schrödinger equation (3.1). The advantages of the SCPOM as compared with the usually used projection-operator methods leading to unphysical results have been discussed in great detail in [9]. Since we are interested only in the spontaneous decay of a state, the virtual transitions contributing to energy-level (Lamb) shifts will be ignored in the following. Then, in the lowest-order approximation our SCPOM yields [3]:

$$\frac{dP_0^{(\varepsilon)}|\Psi(t)\rangle}{dt} = -\frac{1}{\hbar^2} \int_0^t d\tau P_0^{(\varepsilon)} H(t) [I_{(\varepsilon)}^{s(l)} - P_0^{(\varepsilon)}] H(t-\tau) P_0^{(\varepsilon)} |\Psi(t-\tau)\rangle \tag{3.4}$$

with

$$P_0^{(\varepsilon)} = |1(\varepsilon)\rangle_{AA} \langle 1(\varepsilon)| \otimes |V\rangle_{RR} \langle V| \tag{3.5}$$

$$I_{(\varepsilon)}^{s(1)} = |1(\varepsilon)\rangle_{AA} \langle 1(\varepsilon)| \otimes |V\rangle_{RR} \langle V| + \int_0^\infty dk \sum_{\substack{i=2,3 \\ \lambda=\pm 1}} |i\rangle_{AA} \langle i| \otimes |k, \beta_{i(\varepsilon)}, \lambda\rangle_{RR} \langle k, \beta_{i(\varepsilon)}, \lambda| \quad (3.6)$$

$$|2\rangle_A = |n=1, l=0, j=\frac{1}{2}, m=\frac{1}{2}\rangle_A = |1S_{1/2}(\frac{1}{2})\rangle_A \quad (3.7a)$$

$$|3\rangle_A = |1S_{1/2}(-\frac{1}{2})\rangle_A \quad (3.7b)$$

$$\beta_{2(+)} = (J_{2(+)} = 1, M_{2(+)} = 0) \quad \beta_{3(+)} = (J_{3(+)} = 1, M_{3(+)} = 1) \quad (3.8a)$$

$$\beta_{2(-)} = (J_{2(-)} = 1, M_{2(-)} = -1) \quad \beta_{3(-)} = (J_{3(-)} = 1, M_{3(-)} = 0). \quad (3.8b)$$

Here  $I_{(\varepsilon)}^{s(1)}$  is the unit operator in the subspace (containing the one-photon states  $|k, \beta_{i(\varepsilon)}, \lambda\rangle_R$ ) created by a onefold action of the interaction Hamiltonian  $H(t)$  on the initial state vector  $|1(\varepsilon)\rangle_A \otimes |V\rangle_R$  [3], where the virtual-transition matrix elements are ignored. This has the consequence that the only matrix elements which appear in (3.4) are:

$$H_{1, M_{i(\varepsilon)}, \lambda}^{1(\varepsilon), i}(k) \quad i=2, 3 \quad \varepsilon = (+, -) \quad \lambda = \pm 1.$$

The calculation of these matrix elements is carried out in appendix A. By using these results (cf (A.21a) and (A.21b)) a closed equation of motion for the probability amplitude for finding the atom in the initial state  $|1(\varepsilon)\rangle_A$  and zero photons in the radiation field,

$$b_{1(\varepsilon), 0}(t) = {}_A \langle 1(\varepsilon)| \otimes {}_R \langle V| P_0^{(\varepsilon)} |\Psi(t)\rangle \quad \varepsilon = (+, -) \quad (3.9)$$

can be derived:

$$\frac{db_{1(\varepsilon), 0}(t)}{dt} = -\frac{\gamma}{2\pi} \int_0^\infty d\omega F(\omega) \int_0^t dt' e^{i(\omega_0 - \omega)\tau} b_{1(\varepsilon), 0}(t - \tau) \quad b_{1(\varepsilon), 0}(0) = 1 \quad (3.10)$$

with

$$F(\omega) = \frac{2\pi}{\gamma \hbar^2 c} \sum_{i=2}^3 \sum_{\lambda=\pm 1} |H_{1, M_{i(\varepsilon)}, \lambda}^{1(\varepsilon), i}(k)|^2 = \frac{\omega [1 + 4(\omega/\Omega)^2]^2}{[1 + (\omega/\Omega)^2]^6} \quad (3.11)$$

$$\Omega = \frac{3c}{2\alpha_0} \quad \gamma = \gamma_0/\omega_0 \quad \gamma_0 = (\frac{2}{3})^8 \alpha^5 mc^2/\hbar \quad (3.12)$$

where according to (A.1) the atomic transition frequency is given by

$$\omega_0 = \omega_{1(\varepsilon), 2} = \omega_{1(\varepsilon), 3} = \frac{3}{8} \alpha^2 mc^2/\hbar + O(\alpha^4). \quad (3.13)$$

Since, from (3.10) it follows that

$$b_{1(+), 0}(t) = b_{1(-), 0}(t) = b_{1, 0}(t) \quad (3.14)$$

we shall drop the subscript  $\varepsilon = (+, -)$  in the following sections.

