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THE BETHE, BROWN, AND STEHN LAMB SHIFT CALCULATION REVISITED

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Abstract

As applied by Bethe, Brown, and Stehn in 1950, the first theory of the Lamb shift, although it contains many physical and mathematical approximations, is known to be in agreement with experiment (tens of MHz discrepancies). In the present work, thanks to new analytic formulas and computer means, we perform their original method of calculation again, without two approximations in the contribution $\Delta E_{<}$ of the low radiation energies: (i) a mathematical approximation within the Bethe logarithm, and (ii) the neglect of retardation exponentials $e^{i\mathbf{k}\cdot\mathbf{x}}$ in the impulsion matrix elements $< m|e^{i\mathbf{k}\cdot\mathbf{x}}\mathbf{p}|n >$. Applied to the Lamb shift of the $1s$ level of hydrogen, our calculation gives a value of 8526 MHz, which is 352 MHz above the 8174 MHz value deduced from experiments. None of the improvements published in the modern literature, which at most are of the order of tens of MHz, can compensate this huge new discrepancy. The precision of our integration over

the discrete and continuous spectra was tested by a sum rule, and found to be 0.9999991.

1 Introduction

Fifty years ago a numerical calculation of the Lamb shift was published [1] by H. A. Bethe, L. M. Brown, and J. R. Stehn (hereafter BBS), giving a theoretical value of 1051 MHz for the $2p-2s$ quantum transition in the hydrogen atom, close to the experimental value of 1062 MHz. Using the same method, J. M. Harriman [2, 3] found 8127 MHz for the shift of the $1s$ level, in agreement with the value of 8174 MHz now deduced from experiments [4, 5]. This lends further support to the Bethe theoretical formula [1, 6, 7], and its descendants. The theory, which was better explained later [8], involves the integral

$$\Delta E_{<}^{(\nu)} = -\frac{\alpha^3 a^2}{4\pi^2} \sum_n (E_n - E_\nu) \int \frac{d^3\mathbf{k}}{k^2} \frac{\mathbf{T}_{n\nu}^{\perp}(\mathbf{k}) \cdot \mathbf{T}_{\nu n}^{\perp}(-\mathbf{k})}{\frac{E_n - E_\nu}{\hbar c} + k}. \quad (1)$$

More precisely, expression (1) gives the contribution $\Delta E_{<}^{(\nu)}$ of the low radiation energies to the Lamb shift $\Delta E^{(\nu)}$ of a given state ν; the summation Σ_n is to be extended over all the levels (n, l, m) of the discrete and continuous spectra. In Eq. (1) we have denoted by $\mathbf{T}_{\nu n}^{\perp}$ the component perpendicular to $\mathbf{k}$ of the impulsion matrix element (*cf.* Glossary) between the quantum states ν and n, with retardation

$$\mathbf{T}_{n\nu}(\mathbf{k}) \equiv < n|e^{i\mathbf{k}\cdot\mathbf{x}}\nabla|\nu > \equiv \int\int\int d^3\mathbf{x}\ \psi_n^*(\mathbf{x}) e^{i\mathbf{k}\cdot\mathbf{x}} \nabla \psi_\nu(\mathbf{x}). \quad (2)$$

The same theory has been the basis of recent calculations [4, 5, 9, 10, 11, 12, 13, 14], and the complementary terms that are found in the modern literature are small compared to the main term (1) (i.e. tens of MHz vs. thousands).

Because the numerical evaluation of expression (1) is difficult, the BBS calculation involves several approximations, with unknown consequences. The purpose of the present work is to improve the BBS's calculation using state-of-the-art computer facilities and new analytical expressions for handling Eq. (1). To describe the largest variations, we have chosen to report here the calculation of the shift of the $1s$ level of hydrogen.

