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ORDER $\alpha^4(m/M)R_\infty$ CORRECTIONS TO HYDROGEN P LEVELS

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

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ABSTRACT

The order $\alpha^4(m/M)R_\infty$ shift of hydrogen P levels is found. The corrections are predominantly of relativistic origin. Our approach is a straightforward extension of that developed and applied by us previously to positronium P levels. The corrections to the Lamb shift in hydrogen constitute numerically $\delta E(2P_{1/2}) = 0.55$ kHz, $\delta E(2P_{3/2}) = 0.44$ kHz.

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1 Introduction

Measurements of the hydrogen Lamb shift have reached now high accuracy. Experimental values of Lamb shift for $n = 2$ are

1 057 845(9) kHz [1],
1 057 851.4(1.9) kHz [2].

The corresponding theoretical accuracy for the hydrogen Lamb shift would be obviously very useful. In particular, the recoil corrections of the relative order $\alpha^4(m/M)R_\infty$ ($R_\infty = 109\,737.315\,682\,7(48)$ cm^{-1} is the Rydberg constant) may well turn out comparable with the quoted experimental errors. Indeed, in positronium the order $\alpha^4 R_\infty$ corrections calculated in Refs.[3, 4] for the $2S$ state and in Ref.[5] for the $2P$ state reach 1 MHz and 0.6 MHz, respectively. The hydrogen correction addressed in the present paper should differ from those numbers roughly by a factor $8m/M$ where the coefficient 8 reflects the dependence of the positronium result on the reduced mass $m/2$ which enters the shift at least in the third power. In this way we come to the conclusion that the discussed corrections in hydrogen can well constitute few kHz.

The $\alpha^4(m/M)R_\infty$ correction to the hydrogen $2S$ states has been found recently[6], and constitutes -0.92 kHz. As to hydrogen P states, the calculation of their shift can be done easily within the approach developed and applied by us earlier to positronium P states [5]. This is the subject of the present paper.

Recoil corrections emerge from two sources. Some effective operators contain M^{-1} explicitly. When treating other perturbations, independent of M, order m/M corrections originate from the dependence on the reduced mass μ of nonrelativistic wave functions, entering the expectation values.

Major part of corrections is of relativistic nature. As for the true radiative corrections of the order discussed, for the states of nonvanishing orbital angular momentum they originate from the electron anomalous magnetic moment only, as it was assumed in Refs.[7, 4] and proven accurately in Ref.[8].

2 Contributions of irreducible operators

2.1 Relativistic correction to the dispersion law

Let us start with the kinematic correction, generated by the v^4/c^4 term in the dispersion law for the electron,

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

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

To calculate the corresponding expectation value is a simple problem in quantum mechanics. So,

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

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

Here

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

is the hydrogen reduced mass;

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

The result differs from that of Ref.[5] for positronium by a fairly obvious scaling factor.

2.2 Relativistic corrections to the Coulomb interaction

This perturbation operator, as extracted from the $(v/c)^4$ corrections to the Coulomb scattering amplitude for free particles, equals

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

We are neglecting systematically here and below effective operators proportional to $\delta(\vec{r})$ in the coordinate representation, their expectation values vanishing for P states. This energy correction is

$$E^{(1)}_C = \epsilon_n\left\{\frac{5}{16}\left(1-\frac{2}{3n^2}\right) + \frac{3}{4}(\vec{\sigma}\vec{l})\left(1-\frac{13}{12n^2}\right)\right\}. \quad (6)$$

Calculational details pertinent to the problem can be found in Ref.[5].

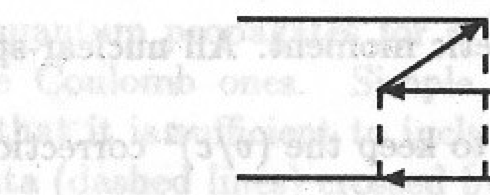

Fig. 1. Z-type double-Coulomb exchange.

