

The $2s_{1/2} \rightarrow 2p_{1/2} +$ one photon transition in hydrogen and hydrogenlike ions*

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The $2s_{1/2} \rightarrow 2p_{1/2} +$ one photon transition rate is calculated and discussed for hydrogen and hydrogenlike ions. It is noted that the induced transition rather than the spontaneous transition is of primary importance since it is the basis of many of the precision Lamb-shift measurements. The lack of a calculation of the transition rate other than a heuristic nonrelativistic derivation which requires a nontrivial assumption motivates the calculation presented here based on the external field approximation to quantum electrodynamics. It is found that the heuristic answer is correct in lowest order. In this derivation we see that the $2s_{1/2} \rightarrow 2p_{1/2} +$ one photon transition gives an apparent contradiction to the often-stated remark that for the electric dipole matrix element there exist three equivalent representations, the "length," "velocity," and "acceleration" forms. The difficulties of an experimental determination of this transition rate using induced transitions in hydrogenlike ions are briefly noted as well as the somewhat different case of heavy muonic atoms where the spontaneous $2s_{1/2} \rightarrow 2p_{1/2} +$ one photon transition has been observed.

I. INTRODUCTION

The spontaneous $2s_{1/2} \rightarrow 2p_{1/2} +$ one photon transition in hydrogen seldom occurs in nature. This decay mode is highly dominated by the principal decay mode of the $2s_{1/2}$ state, the $\frac{1}{7}$ -sec two-photon transition to the ground state. The induced transition is, on the other hand, of great importance in physics because it is the basis of many of the precision experiments on the Lamb shift. Future experimental interest in this transition may occur in measurements of the rate. Viewing the total decay rate as the imaginary part of a complex energy-level shift, the experimental determination of the $2s_{1/2} \rightarrow 2p_{1/2} +$ one photon transition rate in hydrogenlike ions would be a far more severe test of quantum electrodynamics in terms of powers of α and $Z\alpha$ than the real energy-level shift. In Sec. III we briefly comment on such experiments.

There is theoretical interest in this transition because it offers a contradiction to the often-stated contention that there exist three representations for the electric dipole matrix element, the "velocity," "length," and "acceleration" forms and that when one uses the exact wave function the forms are equivalent. The calculation of this decay amplitude appears to have been neglected so far. All we have is the heuristic argument referred to by Bethe and Salpeter.¹ This argument uses nonrelativistic quantum mechanics and an unjustified assumption.

This derivation starts with the nonrelativistic electric dipole transition amplitude²:

$$M_{\mathbf{nr}} = -\frac{e}{(2\omega_q)^{1/2}} \frac{1}{m} \langle 2p_{\mathbf{nr}} | \vec{p} \cdot \vec{\epsilon} | 2s_{\mathbf{nr}} \rangle. \quad (1)$$

$\vec{\epsilon}$ is the polarization vector of the emitted photon. ω_q is the frequency of the emitted photon, and

$|2s_{\mathbf{nr}}\rangle$ and $|2p_{\mathbf{nr}}\rangle$ are the nonrelativistic wave functions.

Using the commutation relation $\vec{p} = -im[\vec{r}, H_{\mathbf{nr}}]$, which involves the nonrelativistic hydrogen Hamiltonian $H_{\mathbf{nr}}$, we obtain

$$M_{\mathbf{nr}} = \frac{ie}{(2\omega_q)^{1/2}} (E_{2s}^{\mathbf{nr}} - E_{2p}^{\mathbf{nr}}) \langle 2p_{\mathbf{nr}} | \vec{r} \cdot \vec{\epsilon} | 2s_{\mathbf{nr}} \rangle, \quad (2)$$

which is zero since the difference in energy of the two degenerate states is zero. As an ansatz the heuristic argument replaces $E_{2s}^{\mathbf{nr}} - E_{2p}^{\mathbf{nr}}$ by the actual energy difference $\Delta E(2s_{1/2}, 2p_{1/2})$, which is the Lamb shift, to obtain the transition amplitude.

$$\tilde{M} = \frac{ie}{(2\omega_q)^{1/2}} \Delta E \langle 2s_{1/2}, 2p_{1/2} | \langle 2p_{\mathbf{nr}} | \vec{r} \cdot \vec{\epsilon} | 2s_{\mathbf{nr}} \rangle. \quad (3)$$

This point of view though engaging is not satisfying. The answer is not justified. Further, we note the "velocity" form of the dipole matrix element in (1) gives a zero result and modified "length" form (2) is definitely nonzero. This procedure appears to contradict the equivalence of the "length" and "velocity" representations.³

In Sec. II we calculate the $2s_{1/2} \rightarrow 2p_{1/2} +$ one photon transition rate using quantum electrodynamics. We find that \tilde{M} the heuristic matrix amplitude is correct up to terms of order α and $(Z\alpha)^2$. In Sec. III we give the spontaneous transition rate and briefly discuss some of the problems in performing a measurement of this rate by using induced transitions.