2 The BBS calculation

Following BBS [1, 8], the Lamb shift of level ν can be computed as the sum

$$\Delta E = \Delta E_{<} + \Delta E_{>} + E_\mu + \textit{other terms}, \quad (3)$$

of electric contributions $\Delta E_<$ of the low radiation energies and $\Delta E_>$ of the high radiation energies, and of a magnetic term E_μ (anomalous magnetic moment), plus other terms. In terms of the radiation wave vectors $\mathbf{k}$, the limit $|\mathbf{k}| = k_c$ of the low and high energies can be defined, for instance, by the inequality

$$k\hbar c < k_c \hbar c \equiv \alpha mc^2. \tag{4}$$

Contribution of the high radiation energies ($k > k_c$) is approximated, according to ref. [8], Eq. (19.2) with (18.2) and (19.3), by

$$\begin{aligned}\Delta E_> &= -(\frac{\hbar}{mc})^2 \frac{\alpha}{3\pi} e < \Delta\phi >_{\nu\nu} \\ &\times \left(-\ln 2 - \ln\alpha - \ln(ak_c) + \frac{5}{6} - \frac{1}{5} - \frac{3}{8} \right). \end{aligned} \tag{5}$$

According to Bethe and Salpeter, the contribution of the low radiation energies (ref. [8], Eq. (19.7)) is

$$\begin{aligned} E_m + \Delta E_< &= -\frac{2\alpha}{3\pi m^2} \int_0^{k_c} dk\ k \left[\frac{< p^2 >_{00}}{kc} \right. \\ &\left. + \sum_n \frac{\mathbf{p}_{\nu n} \cdot \mathbf{p}_{n\nu}(E_\nu - E_n)}{kc(kc + E_n - E_\nu)} \right], \end{aligned} \tag{6}$$

of which the first term E_m is compensated by mass renormalization. The second term of (6)

$$\Delta E_< = -\frac{2\alpha}{3\pi m^2 c} \int_0^{k_c} dk \sum_n \frac{\mathbf{p}_{\nu n} \cdot \mathbf{p}_{n\nu}(E_\nu - E_n)}{kc + E_n - E_\nu}, \tag{7}$$

with

$$\mathbf{p}_{n\nu} \equiv -i\hbar < n|\nabla|\nu >, \tag{8}$$

should be written as expression (1) with a cut-off at $k = k_c$ when the retardation exponentials are not neglected in the impulsion matrix elements $\mathbf{p}_{n\nu}$. Indeed, omitting these exponentials, expression (1) simplifies into Eq. (7), thanks to the identity

$$\int d\varphi \int d\theta \sin\theta \mathbf{T}^\perp \cdot \mathbf{T}^\perp = \frac{2}{3} \int d\varphi \int d\theta \sin\theta\ \mathbf{T} \cdot \mathbf{T}, \tag{9}$$

which holds when $\mathbf{T}$ does not involve $\mathbf{k}$.

To simplify the computation of $E_<$, BBS use the following approximation in the denominator of (7)

$$\ln\left|\frac{E_n - E_\nu}{\hbar c} + k_c\right| \simeq \ln k_c, \tag{10}$$

and obtain

$$\Delta E_< = C\left(-\ln\frac{k_0}{Ry} + \ln 2 - \ln\alpha + \ln(ak_c)\right), \tag{11}$$

where the Bethe logarithm is defined as

$$\ln\left(\frac{k_0}{Ry}\right) \equiv \frac{\sum_n E_{n\nu}\mathbf{p}_{\nu n}\cdot\mathbf{p}_{n\nu}\ln\left(\frac{E_{n\nu}}{Ry}\right)}{\sum_n E_{n\nu}\ \mathbf{p}_{\nu n}\cdot\mathbf{p}_{n\nu}}. \tag{12}$$

The constant C is the same as in Eq. (5).

To check the correctness of our integration method and accuracy of our computer programs, we have first performed the BBS calculation without any change for the $1s$, $2s$, and $2p$ levels, and obtained results identical to those of refs. [1, 2]. We incidentally noticed that the formula given by Stobbe [15] for the oscillator strength was correct (not too large by a factor of 2 as claimed by BBS), and that the integration element over the continuous spectrum used by BBS was too large by a factor of 2. In any case, this does not change the final result, with which we are in perfect agreement.

