Order $(Z\alpha)^4(m/M)R_\infty$ correction to the hydrogen energy levels

A. S. Elkhovskiĭ

G. I. Budker Institute of Nuclear Physics, Siberian Branch of the Russian Academy of Sciences, 630090 Novosibirsk, Russia

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A correction to the hydrogen energy levels that is first-order in m/M and fourth-order in $Z\alpha$ (pure nuclear recoil) is calculated. It consists of two contributions, one building up on the atomic scale and the other at distances of the order of the Compton electron wavelength. The long-distance contribution is found by two different perturbation methods. The source of the perturbation in both is the slow motion of the nucleus. In one the electron is assumed a relativistic particle from the start. In the other the relativistic effects are also considered perturbatively. The short-distance contribution is found in the Feynman and Coulomb gauges. Recent results for P levels are confirmed, in contrast to those for S levels. Numerically, the shift is found to amount to 2.77 kHz for the ground state and 0.51 kHz for the $2S$ state. © *1996 American Institute of Physics.* [S1063-7761(96)00608-7]

1. INTRODUCTION

Reducing the uncertainty in the theoretical prediction of the energy difference of the $2S$ and $2P$ states of the hydrogen atom to about 1 kHz would make it possible, after achieving the same precision in experiments, to determine the proton's charge radius with a one-percent accuracy. Recently completed calculations of the correction of relative-order $(\alpha/\pi)^2(Z\alpha)^3$ (see Ref. 1 and the references cited therein) suggest that among potential sources of this theoretical uncertainty may be the correction of relative order $(Z\alpha)^4 m/M$, which emerges as a result of allowing for nuclear recoil and the relativistic effects in electron motion simultaneously. In the present paper this correction is calculated for an arbitrary energy level of the hydrogen atom.

Earlier the correction of the order discussed here was calculated for P states in Ref. 2. Since in states with nonzero angular momentum the correction builds up on the atomic scale, to calculate this correction one can use the standard quantum mechanical perturbation theory for effective operators describing relativistic effects. Proof of the validity of this approach (for states with nonzero angular momentum in the order in α under discussing) lies in the convergence at small distances of all matrix elements of the effective operators arising in the perturbation theory.

At the same time, an attempt to employ the nonrelativistic approach in calculating the correction to S states, whose wave functions do not vanish at small distances, leads to divergent matrix elements. Indeed, among the effective operators there are those that depend on r as r^{-3} or even as r^{-4} (see Ref. 2). With regard to the latter, for S states an r^{-4} operator is equivalent (to within a nonsingular operator) to the sum of operators with an r^{-3} radial dependence and a $\delta(\mathbf{r})/r$ radial dependence. In Ref. 3 the logarithmically divergent contributions to the shift of S levels were shown to cancel out. This means that the correction for states with a zero angular momentum naturally splits into two contributions, one at long distances and one at short, each building up on its own scale. While in calculating the long-distance contribution we can still use the nonrelativistic approach, for the short-distance contribution (distances of order of the electron Compton wavelength) we must use relativistic techniques.

A closed expression for the first nuclear-recoil correction (linear with respect to the mass ratio) to the energy of a relativistic electron moving in a Coulomb field is given in Sec. 2. It is used in Sec. 3 to evaluate the long-distance contribution. Here again the relativistic approach proves to be more efficient. Section 4 is devoted to finding the short-distance contribution in the Feynman gauge. The results are verified in Sec. 5. Here the long-distance contribution is recalculated using the nonrelativistic approach, and the short-distance contribution is found again in the Coulomb gauge. Finally, in Sec. 6 we discuss the numerical values of the energy shifts and compare the results of the present work with those obtained in Refs. 2 and 4.

Throughout the paper we employ the relativistic system of units: $\hbar = c = 1$. Since we are not considering radiative corrections, Z can also be set equal to unity.

2. THE METHODS OF CALCULATION

As one of the methods for finding the long-distance contribution we use the nonrelativistic approach, which begins with the Schrödinger equation in a Coulomb field. In other words, in this approach both particles are assumed nonrelativistic. To allow for relativistic effects we expand the scattering amplitude for free relativistic particles in a power series in the initial and final velocities. In this way we set up an operator expansion for the effective interaction potential. The difference of the effective potential and the Coulomb potential is then used as a perturbing operator in the ordinary quantum mechanical perturbative approach, which is extremely effective in determining the contribution of atomic distances. Earlier it was used in calculating the logarithmic (in α) corrections in the two-body problem,[5] the order $m\alpha^6$ corrections to the positronium P levels,[6] and the order $m^2\alpha^2/M$ corrections to the hydrogen P levels.[2] Unfortunately, the nonrelativistic approach becomes ineffective when calculating the short-distance contribution.

