LAMB SHIFT OF THE LEVELS OF INNER ELECTRONS IN HEAVY ATOMS

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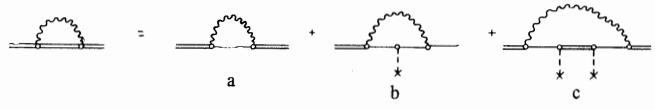
The self-energy of an inner electron in a heavy atom is calculated by expanding the electron propagator in a series in powers of the potential of the nucleus. The terms containing the first and second powers of the potential are isolated; the remainder is calculated with the aid of a variational principle. Calculation of the electron's self-energy in the $1s_{1/2}$ state in an atom with $Z = 137$ is carried out, taking into account the finite size R of the nucleus. The principal terms of order $\alpha \ln^2 R$ are calculated.

1. In article[1] a method of calculating the radiative corrections for inner electrons in heavy atoms was formulated in general terms. The basic goal of the present article is a detailed development of this method and as an example—the execution of the actual calculation for a specific atom. The calculation, however, is not carried out for a real atom but for a hypothetical atom with nuclear charge $Z = 137$. The main reason for such a choice is the fact that for $Z = 137$ the calculations simplify considerably, and they can be carried to completion without the application of numerical methods. This makes it possible to analyze the importance of taking into account individual terms in the expression for the total level shift. Such a calculation is not just of methodological interest. The question of the structure of superheavy atoms has recently been discussed in the literature.[2,3] The radiative corrections in such atoms may turn out to have an appreciable effect on the calculated position of the levels.

Here it is necessary to make an important reservation. In the calculation we have used the Dirac wave functions obtained for a point nucleus. Such functions are singular at the origin, and some of the integrals which appear in the expression for the level shift diverge. In such cases we have carried the integration down to a distance of the order of the nuclear radius $R \approx 0.7 \times 10^{-12}$ cm.[3] This distance is still approximately 100 times smaller than the radius of the first Bohr orbit in an atom with $Z = 137$; therefore in the absence of divergences the correction due to finite size of the nucleus should be of the order of 10^{-2}. However, in divergent integrals the singularities are rather strong, which leads to the appearance of terms of order $\alpha \ln^2 R$ (α is the fine structure constant) in the expression for the shift. The question arises as to whether this result changes if more accurate wave functions, constructed for a finite nucleus, are used. For this reason we compared the values of the Coulomb and more precise wave functions at distances of the order of R. For example, the upper component of the Coulomb function for the $1s_{1/2}$ level associated with $Z = 137$ has the form[1)] $g(r) = 2r^{-1}e^{-r}$ (in units $\hbar = c = 1$), and according to the work of Popov[3] the corrected function is given by $g(r) = r^{-1}K(\sqrt{8r})$ where K is Macdonald's function. For $r = 10^{-2}$, in the first case one obtains $rg(r) \approx 2$, and in the second case $rg(r) \approx 1.4$. Thus, one does not expect substantial differences to occur.



In the calculation we shall follow the general scheme set forth in the article[1]. In fact the whole problem reduces to a calculation of the electron's self-energy. The total level shift breaks up into three terms corresponding to an expansion of the self-energy diagrams in powers of the external potential (see the accompanying figure). In the figure a double line depicts an electron in the Coulomb field of the nucleus, a simple solid line represents a free electron, a wavy line represents a photon, and a dashed line represents an interaction with the nucleus. We shall not take vacuum polarization into account in this article; it gives a contribution which is formally of the same order of smallness in α as the electron's self-energy. Actually the contribution of this diagram is considerably smaller—not more than 10% of the magnitude of the self-energy, judging from the results of the calculations[4] for the mercury atom ($Z = 80$). We emphasize that our calculations are of an approximate nature. In the first place this is due to the fact that the radius of the nucleus with $Z = 137$ is not exactly known. Further, in calculating the contribution from diagram b (see the figure) we restricted our attention to taking account of only the leading terms of order $\alpha \ln^2 R \sim 1/10$. Finally, the contribution of diagram c was also not calculated exactly, but was estimated with the aid of a variational principle.

