Order $\alpha^4(m/M)R_\infty$ corrections to hydrogen P levels

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(Submitted 4 October 1994)
Zh. Eksp. Teor. Fiz. **107**, 393–400 (February 1995)

Order of $\alpha^4(m/M)R_\infty$ corrections to hydrogen P levels have been found. They are predominantly relativistic. The calculation method is a straightforward generalization of the approach previously used by us to find the shift of positronium P levels. The numerical values of the corrections found to the Lamb shift in hydrogen are $\delta E(2P_{1/2})=0.55$ kHz and $\delta E(2P_{3/2})=0.44$ kHz.

1. INTRODUCTION

The high accuracy that has been achieved in measurements of the $2S_{1/2}-2P_{1/2}$ gap in hydrogen, as indicated by the values

1057845(9) kHz (Ref. 1),

1057851.4(1.9) kHz (Ref. 2),

calls for achievement of a corresponding accuracy in theoretical predictions. In particular, the correction for nuclear recoil of relative order $\alpha^4(m/M)R_\infty$ [$R_\infty=109737.3156827(48)$ cm^{-1} is the Rydberg constant] may turn out to be comparable to the experimental error.[2] In fact, in positronium the order α^4R_∞ corrections calculated in Refs. 3 and 4 for the $2S$ state and in Ref. 5 for the $2P$ state are equal to 1 MHz and 0.6 MHz, respectively. The corrections for hydrogen discussed in this paper should be approximately $8m/M$ times smaller. Here the factor of 8 reflects the dependence of the result for positronium on its reduced mass $m/2$, which appears to at least the third power in the shift. Thus, a correction of about 2–3 kHz might be expected in hydrogen.

The order $\alpha^4(m/M)R_\infty$ correction to the energy of the hydrogen $2S$ state was recently calculated in Ref. 6 and is equal to -0.92 kHz. As for the P states, the corresponding corrections can be found in a fairly simple manner by the approach that we developed to calculate the shift of positronium P levels.[5] This is the subject of the present paper.

Energy corrections containing m/M arise in two ways. Some effective perturbation operators contain the reciprocal mass explicitly. In the case of operators not containing the nuclear mass, it appears in the corresponding energy corrections due to the reduced-mass dependence of the nonrelativistic wave functions that we employed as a perturbation-theory basis set.

The bulk of the corrections are relativistic. Radiative corrections of the order under discussion appear for states with a nonzero orbital angular momentum only due to an anomalous electronic magnetic moment.[7,5] This was rigorously proved in Ref. 8.

2. CONTRIBUTIONS OF IRREDUCIBLE OPERATORS

2.1. Relativistic correction to the dispersion law

Let us begin with the kinematic correction to the energy appearing as a result of the averaging of the second correction to the nonrelativistic dispersion law for the electron

$$\sqrt{m^2+p^2}-m=\frac{p^2}{2m}-\frac{p^4}{8m^3}+\frac{p^6}{16m^5}+\dots, \quad (1)$$

$$V_{\rm kin}^{(1)}=\frac{p^6}{16m^5}. \quad (2)$$

Averaging over the nonrelativistic wave functions gives

$$E_{\rm kin}^{(1)}=-\frac{m^2}{M}\frac{\partial}{\partial\mu}\left\langle\frac{p^6}{16m^5}\right\rangle \quad (3)$$

$$=-\frac{\epsilon_n}{5}\left(8-\frac{17}{n^2}+\frac{75}{8n^3}\right). \quad (4)$$

Here

$$\mu=\frac{mM}{M+m}\approx m\left(1-\frac{m}{M}\right)$$

is the reduced mass, and

$$\varepsilon_n\equiv\frac{m^2\alpha^6}{Mn^3}.$$

The correction found differs from the corresponding result for positronium[5] only by an obvious scaling factor.

2.2. Relativistic corrections to the Coulomb interaction

The fourth-order correction in v/c to single Coulomb exchange is derived from the free-particle scattering amplitude and equals

$$V_C=-\frac{\alpha}{32m^4}\frac{4\pi}{q^2}\left\{\frac{5}{4}(p'^2-p^2)^2-3i(\sigma,\mathbf{p}'\mathbf{p})(p'^2+p^2)\right\}, \quad (5)$$

where

$$\mathbf{q}=\mathbf{p}'-\mathbf{p}.$$

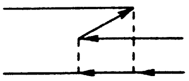

FIG. 1. Z-type diagram with double Coulomb exchange.