#### 4. Analytic treatment of equation (3.10)

By applying the Laplace transformation to (3.10), we obtain

$$\hat{b}_{1, 0}(z) = \int_0^\infty dt e^{-zt} b_{1, 0}(t) = 1 \left[ z + \frac{\gamma}{2\pi} \int_0^\infty \frac{d\omega F(\omega)}{z - i(\omega_0 - \omega)} \right]^{-1} \quad (4.1)$$

The Laplace inversion and substitution  $z = -iu + i\omega_0$  yields

$$b_{1,0}(t) = \frac{e^{i\omega_0 t}}{2\pi i} \int_C du e^{-iu} \hat{B}(u) \tag{4.2}$$

where

$$\hat{B}(u) = \frac{1}{N(u)} \quad N(u) = u - \omega_0 + \frac{\gamma}{2\pi} I(u) \tag{4.3}$$

$$I(u) = \int_0^\infty d\omega \frac{F(\omega)}{\omega - u} \tag{4.4}$$

and the path of integration  $C$  in (4.2) is a horizontal line in the half-plane  $\text{Im}(u) > 0$ , oriented from the right to the left. The evaluation of the integral in (4.4) (see appendix B) yields

$$I(u) = \frac{\Omega}{(1 + \tilde{u}^2)^5} P_{11}(\tilde{u}) + F(u) [-\log(\tilde{u}) + i\pi] \quad \tilde{u} = \frac{u}{\Omega} \tag{4.5}$$

where  $P_{11}(\tilde{u})$  is a polynomial of degree 11 in  $\tilde{u}$ :

$$P_{11}(\tilde{u}) = \frac{167}{512}\pi + \frac{7}{120}\tilde{u} + \frac{77}{512}\pi\tilde{u}^2 + O(\tilde{u}^3) \tag{4.6}$$

and  $\log(u)$  is a multivalued natural logarithm of a complex variable. The integrand of (4.2) is analytic for  $\text{Im}(u) > 0$  and ‘lives’ on the Riemann surface of  $\log(u)$ . Analogously to I, we deform the path integration  $C$  to the path  $K$ . The path  $K$  consists of two rays, both parallel to the line  $\text{Re}(u) + \text{Im}(u) = 0$ ; one of them runs from  $(1 - i)\infty$  to the branch point 0 on the lower Riemann sheet  $-1$ , and the other runs in the opposite direction on sheet 0 (see figure 1 in I).

The number of poles passed in the process of the path deformation as well as their localization can be found directly from the results derived in appendices C and B of I. The only difference is that in the present calculations we have to use the natural cut-off function  $F(u)$  (cf (3.11)) instead of the non-relativistic one

$$f(u) = \frac{u}{[1 + (u/\Omega)^2]^4} \tag{4.7}$$

used in I. It should be taken into account that between these cut-off functions the following relations hold:

$$|F(u)| < 16|f(u)| \quad u = (1 - i)\Omega x \quad 0 \leq x \leq \infty \tag{4.8}$$

(the path of integration  $K$  is parametrized), and

$$|I(u)| < 16|\tilde{I}(u)| \quad \tilde{I}(u) = \int_0^\infty \frac{d\omega f(\omega)}{\omega - u} \tag{4.9}$$

$$|I'(u)| < 16|\tilde{I}'(u)| \quad I'(u) = \frac{dI(u)}{du} \tag{4.10}$$

where the both last relations follow immediately if  $F(\omega) < 16f(\omega)$  is inserted into the expressions for  $I(u)$  and  $I'(u)$ , respectively (cf (4.4)).

In this way we can adopt the localization of the poles, the residue evaluation and the error estimation from appendices B and C in I. The fixed-point method yields the following result for the Weisskopf-Wigner pole  $u_{-1}$  (lying on the Riemann sheet  $-1$ ):

$$u_{-1} = \omega_0 - \frac{167}{1024} \gamma \Omega - \frac{7}{240\pi} \gamma_0 - \frac{\gamma_0}{2\pi} \ln\left(\frac{\Omega}{\omega_0}\right) - i \frac{\gamma_0}{2} + \Delta_u$$

$$\left| \frac{\Delta_u}{u_{-1}} \right| < 10^{-10}. \tag{4.11}$$

Of course, this leads to somewhat larger errors as compared with the results of I, but the errors are still small enough to guarantee the applicability of the fixed-point method as well as the residue calculation and there is no need for a more exact approximation procedure.