2. Let us begin with the calculation of the contribution from diagram a. According to the formula given in[1], this contribution is given by[2)]

$$\Delta E_a = i \int \bar{\psi}_0(\mathbf{p}) \Sigma_R(\mathbf{p}, E_0) \psi_0(\mathbf{p})\, d\mathbf{p}, \tag{1}$$

where $\psi_0(\mathbf{p})$ is the electron's wave function in the

[1)]We consider α to be a rational fraction, i.e., $\alpha = 1/137$. In fact $\alpha = 1/137.037$, i.e., the error is less than 10^{-2}.

[2)]It is not correct that the numerical coefficient in front of the integral in formula (27) in [1] should be the same as in formula (29) for the vertex part. See the present article for the correct coefficients.

momentum representation, E_0 is the energy level, and Σ_R is the regularized self-energy part. Let us substitute the expression for Σ_R taken from[5] into Eq. (1). We note here that the expressions for Σ_R cited in the monographs[6,7] are incorrect. In connection with this, see article[8]. The corrected expression for Σ_R given in[8] agrees with the result available in[5]. In our notation, which is identical to the notation used in the monograph[6], this expression has the form (everywhere we use units such that $\hbar = c = 1$):

$$\Sigma_R(p) = -\frac{\alpha}{4\pi}\hat{p}\frac{p^2-m^2}{p^2}\left\{\frac{p^2+m^2}{p^2}\ln\frac{p^2+m^2}{m^2}-1\right\}$$
$$+\frac{\alpha}{4\pi}im\left\{\frac{4(p^2+m^2)}{p^2}\ln\frac{p^2+m^2}{m^2}-2\right\}+\frac{\alpha i}{2\pi}(i\hat{p}+m)\ln\frac{\lambda^2}{m^2}, \quad (2)$$

where $p \equiv (\mathbf{p}, iE_0)$, m is the electron mass, and λ is the fictitious mass of the photon. The last term in formula (2) contains the infrared divergence which appears as a result of renormalization. As shown in[1], this divergence is cancelled by an analogous divergence in diagram b, so that in what follows one can omit the last term in (2). Substituting (2) into (1) and changing to three-dimensional notation, we obtain (also assuming m = 1)

$$\Delta E_a = -\frac{\alpha}{4\pi}\int \psi_0^+(\mathbf{p})\left\{(\alpha\mathbf{p}-E_0)\frac{\mathbf{p}^2-E_0^2-1}{\mathbf{p}^2-E_0^2}\cdot\right.$$
$$\times\left[\frac{\mathbf{p}^2-E_0^2+1}{\mathbf{p}^2-E_0^2}\ln(\mathbf{p}^2-E_0^2+1)-1\right]$$
$$\left.+2\beta\left[\frac{2(\mathbf{p}^2-E_0^2+1)}{\mathbf{p}^2-E_0^2}\ln(\mathbf{p}^2-E_0^2+1)-1\right]\right\}\psi_0(\mathbf{p})\,d\mathbf{p}, \quad (3)$$

where α and β are the Dirac matrices.

Now let us write down expressions for $\psi_0(\mathbf{p})$ and E_0. According to the Sommerfeld formula, for the $1s_{1/2}$ state we obtain

$$E_0 = \sqrt{1-(Z\alpha)^2}, \quad (4)$$

i.e., for Z = 137 it turns out that $E_0 = 0$. Formula (4) is no longer applicable for $Z > 137$, but for Z = 137 the deviations from (4) should be of the order of 10^{-2} (see the discussion in Sec. 1). In the coordinate representation, the wave function of the $1s_{1/2}$ state has the form[9]

$$\psi_0(r) = \begin{pmatrix} g(r)\,Y_{00}(\Omega) \\ 0 \\ -\frac{i}{\sqrt{3}}f(r)\,Y_{10}(\Omega) \\ i\sqrt{\frac{2}{3}}f(r)\,Y_{11}(\Omega) \end{pmatrix}, \quad (5)$$

for Z = 137

$$g(r) = -f(r) = \frac{2}{r}e^{-r}. \quad (6)$$

We shall use Rubinowicz's article[10] in order to change to the momentum representation. According to[10],

$$\psi_0(\mathbf{p}) = \begin{pmatrix} v(\varkappa)\,Y_{00}(\Omega) \\ 0 \\ \sqrt{1/3}\,u(\varkappa)\,Y_{10}(\Omega) \\ \sqrt{2/3}\,u(\varkappa)\,Y_{11}(\Omega) \end{pmatrix}, \quad (7)$$