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In the alternative approach a relativistic light particle (an electron) moves in the field generated by a slow heavy particle (the nucleus). In the leading approximation the heavy particle is at rest and serves as the source of the Coulomb field. The wave function of the system reduces to the wave function of the light particle satisfying the Dirac equation. To first order in the reciprocal mass of the heavy particle the perturbation operator coincides with the particle's nonrelativistic Hamiltonian:

$$V=\frac{(\mathbf{P}-|e|\mathbf{A}(\mathbf{R}))^2}{2M}. \tag{1}$$

Here $\mathbf{P}$ and $\mathbf{R}$ are, respectively, the momentum and position operators of the nucleus.

Unfortunately, one cannot directly average the perturbation operator (1) over the unperturbed wave function, since the operator depends on the dynamical variables of the nucleus while the unperturbed wave function depends on the electron position coordinates or momentum. To overcome this difficulty we can use the fact that observables in QED are gauge invariant.[7] Being expressed in terms of the electron's variables, the average of (1) must remain gauge invariant. With this requirement, the new form of the average is practically obvious:

$$\Delta E_{\mathrm{rec}}=-\frac{1}{M}\int\frac{d\omega}{2\pi i}\langle(\mathbf{p}-\mathbf{D})G_{E+\omega}(\mathbf{p}-\mathbf{D})\rangle. \tag{2}$$

Here $\mathbf{p}$ is the electron momentum operator, and the integral operator $\mathbf{D}$ describes the exchange of a transverse photon.[1)] The kernel of $\mathbf{D}$ has the form

$$\frac{4\pi\alpha\alpha_k}{k^2-\omega^2},\quad \boldsymbol{\alpha}_k\equiv\boldsymbol{\alpha}-\frac{\mathbf{k}(\boldsymbol{\alpha}\mathbf{k})}{k^2}.$$

In Eq. (2), G is the Green's function of the Dirac equation in a Coulomb field, and E is the energy of the electron state over which the averaging is done. To verify the validity of (2), we note that its part that is quadratic in $\mathbf{D}$ emerges as a result of trivial averaging of the $\mathbf{A}^2$-term of operator (1) over the electromagnetic field fluctuations. All the other terms ensure that (2) is invariant under a gauge transformation:

$$\psi\to\exp[i\phi(\mathbf{r})]\psi,\quad \mathbf{D}\to\mathbf{D}+i[\mathbf{p},\phi]. \tag{3}$$

Clearly, the same result can be obtained from Eq. (11) of Ref. 7 after using the Dirac equation.

The first attempt in deriving an expression for the energy correction that is caused by recoil and is exact in the Coulomb field was made by Braun.[8] Complete expressions for the various contributions in the Coulomb gauge were first obtained in the quasipotential approach in Ref. 9. It can be proved that the sum of these expressions is (2).

3. THE LARGE-DISTANCE CONTRIBUTION

In this section we study the energy contribution that builds up on the atomic scale. To verify the results we use both approaches described above. Here we describe in detail the calculations in the relativistic approach. The procedure for comparing the results with those of the more cumbersome nonrelativistic approach is discussed in Sec. 5.

3.1. The Coulomb contribution

The Coulomb part of the contribution,

$$\Delta E_C=-\frac{1}{M}\int\frac{d\omega}{2\pi i}\langle\mathbf{p}G_{E+\omega}\mathbf{p}\rangle=\frac{1}{2M}\langle\mathbf{p}(\Lambda_+-\Lambda_-)\mathbf{p}\rangle, \tag{4}$$

naturally splits into two terms:[8]

$$\Delta E_C=\left\langle\frac{p^2}{2M}\right\rangle-\frac{1}{M}\langle\mathbf{p}\Lambda_-\mathbf{p}\rangle. \tag{5}$$

