Lamb Shifts in Muonium and Hydrogen Atom

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We present a new calculation of the center of mass (CM) corrections on the Lamb shifts energy in muonium ($\mu^+ \ e^-$ system) and hydrogen atom. It turns out that the good agreement so far obtained for the Lamb shifts energy between theory and experiment is seriously destroyed by the CM effects. This should give rise to a question as to what should be a solution for the Lamb shifts energy in atoms since Bethe's standard calculation has an intrinsic problem of the logarithmic divergence. Also, we discuss some differences between recoil corrections of Barker-Glover model and the center of mass effects of the present calculation. The main difference comes from the fact that the spin-orbit term is missing in the non-hermite Hamiltonian of Barker-Glover model while we make a physically plausible approximation starting from well established Hamiltonian, though not necessarily perturbative.

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I. INTRODUCTION

It is believed that the observed Lamb shifts energy is reproduced very well by Bethe's calculation which is based on the renormalization procedure of the fermion self-energy diagrams [1]. In this case, however, the calculation has the logarithmic divergence as is well-known, but this divergence is removed in terms of the very artificial manipulation, though quite difficult to understand. This theoretical formula with the very "precise Lamb shifts energy" in hydrogen atom is written as [2–4]

$$\Delta E_{2s_{\frac{1}{2}}-2p_{\frac{1}{2}}} = \frac{m\alpha^5}{6\pi}\left[\log\frac{m}{2 < E_I - E_{n=2,\ell=0} >_{av}} + \frac{11}{24} - \frac{1}{5} + \frac{1}{2}\right] \tag{1.1}$$

which is given in most of the field theory textbooks [5]. The experimental value is reported as [6, 7]

$$\Delta E^{\rm exp}_{(2s_{\frac{1}{2}}-2p_{\frac{1}{2}})}(\text{Hydrogen}) = (4.3750 \pm 0.0001) \times 10^{-6} \quad \text{eV} \tag{1.2}$$

while the theoretical prediction of eq.(1.1) becomes

$$\Delta E^{\rm the}_{(2s_{\frac{1}{2}}-2p_{\frac{1}{2}})}(\text{Hydrogen}) = 4.3743 \times 10^{-6} \quad \text{eV} \tag{1.3}$$

which perfectly agrees with experiment, though the agreement looks too good. However, the derivation of eq.(1.1) is extremely difficult to understand as already pointed out in the textbook of Sakurai [5]. The reason of the difficulty in understanding eq.(1.1) is related to the derivation itself since people made use of the infra-red divergence to cancel out the ultra-violet divergence by manipulating them in some way or the other. But the physical origins of the infra-red and ultra-violet divergences are completely different from each other, and therefore it is physically very difficult to accept eq.(1.1) itself.

Now the Lamb shifts energy in muonium is also measured, and the observed value of the Lamb shifts in muonium is found to be [8–10]

$$\Delta E^{\rm exp}_{2s_{\frac{1}{2}}-2p_{\frac{1}{2}}}(\text{Muonium}) = (4.31 \pm 0.09) \times 10^{-6} \quad \text{eV} \tag{1.4}$$

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while the theoretical value of the Lamb shifts energy in muonium becomes

$$\Delta E^{\text{the}}_{2s_{\frac{1}{2}}-2p_{\frac{1}{2}}}(\text{Muonium}) = 4.35 \times 10^{-6} \quad \text{eV} \tag{1.5}$$

where the main deviation from the hydrogen atom case is considered to be due to the vacuum polarization contributions [11–14]. Here, the agreement between theory and experiment is very good indeed.

However, we show below that there exists the contribution to the Lamb shifts energy from the higher order center of mass correction which is always there and an inevitable effect since muonium is indeed composed out of electron and muon. In addition, one body Dirac equation, though solved exactly, is of course, an approximate equation for muonium. In this case, we should add the center of mass correction of the Lamb shifts energy to Bethe's result, and the total Lamb shifts energy of muonium becomes

$$\Delta E^{\text{the}}_{2s_{\frac{1}{2}}-2p_{\frac{1}{2}}} \simeq 4.93 \times 10^{-6} \quad \text{eV} \tag{1.5}$$

which completely destroys the agreement of the theoretical prediction with the muonium experiment of Lamb shifts energy. This is very serious, and it is clear that we should reconsider the basic mechanism of the Lamb shifts energy from the beginning. At least, Bethe's calculation is now inconsistent with experiment, and this strongly suggests that the resolution of the degeneracy in the $2s_{\frac{1}{2}}$ and $2p_{\frac{1}{2}}$ states in hydrogen atom may not necessarily be due to the mass renormalization procedure of the self-energy of fermions [15]. But it is, at present, an open problem.