$$v(\varkappa) = -\frac{1}{2}\sqrt{\frac{1+\gamma}{2\Gamma(2\gamma+1)}}G(0, 2\gamma+1, \gamma-1, 0; \varkappa), \quad (8)$$

$$u(\varkappa) = -\frac{1}{2}\sqrt{\frac{1-\gamma}{2\Gamma(2\gamma+1)}}G(0, 2\gamma+1, \gamma-1, 1; \varkappa), \quad (9)$$

$$G(\nu, \beta, \delta, l; \varkappa) = \frac{1}{\sqrt{\varkappa}}\int_0^\infty e^{-\rho/2}\rho^{\delta+3/2}F(-\nu, \beta; \rho)\,J_{l+1/2}\left(\frac{\rho\varkappa}{2}\right)d\rho, \quad (10)$$

$$\gamma = \sqrt{1-(\alpha Z)^2}, \quad (11)$$

where $F(-\nu, \beta; \rho)$ denotes the degenerate hypergeometric function, $J_{l+1/2}$ is the Bessel function, $\Gamma(2\gamma+1)$ is the Gamma function, and $\varkappa \equiv |\mathbf{p}|$. In[10] a representation is obtained for the function G in terms of a hypergeometric function of complex argument; this representation, however, is not applicable for Z = 137 since it contains $\Gamma(\gamma)$ and $\gamma = 0$ according to Eq. (11). Expressions (8) and (9) nevertheless remain finite even for Z = 137. A direct calculation of the integral (10) gives[11]

$$G(0, 1, -1, 0; \varkappa) = \frac{1}{\sqrt{\pi}}\frac{1}{1+\varkappa^2}, \quad (12)$$

$$G(0, 1, -1, 1; \varkappa) = \frac{\Gamma(3)}{\Gamma(5/2)}\frac{\varkappa}{1+\varkappa^2}F\left(\frac{1}{2}, 1, \frac{5}{2}; -\varkappa^2\right), \quad (13)$$

where F denotes the hypergeometric function. One can simplify expression (13) by a series of transformations (see[11]) and finally we obtain

$$v(\varkappa) = \sqrt{\frac{2}{\pi}}\frac{1}{1+\varkappa^2}, \quad (14)$$

$$u(\varkappa) = \sqrt{\frac{2}{\pi}}\frac{1}{\varkappa}\left\{\frac{\operatorname{arc\,tg}\varkappa}{\varkappa}-\frac{1}{1+\varkappa^2}\right\}. \quad (15)$$

Substituting (7) into (3) and performing a simple integration over angles, for Z = 137 we obtain

$$\Delta E_a = \frac{\alpha}{\pi}\int_0^\infty \varkappa^2\,d\varkappa\left\{(v^2(\varkappa)-u^2(\varkappa))\left[1-2\frac{\varkappa^2+1}{\varkappa^2}\ln(\varkappa^2+1)\right]\right.$$
$$\left.-\frac{4}{3}\varkappa v(\varkappa)u(\varkappa)\frac{\varkappa^2-1}{\varkappa^2}\left(\frac{\varkappa^2+1}{\varkappa^2}\ln(\varkappa^2+1)-1\right)\right\}. \quad (16)$$

Certain terms in the integral (16) give divergences at the upper limit. In such cases we integrate up to the value K = 1/R. Now let us present the final result, which is obtained after substitution of (14) and (15) into (16) and evaluation of the integrals:

$$\Delta E_a = \frac{\alpha}{3\pi}\left\{1-4\ln 2+2\ln K+\frac{4}{\pi}\int_0^\infty\frac{dp}{p^2}\operatorname{arc\,tg}^2 p\ln(1+p^2)\right.$$
$$\left.-\frac{4}{\pi}\int_0^K\frac{dp}{p}\operatorname{arc\,tg} p\ln(1+p^2)\right\}. \quad (17)$$

It is not difficult to see that as $K \to \infty$ the last integral in (17) diverges like $\ln^2 K$.

