Reduced Dirac equation and Lamb shift as off-mass-shell effect in quantum electrodynamics

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Based on the accurate experimental data of energy-level differences in hydrogen-like atoms, especially the 1S–2S transitions of hydrogen and deuterium, the necessity of introducing a reduced Dirac equation with reduced mass as the substitution of original electron mass is stressed. Based on new cognition about the essence of special relativity, we provide a reasonable argument for the reduced Dirac equation to have two symmetries, the invariance under the (newly defined) space–time inversion and that under the pure space inversion, in a noninertial frame. By using the reduced Dirac equation and within the framework of quantum electrodynamics in covariant form, the Lamb shift can be evaluated (at one-loop level) as the radiative correction on a bound electron staying in an off-mass-shell state—a new approach eliminating the infrared divergence. Hence the whole calculation, though with limited accuracy, is simplified, getting rid of all divergences and free of ambiguity.

Keywords: reduced Dirac equation, Lamb shift, off-mass-shell

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1. Introduction

As is well known, the Dirac equation for electron in a hydrogen-like atom is usually treated as a one-body equation with the nucleus being an inert core having infinite mass and exerting a potential $V(r) = -Z\alpha/r$ ($\hbar = c = 1$) on the electron. Then the rigorous solution of energy levels reads[1]

$$E_{nj} = m_e f(n, j), \tag{1}$$

$$f(n,j) = \left[1 + \frac{(Z\alpha)^2}{(n-\beta)^2}\right]^{-1/2}, \tag{2}$$

$$\beta = j + \frac{1}{2} - \sqrt{\left(j+\frac{1}{2}\right)^2 - (Z\alpha)^2}, \tag{3}$$

where j is the total angular momentum. The expansion of $f(n,j)$ to the power of $(Z\alpha)^6$ is given as[1]

$$\begin{aligned} f(n,j) = 1 &- \frac{(Z\alpha)^2}{2n^2} - \frac{(Z\alpha)^4}{2n^3}\left(\frac{1}{j+\frac{1}{2}} - \frac{3}{4n}\right) \\ &- \frac{(Z\alpha)^6}{8n^3}\left[\frac{1}{(j+\frac{1}{2})^3} + \frac{3}{n(j+\frac{1}{2})^2} \right. \\ &\left. + \frac{5}{2n^3} - \frac{6}{n^2(j+\frac{1}{2})}\right] + \cdots . \end{aligned} \tag{4}$$

Obviously, besides the rest energy of the electron given by the first term, the second term has exactly the form of Bohr energy level except that the mass m_e must be replaced by the reduced mass

$$\mu = \frac{m_e m_N}{m_e + m_N} \equiv \frac{m_e m_N}{M}, \tag{5}$$

with m_N being the mass of the nucleus and $M = m_e + m_N$.

However, as discussed in Refs. [1] and [2], the concept of reduced mass in relativistic quantum mechanics (RQM) is ambiguous to some extent. Since the 1950's, a number of authors have made a great effort at the level of two-body RQM and that of quantum electrodynamics (QED) to take account of the recoil effect,[1,3–6] incorporating their results into a compact form (to order of α^4):

$$\begin{aligned} E = M &+ \mu[f(n,j) - 1] - \frac{\mu^2}{2M}[f(n,j) - 1]^2 \\ &+ \frac{(Z\alpha)^4 \mu^3}{2n^3 m_N^2}\left[\frac{1}{j+\frac{1}{2}} - \frac{1}{l+\frac{1}{2}}\right](1 - \delta_{l0}). \end{aligned} \tag{6}$$

A comprehensive review on the theory of hydrogen-like atoms can be found in Ref. [7]. The aim of this paper is two-fold. First, based on the experimental

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data of hydrogen 1S–2S transition frequency[8] and its isotope shifts of hydrogen and deuterium,[9] we stress the necessity of the introduction of reduced mass μ (Section 2) before we are able to argue the reasonableness of introducing a "reduced Dirac equation" with μ as the substitution of $m_{\rm e}$ (Section 3). Second, based on the above conception, we will present a calculation of Lamb shift (LS) as an off-mass-shell effect by performing the evaluation of self-energy diagrams of electron (Section 4) and photon (Section 5) as well as the vertex function (Section 6) at the one-loop level of QED in the covariant form. The new insight of our calculation is focused on the regularization renormalization method (RRM). As initiated by Yang[10,11] and elaborated in a series of papers (Refs. [12]–[17] and references therein), we can get rid of all ultra violet divergences in the calculation of quantum field theory (QFT). Furthermore, in this paper, we will be able to get rid of the annoying infrared divergence in the vertex function by treating the electron moving off its mass-shell to a certain extent which is fixed through the evaluation of self-energy diagram or by the Virial theorem. Based on the above improvements, the one-loop calculation yields values of LS in a simple but semi-quantitative way (Sections 7 and 8). Although the accuracy is limited at one-loop level, we hope our approach could serve as a new starting point for calculations at high-loop order to obtain accurate results at a comparatively low labour cost. The final Section 9 and Appendix will contain a summary and discussion.

2. The 1S–2S transitions of atomic hydrogen and deuterium

In the last decade, thanks to remarkable advances in high resolution laser spectroscopy and optical frequency metrology, the 1S–2S two-photon transition in atomic hydrogen H (or deuterium D) with its natural linewidth of only 1.3 Hz has been measured to a very high accuracy. In 1997, Udem *et al.* determined the 1S–2S interval of H to be[8]

$$f^{(\rm H)}(\rm 1S–2S) = 2466061413187.34(84)\ \rm kHz. \quad (7)$$

Even four years earlier, Schmidt-Kalar *et al.* had measured the isotope-shift of the 1S–2S transition of H and D to an accuracy of 3.7×10^{-8},[9] giving (as quoted in Ref. [18]):

$$\begin{aligned}\Delta f &\equiv f^{(\rm D)}(\rm 2S–1S) - f^{(\rm H)}(\rm 2S–1S)\\ &= 670994337(22)\ \rm kHz. \end{aligned}\quad (8)$$

(in 1998, Huber *et al.*[19] measured a more accurate datum: 670994334.64(15) kHz), which is of the order of 10^{-4} in comparison with Eq. (7). As pointed out in Ref. [9], this 671-GHz isotope-shift can be ascribed almost entirely to the different masses of proton (p) and deuteron (d). And the nuclear volume effects become important because the QED effects cancel considerably in the isotope shift.

Here, we wish to emphasize that in the first approximation, both experimental data (7) and (8) can be well accounted for by simply resorting to Eq. (1), with $m_{\rm e}$ replaced by the reduced mass

$$\mu_{\rm H} = \frac{m_{\rm e}m_{\rm p}}{m_{\rm e}+m_{\rm p}}, \quad \mu_{\rm D} = \frac{m_{\rm e}m_{\rm d}}{m_{\rm e}+m_{\rm d}} \quad (9)$$

for H and D respectively.

Indeed, by adopting the following updated values:[18,20–22]

$$\alpha = (137.03599944)^{-1},$$
$$\alpha^2 = 0.532513542\times10^{-4}, \quad (10)$$
$$\alpha^4 = 0.283570673\times10^{-8},$$
$$\alpha^6 = 0.151005223\times10^{-12}, \quad (11)$$
$$m_{\rm e} = 0.51099906\ \rm MeV = 1.2355897\times10^{20}\ Hz, \quad (12)$$
$$R_\infty = \frac{1}{2}\alpha^2 m_{\rm e} = 3.28984124\times10^{15}\ \rm Hz, \quad (13)$$
$$\frac{m_{\rm p}}{m_{\rm e}} = 1836.1526665, \quad (14)$$

and denoting

$$\frac{m_{\rm e}}{m_{\rm p}} = b_{\rm H} = 5.446170255\times10^{-4},$$
$$\frac{1}{1+b_{\rm H}} = 0.999455679, \quad (15)$$
$$\frac{m_{\rm e}}{m_{\rm d}} = b_{\rm D} = 2.724436319\times10^{-4},$$
$$\frac{1}{1+b_{\rm D}} = 0.99972763, \quad (16)$$

we can calculate the energy difference between 2S and 1S of H through Eq. (1), with $m_{\rm e}$ replaced by $\mu_{\rm H}$ (the superscript RDE refers to the reduced Dirac equation), i.e.

$$\begin{aligned}\Delta E_{\rm H}^{\rm RDE}(\rm 2S–1S) &= \mu_{\rm H}[f(2,1/2)-f(1,1/2)]\\ &= \frac{m_{\rm e}}{1+b_{\rm H}}(1.996950159\times10^{-5})\\ &= 1.2355897\times10^{20}\times0.999455679\\ &\quad\times1.996950159\times10^{-5}\\ &= 2.466067984\times10^{15}\ \rm Hz, \end{aligned}\quad (17)$$

which is only a bit larger than the experimental datum Eq. (7) with an accuracy of 3×10^{-6}. However, a more stringent test of RDE should be the isotope shifts of H and D. We have

$$\frac{1}{1+b_{\rm D}}-\frac{1}{1+b_{\rm H}}=(b_{\rm H}-b_{\rm D})-(b_{\rm H}^2-b_{\rm D}^2)+(b_{\rm H}^3-b_{\rm D}^3)+\cdots=2.719511528\times10^{-4}, \tag{18}$$

$$\Delta E_{\rm D-H}^{\rm RDE}=(\mu_{\rm D}-\mu_{\rm H})[f(2,1/2)-f(1,1/2)]=6.7101527879\times10^{11}\ {\rm Hz}, \tag{19}$$

which has only a discrepancy larger than the experimental datum (Eq. (8)) by 20.941 MHz with an accuracy of 3×10^{-5}. Of course, it is still not satisfactory in an analysis of high accuracy.[9] Now we resort to Eq. (6), where the third term on the right-hand side does provide a further modification, i.e.

$$\begin{aligned}&-\frac{1}{2}m_{\rm e}\left[\frac{b_{\rm D}}{(1+b_{\rm D})^3}-\frac{b_{\rm H}}{(1+b_{\rm H})^3}\right]\{[f(2,1/2)-1]^2-[f(1,1/2)-1]^2\}\\&=\frac{1}{2}m_{\rm e}[(b_{\rm H}-b_{\rm D})-3(b_{\rm H}^2-b_{\rm D}^2)+\cdots](-6.646361554\times10^{-10})=-11.176\ {\rm MHz},\end{aligned} \tag{20}$$

which brings the discrepancy between the theory and the experiment down to less than 10 MHz.

Although the detailed explanation for this discrepancy remains quite complicated,[9] the above comparison is enough to convince us that the inevitable advent of reduced mass in the RDE or Eq. (6) is by no means a simple fortune. It must have a deep reason from a theoretical point of view. Notice further that once the conditions $m_{\rm e}\ll m_{\rm p}$ and $m_{\rm e}\ll m_{\rm d}$ hold, the difference in spin between p and d seems not so important. So in the next section, we will strive to justify the reduced Dirac equation on a reasonable basis. Of course, it is still an approximate one, but seems much better than the original Dirac equation when dealing with hydrogen-like atoms.

3. Reduced mass and reduced Dirac equation

Consider a system of two particles with rest masses m_1 and m_2. Their coordinates in the centre-of-mass (CM) system are $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ respectively as shown in Fig. 1. If there is a potential $V(r)=V(|\boldsymbol{r}_1-\boldsymbol{r}_2|)$ between them, two equations $m_1\ddot{\boldsymbol{r}}_1=-\nabla_r V(\boldsymbol{r})$ and $m_2\ddot{\boldsymbol{r}}_2=\nabla_r V(\boldsymbol{r})$ will reduce into one, i.e.,

$$\mu\frac{{\rm d}^2\boldsymbol{r}}{{\rm d}t^2}=-\nabla_r V(\boldsymbol{r}),\quad\left(\mu=\frac{m_1m_2}{m_1+m_2}\right). \tag{21}$$

At first sight, the definition of centre-of-mass (CM) in classical mechanics $m_1r_1=m_2r_2$ becomes doubtful in the theory of special relativity (SR) because the mass is no longer a constant. But actually, we can still introduce the coordinate of CM in the laboratory coordinate system (LCS) (with $\boldsymbol{r}_1'$ and $\boldsymbol{r}_2'$ being the coordinates of m_1 and m_2):

$$\begin{aligned}&R=\frac{1}{M}(m_1\boldsymbol{r}_1'+m_2\boldsymbol{r}_2')=(X,Y,Z),\\&(M=m_1+m_2)\end{aligned} \tag{22}$$

and the relative coordinate of m_1 and m_2 ($\boldsymbol{r}_i=\boldsymbol{r}_i'-\boldsymbol{R}$, $i=1,2$):

$$\boldsymbol{r}=\boldsymbol{r}_1'-\boldsymbol{r}_2'=\boldsymbol{r}_1-\boldsymbol{r}_2=(x,y,z). \tag{23}$$

Here the motion of CM in the LCS is assumed to be slow and so

$$\frac{\partial}{\partial x_1'}=\frac{m_1}{M}\frac{\partial}{\partial X}+\frac{\partial}{\partial x},\quad\frac{\partial}{\partial x_2'}=\frac{m_2}{M}\frac{\partial}{\partial X}-\frac{\partial}{\partial x}. \tag{24}$$

Notice that the momentum $\boldsymbol{P}$ of CM and the relative momentum $\boldsymbol{p}_r$ become operators in quantum mechanics (QM) without explicit dependence on mass:

$$\boldsymbol{P}=-{\rm i}\,\hbar\nabla_{\boldsymbol{R}},\quad\boldsymbol{p}_r=-{\rm i}\,\hbar\nabla_{\boldsymbol{r}}. \tag{25}$$

Thus the momenta of m_1 and m_2 in laboratory coordinate system (LCS) read

$$\begin{aligned}\boldsymbol{p}_1'&=-{\rm i}\,\hbar\nabla_{\boldsymbol{r}_1'}=\frac{m_1}{M}\boldsymbol{P}+\boldsymbol{p}_r,\\\boldsymbol{p}_2'&=-{\rm i}\,\hbar\nabla_{\boldsymbol{r}_2'}=\frac{m_2}{M}\boldsymbol{P}-\boldsymbol{p}_r.\end{aligned} \tag{26}$$

Since the centre-of-mass coordinate system (CMCS) is also an inertial frame which can be transformed from the LCS via a linear Lorentz transformation, it is defined by the condition that $\boldsymbol{P}=0$ in CMCS. In other words, CMCS is defined by the condition $\boldsymbol{p}_1+\boldsymbol{p}_2=0$, or (from Eq. (26))

$$\boldsymbol{p}_1'=-{\rm i}\,\hbar\nabla_{\boldsymbol{r}_1'}=\boldsymbol{p}_r,\quad\boldsymbol{p}_2'=-{\rm i}\,\hbar\nabla_{\boldsymbol{r}_2'}=-\boldsymbol{p}_r. \tag{27}$$

Evidently, the above definition of CMCS remains valid in the realm of relativistic QM (RQM) even the exact meaning of CM seems obscure to some extent due to the conjugation relation of a particle's position and its momentum, see Fig. 1.

