Logarithmic radiative corrections to the dipole matrix elements in the hydrogen atom

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Results are obtained in numerical and analytic form for the radiative corrections to the dipole matrix elements, level widths, and line intensities in hydrogenlike systems. These results have the relative order of magnitude $\alpha(Z\alpha)^2 \ln Z\alpha$. The analytic expression has the form of a finite sum. The correction to the corresponding matrix elements in parabolic coordinates is also found. [S1063-7761(96)01004-9]

1. INTRODUCTION

The calculation of radiative corrections to dipole matrix elements has become of a topic of current interest in connection with precise measurements of the ratio of the $2p_{1/2}$ line width and Lamb splitting in the hydrogen atom[1] and studies of the Stark effect in the hydrogen atom performed with the goal of refining the value of the fine structure constant.[2,3] Radiative corrections in the logarithmic approximation were found for the $2p_{1/2}$ level numerically[4,5] and then in Ref. 6 a general formalism was constructed, based on representing the Green's function of the electron in the Coulomb field of the nucleus in the form of a sum over states and leading to an integral which can be easily evaluated numerically.

The present paper is a direct continuation of Ref. 6. Within the framework of the formalism developed in Ref. 6 we obtain numerical results for the corrections to the various dipole matrix elements and delineate which intermediate states give the main contribution. With the help of the sum rule found in Refs. 5 and 6 we rearrange the sum, which in a number of cases allows us to sum up a substantial number of terms. We also develop a formalism for obtaining corrections in analytic form with the help of a closed representation[7,8] of the Coulomb Green's function in the form of a combination of Whittaker functions. We also obtain a general expression for the corrections to the dipole matrix elements in the form of a finite double sum. The results for the corrections to the dipole matrix elements for the levels with $n=1-4$ as well as the results for some asymptotic limits are represented in explicit form. A simple expression for the diagonal matrix elements in n is obtained for arbitrary levels. We succeeded in finding it by using one more representation[8–10] for the Coulomb Green's function in the form of a Sturm expansion over Laguerre polynomials. We have also found corrections to the dipole matrix elements in parabolic coordinates.

The paper is organized as follows: first, we obtain a general expression in the Yennie gauge for the radiative corrections to the dipole matrix elements for the hydrogen atom in the logarithmic approximation, which reduces to allowing for an effective δ-function potential. The following three Sections are dedicated to direct calculations of the corrections to the dipole matrix elements, induced by the δ-function perturbation to the Coulomb potential. In each of these three Sections we consider different representations for the Coulomb Green's function. Section VI discusses the results. The Appendices derive the sum rule, which is linear in the dipole matrix elements for arbitrary value of the orbital angular momentum, and the reduced Green's functions for some lower levels. They also include a calculation of the asymptotic limits of the corrections to the dipole matrix elements.

2. RADIATIVE CORRECTIONS IN THE YENNIE GAUGE

It is convenient to calculate the radiative corrections in the Yennie gauge[11–13]

$$D^{Y}_{\mu\nu}(k)=\frac{1}{k^2}\left(g_{\mu\nu}+2\frac{k_\mu k_\nu}{k^2}\right), \tag{1}$$

in which the low-energy asymptotic limits of the radiative insertions to the electron line have the gentlest behavior and are free of fictitious infrared divergences,[14,15] which are subtracted out in the standard gauges only in the final answer. It is not hard to convince oneself[4–6] that all radiative corrections in the logarithmic approximation are described in the Yennie gauge (1) by the δ-function potential

$$V=A\,\delta(\mathbf{r}), \tag{2}$$

where

$$A=\frac{4}{3}\frac{\alpha(Z\alpha)}{m^2}\ln\frac{1}{(Z\alpha)^2}, \tag{3}$$

$\alpha=e^2$ is the fine structure constant, and Z is the nuclear charge in units of the proton charge; here and below we use relativistic units, in which $\hbar=c=1$.

The correction to the radiation operator does not contain a low-energy logarithm $[\ln(Z\alpha)]$. The same is true of the corrections to the wave functions of the states $l\neq 0$.[4–6] It suffices to consider only the correction to the wave function of the s-levels

$$|ns\rangle^{V}=\bar{G}_n(E_n)V|ns\rangle, \tag{4}$$

where the reduced Green's function $\bar{G}_n(E)$ is obtained from the total Green's function $G(E)$ by subtracting the pole:

TABLE I. Analytic and numerical values of $S_{n'n}$.