Now, due to the Coulomb interaction electron can go over into a negative-energy intermediate state. The corresponding contributions are described by Z-diagram presented in Fig.1. The corresponding perturbation operator is

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

The energy correction generated in this way equals

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

2.3 Single magnetic exchange

In the noncovariant perturbation theory the electron-proton scattering amplitude due to the exchange by one magnetic quantum is

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

In the dispersion law for electron it is sufficient here to confine to the nonrelativistic approximation. The proton current to our accuracy reduces to

$$\vec{J}(-\vec{p}\,',-\vec{p}) = -\frac{1}{2M}(\vec{p}\,' + \vec{p}) \quad (10)$$

We omit at the moment the hyperfine contributions induced by the spin part of this current

$$\vec{J}^s(-\vec{p}\,',-\vec{p}) = -\frac{1}{2M} ig[\vec{\sigma}_p \times (\vec{p}\,' - \vec{p})],$$

where $g = 2.79$ is the proton magnetic moment. All nuclear-spin-dependent effects will be discussed below.

In the electron current we have to keep the $(v/c)^2$ corrections:

$$\begin{aligned} \vec{j}(\vec{p}\,',\vec{p}) &= \frac{1}{2m}\{\vec{p}\,' + \vec{p} + i[\vec{\sigma} \times (\vec{p}\,' - \vec{p})]\} \\ &\times \left(1 - \frac{p'^2 + p^2}{4m^2}\right) - \frac{(p'^2 - p^2)^2}{16m^3} i[\vec{\sigma} \times (\vec{p}\,' + \vec{p})]. \end{aligned} \quad (11)$$

They produce the following energy shift:

$$\begin{aligned} E^{(1)}_{curr} &= \left\langle \frac{\alpha}{4mM}\frac{4\pi}{q^2}\left\{\frac{(p'^2 - p^2)^2}{4m^2}\frac{i(\vec{\sigma},\vec{q}\times\vec{p})}{q^2} \right.\right. \\ &\left.\left. + \frac{p'^2 + p^2}{2m^2}\left(2\frac{(\vec{q}\times\vec{p})^2}{q^2} + i(\vec{\sigma},\vec{q}\times\vec{p})\right)\right\}\right\rangle, \quad (12) \\ &= \epsilon_n\left\{\frac{7}{15} - \frac{31}{30n^2} + \frac{1}{2n^3} - \frac{\vec{\sigma}\vec{l}}{4}\left(1 - \frac{1}{n^2}\right)\right\}. \end{aligned}$$

Let us consider now the retardation effect. To this end the currents can be taken in the leading approximation, while the perturbation of interest originates from the second-order term of the expansion of the factor $[E_n - p^2/2m - q]^{-1}$ in (2.3) in powers of $(E_n - p^2/2m)/q$,

$$E^{(1)}_{ret} = \left\langle -\frac{\alpha}{4mM}\frac{4\pi}{q^2}\frac{(E_n - p^2/2m)^2 + (E_n - p'^2/2m)^2}{q^2}\right.$$

$$\left.\times\left\{2\frac{(\vec{q}\times\vec{p})^2}{q^2} + i(\vec{\sigma},\vec{q}\times\vec{p})\right\}\right\rangle, \quad (13)$$

$$= \epsilon_n\left\{\frac{2}{5} - \frac{1}{4n} + \frac{3}{20n^2} + \frac{\vec{\sigma}\vec{l}}{30}\left(4 - \frac{1}{n^2}\right)\right\}. \quad (14)$$

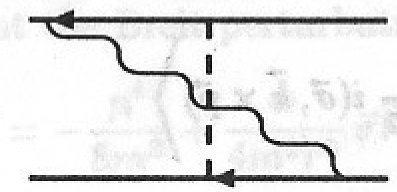

Fig.2. Single-magnetic-single-Coulomb exchange.

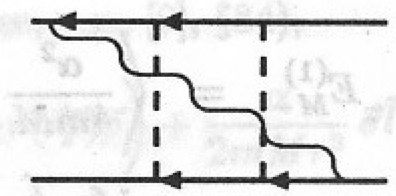

Fig.3. Single-magnetic-double-Coulomb exchange.