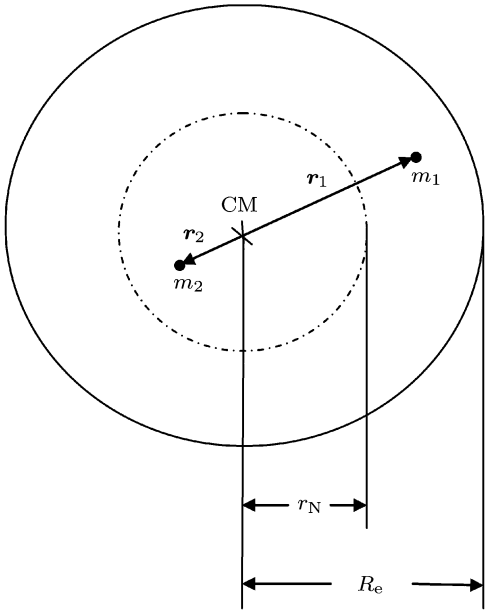


Fig. 1. Hydrogen-like atom in quantum mechanical description. The nucleus with mass m_2 occupies a small sphere with radius $r_{\rm N}$ (greatly exaggerated in the diagram) while the electron with mass m_1 spreads over a larger sphere with radius $R_{\rm e}$ (i.e. atomic radius). Their common centre is the atom's centre of mass (CM). The wavefunction $\psi(\boldsymbol{r})\mathrm{e}^{-\mathrm{i}Et}$ with $\boldsymbol{r} = \boldsymbol{r}_1 - \boldsymbol{r}_2$ shows the electron amplitude under a "fictitious measurement",[24] during which the electron and the nucleus shrink into two "fictitious point particles" located at $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ simultaneously. The Coulomb potential $V(r) = -Ze^2/r$ between them is a static one. The probability to find the electron at $\boldsymbol{r}$ is $|\psi(\boldsymbol{r})|^2$ while that to find its momentum being $\boldsymbol{p}$ is $|\phi(\boldsymbol{p})|^2$ with $\phi(\boldsymbol{p})$ being the Fourier transform of $\psi(\boldsymbol{r})$.

Now, from Eq. (27), it is natural to replace $\boldsymbol{p}_1$ and $\boldsymbol{p}_2$ by $\boldsymbol{p}_r$, thereby reducing the two-particle degrees of freedom to one. In the meantime, the origin of CMCS is discarded, it is substituted by the position of m_2 ($\boldsymbol{r} = \boldsymbol{r}_1 - \boldsymbol{r}_2$). We will call the system associated with $\boldsymbol{r}$ the relative motion coordinate system (RMCS), which should be viewed as a variant of CMCS. The transformation from CMCS to RMCS is by no means a linear one. Rather, the origin of RMCS (m_2) is moving non-uniformly in the CMCS. Therefore, while rest masses m_1 and m_2 remain the same in both LCS and CMCS, they reduce to one mass $\mu = (m_1m_2)/(m_1 + m_2)$ for m_1 in RMCS (or for m_2 if m_1 is chosen as the origin of RMCS).

We express the total energy $E = E_1 + E_2$ in CMCS in terms of p_r and reduced mass μ ($\mu = (m_1m_2)/M$, $M = m_1 + m_2$), where

$$E_1 = \sqrt{m_1^2 + p_1^2} = \sqrt{m_1^2 + p_r^2},$$
$$E_2 = \sqrt{m_2^2 + p_2^2} = \sqrt{m_2^2 + p_r^2}. \qquad (28)$$

Treating all p_1, p_2 and p_r as c-numbers, we have

$$\begin{aligned} E^2 &= (E_1 + E_2)^2 \\ &= M^2 + \frac{M}{\mu}p_r^2 + \frac{1}{4\mu^2}p_r^4\left(4 - \frac{M}{\mu}\right) + \cdots, \qquad (29) \end{aligned}$$

where the expansion in p_r is kept to the order of p_r^4. Two extreme cases will be considered separately:

Case 1 $m_2 \gg m_1$, $\mu \lesssim m_1$, and $M \gg \mu$

$$\begin{aligned} E^2 &= M^2\left[1 + \frac{1}{\mu M}p_r^2 - \frac{1}{4M\mu^3}p_r^4\left(1 - \frac{4\mu}{M}\right) + \cdots\right], \\ E &= M\left[1 + \frac{1}{2\mu M}p_r^2 - \frac{1}{8M\mu^3}p_r^4\left(1 - \frac{3\mu}{M}\right) + \cdots\right] \\ &= M + \frac{1}{2\mu}p_r^2 - \frac{1}{8\mu^3}p_r^4 + \cdots \\ &\simeq M - \mu + \sqrt{\mu^2 + p_r^2} \\ &\simeq m_2 + (m_1 - \mu) + \sqrt{\mu^2 + p_r^2}, \qquad (30) \\ E' &\equiv E - m_2 = (m_1 - \mu) + \sqrt{\mu^2 + p_r^2}. \qquad (31) \end{aligned}$$

Case 2 $m_1 = m_2 = m$, and $\mu = m/2$, $M = 2m = 4\mu$. Then to the accuracy of p_r^4, we have

$$\begin{aligned} E^2 &= M^2 + \frac{M}{\mu}p_r^2 = 4m^2 + 4p_r^2, \\ E &= 2m + \frac{1}{2\mu}p_r^2 - \frac{1}{32\mu^3}p_r^4 + \cdots, \\ E' &\equiv E - M = \frac{1}{2\mu}p_r^2 - \frac{1}{32\mu^3}p_r^4 \simeq \frac{1}{2\mu}p_r^2, \\ &\quad (\text{if } \ p_r^2 \ll \mu^2). \qquad (32) \end{aligned}$$

It is interesting to see that after introducing μ and p_r, the energy E' in RMCS looks quite "relativistic" in the Case 1 whereas it looks rather "non-relativistic" in the Case 2 even both of them are derived from the same relativistic expression, Eq. (28), approximately.

Since the RMCS is not an inertial system, the original mass of m_1 in CM changes abruptly to μ as shown in Eq. (31). How can we derive the reduced Dirac equation (RDE) in RMCS? Fortunately, we already found a basic symmetry, the space–time inversion symmetry, which serves as not only revealing the essence of special relativity (SR), but also deriving the original Dirac equation and the tachyon theory for neutrinos.[23–26] Based on this symmetry, we are going to derive the equation in RQM for either Case 1 or Case 2.

We consider Case 2 ($m_1 \simeq m_2$) first. The motivation is stemming from the success in applying the Schrödinger equation to heavy-quarkoniums like $c\bar{c}$ and $b\bar{b}$ in particle physics (Ref. [27], see also Ref. [24] §9.5 D). Ignoring the spins of both m_1 and m_2, we assume the coupling equations in laboratory system for the two-particle system as

$$\begin{cases} \mathrm{i}\,\hbar\dfrac{\partial\varphi}{\partial t} = (m_1+m_2)c^2\varphi + V(|\boldsymbol{r}'_1-\boldsymbol{r}'_2|)(\varphi+\chi) - \left(\dfrac{\hbar^2}{2m_1}\nabla^2_{\boldsymbol{r}'_1}+\dfrac{\hbar^2}{2m_2}\nabla^2_{\boldsymbol{r}'_2}\right)(\varphi+\chi), \\ \mathrm{i}\,\hbar\dfrac{\partial\chi}{\partial t} = -(m_1+m_2)c^2\chi - V(|\boldsymbol{r}'_1-\boldsymbol{r}'_2|)(\varphi+\chi) + \left(\dfrac{\hbar^2}{2m_1}\nabla^2_{\boldsymbol{r}'_1}+\dfrac{\hbar^2}{2m_2}\nabla^2_{\boldsymbol{r}'_2}\right)(\varphi+\chi), \end{cases} \tag{33}$$

where $\varphi=\varphi(\boldsymbol{r}'_1,\boldsymbol{r}'_2,t)$ and $\chi=\chi(\boldsymbol{r}'_1,\boldsymbol{r}'_2,t)$ are hidden "particle" and "antiparticle" fields of the two-particle system. From now on, the $\boldsymbol{r}'_i$ $(i=1,2)$ is the flowing coordinate of "fields" in QM, i.e., that of "fictitious point particles". See Fig. 1. Equation (33) remains invariant under the (newly defined) space–time inversion $(\boldsymbol{r}'_1\to-\boldsymbol{r}'_1,\boldsymbol{r}'_2\to-\boldsymbol{r}'_2,t\to-t)$:

$$\begin{cases} \varphi(-\boldsymbol{r}'_1,-\boldsymbol{r}'_2,-t) \longrightarrow \chi(\boldsymbol{r}'_1,\boldsymbol{r}'_2,t), \\ \chi(-\boldsymbol{r}'_1,-\boldsymbol{r}'_2,-t) \longrightarrow \varphi(\boldsymbol{r}'_1,\boldsymbol{r}'_2,t), \end{cases} \tag{34}$$

$$V(-\boldsymbol{r}'_1,-\boldsymbol{r}'_2,-t)\longrightarrow V(\boldsymbol{r}'_1,\boldsymbol{r}'_2,t). \tag{35}$$

Note that, however, the time t is not contained in V explicitly. Equation (35) merely means that both m_1 and m_2 $(m_1\approx m_2)$ transform into those of their antiparticles under the space–time inversion. Actually, the strengths of hidden antiparticle field χ are enhanced almost equally in m_1 and m_2 when fictitious particles' velocities increase with the enhancement of attractive potential $V(r)$.

After introducing the CM coordinate $\boldsymbol{R}=M^{-1}(m_1\boldsymbol{r}'_1+m_2\boldsymbol{r}'_2)$, $(M=m_1+m_2)$ and relative coordinate $\boldsymbol{r}=\boldsymbol{r}'_1-\boldsymbol{r}'_2$, and setting

$$\varphi=\Phi+\mathrm{i}\,\frac{\hbar}{Mc^2}\,\dot{\Phi},\quad \chi=\Phi-\mathrm{i}\,\frac{\hbar}{Mc^2}\,\dot{\Phi}, \tag{36}$$

we find $(\mu=m_1m_2/M)$

$$\ddot{\Phi}-c^2\nabla^2_{\mathrm{R}}\Phi-c^2\frac{M}{\mu}\nabla^2_r\Phi + \frac{1}{\hbar^2}(M^2c^4+2VMc^2)\Phi=0. \tag{37}$$

Its stationary solution reads

$$\Phi(\boldsymbol{R},\boldsymbol{r},t)=\psi(\boldsymbol{r})\exp\left[\frac{\mathrm{i}}{\hbar}(\boldsymbol{P}\cdot\boldsymbol{R}-Et)\right], \tag{38}$$

where E is the total energy of the system while $\boldsymbol{P}$ the momentum of CM. The reduced "one-body" equation for $\psi(\boldsymbol{r})$ turns out to be[1)]

$$\begin{cases} \left[-\dfrac{\hbar^2}{2\mu}\nabla^2_{\boldsymbol{r}}+V(\boldsymbol{r})\right]\psi(\boldsymbol{r})=\varepsilon\psi(\boldsymbol{r}), \\ \varepsilon=\dfrac{1}{2Mc^2}(E^2-M^2c^4-\boldsymbol{P}^2c^2). \end{cases} \tag{39}$$

We set $\boldsymbol{P}=0$ (i.e. turn to CMCS) and denote the binding energy $B=Mc^2-E$, yielding

$$B = Mc^2\left[1-\left(1+\frac{2\varepsilon}{Mc^2}\right)^{1/2}\right] = -\varepsilon+\frac{1}{2}\frac{\varepsilon^2}{Mc^2}-\cdots. \tag{40}$$

Notice that although equation (39) looks like a "non-relativistic" stationary Schrödinger equation, it is essentially relativistic. This can be seen from its remarkable property that the eigenvalue ε has a lower bound $-\frac{1}{2}Mc^2$, corresponding to $E_{\min}=0$ $(B_{\max}=M)$!

An example is to consider "positronium" composed of e^+ and e^- with charge Ze and $-Ze$ respectively. Once when the "fictitious charge number" Z increases from 1 to $Z_{\max}=(4/\alpha^2)^{1/4}=16.555$, the whole bound system will have a lowest ground energy $E_{\min}=0$! So equation (39) is really a relativistic QM equation capable of giving a nonperturbative solution under the strong coupling.

Equation (39) provides a justification (realization) of conjecture Eq. (32) relevant to Case 2 $(m_1\simeq m_2)$ where the spins of both particles are merely of second importance.

Now we turn to Case 1 where $m_2\gg m_1$, taking the spin of m_1 into account but ignoring that of m_2 as before. Based on the experience in Case 2, also because of great difficulty in deriving the equation starting from the laboratory system for Case 1, we directly introduce the reduced Dirac equation (RDE) in the RMCS as a pair of coupled equations of two-component spinors $\varphi(\boldsymbol{r},t)$ and $\chi(\boldsymbol{r},t)$, $(c=\hbar=1)$

$$\begin{cases} \mathrm{i}\,\dot{\varphi} = \mathrm{i}\,\boldsymbol{\sigma}_1\cdot\nabla_{\boldsymbol{r}}\chi+\mu\varphi+V(\boldsymbol{r})\varphi, \\ \mathrm{i}\,\dot{\chi} = \mathrm{i}\,\boldsymbol{\sigma}_1\cdot\nabla_{\boldsymbol{r}}\varphi-\mu\chi+V(\boldsymbol{r})\chi \end{cases} \tag{41}$$

with μ replacing m_1. Here $\boldsymbol{\sigma}_1$ is Pauli matrix acting on the spin space of particle m_1. Equation (41) is invariant under the space–time inversion $(\boldsymbol{r}\to-\boldsymbol{r},t\to$

[1)] With equation (35), equation (37) is invariant under the space–time inversion $(\boldsymbol{r}\to-\boldsymbol{r},t\to-t)$. Equivalently, under the mass inversion $(m_1\to-m_1,m_2\to-m_2)$, equations (37) and (39) remain invariant in the sense that not only $\mu\to-\mu,M\to-M$, but also $V(\boldsymbol{r})\to-V(\boldsymbol{r}),\varepsilon\to-\varepsilon$. Notice that, however, the simultaneous inversion of m_1 and m_2 implies $m_1\simeq m_2$, so both particles change under their mutual interaction $V(\boldsymbol{r})$ simultaneously. Here V, the "internal potential energy" of two-body system, is called a "scalar potential". We see that either the invariance under the space–time inversion or that under the mass inversion is capable of showing the particle–antiparticle symmetry (i.e., relativistic nature) of a system essentially.

$-t)$, $\varphi(-\boldsymbol{r},-t)\to\chi(\boldsymbol{r},t)$, and $\chi(-\boldsymbol{r},-t)\to\varphi(\boldsymbol{r},t)$ whereas we assume

$$V(-\boldsymbol{r},-t)\longrightarrow -V(\boldsymbol{r},t), \tag{42}$$

which is in contrast to Eq. (35) for the Case 2.[2)]

The reasons are as follows. (i) Equation (41) should degenerate into the original Dirac equation when $m_2\to\infty$, and $\mu=m_1m_2/(m_1+m_2)\to m_1$. (ii) Since now $m_2\gg m_1$ (but $m_2\neq\infty$), m_1 moves much faster than m_2 in the CMCS. Hence the antiparticle field χ is enhanced much appreciably in m_1 than in m_2, which is a situation totally different from that in the Case 2 where $m_1\approx m_2$. (iii) If instead of Eq. (42), we still assume $V(-\boldsymbol{r},-t)\longrightarrow V(\boldsymbol{r},t)$ like Eq. (35) and change the sign before $V(\boldsymbol{r})$ in the second equation of Eq. (41) to keep its invariance under the space–time inversion, then we obtain an equation which can lead to a reversed fine-structure of atom (e.g., the $\mathrm{P}_{1/2}$ state lies above the $\mathrm{P}_{3/2}$ state), a wrong prediction obviously excluded by experiments.