The above path deformation of the integration in (4.2) and the theory of the residue calculus yields

$$b_{1,0}(t) = R_1(t) + D_1(t) \tag{4.12}$$

where

$$R_1(t) = \text{Res}[e^{i\omega_0 t} e^{-iu t} \hat{B}(u), u_{-1}] \tag{4.13}$$

is the residue of the Weisskopf-Wigner pole describing the Markovian behaviour (exponential decay) and

$$D_1(t) = \frac{e^{i\omega_0 t}}{2\pi i} \int_K du \hat{B}(u) e^{-iu t} \tag{4.14}$$

describes the non-Markovian behaviour (deviation from exponential decay). By using appendix B in I, it is easy to calculate the residue in (4.13):

$$R_1(t) = (1 + \Delta_R) e^{i\omega_0 t} e^{-iu_{-1} t} \quad |\Delta_R| < 1.6 \times 10^{-6}. \tag{4.15}$$

By parametrizing the path of integration  $K$ , (4.14) takes the following form:

$$D_1(t) = -\frac{e^{i\omega_0 t}}{2\pi i} \int_0^\infty e^{-iu t} \left[ \frac{1}{N_0(u)} - \frac{1}{N_{-1}(u)} \right] du \quad u = (1-i)\Omega x$$

$$= \frac{e^{i\omega_0 t}}{2\pi} (1-i) \int_0^\infty \frac{\gamma F(u) e^{-iu t} \Omega dx}{N_0(u) N_{-1}(u)} \tag{4.16}$$

with

$$N_0(u) = u - \omega_0 + \frac{\gamma}{2\pi} I_0(u) \quad N_{-1}(u) = N_0(u) + i\gamma F(u) \tag{4.17}$$

where the subscripts 0 and  $-1$  denote different branches of the functions on the Riemann surface of  $\log(u)$ . According to Abel's asymptotic the main asymptotic contribution to  $D_1(t)$  in (4.16) stems from the first term in a geometric series development around  $x = 0$ :

$$\frac{F[(1-i)\Omega x]}{N_0[(1-i)\Omega x] N_{-1}[(1-i)\Omega x]} = \frac{(1-i)\Omega x}{N_0^2(0)} + O(x^2). \tag{4.18}$$

Thus, the asymptotic result for  $D_1(t)$  reads as

$$D_1(t \rightarrow \infty) = -\frac{\gamma}{2\pi N_0^2(0)} \frac{1}{t^2} e^{i\omega_0 t} \tag{4.19}$$

where according to (4.3), (4.5) and (4.6) it holds that

$$N_0(0) = -\omega_0 + \frac{\gamma\Omega}{2\pi} P_{11}(0) = -\omega_0 + \gamma\Omega \frac{167}{1024} \approx -\omega_0. \tag{4.20}$$

Analogously to I, the integral in (4.16) can be solved by an approximation procedure based on accurate error estimates. This procedure shows that the asymptotic main term

$$M(t) = -\frac{\gamma}{2\pi(-\omega_0 + \gamma\Omega(167/1024))^2} \frac{e^{i\omega_0 t}}{t^2} \approx -\frac{\gamma}{2\pi\omega_0^2} \frac{e^{i\omega_0 t}}{t^2} \tag{4.21}$$

describes the non-Markovian behaviour for *finite times* as well, within some error bounds:

$$D_1(t) = M(t) + \Delta_D(t) \tag{4.22}$$

$$\left| \frac{\Delta_D(t)}{M(t)} \right| < 25 \times 10^{-3} \quad t \geq 10^{-12} \text{ s.} \tag{4.23}$$

### 5. Radiative lineshape

The radiative lineshape or frequency spectrum, describing the probability for finding the emitted photon in the frequency interval  $[\omega, \omega + d\omega]$ , can be obtained from (4.2) in the following way. The path of integration  $C$  in (4.2) should be deformed to the path  $C^*$ . The path  $C^*$  consists of two horizontal rays, emanating from 0 and tending to  $+\infty$ , so that  $C^*$  starts on the upper half-plane of the zeroth Riemann sheet at  $+\infty$ , then winds around the branch point 0 and tends to  $+\infty$  on the lower half-plane of the same zeroth Riemann sheet.