3. Now let us consider the contribution from diagram b. According to[1], this contribution is given by the formula

$$\Delta E_b = -\frac{\alpha Z}{2\pi^2}\int \psi_0^+(\mathbf{p})\gamma_4\Lambda_4(\mathbf{p}E_0; \mathbf{q}E_0)\frac{1}{(\mathbf{p}-\mathbf{q})^2}\psi_0(\mathbf{q})\,d\mathbf{p}\,d\mathbf{q}, \quad (18)$$

where Λ_4 is the component of the regularized vertex part. Let us borrow the expression for Λ_4 from[5]. In our notation

$$\gamma_4\Lambda_4 = \frac{\alpha}{4\pi}\left\{2\int_0^1 dx\ln\left|\frac{m^2}{m^2+x(1-x)(\mathbf{p}-\mathbf{q})^2}\right| - \frac{11}{2} - 2\ln\frac{\lambda^2}{m^2}\right.$$

$$+\int_0^1 dx\int_0^{1-x} dy\,\frac{2\gamma_4 A_4+4i\gamma_4\hat{Q}Q_4-2\gamma_4 R_4}{Z(\mathbf{p},\mathbf{q},x,y)}-2\int_0^1 dx\int_0^{1-x} dy\ln\left|\frac{(x+y)m^2}{Z(\mathbf{p},\mathbf{q},x,y)}\right|\Big\} \tag{19}$$

$$\gamma_4 A_4=(i\hat{q}-m)\,i\hat{p}-\gamma_4(i\hat{p}+m)(i\hat{q}-m)\,\gamma_4-\gamma_4(i\hat{p}+m)\,\gamma_4(i\hat{q}+2m), \tag{20}$$

$$\gamma_4 R_4=-\gamma_4\hat{Q}\,(\hat{p}-\hat{q})\,\gamma_4+(\hat{p}-\hat{q})\,\hat{Q}-i\gamma_4(i\hat{p}+2m)\,\gamma_4\hat{Q}-i\gamma_4\hat{Q}\gamma_4(i\hat{q}+2m), \tag{21}$$

$$\hat{Q}=x\hat{q}+y\hat{p}, \tag{22}$$

$$Z(\mathbf{p},\mathbf{q},x,y)=-(1-x-y)yp^2-(1-x-y)xq^2-xy(\mathbf{p}-\mathbf{q})^2 -m^2(x+y)-(1-x-y)\lambda^2, \tag{23}$$

where as before $p\equiv(\mathbf{p}, iE_0)$ and λ is the fictitious photon mass. The presence of λ in the expression for $Z(\mathbf{p},\mathbf{q},x,y)$ corresponds to the fact that the vertex part in general may contain infrared divergences even before regularization. However, such divergences will appear only in that case when the electron states corresponding to the ends of the diagram b are free. Therefore, in our case we may set $\lambda=0$ in the expression for $Z(\mathbf{p},\mathbf{q},x,y)$. After this in (19) there remains only the dependence on $\ln(\lambda^2/m^2)$ which arises as a result of regularization. This divergence is cancelled by the corresponding term in (2).

Now let us go over to the three-dimensional notation, and let us transform the numerator of the second integral in (19). The transformations lead to the following result (m = 1):

$$\begin{aligned}2\gamma_4 A_4+4i\gamma_4\hat{Q}Q_4-2\gamma_4 R_4&=2\mathbf{qp}(x+y-1)+2i\alpha[\mathbf{qp}](x+y+1)\\&+2E_0\boldsymbol{\alpha}\mathbf{p}[3-x-3y+2y(x+y)]\\&+2E_0\boldsymbol{\alpha}\mathbf{q}[-1-3x-y+2x(x+y)]+8\beta E_0(1-x-y)\\&+2\mathbf{p}^2y+2\mathbf{q}^2x-2-2E_0^2[1-2(x+y)+2(x+y)^2],\end{aligned} \tag{24}$$

where α and β are the Dirac matrices. With the aid of (19) and (24) it is convenient to represent the entire expression (18) in the form (for Z = 137, i.e., for E_0 = 0)

$$\Delta E_b=\frac{\alpha(Z\alpha)}{(2\pi)^3}\sum_{k=0}^{4} I_k, \tag{25}$$

$$I_0=-\frac{11}{2}\int\psi_0^+(\mathbf{p})\frac{1}{(\mathbf{p}-\mathbf{q})^2}\psi_0(\mathbf{q})\,d\mathbf{p}\,d\mathbf{q}, \tag{26}$$

$$I_1=-2\int_0^1 dx\int\psi_0^+(\mathbf{p})\frac{\ln|1+x(1-x)(\mathbf{p}-\mathbf{q})^2|}{(\mathbf{p}-\mathbf{q})^2}\psi_0(\mathbf{q})\,d\mathbf{p}\,d\mathbf{q}. \tag{27}$$