However, one kind of invariance is not enough to fix an equation. Indeed, the beauty of Dirac equation or RDE is hidden in two symmetries: besides the symmetry of space–time inversion, it has another left–right (parity) symmetry. To see it, we define

$$\xi=\frac{1}{\sqrt{2}}(\varphi+\chi),\quad \eta=\frac{1}{\sqrt{2}}(\varphi-\chi), \tag{43}$$

and recast Eq. (41) into

$$\begin{cases}\mathrm{i}\,\dot{\xi}\ =\mathrm{i}\,\boldsymbol{\sigma}_1\cdot\nabla_{\boldsymbol{r}}\xi+\mu\eta+V(\boldsymbol{r})\xi,\\ \mathrm{i}\,\dot{\eta}\ =-\mathrm{i}\,\boldsymbol{\sigma}_1\cdot\nabla_{\boldsymbol{r}}\eta+\mu\xi+V(\boldsymbol{r})\eta,\end{cases} \tag{44}$$

which is invariant under a pure space inversion ($\boldsymbol{r}\to-\boldsymbol{r},t\to t$) under the assumption of

$$\begin{aligned}&\xi(-\boldsymbol{r},t)\to\eta(\boldsymbol{r},t),\quad \eta(-\boldsymbol{r},t)\to\xi(\boldsymbol{r},t),\\ &V(-\boldsymbol{r})\to V(\boldsymbol{r})=V(r).\end{aligned} \tag{45}$$

The parity invariance of Dirac equation or RDE has a far-reaching consequence that the Dirac particle is always a subluminal one. By contrast, once the parity is violated to maximum, a superluminal particle (tachyon) will emerge. Interestingly enough, any theory capable of treating particle and antiparticle on an equal footing must respect the common basic symmetry—the invariance of space–time inversion. The new insight of this section is this symmetry can be applied even in a noninertial frame—the RMCS. Of course, the validity of RDE can be verified only by experiments as discussed in Section 2, although it is still an approximate description of nature like any other theory in physics. For further discussion, see Section 9.

4. Self-energy correction of a bound electron in atom

In our understanding, one important reason why the calculation of QED for electron in a hydrogen-like atom is so complicated lies in the fact that while calculations are performed in the CMCS, the centre of potential (the nucleus with mass $m_2=m_{\mathrm{N}}$) undergoes a complex motion. So the recoil effect interwinds with the high-loop correction of QED as discussed in many chapters of the books [1] and [2]. We will try to find an alternative approach by adopting the RDE and performing calculation in the RMCS. We begin with the Feynman diagram integral (FDI) of electron self-energy at one-loop level, adopting the Bjorken–Drell metric and rationalized Gaussian units with electron charge $-e$ ($e>0$), see Fig. 2(a) (Ref. [16]), as follows:

$$-\mathrm{i}\,\Sigma(p)=(\mathrm{i}\,e)^2\int\frac{\mathrm{d}^4k}{(2\pi)^4}\frac{g_{\mu\nu}}{\mathrm{i}\,k^2}\gamma^\mu\frac{\mathrm{i}}{\not p-\not k-\mu}\gamma^\nu. \tag{46}$$

Here a free electron with reduced mass μ moves with a four-dimensional momentum p, whose spatial component is just the relative momentum $\boldsymbol{p}_r$ discussed in the previous section, k is the momentum of virtual photon. As usual, a Feynman parameter x will bring Eq. (46) into

$$-\mathrm{i}\,\Sigma(p)=-e^2\int\frac{\mathrm{d}^4k}{(2\pi)^4}\frac{N}{D}, \tag{47}$$

$$\begin{aligned}&\frac{1}{D}=\int_0^1\frac{\mathrm{d}x}{[k^2-2p\cdot kx+(p^2-\mu^2)x]^2},\\ &N=-2(\not p-\not k)+4\mu,\end{aligned} \tag{48}$$

($\not p=p^\mu\gamma_\mu$, $p\cdot k=p^\mu k_\mu$). A shift in momentum integration: $k\to K=k-xp$ recasts Eq. (47) into

$$-\mathrm{i}\,\Sigma(p)=-e^2\int_0^1\mathrm{d}x[-2(1-x)\ \not p+4\mu]I \tag{49}$$

[2)] For a hydrogen-like atom, $V(r)=-Ze^2/r$ does not contain time t explicitly. Equation (42) merely means that under the space–time inversion, the electron transforms into a position whereas the nucleus remains unchanged. See point i) of Section 9. Previously, the V in Eq. (42) was called a "vector potential", meaning the "potential energy" of the electron in an "external field" of nucleus. Note that, formally, equation (41) remains invariant under a mass inversion as $\mu\to-\mu,\phi\to\chi$ and $\chi\to\phi$ ($V(\boldsymbol{r})$ remains unchanged) in a noninertial frame RMCS. Actually, since $m_1=m_{\mathrm{e}}\to-m_{\mathrm{e}}$, but $m_2=m_{\mathrm{N}}\to m_{\mathrm{N}},\mu\to-\mu(1+2m_{\mathrm{e}}/M)$. So equation (41) has an inaccuracy up to $2m_{\mathrm{e}}/M$ ($<1.1\times10^{-3}$ for H).

with a logarithmically divergent integral (in Minkowski momentum space) being

$$I = \int \frac{d^4K}{(2\pi)^4} \frac{1}{[K^2 - M^2]^2},$$
$$M^2 = p^2x^2 + (\mu^2 - p^2)x. \tag{50}$$

Our new regularization–renormalization method (RRM) is based on a cognition that the virtual process in the self-energy diagram does provide a radiative correction to the electron mass but only when the electron is off the mass shell, i.e., $p^2 \neq \mu^2$. When it is on the mass shell, $p^2 = \mu^2$, the appearance of a divergent integral like I in Eq. (50) is essentially a warning to the fact that to calculate the mass of electron is beyond the ability of perturbative QED.

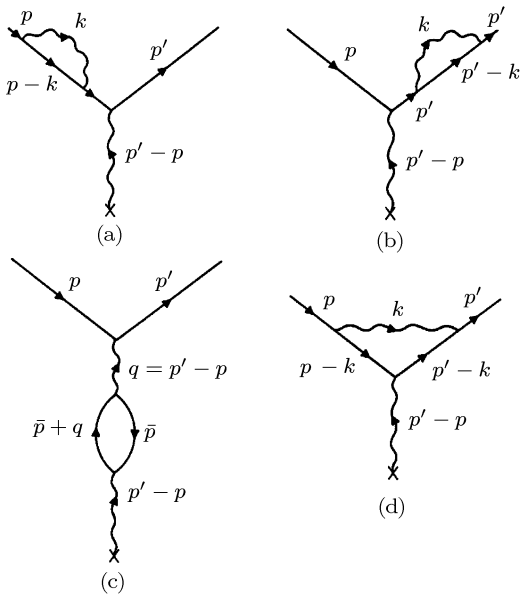


Fig. 2. Four Feynman diagrams at one-loop level (in covariant form). Panels (a) and (b) are self-energy diagrams of the electron, panel (c) shows vacuum polarization, and panel (d) displays vertex function. Solid lines and wavy lines refer to electron and photon respectively, while X denotes the nucleus. Here p, q and k denote four-dimensional momenta.

We consider the converse: if $\Sigma(p)$ does modify the electron mass μ to some extent, it must comes from the divergent integral I. However, the latter is a dimensionless number, we can change the unit of M (and k) at our disposal without any change in the value of I. So any real change of μ (on the mass shell) is incredible. The deeper reason lies in a "principle of relativity" in epistemology: everything is moving and becomes recognizable only in relationship with other things. What we can understand is either no mass scale or two mass scales, but never one mass scale. For instance, in the famous Gross–Neveu model,[28] a massive fermion is created only to the accompaniment of the change (phase transition) of its environment (vacuum) which provides another mass scale (a standard weight). Another example is just the change of electron mass from $m_{\rm e}$ to $\mu_{\rm H}$ in a hydrogen atom due to the coexistence of atom nucleus—the proton, and this change is also a nonperturbative effect.

Therefore, we expected too much in the past. There is no way to evaluate Eq. (50) unambiguously or pick out some finite and fixed modifications to the mass μ. What we can do is to separate the valuable information carried by Eq. (50) from an arbitrary constant which will be introduced by a simple trick and then fixed by the experimental data of μ. We will see the information about how the value of I exactly changes when the electron moves off the mass shell.

To handle Eq. (50), we perform a differentiation with respect to the mass-square parameter M^2, then the integration with respect to K becomes convergent, yielding

$$\frac{\partial I}{\partial M^2} = \frac{-\,{\rm i}}{(4\pi)^2} \frac{1}{M^2}, \tag{51}$$

which indicates that while the exact value of I remains obscure, its change linked with M^2 has a definite meaning. So we re-integrate Eq. (51) with respect to M^2 and arrive at

$$I = \frac{-\,{\rm i}}{(4\pi)^2}(\ln M^2 + C_1) = \frac{-\,{\rm i}}{(4\pi)^2} \ln \frac{M^2}{\mu_2^2}, \tag{52}$$

where an arbitrary constant $C_1 = -\ln \mu_2^2$ is introduced (μ_2 should not be confused with the reduced mass μ). Further integration with respect to Feynman parameter x leads to

$$\Sigma(p) = A + B\ \not{p},$$
$$A = \frac{\alpha}{\pi}\mu \left[2 - 2\ln \frac{\mu}{\mu_2} + \frac{(\mu^2 - p^2)}{p^2} \ln \frac{(\mu^2 - p^2)}{\mu^2}\right],$$
$$B = \frac{\alpha}{4\pi}\left\{2\ln \frac{\mu}{\mu_2} - 3 - \frac{(\mu^2 - p^2)}{p^2} \times \left[1 + \frac{(\mu^2 + p^2)}{p^2} \ln \frac{(\mu^2 - p^2)}{\mu^2}\right]\right\}. \tag{53}$$

Using the chain approximation, we can derive the modification of electron propagator as

$$\frac{\rm i}{\not{p} - \mu} \to \frac{\rm i}{\not{p} - \mu} \frac{1}{1 - \Sigma(p)/(\not{p} - \mu)} = \frac{{\rm i}\, Z_2}{\not{p} - \mu_{\rm R}}, \tag{54}$$

where

$$Z_2 = \frac{1}{1 - B} \tag{55}$$

is the renormalization factor for wave function of electron and

$$\mu_{\rm R} = \frac{\mu + A}{1 - B} \tag{56}$$

is the renormalized mass of μ. The increment of mass reads

$$\delta\mu = \mu_{\rm R} - \mu = \frac{A + \mu B}{1 - B}. \tag{57}$$

For a free electron (in the atom), the mass-shell condition $p^2 = \mu^2$ should lead to

$$\delta\mu|_{p^2=\mu^2} = \frac{\alpha\mu}{4\pi}\left(5 - 6\ln\frac{\mu}{\mu_2}\right) = 0 \tag{58}$$

as discussed above.[3)] So we must set $\mu_2 = \mu e^{-5/6}$ which in turn fixes

$$Z_2|_{p^2=\mu^2} = \frac{1}{1 + \alpha/3\pi} \approx 1 - \frac{\alpha}{3\pi}. \tag{59}$$

However, the above evaluation further provides us with important knowledge of $\delta\mu$ when electron moves off the mass-shell. Consider a similar diagram in Fig. 2(b), we can set on an average meaning that

$$p^2 = \mu^2(1 - \zeta) \tag{60}$$

with $\zeta > 0$, which implies from Eq. (57) with Eq. (53) that:[29]

$$\delta\mu = \frac{\alpha\mu}{4\pi}\frac{(-\zeta + 2\zeta\ln\zeta)}{1 + \alpha/3\pi}, \tag{61}$$

where some terms of the order of ζ^2 or $\zeta^2\ln\zeta$ are neglected since $\zeta \ll 1$. Equation (61) establishes the correspondence between the mass modification $\delta\mu$ and the parameter ζ describing the off-mass-shell extent of electron in the bound state. For a hydrogen-like atom, we may ascribe $\delta\mu$ to the (minus) binding energy of electron in the Bohr theory and express it as

$$\delta\mu = \varepsilon_n = -\frac{Z^2\alpha^2}{2n^2}\mu. \tag{62}$$

Then equation (61) gives the value of ζ for fixed values Z and n. We will see from the vertex function that these values of ζ are crucial to the calculation of Lamb shift (Sections 7 and 8).

5. Photon self-energy

As discussed in various text books,[30−32] we encounter the FDI of vacuum polarization Fig. 2(c) as:[16]

$$\begin{aligned}\Pi_{\mu\nu}(q) =& \frac{8\,\mathrm{i}\,e^2}{(4\pi)^2}(q_\mu q_\nu - g_{\mu\nu}q^2) \\ &\times \int_0^1 \mathrm{d}x(x^2 - x)\ln\frac{m^2 + q^2(x^2 - x)}{\mu_3^2}\end{aligned}$$

$$\begin{aligned}\Pi_{\mu\nu}(q) =& -(-\,\mathrm{i}\,e)^2\,\mathrm{Tr}\int\frac{\mathrm{d}^4\bar{p}}{(2\pi)^4} \\ &\times \gamma_\mu\frac{\mathrm{i}}{\not{\bar{p}} - m}\gamma_\nu\frac{\mathrm{i}}{\not{\bar{p}} + \not{q} - m}.\end{aligned} \tag{63}$$

Here q is the momentum transfer along the photon line and m the mass of electron. Introducing the Feynman parameter x as in previous section and performing a shift in momentum integration: $\bar{p} \to K = \bar{p} + xq$, we obtain

$$\Pi_{\mu\nu}(q) = -4e^2\int_0^1 \mathrm{d}x(I_1 + I_2), \tag{64}$$

where

$$I_1 = \int\frac{\mathrm{d}^4K}{(2\pi)^4}\frac{2K_\mu K_\nu - g_{\mu\nu}K^2}{(K^2 - M^2)^2} \tag{65}$$

with

$$M^2 = m^2 + q^2(x^2 - x) \tag{66}$$

is quadratically divergent while

$$I_2 = \int\frac{\mathrm{d}^4K}{(2\pi)^4}\frac{(x^2 - x)(2q_\mu q_\nu - g_{\mu\nu}q^2) + m^2 g_{\mu\nu}}{(K^2 - M^2)^2} \tag{67}$$

is only logarithmically divergent like that in Eq. (50). An elegant way to handle I_1, equation (65), is to modify M^2 into

$$M^2(\sigma) = m^2 + q^2(x^2 - x) + \sigma \tag{68}$$

and differentiating I_1 with respect to σ. After integration with respect to K, we reintegrate it with respect to σ twice, arriving at the limit $\sigma \to 0$,

$$\begin{aligned}I_1 =& \frac{\mathrm{i}\,g_{\mu\nu}}{(4\pi)^2}\Big\{[m^2 + q^2(x^2 - x)] \\ &\times \ln\frac{m^2 + q^2(x^2 - x)}{\mu_3^2} + C_2\Big\}\end{aligned} \tag{69}$$

with two arbitrary constants: $C_1 = -\ln\mu_3^2$ and C_2. Combining I_1 and I_2 together, we find

$$-\frac{4\,\mathrm{i}\,e^2}{(4\pi)^2}g_{\mu\nu}C_2. \tag{70}$$

The continuity equation of current induced in the

[3)] We will keep the same mass symbol μ throughout high-loop calculations of QED and reconfirm (renormalize) it at every step by experiment. Just as one has to reconfirm his plane ticket before his departure from the airport, he must use the same name throughout his entire journey.[17]

vacuum polarization[30]

$$q^\mu \Pi_{\mu\nu}(q) = 0 \tag{71}$$

is ensured by the factor $(q_\mu q_\nu - g_{\mu\nu}q^2)$. So we set $C_2 = 0$. Consider the scattering between two electrons via the exchange of a photon with momentum transfer $q \to 0$. Adding the contribution of $\Pi_{\mu\nu}(q)$ to the tree diagram amounts to modifying the charge square:

$$\begin{aligned} & e^2 \longrightarrow e_{\rm R}^2 = Z_3 e^2, \ \text{ with} \\ & Z_3 = 1 + \frac{\alpha}{3\pi}\left(\ln\frac{m^2}{\mu_3^2} - \frac{q^2}{5m^2} + \cdots\right). \end{aligned} \tag{72}$$