In the sum $\Delta E_< + \Delta E_>$ the cut-off value k_c cancels between Eqs. (11) and (5). A change in k_c adds opposite quantities to columns 1 and 2 (Table 1, Section 2). For the $1s$ state we have found $\Delta E_< + \Delta E_> = 7721$ MHz (Table 1, col. 3). Including the magnetic term 406.93 MHz of Eq. (3), the BBS calculation gives for the $1s$ level $\Delta E = 7721 + 407 = 8128$ MHz. This is the shift obtained by Harriman [2] (8127 MHz), witnessing that this primeval formulation of the theory was already roughly in agreement with experiments (8174 MHz [4, 5] for the $1s$ Lamb shift).

3 Using the exact denominator

We have also performed a calculation identical to that of Section 2, but without the approximation (10). The retardation was still neglected, i.e., we have used the matrix elements (8). Expression (11) remains valid, provided that the Bethe logarithm is redefined as

$$\ln\left(\frac{k_0}{Ry}\right) = -\frac{\sum_n E_{n\nu}\mathbf{p}_{\nu n}\cdot\mathbf{p}_{n\nu}\ln(\frac{\alpha}{2k_c a}+\frac{Ry}{E_{n\nu}})}{\sum_n E_{n\nu}\mathbf{p}_{\nu n}\cdot\mathbf{p}_{n\nu}}. \tag{13}$$

We found that approximation (10) has little influence on the contribution of the discrete spectrum (428.07 MHz in Table 1, Section 3, *vs.* 427.86 MHz in Table 1, Section 2). However, it does have a strong effect on the contribution of the continuous spectrum which is increased by 2869 MHz (Table 1, Section 3) − 2425 MHz (Table 1, Section 2) = 444 MHz.

In the preceding calculations (Sections 2 and 3), an analytic integration was performed over **k**, and then a second integration was carried out over the discrete and continuous spectra.

For the discrete spectrum, and small quantum numbers $n \leq 11$, we have used exact impulsion matrix elements, thanks to computer subroutines working in integer numbers, able to simplify the rational fractions. For large n ($n \geq 12$ here, *vs.* $n \geq 6$ in BBS), we have approximated the matrix elements by expanding the wave functions in n^{-1} [16, 17, 18, 19], like in BBS.

Furthermore, for the continuous spectrum, a numerical integration was performed over the energy E_n of the wave functions (continuous n), with the change of variable

$$E_n \mapsto \ln(\frac{E_n - E_\nu}{a.u.}). \tag{14}$$

The precision of the spectral integration was tested on the sum rule

$$\sum_n \mathbf{p}_{\nu n}\cdot\mathbf{p}_{n\nu}(E_n - E_\nu) = \frac{\hbar^2 e^2}{2\epsilon_0}|\psi_\nu(\mathbf{0})|^2, \tag{15}$$

yielding a left-hand-side to right-hand-side ratio equal to 0.9999991.

In order to prepare the calculations of Section 4, where an analytic integration over k would be impossible because of the retardation exponentials, we have also performed the calculations of Sections 2 and 3, using a numerical integration over k. We have used the change of variable

$$k \mapsto \ln(ka), \tag{16}$$

and obtained results similar to those found above.

4 Keeping the retardation exponentials

Finally, we performed the same calculation as in Section 3, while keeping the retardation exponentials, i.e., according to Eqs. (1) and (2).

In Sections 2 and 3, the matrix elements (8) between states (n, l, m) and (ν, λ, μ) were nonzero only for $l - \lambda = \pm 1$ and $m - \mu = -1, 0, 1$. These selection rules no longer hold for the matrix elements (2). However, the matrix elements (2) which do not satisfy the selection rules are small [20]. To avoid lengthy calculations, they will be neglected hereafter.