$$I_2=2i\int_0^1 dx\int_0^{1-x} dy\int\psi_0^+(\mathbf{p})\frac{(x+y+1)\alpha[\mathbf{qp}]}{Z(\mathbf{p},\mathbf{q},x,y)(\mathbf{p}-\mathbf{q})^2}\psi_0(\mathbf{q})\,d\mathbf{p}\,d\mathbf{q}, \tag{28}$$

$$I_3=2\int_0^1 dx\int_0^{1-x} dy\int\psi_0^+(\mathbf{p})\frac{\mathbf{p}^2y+\mathbf{q}^2x-2}{Z(\mathbf{p},\mathbf{q},x,y)(\mathbf{p}-\mathbf{q})^2}\psi_0(\mathbf{q})\,d\mathbf{p}\,d\mathbf{q}, \tag{29}$$

$$I_4=-2\int_0^1 dx\int_0^{1-x} dy\int\psi_0^+(\mathbf{p})\frac{1}{(\mathbf{p}-\mathbf{q})^2}\ln\left|\frac{x+y}{Z(\mathbf{p},\mathbf{q},x,y)}\right|\psi_0(\mathbf{q})\,d\mathbf{p}\,d\mathbf{q}. \tag{30}$$

Now let us carry out the angular integrations in Eqs. (26)—(30). We shall indicate how this is done for the example of I_0. Substituting (7) into (26) we obtain

$$\begin{aligned}I_0=\int d\mathbf{p}\,d\mathbf{q}\{&v(\varkappa_p)v(\varkappa_q)Y_{00}^*(\Omega_p)Y_{00}(\Omega_q)+{}^1/_3u(\varkappa_p)u(\varkappa_q)Y_{10}^*(\Omega_p)Y_{10}(\Omega_q)\\&+{}^2/_3u(\varkappa_p)u(\varkappa_q)Y_{11}^*(\Omega_p)Y_{11}(\Omega_q)\}f_0(\varkappa_p,\varkappa_q,\cos\gamma_{pq}),\end{aligned} \tag{31}$$

where $\varkappa_p\equiv|\mathbf{p}|$, $\varkappa_q\equiv|\mathbf{q}|$, and $\cos\gamma_{pq}=\cos(\widehat{\mathbf{p},\mathbf{q}})$. Since it is not necessary for us to use the four-momenta p and q any more, for convenience in what follows we shall use the notation $|\mathbf{p}|\equiv p$ and $|\mathbf{q}|\equiv q$. The function f_0 has the form

$$f_0(p,q,\cos\gamma_{pq})=-\frac{11}{2}\frac{1}{p^2+q^2-2pq\cos\gamma_{pq}}. \tag{32}$$

Let us expand f_0 in terms of spherical harmonics:

$$f_0(p,q,\cos\gamma_{pq})=\sum_{lm}a_l^{(0)}(p,q)\,Y_{lm}^*(\Omega_p)\,Y_{lm}(\Omega_q). \tag{33}$$

The coefficients in this expansion are determined by the formula

$$a_l^{(0)}=2\pi\int_{-1}^{1}P_l(z)f_0(p,q,z)\,dz, \tag{34}$$

where $P_l(z)$ is the Legendre polynomial. Substituting the expansion (33) into (31) and integrating over angles we obtain

$$I_0=\int_0^\infty p^2\,dp\int_0^\infty q^2\,dq\,\{v(p)v(q)a_0^{(0)}(p,q)+u(p)u(q)a_1^{(0)}(p,q)\}. \tag{35}$$

Calculation of the coefficients according to formula (34) gives

$$a_0^{(0)}(p,q)=-\frac{11}{2}\frac{\pi}{pq}\ln\frac{(p+q)^2}{(p-q)^2}, \tag{36}$$

$$a_1^{(0)}(p,q)=-\frac{11}{2}\frac{\pi}{pq}\left[\frac{p^2+q^2}{2pq}\ln\frac{(p+q)^2}{(p-q)^2}-2\right]. \tag{37}$$