As in Ref. [17], we will set $\mu_3 = m$ so that at the Thomson limit we have $\lim_{q\to 0} e_{\rm R}^2 = e^2$. However, for the purpose of calculating Lamb shift (LS) below, the second term in the parenthesis of Z_3 is important because for a bound state it contributes a term of effective potential (adding to Coulomb potential), called the Uehling potential (Ref. [32], p. 253):

$$-\frac{4\alpha^2}{15m^2}\delta(\boldsymbol{r}). \tag{73}$$

6. Off-mass-shell vertex function

Consider an electron (see Fig. 2(d)) moving in a hydrogen atom, its momentum changes from p to p' via the scattering by the proton and an exchange of virtual photon with momentum k. The FDI at one-loop level reads

$$\begin{aligned} \Lambda_\mu(p',p) = {} & (-\mathrm{i}\,e)^2 \int \frac{\mathrm{d}^4k}{(2\pi)^4}\frac{-\mathrm{i}}{k^2}\gamma_\nu \frac{\mathrm{i}}{\not{p}' - \not{k} - \mu} \\ & \times \gamma_\mu \frac{\mathrm{i}}{\not{p} - \not{k} - \mu}\gamma^\nu. \end{aligned} \tag{74}$$

However, different from Ref. [17] and many other reports, not only the reduced mass μ (instead of m) of electron is used, but also a new approach will be adopted. We assume that the electron moves off-mass-shell in the sense of (as in Section 4):

$$p^2 = p'^2 = \mu^2(1-\zeta). \tag{75}$$

We still have

$$p' - p = q, \quad p\cdot q = -\frac{1}{2}q^2. \tag{76}$$

Introducing Feynman parameters $u = x + y$ and $v = x - y$, we perform a shift in the momentum integration: $k \to K = k - (p + q/2)u - (q/2)v$, thus

$$\Lambda_\mu = -\mathrm{i}\,e^2[I_3\gamma_\mu + I_4] \tag{77}$$

with

$$I_3 = \int_0^1 \mathrm{d}u \int_{-u}^{u} \mathrm{d}v \int \frac{\mathrm{d}^4K}{(2\pi)^4}\frac{K^2}{(K^2-M^2)^3}, \tag{78}$$

$$M^2 = \left[\mu^2(1-\zeta) - \frac{q^2}{4}\right]u^2 + \frac{q^2}{4}v^2 + \zeta\mu^2 u, \tag{79}$$

$$I_4 = \int_0^1 \mathrm{d}u \int_{-u}^{u} \mathrm{d}v \int \frac{\mathrm{d}^4K}{(2\pi)^4}\frac{A_\mu}{(K^2-M^2)^3}, \tag{80}$$

$$\begin{aligned} A_\mu = {} & (4-4u-2u^2)\mu^2(1-\zeta)\gamma_\mu + 2\,\mathrm{i}(u^2-u)\mu q^\nu \sigma_{\mu\nu} \\ & - \left(2 - 2u + \frac{u^2}{2} - \frac{v^2}{2}\right)q^2\gamma_\mu \\ & - (2+2u)v\mu q_\mu. \end{aligned} \tag{81}$$

Set $K^2 = K^2 - M^2 + M^2$, then $I_3 = I_3' - \mathrm{i}/32\pi^2$, where I_3' is only logarithmically divergent and so can be treated as in previous sections, thereby yielding

$$I_3' = \frac{-\mathrm{i}}{(4\pi)^2}\int_0^1 \mathrm{d}u \int_{-u}^{u} \mathrm{d}v \ln\frac{M^2}{\mu_1^2} \tag{82}$$

with μ_1 an arbitrary constant.

However, unlike Ref. [17] where the calculation was conducted on the mass-shell, now the off-mass-shell integration in Eq. (82) can be performed in the approximation that $Q^2/4\mu^2 \ll 1$ and $\zeta \ll 1$ ($Q^2 = -q^2$, Q is the three-dimensional momentum transfer) which will be enough to calculate the Lamb shift (LS). Denoting

$$a = \left[\mu^2(1-\zeta) + \frac{Q^2}{4}\right]u^2 + \zeta\mu^2 u, \quad b = \frac{Q^2}{4}, \tag{83}$$

we perform the integration with respect to v and u rigorously as follows:

$$\begin{aligned} & \int_{-u}^{u} \mathrm{d}v \ln(a - bv^2) \\ & = 2u\{\ln\mu^2 + \ln u + \ln[(1-\zeta)u + \zeta\} \\ & \quad - 4u + 2\sqrt{\frac{4a}{Q^2}}\ln\frac{1+\sqrt{Q^2/4a}u}{1-\sqrt{Q^2/4a}u}. \end{aligned} \tag{84}$$

Expanding the last term and keeping only up to the order of ζ and $Q^2/4\mu^2$, we obtain

$$\begin{aligned} & \int_0^1 \mathrm{d}u \int_{-u}^{u} \mathrm{d}v \ln(a - bv^2) \\ & \simeq \ln\mu^2 - 1 + \zeta + \frac{Q^2}{6\mu^2}(1-\zeta). \end{aligned} \tag{85}$$

To our great pleasure, throughout the evaluation of I_4, there is no infrared divergence which appeared in previous reports when integrated with respect to u with lower limit zero. To avoid the infrared divergence, e.g., in Ref. [17], a cutoff was introduced at

the lower limit. Now the infrared divergence disappears due to the existence of off-mass-shell parameter ζ. For example, we encounter the following integral, in which no cutoff is needed ($\lambda = (1-\zeta) + Q^2/4\mu^2 \sim 1$):

$$\int_0^1 \frac{\mathrm{d}u}{u+\zeta/\lambda} = \frac{\zeta}{\lambda} - \ln\frac{\zeta}{\lambda}. \tag{86}$$

Hence, after elementary but tedious calculation, we find

$$\begin{aligned}\Lambda_\mu(p',p) = {} & \frac{\alpha}{4\pi}\left[\frac{11}{2} - \ln\frac{\mu^2}{\mu_1^2} - 3\zeta + 4(1+\zeta)\ln\zeta\right]\gamma_\mu \\ & + \frac{\alpha}{4\pi}\frac{Q^2}{\mu^2}\gamma_\mu\left(\frac{1}{6} + \frac{1}{2}\zeta + \frac{4}{3}\ln\zeta + 2\zeta\ln\zeta\right) \\ & + \mathrm{i}\,\frac{\alpha}{4\pi}\frac{q^\nu}{\mu}\sigma_{\mu\nu}(1 + 3\zeta + 2\zeta\ln\zeta). \end{aligned} \tag{87}$$

7. Calculation of Lamb shift as an off-mass-shell effect at one-loop level

There are three parts on the right-hand side of Eq. (87). The first part in combination with the vertex γ_μ at tree level provides a renormalization factor as

$$Z_1^{-1} = 1 + \frac{\alpha}{4\pi}\left[\frac{11}{2} - \ln\frac{\mu^2}{\mu_1^2} - 3\zeta + 4(1+\zeta)\ln\zeta\right]. \tag{88}$$

Further combination with Z_2 in Eq. (55) and Z_3 in Eq. (72) leads to a renormalized charge (at one-loop level, see Fig. 2),

$$e_{\mathrm{R}} = \frac{Z_2}{Z_1} Z_3^{1/2} e. \tag{89}$$

However the Ward identity implies that[30–32]

$$Z_1 = Z_2. \tag{90}$$

Therefore

$$\alpha_{\mathrm{R}} = \frac{e_{\mathrm{R}}^2}{4\pi} = Z_3\alpha. \tag{91}$$

Note that the Ward identity holds not only for an electron on the mass-shell, but also for off-mass-shell case. Hence for every bound state in hydrogen-like atom with a definite value of ζ (Z_1 and Z_2 are functions of ζ), the arbitrary constant μ_1 in Eq. (88) plays a flexible role in guaranteing the validity of Eq. (90) (other two constants μ_2 and μ_3 have been fixed in Eqs. (58) and (72) respectively). For further discussion, see Section 9.

The second part of Eq. (87) contains $Q^2\gamma_\mu$. Just like the Uehling potential in Eq. (72) (with $q^2 = -Q^2$), it contributes an effective potential of δ function type as

$$\frac{\alpha^2}{\mu^2}\left[-\frac{1}{6} - \frac{1}{2}\zeta - \frac{4}{3}\ln\zeta - 2\zeta\ln\zeta\right]\delta(\boldsymbol{r}). \tag{92}$$

Finally, the third part of Eq. (87) amounts to a modification of electron magnetic moment in the atom, and the gyromagnetic ratio of electron reads

$$g = 2\left[1 + \frac{\alpha}{2\pi}(1 + 3\zeta + 2\zeta\ln\zeta)\right]. \tag{93}$$

We will call the anomalous part of magnetic moment $a = \tilde{\alpha}/2\pi$, where $\tilde{\alpha} = \alpha(1 + 3\zeta + 2\zeta\ln\zeta)$. The radiative correction on the magnetic moment of an electron has two consequences. One is a modification to the L–S coupling in a hydrogen-like atom (with charge number Z):[30,31]

$$H_{LS}^{\mathrm{rad}} = 2\left(\frac{\tilde{\alpha}}{2\pi}\right)\frac{\alpha Z}{4\mu^2 r^3}\boldsymbol{\sigma}\cdot L. \tag{94}$$

Here, the electron mass has been modified from m (see, e.g., Ref. [24]) to μ which can be derived from the reduced Dirac equation.

Another consequence of anomalous magnetic moment of electron exhibits itself as an additional potential of δ function type like Eq. (73)[30,31]

$$\frac{Z\alpha\tilde{\alpha}}{2\mu^2}\delta(\boldsymbol{r}). \tag{95}$$

Note that expressions (94) and (95) are effective only to states with $L \neq 0$ and S state with $L = 0$ respectively.

Adding the results of expressions (94) and (95) and the sum of expressions (73) and (92) multiplied by Z together to obtain all radiative corrections (at one-loop level) on electron in the hydrogen-like atom, then we have the effective potential as

$$\begin{aligned} V_{\mathrm{eff}}^{\mathrm{rad}} = {} & \frac{Z\alpha^2}{\mu^2}\left[-\frac{4}{3}\ln\zeta - \frac{1}{2}\zeta - 2\zeta\ln\zeta - \frac{1}{6} - \frac{4}{15}\frac{\mu^2}{m^2}\right. \\ & \left. + \frac{1}{2}(1 + 3\zeta + 2\zeta\ln\zeta)\right]\delta(\boldsymbol{r}) \\ & + \frac{Z\alpha^2}{4\pi\mu^2 r^3}(1 + 3\zeta + 2\zeta\ln\zeta)\boldsymbol{\sigma}\cdot\boldsymbol{L} \\ \simeq {} & \frac{Z\alpha^2}{\mu^2}\left[-\frac{4}{3}\ln\zeta + \frac{1}{15} + \zeta - \zeta\ln\zeta\right]\delta(\boldsymbol{r}) \\ & + \frac{Z\alpha^2}{4\pi\mu^2 r^3}(1 + 3\zeta + 2\zeta\ln\zeta)\boldsymbol{\sigma}\cdot\boldsymbol{L}, \end{aligned} \tag{96}$$

where we take $\mu^2/m^2 \approx 1$ in the Uehling potential to make the formula simpler for a semi-quantitative

calculation. Equation (96) leads to the energy modification of a bound state (with quantum numbers n, l, j) in a hydrogen-like atom:

$$\delta(\boldsymbol{r}) \longrightarrow |\psi_{ns}(0)|^2 = \frac{Z^3\alpha^3}{\pi n^3}\mu^3, \quad (l=0), \tag{97}$$

$$\Delta E^{\rm rad} = \Delta E^{\rm rad}(ns) + \Delta E^{\rm rad}_{LS}, \tag{98}$$

$$\Delta E^{\rm rad}(ns) = \frac{Z^4\alpha^3}{\pi n^3}R_y\left[\frac{8}{3}\ln\frac{1}{\zeta} + \frac{2}{15} + 2\zeta(1-\ln\zeta)\right]\delta_{l0}, \tag{99}$$

$$\Delta E^{\rm rad}_{LS} = \frac{Z^4\alpha^3}{\pi n^3}R_y\frac{1+\zeta(3+2\ln\zeta)}{l(2l+1)(l+1)} \times \begin{cases} l, & (j=l+1/2), \\ -(l+1), & (j=l-1/2), \end{cases} \tag{100}$$

where

$$R_y = \frac{1}{2}\alpha^2\mu = \frac{\mu}{m}R_\infty. \tag{101}$$

8. Energy-level difference in hydrogen-like atom: theory vs. experiment

We will study some energy-level differences near the ground state of hydrogen-like atoms, where accurate experimental data are available. Theoretically, the energy level is fixed primarily by the formula derived from the reduced Dirac equation (RDE), i.e., Eq. (1) with $m_{\rm e}$ substituted by μ_A where the subscript A refers to atoms H, D or ion $\rm He^+$, and so on,

$$E^{\rm RDE}_A = \mu_A[f(n,j)-1] = \frac{m_{\rm e}}{1+b_A}[f(n,j)-1] = \frac{1}{1+b_A}(1.2355897\times10^{20})\left[-\frac{(Z\alpha)^2}{2n^2} - \frac{(Z\alpha)^4}{3n^3}\left(\frac{1}{j+1/2}-\frac{3}{4n}\right)-\cdots\right] \text{Hz}. \tag{102}$$

Further recoil corrections Eq. (6) derived by previous authors will be divided into two terms:

$$\Delta E^{\rm recoil-1}_A(n,j) = -\frac{\mu_A^2}{2M_A}[f(n,j)-1]^2 = -\frac{m_{\rm e}b_A}{2(1+b_A)^3}[f(n,j)-1]^2, \tag{103}$$

$$\Delta E^{\rm recoil-2}_A(n,j,l) = \frac{(Z\alpha)^4\mu_A^3}{2n^3m_{\rm N}^{(A)^2}}\left(\frac{1}{j+\frac{1}{2}}-\frac{1}{l+\frac{1}{2}}\right)(1-\delta_{l0}). \tag{104}$$

Next comes the radiative correction calculated by QED at one-loop level, Eq. (98),

$$\Delta E^{\rm rad}_A(n,j,l) = \frac{1}{1+b_A}\frac{Z^4}{n^3}\left(\frac{\alpha^3}{\pi}R_\infty\right)\left[\left(-\frac{8}{3}\ln\zeta+\frac{2}{15}+2\zeta(1-\ln\zeta)\right)\delta_{l0} + \frac{1+\zeta(3+2\ln\zeta)}{2l+1}C_{jl}(1-\delta_{l0})\right], \tag{105}$$

where

$$C_{jl} = \begin{cases} \dfrac{1}{l+1}, & j=l+\dfrac{1}{2}, \\ -\dfrac{1}{l}, & j=l-\dfrac{1}{2}. \end{cases} \tag{106}$$

Finally, the finite nucleus size (NS) with radius $r_{\rm N}^{(A)}$ brings a correction[18]

$$\Delta E^{\rm NS}_A(n,j) = \frac{4}{3}\left(\frac{\mu_A}{m_{\rm e}}\right)^3\frac{Z^4}{n^3}\left(\frac{r_{\rm N}^{(A)}}{a_\infty}\right)^2 R_\infty\delta_{l0} = \left(\frac{1}{1+b_A}\right)^3\frac{Z^4}{n^3}(4.386454987\times10^7) \times\left[\frac{r_{\rm N}^{(A)}(\text{fm})}{5.2917725}\right]^2\delta_{l0}\ \text{Hz}. \tag{107}$$

As explained in Eqs. (61) and (62), the value of off-mass-shell parameter ζ in Eq. (105) can be calculated from the electron self-energy at one-loop level as

$$\frac{Z^2\alpha}{n^2} = \frac{1}{2\pi}\frac{(\zeta^{\langle S\rangle} - 2\zeta^{\langle S\rangle}\ln\zeta^{\langle S\rangle})}{1+\alpha/3\pi}, \tag{108}$$

where the superscript $\langle S\rangle$ refers to "self-energy". However, we may derive the value of ζ in an alternative way. Divide the square average of four-dimensional momentum p into two parts:

$$\langle p^2\rangle = \langle E^2\rangle - \langle \boldsymbol{p}^2\rangle, \tag{109}$$

where

$$\langle E^2\rangle = E^2 = (\mu - B)^2 \simeq \mu^2 - 2\mu B, \tag{110}$$

since the binding energy

$$B = \frac{Z^2\alpha^2}{2n^2}\mu \ll \mu. \tag{111}$$

The square average of three-dimensional momentum $\boldsymbol{p}$, $\langle \boldsymbol{p}^2\rangle$, can be evaluated by the Virial theorem (e.g., Ref. [24]). In a Coulomb field, an electron has potential energy $V = -Ze^2/4\pi r$ and kinetic energy $T = \frac{1}{2\mu}\boldsymbol{p}^2$. Then

$$\begin{aligned}\langle \boldsymbol{p}^2\rangle &= 2\mu\langle T\rangle = 2\mu[-B - \langle V\rangle] = 2\mu B,\\ \langle p^2\rangle &= \mu^2 - 4\mu B = \mu^2\left(1 - \frac{4B}{\mu}\right).\end{aligned} \tag{112}$$

Comparing Eq. (112) with $\langle p^2\rangle = \mu^2(1-\zeta^{\langle V\rangle})$, we find

$$\zeta^{\langle V\rangle} = \frac{4B}{\mu} = \frac{2Z^2\alpha^2}{n^2}, \tag{113}$$

where the superscript $\langle V\rangle$ refers to "Virial theorem". Table 1 gives the values of $\zeta^{\langle S\rangle}$ and $\zeta^{\langle V\rangle}$ with their logarithm values as well as two kinds of "average", $\zeta^{\langle S+V\rangle} = \frac{1}{2}(\zeta^{\langle S\rangle} + \zeta^{\langle V\rangle})$ and $\zeta^{\langle SV\rangle} = \sqrt{\zeta^{\langle S\rangle}\zeta^{\langle V\rangle}}$, to be used in Eq. (105).