II. BARKER-GLOVER MODEL ON LAMB SHIFTS

Barker and Glover first obtained the one body reduced Hamiltonian starting from the two body Dirac equation [16]. However, they used the approximation scheme of Bethe-Salpeter equation [17] which does not necessarily give an hermite Hamiltonian [18, 19]. The validity of the Bethe-Salpeter equation is discussed in detail in terms of the two dimensional field theory model calculations [20], and one sees that the Bethe-Salpeter approximation does not agree with the exact diagonalization result when the relativity becomes important [20, 21].

A. Negative Energy State

In the Bethe-Salpeter equation, one takes into account the negative energy states explicitly. However, the particle and anti-particle pair creations are calculated in such a way that the transformation is not unitary, and thus this method should naturally give rise to the non-hermite Hamiltonian. On the other hand, the Bogoliubov transformation of one vacuum to the other is unitary, and thus this does not have such a difficulty. In order to see it more explicitly, we define the vacuum states $|0\rangle_{BS}$ in the Bethe-Salpeter equation as

$$\hat{Q}|0\rangle_{BS} = 0 \tag{2.1}$$

with

$$\hat{Q}^\dagger = \sum_n (X_n a_n^\dagger b_{-n}^\dagger + Y_n b_{-n} a_n) \tag{2.2}$$

where $a_n^\dagger$ and $b_n^\dagger$ denote the creation operators of the particle and anti-particle states, respectively. We see that this transformation of the original vacuum $|0\rangle$ to the Bethe-Salpeter vacuum $|0\rangle_{BS}$ is not necessarily unitary. On the other hand, the Bogoliubov vacuum state $|\Omega\rangle$ is defined as

$$|\Omega\rangle = e^{-\sum_n \theta_n (a_n^\dagger b_{-n}^\dagger - b_{-n} a_n)}|0\rangle \tag{2.3}$$

where θ_n are variational parameters. As one sees, the Bogoliubov transformation is unitary, and therefore the Hamiltonian one obtains after the variational principle should be hermite.

B. Missing of Spin-Orbit Effects

The Hamiltonian obtained by Barker and Glover does not have any spin-orbit terms from the proton recoil corrections. This can be understood in the following way. In the non-relativistic expansion, the correction terms due to the motion of electron and proton should appear in terms of $\frac{\boldsymbol{p}}{m}$ and $\frac{\boldsymbol{P}}{M_p}$, respectively, and therefore the spin-orbit term should have the following shape for electron

$$H_{so}^{e} \simeq c_0 e \left(\boldsymbol{\sigma} \cdot \frac{\boldsymbol{E}}{m}\right)\left(\boldsymbol{\sigma} \cdot \frac{\boldsymbol{p}}{m}\right) \simeq -\frac{e}{4m^2}\boldsymbol{\sigma} \cdot \boldsymbol{E} \times \boldsymbol{p} \tag{2.4}$$

where $\boldsymbol{\sigma}$ denotes the spin operator of electron and c_0 is a numerical constant. In the case of proton motion, we may obtain

$$H_{so}^{p} \simeq c_1 e \left(\boldsymbol{\sigma}_p \cdot \frac{\boldsymbol{E}}{M_p}\right)\left(\boldsymbol{\sigma}_p \cdot \frac{\boldsymbol{P}}{M_p}\right) \simeq \frac{e}{4M_p^2}\boldsymbol{\sigma}_p \cdot \boldsymbol{E} \times \boldsymbol{p}. \tag{2.5}$$

However, this spin-orbit interaction is smaller of the order $\left(\frac{m}{M_p}\right)^2$ than the normal spin-orbit interaction and, it is obviously much too small as a correction term of the center of mass effect. At this point, a question may arise as to whether we may find the following shape for the spin-orbit interaction term or not

$$H'_{so} \simeq c_2 e \left(\boldsymbol{\sigma}_p \cdot \frac{\boldsymbol{E}}{M_p}\right)\left(\boldsymbol{\sigma} \cdot \frac{\boldsymbol{p}}{m}\right). \tag{2.6}$$

However, this term cannot induce the normal spin-orbit force, and thus the recoil correction of proton cannot give rise to the spin-orbit interaction at the correction factor of $\frac{m}{M_p}$, and this is just consistent with the calculated results of Barker and Glover. In fact, they could not find any spin-orbit interaction terms at the correction factor of $\frac{m}{M_p}$ in comparison with the normal spin-orbit term.