The discrete spectrum is considered first. For the discrete levels n, the matrix elements (2) have been given previously [20], together with their contribution to Eq. (1), namely

$$\begin{aligned}\Delta E_{1s,np} &= \alpha^5 mc^2 \frac{4}{n^3\pi}\int_0^\infty \frac{dk}{k^4(a\omega+k)}\rho^{2n} \\ &\quad\times\left[\cos(n\theta)+\sin(n\theta)\left(-\frac{ah}{nk}+\frac{a^2h^2+k^2}{2k}\right)\right]^2, \qquad (17)\end{aligned}$$

with the definitions

$$\omega \equiv \frac{\alpha}{2a}\left(1-\frac{1}{n^2}\right) \qquad (18)$$

$$h \equiv \frac{1}{a}\left(1+\frac{1}{n}\right) \qquad (19)$$

$$\rho^2 \equiv 1-\frac{4}{n(a^2h^2+k^2)} \qquad (20)$$

$$\theta \equiv \tan^{-1}\left[\frac{k}{ah-\frac{n}{2}(a^2h^2+k^2)}\right]. \qquad (21)$$

For $n > 11$, the integral over k can be approximated by

$$\int_0^\infty \frac{dk}{k^4(a\omega+k)}\exp\left[-\frac{4}{1+k^2}\right]\left(\cos\gamma-\frac{1}{\gamma}\sin\gamma\right)^2 = 0.175, \qquad (22)$$

with

$$\gamma \equiv -\frac{2k}{1+k^2}. \qquad (23)$$

Levels 1 to 11 contribute 383.5 MHz to $\int_0^{k_c}$, while levels 12 to infinity contribute 6.3 MHz.

Next the continuous spectrum is taken up. We substitute for $\|\mathbf{T}^{\perp}\|^2$ from Eq. (62) into Eq. (1), and integrate over k and over E numerically, with the change of variables (14) and (16). We thus obtain 2863 MHz for the contribution of the continuous spectrum, and get $\int_0^{k_c} = 390 + 2863 = 3252$ MHz for the whole spectrum (Table 1, Section 4).

Note that, from the BBS theoretical point of view, Eq. (1) must not be used to compute the contribution $E_>$ of the high radiation energies. However, to examine the convergence of integral (1) for infinite k, we have also computed its integral from k_c to ∞, which is 1894 MHz (Table 1, col. 2). The sum 3252 + 1894 = 5146 MHz (Table 1, col. 3) is the value of integral (1) without a cut-off. It has no physical meaning in the BBS theory.

5 Conclusion

We have shown how two approximations made by BBS (approximation (10); and the neglect of the retardation exponentials) can be avoided. We have applied this to the Lamb shift of the 1s level of the hydrogen atom (Table 1), and obtained $\Delta E_< = 3252$ MHz, a value 399 MHz higher than the result 2853 MHz of the BBS calculation. Approximation (10) is responsible for $3297 - 2853 = 444$ MHz. Retardation has an effect of $3252 - 3297 = -45$ MHz, much smaller than the effect of approximation (10). However, intrinsically, 45 MHz is large from a spectroscopic point of view, and contradicts Dyson's assumption [21] that retardation had little influence below αmc^2.

Following Eq. (3) let us add, to our new value of $E_<$, the BBS value of $E_>$ given by Eq. (5), and the anomalous magnetic moment term E_μ. The result is

$$\Delta E = 3252 + 4867 + 407 = 8526 \text{ MHz}, \tag{24}$$

a value which is 352 MHz above the experimental value of 8174 MHz. This is a huge discrepancy between theory and experiment, and its order of magnitude is large compared to all the complementary terms (tens of MHz) that have been introduced after the BBS calculation.

For explaining the unexpected numerical results obtained with and without approximation (10), one is led down one of the following two paths:

- The theory of $\Delta E_<$ leading to $ln|k_c + (E_n - E_\nu)/\hbar c|$ is correct and, consequently, the value $\Delta E_< = 3297$ MHz is better than $\Delta E_< = 2853$ MHz. But then, the other terms of Eq. (3) are wrong by about 352 MHz. Certainly in this case the contribution $\Delta E_>$ of the high radiation energies must be reconsidered, since one has lost the balance

$$\Delta E_< = -C\ ln\ k_c + \ldots, \tag{25}$$

$$\Delta E_> = +C\ ln\ k_c + \ldots, \tag{26}$$

  thanks to which the result of BBS was independent of the choice of the cut-off k_c.