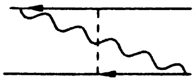

FIG. 2. Magnetic quantum crossed by a Coulomb quantum.

Here and below we omit the operators which are proportional to $\delta(\mathbf{r})$ in the coordinate representation, since their averages in the P state are equal to zero. As a result, for the energy correction we obtain

$$E_C^{(1)}=\epsilon_n\left\{\frac{5}{16}\left(1-\frac{2}{3n^2}\right)+\frac{3}{4}(\sigma\mathbf{l})\left(1-\frac{13}{12n^2}\right)\right\}. \tag{6}$$

The details of the calculations can be found in Ref. 5.

Now, as a result of the interaction the electron can undergo a transition to a state with a negative energy. This contribution is described by the Z-type diagram presented in Fig. 1. The corresponding perturbation operator,

$$V_{C-}=-\frac{(4\pi\alpha)^2}{8m^3}\int\frac{d^3k}{(2\pi)^3}\frac{\mathbf{k}(\mathbf{q}-\mathbf{k})}{k^2(\mathbf{q}-\mathbf{k})^2}, \tag{7}$$

gives the energy shift

$$E_{C-}^{(1)}=-\frac{\epsilon_n}{5}\left(1-\frac{2}{3n^2}\right). \tag{8}$$

2.3. Single magnetic exchange

In noncovariant perturbation theory the amplitude for scattering of an electron on a proton with single magnetic exchange has the form

$$A_M=-\frac{4\pi\alpha}{2q}j_i(\mathbf{p}',\mathbf{p})J_j(-\mathbf{p}',-\mathbf{p})\left(\frac{1}{E_n-q-p^2/2m}+\frac{1}{E_n-q-p'^2/2m}\right)\left(\delta_{ij}-\frac{q_iq_j}{q^2}\right). \tag{9}$$

In the dispersion law for the electron it is now sufficient to restrict ourselves to the leading nonrelativistic approximation. The proton current may be written with the required accuracy in the form

$$\mathbf{J}(-\mathbf{p}',-\mathbf{p})=-\frac{1}{2M}(\mathbf{p}'+\mathbf{p}). \tag{10}$$

Below we shall discuss the hyperfine interaction caused by the spin current of the proton

$$\mathbf{J}^s(-\mathbf{p}',-\mathbf{p})=-\frac{1}{2M}ig\sigma_p\mathbf{q}, \tag{11}$$

where $g=2.79$ is the proton magnetic moment.

The $(v/c)^2$ corrections in the expression for the electronic current must be retained:

$$\mathbf{j}(\mathbf{p}',\mathbf{p})=\frac{1}{2m}\{\mathbf{p}'+\mathbf{p}+i[\sigma\mathbf{q}]\}\left(1-\frac{p'^2+p^2}{4m^2}\right)-\frac{(p'^2-p^2)}{16m^3}i[\sigma\times(\mathbf{p}'+\mathbf{p})]. \tag{12}$$

They give the following contribution to the energy

$$E_{\text{curt}}^{(1)}=\left\langle\frac{\alpha}{4mM}\frac{4\pi}{q^2}\left\{\frac{(p'^2-p^2)^2}{4m^2}\frac{i(\sigma[\mathbf{qp}])}{q^2}+\frac{p'^2+p^2}{2m^2}\left(2\frac{[\mathbf{qp}]^2}{q^2}+i(\sigma,[\mathbf{qp}])\right)\right\}\right\rangle$$
$$=\epsilon_n\left\{\frac{7}{15}-\frac{31}{30n^2}+\frac{1}{2n^3}-\frac{\sigma\mathbf{l}}{4}\left(1-\frac{1}{n^2}\right)\right\}. \tag{13}$$

Let us now consider the retardation effect. As for the currents, we can restrict ourselves to the leading nonrelativistic approximation; the perturbation of the order of interest to us arises from the second term in the expansion of the energy factor in (9) in powers of $(E_n-p^2/2m)/q$:

$$E_{\text{ret}}^{(1)}=\left\langle-\frac{\alpha}{4mM}\frac{4\pi}{q^2}\frac{(E_n-p^2/2m)^2+(E_n-p'^2/2m)^2}{q^2}\times\left\{2\frac{[\mathbf{qp}]^2}{q^2}+i(\sigma[\mathbf{qp}])\right\}\right\rangle \tag{14}$$

$$=\epsilon_n\left\{\frac{2}{5}-\frac{1}{4n}+\frac{3}{20n^2}+\frac{\sigma\mathbf{l}}{30}\left(4-\frac{1}{n^2}\right)\right\}. \tag{15}$$