n	$n'=2$	$n'=3$	$n'=4$	$n'=\infty$
1	$\frac{131}{48}+\ln\frac{4}{3}$	$\frac{55}{36}+\ln\frac{3}{2}$	$\frac{1103}{960}+\ln\frac{8}{5}$	$\ln 2-\frac{3}{8}-\mathcal{E}_2+\frac{5}{8}e^2$
	3.0168	1.9332	1.6190	1.2542
2	$\frac{1}{12}$	$\frac{2351}{720}+\ln\frac{6}{5}$	$\frac{1843}{960}+\ln\frac{4}{3}$	$\ln 2-\frac{235}{128}-\mathcal{E}_4+\frac{47}{128}e^4$
	0.0833	3.4476	2.2075	1.2376
3	$-\frac{451}{80}-\ln\frac{5}{4}$	$\frac{1}{8}$	$\frac{676223}{190400}+\ln\frac{8}{7}$	$\ln 2-\frac{541}{216}-\mathcal{E}_6+\frac{325}{1512}e^6$
	−5.8606	0.0556	3.6851	1.2836
4	$-\frac{875}{192}-\ln\frac{3}{2}$	$-\frac{21107}{4032}-\ln\frac{7}{6}$	$\frac{1}{24}$	$\ln 2-\frac{413551}{141312}-\mathcal{E}_8+\frac{6973}{47104}e^8$
∞	$\mathcal{E}'_4-\frac{7}{16}e^4$	$\mathcal{E}'_6-\frac{2}{9}e^6$	0.0417	
	−4.9628	5.3890	$\mathcal{E}'_8-\frac{181}{1216}e^8$	1.3269
	−4.2558	−3.6611	−3.3318	

Thus, the correction to the dipole matrix element

$$\mathbf{d}_{n'm'n}=\langle n'pm'|e\mathbf{r}|ns\rangle \tag{6}$$

is equal to

$$\delta\mathbf{d}_{n'm'n}=eA\psi_{ns}(0)\int d^3r\,\psi_{n'pm'}(\mathbf{r})\mathbf{r}\bar{G}_n(E_n;\mathbf{r},0). \tag{7}$$

The corrections to the matrix elements between the other states do not contain logarithms and in this approximation are equal to zero. It is not hard to convince oneself that in the case of a perturbation of a central field the angular integrals can always be separated and the correction $\delta\mathbf{d}_{n'm'n}$ as a three-dimensional vector is aligned with the original matrix element $\mathbf{d}_{n'm'n}$. To avoid complications, we present the results in terms of $d_{zn'm'n}$ (for $m'=0$), dropping the subscript m', or in terms of corrections to the reduced matrix element $\langle n'p\|r\|ns\rangle$.

3. CALCULATIONS WITH THE GREEN'S FUNCTION IN THE FORM OF A SUM OVER STATES

We represent the Coulomb function as a sum over states of the discrete and continuous spectra:

$$\bar{G}_n(E)=\sum_{q\neq n}\frac{|qs\rangle\langle qs|}{E-E_q}. \tag{8}$$

The correction to the dipole matrix element reduces to

$$\delta d_{zn'n}=\sum_{q\neq n}\frac{\langle n'p|ez|qs\rangle\langle qs|V|ns\rangle}{E_n-E_q}, \tag{9}$$

where the matrix elements for the effective potential (2) and the dipole interaction are known. As a result, we obtain

$$\delta d_{zn'n}=-\frac{2A(Z\alpha)m^2}{\pi}d_{zn'n}\left[\sum_{n''\neq n}\frac{1}{n''^2}\frac{1}{1/n^2-1/n''^2}\frac{\mathcal{D}_{n''n'}}{\mathcal{D}_{nn'}}+\int_0^\infty\frac{dt}{t^3(1/n^2+1/t^2)}\frac{1}{1-e^{-2\pi t}}\frac{\mathcal{D}_{tn'}}{\mathcal{D}_{nn'}}\right], \tag{10}$$

where the variable t is a continuous analog of the principal quantum number and for the states of the continuous spectrum with wave number k we have $k=Z\alpha m/t$, and explicit expressions for the quantities

$$\mathcal{D}_{qn}=\frac{d_{znq}}{d_{zn1}}\frac{\psi_{1s}(0)}{\psi_{qs}(0)} \tag{11}$$

are given in Ref. 6. The quantities $\mathcal{D}_{qn}$ allow simple analytic continuation from the discrete states to the continuous states and are convenient for calculation, in particular for the reason that they do not depend on the definitions of the phase factors in the spherical harmonics. In those cases in which this is important, we will use wave functions with phases defined according to Ref. 16.

Calculating the corrections (10) does not present any difficulty. With reference to expression (10), it is convenient to present all numerical values in relative units:

$$\delta d_{zn'n}=\frac{A(Z\alpha)m^2}{\pi}d_{zn'n}S_{n'n}. \tag{12}$$

Numerical results for $n=1-4$ and some asymptotic cases are laid out in Table I. The values for the matrix elements of the $1s-2p$ and $2s-2p$ transitions coincide with those found earlier.[4–6]

The main advantage of calculating with the sum over states is the transparent physical meaning of each individual term. The continuous spectrum does not make too large a contribution (see Table II), and the sum over states of the discrete spectrum is gathered mainly from the first few terms. This often allows us to estimate the contributions after fairly simple calculations, restricting ourselves to the first few terms.