- Otherwise, there exists a better theory for $\Delta E_<$ giving directly $ln|k_c|$ (and not $ln|k_c + (E_n - E_\nu)/\hbar c|$), and the value $\Delta E_< = 2853$ MHz is better than $\Delta E_< = 3297$ MHz. Then the other terms of Eq. (3), especially expression (5), are correct a priori.

Appendix: Impulsion matrix elements including a retardation exponential

As a consequence of the retardation of the electromagnetic potential, many calculations of electrodynamics [21, 22, 23, 24, 25, 26, 27, 28] involve impulsion matrix elements with retardation $\mathbf{T}_{\nu n}$ defined by Eq. (2), where $\mathbf{k}$ is a wave vector ($k \equiv \|\mathbf{k}\|$ inverse wavelength).

For wave functions ν, n that are solutions of the Schrödinger equation, and thanks to

$$< \nu|\nabla|n >= \frac{m_e}{\hbar^2}(E_n - E_\nu) < \nu|\mathbf{x}|n >, \tag{27}$$

the impulsion matrix elements $\mathbf{p}_{\nu n}$ can be replaced by those of the position $\mathbf{x}$ of the electron, which are simpler to evaluate. For the $\mathbf{T}_{\nu n}$'s, we have the similar relationship

$$< \nu|e^{i\mathbf{k}\cdot\mathbf{x}}\nabla|n > +i < \nu|\mathbf{x}e^{i\mathbf{k}\cdot\mathbf{x}}\nabla|n > \cdot\mathbf{k} = -i\mathbf{k} < \nu|e^{i\mathbf{k}\cdot\mathbf{x}}|n > + \left[\frac{k^2}{2} + \frac{m_e}{\hbar^2}(E_n - E_\nu)\right] \times < \nu|\mathbf{x}e^{i\mathbf{k}\cdot\mathbf{x}}|n >, \tag{28}$$

and the component of $\mathbf{T}_{\nu n}$ parallel to $\mathbf{k}$ is

$$\mathbf{k}\cdot < \nu|e^{i\mathbf{k}\cdot\mathbf{x}}\nabla|n >= -i\left[\frac{k^2}{2}+\frac{m_e}{\hbar^2}(E_n-E_\nu)\right] < \nu|e^{i\mathbf{k}\cdot\mathbf{x}}|n > . \quad (29)$$

These equations are obtained by integrating the Schrödinger equation

$$\Delta\psi_\nu^* + \frac{2m_e}{\hbar^2}[E_\nu + e\phi(\mathbf{x})]\psi_\nu^* = 0, \quad (30)$$

multiplied by $\psi_n e^{i\mathbf{k}\cdot\mathbf{x}}$.

For hydrogenlike wave functions $n \equiv (n, l, m)$ and $\nu \equiv (\nu, \lambda, \mu)$ both belonging to the discrete spectrum, a method for computing $\mathbf{T}_{\nu n}$ has been given previously [20]. Now we deal with the case where ν belongs to the discrete spectrum, and n to the continuous spectrum [29]. For simplicity, we shall take $\nu \equiv 1s \equiv (\nu = 1, \lambda = 0, \mu = 0)$ and $n \equiv np \equiv (E, l = 1, m = 0)$, but the method can be extended to other levels. The state np has the positive energy $E = 1/2n^2$ a.u.

The simpler integrals $< np|\nabla|\nu >$ have been obtained starting from the expression

$$R_{n1}(r) = D\, r^{-l-1}\int d\xi e^{-(2ir/na)\xi}(\xi+\frac{1}{2})^{-in-l-1}(\xi-\frac{1}{2})^{in-l-1}, \quad (31)$$

of the radial part of the wave function ψ_{np} of the continuous spectrum (ref. [8], Eq. (4.22); D is a constant). Applied to the calculation of $\mathbf{T}_{n\nu}(\mathbf{k})$ as defined by (2), Eq. (31) leads to difficult integration operations. Instead of (31), we shall adopt the hypergeometric representation of ψ_{np} (ref. [8], Eq. (4.23)), and convert it into a contour integral different from (31).