Owing to the finite character of the propagation time of a magnetic quantum, it can cross an arbitrary number of Coulomb quanta. A simple count of the powers of the momenta reveals that, apart from the contribution calculated above, it is sufficient for us to take into account diagrams with one or two Coulomb quanta (dashed lines) crossed by a magnetic quantum (wavy line). In the former case (Fig. 2) the perturbation operator is obtained as the product of the Pauli currents and the first term in the expansion in $(E_n-p^2/2m)/q$:

$$E_{MC}^{(1)}=\left\langle-(4\pi\alpha)^2\int\frac{d^3k}{(2\pi)^3}\frac{\delta_{ij}-\frac{k_ik_j}{k^2}}{2k(\mathbf{q}-\mathbf{k})^2}\left(J_i(\mathbf{p},\mathbf{p}+\mathbf{k})j_j(\mathbf{p}',\mathbf{p}'+\mathbf{k})\frac{2E_n-(\mathbf{p}'-\mathbf{k})^2/2m-p^2/2m}{k^3}+J_i(\mathbf{p}',\mathbf{p}'+\mathbf{k})j_j(\mathbf{p},\mathbf{p}+\mathbf{k})\frac{2E_n-(\mathbf{p}+\mathbf{k})^2/2m-p'^2/2m}{k^3}\right)\right\rangle \tag{16}$$

$$=\epsilon_n\left\{-\frac{13}{20}+\frac{1}{2n}-\frac{3}{20n^2}-\sigma\mathbf{l}\left(\frac{7}{60}+\frac{1}{30n^2}\right)\right\}. \tag{17}$$

In the latter case it is sufficient to take all the elements of the diagram (Fig. 3) in the leading nonrelativistic approximation:

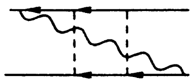

FIG. 3. Magnetic quantum crossed by two Coulomb quanta.

$$E^{(1)}_{\text{MCC}}=\Bigg\langle -(4\pi\alpha)^3\int\frac{d^3k}{(2\pi)^3}\int\frac{d^3k'}{(2\pi)^3}\times\frac{\delta_{ij}-k_ik_j/k^2}{2k^4(\mathbf{q}-\mathbf{k}')^2(\mathbf{k}'-\mathbf{k})^2}\{J_i(\mathbf{p},\mathbf{p}+\mathbf{k})j_j(\mathbf{p}',\mathbf{p}'+\mathbf{k})+J_i(\mathbf{p}',\mathbf{p}'+\mathbf{k})j_j(\mathbf{p},\mathbf{p}+\mathbf{k})\}\Bigg\rangle \tag{18}$$

$$=\frac{\epsilon_n}{4}\left\{\frac{5}{3}-\frac{1}{n}+\frac{\sigma\mathbf{l}}{3}\right\}. \tag{19}$$

One more contribution of order $\alpha^4(m/M)R_\infty$ to the energy arises from the Z-type diagrams with single magnetic exchange (see Fig. 4). In the leading nonrelativistic approximation it is not difficult to obtain

$$E^{(1)}_{M-}=\left\langle\frac{\alpha^2}{4mM}\int\frac{d^3k}{(2\pi)^3}\frac{(4\pi)^2}{k^2(\mathbf{q}-\mathbf{k})^2}i(\sigma[\mathbf{kp}])\right\rangle \tag{20}$$

$$=-\frac{\epsilon_n}{10}\left(1-\frac{2}{3n^2}\right)\sigma\mathbf{l}. \tag{21}$$

2.4. Double magnetic exchange

We should still examine irreducible diagrams with two magnetic quanta. A contribution of the required order to the energy arises only from diagrams of the type shown in Fig. 5. Their sum reduces to

$$E^{(1)}_{MM}=\Bigg\langle\frac{\alpha^2}{2m^2M}\int\frac{d^3k}{(2\pi)^3}\frac{(4\pi)^2}{k^2k'^2}\Bigg\{\mathbf{pp}'-2\frac{(\mathbf{kp})(\mathbf{kp}')}{k^2}+\frac{(\mathbf{kp})(\mathbf{kk}')(\mathbf{kp}')}{k^2k'^2}-\frac{\mathbf{kk}'}{2}+i\sigma\Bigg([\mathbf{k}'\mathbf{p}]-\frac{\mathbf{k}'\mathbf{k}(\mathbf{kp})}{k^2}\Bigg)\Bigg\}\Bigg\rangle \tag{22}$$

$$=\epsilon_n\left\{\frac{1}{3}\left(1-\frac{1}{n^2}\right)-\frac{\sigma\mathbf{l}}{10}\left(1-\frac{2}{3n^2}\right)\right\}, \tag{23}$$

where $\mathbf{k}'=\mathbf{q}-\mathbf{k}$.