Note that the energy of the higher excited states is small and therefore it may be expected that by neglecting it in the denominator

$$\frac{1}{E_n-E_q}\to\frac{1}{E_n}.$$

it will be possible to obtain an answer close to the right one. For the ground level this is reasonable for the entire discrete spectrum, and also for the continuous spectrum. The contribution with the simplified denominator is easily found with the help of the sum rule[5,6]

$$\sum\psi_{qs}(0)\langle n'p|ez|qs\rangle=0. \tag{13}$$

TABLE II. Contributions of individual terms to $S_{n'n}$.

$n-n'$	Discrete spectrum: Individual terms 1	2	3	4	5	$6,\ldots\infty$	Sum $1,\ldots\infty$	Continuum
1-2	–	3.7969	−0.3149	−0.0790	−0.0329	−0.0555	3.3145	−0.2977
1-3	–	−5.5924	10.6667	−1.2611	−0.3497	−0.4485	3.0149	−1.0817
1-4	–	−3.9692	−7.7755	20.3451	−2.8144	−1.9765	3.8095	−2.1905
2-2	−0.2341	–	0.1769	0.0347	0.0132	0.0206	0.0113	0.0720
2-3	0.1589	–	4.0690	−0.3758	−0.0953	−0.1132	3.6436	−0.1960
2-4	0.2239	–	−4.1792	8.5430	−1.0805	−0.7062	2.8011	−0.5936
3-2	0.5954	−5.4253	–	−0.4032	−0.1176	−0.1545	−5.5053	−0.3553
3-3	−0.0176	−0.2359	–	0.1900	−0.0369	0.1109	0.0106	0.0450
3-4	0.0241	0.2297	–	4.2052	−0.4072	−0.2279	3.8239	−0.1388
4-2	0.9000	−6.4072	2.4294	–	−0.5928	−0.5244	−4.1949	−0.7679
4-3	0.0564	0.5913	−5.1554	–	−0.3943	−0.2703	−5.1724	−0.2166
4-4	−0.0035	−0.0260	−0.2329	–	0.1967	0.0761	0.0104	0.0313

This contribution is equal to

$$[\delta d_{zn'n}]_S=-\frac{1}{E_n}\langle n'p|e\ z|ns\rangle\langle ns|V|ns\rangle, \tag{14}$$

or

$$[\delta d_{zn'n}]_R=\frac{2AZ\alpha m^2}{\pi n}\ d_{zn'n}. \tag{15}$$

The remainder can be represented in the form of a new sum:

$$[\delta d_{zn'n}]_R=\sum_{q\neq n}\langle n'p|e\ z|qs\rangle\langle qs|V|ns\rangle\frac{E_q}{E_n(E_n-E_q)}. \tag{16}$$

The contributions of individual terms to the remainder for transitions to the ground state are given in Table III. It can be seen that for the ground state use of the sum rule (13) substantially improves the quality of the estimates from the first few terms.

We note also that, as is well known from standard sum rules (see, for example, Refs. 17 and 18), the diagonal matrix element ($q=n'$) is always significantly larger than all the remaining matrix elements (for fixed value of n') and, as a rule, determines the sign of the total sum (9). At the same time, according to the sum rule (13) not all the matrix elements (after taking out the phase factor) can be of the same sign. We convinced ourselves in a number of particular cases (the elements between ns, $n=1-8$, and arbitrary discrete and continuous p and the elements between np, $n=2-7$, and arbitrary s) that for the standard definitions of the phases [1)] all the nondiagonal matrix elements have the opposite sign of the diagonal term.[2)] In this case it is easily shown that when using the sum rule the contribution of the continuous spectrum changes sign and, summing the discrete spectrum in Eqs. (9) and (16), one can obtain upper and lower estimates.

However, we do not have a proof that the signs of the nondiagonal terms are always identical. It should be mentioned that the form of the standard expression for the reduced diagonal matrix element between states of the discrete and continuous spectra is such that it is not obviously real (see, for example, Ref. 18).

In addition, it is not clear to what extent definiteness is connected with the values of the orbital angular momentum. An argument based on the standard sum rule and indicating that the diagonal element is the largest does not only apply at high values of the orbital angular momentum. Appendix A derives a sum rule for arbitrary l, from which it is clear that the signs of the matrix elements $\langle n,l+1\|r\|ql\rangle$ for fixed n and arbitrary q cannot all be identical. We have also found that for the corresponding definition of the phases in the case of the dipole elements[3)] between nd ($n=3-6$) and any discrete or continuous p and between np ($n=2-6$) and any discrete or continuous d the signs of the nondiagonal elements are identical and opposite the sign of the corresponding diagonal element.

TABLE III. Contributions of individual terms to the remainder (16) for $S_{n'1}$ arising after application of the sum rule. (The terms in parentheses are also included in the sum "$n',\ldots,\infty$.")