We choose a direct orthonormal frame $(\mathbf{i}', \mathbf{j}, \mathbf{e_3})$ so that $\mathbf{e}_3$ is the axis of the np orbital, and the wave vector $\mathbf{k}$ is contained in the plane of $\mathbf{i}'$ and $\mathbf{e}_3$. There are two opposite solutions for $\mathbf{i}'$. Let us choose $\mathbf{i}'$ so that $\mathbf{e}_3$ is between $\mathbf{i}'$ and $\mathbf{k}$. We have

$$\mathbf{T} = \int d^3\mathbf{x}\; \psi_{np}^*(\mathbf{x})e^{i\mathbf{k}\cdot\mathbf{x}}\nabla\psi_{1s}(\mathbf{x}), \quad (32)$$

with

$$\psi_{1s} = \frac{a^{-3/2}}{\sqrt{\pi}} e^{-\frac{r}{a}}, \tag{33}$$

$$\nabla\psi_{1s} = -\frac{a^{-5/2}}{\sqrt{\pi}} e^{-r/a}\frac{\mathbf{x}}{r}, \tag{34}$$

$$\psi_{np} = a^{-3/2}\frac{\sqrt{3}}{2\sqrt{\pi}} R_{n1}(r)\cos\theta', \tag{35}$$

$$\theta' \equiv \angle(\mathbf{e}_3, \mathbf{x}); \quad \theta \equiv \angle(\mathbf{k}, \mathbf{x}); \quad \beta \equiv \angle(\mathbf{e}_3, \mathbf{k}), \tag{36}$$

$$R_{n1}(r) = C_{n1}\frac{r}{a} e^{-\frac{ir}{na}} F(in+2, 4, \frac{2ir}{na}), \tag{37}$$

$$C_{n1} = \frac{2}{3n}\frac{\sqrt{1+n^2}}{\sqrt{1-e^{-2\pi n}}}. \tag{38}$$

Let $\mathbf{i}$ be the unit vector orthogonal to $\mathbf{k}$ and contained in the half-plane of edge $\mathbf{k}$ and containing $\mathbf{e}_3$. Then, $\cos\theta'$ may easily be expressed as a function of the spherical coordinates (r, θ, φ) of $\mathbf{x}$ in the direct orthonormal frame $(\mathbf{i}, \mathbf{j}, \mathbf{w} \equiv \mathbf{k}/|\mathbf{k}|)$

$$\cos\theta' = \cos\theta\cos\beta + \sin\theta\cos\varphi\sin\beta. \tag{39}$$

We notice that

$$\mathbf{T} = \nabla_{\mathbf{k}}\left[\frac{ia^{-5/2}}{\sqrt{\pi}}\int d^3\mathbf{x}\psi_n^* e^{i\mathbf{k}\cdot\mathbf{x}}\frac{e^{-r/a}}{r}\right]. \tag{40}$$

The term within square brackets in (40) is equal to

$$[\,] = ia^{-4}\sqrt{3}\ \cos\beta A(k), \tag{41}$$

with

$$A(k) \equiv \int_0^\infty dr\ re^{-r/a}R_{n1}(r)\int_0^\pi d\theta\sin\theta\cos\theta e^{ikr\cos\theta}. \tag{42}$$

Substitution of (41) into (40) gives, for the component of $\mathbf{T}$ orthogonal to $\mathbf{k}$, the value

$$\mathbf{T}^\perp = \mathbf{i}\ i\ a^{-4}\sqrt{3}\ C_{n1}\sin\beta\ \frac{A(k)}{k}. \tag{43}$$

We now have to compute A(k). The integral over k is

$$\int_\theta = -\frac{1}{kr}\left[e^{ikr}\left(i-\frac{1}{kr}\right)+e^{-ikr}(i+\frac{1}{kr})\right]. \tag{44}$$

The hypergeometric function F in R_{n1} is equal ([30], Eq. (d.9)) to

$$F = \frac{3}{\pi n(1+n^2)}\oint_{C'} dt\; e^{2itr/na}(-t)^{in+1}(1-t)^{1-in}. \tag{45}$$

The contour C' in the complex plane encloses the points $t=0$ and $t=1$, and is run in the positive sense. The integrand is holomorphic in the complex plane except in 0 and 1, which are branch points. The discontinuity reduces to the segment $[0,1]$.