II. CALCULATION

In this section we will calculate the $2s_{1/2} \rightarrow 2p_{1/2} +$ one photon transition rate. The techniques used and simplifications noted are applicable to the other

electric dipole transitions between states of the same principal quantum number and total angular momentum. These states have the same energy when calculated by the Dirac equation. Radiative corrections split this degeneracy.

The calculation we perform starts from the external field approximation in quantum electrodynamics. The notation and some of the procedure comes from Lin and Feinberg's work⁴ on the radiative corrections to the $2s_{1/2} \rightarrow 1s_{1/2}$ + one photon transition rate for hydrogenlike ions. The diagrams we need to evaluate are shown in Fig. 1. The sum of the graphs 1(a)–1(d) gives rise to the expression⁵

$$M^D = \frac{e}{(2\omega_q)^{1/2}} \left\langle f \left| \Sigma_{\text{tot}} \frac{1}{\not{p} - m + i\eta} \not{\epsilon} + \not{\epsilon} \frac{1}{\not{p} - m + i\eta} \Sigma_{\text{tot}} \right| i \right\rangle \quad (4)$$

where $\Sigma_{\text{tot}} = \Sigma^{\text{el}} + \Sigma^{\gamma}$ is the total self-energy operator. Σ^{el} is the electron-self-energy term which is shown in Fig. 2(a), minus its mass counterterm. Σ^{γ} is the vacuum polarization operator which is displayed in Fig. 2(b). The initial and final states are degenerate solutions of the Dirac equation with eigenenergy E and as such have the property

$$\begin{aligned} (\not{p} - m)|n\rangle &= 0, \\ \langle n | (\not{p} - m) &= 0, \end{aligned} \quad (5)$$

where, here, $\langle n |$ represents the Dirac adjoint vector $\langle n | = u_n^\dagger \beta$ rather than the Hermitian conjugate vector. The mechanical momentum is $\pi = (E + Z\alpha/r, \vec{p})$ and $\epsilon_\mu = (0, \vec{\epsilon})$ is the emitted photon's polarization vector. The frequency ω_q corresponds to the photon's energy which is the actual difference in energy between the $2s_{1/2}$ and $2p_{1/2}$ states.

We expand the energy denominators in a complete set of solutions to the Coulomb problem in the Dirac equation neglecting those states i and f which are projected out by the use of $i\eta$ in the denominators:

$$\begin{aligned} M^D &= \frac{e}{(2\omega_q)^{1/2}} \\ &\times \sum_{n \neq i, f} \left\langle f \left| \Sigma_{\text{tot}} \frac{|n\rangle\langle n|}{E - E_n} \not{\epsilon} + \not{\epsilon} \frac{|n\rangle\langle n|}{E - E_n} \Sigma_{\text{tot}} \right| i \right\rangle. \end{aligned} \quad (6)$$

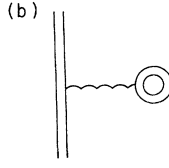
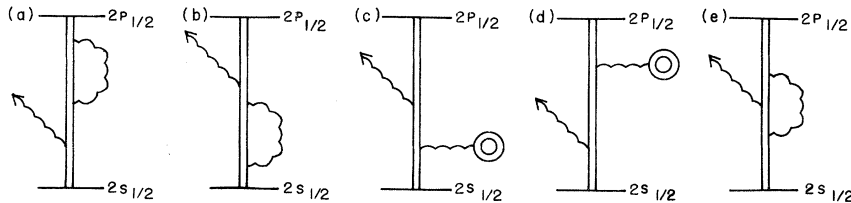


FIG. 2. (a) Electron self-energy operator; (b) vacuum polarization operator.