By using the argument principle of appendix C in I, it can be shown that in the process of the path deformation no poles are passed and, therefore, (4.2) takes the following form:

$$b_{1,0}(t) = \frac{e^{i\omega_0 t}}{2\pi i} \int_{C^*} du e^{-itu} \hat{B}(u). \tag{5.1}$$

By parametrizing the path of integration  $C^*$  we obtain

$$\begin{aligned} b_{1,0}(t) &= \frac{e^{i\omega_0 t}}{2\pi i} \int_0^\infty d\omega e^{-i\omega t} \left[ \frac{1}{N_0(\omega - i0)} - \frac{1}{N_0(\omega + i0)} \right] \\ &= \frac{e^{i\omega_0 t}}{2\pi i} \int_0^\infty d\omega e^{-i\omega t} \frac{i\gamma F(\omega)}{N_0^2(\omega + i0) - i\gamma F(\omega) N_0(\omega + i0)} \\ &= e^{i\omega_0 t} \int_0^\infty d\omega e^{-i\omega t} \frac{(\gamma/2\pi)F(\omega)}{[N_0(\omega) - i(\gamma/2)F(\omega)]^2 + [(\gamma F(\omega))/2]^2} \end{aligned} \tag{5.2}$$

where we used

$$N_0(\omega - i0) = N_0(\omega + i0) - i\gamma F(\omega). \tag{5.3}$$

For  $t = 0$ , the integrand of (5.2) is identical with the frequency spectrum function:

$$S(\omega) = \frac{\gamma}{2\pi} \frac{F(\omega)}{[\omega - \omega_0 + (\gamma/2\pi)J(\omega)]^2 + (\gamma^2/4)F^2(\omega)} \tag{5.4}$$



where

$$J(\omega) = I_0(\omega) - i\pi F(\omega). \quad (5.5)$$

The function  $S(\omega)$  is quasi-Lorentzian with the decay rate  $\gamma F(\omega)$  and the frequency shift  $(\gamma/2\pi)J(\omega)$ , both depending on the frequency  $\omega$ . This result differs from the usual Lorentzian spectrum used in the literature [10]. Namely, in the Lorentzian spectrum of the spontaneously emitted radiation, the decay rate as well as the frequency shift depend on the atomic transition frequency  $\omega_0$  and not on the frequency  $\omega$ .

## 6. Discussion

In the present paper, for the first time to our knowledge, a non-Markovian treatment of the time-dependent spontaneous Lyman- $\alpha$  emission process in the case of a Dirac hydrogen atom has been achieved. In the literature the relativistic treatment of the spontaneous emission was usually restricted to the calculation of time-independent transition probabilities without giving any result for the time-dependent behaviour of a spontaneous decaying atom.

The relativistic transition probabilities were calculated numerically not only for one-electron atoms beyond the dipole approximation (making use of expansions in terms of electric and magnetic multipoles), but for many-electron atoms as well (see e.g. the papers by Johnson *et al* [11-13] and Scofield [14, 15]). In spite of all this, apart from general expressions for transition matrix elements, we have not found any analytic result for the matrix elements of the  $2P_{1/2}(\pm 1/2) \rightarrow 1S_{1/2}(\pm 1/2)$  transitions in the literature. Since such analytic results, which take into account retardation effects, are absolutely necessary in our treatment, the transition matrix elements of interest were calculated in appendix A.

In other words, a correct non-Markovian treatment of the problem requires the inclusion of the retardation effects as well as the application of an SCPOM. Namely, as a consequence of ignoring retardation effects, not only do divergent results, making the introduction of unnatural cut-off frequencies, appear, but incorrect cut-off-dependent deviations from exponential decay emerge as well (for more details see [1]). Further, as was demonstrated in [9], the usually used projection-operator method yields unphysical results (negative probabilities) for the deviations from exponential decay, since the Born approximation without the Markov approximation leads to the violation of a consistency condition.

In order not to make further calculations unnecessarily complicated and analytically unfeasible, in the radial part of the transition matrix elements, terms of order of  $\alpha^3$  were ignored in appendix A (cf (A.15)). The neglect of these terms is justified in the present treatment, since these terms do not influence the non-Markovian time behaviour, but only contribute to corrections of the Einstein coefficient  $\gamma_0$  for the spontaneous emission, which are of order of magnitude  $\gamma_0\alpha^2$ . However, despite the fact that higher-order- $\alpha$  relativistic effects were ignored, it is obvious that the present treatment is superior to that of the non-relativistic one used in I, since, contrary to I, the effect of the electron spin and terms like  $(e^2/2mc^2)A^2$  are taken into account (in this sense similarity to the Pauli approximation arises).

By comparing the present treatment to that of I, the following can be deduced:

(i) Instead of a single transition  $2P \rightarrow 1S$  (see I) two different transitions  $2P_{1/2}(\pm 1/2) \rightarrow 1S_{1/2}(1/2)$  and  $2P_{1/2}(\pm 1/2) \rightarrow 1S_{1/2}(-1/2)$  occur.