In (45) we make the change of variable $z \equiv t - 1/2$, which transforms contour C' into a contour C enclosing the points $t=-1/2$ and $t=1/2$. Then we substitute (37), (44) and (45) into (42), and permute the integrals in (42). This gives

$$A(k) = -\frac{3C_{n1}}{\pi n(1+n^2)ka}\oint_C dz(z+\frac{1}{2})^{in+1}(z-\frac{1}{2})^{1-in}\int_r, \tag{46}$$

where

$$\int_r \equiv \sum_{+,-}\left(i\int drre^{\gamma r} \mp \frac{1}{k}\int dre^{\gamma r}\right); \quad \gamma \equiv -\frac{1}{a}+\frac{2iz}{na}\pm ik. \tag{47}$$

Using

$$\int_0^\infty drre^{\gamma r} = \frac{1}{\gamma^2}, \tag{48}$$

since $Re(\gamma) < 0$, we obtain

$$\int_r = -\frac{4ik^2}{[(-\frac{1}{a}+\frac{2iz}{na})^2+k^2]^2}, \tag{49}$$

hence

$$\begin{aligned} A(k) \;&=\; \frac{12ikC_{n1}}{\pi n(1+n^2]a}\oint_C dz(z+\frac{1}{2})^{1+in}(z-\frac{1}{2})^{1-in} \\ &\quad\times\left[\left(\frac{1}{a}-\frac{2iz}{na}\right)^2+k^2\right]^{-2}. \end{aligned} \tag{50}$$

The two double poles

$$b \equiv b(\pm) = \frac{n}{2}(-i \pm ka), \tag{51}$$

of A are situated outside of contour C. In addition, the integral over a contour going to infinity is zero, since the integrand behaves like z^{-2} for large $\|z\|$. Therefore, we have

$$\oint_C = -2\pi i \sum residues, \tag{52}$$

hence

$$\begin{aligned} A(k) &= \frac{3kn^3a^3C_{n1}}{1+n^2} \sum_{+,-} \left[(z-b)^{-2} \left(\frac{z+1/2}{z-1/2} \right)^{in} \right. \\ &\quad \left. \times \left(-\frac{z^2 - 1/4}{z-b} + z - \frac{in}{2} \right) \right], \end{aligned} \tag{53}$$

for each term in $\sum_{+,-}$, the pole b is given by (51), and z is taken at the other pole as

$$z \equiv z(\pm) = \frac{n}{2}(-i \mp ka). \tag{54}$$

Rearranging (53), and substituting into (43) gives

$$\mathbf{T}^{\perp} = \mathbf{i}a^{-3}\frac{\sqrt{3}}{2}\frac{\sin\beta}{\sqrt{1+n^2}\sqrt{1-e^{-2\pi n}}k^2}\sum_{+,-} C(\pm)B(\pm), \tag{55}$$

where we have introduced the real parameters C, B, ρ, θ, η, and ϕ by

$$C(\pm) \equiv \left(\frac{z+1/2}{z-1/2} \right)^{in} = e^{-n\theta}\rho^{\pm in}, \tag{56}$$

$$B(\pm) \equiv \eta e^{\pm i\phi} \equiv \mp i \left(\frac{n}{ka} + \frac{1}{kna} + nka \right) + 2n, \tag{57}$$

$$\rho e^{i\theta} \equiv \frac{-i + ka + n^{-1}}{-i + ka - n^{-1}}. \tag{58}$$

Finally, Eqs.(55)-(57) can be re-written in the form

$$\begin{aligned} \mathbf{T}^{\perp} &= \mathbf{i}\frac{\sqrt{3}\sin\beta}{2a^3k^2\sqrt{1+n^2}\sqrt{1-e^{-2\pi n}}} \\ &\quad \times \sum_{+,-} \left[\left(\frac{\pm ka + n^{-1} - i}{\pm ka - n^{-1} - i} \right)^{in} (2n \pm iG) \right], \end{aligned} \tag{59}$$