Here Λ_+ and Λ_- are the projection operators onto the sets of positive- and negative-frequency solutions of the Dirac equation in the Coulomb field. Using this fact we can represent the expectation value of the operator $p^2/2M$ in the following form:[9]

$$\left\langle\frac{p^2}{2M}\right\rangle=\frac{m^2-E^2}{2M}+\frac{m^2}{2M}\left\langle 2(E-m\beta)\frac{\alpha}{r}+\frac{\alpha^2}{r^2}\right\rangle. \tag{6}$$

As for the second term in Eq. (5), responsible for virtual transitions into negative-frequency states, on the atomic scale it contributes practically nothing to the order of interest to us, as can easily be verified. Indeed, simply counting the powers of α on the right-hand side of the obvious inequality

$$|\langle\mathbf{p}\Lambda_-\mathbf{p}\rangle|<\left|\frac{1}{4m^2}\langle[\mathbf{p},C]\Lambda_-[\mathbf{p},C]\rangle\right|, \tag{7}$$

where C is the Coulomb potential, we find that at large distances the product of commutators already contains the sixth power of α. Hence all the other cofactors on the right-hand side can be replaced by their nonrelativistic limits. Since the nonrelativistic region contains no negative-frequency states, the large-distance contribution to the second term vanishes in the order considered here.

3.2. The magnetic contribution

After integrating with respect to frequency, the expression for the single transverse, or magnetic, contribution,

$$\Delta E_M=\frac{1}{M}\int\frac{d\omega}{2\pi i}\langle\mathbf{p}G\mathbf{D}+\mathbf{D}G\mathbf{p}\rangle, \tag{8}$$

assumes the form

$$\Delta E_M=-\frac{\alpha}{M}\,\mathrm{Re}\left\langle\mathbf{p}\left(\sum_+\frac{|m\rangle\langle m|}{k+E_m-E}-\sum_-\frac{|m\rangle\langle m|}{E-E_m+k}\right)\frac{4\pi\alpha_k}{k}\right\rangle, \tag{9}$$

where Σ_+ stands for the sum over the discrete spectrum and the integral over the positive-frequency part, and Σ_- stands for the integral over the negative-frequency part.

If the transverse-photon momentum is in the atomic range, $k\sim ma$, we can expand the first term on the right-hand side of Eq. (9) in a power series in $(E-E_m)/k$. In the zeroth approximation (the instantaneous exchange approximation) we have

$$-\frac{\alpha}{M}\mathrm{Re}\left\langle\frac{4\pi\boldsymbol{\alpha}_k}{k^2}\Lambda_+\mathbf{p}\right\rangle$$

$$=-\frac{1}{2M}\left\langle 2(E-m\beta)\frac{\alpha}{r}+\frac{\alpha^2}{r^2}\right\rangle+\frac{\alpha}{M}\mathrm{Re}\left\langle\frac{4\pi\boldsymbol{\alpha}_k}{k^2}\Lambda_-\mathbf{p}\right\rangle. \tag{10}$$

Adding the first term to (6) yields the simple result[9]

$$\frac{m^2-E^2}{2M}=\frac{m^2\alpha^2}{2MN^2}, \tag{11}$$

where the standard notation of the Dirac–Coulomb problem are used,

$$N=\sqrt{(\gamma+n_r)^2+\alpha^2},\quad \gamma=\sqrt{\kappa^2-\alpha^2},$$

with n_r the radial quantum number, and $\kappa=-1-\boldsymbol{\sigma}\mathbf{l}$. Note that (11) coincides with its nonrelativistic limit only for states with $n_r=0$.

Since we are interested only in corrections of even order in α, we immediately proceed with the second term in the expansion, which describes the retardation effect:

$$\Delta E_{\mathrm{ret}}=-\frac{\alpha}{M}\mathrm{Re}\left\langle\mathbf{p}\sum_+(E_m-E)^2|m\rangle\langle m|\frac{4\pi\boldsymbol{\alpha}_k}{k^4}\right\rangle$$

$$=-\frac{\alpha}{M}\mathrm{Re}\left\langle[H,[H,\mathbf{p}]]\Lambda_+\frac{4\pi\boldsymbol{\alpha}_k}{k^4}\right\rangle. \tag{12}$$

Here $H=\boldsymbol{\alpha}\mathbf{p}+\beta m+C$ is the Dirac Hamiltonian in a Coulomb field. Replacing the corresponding operator by its kernel, we obtain

$$[H,\mathbf{p}]=\alpha\frac{4\pi\mathbf{k}}{k^2},\quad [H,[H,\mathbf{p}]]=\alpha\frac{4\pi\mathbf{k}(\boldsymbol{\alpha}\mathbf{k})}{k^2}.$$