(ii) Instead of non-relativistic cut-off and level-shift functions  $f(\omega)$  (cf (4.7)) and  $\tilde{I}(\omega)$  (cf (4.9) and in I see (2.5)) new functions  $F(\omega)$  (cf (3.11)) and  $I(\omega)$  (cf (4.4) and (4.5)) are obtained.

From (i) and (ii) it follows that if we are only interested in the total result for the non-decay probability amplitude of the state  $2P_{1/2}$ , where both transitions mentioned in (i) are included, the only difference between the present results and that of I exists in small corrections in the real part of the Weisskopf-Wigner pole (level shift) (compare (4.11) with (2.9) in I) and in the frequency  $\omega_0$  appearing in the coefficient of the denominator of the asymptotic main term  $M(t)$  (compare (4.21) with (2.22) in I).

Finally, from all this it can be concluded that the relativistic treatment of the problem leads only to small corrections in the constant coefficients (Einstein coefficient for the spontaneous emission, transition frequency and level shift) but no correction in the Markovian and non-Markovian time behaviour arises.

Now a few words should be spent on the radiative lineshape treated in section 5. The present non-Markovian treatment leads to a new quasi-Lorentzian spectrum (cf (5.4)) in which instead of constant decay rate  $\gamma F(\omega_0)$  and frequency shift  $J(\omega_0)$  (see e.g. [10]) frequency-dependent functions  $\gamma F(\omega)$  and  $J(\omega)$  (whose non-relativistic expressions are given by (4.7) and (4.9)) appear. However, since these frequency-dependent functions are multiplied by a very small factor  $\gamma \approx 10^{-8}$ , the effect of the frequency dependence is extremely weak and the Lorentzian spectrum used in the literature can be considered as a very good approximation in a large frequency interval around the transition frequency  $\omega_0$ .

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**Appendix A: Analytic results for the transition matrix elements without dipole approximation**

The discrete energy eigenvalues of an electron in a Coulomb potential [7] read as

$$\begin{aligned}
 E_s = E_{nj} &= mc^2 \left\{ 1 + \frac{\alpha^2}{[n - (j + \frac{1}{2}) + \sqrt{(j + \frac{1}{2})^2 - \alpha^2}]^2} \right\}^{-1/2} \\
 &= mc^2 \left[ 1 - \frac{1}{2} \frac{\alpha^2}{n^2} + O(\alpha^4) \right].
 \end{aligned}
 \tag{A.1}$$

By the subscripts  $s = (n, l, j, m)$  we denote collectively the principal quantum number  $n$  as well as the angular momentum quantum numbers  $l, j, m$  and  $\alpha$  is the fine structure constant. The Dirac eigenfunctions corresponding to the eigenvalues  $E_s$  read as

$$u_s(\mathbf{r}) = \begin{pmatrix} g_s(\mathbf{r})\phi_s(\Omega) \\ -if_s(\mathbf{r})\tilde{\phi}_s(\Omega) \end{pmatrix}
 \tag{A.2}$$

where  $g_s(r) = g_{nlj}(r)$ ,  $f_s(r) = f_{nlj}(r)$  are the radial parts and  $\phi_s(\Omega)$ ,  $\tilde{\phi}_s(\Omega)$  are the angular parts given by

$$\phi_{l,j=l+\frac{1}{2},m}(\Omega) = \begin{pmatrix} \sqrt{(l+m+1/2)/(2l+1)} & Y_{l,m-\frac{1}{2}}(\Omega) \\ \sqrt{(l-m+1/2)/(2l+1)} & Y_{l,m+\frac{1}{2}}(\Omega) \end{pmatrix} \tag{A.3a}$$

$$\tilde{\phi}_{l,j=l+\frac{1}{2},m}(\Omega) = \begin{pmatrix} \sqrt{(l-m+3/2)/(2l+3)} & Y_{l+1,m-\frac{1}{2}}(\Omega) \\ -\sqrt{(l+m+3/2)/(2l+3)} & Y_{l+1,m+\frac{1}{2}}(\Omega) \end{pmatrix} \tag{A.3b}$$

$$\phi_{l,j=l-\frac{1}{2},m}(\Omega) = \begin{pmatrix} \sqrt{(l-m+1/2)/(2l+1)} & Y_{l,m-\frac{1}{2}}(\Omega) \\ -\sqrt{(l+m+1/2)/(2l+1)} & Y_{l,m+\frac{1}{2}}(\Omega) \end{pmatrix} \tag{A.3c}$$

$$\tilde{\phi}_{l,j=l-\frac{1}{2},m}(\Omega) = \begin{pmatrix} \sqrt{(l+m-1/2)/(2l-1)} & Y_{l-1,m-\frac{1}{2}}(\Omega) \\ \sqrt{(l-m-1/2)/(2l-1)} & Y_{l-1,m+\frac{1}{2}}(\Omega) \end{pmatrix} \tag{A.3d}$$