with

$$G \equiv \frac{n}{ka} + \frac{1}{nka} + nka. \tag{60}$$

The sum $\sum$ in (55), squared, is

$$|\sum_{+,-}|^2 = 4|C|^2|B|^2 \cos^2[\arg C(+) + \arg B(+)]. \tag{61}$$

Therefore, the magnitude of $\mathbf{T}^\perp$ squared is

$$\|\mathbf{T}^\perp\|^2 = \frac{3\sin^2\beta}{a^6k^4(1+n^2)(1-e^{-2\pi n})} e^{-2n\theta}\eta^2\cos^2(n\ln\rho + \phi), \tag{62}$$

with the notations

$$\theta \equiv \tan^{-1}\left[\frac{2}{n(1+k^2a^2-n^{-2})}\right], \tag{63}$$

$$\rho^2 \equiv \frac{1+(ka+n^{-1})^2}{1+(ka-n^{-1})^2}, \tag{64}$$

$$\eta^2 \equiv 4n^2 + G^2, \tag{65}$$

$$\phi \equiv \tan^{-1}\left(\frac{G}{2n}\right). \tag{66}$$

Note that expressions (59) and (62) of the matrix elements (2) are compatible with known expressions of the matrix elements (8) without an exponential [8, 15]. Indeed, starting from Eq. (62), it is possible to verify that, in the limit $k \to 0$, one has

$$\begin{aligned} \| < E|e^{i\mathbf{k}\cdot\mathbf{x}}\nabla|1s >^\perp \| &\to \| < E|\nabla|1s > \| \sin\beta \\ &= \frac{2^3n^3e^{-2n\cot^{-1}n}\sin\beta}{a\sqrt{3(1+n^2)^3(1-e^{-2\pi n})}}. \end{aligned} \tag{67}$$

Glossary

Values of the physical constants were taken from ref. [31, 32].

a Bohr radius

$-e$ electron charge

$\mathbf{e}_3$ axis of the p orbital

$E_{n\nu} = E_n - E_\nu$ energy difference between states
F confluent hypergeometric function
$k = \|\mathbf{k}\|$ radiation inverse wavelength λ^{-1}
$k_c = a^{-1}$ cut-off value of k, corresponding to a maximum value αmc^2 for the energy $k\hbar c$ involved in the denominator of (1). Note that k_c differs from the inverse wavelength $(2\pi a)^{-1}$ corresponding to the energy αmc^2.
m_e electron mass
n eigenstate of the hamiltonian, corresponding to the energy $E_n = \mp 1/(2n^2)$ a.u. (- for the discrete spectrum, + for the continuous spectrum)
$\mathbf{T}^\perp$ component perpendicular to $\mathbf{k}$ of the impulsion matrix element with retardation $\mathbf{T}$ (Eq. (2)), divided by $\hbar/i$.
α fine structure constant
β angle between $\mathbf{e}_3$ and the wave vector $\mathbf{k}$
$\phi = e/(4\pi\epsilon_0 r)$ scalar electric potential created by the proton.

		Interval of integration in $\int dk$ in Eq. (1)		
	Spectrum in $\sum_n$ in (1)	$0 < k\hbar c < \alpha mc^2$ col. 1	$\alpha mc^2 < k\hbar c < \infty$ col. 2	$0 < k\hbar c < \infty$ col3=col1+ col2
Section 2 (BBS)	discrete	428.	∞	∞
no retardation	continuous	2425.	∞	∞
approx (46)	whole	2853.	∞	∞
(i.e. Eqs. (1),(8),(10))			Eq. (5) 4867.	7721.
Section 3	discrete	428.	∞	∞
no retardation	continuous	2869.	∞	∞
	whole	3297.	∞	∞
(i.e. Eqs. (1), (8))			Eq. (5) 4867.	8165.
Section 4	discrete	390.	6.	396.
retardation	continuous	2863.	1888.	4750.
(i.e. Eqs. (1), (2))	whole	3252.	1894.	5146.
			Eq. (5) 4867.	8119.

Table 1: *The Bethe integral (1) for the Lamb shift (MHz) of the* $1s$ *level of the hydrogen atom, with or without approximation (10), and without or with retardation (Eq. (8) or (2)).*

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