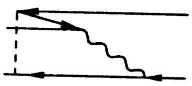

FIG. 4. Z-type diagram with single magnetic exchange.

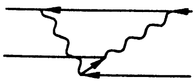

FIG. 5. Double magnetic exchange.

3. ITERATION OF THE BREIT HAMILTONIAN

The next class of order $\alpha^4(m/M)R_\infty$ corrections arises from iteration of the usual second-order Breit Hamiltonian V with respect to v/c.

Omitting the terms containing $\delta(\mathbf{r})$ and the proton spin, we write the Breit potential (Ref. 9, Sec. 84)

$$V=-\frac{p^4}{8m^3}+\frac{\alpha}{4m^2r^3}\sigma\mathbf{l}-\frac{\alpha}{2mMr}\left(p^2+\frac{1}{r^2}\mathbf{r}(\mathbf{rp})\mathbf{p}\right)+\frac{\alpha}{2mMr^3}\sigma\mathbf{l}, \tag{24}$$

in the form

$$V=m\alpha^4v, \tag{25}$$

$$v=a\left\{h,\frac{1}{r}\right\}+b[h,ip_r]+c\frac{1}{r^2}. \tag{26}$$

Here

$$a=-\frac{1}{2}+\frac{m}{M},\quad b=\frac{\sigma\mathbf{l}}{8}+\frac{m}{M}\left(\frac{1}{2}-\frac{\sigma\mathbf{l}}{8}\right),\quad c=-\frac{1}{2}+b; \tag{27}$$

$p_r=-i(\partial_r+1/r)$ is the radial momentum, and

$$h=\frac{p_r^2}{2}+\frac{1}{r^2}-\frac{1}{r}$$

is the unperturbed Hamiltonian for radial motion with $L=1$ in the Coulomb field.

Expression (26) makes it possible to find an energy correction without using the explicit form of the Coulomb Green's function. The details of the derivation as applied to positronium can be found in Ref. 5. The result for hydrogen has the form

$$\Delta E=\frac{m^2\alpha^6}{4\mu n^3}\left\{-\frac{3a^2+14ab+13b^2}{15}-\frac{2c(2c+9a+9b)}{27}-\frac{2c^2}{3n}+\frac{2}{3n^2}\left(\frac{11a^2+13ab+6b^2}{5}+4ac\right)-\frac{5a^2}{2n^3}\right\}. \tag{28}$$

Substituting the expressions for a, b, and c (27) and isolating the terms proportional to M^{-1}, we find

$$E^{(2)}=\varepsilon_n\left\{\frac{467}{480}+\frac{3}{16n}-\frac{347}{120n^2}+\frac{15}{8n^3}-\sigma\mathbf{l}\left(\frac{419}{960}+\frac{3}{32n}-\frac{53}{80n^2}\right)\right\}. \tag{29}$$

4. CORRECTIONS TO THE HYPERFINE INTERACTION

The complete relativistic expression for the hyperfine splitting of the levels of the hydrogen atom reduces to the average potential of the interaction of the relativistic electron with the nuclear magnetic moment for the Dirac wave functions in the Coulomb field:

$$\delta E_{hfs}(nlj;F)=\alpha\boldsymbol{\mu}\left\langle nlj\left|\frac{\mathbf{r}}{r^3}\times\boldsymbol{\alpha}\right|nlj\right\rangle, \qquad (30)$$

where $\boldsymbol{\mu}$ is the nuclear magnetic moment operator, which contains $1/M$, and $\boldsymbol{\alpha}$ denotes Dirac matrices. This expression can be obtained[10] from an analysis of Feynman diagrams in analogy with the derivation of the Dirac equation in a Coulomb field.