III. REALISTIC CALCULATIONS OF CENTER OF MASS EFFECTS

The most important point is that we do not know how we can solve the Dirac equation properly for the two body system, and therefore, we should develop a reliable method to evaluate the center of mass corrections for the $2s_{\frac{1}{2}}$ and $2p_{\frac{1}{2}}$ states. As we see above, the model calculation of Barker and Glover cannot give rise to a correct center of mass effect, and therefore we present a new evaluation of the center of mass effects.

Here, we start from the higher order Hamiltonian of the non-relativistic expansion in the Foldy-Wouthuysen transformation for lepton and proton [22]

$$H = m + M_p + \frac{\boldsymbol{P}^2}{2M_p} + \frac{1}{2m}(\boldsymbol{p} - e\boldsymbol{A})^2 + e\Phi - \frac{e}{2m}\boldsymbol{\sigma} \cdot \boldsymbol{B} \tag{3.1a}$$

$$H' = -\frac{\boldsymbol{p}^4}{8m^3} - \frac{e}{4m^2}\boldsymbol{\sigma} \cdot \boldsymbol{E} \times \boldsymbol{p} - \frac{e}{8m^2}\boldsymbol{\nabla} \cdot \boldsymbol{E} \tag{3.1b}$$

where H' term denotes the higher order effects which are relevant to the present discussion. This Hamiltonian is well examined and there is no doubt that this is a correct Hamiltonian which can describe the spectrum of the hydrogen-like atoms. Now, we define the reduced mass μ as

$$\mu = \frac{mM_p}{m + M_p} = m\left(1 + \frac{m}{M_p}\right)^{-1} \tag{3.2a}$$

and thus m can be written as

$$m = \mu\left(1 + \frac{m}{M_p}\right). \tag{3.2b}$$

Therefore, we can rewrite all the Hamiltonian in terms of μ as

$$H_{NR} = \frac{1}{2\mu}(\boldsymbol{p} - e\boldsymbol{A})^2 - \frac{e^2}{r} - \frac{e}{2\mu}\boldsymbol{\sigma}\cdot\boldsymbol{B} - \frac{\boldsymbol{p}^4}{8\mu^3} - \frac{e}{4\mu^2}\boldsymbol{\sigma}\cdot\boldsymbol{E}\times\boldsymbol{p} - \frac{e}{8\mu^2}\boldsymbol{\nabla}\cdot\boldsymbol{E} \tag{3.3}$$

where the mass term and the center of mass motion term are not written here. It is important to examine that this Hamiltonian should indeed give the degenerate energy spectrum of $2s_{\frac{1}{2}}$ and $2p_{\frac{1}{2}}$, and in fact, one can easily reproduce the degeneracy of the two states. Therefore, we should note that eqs.(3.1) is indeed a correct Hamiltonian which is well examined experimentally.

In addition, there are new terms which should be of the order of $\mathcal{O}\left(\frac{m}{M_p}\right)$ higher than H_{NR} of eq.(3.3), and these terms correspond to the higher order center of mass correction effects.

IV. HIGHER ORDER CENTER OF MASS CORRECTIONS IN MUONIUM

Now we discuss the higher order center of mass effects in muonium. In this case, the mass of muon is 105.66 MeV while electron is 0.511 MeV. This clearly indicates that the higher order center of mass effect in muonium must be much more important than the hydrogen atom case. Here, we start from the higher order Hamiltonian of the non-relativistic expansion in the Foldy-Wouthuysen transformation for electron and muon as given in eqs.(3.1) where M_p should be replaced by m_μ [22, 23].

A. Higher Order Center of Mass Corrections in Muonium

Now, there should be left some important terms which must be of the order of $\frac{m}{m_\mu}$. This is a correction term which should come from the H' Hamiltonian when replacing m by μ using eq.(3.2b), and we can write it as

$$H'_{\rm CM} = \left(\frac{3m}{m_\mu}\right)\frac{\boldsymbol{p}^4}{8\mu^3} + \left(\frac{2m}{m_\mu}\right)\frac{e}{4\mu^2}\boldsymbol{\sigma}\cdot\boldsymbol{E}\times\boldsymbol{p} + \left(\frac{2m}{m_\mu}\right)\frac{e}{8\mu^2}\boldsymbol{\nabla}\cdot\boldsymbol{E} \tag{4.1}$$

which corresponds to the higher order corrections for the kinetic energy, spin-orbit and the Darwin terms arising from the center of mass replacement. In some sense, the procedure of obtaining this Hamiltonian from the replacement of eq.(3.2) should be neither perturbative nor due to the non-relativistic reduction, and therefore, it is quite natural that the correction terms are very different from the Barker-Glover result. But it is clear that the effect should be there.