In the leading nontrivial approximation, the matrix elements of the Dirac matrices $\boldsymbol{\alpha}$ over positive-frequency states can be replaced by the appropriate Pauli currents:

$$\Delta E_{\mathrm{ret}}\approx-\frac{\alpha^2}{M}\left\langle\frac{4\pi\mathbf{k}'}{k'^2}\frac{2\mathbf{p}'\mathbf{k}'-k'^2}{2m}\frac{4\pi}{k^4}\frac{2\mathbf{p}_k+i[\boldsymbol{\sigma}\mathbf{k}]}{2m}\right\rangle. \tag{13}$$

Here $\mathbf{k}'=\mathbf{q}-\mathbf{k}$, $\mathbf{q}=\mathbf{p}'-\mathbf{p}$, and $\mathbf{p}$ and $\mathbf{p}'$ are the arguments of the wave function and its conjugate counterpart, respectively. After going over to the spatial representation, we obtain

$$\Delta E_{\mathrm{ret}}=\frac{\alpha^2}{4m^2M}\left\langle-2\mathbf{p}\frac{1}{r^2}\mathbf{p}+\frac{7\mathbf{l}^2+2\boldsymbol{\sigma}\mathbf{l}}{2r^4}\right\rangle. \tag{14}$$

Actually, the integral with respect to $\mathbf{k}$ in (13) contains an infrared divergence. It is dropped from (14) because photons of low virtuality (with $k\sim m\alpha^2$) are responsible for radiative corrections in the odd orders in α. To verify this fact, we regularize the divergence by introducing a photon mass λ, with $m\alpha^2\ll\lambda\ll m\alpha$. Then the term omitted in (14), proportional to $1/\lambda$, is canceled out by the corresponding term in the difference of (9) and an expression obtained from (9) by substituting $\sqrt{k^2+\lambda^2}$ for k. On the other hand, this difference determines the low-frequency contribution to the order $m\alpha^5/M$ correction.

Finally, the virtual transitions into negative-frequency states caused by emission of a single magnetic quantum are described by the last terms in (9) and (10). The expansion of the last term in (9) at large distances starts with the seventh power of α. This can easily be verified by using an inequality similar to (7). As for the negative-frequency contribution to (10), in the first nontrivial approximation it is reduced to

$$-\frac{\alpha^2}{2mM}\left\langle\frac{4\pi\boldsymbol{\alpha}_{k'}}{k'^2}\lambda_-(\mathbf{p}+\mathbf{k})\frac{4\pi\mathbf{k}}{k^2}\right\rangle$$

$$\approx\frac{\alpha^2}{4m^2M}\left\langle\frac{4\pi\boldsymbol{\alpha}_{k'}\mathbf{k}}{k'^2}\frac{4\pi\boldsymbol{\alpha}\mathbf{k}}{k^2}\right\rangle, \tag{15}$$

which after going over to the spatial representation yields

$$\Delta E_{M-}=-\frac{\alpha^2}{4m^2M}\left\langle\frac{1}{r^4}-\frac{4\pi\delta(\mathbf{r})}{r}\right\rangle. \tag{16}$$

In S states this average is logarithmically divergent at small distances (linear divergences cancel out). The ultraviolet divergence in the large-distance contribution to the correction to the S levels will be discussed after we find the total large-distance contribution. Indeed, in view of the gauge invariance of individual terms [e.g., (16)], the divergences contained in these terms have no physical meaning when considered individually.

3.3. The seagull contribution

As in Sec. 3.2, taking the integral with respect to ω in the expression for the double-transverse, or seagull, contribution

$$\Delta E_S=-\frac{1}{M}\int\frac{d\omega}{2\pi i}\langle\mathbf{D}G_{E+\omega}\mathbf{D}\rangle \tag{17}$$

yields

$$\Delta E_S=\frac{\alpha^2}{2M}\left\langle\frac{4\pi\boldsymbol{\alpha}_{k'}}{k'}\sum_+\frac{|m\rangle\langle m|[1+(E_m-E)/(k'+k)]}{(E_m-E+k')(E_m-E+k)}\right.$$

$$\left.\times\frac{4\pi\boldsymbol{\alpha}_k}{k}+\ldots\right\rangle, \tag{18}$$