$n-n'$	Discrete spectrum: Individual terms 1	2	3	4	5	$n',\ldots\infty$	Sum $1,\ldots\infty$	Continuum
1-2	–	0.9492	(−0.0350)	(−0.0049)	(−0.0013)	−0.0422	0.9070	0.1098
1-3	–	−1.3981	1.1852	(−0.0788)	(−0.0140)	−0.1008	−0.3137	0.2469
1-4	–	−0.9923	−0.8639	1.2716	(−0.1126)	−0.1506	−0.7352	0.3542

4. CALCULATIONS WITH THE GREEN'S FUNCTION IN THE HOSTLER REPRESENTATION

The representation of the Coulomb Green's function considered above is easily visualizable; however, it does not allow us to obtain answers in closed analytic form. This can be done by representing the nonrelativistic Coulomb Green's function in the form of a sum over partial waves:

$$G(E;\mathbf{r},\mathbf{r}')=\sum_{lm} g_l(E;r,r')Y_{lm}\left(\frac{\mathbf{r}}{r}\right)Y^*_{lm}\left(\frac{\mathbf{r}}{r'}\right). \quad (17)$$

In the case of a δ-function perturbation, only the value of $G(\mathbf{r},\mathbf{r}')$ at $\mathbf{r}'=0$ matters, and only the s-wave remains in the sum (17). Substituting explicit expressions for the partial Green's function g_0, we obtain for the total (unreduced) function[7,8]

$$G(E;\mathbf{r},0)=-\frac{1}{4\pi}\Gamma(1-\nu)\frac{2m}{r}W_{\nu,1/2}\left(\frac{2Z\alpha mr}{\nu}\right), \quad (18)$$

where we have introduced the analog of the principal quantum number

$$\nu=\sqrt{-(Z\alpha)^2m/2E}.$$

The Whittaker function $W_{\nu,m}(z)$, defined in Ref. 20, can be represented in the form of an asymptotic expansion (see the last equation (unnumbered) in Sec. 16.3 of Ref. 20):

$$W_{\nu,1/2}(z)$$

$$=e^{-z/2}z^{\nu}\left\{1+\sum_{s=1}^{\infty}\frac{1}{s!z^s}\prod_{p=1}^{s}\left[\frac{1}{4}-\left(\nu+\frac{1}{2}-p\right)^2\right]\right\}. \quad (19)$$

To calculate the corrections, we need the reduced Green's function at $E=E_n$, and, in order to subtract the pole as in Eq. (5), it is necessary to consider the values of ν near integers n. In the case of integer values of ν the sum in expression (19) terminates and only a finite number of terms contribute. It is also readily grasped that for near-integer values of ν $(\nu=n+\varepsilon)$ only a finite number of terms of the series can be of order not higher than ε. For a correct account of the pole, it suffices to restrict ourselves to nonzero terms linear in the small parameter ε. That the asymptotic expansion cuts off at a finite number of terms,

$$W_{n+\varepsilon,1/2}(z)=e^{-z/2}z^{n+\varepsilon}\sum_{s=0}^{n}\frac{(-1)^s}{s!z^s}$$

$$\times\left[\frac{\Gamma(n+1+\varepsilon)}{\Gamma(n+1-s+\varepsilon)}\right]^2\frac{n-s+\varepsilon}{n+\varepsilon}+O(\varepsilon^2), \quad (20)$$

does not mean that their sum coincides with the function being expanded. However, it is not hard to convince oneself that in the given case the finite sum (20) indeed reproduces the Whittaker function $W_{n+\varepsilon,1/2}(z)$ with the necessary accuracy (see the derivation of the expansion in Section 16.3 of Ref. 20).

It is not difficult to isolate the pole term in expression (18), and after subtracting it out we obtain the reduced Coulomb Green's function:

$$\bar{G}_n(E_n;0,\mathbf{r})=-\frac{Z\alpha m^2}{2\pi r}\frac{e^{-z_n/2}}{n!}\sum_{s=0}^{n}\frac{(-z_n)^{n-s}}{s!}\left[\frac{n!}{(n-s)!}\right]^2$$

$$\times\left\{(n-s)\left[(\psi(n+1)-2\psi(n-s+1))\right.\right.$$

$$\left.\left.-\frac{2(n-s)+3-z_n}{2n}z_n\right]+1\right\}, \quad (21)$$

where $\psi(z)$ is the logarithmic derivative of the Γ-function and we have introduced the notation

$$z_n=2Z\alpha mr/n. \quad (22)$$

Some partial expressions for the reduced function (21) of some of the lower levels are given in Appendix B.