Next, we employ the relativistic commutation relation

$$\not{\epsilon} = i[\not{p}, \vec{r} \cdot \vec{\epsilon}], \quad (7)$$

which enables us to cancel the energy denominators.

$$\begin{aligned} M^D &\approx \frac{ie}{(2\omega_q)^{1/2}} \sum_{n \neq i, f} \left(\langle f | \Sigma_{\text{tot}} | n \rangle \langle n | \beta \vec{r} \cdot \vec{\epsilon} | i \rangle \right. \\ &\quad \left. - \langle f | \beta \vec{r} \cdot \vec{\epsilon} | n \rangle \langle n | \Sigma_{\text{tot}} | i \rangle \right). \end{aligned} \quad (8)$$

After adding and subtracting the i and f states to the intermediate states, we sum over a complete set of states:

$$\begin{aligned} M^D &\approx \frac{ie}{(2\omega_q)^{1/2}} \left[\langle f | \beta \vec{r} \cdot \vec{\epsilon} | i \rangle \langle i | \Sigma_{\text{tot}} | i \rangle - \langle f | \Sigma_{\text{tot}} | f \rangle \right. \\ &\quad \left. + \langle f | \Sigma_{\text{tot}} \vec{r} \cdot \vec{\epsilon} - \vec{r} \cdot \vec{\epsilon} \Sigma_{\text{tot}} | i \rangle \right]. \end{aligned} \quad (9)$$

The first term in the square brackets in (9) consists of the transition amplitude $\langle f | \beta \vec{r} \cdot \vec{\epsilon} | i \rangle$ multiplied by the lowest-order contribution to the Lamb shift $\Delta E^{(1)}(2s_{1/2}, 2p_{1/2}) = \langle i | \Sigma_{\text{tot}} | i \rangle - \langle f | \Sigma_{\text{tot}} | f \rangle$. It is this term which gives rise to the amplitude \bar{M} in (3). The second term in the brackets contains a part $\langle f | \Sigma^{\gamma} \vec{r} \cdot \vec{\epsilon} - \vec{r} \cdot \vec{\epsilon} \Sigma^{\gamma} | i \rangle$ which cancels through relative order α in (9) because the leading order of the the vacuum polarization operator $\Sigma^{\gamma} \sim \beta Z\alpha \nabla^2(1/r)$ commutes with $\vec{r} \cdot \vec{\epsilon}$. The remaining part of the second term in (9) cancels exactly the entire vertex amplitude M^A as we will show in the next few paragraphs:

$$\begin{aligned} M^D &\approx \frac{ie}{(2\omega_q)^{1/2}} \Delta E^{(1)}(2s_{1/2}, 2p_{1/2}) \langle f | \beta \vec{r} \cdot \vec{\epsilon} | i \rangle \\ &\quad - \frac{ie}{(2\omega_q)^{1/2}} \langle f | \vec{r} \cdot \vec{\epsilon} \Sigma^{\text{el}} - \Sigma^{\text{el}} \vec{r} \cdot \vec{\epsilon} | i \rangle. \end{aligned} \quad (10)$$

FIG. 1. (a) and (b) Electron self-energy contribution to transition amplitude; (c) and (d) vacuum polarization contribution to transition amplitude; (e) vertex contribution to transition amplitude.

The vertex graph is drawn in Fig. 1(e), and its matrix element is written below⁵:

$$M^A = \frac{e}{(2\omega_q)^{1/2}} \left\langle f \left| \frac{\alpha}{4\pi^3} \int \frac{d^4k}{ik^2} \gamma_\lambda \frac{1}{\not{k} - \not{m}} \not{\epsilon} \frac{1}{\not{k} - \not{m}} \gamma^\lambda \right| i \right\rangle. \quad (11)$$

Using the commutation relation $i[\not{k} - \not{m}, \vec{\Gamma} \cdot \vec{\epsilon}] = \not{\epsilon}$, we simplify M^A :

$$M^A \approx \frac{ie}{(2\omega_q)^{1/2}} \frac{\alpha}{4\pi^3} \int \frac{d^4k}{ik^2} \left\langle f \left| \vec{\Gamma} \cdot \vec{\epsilon} \gamma_\lambda \frac{1}{\not{k} - \not{m}} \gamma^\lambda - \gamma_\lambda \frac{1}{\not{k} - \not{m}} \gamma^\lambda \vec{\Gamma} \cdot \vec{\epsilon} \right| i \right\rangle. \quad (12)$$

Next, inside the matrix element and regulated integral over k we add and subtract $\delta m \vec{\Gamma} \cdot \vec{\epsilon}$, where δm is the mass counterterm, and finish with an expression for M^A containing Σ^{e1} :

$$M^A \approx \frac{ie}{(2\omega_q)^{1/2}} \left\langle f \left| \vec{\Gamma} \cdot \vec{\epsilon} \Sigma^{e1} - \Sigma^{e1} \vec{\Gamma} \cdot \vec{\epsilon} \right| i \right\rangle. \quad (13)$$

This expression for M^A exactly cancels the second term of M in (10).