By using (2.3)-(2.10), (A.2) and (A.3) the transition matrix elements of (2.2) take the following form:

$$\begin{aligned} H_{J,M,\lambda}^{s,s'}(k) = & e[2\hbar ck/(2J+1)]^{1/2} i^{J+1} \{i\lambda[\sqrt{J}R_{J+1}^{s,s'}(k)N_{J,J+1,M}^{s,s'} \\ & -\sqrt{J+1}R_{J-1}^{s,s'}(k)N_{J,J-1,M}^{s,s'} -\sqrt{J}R_{J+1}^{s,s'}(k)\tilde{N}_{J,J+1,M}^{s,s'} \\ & +\sqrt{J+1}R_{J-1}^{s,s'}(k)\tilde{N}_{J,J-1,M}^{s,s'}] + R_J^{s,s'}(k)N_{J,J,M}^{s,s'} - R_J^{s,s'}(k)\tilde{N}_{J,J,M}^{s,s'} \} \end{aligned} \tag{A.4}$$

where we used

$$N_{J,L,M}^{s,s'} = \int d\Omega Y_{J,L,M}(\Omega) \cdot \mathbf{B}_{s,s'}(\Omega) \tag{A.5a}$$

$$\tilde{N}_{J,L,M}^{s,s'} = \int d\Omega Y_{J,L,M}(\Omega) \cdot \tilde{\mathbf{B}}_{s,s'}(\Omega) \tag{A.5b}$$

$$\mathbf{B}_{s,s'}(\Omega) = \sum_{q=-1}^1 \mathbf{e}_q \phi_s^+(\Omega) \sigma_q \tilde{\phi}_{s'}(\Omega) \tag{A.6a}$$

$$\tilde{\mathbf{B}}_{s,s'}(\Omega) = \sum_{q=-1}^1 \mathbf{e}_q \tilde{\phi}_s^+(\Omega) \sigma_q \phi_{s'}(\Omega) \tag{A.6b}$$

$$R_J^{s,s'}(k) = \int_0^\infty dr r^2 j_J(kr) g_s(r) f_{s'}(r). \tag{A.7}$$

According to calculations of section 3 the only matrix elements of interest are:

$$\begin{aligned} H_{1,M_{i(\epsilon)},\lambda}^{1(\epsilon),i} = & -(2\hbar ck/3)^{1/2} i\lambda [R_2^{1(\epsilon),i}(k)N_{1,2,M_{i(\epsilon)}}^{1(\epsilon),i} -\sqrt{2}R_0^{1(\epsilon),i}(k)N_{1,0,M_{i(\epsilon)}}^{1(\epsilon),i} \\ & -R_2^{i(1\epsilon)}(k)\tilde{N}_{1,2,M_{i(\epsilon)}}^{i(1\epsilon),i} +\sqrt{2}R_0^{i(1\epsilon)}(k)\tilde{N}_{1,0,M_{i(\epsilon)}}^{i(1\epsilon),i}] \\ i = 2, 3 \quad & M_{2(+)} = M_{3(-)} = 0 \quad M_{2(-)} = -M_{3(+)} = -1 \end{aligned} \tag{A.8}$$

where in our case the two last terms in (A.4), (stemming from magnetic multipole transitions) vanish, since only electric dipole transitions are possible.

By using (A.5), (A.6), (A.3), (2.7) and the orthogonality properties of the spherical harmonics, a lengthy calculation yields the following result for the angular parts of the transition matrix elements appearing in (A.8):

$$N_{1,2,0}^{1(+),2} = \frac{1}{\sqrt{2}} N_{1,2,-1}^{1(-),2} = -\frac{1}{\sqrt{2}} N_{1,2,1}^{1(+),3} = -N_{1,2,0}^{1(-),3} = -\frac{\sqrt{2}}{3\sqrt{\pi}} \tag{A.9a}$$

$$N_{1,0,0}^{1(+),2} = \frac{1}{\sqrt{2}} N_{1,0,-1}^{1(-),2} = -\frac{1}{\sqrt{2}} N_{1,0,1}^{1(+),3} = -N_{1,0,0}^{1(-),3} = -\frac{1}{6\sqrt{\pi}} \tag{A.9b}$$

$$\tilde{N}_{1,0,0}^{1(+),2} = \frac{1}{\sqrt{2}} \tilde{N}_{1,0,-1}^{1(-),2} = -\frac{1}{\sqrt{2}} \tilde{N}_{1,0,1}^{1(+),3} = -\tilde{N}_{1,0,0}^{1(-),3} = \frac{1}{2\sqrt{\pi}} \quad \tilde{N}_{1,2,M_{l(\epsilon)}}^{1(\epsilon),j} = 0. \tag{A.9c}$$