where the dots stand for the contribution of negative-frequency states, which differs from that of the positive-frequency states in the overall sign and the signs of k and k'. It can easily be verified that the terms linear in $k/2m$ in the expansion of the negative-frequency part cancel out. But these are precisely the terms that lead on the atomic scale to the contribution of the sought order. We are, therefore, forced to examine the expression explicitly written in (18). In the leading nonrelativistic approximation

$$\Delta E_{S+}=\frac{\alpha^2}{2M}\left\langle\frac{4\pi\boldsymbol{\alpha}_{k'}}{k'^2}\Lambda_+\frac{4\pi\boldsymbol{\alpha}_k}{k^2}\right\rangle \tag{19}$$

we again replace the matrix elements of $\boldsymbol{\alpha}$ over positive-frequency states by the Pauli currents,

$$\Delta E_{S+}=\frac{\alpha^2}{2M}\left\langle\frac{4\pi}{k'^2}\frac{2\mathbf{p}'_{k'}+i[\boldsymbol{\sigma}\mathbf{k}']}{2m}\frac{4\pi}{k^2}\frac{2\mathbf{p}_k+i[\boldsymbol{\sigma}\mathbf{k}]}{2m}\right\rangle, \tag{20}$$

and go to the spatial representation. The result is

$$\Delta E_{S+}=\frac{\alpha^2}{4m^2M}\left\langle 2\mathbf{p}\frac{1}{r^2}\mathbf{p}+\frac{1}{r^4}-\frac{3\mathbf{l}^2+2\boldsymbol{\sigma}\mathbf{l}}{2r^4}\right\rangle. \tag{21}$$

3.4. The total large-distance contribution

Summing (14), (16), and (21), we get

$$\frac{\alpha^2}{4m^2M}\left\langle 2\frac{\mathbf{l}^2}{r^4}+\frac{4\pi\delta(\mathbf{r})}{r}\right\rangle. \tag{22}$$

Expanding (11) in a power series in α^2 and calculating the average in (22), we obtain the large-distance contribution for states with nonzero l:

$$\Delta E_{l>0}=\frac{m^2\alpha^6}{Mn^3}\left\{\frac{1}{8|\kappa|^3}+\frac{6\kappa}{|\kappa|(4\kappa^2-1)(2\kappa+3)}+\frac{3}{8n\kappa^2}-\frac{1}{n^2|\kappa|}\left[1+2\frac{\kappa^2(\kappa+1)}{(4\kappa^2-1)(2\kappa+3)}\right]+\frac{1}{2n^3}\right\}. \tag{23}$$

For $l=1$ this is reduced to the result obtained in Ref. 2. As mentioned in the Introduction, the effective operators that emerge in the order under consideration are not sufficiently singular to balance the vanishing of the wave function for states with nonzero angular momenta as $r\to 0$. For this reason, the expression (23) constitutes the total correction of the order under consideration to levels with $l>0$.

In S states the first term vanishes due to the action of the operator $\mathbf{l}$. Note that direct generalization of the result for states with nonzero angular momentum to S states leads to an erroneous final contribution: the vanishing of the angular matrix element is balanced by a linear divergence in the radial matrix element.

As for the second term, which formally contains a linear divergence, it is a remnant of the small-distance contribution to the previous order correction (fifth in α). To verify this, we again regularize the divergence at small distances by subtracting the potential for the exchange of a transverse photon of mass $\lambda\gg m\alpha$ from the instant transverse exchange potential in (15):

$$\frac{4\pi\boldsymbol{\alpha}_{k'}}{k'^2}\to\frac{4\pi\boldsymbol{\alpha}_{k'}}{k'^2}-\frac{4\pi\boldsymbol{\alpha}_{k'}}{k'^2+\lambda^2}. \tag{24}$$

By going to the spatial representation, instead of a singular operator we get its regularized version,

$$\frac{4\pi\delta(\mathbf{r})}{r}\to\frac{2\lambda}{3}4\pi\delta(\mathbf{r}),$$

whose expectation value yields the energy correction of order $m\lambda\alpha^5/M$. This correction is canceled out by the linear-in-λ term in the expansion of the small-distance contribution to the order $m^2\alpha^5/M$ correction, calculated with the massive propagator of the transverse photon (now we must use the fact that λ is small compared to the electron mass). Along with the correction to the order $m^2\alpha^5/M$ contribution, which is linear in λ/m one could expect a correction linear in $\alpha=m\alpha/m$. It is obvious, however, that at large distances the expansion parameter is actually $(p/m)^2\sim\alpha^2$, so that the operator under discussion contributes nothing to the order of interest to us. On the other hand, the correction to the local operator which is linear in α ($\propto\delta(\mathbf{r})$) may occur as an ordinary radiative correction. In this case it acquires its value entirely at small distances. Section 5 is devoted to the calculation of such corrections.