Magnetic quantum propagates for a finite time and can cross arbitrary number of the Coulomb ones. Simple counting of the momenta powers demonstrates that it is sufficient to include the diagrams with one and two Coulomb quanta (dashed lines) crossed by the magnetic photon (wavy line). In the first case, Fig.2, the perturbation operator arises as a product of the Pauli currents and the first-order term in the expansion in $(E_n - p^2/2m)/q$:

$$\begin{aligned} E^{(1)}_{MC} &= \left\langle -(4\pi\alpha)^2 \int \frac{d^3k}{(2\pi)^3}\frac{\delta_{ij} - \frac{k_i k_j}{k^2}}{2k(\vec{q} - \vec{k})^2} \right. \quad (15) \\ &\times \left(J_i(\vec{p},\vec{p} + \vec{k})\, j_j(\vec{p}\,',\vec{p}\,' + \vec{k})\,\frac{2E_n - (\vec{p}\,' - \vec{k})^2/2m - p^2/2m}{k^3} \right. \\ &\left.\left. + J_i(\vec{p}\,',\vec{p}\,' + \vec{k})\, j_j(\vec{p},\vec{p} + \vec{k})\,\frac{2E_n - (\vec{p} + \vec{k})^2/2m - p'^2/2m}{k^3}\right)\right\rangle, \\ &= \epsilon_n\left\{-\frac{13}{20} + \frac{1}{2n} - \frac{3}{20n^2} - \vec{\sigma}\vec{l}\left(\frac{7}{60} + \frac{1}{30n^2}\right)\right\} \quad (16) \end{aligned}$$

In the second case all the elements of diagram 3 should be taken to leading nonrelativistic approximation:

$$\begin{aligned} E^{(1)}_{MCC} &= \left\langle -(4\pi\alpha)^3 \int \frac{d^3k}{(2\pi)^3}\int \frac{d^3k'}{(2\pi)^3}\frac{\delta_{ij} - k_i k_j/k^2}{2k^4(\vec{q} - \vec{k}\,')^2(\vec{k}\,' - \vec{k})^2} \right. \quad (17) \\ &\left. \times\left\{J_i(\vec{p},\vec{p} + \vec{k})\, j_j(\vec{p}\,',\vec{p}\,' + \vec{k}) + J_i(\vec{p}\,',\vec{p}\,' + \vec{k})\, j_j(\vec{p},\vec{p} + \vec{k})\right\}\right\rangle, \end{aligned}$$

$$= \frac{\epsilon_n}{4}\left\{\frac{5}{3}-\frac{1}{n}+\frac{\vec{\sigma}\vec{l}}{3}\right\} \qquad (18)$$

One more energy correction of the $\alpha^4 R_\infty m/M$ order at the single magnetic exchange is due to the electron transitions to negative-energy intermediate states (see Fig.4). To leading approximation one gets easily

$$E^{(1)}_{M-} = \left\langle \frac{\alpha^2}{4mM}\int \frac{d^3k}{(2\pi)^3}\,\frac{(4\pi)^2}{k^2(\vec{q}-\vec{k})^2}\, i(\vec{\sigma},\vec{k}\times\vec{p})\right\rangle, \qquad (19)$$

$$= -\frac{\epsilon_n}{10}\left(1-\frac{2}{3n^2}\right)\vec{\sigma}\vec{l}. \qquad (20)$$

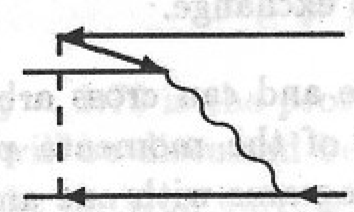

Fig.4. Z-type single-magnetic-single-Coulomb exchange.

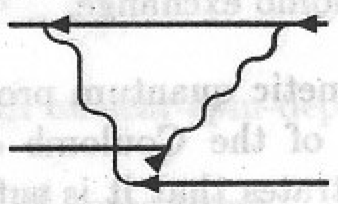

Fig.5. Double-magnetic exchange.