The radial matrix elements appearing in (A.8) are

$$R_J^{1(\epsilon),i}(k) = \int_0^\infty dr r^2 j_J(kr) g_{1(\epsilon)}(r) f_i(r) \quad J = 0, 2 \quad i = 2, 3 \tag{A.10a}$$

$$R_2^{1/2(\epsilon)}(k) = \int_0^\infty dr r^2 j_2(kr) g_i(r) f_{1(\epsilon)}(r) \quad i = 2, 3 \tag{A.10b}$$

where the spherical Bessel functions are given by

$$j_J(x) = (-i)^J \frac{1}{2} \int_{-1}^1 dy e^{ixy} P_J(y) \tag{A.11a}$$

$$j_J(x) = (-1)^J x^J \frac{d^J}{(x dx)^J} \left( \frac{\sin x}{x} \right) \tag{A.11b}$$

with  $P_J(y)$  as the Legendre polynomials.

The normalized radial Dirac eigenfunctions can be found in [7] and read as

$$g_{1(\epsilon)} = \left( \frac{2}{Na_0} \right)^{3/2} \left[ \frac{2\eta + 1}{\Gamma(2\eta + 1)} \right]^{1/2} \left[ \frac{1 + \delta_2}{4N(N-1)} \right]^{1/2} e^{-1/2\rho} \left[ (N-2)\rho^{\eta-1} - \frac{N-1}{2\eta+1} \rho^\eta \right] \tag{A.12a}$$

$$f_{1(\epsilon)} = - \left( \frac{1 - \delta_2}{1 + \delta_2} \right)^{1/2} \frac{(2\eta + 1)N - (N-1)\rho}{(2\eta + 1)(N-2) - (N-1)\rho} g_{1(\epsilon)} \tag{A.12b}$$

$$g_i = \left( \frac{2}{a_0} \right)^{3/2} \left[ \frac{1 + \delta_1}{2\Gamma(2\eta + 1)} \right]^{1/2} e^{-r/a_0} \left( \frac{2r}{a_0} \right)^{\eta-1} \quad i = 2, 3 \tag{A.13a}$$

$$f_i = \left( \frac{1 - \delta_1}{1 + \delta_1} \right) g_i \tag{A.13b}$$

$$\eta = (1 - \alpha^2)^{1/2} \quad N = \sqrt{2(1 + \eta)} \quad \rho = \frac{2r}{Na_0} \tag{A.14a}$$

$$\delta_1 = \left[ 1 + \left( \frac{\alpha}{\eta} \right)^2 \right]^{-1/2} \quad \delta_2 = \left[ 1 + \left( \frac{\alpha}{1 + \eta} \right)^2 \right]^{-1/2} \tag{A.14b}$$

where  $\alpha_0 \approx 10^{-9}$  cm is the Bohr radius and  $\alpha \approx 1/137$  is the fine structure constant. By using (A.12)–(A.14) we obtain

$$g_i f_{1(\epsilon)} = \frac{K_0^3}{\sqrt{6}} e^{-Kr} \left[ \frac{K_0 r - 6}{4} \alpha + O(\alpha^3) \right] \tag{A.15a}$$

$$K_0 = \frac{1}{a_0} \quad K = \frac{3}{2} K_0 \quad i = 2, 3$$

$$g_{1(\epsilon)} f_i = \frac{K_0^3}{2\sqrt{6}} e^{-Kr} [K_0 r \alpha + O(\alpha^3)] \quad i = 2, 3. \tag{A.15b}$$

Further, by making use of (A.15) (where the terms of the order of  $\alpha^3$  are ignored) the radial matrix elements of (A.10) can be written as

$$R_l^{1(\varepsilon),i}(k) = \frac{K_0^4 \alpha}{2\sqrt{6}} J^{l,3}(k, K) \quad l=0, 2 \quad (\text{A.16a})$$

$$R_0^{i,1(\varepsilon)}(k) = \frac{K_0^4 \alpha}{4\sqrt{6}} J^{0,3}(k, K) - \frac{\sqrt{6}}{4} K_0^3 \alpha J^{0,2}(k, K) \quad (\text{A.16b})$$

with

$$\begin{aligned} J^{l,m}(k, K) &= \int_0^\infty dr j_l(kr) e^{-Kr} r^m \\ &= \frac{(-i)^l}{2} \Gamma(m+1) \int_{-1}^1 dx \frac{P_l(x)}{(K - ikx)^{m+1}} \\ l, m \in \mathbb{N}_0 \quad k, K \in \mathbb{R} \end{aligned} \quad (\text{A.17})$$

$$J^{l,m+1}(k, K) = -\frac{\partial}{\partial K} J^{l,m}(k, K) \quad (\text{A.18})$$

where we applied (A.11a). Further, because of (A.11b), it holds that

$$J^{l+1,m+1}(k, K) = \frac{l}{k} J^{l,m}(k, K) - \frac{\partial}{\partial k} J^{l,m}(k, K). \quad (\text{A.19})$$