Table 1. Off-mass-shell parameter ζ and $\ln\zeta$.

Z^2/n^2	$\zeta^{\langle S\rangle}\times 10^4$	$-\ln\zeta^{\langle S\rangle}$	$\zeta^{\langle V\rangle}\times 10^6$	$-\ln\zeta^{\langle V\rangle}$	$\zeta^{\langle S+V\rangle}\times 10^5$	$-\ln\zeta^{\langle S+V\rangle}$	$\zeta^{\langle SV\rangle}\times 10^5$	$-\ln\zeta^{\langle SV\rangle}$
$\frac{1}{16}$	1.546093458	8.77461	$\frac{\alpha^2}{8} = 6.6564192$	11.91992886	8.0632	9.425609	3.2080284	10.34727
$\frac{1}{4}$	7.446539697	7.20259	$\frac{\alpha^2}{2} = 26.6256771$	10.5336345	38.5639	7.860609	14.0808	8.86816225
1	37.73719345	5.57969	$2\alpha^2 = 106.502$	9.147340142	194.011	6.2450103	63.39626	7.36351521

Now we are in a position to discuss a number of cases.

(I) The so-called classic Lamb shift of hydrogen atom, which was measured experimentally as[18]

$$\begin{aligned}L_{\rm H}^{\rm exp}(2{\rm S}\text{–}2{\rm P}) &\equiv E_{\rm H}(2{\rm S}_{1/2}) - E_{\rm H}(2{\rm P}_{1/2})\\ &= 1057.845\ {\rm MHz}.\end{aligned} \tag{114}$$

Theoretically, in this case ($b_{\rm H} = 5.446170255\times 10^{-4}$, $r_{\rm N}^{\rm H} = r_{\rm p} = 0.862$ fm, 1 fm=10^{-15} m), equations (102) and (103) make no contributions while euqations (104) and (107) only contribute

$$\begin{aligned}\Delta E_{\rm H}^{{\rm recoil}-2}(2{\rm S}_{1/2}\text{–}2{\rm P}_{1/2}) &= -E_{\rm H}^{{\rm recoil}-2}(2,1/2,1)\\ &= -2.16156\ {\rm kHz},\end{aligned} \tag{115}$$

and

$$\Delta E_{\rm H}^{\rm NS}(2{\rm S}\text{–}2{\rm P}) = 0.14525347\ {\rm MHz} \tag{116}$$

respectively. The dominant contribution comes from Eq. (105). If using $\zeta^{\langle S\rangle}$, we obtain

$$\begin{aligned}&\Delta E_{\rm H}^{{\rm rad}\langle S\rangle}(2{\rm S}\text{–}2{\rm P})\\ &= \frac{1}{1+b_{\rm H}}\frac{1}{8}(4.06931316\times 10^8)\\ &\quad\times\left[-\frac{8}{3}\ln\zeta^{\langle S\rangle} + \frac{7}{15} + 3\zeta^{\langle S\rangle} - \frac{4}{3}\zeta^{\langle S\rangle}\ln\zeta^{\langle S\rangle}\right]\\ &= 1000.6567\ {\rm MHz}.\end{aligned} \tag{117}$$

If we use other three values of $\ln\zeta$ in Table 1, correspondingly we obtain

$$\Delta E_{\rm H}^{{\rm rad}\langle V\rangle}(2{\rm S}\text{–}2{\rm P}) = 1451.7912\ {\rm MHz}, \tag{118}$$

$$\Delta E_{\rm H}^{{\rm rad}\langle S+V\rangle}(2{\rm S}\text{–}2{\rm P}) = 1089.6513\ {\rm MHz}, \tag{119}$$

$$\Delta E_{\rm H}^{{\rm rad}\langle SV\rangle}(2{\rm S}\text{–}2{\rm P}) = 1226.0871\ {\rm MHz}. \tag{120}$$

It seems that the value in Eq. (117) is smaller whereas the value in Eq. (118) too large. So as an empirical rule in our semiquantitative calculation, we may use Eq. (119) to obtain

$$\begin{aligned}L_{\rm H}^{\rm theor.}(2{\rm S}\text{–}2{\rm P}) &= 1089.651 + 0.145 - 0.002\\ &= 1089.794\ {\rm MHz},\end{aligned} \tag{121}$$

which is 3% larger than the value in Eq. (114).

(II) The Lamb shift of He^+ atom, which has been measured as (quoted from Ref. [7])

$$L_{\rm He^+}^{\rm exp}(2{\rm S}\text{–}2{\rm P}) = 14041.13(17)\ {\rm MHz}. \tag{122}$$

Similar to the case of hydrogen atom but with $Z = 2$ and $b_{\rm He^+} = m_{\rm e}/m_\alpha = 0.0001371$, we find

$$\begin{aligned}&\Delta E_{\rm He^+}^{{\rm rad}\langle S\rangle}(2{\rm S}\text{–}2{\rm P}) = 1.252680693\times 10^{10}\ {\rm Hz},\\ &\Delta E_{\rm He^+}^{{\rm rad}\langle V\rangle}(2{\rm S}\text{–}2{\rm P}) = 2.023083608\times 10^{10}\ {\rm Hz},\\ &\Delta E_{\rm He^+}^{{\rm rad}\langle S+V\rangle}(2{\rm S}\text{–}2{\rm P}) = 1.369980830\times 10^{10}\ {\rm Hz},\\ &\Delta E_{\rm He^+}^{{\rm rad}\langle SV\rangle}(2{\rm S}\text{–}2{\rm P}) = 1.636521214\times 10^{10}\ {\rm Hz}.\end{aligned} \tag{123}$$

As in the case of H atom, we take the $\langle S+V\rangle$ scheme and add

$$\Delta E_{\rm He^+}^{{\rm recoil}-2}(2{\rm S}\text{–}2{\rm P}) = -2.165\ {\rm kHz}, \tag{124}$$

$$\Delta E_{\rm He^+}^{\rm NS}(2{\rm S}\text{–}2{\rm P}) = 4.514\ {\rm MHz}, \tag{125}$$

($r_\alpha \simeq 1.2$ fm), to find the theoretical value to be

$$L^{\rm theor.}_{\rm He^+}(2{\rm S}\text{–}2{\rm P}) = 13704.220 \text{ MHz}, \tag{126}$$

which is 2.41% smaller than the value in Eq. (122).

(III) The following energy-level difference, which is related to the "hyper Lamb shift (HLS)" as follows:[18]

$$\begin{aligned}\Delta^{\rm exp}_{\rm H} &\equiv E_{\rm H}(4{\rm S}) - E_{\rm H}(2{\rm S}) - \frac{1}{4}[E_{\rm H}(2{\rm S}) - E_{\rm H}(1{\rm S})] \\ &= 4797.338(10) \text{ MHz}.\end{aligned} \tag{127}$$

Theoretically, now equation (102) makes the main contribution as follows:

$$\Delta E^{\rm RDE}_{\rm H}\left[(4{\rm S}) - \frac{5}{4}(2{\rm S}) + \frac{1}{4}(1{\rm S})\right] = 3923.95 \text{ MHz}. \tag{128}$$

(The notation in parenthesis is self-evident). Equations (103) and (105) contribute

$$\Delta E^{\rm recoil-1}_{\rm H}\left[(4{\rm S}) - \frac{5}{4}(2{\rm S}) + \frac{1}{4}(1{\rm S})\right] = -4.186 \text{ MHz}, \tag{129}$$

and

$$\begin{aligned}\Delta E^{{\rm rad}\langle S\rangle}_{\rm H} &= 451.229097 \text{ MHz}, \\ \Delta E^{{\rm rad}\langle S+V\rangle}_{\rm H} &= 529.288296 \text{ MHz}, \\ \Delta E^{{\rm rad}\langle SV\rangle}_{\rm H} &= 675.907131 \text{ MHz}, \\ \Delta E^{{\rm rad}\langle V\rangle}_{\rm H} &= 903.266275 \text{ MHz},\end{aligned} \tag{130}$$

respectively. Adding a small contribution from Eq. (107)

$$\Delta E^{\rm NS}_{\rm H}\left[(4{\rm S}) - \frac{5}{4}(2{\rm S}) + \frac{1}{4}(1{\rm S})\right] = 0.1270967854 \text{ MHz}, \tag{131}$$

we have

$$\begin{aligned}\Delta^{{\rm theor.}\langle S\rangle}_{\rm H} &= 4371.120197 \text{ MHz}, \\ \Delta^{{\rm theor.}\langle S+V\rangle}_{\rm H} &= 4449.179396 \text{ MHz}, \\ \Delta^{{\rm theor.}\langle SV\rangle}_{\rm H} &= 4595.798231 \text{ MHz}, \\ \Delta^{{\rm theore.}\langle V\rangle}_{\rm H} &= 3923.95 - 4.186 \\ &\quad + 903.266275 + 0.1271 \\ &= 4823.1574 \text{ MHz}.\end{aligned} \tag{132}$$

The $\langle V\rangle$ scheme is only 0.54% larger than Eq. (127). All other schemes each would give too small a value. So we guess that for S states $\langle V\rangle$ scheme is better than $\langle S\rangle$ scheme.

(IV) The following energy-level difference, which was also measured as[18]

$$\begin{aligned}\Delta'^{\rm exp}_{\rm H} &\equiv E_{\rm H}(4{\rm D}_{5/2}) - E_{\rm H}(2{\rm S}) \\ &\quad - \frac{1}{4}[E_{\rm H}(2{\rm S}) - E_{\rm H}(1{\rm S})] \\ &= 6490.144(24) \text{ MHz}.\end{aligned} \tag{133}$$

Theoretically, equation (102) also makes the main contribution

$$\Delta E^{\rm RDE}_{\rm H}\left[(4{\rm D}_{5/2}) - \frac{5}{4}(2{\rm S}) + \frac{1}{4}(1{\rm S})\right] = 5747.92 \text{ MHz}, \tag{134}$$

while

$$\Delta E^{\rm recoil-1}_{\rm H}\left[(4{\rm D}_{5/2}) - \frac{5}{4}(2{\rm S}) + \frac{1}{4}(1{\rm S})\right] = -4.18611 \text{ MHz}, \tag{135}$$

$$\Delta E^{\rm recoil-2}_{\rm H}[(4{\rm D}_{5/2})] = \alpha^4 m_{\rm e}(5.446170255 \times 10^{-4})^2\left(\frac{1}{3} - \frac{2}{5}\right) = -6.9283 \text{ kHz} \tag{136}$$

are all small, and we will have

$$\begin{aligned}\Delta' E^{{\rm rad}\langle S\rangle}_{\rm H}\left[(4{\rm D}_{5/2}) - \frac{5}{4}(2{\rm S}) + \frac{1}{4}(1{\rm S})\right] &= 302.088631 \text{ MHz}, \\ \Delta' E^{{\rm rad}\langle V\rangle}_{\rm H}\left[(4{\rm D}_{5/2}) - \frac{5}{4}(2{\rm S}) + \frac{1}{4}(1{\rm S})\right] &= 700.843464 \text{ MHz}, \\ \Delta' E^{{\rm rad}\langle S+V\rangle}_{\rm H}\left[(4{\rm D}_{5/2}) - \frac{5}{4}(2{\rm S}) + \frac{1}{4}(1{\rm S})\right] &= 369.124660 \text{ MHz}, \\ \Delta' E^{{\rm rad}\langle SV\rangle}_{\rm H}\left[(4{\rm D}_{5/2}) - \frac{5}{4}(2{\rm S}) + \frac{1}{4}(1{\rm S})\right] &= 500.131264 \text{ MHz}.\end{aligned} \tag{137}$$

Finally, the nucleus size effect gives

$$\Delta' E^{\rm NS}_{\rm H}\left[(4{\rm D}_{5/2}) - \frac{5}{4}(2{\rm S}) + \frac{1}{4}(1{\rm S})\right] = 11.62027752 \times 10^5\left(\frac{1}{4} - \frac{5}{4} \times \frac{1}{8}\right) = 0.10894 \text{ MHz}. \tag{138}$$

In summary, we have

$$\begin{aligned}
&\Delta'^{\langle S\rangle}_{\rm H} = \Delta' E^{\rm RDE}_{\rm H} + \Delta' E^{\rm recoil-1}_{\rm H} + \Delta' E^{\rm recoil-2}_{\rm H} + \Delta' E^{\rm rad\langle S\rangle}_{\rm H} + \Delta' E^{\rm rad\langle NS\rangle}_{\rm H} = 6045.925 \text{ MHz},\\
&\Delta'^{\langle V\rangle}_{\rm H} = 6444.679 \text{ MHz}, \quad \Delta'^{\langle S+V\rangle}_{\rm H} = 6112.961 \text{ MHz},\\
&\Delta'^{\langle SV\rangle}_{\rm H} = 6243.967 \text{ MHz}.
\end{aligned} \tag{139}$$

which are 6.8%, 0.7%, 5.8% and 3.8% smaller than the experimental value in Eq. (133) respectively.