Integrating over the coordinate does not pose any difficulty:

$$\delta d_{zn'n}=-\frac{meA}{4\pi}\sqrt{\frac{n'^3(n'^2-1)}{3n^3}}$$

$$\times\sum_{s'=0}^{n}\sum_{t=0}^{n'-2}\frac{(-1)^{t+s'}s'n!}{t!(n-s')!s'!^2}\frac{(n'-2)!}{(n'-2-t)!}$$

$$\times\frac{(t+s'+3)!}{(t+3)!}\left(\frac{2n'}{n+n'}\right)^{s'}\left(\frac{2n}{n+n'}\right)^{t+4}$$

$$\times\left([\psi(s'+t+4)+\psi(n+1)-2\psi(s'+1)]\right.$$

$$\left.+\ln\frac{2n'}{n+n'}+\frac{n'(t+4)-s'n}{n(n+n')}+\frac{n-3s'/2}{ns'}\right). \quad (23)$$

Results for particular cases, including some asymptotic limits, are given in Table I. The analytic results coincide with the numerical, and the asymptotic limits are calculated in analytic form in Appendix C.

5. CALCULATIONS WITH THE STURM EXPANSION OF THE GREEN'S FUNCTION

Expression (23) is quite cumbersome, and it is not clear how it can be simplified. At the same time, however, in the case of the matrix elements diagonal in the principal quantum number, it is possible to obtain a simple answer. In this case we represent the partial Green's functions in the form of a Sturm expansion over the Laguerre polynomials[9] (see also Refs. 8 and 10):

$$\bar{g}_{ln}(E_n,r,r')=-\frac{4(Z\alpha)m^2}{n}$$

$$\times\left\{(z_nz_n')^l\exp\left(-\frac{z_n+z_n'}{2}\right)\right.$$

$$\times\sum_{\substack{n'=l+1\\n'\neq n}}^{\infty}\frac{(n'-l-1)!L^{2l+1}_{n'+l}(z_n)L^{2l+1}_{n'+l}(z_n')}{(n'+l)!(n'-n)}$$

$$+\frac{(n-l-1)!}{n[(n+l)!]^2}\left[\frac{5}{2}+z_n\frac{\partial}{\partial z_n}+z_n'\frac{\partial}{\partial z_n'}\right](z_nz_n')^l$$

$$\times\exp\left(-\frac{z_n+z_n'}{2}\right)L_{n+l}^{2l+1}(z_n)L_{n+l}^{2l+1}(z_n')\Bigg\}.$$

The generalized Laguerre polynomials in Eq. (24) are defined (in contrast to Refs. 8 and 10) as in Refs. 17 and 19:

$$L_n^m(z)=(-1)^m\frac{n!}{(n-m)!}e^z z^{-m}\left[\frac{d}{dz}\right]^{n-m}(e^{-z}z^n). \quad (25)$$

For the corrections to the diagonal matrix elements ($n'=n$) the arguments of the Laguerre polynomials (z_n) in Eq. (24) coincide with the general argument of the Laguerre polynomial in the radial wave function $R_{n'1}(r)$, and in the calculation of correction (7) radial integrals arise analogous to those considered in detail in Ref. 19 in the discussion of diagonal dipole matrix elements. After calculating them we get the finite sum

$$\delta d_{znn}=-\frac{eAm}{4\sqrt{3}\pi}\sqrt{n^2-1}\left\{\frac{(-1)^n}{(n+1)!}\right.$$
$$\left.\times\sum_{\substack{k=0\\k\neq n-1}}^{n+1}\frac{(k+1)!}{d+1-n}\sum_{p=0}^{k}\frac{(-1)^p(p+4)!}{p!(k-p)!(p+3-n)!}-5\right\}. \quad (26)$$

The summation limits of this sum are dictated by the requirement that the arguments of the factorials in the denominator be nonnegative; for $n\geqslant 3$ both lower limits can be replaced by $n-3$. One can convince oneself by direct summation that the quantity in braces is equal to unity. We finally obtain

$$\delta d_{znn}=\frac{1}{6n}\frac{AZ\alpha m^2}{\pi}d_{znn}. \quad (27)$$

It is not hard to make the transformation to parabolic coordinates (see Ref. 6), in which the corrections to the dipole matrix elements have the form

$$\delta(\langle n_1n_2m|z|n_1n_2m\rangle)=\frac{AZ\alpha m^2}{3\pi n^2}\langle n_1n_2 0|z|n_1n_2 0\rangle\delta_{m0}. \quad (28)$$

6. DISCUSSION OF RESULTS

Let us now discuss the quantities that can be measured. Besides the level splitting in the Stark effect, the line widths (lifetimes) and line intensities, or rather their ratios, can be measured with high accuracy. We assume that in the measurement of the ratio of intensities of the transition from one level to another it is possible to achieve sufficient experimental accuracy.