The radial part of average (30) is calculated most simply using virial relations (see, for example Ref. 11). The final result has the form

$$\delta E_{hfs}(nlj;F)=\frac{\boldsymbol{\mu}\mathbf{j}}{j(j+1)}\,[j(j+1)-l(l+1)+1/4]\alpha^2\,\frac{\partial E_{nj}}{\partial\kappa}\,\frac{E_{nj}-m/2\kappa}{j(j+1)-\alpha^2}, \qquad (31)$$

where E_{nj} is the energy of the bound state in the relativistic Coulomb problem and $\kappa=(l-j)(2j+1)$.

Of course, the relativistic correction to the hyperfine interaction under discussion can be found just like the contribution which is not dependent on the nuclear spin (see the preceding sections). Then the contributions due to retardation in the case of single magnetic exchange and to diagrams 2 and 3 cancel out one another, in agreement with the instantaneous nature of the interaction described by Eq. (30). The final result of the calculation (which is presented in the next section) coincides with the corresponding order of the α^2 expansion of the exact expression (31).

5. TRUE RADIATIVE CORRECTIONS

Even the true radiative corrections of order $\alpha^4 R_\infty(m/M)$ to the energy of the P levels can be represented in a simple form with practically no special calculations. As was postulated in Refs. 7 and 5 and rigorously proved in Ref. 8, all the true radiative corrections to levels with $l\neq 0$ reduce to the contribution of the anomalous electronic magnetic moment to single magnetic exchange and spin-orbit coupling.[1]

It can easily be shown that only the second-order correction to the electron magnetic moment, $-0.328\alpha^2/\pi^2$, influences the shift $\sim\alpha^4(m/M)R_\infty$ of the levels with $l\neq 0$. In particular, as in positronium, the contributions of the anomalous magnetic moment to the retardation also cancel out one another in diagram 2.

Thus, we arrive at the following expression for the radiative shift of the hydrogen nP levels:

$$E_{\rm rad}^{(1)}=\epsilon_n\,\frac{0.328}{\pi^2}\left\{\frac{1}{3}\,\boldsymbol{\sigma}\mathbf{l}+2.79\,\frac{(\boldsymbol{\sigma}\mathbf{l})(\mathbf{j}\boldsymbol{\sigma}_{\rm p})}{12j(j+1)}\right\}. \qquad (32)$$

6. RESULTS

The total correction to the hydrogen P levels without consideration of the nuclear spin is

$$\delta E(nP_j)=\epsilon_n\left\{\frac{217}{480}+\frac{3}{16n}-\frac{14}{15n^2}+\frac{1}{2n^3}-\boldsymbol{\sigma}\mathbf{l}\left(\frac{7}{192}+\frac{3}{32n}-\frac{1}{6n^2}-\frac{1}{3}\,\frac{0.328}{\pi^2}\right)\right\}. \qquad (33)$$

The numerical values of this correction for $n=2$ are

$$\delta E(2P_{1/2})=0.55\ \text{kHz},$$

$$\delta E(2P_{3/2})=0.44\ \text{kHz}.$$

They are somewhat smaller than the rough estimate given at the beginning of this paper.

The corrections to the hyperfine structure in states with a fixed total angular momentum F can be represented in an analogous form:

$$\delta E(nP_j;F)=\epsilon_n 2.79\,\frac{\mathbf{j}\boldsymbol{\sigma}_{\rm p}}{2j(j+1)}\left\{\frac{157}{270}+\frac{2}{3n}-\frac{7}{5n^2}-\boldsymbol{\sigma}\mathbf{l}\left(\frac{173}{540}+\frac{1}{6n}-\frac{2}{15n^2}-\frac{1}{6}\,\frac{0.328}{\pi^2}\right)\right\}. \qquad (34)$$

The numerical values of the contributions to the hyperfine splitting of the $2P_j$ levels equal

$$\Delta_{hf}(2P_{1/2})=6.12\ \text{kHz},$$

$$\Delta_{hf}(2P_{3/2})=0.38\ \text{kHz}.$$

We thank H. Grotch for supplying the results reported in Ref. 6 before publication. This research was partially financed by the "Universities of Russia" Program, grant No. 94-6.7-2053.

[1)]Unfortunately, the contribution of the anomalous magnetic moment to the spin-orbit coupling was omitted in Ref. 5. The corresponding correction to the positronium P levels is $-(0.328/\pi^2)(m\alpha^6/24n^3)$ **LS**, which gives 0.0032, 0.0016, and −0.0016 MHz for $j=0$, 1, and 2, respectively, and has practically no influence on the final numerical results.

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Translated by P. Shelnitz