(V) The combination of Eq. (127) with Eq. (133), which experimentally yields

$$\Delta''^{\rm exp}_{\rm H} \equiv E(4{\rm D}_{5/2}) - E(4{\rm S}_{1/2}) = 1692.806 \text{ MHz}. \tag{140}$$

Then, theoretically, we have

$$\Delta''^{\rm RDE}_{\rm H}(4{\rm D}_{5/2}{-}4{\rm S}) = 1.823886903 \times 10^9 \text{ Hz}, \tag{141}$$

$$\Delta''^{\rm recoil-1}_{\rm H}(4{\rm D}_{5/2}{-}4{\rm S}) = 1.1008 \text{ Hz}, \tag{142}$$

$$\Delta''^{\rm recoil-2}_{\rm H}(4{\rm D}_{5/2}{-}4{\rm S}) = -6.9283 \text{ kHz}, \tag{143}$$

$$\Delta''^{\rm NS}_{\rm H}(4{\rm D}_{5/2}{-}4{\rm S}) = -0.0181605862 \text{ MHz}, \tag{144}$$

and

$$\Delta''^{\rm rad\langle S\rangle}_{\rm H}(4{\rm D}_{5/2}{-}4{\rm S}) = -149.1404661 \text{ MHz}, \tag{145}$$

$$\Delta''^{\rm rad\langle V\rangle}_{\rm H}(4{\rm D}_{5/2}{-}4{\rm S}) = -202.4228107 \text{ MHz}, \tag{146}$$

$$\Delta''^{\rm rad\langle S+V\rangle}_{\rm H}(4{\rm D}_{5/2}{-}4{\rm S}) = -160.1636366 \text{ MHz}, \tag{147}$$

$$\Delta''^{\rm rad\langle SV\rangle}_{\rm H}(4{\rm D}_{5/2}{-}4{\rm S}) = -175.7758676 \text{ MHz}. \tag{148}$$

Altogether, we have

$$\begin{aligned}
&\Delta''^{\rm theor.\langle S\rangle}_{\rm H}(4{\rm D}_{5/2}{-}4{\rm S}) = 1674.721349 \text{ MHz}, \quad \Delta''^{\rm theor.\langle S+V\rangle}_{\rm H}(4{\rm D}_{5/2}{-}4{\rm S}) = 1663.716339 \text{ MHz},\\
&\Delta''^{\rm theor.\langle SV\rangle}_{\rm H}(4{\rm D}_{5/2}{-}4{\rm S}) = 1648.104108 \text{ MHz}, \quad \Delta''^{\rm theor.\langle V\rangle}_{\rm H}(4{\rm D}_{5/2}{-}4{\rm S}) = 1621.439105 \text{ MHz},
\end{aligned} \tag{149}$$

which are 1.1%, 1.7%, 2.6% and 4.2% smaller than the value in Eq. (140) respectively.

(VI) The accurate data of 2S–1S transition in hydrogen atom as discussed in Section 2, which are obtained by rewriting Eq. (7) as (see also Ref. [33]):

$$\Delta E^{\rm exp}_{\rm H}(2{\rm S}{-}1{\rm S}) = 2.46606141318734 \times 10^{15} \text{ Hz}. \tag{150}$$

Theoretically, we have [see Eq. (17)]

$$\Delta E^{\rm RDE}_{\rm H}(2{\rm S}{-}1{\rm S}) = 2.466067984 \times 10^{15} \text{ Hz}, \tag{151}$$

$$\Delta E^{\rm recoil-1}_{\rm H}(2{\rm S}{-}1{\rm S}) = 22.32598676 \text{ MHz}, \tag{152}$$

$$\begin{aligned}
&\Delta E^{\rm rad\langle S\rangle}_{\rm H}(2{\rm S}{-}1{\rm S}) = -5142.081146 \text{ MHz}, \quad \Delta E^{\rm rad\langle S+V\rangle}_{\rm H}(2{\rm S}{-}1{\rm S}) = -5765.958928 \text{ MHz},\\
&\Delta E^{\rm rad\langle SV\rangle}_{\rm H}(2{\rm S}{-}1{\rm S}) = -6835.535314 \text{ MHz}, \quad \Delta E^{\rm rad\langle V\rangle}_{\rm H}(2{\rm S}{-}1{\rm S}) = -8541.095068 \text{ MHz},
\end{aligned} \tag{153}$$

$$\Delta E^{\rm NS}_{\rm H}(2{\rm S}{-}1{\rm S}) = 11.62027752 \times 10^5 \left(\frac{1}{8} - 1\right) = -1.016774283 \text{ MHz}. \tag{154}$$

Taking the value of $\Delta E^{\rm rad}_{\rm H}(2{\rm S}{-}1{\rm S})$, we have

$$\begin{aligned}
&\Delta E^{\rm theor.\langle S\rangle}_{\rm H}(2{\rm S}{-}1{\rm S}) = 2.466062836 \times 10^{15} \text{ Hz}, \quad \Delta E^{\rm theor.\langle S+V\rangle}_{\rm H}(2{\rm S}{-}1{\rm S}) = 2.466062239 \times 10^{15} \text{ Hz},\\
&\Delta E^{\rm theor.\langle SV\rangle}_{\rm H}(2{\rm S}{-}1{\rm S}) = 2.466061169 \times 10^{15} \text{ Hz}, \quad \Delta E^{\rm theor.\langle V\rangle}_{\rm H}(2{\rm S}{-}1{\rm S}) = 2.466059464 \times 10^{15} \text{ Hz}.
\end{aligned} \tag{155}$$

They are 1450 MHz and 826 MHz larger than the value in Eq. (150) and 244 MHz and 1949 MHz smaller than the value in Eq. (150) respectively. Or, their discrepancies are $+5.9\times10^{-7}$, $+3.3\times10^{-7}$, -1.0×10^{-7}, -7.9×10^{-7}, respectively. These discrepancies basically stem from the uncertainty in the calculation of $\Delta E^{\rm rad}_{\rm H}(2{\rm S}{-}1{\rm S})$.

(VII) The isotope-shift of 2S–1S transition, which is obtained by rewriting Eq. (8) as

$$\Delta E^{\rm exp}_{\rm D-H}(2{\rm S}\text{–}1{\rm S}) = 6.70994337 \times 10^{11}\ {\rm Hz}. \tag{156}$$

Theoretically, rewriting Eqs. (19) and (20) yields

$$\Delta E^{\rm RDE}_{\rm D-H}(2{\rm S}\text{–}1{\rm S}) = 6.7101527879 \times 10^{11}\ {\rm Hz}, \tag{157}$$

and

$$\Delta E^{{\rm recoil}-1}_{\rm D-H}(2{\rm S}\text{–}1{\rm S}) = -11.176\ {\rm MHz}, \tag{158}$$

$$\Delta E^{{\rm rad}\langle S\rangle}_{\rm D-H}(2{\rm S}\text{–}1{\rm S}) = -1.399158\ {\rm MHz}, \quad \Delta E^{{\rm rad}\langle V\rangle}_{\rm D-H}(2{\rm S}\text{–}1{\rm S}) = -2.324028\ {\rm MHz},$$

$$\Delta E^{{\rm rad}\langle S+V\rangle}_{\rm D-H}(2{\rm S}\text{–}1{\rm S}) = -1.568915\ {\rm MHz}, \quad \Delta E^{{\rm rad}\langle SV\rangle}_{\rm D-H}(2{\rm S}\text{–}1{\rm S}) = -1.859945\ {\rm MHz}, \tag{159}$$

$$\Delta E^{\rm NS}_{\rm D-H}(2{\rm S}\text{–}1{\rm S}) = -5.11384949\ {\rm MHz}. \tag{160}$$

Altogether, we find [using $\langle V\rangle$ scheme in Eq. (159)]

$$\Delta E^{{\rm theor.}\langle V\rangle}_{\rm D-H}(2{\rm S}\text{–}1{\rm S}) = 6.709966701 \times 10^{11}\ {\rm Hz}, \tag{161}$$

which is 2.333 MHz larger than the value in Eq. (156) or has a deviation of only 3.5×10^{-6}. Evidently, even equation (157) solely deviates from Eq. (156) by 3×10^{-5} only. And as expected, the differences among schemes for $\Delta E^{\rm rad}_{\rm D-H}(2{\rm S}\text{–}1{\rm S})$ have little influence on the theoretical value, because any of the values in Eq. (159) are much smaller than the value induced by the nucleus size effect Eq. (160) ($r^{\rm D}_{\rm N} = r_{\rm d} = 2.115$ fm).

(VIII) The so-called absolute Lamb-shift of 1S state in hydrogen atom, which was determined by Weitz *et al.*[18] from the measured value in Eq. (127) or Eq. (133). In our notation, using Eq. (133), we will write it as follows:

$$L_{\rm H}(1{\rm S}) = 4\Big\{\Delta'^{\rm exp}_{\rm H} - \Delta E^{\rm RDE}_{\rm H}\Big[(4{\rm D}_{5/2}) - \frac{5}{4}(2{\rm S}) + \frac{1}{4}(1{\rm S})\Big] - \Delta E^{{\rm recoil}-1}_{\rm H}\Big[(4{\rm D}_{5/2}) - \frac{5}{4}(2{\rm S}) + \frac{1}{4}(1{\rm S})\Big]$$
$$- \Delta E^{{\rm recoil}-2}_{\rm H}(4{\rm D}_{5/2}) + \frac{5}{4}L_{\rm H}(2{\rm S}) - L_{\rm H}(4{\rm D}_{5/2})\Big\}. \tag{162}$$

Here the Lamb shift of 2S state $L_{\rm H}(2{\rm S})$ can be determined from the experimental value of Eq. (114) with $L_{\rm H}(2{\rm P}_{1/2})$ being calculated from Eq. (105),

$$L_{\rm H}(2{\rm S}) = L^{\rm exp}_{\rm H}(2{\rm S}\text{–}2{\rm P}) - \Delta E^{{\rm recoil}-2}_{\rm H}(2{\rm S}\text{–}2{\rm P}_{1/2}) + L_{\rm H}(2{\rm P}_{1/2}) = 1040.901\ {\rm MHz}. \tag{163}$$

And $L_{\rm H}(4{\rm D}_{5/2})$ can also be calculated from Eq. (105), so

$$L_{\rm H}(1{\rm S}) = 8188.478\ {\rm MHz}, \tag{164}$$

which is in agreement with 8172.874(60) MHz given by Ref. [18] within an accuracy of $\lesssim 0.2\%$. If we use Eq. (27) to derive $L_{\rm H}(1{\rm S})$, we need to calculate $L_{\rm H}(4{\rm S})$ which is much larger than $L_{\rm H}(4{\rm D}_{5/2})$ and its derivation from Eq. (105) seems not reliable. Similarly, the theoretical value of $L_{\rm H}(1{\rm S})$ turns out to be

$$L^{\rm theor.}_{\rm H}(1{\rm S}) = \Delta E^{\rm rad}_{\rm H}(1{\rm S}) + \Delta E^{\rm NS}_{\rm H}(1{\rm S}) \tag{165}$$

with $\Delta E^{\rm NS}_{\rm H}(1{\rm S}) = 0.14525347$ MHz. However, the value of $\Delta E^{\rm rad}_{\rm H}(1{\rm S})$ strongly depends on the scheme we used in Eq. (105), which must be narrowed in a high-loop calculation. The theoretical prediction was given in Ref. [7] as

$$L^{\rm theor.}_{\rm H}(1{\rm S}) = 8172754(14)(32)\ {\rm kHz}. \tag{166}$$

Further discussion can be found in Refs. [8], [34] and [35].

9. Summary and discussion

The remarkable progress of the experimental research on energy-level differences in hydrogen-like atoms has been making this field an ideal theoretical laboratory for physics.

i) The inevitable and successful application of reduced Dirac equation (RDE) to hydrogen-like atoms,

especially to the isotope-shift of 2S–1S transition as reflected by Eq. (156) through Eq. (161), is by no means an accidental fortune. It implies that the argument in Section 3 for introducing RDE, Eq. (41), is correct to a high accuracy. In particular, the basic principle of invariance under space–time inversion Eq. (42) (with original mass m) could remain valid even for a noninertial frame. This implication has a far-reaching consequence that a generalization at the above symmetry to a localized curved space–time may serve as a possible road to the quantization of the general theory of relativity.[25]

However, there are two realizations of potential V under the space–time inversion: Eq. (35) ("scalar" type) and Eq. (42) ("vector" type). While equation (42) is dominant in an atom like H with $m_{\rm p} \gg m_{\rm e}$, the remaining discrepancy of 2.333 MHz between theory and experiment [Eq. (161) versus Eq. (156)] strongly hints that an important and subtle effect has been ignored. (To consider the contribution of the deuteron polarizability merely accounts for about 20 kHz[9]). We think what may be neglected must be a tiny excitation of antiparticle field in the nucleus due to its interaction with electron in the CMCS. So when we reduce the degrees of freedom of two-body system from two to one, the RDE should be modified to take account of the tiny mixture of "scalar" potentials (see the page note after Eq. (42)). The modified RDE (MRDE) should still respect to the basic symmetry of space time inversion ad may lead to further corrections similar to but different from Eq. (103) and Eq. (104). We have not found the MRDE yet. However, an experimental evidence for the above conjecture could be the following prediction: the discrepancy between the present theory (with RDE) and the experiment must be smaller for the isotope shift in 2S–1S transition of atoms ^{4}He and ^{3}He than that of atoms H and D.

Recently, by using the Dirac's method, Marsch rigorously studied the hydrogen atom as a two-Dirac particle system bound by Coulomb force.[36] His solutions are composed of positive and negative pairs, corresponding respectively to hydrogen and antihydrogen as expected. However, surprisingly, in the hydrogen spectrum, besides the normal type-1 solution with reduced mass μ, there is another anomalous type-2 solution with energy levels: $E'_n = Mc^2 - 2\mu c^2 + \frac{1}{2}\mu c^2(\alpha/n)^2 + \cdots$ $(n = 1, 2, \ldots)$ and "strange enough, the type-2 ground state $(n = 1)$ does not have the lowest energy but the continuum $(n = \infty)$". In our opinion, based on what we learnt from the Dirac equation and RDE, these anomalous solutions imply a positron moving in the field of proton. So all discrete states with energy E'_n are actually unbound, and they should be and can be ruled out in physics either by the "square integrable condition" or the "orthogonality criterion" acting on their rigorous wave functions (for one-body Dirac equation, see Ref. [37], also pp. 28–31, 50 of Ref. [38]). On the other hand, all continuum states $(n = \infty)$ with energies lower than $Mc^2 - 2\mu c^2$ correspond to scattering wave functions with negative phase shifts , showing the repulsive force between positron and proton. (see Ref. [39], Subsection 1.5 in Ref. [38] or Subsection 9.5 of Ref. [24]). Marsch's discovery accurately reflects two things: a) the negative energy state of a particle just describes its antiparticle state; b) the Coulomb potential allows a complete set of solutions comprised of two symmetric sectors, i.e., hydrogen and antihydrogen. In the hydrogen sector, the proton remains unchanged regardless of the process of electron changing into positron under the Coulomb interaction.

The above particle–antiparticle symmetry (including Eq. (42) showing the unequal treatment between electron and nucleus), together with the parity symmetry, is hidden in the Dirac's four-component theory in covariant form, so they were overlooked to some extent in the past. The advantage or flexibility of two-component noncovariant form of Dirac equation or RDE (as discussed in this paper) lies in the fact that the above two symmetries become accurate and so easy to be extended (or violated) in an explicit manner. For completeness, we stress again that for antiparticle, one should use momentum and energy operators $\boldsymbol{p}_{\rm c} = {\rm i}\nabla$ and $E_{\rm c} = -{\rm i}\partial/\partial t$ instead of $\boldsymbol{p} = -{\rm i}\nabla$ and $E = {\rm i}\partial/\partial t$ for particle as required by the space–time inversion symmetry. The historical mission of the conception to imagine the positron as a "hole" in the sea of negative energy electrons is already over. Since the CPT invariance was further verified,[40] the relation between a particle $|a\rangle$ and its antiparticle $|\bar{a}\rangle$ has been well-established as[4)]

$$|\bar{a}\rangle = CPT|a\rangle \tag{167}$$

with their wave-functions (in free motion) being respectively

$$\langle \boldsymbol{x}, t|a\rangle \sim \exp\left[\frac{\rm i}{\hbar}(\boldsymbol{p}\cdot\boldsymbol{x} - Et)\right], \tag{168}$$

$$\langle \boldsymbol{x}, t|\bar{a}\rangle \sim \exp\left[-\frac{\rm i}{\hbar}(\boldsymbol{p}\cdot\boldsymbol{x} - Et)\right]. \tag{169}$$

[4)] To our knowledge, the correct definition, Eq. (167), was first given by T. D. Lee and C. S. Wu at *Ann. Rev. Nucl. Sci.* **15**, 381 (1965). See also G. J. Ni at *J. Fudan University* (Natural Science) No. 3–4, 125 (1974).