After some calculation, from (A.17)–(A.19), it follows that

$$J^{0,2}(k, K) = \frac{2}{K^3} \frac{1}{[1 + (k/K)^2]^2} \quad (\text{A.20a})$$

$$J^{0,3}(k, K) = \frac{2}{K^4} \frac{3 - (k/K)^2}{[1 + (k/K)^2]^3} \quad (\text{A.20b})$$

$$J^{2,3}(k, K) = \frac{1}{K^4} \frac{8(k/K)^2}{[1 + (k/K)^2]^3}. \quad (\text{A.20c})$$

By inserting (A.9), (A.16) and (A.20) into (A.8), we finally obtain for the transition matrix elements:

$$\begin{aligned} H_{1,0,\lambda}^{1(+),2}(k) &= -\lambda i \hbar (c\alpha)^{1/2} \frac{(k/K)^{1/2} [1 + 4(k/K)^2]}{[1 + (k/K)^2]^3} \\ \lambda = \pm 1 \quad \alpha &= \left(\frac{2}{3}\right)^9 \alpha^4 mc^2 / (2\pi\hbar) \end{aligned} \quad (\text{A.21a})$$

$$H_{1,1,\lambda}^{1(+),3}(k) = -H_{1,-1,\lambda}^{1(-),2}(k) = \sqrt{2} H_{1,0,\lambda}^{1(-),3}(k) = -\sqrt{2} H_{1,0,\lambda}^{1(+),2}(k). \quad (\text{A.21b})$$

## Appendix B: Evaluation of the integral in equation (4.4)

The integral in (4.4) can be evaluated by a method similar to that described in appendix A of I. Namely, the partial fraction decomposition yields

$$\frac{\mathcal{F}(x, a)}{x - u} = \frac{\mathcal{P}_{11}(x, u, a)}{(1 + x^2)^6} + \frac{\mathcal{F}(u, a)}{x - u} \quad (\text{B.1})$$

where

$$\mathcal{F}(x, a) = \frac{x(1+ax^2)}{(1+x^2)^6} \tag{B.2}$$

and  $\mathcal{P}_{11}(x, u, a)$  is a polynomial of degree 11 in  $x$  as well as in  $u$ , since it holds that

$$x(1+ax^2) = \frac{\mathcal{P}_{11}(x, u, a)(x-u) + u(1+au^2)(1+x^2)^6}{(1+u^2)^6}. \tag{B.3}$$

Then, by using (B.1) and applying the method used in appendix A of I, it can be shown that integrals of the form

$$\mathcal{I}(u, a) = \int_0^\infty dx \frac{\mathcal{F}(x, a)}{x-u} \quad \mathcal{F}(x, a) = \frac{x(1+ax^2)}{(1+x^2)^6} \tag{B.4}$$

have the following exact solution:

$$\mathcal{I}(u, a) = \frac{P_{11}(u, a)}{(1+u^2)^6} + \mathcal{F}(u, a)[- \log(u) + i\pi] \tag{B.5}$$

where  $P_{11}(u, a)$  is a polynomial of degree 11 in  $u$ :

$$\begin{aligned} P_{11}(u, a) = & \pi[63 + 14a + 3a^2]/512 + u[-137 + 24a + 3a^2]/120 \\ & + u^2\pi[-315 + 210a + 25a^2]/512 + u^3[-30 - 13a + 3a^2]/12 \\ & + u^4\pi[-105 - 210a + 75a^2]/512 + u^5[-15 - 12a - a^2]/6 \\ & + u^6\pi[-63 - 70a - 75a^2]/256 + u^7[-10 - 6a - 3a^2]/6 \\ & + u^8\pi[-45 - 42a - 25a^2]/512 + u^9[-15 - 8a - 3a^2]/24 \\ & + u^{10}\pi[-7 - 6a - 3a^2]/512 + u^{11}[-6 - 3a - a^2]. \end{aligned} \tag{B.6}$$

From (B.5) and (B.6) the results (4.5) and (4.6) can be deduced immediately for  $a = 4$ .

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