2.4 Double magnetic exchange

Let us consider now irreducible diagrams with two magnetic quanta. To our approximation they are confined to the type presented in Fig.5. Their sum reduces to

$$E^{(1)}_{MM} = \left\langle \frac{\alpha^2}{2m^2M}\int \frac{d^3k}{(2\pi)^3}\,\frac{(4\pi)^2}{k^2k'^2}\left\{\vec{p}\vec{p}\,'-2\frac{(\vec{k}\vec{p})(\vec{k}\vec{p}\,')}{k^2}+\frac{(\vec{k}\vec{p})(\vec{k}\vec{k}\,')(\vec{k}\vec{p}\,')}{k^2k'^2}\right.\right.$$

$$\left.\left. -\frac{\vec{k}\vec{k}\,'}{2}+i\vec{\sigma}\left(\vec{k}\,'\times\vec{p}-\frac{\vec{k}\,'\times\vec{k}\,(\vec{k}\vec{p})}{k^2}\right)\right\}\right\rangle, \qquad (21)$$

$$= \epsilon_n\left\{\frac{1}{3}\left(1-\frac{1}{n^2}\right)-\frac{\vec{\sigma}\vec{l}}{10}\left(1-\frac{2}{3n^2}\right)\right\}, \qquad (22)$$

Here $\vec{k}\,'=\vec{q}-\vec{k}$.

3 Corrections of second order in the Breit Hamiltonian

Next class of the order $\alpha^4 R_\infty$ corrections originates from the iteration of the usual Breit Hamiltonian V of second order in v/c.

Omitting again nuclear-spin-dependent terms and those with $\delta(\vec{r})$, we present the Breit perturbation for hydrogen (see, e.g., [9], §84),

$$V = -\frac{p^4}{8m^3}+\frac{\alpha}{4m^2r^3}\vec{\sigma}\vec{l}-\frac{\alpha}{2mMr}\left(p^2+\frac{1}{r^2}\vec{r}(\vec{r}\vec{p})\vec{p}\right)+\frac{\alpha}{2mMr^3}\vec{\sigma}\vec{l} \qquad (23)$$

as:

$$V = m\alpha^4 v, \qquad (24)$$

$$v = a\left\{h,\frac{1}{r}\right\}+b\,[h,ip_r]+c\,\frac{1}{r^2}. \qquad (25)$$

Here

$$a=-\frac{1}{2}+\frac{m}{M},\quad b=\frac{\vec{\sigma}\vec{l}}{8}+\frac{m}{M}\left(\frac{1}{2}-\frac{\vec{\sigma}\vec{l}}{8}\right),\quad c=-\frac{1}{2}+b; \qquad (26)$$

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

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

is the unperturbed hydrogen Hamiltonian for the radial motion with $L=1$, written in atomic units.

It is a simple quantum-mechanical exercise now to derive the second-order energy correction from perturbation (24). The details of derivation, as applied to positronium, are presented in Ref.[5]. In the hydrogen case the result reads

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

$$\left.-\frac{2c^2}{3n}+\frac{2}{3n^2}\left(\frac{11a^2+13ab+6b^2}{5}+4ac\right)-\frac{5a^2}{2n^3}\right\}. \qquad (27)$$

We substitute now into this expression values (26) for a, b, c and single out terms $\sim M^{-1}$ of interest to us. The result is

$$E^{(2)} = \epsilon_n\left\{\frac{467}{480}+\frac{3}{16n}-\frac{347}{120n^2}+\frac{15}{8n^3}-\vec{\sigma}\vec{l}\left(\frac{419}{960}+\frac{3}{32n}-\frac{53}{80n^2}\right)\right\}. \qquad (28)$$

4 Corrections to the hyperfine interaction

Let us discuss now the energy corrections induced by the magnetic interaction with the proton magnetic moment, i.e. relativistic corrections to the hyperfine interaction. The complete relativistic expression for the hyperfine level splitting in hydrogen reduces to the expectation value of the interaction between the relativistic electron and nuclear magnetic moment calculated with the Dirac wave functions:

$$\delta E_{hfs}(nlj;F) = \alpha\vec{\mu}\left\langle nlj\left|\frac{\vec{r}}{r^3}\times\vec{\alpha}\right|nlj\right\rangle \tag{29}$$

(here $\vec{\mu}$ is the nuclear magnetic moment operator, which is by itself $\sim 1/M$, $\vec{\alpha}$ are the Dirac α-matrices. This formula can be derived[10], practically in the same way as the Dirac equation itself, from the analysis of the Feynman diagrams.