Integration over the angles in I_2 leads to the result $I_2=0$. For I_1, I_3, and I_4 we obtain (k = 1, 3, 4)

$$I_k=\int_0^\infty p^2\,dp\int_0^\infty q^2\,dq\,\{v(p)v(q)a_0^{(k)}(p,q)+u(p)u(q)a_1^{(k)}(p,q)\}\equiv I_k^0+I_k^1, \tag{38}$$

$$a_l^{(1)}=-4\pi\int_0^1 dx\int_{-1}^1 dz\frac{P_l(z)}{p^2+q^2-2pqz}\ln|1+x(1-x)(p^2+q^2-2pqz)|, \tag{39}$$

$$a_l^{(3)}=2\pi\int_0^1 dx\int_0^{1-x} dy\int_{-1}^1 dz\frac{P_l(z)}{p^2+q^2-2pqz} \times\frac{2pqz(x+y-1)+2p^2y+2q^2x-2}{2xypqz-(1-y)yp^2-(1-x)xq^2-(x+y)}, \tag{40}$$

$$a_l^{(4)}=-4\pi\int_0^1 dx\int_0^{1-x} dy\int_{-1}^1 dz\frac{P_l(z)}{p^2+q^2-2pqz} \times\ln\left|\frac{x+y}{2xypqz-(1-y)yp^2-(1-x)xq^2-(x+y)}\right|. \tag{41}$$

Of the integrals written down, only I_0 is calculated to the very end; the remaining integrals are still too complicated. Therefore we shall be occupied with the selection of the terms which diverge as $p, q\to\infty$, and we confine our attention to the leading terms of order $\ln^2 K$. One can immediately verify that I_0 does not contain any such terms; therefore we immediately go on to I_1. First let us analyze I_1^0. By virtue of the symmetric nature of the integrand in (38) with respect to p and q, we shall integrate over the region $(0\le p\le\infty,\ 0\le q\le p)$, having multiplied the entire integral by 2. Introducing the variable $\xi=q/p$ we obtain

$$I_1^0=-16\int_0^K\frac{p^3\,dp}{1+p^2}\int_0^1\frac{\xi^2\,d\xi}{1+p^2\xi^2}\int_0^1 dx\int_{-1}^1 dz\frac{\ln|1+p^2(1-x)x(1+\xi^2-2\xi z|}{1+\xi^2-2\xi z}. \tag{42}$$

Since the region of large values of p introduces the major contribution to the integral (42), we replace the integrand in (42) by its asymptotic form as $p\to\infty$.

Then we obtain the major term in I_1^0 in the form

$$I_1^0 \approx -16\int_0^K \frac{p\ln p^2}{1+p^2}dp\int_0^1 d\xi\int_0^1 dx\int_{-1}^1 \frac{dz}{1+\xi^2-2\xi z} \approx -4\pi^2\ln^2 K. \quad (43)$$

The remaining integrals are analyzed in exactly the same fashion. Now let us present the final results:

$$I_1 \approx -8\pi^2\ln^2 K, \quad (44)$$

$$I_4 \approx 4\pi^2\ln^2 K. \quad (45)$$

The integral I_3 does not contain any terms of order $\ln^2 K$. Thus

$$\Delta E_b = \frac{\alpha}{2\pi}\ln^2 K. \quad (46)$$

4. Now let us go on to the last part of the calculation, that is, to diagram c. We estimate the contribution corresponding to this diagram with the aid of the variational principle proposed in[1]. According to[1],

$$\Delta E_c = \Delta E_c' - \Delta E_c''$$
$$\Delta E_c' = \frac{\alpha(Z\alpha)^2}{\pi(4\pi)^2 i}\int_{-\infty}^{\infty} d\omega\cdot \quad (47)$$

$$\times\sum_n \frac{\langle\psi_0^{(1)+}(\mathbf{r}_4)\psi_n^{(2)+}(\mathbf{r}_3)U^{(12)}(\mathbf{r}_1,\ldots,\mathbf{r}_4;\omega)\psi_n^{(1)}(\mathbf{r}_2)\psi_0^{(2)}(\mathbf{r}_4)\rangle}{E_n(1-i0)+\omega}, \quad (48)$$

$$U^{(12)}(\mathbf{r}_1,\ldots,\mathbf{r}_4;\omega) = U^{(1)}(\mathbf{r}_3,\mathbf{r}_4;\omega)U^{(2)}(\mathbf{r}_1,\mathbf{r}_2;\omega)v(\mathbf{r}_1,\mathbf{r}_4;\omega), \quad (49)$$