Thus, in S states the large-distance contribution is exhausted by the order $m^2\alpha^6/M$ term from the expansion of (11):

$$\Delta E^{LD}_{l=0}=\frac{m^2\alpha^6}{2Mn^3}\left(\frac{1}{4}+\frac{3}{4n}-\frac{2}{n^2}+\frac{1}{n^3}\right). \tag{25}$$

Only in the ground state does this contribution vanish.

4. THE SMALL-DISTANCE CONTRIBUTION

As mentioned in the Introduction, in S states in addition to the large-distance contribution there can be a contribution originating at distances on the order of the electron Compton wavelength. Since the two contributions are well-separated in scale, each is gauge invariant. This makes it possible to use the most suitable gauge when calculating the small-distance contribution. The Feynman gauge has proved convenient. The main formula (2) can either be written in this gauge by employing the Dirac equation or can be derived directly from Eq. (11) of Ref. 7:

$$\Delta E_{\rm tot}=-\frac{\alpha^2}{M}\int\frac{d\omega}{2\pi i}\left\langle\frac{4\pi}{k'^2+\lambda^2-\omega^2}\left(\boldsymbol{\alpha}+\frac{\mathbf{k}'}{\omega}\right)G_{E+\omega}\times\left(\boldsymbol{\alpha}-\frac{\mathbf{k}}{\omega}\right)\frac{4\pi}{k^2+\lambda^2-\omega^2}\right\rangle. \tag{26}$$

The momenta of both photons are assumed to be directed from the nucleus to the electron. The photon mass λ is introduced to establish control over the infrared divergences, which emerge in perturbational calculations of the small-distance contribution as remnants of contributions of previous orders in α or of the large-distance contribution of the order considered.

Replacing the wave functions in the integrand by their values at zero and the Green's function by the term in its expansion (the term must be linear in the Coulomb potential), we obtain

$$\Delta E_G=\frac{\alpha^3\psi^2}{M}\int\frac{d\omega}{2\pi i}\left\langle\frac{4\pi}{p'^2-\mathscr{K}^2}\left(\boldsymbol{\alpha}-\frac{\mathbf{p}'}{\omega}\right)\times\frac{m+\omega+\beta m+\boldsymbol{\alpha}\mathbf{p}'}{p'^2-\Omega^2}\frac{4\pi}{q^2}\frac{m+\omega+\beta m+\boldsymbol{\alpha}\mathbf{p}}{p^2-\Omega^2}\times\left(\boldsymbol{\alpha}-\frac{\mathbf{p}}{\omega}\right)\frac{4\pi}{p^2-\mathscr{K}^2}\right\rangle. \tag{27}$$

Here $\psi^2\equiv|\psi(0)|^2$, the angle brackets stand for integration with respect to $\mathbf{p}$ and $\mathbf{p}'$, $\mathbf{q}=\mathbf{p}'-\mathbf{p}$, and we have introduced the notation

$$\mathscr{K}\equiv\sqrt{\omega^2-\lambda^2},\quad \Omega\equiv\sqrt{2m\omega+\omega^2}.$$

Contrary to the case of large distances, in the relativistic region the opposite order of integration has proved more suitable: first with respect to $\mathbf{p}$ and $\mathbf{p}'$, and then with respect to ω. As for the first integral, its calculation becomes trivial

after going over to the spatial representation. As a preparatory step, it is convenient to express all scalar products of momenta in terms of their squares. This leads to terms that do not contain Ω in their denominators and can be discarded since λ is the only scale in such terms, while we are interested in contributions that build up their values on momenta of order of the electron mass. After we go over to ordinary space, the two-loop integral with zero external momenta is transformed into a simple one-dimensional integral with respect to r. As a result of this integration we are left with an integral in the complex ω plane, with the integration contour encompassing the cut connecting the points $-2m$ and $-\lambda$. The final result is

$$\Delta E_G=\frac{\pi\alpha^3\psi^2}{Mm}\left(\frac{1}{\varepsilon}-\frac{8}{3\pi\sqrt{\varepsilon}}\int_1^\infty\frac{dx}{\sqrt{x(x^2-1)}}+4\ln 2-\frac{5}{2}\right), \tag{28}$$

where $\varepsilon=\lambda/2m$.