Note that in Eqs. (168) and (169), they have the same momentum $\boldsymbol{p}$ and positive energy E. Either a newly defined space–time inversion ($\boldsymbol{x} \to -\boldsymbol{x}$, $t \to -t$) or a simple change of $\mathrm{i} \to -\mathrm{i}$ will transform Eq. (168) into Eq. (169) (or *vice versa*).

ii) Throughout this paper, the electron bound in an atom is just treated as a stationary "ball" with nucleus at its centre and a (Bohr) radius of $\sim 1/\alpha m_{\rm e}$. However, it is in an off-mass-shell state (in some sense, our atom model is just opposite to J. J. Thomson's atom model suggested 100 years ago). In fact, the electron mass is reduced suddenly from $m_{\rm e}$ to μ in the RMCS when it is captured by a nucleus at the far remote orbit with quantum number $n \longrightarrow \infty$ and further reduced to $\mu + \delta\mu \simeq \mu - (Z^2\alpha^2/2n^2)\mu$ until n decreases to the lowest limit $n = 1$. The Lamb shift should be viewed as a further modification to the mass of an off-mass-shell electron due to radiative correction.

Notice that the parameter Q^2 in the vertex function, Eq. (87), means the square of (three-dimensional) momentum transfer when a free electron is on its mass-shell and collides with some other particles as discussed in Ref. [14]. By contrast, now Q^2 exhibits itself as an effective potential of δ-function type exerted by the nucleus on the bound (and so off-mass-shell) electron as shown by Eq. (92). To bind an electron to a nucleus is by a nonperturbative effect. Hence we can understand why the discrepancy between $\zeta^{\langle S\rangle}$ (calculated by perturbative QED at one-loop order) and $\zeta^{\langle V\rangle}$ (evaluated via nonperturbative Virial theorem) is so large. Fortunately, they lead discrepancies in the calculated values of Lamb shift to be not so large as those shown in Section 8. When $\zeta^{\langle V\rangle}$ or $\zeta^{\langle S+V\rangle}$ (or $\zeta^{\langle SV\rangle}$) is substituted into Eq. (105) which is derived from perturbative ($L = 1$) theory, we should always be aware of some theoretical inconsistency in such a semi-empirical treatment. But as a whole, we believe that the concept of Lamb shift as an off-mass-shell effect in covariant QED is basically correct.

iii) For a free on-mass-shell electron, its charge square $e_{\rm R}^2$ will increase with the increase of Q^2 as shown by Eq. (72) (with $\mu_3 = m_{\rm e}$, $q^2 = -Q^2$) and was calculated in detail in Ref. [17]. The calculation results are in agreement with the experimental data. Note that, however, the Ward identity $Z_1 = Z_2$ has been used. An interesting question arises for a bound electron: as its $e_{\rm R}^2$ is not a function of Q^2, will $e_{\rm R}^2$ change with quantum number n? To answer this question, we put Ward identity aside for a while and write down the renormalized $\alpha_{\rm R} = e_{\rm R}^2/4\pi$ as

$$\alpha_{\rm R} = \frac{Z_2^2}{Z_1^2} Z_3 \alpha \longrightarrow \frac{Z_2^2}{Z_1^2}\alpha. \tag{170}$$

We work in the CMCS, so $Z_2 = 1/(1-B)$ and B is shown in Eq. (53) but with μ replaced by $m_{\rm e} = m$. Similarly, Z_1 is given by the first part on the right-hand side of Eq. (87) with $\mu \longrightarrow m$:

$$Z_1 \simeq 1 + \frac{\alpha}{4\pi}\left[\frac{11}{2} - \ln\frac{m^2}{\mu_1^2} - 3\xi + 4(1+\xi)\ln\xi\right], \tag{171}$$

where the off-mass-shell parameter ξ in CMCS is defined by

$$\begin{aligned} p^2 &= m^2(1-\xi) = m^2(1-\eta-\zeta') = m^2(1-\eta) - m^2\zeta' \\ &= \mu^2 - m^2\zeta' = \mu^2(1-\zeta) \end{aligned} \tag{172}$$

with

$$m^2(1-\eta) = \mu^2, \quad \eta = 1 - \frac{\mu^2}{m^2}, \quad \zeta' = \frac{\mu^2}{m^2}\zeta, \tag{173}$$

and ζ is exactly that in Eq. (88). If we ignore the dependence of $(1-B)$ on ζ, equation (170) would give ($\zeta \ll 1$)

$$\alpha_{\rm R} = \alpha\left[1 + \frac{2\alpha}{\pi}\ln\left(1 + \frac{\zeta}{\eta}\right)\right] \tag{174}$$

after renormalization by adjusting the arbitrary constant μ_1 so that

$$\alpha_{\rm R}|_{\zeta\to 0} = \alpha, \tag{175}$$

which is related to the Thomson limit $\alpha_{\rm R}|_{Q\to 0} = \alpha$ for a free electron continuously but not smoothly. Then for two lowest bound states with $n = 1$ and $n = 2$, we would have (in $\langle V\rangle$ scheme)

$$\begin{aligned} &\alpha_{\rm R}|_{n=1} \simeq \alpha(1.000433832), \\ &\alpha_{\rm R}|_{n=2} \simeq \alpha(1.0001123). \end{aligned} \tag{176}$$

This would modify the Bohr energy level in hydrogen-like atom A into

$$\tilde{E}_A^{\rm Bohr}(n) = -\frac{Z^2\alpha_n^2}{2n^2}\mu_A, \tag{177}$$

and make an extra contribution to the isotope-shift as

$$\Delta\tilde{E}_{\rm D-H}^{\rm Bohr}(\text{2S–1S}) \simeq 726\ \text{MHz}, \tag{178}$$

which is definitely excluded in experiment. Hence the above consideration from Eq. (170) to Eq. (178) is wrong. We learn concretely once again that the Ward identity $Z_1 = Z_2$ is valid not only for an electron on its mass-shell, but also for off-mass-shell case. Thus

we use the same value of α throughout the whole calculation.

iv) In Ref. [17], using our RRM and new renormalization group equation (RGE) for QCD derived from it and keeping all masses of 6 quarks ($m_{\rm c}$ = 1.031 GeV, $m_{\rm b}$ = 4.326 GeV, $m_{\rm t}$ = 175 GeV, $m_{\rm s}$ = 200 MeV, $m_{\rm u}$ = 8 MeV, $m_{\rm d}$ = 10 MeV), we calculate the values of strong coupling constant $\alpha_{{\rm s}_i}(Q)$ for i=u, d, s, c, b respectively. Their running curves (starting from the common renormalization point $\alpha_{\rm s}$ ($M_{\rm Z}$) = 0.118) follow the trend of experimental data (as shown on p. 158 of Ref. [40]) quite well but separate in the low Q region. Interesting enough, each of them rises to a maximum $\alpha_{{\rm s}_i}^{\max}$ and then suddenly drops to zero at $Q = 0$ corresponding to a threshold energy scale $E_i^{\rm th}$ which could be explained as the excitation energy scale for breaking the quark pair. For example, we find $E_{\rm b}^{\rm th}$ = 1.13 GeV which is just the hadronization energy scale of upsilon $\Upsilon({\rm b\bar{b}})$ against its dissociation into two bosons. Experimentally, $M(\Upsilon(4{\rm s})) - M(\Upsilon)$ = 1.12 GeV and $\Upsilon(4{\rm s}) \to {\rm B^+B^-}$ or ${\rm B^0\bar{B}^0}$. Similarly, $E_{\rm c}^{\rm th} = 0.398$ GeV while $M(\psi(3770)) - M(\psi(3097))$ = 673 MeV and $\psi(3770) \to {\rm D^+D^-}$ or ${\rm D^0\bar{D}^0}$. It seems that $E_{\rm s}^{\rm th} \sim$ 90 MeV and $E_{\rm u,d}^{\rm th} \sim 0.4$ MeV are not so reliable but still reasonable.

Actually, our calculation on QCD is backed by that on QED. In Ref. [17], using our RRM and improved RGE, keeping all contributions from 9 charged leptons and quarks we are able to calculate the running fine-structure constant $\alpha_{\rm R}(Q)$ from the renormalization point $\alpha_{\rm R}(Q)|_{Q=0} = \alpha = (137.036)^{-1}$ until it coincides with the experimental value of $\alpha_{\rm exp}(M_{\rm Z}) = (128.89)^{-1}$. We fit quark masses as mentioned above and find no further room left for extra charged elementary particles (say, of 4th generation).

v) In 1989, we estimated the upper and the lower bounds on Higgs mass $M_{\rm H}$ by using a nonperturbative approach in QFT — the Gaussian effective potential (GEP) method, yielding:[41]

$$76 \text{ GeV} < M_{\rm H} < 170 \text{ GeV}. \tag{179}$$

Like many other authors, we were bothered a lot by divergences. After a deeper study on the $\lambda\phi^4$ model by using our new RRM,[16] we cope with this problem by combination GEP with RRM, yielding[13]

$$M_{\rm H} = 138 \text{ GeV}. \tag{180}$$

This is not an upper or a lower bound but a prediction based on the input of experimental data:

$$M_{\rm W} = 80.359 \text{ GeV}, \quad M_{\rm Z} = 91.1884 \text{ GeV},$$
$$\alpha^{-1} = \frac{4\pi}{g^2 \sin^2\theta_{\rm W}} = 128.89,$$
$$\sin^2\theta_{\rm W} = \frac{g'^2}{g^2 + g'^2} = 0.2317, \tag{181}$$

where $\theta_{\rm W}$ is the weak mixing (Weinberg) angle. Because of getting rid of all divergences, our calculation is well under control at each step. As now the search for Higgs particle becomes so urgent experimentally but the theoretical estimation about its mass still remains uncertain,[40] we think our approach with the prediction Eq. (180) deserves to be reconsidered.

vi) Moreover, our RRM can be used in $(D+1)$-dimensional space–time without limitation on the space dimension number D. A detailed analysis of sinh(sine)-Gordon models with $D = 1, 2$ and 3 (also using GEPM) was given by Ref. [14]. Another example is again the Lamb shift but calculated by QED in noncovariant form and by using RRM similar to that in this paper, see Appendix (Ref. [15], see also the Appendix 9A in Ref. [24]). The theoretical value of Eq. (A20) in Appendix seems better than the value in expression Eq. (121), showing that for dealing with the Lamb shift, the noncovariant theory may be more suitable than the covariant one at least in the lowest order.

vii) Previously, the theories for Lamb shift or generally for calculating energy levels in hydrogen-like atoms are rather complicated as reviewed in Refs. [1], [2] and [7], some of which have been discussed in the Appendix of this paper. For further clarity, we try to summarize the main obstacles, or challenges in four points: 1) different masses of nuclei must be taken into account; 2) relativistic effects of the electron (not nucleus) are important; 3) in calculating radiative corrections, the divergence becomes severer and severer with the increase of loop number; 4) since nuclei properties are different from one atom to another, to treat each atom as a two-body system individually would be a daunting task, it cannot be rigorous eventually either. This can be clearly seen from the recent work by Marsch.[36]

Facing these challenges and learning from lessons and experiences of previous authors, we see that the clue point is to replace the electron mass m by reduced mass μ and work in the noninertial frame (RMCS) throughout the entire calculation. As is well known, this can be handled in nonrelativistic QM by a mathematical trick but is impossible in relativistic case. So what we need is a new understanding of the essence of special relativity — the invariance (of theory) under the (newly defined) space–time inversion in one

inertial frame. Then we are able to claim the same invariance in the RMCS with μ replacing m for establishing the RDE, merely by ignoring a tiny centripetal acceleration of the nucleus in CMCS (see page note after Eq. (42)). The approximation in RDE is just a little price paid for the much bigger gain—improving the original Dirac equation (unable to treat different nuclei) and avoiding the confusion in QED calculation because of the entanglement of the centre-of-mass frames with RMCS (i.e., the radiative corrections are entangled with the recoil effect as we can see from previous literatures). In some senses, we jump over obstacles 1), 2) and 4) at the least labour cost (by constructing RDE). In the meantime, we hope that the RDE would be conducive to easing the difficulty in point 3). And it is a great pleasure to see that the essential correctness of our understanding is accurately validated by Marsch's work as well as puzzles raised in his paper.[36] Please see also Ref. [42].

As to challenge 3), only after we puzzled over the "divergence" for decades, could we suddenly realize that we misread its implication as a "large number". Rather, it means the "uncertainty". Now we look at the calculation in Section 4 again. Previously, many authors treated the divergent integral I in Eq. (50) by different tricks of regularization, arriving at Eq. (56). Because both A and B are divergent, it was thought that the original mass (μ here) did receive some radiative corrections (via the self-energy diagrams in Figs. 2(a) and 2(b)) and became a "renormalized" mass ($\mu_{\rm R}$ here). The latter should be the observed mass in experiment or physical mass (of electron). So the original mass is called the "bare mass", which is written into the Lagrangian density as an input parameter of QFT. Then in constructing Feynman diagrams of certain perturbative calculation, one needs to further introduce some (divergent) "counter terms" for cancelling the divergence stemming from the bare mass. Based on that understanding, the renormalization factor for wavefunction, Z_2 in Eq. (55), is a divergent quantity too (in sharp contrast to here Eq. (59) being a fixed and finite number). Previously, in Eq. (72), the $e_{\rm R}$ on the left-hand side was the observed charge which should be finite, but the e on the right-hand side was regarded as a "bare charge" which, together with the Z_3, was a divergent quantity. (see Figs. 7.8 in Ref. [32]. By contrast, here both Z_3 and e are finite. Actually, here e is defined as the physical charge observed at the Thomson limit in experiment).

In our opinion, the reason why we encountered so many superfluous troubles in the past is because we overlooked what Bethe said in 1947.[43] Please read his words quoted after Eq. (A2) in the Appendix. We explain it via our Eq. (46). The (reduced) mass (μ) already contains some contributions from self-energy diagrams like Figs. 2(a) and 2(b). When we evaluate the (divergent) integral, Eq. (50), trying to find the radiative corrections on the electron, the latter is bound to confuse with that already contained in the mass. In other words, the dividing line between them is blurred inevitably. The emergence of explicit divergence is essentially a warning to the fact that the effect you want to evaluate has been entangled with the mass itself, rendering both of them uncertain. Hence the aim of the so-called renormalization is nothing but to redraw a dividing line between them such that the values of masses reconfirmed by the experiment and the new effect (e.g., the mass increment when the electron moves off-mass-shell, Eq. (61)) can be clearly separated. In short, what we have been learning in the past decade is that at the level of QM, in the Hamiltonian like Eq. (A1) in Appendix, the parameters m and e can be regarded as being well-defined. But they are not so at the level of QFT. Once the calculation is made beyond the tree level, i.e., with loop number $L \geq 1$, the divergence occurs and the meaning of parameters becomes obscure immediately.

We need to reconfirm all parameters contained in the Lagrangian density before they can be linked with experiments. In this sense, a model of QFT is at most an "effective field theory". According to the above point of view, we believe that our RRM just provides a natural way to carry out these processes of reconfirmation,[16] getting rid of divergences and ambiguities. Please see also Ref. [44].

viii) Last but not least, during the learning and teaching of graduate courses on QFT for decades, we share the joy and puzzle with our students at all times. We hope that the presentation of this paper could be useful as being a teaching reference to render the QFT course more understandable, interesting and attractive.