In the Schrödinger approximation the width and intensity are equal to

$$\Gamma_0(\lambda'\to\lambda)=\frac{4\omega_{\lambda'\lambda}^3}{3}|\mathbf{d}_{\lambda'\lambda}|^2, \quad (29)$$

$$I_0(\lambda'\to\lambda)=\frac{4\omega_{\lambda'\lambda}^4}{3}|\mathbf{d}_{\lambda'\lambda}|^2. \quad (30)$$

There are a number of corrections to this expression: relativistic corrections of relative order $(Z\alpha)^2$ and $(Z\alpha)^4$ are known (see, for example, Refs. 8 and 21), as well as corrections to the yield.[22] The leading contributions still unknown at the present time are the radiative corrections. In the logarithmic approximation in the Yennie gauge the leading radiative correction can be considered nonrelativistically as a correction directly to expressions (29) and (30). The perturbation of the frequency is completely determined by the Lamb shift of the s-level taking part in the transition. The corrections to the dipole matrix elements were found above, and it is not hard now to find the corrections to the intensities and widths. Note that the corrections to the decay width of the $2p$ level

$$\delta\Gamma(2p\to 1s)=-\Gamma_0(2p\to 1s)\cdot\frac{4}{3\pi}\alpha(Z\alpha)^2$$
$$\times\ln\frac{1}{(Z\alpha)^2}\left(-2\ln\frac{4}{3}+\frac{61}{24}\right), \quad (31)$$

found in Refs. 4–6 numerically,[4)] are in agreement with an unpublished result by K. Pachucki, obtained by a fundamentally different approach.

The correction to the frequency

$$\frac{\delta\omega_{\lambda'\lambda}}{\omega_{\lambda'\lambda}}=\frac{(Z\alpha)m^2A}{\pi}\frac{2n_p^2}{n_s(n_s^2-n_p^2)}, \quad (32)$$

where the index n_s pertains to the s-level, and the index n_p, to the p-level, always has opposite sign in comparison with the dipole matrix element. This can be understood from considerations of the sum rule (14), which determines the sign and scale of the ground level, and by observing the sign of the contribution of the diagonal matrix element to the sum (9). We also present an analytic expression for the correction to the width of the $3s$ level in the hydrogen atom:

$$\delta\Gamma(3s\to 2p)=-\Gamma_0(3s\to 2p)\cdot\frac{4}{3\pi}\alpha(Z\alpha)^2$$
$$\times\ln\frac{1}{(Z\alpha)^2}\left(2\ln\frac{5}{4}+\frac{387}{40}\right). \quad (33)$$

The remaining states can decay in several different ways, and therefore closed expressions for the corrections are quite cumbersome. Table IV gathers together the corrections to the line intensities and also to the partial and total line widths for transitions between the lower levels. The corrections to the transitions not including the levels with $l=0$ as either initial or final state are equal in the logarithmic approximation to zero.

Important for applications is the fact that the sum (9) is determined by the first few terms (see Table II), and therefore for estimates it is possible to use the above formulas not other than δ-function potentials. The estimate of the error of the logarithmic approximation that we have used in the present work is also connected with a consideration of potentials that are not described by a δ-function and, strictly speaking, are non-local. It is possible to apply our results to this case if we introduce an effective value for the parameter A in Eq. (2) according to the equality

TABLE IV. Corrections to the line intensities and partial and total line widths corresponding to transitions in the lower levels, in units of $A(Z\alpha)m^2/\pi$.

Level	Transition	$\delta I/I$	Partial and total $\delta\Gamma/\Gamma$	
	Corrections to the intensities and widths			
$2p$	$2p\to 1s$	-4.6331	-1.9664	-1.9664
$3s$	$3s\to 2p$	-9.5879	-10.121	-10.121
$3p$	$3p\to 1s$	-5.1336	-2.8836	-2.3654
	$3p\to 2s$	-0.3048	1.4952	
$4s$	$4s\to 2p$	-9.2589	-9.4256	-9.1860
	$4s\to 3p$	-8.2066	-8.8494	
$4p$	$4p\to 1s$	-5.2952	-3.1620	-2.4981
	$4p\to 2s$	-0.9183	0.4150	
	$4p\to 3s$	1.2750	2.7988	
	$4p\to 3d$	0	0	

$$A=\frac{\Delta E_L(1s)}{(\psi_{1s}(0))^2} \tag{34}$$

in which case an estimate of its relative error is given by

$$\frac{\Delta E_L(1s)-8\Delta E_L(2s)}{\Delta E_L(1s)} \quad \text{or} \quad \frac{\Delta E_L(2p)}{\Delta E_L(2s)}. \tag{35}$$

In the case of a δ-function potential the ratios in (35) are equal to zero. The similarly defined dimensionless quantity $A(Z\alpha)m^2/\pi$, in units of which all the corrections are given in Tables I–IV, in the case of single-loop radiative contributions to the Lamb shift vary from $1.24(3)\cdot 10^{-6}$ and $4.0(1)\cdot 10^{-6}$ for $Z=1$, 2 to $1.5(1)\cdot 10^{-4}$ and $2.6(3)\cdot 10^{-4}$ for $Z=20$, 30, where the results for large Z were obtained from the numerical calculations of Mohr.[23]

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APPENDIX A: SUM RULES FOR THE DIPOLE MATRIX ELEMENTS BETWEEN LEVELS WITH $l>1$