But if we ignore the interaction in the Green's function entirely, we must use the Dirac equation to properly account for the behavior of the wave function at small distances:

$$\Delta E_\psi=2\frac{\alpha^3\psi^2}{M}\int\frac{d\omega}{2\pi i}\left\langle\frac{4\pi}{p'^4}(2m+\boldsymbol{\alpha}\mathbf{p}')\frac{4\pi}{q^2-\mathscr{K}^2}\right.$$
$$\left.\times\left(\boldsymbol{\alpha}+\frac{\mathbf{q}}{\omega}\right)\frac{m+\omega+\beta m+\boldsymbol{\alpha}\mathbf{p}}{p^2-\Omega^2}\left(\boldsymbol{\alpha}-\frac{\mathbf{p}}{\omega}\right)\frac{4\pi}{p^2-\mathscr{K}^2}\right\rangle. \tag{29}$$

Using the same procedure, we take $-r/2$ as the Fourier transform of $4\pi/p^4$. The linearly divergent constant discarded in the process is actually proportional to $1/\alpha$ and therefore constitutes a part of the correction of the previous order. As a result we get

$$\Delta E_\psi=\frac{\pi\alpha^3\psi^2}{Mm}\left(-\frac{1}{2\varepsilon^2}+\frac{1}{\varepsilon}-\frac{8}{3\pi\sqrt{\varepsilon}}\int_1^\infty\frac{dx}{\sqrt{x(x^2-1)}}\right). \tag{30}$$

The terms in (28) and (30) that depend on the photon mass arise from integration over the range of momenta $p\sim\lambda$ and frequencies $\omega\sim\lambda$ (or $\sqrt{m\lambda}$) and therefore do not belong to the small-distance contribution, which is determined by the range $p\sim\omega\sim m$ and is independent of the infrared cutoff parameter:

$$\Delta E^{SD}=\frac{m^2\alpha^6}{Mn^3}\left(4\ln 2-\frac{5}{2}\right)\delta_{l0}. \tag{31}$$

Note that the result contains no hidden large-distance contributions that could emerge as a result of dividing all common (nonzero) powers of the photon mass out of numerator and denominator: all terms proportional to positive powers of α were set equal to zero in the process of calculation. Clearly, the emergence of such contributions would be self-contradictory because the convergence of the integral at distances of order $1/\lambda$ means that at $p\sim\lambda$ the total sum of powers of momenta in the denominator of the integrand is at least one unit greater than the total power of the numerator and measure of integration. In other words, all contributions of "large" distances (of order $1/\lambda$) have to contain a positive power of the photon mass in the denominator.

5. VERIFYING THE RESULTS

5.1. The large-distance contribution

To verify the validity of the results for the different terms constituting the large-distance contribution, all were obtained within the framework of the nonrelativistic approach, which uses the Schrödinger equation as the starting point. For states with nonzero angular momenta we adopted the following procedure. Since all the contributions exhibit the same analytical structure,

$$\Delta E=\frac{m^2\alpha^6}{Mn^3}\Sigma,$$

where

$$\Sigma=\frac{1}{|\kappa|^3}\left(a_\infty+\frac{a_{1/2}}{\kappa-1/2}+\frac{a_{-1/2}}{\kappa+1/2}+\frac{a'_{-1/2}}{(\kappa+1/2)^2}+\frac{a_{-1}}{\kappa+1}\right.$$
$$\left.+\frac{a_{-3/2}}{\kappa+3/2}\right)+\frac{1}{n\kappa^2}\left(b_\infty+\frac{b_{-1/2}}{\kappa+1/2}\right)+\frac{1}{n^2|\kappa|}$$
$$\times\left(c_\infty+\frac{c_{1/2}}{\kappa-1/2}+\frac{c_{-1/2}}{\kappa+1/2}+\frac{c_{-3/2}}{\kappa+3/2}\right)+\frac{d}{n^3}, \tag{32}$$

the constants a, b, c, and d for each contribution were first calculated in the nonrelativistic setting from their asymptotic behavior as $\kappa\to\infty$ or as the residues at the corresponding poles in the complex κ plane, and then compared with the values obtained in the relativistic setting. In the process of comparison, the set of the "nonrelativistic" terms was broken down into groups according to the meaning of the respective "relativistic" contributions. For instance, the retardation part (14) of the magnetic contribution consists of three terms in the nonrelativistic setting: $\Delta E^{(1)}_{MC}$, $\Delta E^{(1)}_{MCC}$, and $\Delta E^{(1)}_{\rm ret}$ (in the notation of Ref. 2).