$$U^{(1)}(\mathbf{r}_3,\mathbf{r}_4;\omega) = \frac{1}{r_3}[(\alpha^{(1)}\mathbf{p}_3)+\beta^{(1)}m+\omega]\frac{1}{r_{34}}e^{i\sqrt{\omega^2-m^2}\,r_{34}}, \quad (50)$$

$$U^{(2)}(\mathbf{r}_1,\mathbf{r}_2;\omega) = \frac{1}{r_2}[(\alpha^{(2)}\mathbf{p}_2)+\beta^{(2)}m+\omega]\frac{1}{r_{12}}e^{i\sqrt{\omega^2-m^2}\,r_{12}}, \quad (51)$$

$$v(\mathbf{r}_1,\mathbf{r}_4;\omega) = \frac{1}{r_{14}}e^{i|\varepsilon_0-\omega|r_{14}}, \quad (52)$$

where $r_{ik} = |\mathbf{r}_i - \mathbf{r}_k|$ and $\mathbf{p}_i = -\nabla_i$. The expression for $\Delta E_c''$ differs from $\Delta E_c'$ by the replacement of $U^{(1)}$ by $\alpha^{(1)}U^{(1)}$ and $U^{(2)}$ by $\alpha^{(2)}U^{(2)}$. The upper indices on the matrices and functions indicate which matrices operate on different functions. The summation in (48) is carried out over the entire spectrum of the Dirac equation for an electron in the field of the nucleus.

As is shown in[1], the expression standing in (48) under the sign of the integral over ω turns into the following matrix element:

$$J(\omega) \equiv \left\langle \psi_0^+(4)U(24;\omega)\frac{1}{H(2)(1-i0)+\omega}U(12;\omega)v(14;\omega)\psi_0(1)\right\rangle, \quad (53)$$

where H is the Dirac operator for the electron in the field of the nucleus. The following variational principle is written down for this matrix element in[1]:

$$I[\psi_1,\psi_2] = \langle\psi_0^+(4)U(24;\omega)\psi_1(124)\rangle + \langle\psi_2(124)U(12;\omega)v(14;\omega)\psi_0(1)\rangle - \langle\psi_2(124)[H(2)(1-i0)+\omega]\psi_1(124)\rangle = \text{extr}, \quad (54)$$

where ψ_1 and ψ_2 are trial functions. The extremal value of the functional (54) coincides with $J(\omega)$, and the equations for the extrema have the form

$$[H(2)(1-i0)+\omega]\psi_1(124) = U(12;\omega)v(14;\omega)\psi_0(1), \quad (55)$$

$$[H(2)(1-i0)+\omega]\psi_2^+(124) = U^+(24;\omega)\psi_0(4). \quad (56)$$

The success associated with the application of variational methods is always determined by an appropriate choice of the trial functions. We use the trial functions

$$\psi_1(124) = c_1\delta(1-2)\psi_0(1), \quad (57)$$

$$\psi_2(124) = c_2\rho_0(4)\psi_0^+(2)r_{14}, \quad (58)$$

where $\rho_0(4) \equiv \psi_0^+(4)\psi_0(4)$ and c_1 and c_2 are variable parameters. It is essential that these functions lead to matrix elements containing the same singularities as for the extrema. Substituting the trial functions into the functional (54), we obtain

$$I(c_1, c_2) = c_1A + c_2B - c_1c_2(E_0 - \omega - i0)C, \quad (59)$$

where

$$A(\omega) = \langle\psi_0^+(2)U(12;\omega)\psi_0(1)\rangle, \quad (60)$$

$$B(\omega) = \langle\rho_0(4)\psi_0^+(2)U(12;\omega)e^{i|\omega|r_{14}}\psi_0(1)\rangle, \quad (61)$$

$$C = \langle\rho_0(2)r_{12}\rho_0(1)\rangle. \quad (62)$$

Variation of the parameters in (59) gives

$$I = \frac{A(\omega)B(\omega)}{C(E_0+\omega-i0)}. \quad (63)$$

Hence

$$\Delta E_c' = \frac{\alpha(Z\alpha)^2}{\pi(4\pi)^2 i}\frac{1}{C}\int_{-\infty}^{\infty}\frac{A(\omega)B(\omega)d\omega}{E_0+\omega-i0}. \quad (64)$$