Let us consider a central potential of the form

$$V_l(\mathbf{r})=\frac{1}{(2l+2)!}\frac{1}{m^2}\left(\frac{1}{m}\frac{\partial}{\partial r}\right)^{2l+2}\delta(r)$$

and the quantity

$$\langle nl\|V_l(r)r\|n'(l+1)\rangle.$$

The latter quantity is obviously equal to zero. It can be rewritten as a sum over intermediate states with orbital momentum l. We then obtain the sum rule

$$\sum_q B_{ql}\langle ql\|r\|n'(l+1)\rangle=0,$$

where

$$B_{ql}=\psi_{q0}(0)\prod_{s=1}^{l}\left(1-\frac{s^2}{n^2}\right)^{1/2}.$$

For states of the continuous spectrum with wave number k we need only substitute $+k^2/(Z\alpha m)^2$ for $-1/n^2$ in the product in the latter expression.

The potential

$$V_l(\mathbf{r})=\frac{1}{(2l)!}\frac{1}{m^2}\left(\frac{\Delta}{m^2}\right)^{2l}\delta(\mathbf{r}),$$

which for $l=0$ is analogous to the potential considered in this paper, also leads to the same results.

APPENDIX B: EXPLICIT EXPRESSIONS FOR THE COULOMB GREEN'S FUNCTION

Here we present the result for the reduced Green's function (21) of the first four levels:

$$\bar{G}_{1s}(E_1;\mathbf{r},0)=\frac{Z\alpha m^2}{4\pi}\frac{2e^{-z_1/2}}{z_1}\times[2z_1(\ln z_1+C)+z_1^2-5z_1-2],$$

$$\bar{G}_{2s}(E_2;\mathbf{r},0)=-\frac{Z\alpha m^2}{4\pi}\frac{e^{-z_2/2}}{2z_2}[4z_2(z_2-2)(\ln z_2+C)+z_2^3-13z_2^2+6z_2+4],$$

$$\bar{G}_{3s}(E_3;\mathbf{r},0)=\frac{Z\alpha m^2}{4\pi}\frac{2e^{-z_3/2}}{9z_3}[6z_3(z_3^2-6z_3+6)\times(\ln z_3+C)+z_3^4-24z_3^3+72z_3^2-12],$$

$$\bar{G}_{4s}(E_4;\mathbf{r},0)=-\frac{Z\alpha m^2}{4\pi}\frac{e^{-z_4/2}}{144z_4}\times[24z_4(z_4^3-12z_4^2+36z_4-24)(\ln z_4+C)$$

$$+3z_4^5-113z_4^4+792z_4^3-1188z_4^2-264z_4+144],$$

where $C=0.5772\ldots$ is the Euler constant. The result for the ground state agrees with the results presented in different form by many authors (see, for example, Ref. 24).

APPENDIX C: SOME ASYMPTOTIC LIMITS OF THE CORRECTIONS TO THE DIPOLE MATRIX ELEMENTS

A. In the calculation of the asymptotic limits for $n'\to\infty$ (for fixed value of n) the following representation can be useful:

$$\delta d_{znn'}=\frac{meA}{\pi}\frac{(-1)^{n+1}}{24\sqrt{3}}\sqrt{\frac{n'^3(n'^2-1)}{n^3}}\times\left(\left[\frac{\partial Q_{\nu n'}}{\partial\nu}\right]_{\nu=n}-\frac{3}{2n}Q_{nn'}\right),$$

where

$$Q_{\nu n'}=\sum_{s=0}^{n}\frac{(-1)^s(\nu-s)\xi_\nu^4\eta_\nu^{\nu-s}}{s!}\frac{\Gamma(\nu+1)\Gamma(\nu-s+4)}{[\Gamma(\nu+1-s)]^2}\times{}_2F_1(\nu-s+4,2-n',4,\xi_\nu)$$

and we have introduced the notation

$$\xi_\nu=\frac{2\nu}{\nu+n'},\quad \eta_\nu=\frac{2n'}{\nu+n'}.$$

Note that in these terms

$$d_{znn'}=\frac{e}{Z\alpha m}\frac{(-1)^{n+1}}{24\sqrt{3}}\sqrt{\frac{n'^3(n'^2-1)}{n^3}}Q_{nn'}.$$

The confluent hypergeometric function appears in expression (C1) in the limit $n'\gg n$:

$$Q_{nn'}\underset{n'\to\infty}{\to}\left(\frac{2n}{n'}\right)^4\times\sum_{s=0}^{n}\frac{(-1)^s(n-s)2^{n-s}}{s!}\frac{\Gamma(n+1)\Gamma(n-s+4)}{[\Gamma(n+1)-s)]^2}\times{}_1F_1(n-s+4,4,-2n),$$

$$\left[\frac{\partial Q_{\nu n'}}{\partial\nu}\right]_{\nu=n n'\to\infty}\to\left(\frac{2n}{n'}\right)^4\sum_{s=0}^{n}\frac{(-1)^s(n-s)2^{n-s}}{s!}\times\frac{\Gamma(n+1)\Gamma(n-s+4)}{[\Gamma(n+1-s)]^2}\left\{\left[\psi(n-s+4)+\psi(n+1)-2\psi(n+1-s)+\ln 2+\frac{5n-4s}{n(n-s)}\right]_1F_1(n-s+4,4,-2n)+\left[\frac{\partial_1F_1(a,4,-2n)}{\partial a}\right]_{a=n-s+4}-\frac{n-s+4}{2}{}_1F_1(n-s+5,5,-2n)\right\}.$$