The non-trivial, radial part of this expectation value can be conveniently calculated by means of a virial relation (see, e.g., Ref.[11]), and the final result reads

$$\delta E_{hfs}(nlj;F) = \frac{\vec{\mu}\cdot\vec{j}}{j(j+1)}\left[j(j+1) - l(l+1) + 1/4\right]\alpha^2\frac{\partial E_{nj}}{\partial\kappa}\,\frac{E_{nj}-m/2\kappa}{j(j+1)-\alpha^2} \tag{30}$$

Here E_{nl} is the eigenvalue of the Dirac Coulomb problem, $\kappa = (l-j)(2j+1)$.

Of course, the discussed relativistic correction to the hyperfine interaction can be derived also in the same way as that independent of nuclear spin (see the previous sections). In such an approach the contributions due to the retardation of the magnetic interaction and to diagrams 2 and 3 cancel out, which just corresponds to the instantaneous nature of the magnetic interaction implied by formula (29). The final result of this calculation (it is presented in the last section) coincides of course with the α^2-expansion of formula (30).

5 True radiative corrections

Even the true radiative corrections of the $\alpha^4 R_\infty m/M$ order to P-levels can be presented in a simple form practically without special calculation. It was suggested in Refs.[7, 5] and accurately proven in Ref.[8] that all true radiative corrections to levels of $l \neq 0$ are confined to the electron anomalous magnetic moment contributions to the single magnetic exchange and to the spin-orbit interaction[5].

It can be easily demonstrated that only the second-order correction to the electron anomalous magnetic moment, $-0.328\alpha^2/\pi^2$, contributes to the order $\alpha^4(m/M)R_\infty$ shifts of hydrogen levels with $l \neq 0$. In particular, as well as in positronium, the anomalous magnetic moment contributions to the first-order retardation effect and to diagram 2 cancel.

In this way we come to the following expression for the radiative shift of hydrogen nP levels

$$E^{(1)}_{rad} = \epsilon_n\,\frac{0.328}{\pi^2}\left\{\frac{1}{3}\vec{\sigma}\vec{l} + 2.79\,\frac{(\vec{\sigma}\vec{l})(\vec{j}\vec{\sigma}_p)}{12j(j+1)}\right\}. \tag{31}$$

6 Results

The total correction to hydrogen P-levels independent of nuclear spin is

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

Its numerical values at $n = 2$ constitute

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

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

They are somewhat smaller than our crude estimates outlined in Introduction.

The hyperfine corrections at given total atomic angular momentum F can be presented in an analogous form:

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[5] Unfortunately, in the paper[5] on positronium by three of us, the contribution of the electron anomalous magnetic moment to the spin-orbit interaction was lost. This correction to positronium P-levels equals

$$-\frac{0.328}{\pi^2}\frac{m\alpha^6}{24n^3}\vec{L}\vec{S}.$$

It constitutes 0.0032, 0.0016 and –0.0016 MHz at j=0, 1 and 2 respectively, which is too small to influence the overall numerical results.

$$\delta E(nP_j;F) = \epsilon_n 2.79 \frac{\vec{j}\vec{\sigma}_p}{2j(j+1)} \left\{ \frac{157}{270} + \frac{2}{3n} - \frac{7}{5n^2} - \vec{\sigma}\vec{l} \left(\frac{173}{540} + \frac{1}{6n} - \frac{2}{15n^2} - \frac{1}{6}\frac{0.328}{\pi^2} \right) \right\}. \quad (33)$$

Numerically these contributions to the hyperfine splitting of $2P_j$-levels constitute

$$\Delta_{hf}(2P_{1/2}) = 6.12\,\text{kHz},$$
$$\Delta_{hf}(2P_{3/2}) = 0.38\,\text{kHz}.$$

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Поправки порядка $\alpha^4(m/M)R_\infty$ к P-уровням водорода

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