It is now convenient to perform the integration over ω. For Z = 137 ($E_0 = 0$) it is necessary for us to integrate the following expressions (m = 1):

$$\int_{-\infty}^{\infty}\frac{\omega^l d\omega}{\omega-i\delta}\exp\{ia\sqrt{\omega^2-1}+ib|\omega|\} \equiv S_l, \quad l = 0,1,2, \quad (65)$$

where $a = r_{12} + r_{12}'$, $b = r_{14}$, and $\delta \to +0$. Using the formula

$$\frac{1}{\omega-i\delta} = \mathrm{P}\frac{1}{\omega} + \pi i\delta(\omega), \quad (66)$$

we at once obtain

$$S_0 = \pi i e^{-a}, \quad (67)$$

$$S_1 = \mathrm{P}\int_{-\infty}^{\infty}\exp\{ia\sqrt{\omega^2-1}+ib|\omega|\}\,d\omega, \quad (68)$$

and in addition $S_2 = 0$. One can evaluate the integral S_1 by differentiating with respect to the integral parameter cited in the monograph[5]:

$$S_1 = \frac{1}{i}\frac{\partial}{\partial a}\int_{-\infty}^{\infty}\frac{d\omega}{\sqrt{\omega^2-1}}\exp\{ia\sqrt{\omega^2-1}+ib|\omega|\}$$
$$\begin{cases} \pi i\dfrac{a}{\sqrt{a^2-b^2}}N_0'(\sqrt{a^2-b^2}) - \dfrac{1}{2}\varepsilon(a)\dfrac{a}{\sqrt{a^2-b^2}}J_0'(\sqrt{a^2-b^2}) \\ \qquad -\dfrac{1}{2}\delta(a)J_0(\sqrt{a^2-b^2}), & a>b, \\ 2i\dfrac{a}{\sqrt{b^2-a^2}}K_0'(\sqrt{b^2-a^2}), & a<b, \end{cases} \quad (69)$$

where J_0, N_0, and K_0 denote the Bessel, Neumann, and Macdonald functions, the prime denotes derivative, and

$$\varepsilon(a) = \begin{cases} 1, & a>0, \\ -1, & a<0. \end{cases} \quad (70)$$

The matrix elements (60) and (61) diverge at small distances from the nucleus; therefore we shall integrate down to R and retain the leading divergent terms, just as earlier. Since the integral with respect to the variable 4 in Eq. (61) does not give any divergences, we are interested in the integration region $r_{12} \to 0$,

$r_{14} \to r_4$, that is, $a \ll b$ ($b \sim 1$). As is clear from Eqs. (67) and (69), in this limit only the integral $S_0 = \pi i$ does not vanish.

Thus, after integration over ω we arrive at the expression

$$\Delta E_c' = \frac{\alpha}{(4\pi)^2}\frac{AB}{C}, \tag{71}$$

where

$$A = \int \psi_0^+(\mathbf{r}_2)\frac{1}{r_1}\left(\alpha \mathbf{p}_1 \frac{1}{r_{12}}\right)\psi_0(\mathbf{r}_1)\,d\mathbf{r}_1\,d\mathbf{r}_2, \tag{72}$$

and

$$B = A\int \rho_0(\mathbf{r})\,d\mathbf{r} = A, \tag{73}$$

since the function $\psi_0(\mathbf{r})$ is normalized to unity. The integrals A and C remain to be evaluated. Here the integration is elementary to perform, and we obtain

$$A = 12\pi \ln R, \tag{74}$$

$$C = {}^{16}/_3(1 + 2\ln 2), \tag{75}$$

$$\Delta E_c' = \frac{27}{16(1+2\ln 2)}\alpha \ln^2 R. \tag{76}$$

Finally, for the second part of expression (47) the angular integration gives $\Delta E_c'' = 0$.

From formulas (17), (46), and (72) we obtain the following result for the level shift:

$$\Delta E = \Delta E_a + \Delta E_b + \Delta E_c = (-0.205 + 0.160 + 0.705)\alpha \ln^2 R \approx 0.1\ mc^2.$$

According to the estimates given in Section 1, the change in the wave functions associated with taking the finite size of the nucleus into account should decrease this result by roughly a factor of two. Finally, we note that the error given by variational principles of the type (54) in nonrelativistic atomic theory usually amounts to 20 or 30% upon using one or two parameters.

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246