It should be noted that the term with the derivative in the last formula does not reduce to a polynomial and thus the correction contains an infinite series. In the case $n=1$ we have

$$\frac{\delta d_{z1n'}}{d_{z1n'}}\underset{n'\to\infty}{\to}\frac{Z\alpha m^2A}{\pi}\left(\ln 2-\frac{3}{8}-\mathscr{E}_2+\frac{5}{8}e^2\right),$$

where we have introduced the notation

$$\mathscr{E}_n=\sum_{k=1}^{\infty}\frac{n^k}{kk!}$$

and for large values of the principal quantum number the matrix elements have the asymptotic limit

$$d_{z1n'}\underset{n'\to\infty}{\to}\frac{16e^{-2}}{\sqrt{3}(n')^{3/2}}.$$

The relative magnitude of the correction tends toward a finite limit. Explicit expressions for the asymptotic limits of the lower levels ($n'=1-4$) are given in Table I.

B. In the limit $n\to\infty$ (for fixed value of n'), using the expression

$$Q_{\nu n'}=\xi_\nu^4\sum_{t=0}^{n'-2}\frac{(-1)^t\xi_\nu^t}{t!}\frac{\Gamma(n'-1)}{\Gamma(n'-1+t)}\frac{\Gamma(4)}{\Gamma(t+4)}\times\sum_{s=0}^{n}\frac{(-1)^s(\nu-s)\eta_\nu^{\nu-s}}{s!}\frac{\Gamma(\nu+1)\Gamma(\nu-s+4-t)}{[\Gamma(\nu+1-s)]^2}$$

and operating in a similar way, we obtain

$$\delta d_{znn'}\underset{n\to\infty}{\to}-\frac{4}{\sqrt{3}}\frac{meA}{\pi}\sqrt{\frac{n'^3(n'^2-1)}{n^3}}\times\sum_{t=0}^{n'-2}\frac{2^t}{t!}(-1)^t\frac{\Gamma(n'-1)}{\Gamma(n'-t-1)}\left\{[\ln(2n')+C+\psi(t+4)-\psi(1)](-2n')(t+4){}_1F_1(t-5,2,-2n')-2n'\left[{}_1F_1(t+5,2,-2n')+(t+4)\times\left[\frac{\partial}{\partial a}{}_1F_1(a,2,-2n')\right]_{a=t+5}\right]+2n'(t+4)\left[{}_1F_1(t+5,2,-2n')-\left[\frac{\partial}{\partial c}{}_1F_1(t+5,c,-2n')\right]_{c=2}\right]+{}_1F_1(t+4,1,-2n')\right\}.$$

The asymptotic limits of the lower levels ($n=1-4$) are shown in Table I in explicit form. The quantities $\mathscr{E}_{2n}$ and

$$\mathscr{E}'_n=\mathscr{E}_n+C+\ln n$$

appearing in them grow rapidly; for example, $\mathscr{E}_8=437.72$. The asymptotic behavior of $\mathscr{E}_{2n}$ for large n is given by

$e^{2n}/2n$ (Ref. 25), and the combination appearing directly in the answers (see Table I) turns out to be extremely slowly varying with n.

[1)]The phase factor of the radial wave function is constructed in such a way that all values at zero for the ns-states should be real and positive and likewise the first derivatives with respect to the radius for the np-states. For large values of l the first nonzero derivative of the radial wave function with respect to the radius is required to be real and positive. Real dipole matrix elements in the definitions of Ref. 16 corresponds to imaginary ones in the definitions of Refs. 18 and 19.

[2)]It is usually given in monographs (e.g., Refs. 16–18) with the wrong sign (see Ref. 6).

[3)]Note that in the expression for the $2p-nd$ matrix elements in Ref. 18 there is a typographical error (formula (52,4)): 2^{20} should read 2^{19}.

[4)]Reference 6, of which the present paper is a direct continuation (see also Refs. 4 and 5), gives a detailed treatment of the discrepancy between the result for the width of the $2p_{1/2}$ level obtained in the works of one of the authors (C. G. K.)[4–6] and the result presented in earlier papers by V. G. Pal'chikov, Yu. L. Sokolov, and V. P. Yakovlev (Pis'ma Zh. Éksp. Teor. Fiz. **38**, 347 (1983) [JETP Lett. **38** (1983)]; Metrologia **21**, 99 (1985)). The latter result took account of only some of the contributions, and differs from expression (31).

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