As noted earlier, S states should be treated separately to avoid fictitious contributions arising from the fact that vanishing angular matrix element are balanced by linearly divergent radial matrix elements. It appears that all divergences at small distances cancel out: the final result is independent of the parameter introduced for regularization of the effective potentials whose singularity is too strong at zero.

5.2. The small-distance contribution

To compare the results of the present work with those of Ref. 4, the small-distance contributions was also calculated in the Coulomb gauge. The calculation method was similar to the one used in the case of the Feynman gauge. The resulting small-distance contributions are

$$C_G=C_\psi=\frac{\pi\alpha^3\psi^2}{Mm}\frac{1}{2}; \tag{33}$$

$$M_G=-\frac{\pi\alpha^3\psi^2}{Mm}\left(\ln\frac{\lambda}{2m}+\frac{3}{2}\right), \tag{34}$$

$$M_\psi = -\frac{\pi\alpha^3\psi^2}{Mm}\ln\frac{\lambda}{2m}; \tag{35}$$

$$S_G = \frac{\pi\alpha^3\psi^2}{Mm}(4\ln 2 - 2), \tag{36}$$

$$S_\psi = \frac{\pi\alpha^3\psi^2}{Mm}2\ln\frac{\lambda}{2m}. \tag{37}$$

Here by C, M, and S we denote the Coulomb, magnetic, and seagull contributions, respectively. It can easily be verified that the sum of these contributions coincides with (31).

6. CONCLUSION

The numerical values of the contributions to the energy are 2.77 kHz for the ground state and 0.51 kHz for the $2S$ state. This is somewhat lower than the value given by a direct estimate ($m^2\alpha^6/M \approx 10.2$ kHz) but is still comparable to the accuracy of the measurements that are to be carried out soon. Interestingly, the corrections to the $2S$ and $2P$ levels (with allowance for the radiative correction of the same order to the $2P$ level[2)]) prove to be very close, so that the correction of 0.04 kHz to their difference is negligible compared to experimental errors.[10]

Now let us see how the results of the present work compare to those obtained in other papers. Apparently, the results for levels with nonzero angular momenta are firmly established.[2,11] The situation with S levels[4,11] merits further discussion, however.

The results of the present work for S levels contradict those of the analytical calculation done by Pachucki and Grotch.[4] But what are the reasons for this discrepancy? Clearly, all the small-distance contributions (33)–(37) are in exact agreement with the "high-energy" contributions of Ref. 4. The same can be said about large-distance contributions (low- and intermediate-energy contributions in the terminology of Ref. 4) with one exception: the retardation contribution in single magnetic exchange. The -2 factor in Eq. (68) of Ref. 4 corresponding to the intermediate-energy contribution in the sixth order in α differs from our result of -1 (in the same units of $m^2\alpha^6/M$), which appears as a result of trivial averaging in (14) over the ground state. Unfortunately, we were unable to reproduce the -2 factor starting with Eq. (67) of Ref. 4. Moreover, several arguments suggest that the result (68) of Ref. 4 for the retardation contribution appears dubious, to say the least. It is known, in particular, that the logarithmic divergence that appears in the order $m^2\alpha^6/M$ arises due to the relativistic corrections to the instant transverse exchange. The corresponding result of the present work is contained in (16) and agrees fully with the results of Refs. 5 and 12. At the same time, allowing for retardation leads only to a finite contribution [in accordance with (14)]. Judging by the result of Ref. 4, the retardation effect is a source not only of a logarithmic divergence but also of a linear divergence at small distances, while the relativistic correction to instant magnetic exchange contributes nothing to the given order.

As for the results of the numerical calculations of Ref. 11, the calculation error for the contribution of single magnetic exchange is greater[2)] than the discrepancy between the analytical results being discussed.

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[1)]For the sake of brevity we write the kernel of an operator instead of the operator proper.
[2)]V. M. Shabaev (private communication).

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