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Appendix: Comparison between noncovariant and covariant theories for Lamb shift

To our knowledge, the exact theory for Lamb shift was based on a combination of noncovariant (nonrelativistic or old-fashioned) QED with covariant (or relativistic) QED as discussed in Ref. [7]. As explained clearly by Sakurai in Ref. [30], in perturbative QFT of noncovariant form, all virtual particles are "on-mass-shell". Here we wish to emphasize that a rigorous reconfirmation procedure of mass parameter is often overlooked in the previous literature. The theory for hydrogen-like atom begins with a Hamiltonian

$$H_0 = \frac{1}{2m}\boldsymbol{p}^2 + \frac{1}{2m_{\rm N}}\boldsymbol{p}^2 - \frac{Z\alpha}{r}, \tag{A1}$$

where $\boldsymbol{p} = -\,\mathrm{i}\,\nabla$ (see Eq. (34) in Ref. [7]). As Bethe[43] first pointed out that the effect of electron interaction with the vector potential $\boldsymbol{A}$ of radiation field (see Refs. [30] and [24])

$$H_{\rm int}^{(1)} = \frac{e}{mc}\boldsymbol{A}\cdot\boldsymbol{p} \tag{A2}$$

should properly be regarded as being already included in the observed mass $m_{\rm obs}$ of the electron, which is denoted by m in Eq. (A1). However, once a concrete calculation is made with Eq. (A2) being taken into account, the divergence emerges immediately. What does it mean? Mathematicians show that there are three implications for a divergence:

I) it is a dimensionless number;

II) it is a large number;

III) it is uncertain.

While we physicists often emphasize the point II), we do not pay enough attention to the points I) and III). We often talked about a quadratically (or linearly) divergent integral without noticing that it has a dimension (say, mass dimension) and thus meaningless in mathematics unless a mass parameter (say, m) in the integral is already fixed as a mass "unit" so that the integral can be divided by m^2 (or m) to become dimensionless. Alternatively, a logarithmically divergent integral is dimensionless and thus unaffected by the choice of unit [like Eq. (50), see also Eq. (A6) below], which just implies an uncertainty to be determined. The implication of uncertainty of a divergence will never vanish even after we have introduced a cutoff manipulatively to curb it. For example, in a pioneering paper to explain the Lamb shift, Welton (Ref. [45], see Subsection 9.6B in Ref. [24]) encountered an integral $I = \int_{\omega_{\rm min}}^{\omega_{\rm max}} \frac{\mathrm{d}\omega}{\omega}$ with ω being the (angular) frequency of virtual photon (vacuum fluctuation). He simply set $\omega_{\rm min} \sim mZ\alpha = Z/a$, ($a$ is Bohr radius) and $\omega_{\rm max} \sim m$ so that $I \simeq \ln(1/Z\alpha) = 4.92$ (for $Z = 1$) which leads to the estimation of Lamb shift $L_{\rm H}^{\rm theor.}(2{\rm S}_{1/2}$–$2{\rm P}_{1/2}) \simeq 668$ MHz. If instead of Bohr radius, the lower cutoff is provided by the electron binding energy, one should obtain $I \simeq \ln(Z\alpha)^{-2}$ and $L_{\rm H}^{\rm theor.} \simeq 1336$ MHz. (see Eq. (30) in Ref. [7]). The above arbitrariness just reflects what is essential in a divergent integral is not its large magnitude ($\ln(1/Z\alpha)$ is merely of the order of 10) but its uncertainty. So what is important in handling the integral is not to curb (or to hide) its divergence but let the divergence exhibit itself as some arbitrary constants explicitly (as shown in Sections 4–6). We will show later how to do this way for noncovariant QED.

While equations (A1) and (A2) only describe a spinless particle, the electron has spin which is endowed with the relativistic nature as shown by Eqs. (41)–(45). For a two-particle system, based on Bethe–Salpeter equation, an effective Dirac equation (EDE) was derived as shown by Eq. (23) in Ref. [7]. When the electromagnetic field interaction is taken into account, the Breit potential $V_{\rm Br}$ was derived as shown by Eq. (35) in Ref. [7]. Then the total Breit Hamiltonian reads (Eq. (36) in Ref. [7])

$$H_{\rm Br} = H_0 + V_{\rm Br}. \tag{A3}$$

However, the electron mass m' (in our notation here) appearing in EDE or $V_{\rm Br}$ should be that in the Dirac equation, also that in the definition of reduced mass $\mu = m'm_{\rm N}/(m' + m_{\rm N})$. Eventually m' could be identified with the observed mass $m_{\rm obs}$, which is not equal to m in Eq. (A1). This is because besides (A2) there is an extra interaction of electron spin with the radiation field:

$$H_{\rm int}^{(2)} = \frac{ge\hbar}{4\mu c}\boldsymbol{\sigma}\cdot\boldsymbol{\nabla}\times\boldsymbol{A}, \tag{A4}$$

where $g = 2\times 1.0011596522$ is the gyromagnetic ratio of electron, see Eq. (9A.15) in Ref. [24]. The difference between m and m' will be calculated in Eq. (A16) below. It turns out to be of the order of αm and cannot be ignored at the level of QED, especially for the explanation of Lamb shift. We guess that this must be one of the reasons why all calculations based on Eq. (A3) became so complicated.

In noncovariant theory, the leading contribution to the Lamb shift comes from the one-photon electron self-energy. The nomenclature here is different from that in the covariant theory. Roughly speaking, the so-called electron self-energy often corresponds to the vertex function in covariant theory (Fig. 2(d) in

this paper) or to Figs. 8 and 11 in Ref. [7] and its evaluations have extended over 50 years.[46] More accurately, it is identified with the radiative insertions in the electron line and the Dirac form factor contribution. Further contributions from the Pauli form factor and the vacuum polarization[7] will be added to a theoretical value of classic Lamb shift, 1050.559 MHz. If more high-order corrections are taken into account, the theoretical value coincides with the experimental value 1057.845 MHz rather accurately (see Table 20 in Ref. [7]). However, the above calculation looks quite complicated due to two reasons: one is the difficulty in dealing with two masses in two coordinate systems, i.e., the electron mass m and the reduced mass μ; another is the introduction of an auxiliary parameter σ $[m(Z\alpha) \gg \sigma \gg m(Z\alpha)^2]$ in order to separate the radiative photon integration region into two parts. In the low momentum region, the Bethe logarithm[47] in noncovariant form makes the main contribution. In the high momentum region, the evaluation resorts to some relativistic covariant form.[31] Then two expressions are matched together to obtain the correct result. It seems to us that the matching trick used is doubtful because both ultraviolet and infrared divergences were ambiguously handled by some cutoff which missed the main point of renormalization—to reconfirm the mass parameter in the presence of radiative corrections as shown in Section 4 (covariant form) or below.

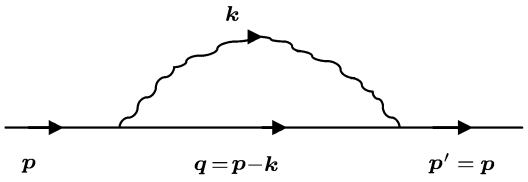


Fig. 3. Electron self-energy (radiative correction) diagram at one-loop level of perturbative QCD in noncovariant form. $H_{\rm int}^{(1)}$ (A2) or $H_{\rm int}^{(2)}$ (A4) is inserted into two vertices. Here $\boldsymbol{p}$, $\boldsymbol{q}$ and $\boldsymbol{k}$ denote three-dimensional momenta.

A simple calculation for Lamb shift in noncovariant form was proposed in Ref. [15] (see also Appendix 9A of Ref. [24]). Consider the self-energy diagram of an electron with reduced mass μ and (three-dimensional) momentum $\boldsymbol{p}$ in the RMCS of a hydrogen-like atom. Similar to, but also different in virtual state from Fig. 2(a), now a photon has energy $\omega_k = k = |\boldsymbol{k}|$ while the electron has momentum $\boldsymbol{q} = \boldsymbol{p} - \boldsymbol{k}$ and energy $\varepsilon_q = (1/2\mu)q^2$. The electron in plane-wave state $|\boldsymbol{p}\rangle$ has two interactions with the radiative field at each vertex as shown by Eqs. (A2) $(m \to \mu)$ and (A4), acquiring an increase in energy respectively (see Fig. 3):

$$\Delta E_p^{(j)} = \sum_i \frac{|\langle i|H_{\rm int}^{(j)}|\boldsymbol{p}\rangle|^2}{\varepsilon_p - \varepsilon_i}, \quad (j = 1, 2). \tag{A5}$$

Here $\varepsilon_i = \varepsilon_q + \omega_k$ is the energy of the intermediate virtual state $|i\rangle$. Simple evaluation leads to

$$\Delta E_p^{(1)} = -\frac{\alpha p}{\pi\mu}\int_{-1}^{1} {\rm d}\eta(1-\eta^2)I,$$
$$I = \int_0^\infty \frac{{\rm d}k}{k+\xi}, \tag{A6}$$

where $\eta = \cos\theta$ with θ being the angle between $\boldsymbol{k}$ and $\boldsymbol{p}$, $\xi = 2(\mu - p\eta)$. Like Eq. (50), we take partial derivative of the divergent integral I with respect to ξ (then the integration of k) and integrate back to I again, yielding

$$\Delta E_p^{(1)} = b_1^{(1)}p^2 + b_2^{(1)}p^4 + \cdots, \tag{A7}$$

$$b_1^{(1)} = \frac{\alpha}{\pi\mu}\left(\frac{4}{3}\ln 2 + \frac{4}{3}\ln\mu - \frac{4}{3}C_1\right), \tag{A8}$$

$$b_2^{(1)} = \frac{\alpha}{\pi\mu^3}\left(-\frac{2}{15}\right). \tag{A9}$$

Note that the term $b_1^{(1)}p^2$ will combine with the kinetic energy $(1/2\mu)p^2$ of a ("spinless") electron, they are indistinguishable. The appearance of an arbitrary constant C_1 accurately reflects the fact that we cannot find the reduced mass via the valuation of $\Delta E_p^{(1)}$ in perturbation theory. So we must choose $b_1^{(1)} = 0$ to reconfirm the value of μ (which is still not the final observed mass, see below). A similar evaluation on $H_{\rm int}^{(2)}$ (of the real electron with spin 1/2) which would induce the spin flip process between states $|\boldsymbol{p}, \pm\frac{1}{2}\rangle$ and $|\boldsymbol{q}, \pm\frac{1}{2}\rangle$, leads to

$$\Delta E_p^{(2)} = \frac{1}{2}\sum_{i,s_z=\pm 1/2}\frac{|\langle i|H_{\rm int}^{(2)}|\boldsymbol{p}, s_z\rangle|^2}{\varepsilon_p - \varepsilon_i}$$
$$= -\frac{\alpha g^2}{8\pi\mu}\int_{-1}^{1}{\rm d}\eta J$$

with

$$J = \int_0^\infty \frac{k^2{\rm d}k}{k+\xi} \tag{A10}$$

being a quadratically divergent integral, J needs partial derivative of third order with respect to ξ, yielding

$$\Delta E_p^{(2)} = b_0^{(2)} + b_1^{(2)}p^2 + b_2^{(2)}p^4 + \cdots, \tag{A11}$$

$$b_0^{(2)} = \frac{g^2}{4}\frac{\alpha\mu}{\pi}\left[4(\ln 2 + \ln\mu) - 4C_2 - \frac{2C_3}{\mu} - \frac{C_4}{\mu^2}\right], \tag{A12}$$

$$b_1^{(2)} = \frac{g^2}{4}\frac{\alpha}{\pi\mu}\left(\frac{4}{3}\ln 2 + 2 + \frac{4}{3}\ln\mu - \frac{4}{3}C_2\right), \tag{A13}$$

$$b_2^{(2)} = \frac{g^2}{4}\frac{\alpha}{\pi\mu^3}\Big(-\frac{1}{15}\Big). \tag{A14}$$

We manage to fix three arbitrary constants C_2, C_3 and C_4. First, the term $b_1^{(2)}p^2$ should be combined with $(1/2\mu)p^2$ term. Since μ is already fixed, further modification to μ due to electron spin should be finite and fixed. So the only possible choice of C_2 is to cancel $\ln\mu$ which is ambiguous in dimension: $C_2 = \ln\mu$, yielding

$$b_1^{(2)} = \frac{\beta}{2\mu}, \quad \beta = \frac{g^2\alpha}{2\pi}\Big(\frac{4}{3}\ln 2 + 2\Big). \tag{A15}$$

Then the dimensional constants C_3 and C_4 must be chosen such that $b_0^{(2)} = 0$, implying that the starting point of this theory is the nonrelativistic Hamiltonian H_0 in Eq. (A1) without rest energy term while both masses of the nucleus and the electron (with spin) are fixed by experiment. Hence now μ acquires a modification via $b_1^{(2)}p^2$ term and becomes an observable one

$$\mu \longrightarrow \mu_{\rm obs} = \frac{\mu}{1+\beta}. \tag{A16}$$

However, we need to consider the relativistic energy of electron shown in Eq. (30), where the term $(-(1/8\mu^3)p^4)$ goes beyond Eq. (A1). Yet the modification of μ as shown in Eq. (A16) does induce a corresponding change $-\frac{1}{8}(1/\mu_{\rm obs}^3 - 1/\mu^3)p^4$, which should be regarded as being an invisible "background" and subtracted from the p^4 term induced by radiative corrections. (The relativistic correction is brought in via the RDE as discussed in Section 8). As a whole, the combination of contributions from $H_{\rm int}^{(1)}$ and $H_{\rm int}^{(2)}$ leads to

$$b_1 = b_1^{(1)} + b_1^{(2)} = b_1^{(2)} \tag{A17}$$

and a "renormalized" b_2

$$\begin{aligned} b_2^{\rm R} &= b_2^{(1)} + b_2^{(2)} + \frac{1}{8\mu^3}(3\beta + 3\beta^2 + \beta^3) \\ &\simeq \frac{\alpha}{\pi\mu_{\rm obs}^3}(1.99808). \end{aligned} \tag{A18}$$

Here we only keep the lowest approximation at the last step. Hence the electron self-energy-diagram contributes a radiative correction to the energy level of the stationary state $|Z,n,l\rangle$ in a hydrogen-like atom

$$\begin{aligned} \Delta E^{\rm rad}(Z,n,l) &= \langle Z,n,l|b_2^{\rm R}p^4|Z,n,l\rangle \\ &= \Big[\frac{8n}{2l+1} - 3\Big]\frac{b_2^{\rm R}Z^4\alpha^4}{n^4}\mu_{\rm obs}^4. \end{aligned} \tag{A19}$$

This form, together with contributions from the vacuum polarization and the nuclear size effect, gives a theoretical value for classic Lamb shift as

$$L_{\rm H}^{\rm theor.}(2{\rm S}_{1/2}\text{–}2{\rm P}_{1/2}) \approx 1056.52 \text{ MHz}, \tag{A20}$$

which is 0.13% smaller than the experimental value. Despite its approximation involved, the above method clearly shows that the so-called renormalization is nothing but a reconfirmation process of mass. We must reconfirm the mass before it can be modified via radiative corrections. Either "skipping over the first step" or "combining two steps into one" is not allowed.

In noncovariant theory, the (three-dimensional) momentum $\boldsymbol{p}$ is combined with the reduced mass μ to form a kinetic energy term $(1/2\mu)\boldsymbol{p}^2$ on the mass shell. Once the energy is modified whereas $\boldsymbol{p}$ is conserved at the vertex, μ is bound to be modified. On the other hand, in covariant theory, the electron energy turns into a component of four-dimensional momentum p and the latter is conserved at the vertex. So the (reduced) mass μ cannot be modified on the mass shell ($p^2 = \mu^2$). Therefore, the renormalization as some reconfirmation has a different meaning in covariant theory from that in noncovariant theory. We guess that this is why the matching procedure of these two formalisms into one theory for Lamb shift proves so difficult.

The establishment of every theory in physics implies not only a discovery of natural law, but also an invention of human being.[48] Hence the comparison among various theories, in many cases, is not about a problem of being right or wrong. Rather, it is about a choice of simplicity, harmony (self-consistency) and beauty. Only time can tell what will be in the future.

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