The lowest-order part of the transition amplitude $M = M^E + M^A$ is given by

$$M \approx \frac{ie}{(2\omega_q)^{1/2}} \Delta E^{(1)}(2s_{1/2}, 2p_{1/2}) \left\langle f \left| \beta \vec{\Gamma} \cdot \vec{\epsilon} \right| i \right\rangle. \quad (14)$$

We may replace relativistic states i and f by the nonrelativistic states $2s_{nr}$ and $2p_{nr}$ with a relative error of $(Z\alpha)^2$. As a result, the lowest order of the transition amplitude M which we derived from quantum electrodynamics agrees with the heuristic nonrelativistic calculation of \tilde{M} in (3).

III. CONCLUSION

From (14) we obtain the lowest-order spontaneous transition rate for $2s_{1/2} \rightarrow 2p_{1/2} + \text{one photon transitions}$:

$$R = \frac{12}{Z^2 \alpha} \frac{[\Delta E^{(1)}(2s_{1/2}, 2p_{1/2})]^3}{m^2}. \quad (15)$$

There are several difficulties in measuring this quantity. We would apply to a known amount of hydrogenic ions in their $2s_{1/2}$ state a known amount of radiation with a frequency corresponding to the $2s_{1/2} - 2p_{1/2}$ separation. From the measurement of the number of subsequent $2p_{1/2} - 1s_{1/2}$ transitions we would infer the amount of induced $2s_{1/2} \rightarrow 2p_{1/2}$

+ one photon transitions. From this quantity we could determine the value of the spontaneous $2s_{1/2} \rightarrow 2p_{1/2} + \text{one photon transition rate}$. These experimental considerations are hampered somewhat by the finite width of the $2p_{1/2}$ state which is about one tenth the size of the $2s_{1/2} - 2p_{1/2}$ splitting for hydrogen.

In addition, it should be noted that the spontaneous $2s_{1/2} \rightarrow 2p_{1/2} + \text{one photon transition}$ has been observed in heavy muonic atoms.⁶ A major change in the derivation of the transition rate results in this case from allowing for the finite size of the nucleus which produces shifts of order $(Z\alpha)^4 M_\mu$ to the energy levels where M_μ is the mass of the muon. For heavy atoms such as Pb^{208} this term is not small and therefore is generally taken into account in the Dirac equation for the wave functions $|i'\rangle$ and $|f'\rangle$ by choosing a model for the nuclear charge distribution such as a uniform distribution.⁷ This alteration splits the $2s_{1/2} - 2p_{1/2}$ degeneracy. For this process the transition matrix element is $[e/(2\omega_q)^{1/2}] \langle f' | \not{\epsilon} | i' \rangle$ where we have neglected retardation. Using Eq. (7) we may write this transition matrix element as $[ie/(2\omega_q)^{1/2}] (E_{i'} - E_{f'}) \times \langle f' | \vec{\Gamma} \cdot \vec{\epsilon} \beta | i' \rangle$ which is here nonzero. The transition rate itself depends on the model and the atom. The radiative correction principally the order $\alpha(Z\alpha)M_\mu$ vacuum polarization contribution to the energy levels are not of much consequence and may be neglected in lowest order.⁸

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¹H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of One and Two Electron Atoms* (Springer-Verlag, Berlin, 1957), pp. 263, 274-275, 285.

²We use the set of units where $\hbar = c = 1$ and $\alpha = e^2/4\pi \approx 1/137$.

³If we reconsider and add the self-interactions to obtain in some sense the "exact" wave functions, we still do not get the two equivalent forms of the electric dipole matrix element because we are neglecting the vertex diagram [See Fig. 1(e)] which is of the same nominal order as the rest of the lowest-order contribution to the amplitude. Likewise, if we use the Dirac relativistic version of the electric dipole matrix element, the transition amplitude would have to be put in a heuristic

tic "length" form; the "velocity" form gives a zero answer.

⁴D. L. Lin and G. Feinberg, Phys. Rev. A 10, 1425 (1974).

⁵In lowest order we consider the emission of a photon between the two states of the same energy which have the vertex and self-energy corrections acting upon them. Accounting for the effect of the radiative corrections only once, we include just the dipole term

$\not{\epsilon}$ of $\not{\epsilon} \exp(-i\vec{q}\cdot\vec{x})$, the photon emission operator.

⁶H. L. Anderson, C. K. Hargrove, E. P. Hincks, J. D. McAndrew, R. J. McKee, and D. Kessler, Phys. Rev. Lett. 22, 221 (1969).

⁷H. A. Bethe and J. W. Negele, Nucl. Phys. A 117, 575 (1968).

⁸Another option which must be used for lower- Z muonic atoms is to include the order $\alpha(Z\alpha)M_\mu$ vacuum polarization term in the construction of the wave function.