As can be seen, this Hamiltonian from the center of mass corrections should be repulsive. Now, we can carry out the calculations of the above Hamiltonian in muonium, and the calculated results for the $2s_{\frac{1}{2}}$ and $2p_{\frac{1}{2}}$ states become

$$\begin{cases} \Delta E_{2s}^{\rm CM} = \frac{23}{64}\frac{m}{m_\mu}\frac{\mu\alpha^4}{2} & \text{for} \quad 2s_{\frac{1}{2}} \\ \Delta E_{2p}^{\rm CM} = \frac{13}{192}\frac{m}{m_\mu}\frac{\mu\alpha^4}{2} & \text{for} \quad 2p_{\frac{1}{2}}. \end{cases} \tag{4.2}$$

In this case, the higher order center of mass correction effect on the Lamb shifts in muonium amounts to

$$\Delta E_{2s_{\frac{1}{2}}-2p_{\frac{1}{2}}}^{\rm CM} \simeq 0.58\times 10^{-6} \quad \text{eV}. \tag{4.3}$$

Therefore, the total Lamb shifts energy in muonium becomes

$$\Delta E_{(2s_{\frac{1}{2}}-2p_{\frac{1}{2}})}^{\rm the}(\text{Muonium}) \simeq 4.93\times 10^{-6} \quad \text{eV} \tag{4.4}$$

which should be compared with the experimental value as shown in eq.(1.4)

$$\Delta E_{2s_{\frac{1}{2}}-2p_{\frac{1}{2}}}^{\rm exp}(\text{Muonium}) = (4.31\pm 0.09)\times 10^{-6} \quad \text{eV}.$$

As one sees, the agreement is now completely destroyed by the center of mass effect which should be just the most fundamental term in the Lamb shifts energy in muonium. This shows that we have to reconsider the basic mechanism of the Lamb shifts energy in some way or the other. At present, we do not know any possible mechanism for explaining the discrepancy.

B. Higher Order Center of Mass Corrections in Hydrogen Atom

Here, we should make a comment on the effect of higher order center of mass corrections in hydrogen atom even though the effect is not so large as the muonium case. The calculation of the center of mass effect on the Lamb shifts energy in hydrogen atom can be carried out, and the calculated result becomes

$$\Delta E^{\rm CM}_{(2s_{\frac{1}{2}}-2p_{\frac{1}{2}})}(\text{Hydrogen}) = 0.067\times 10^{-6} \quad \text{eV} \tag{4.5}$$

and, therefore, the total Lamb shifts energy in hydrogen atom becomes

$$\Delta E^{\rm the}_{(2s_{\frac{1}{2}}-2p_{\frac{1}{2}})}(\text{Hydrogen}) = 4.441\times 10^{-6} \quad \text{eV} \tag{4.6}$$

which should be compared with the observed value

$$\Delta E^{\rm exp}_{(2s_{\frac{1}{2}}-2p_{\frac{1}{2}})}(\text{Hydrogen}) = (4.3750\pm 0.0001)\times 10^{-6} \quad \text{eV}. \tag{4.7}$$

We see now that the center of mass correction term also destroys the excellent agreement so far obtained for the Lamb shifts energy in hydrogen atom, even though it is much less pronounced than the muonium case.

V. INFRA-RED AND ULTRA-VIOLET DIVERGENCES IN LAMB SHIFTS

Here we should make a comment on the treatment of the divergences in the Lamb shifts in connection with Bethe's calculation. The calculation by Bethe has a logarithmic divergence and therefore Bethe himself realized this difficulty since physical observables should not have any divergences. On the other hand, people made some special manipulations which are not understandable at all. This is concerned with the method that the ultra-violet divergence (logarithmic divergence) should be canceled out by the infra-red divergence and people obtained the following Lamb shifts energy as [2–5]

$$\Delta E_{2s_{\frac{1}{2}}-2p_{\frac{1}{2}}} = \frac{m\alpha^5}{6\pi}\left[\log\frac{m}{2< E_I - E_{n=2,\ell=0} >_{av}} + \frac{11}{24} - \frac{1}{5} + \frac{1}{2}\right]. \tag{1.1}$$

However, this equation cannot be accepted physically whatever one invents any mathematics which enables to cancel out the two divergences with each other. The basic physical mistake of this calculation is concerned with the fact that the logarithmic infinity of the ultra-violet divergence is originated from the infinite number of states of photon in the free photon Fock space while the infra-red divergence comes from the following energy denominator when one makes field quantization of vector potential $\boldsymbol{A}$ as

$$\boldsymbol{A} = \sum_{\boldsymbol{k},\lambda}\frac{\boldsymbol{\epsilon}(\boldsymbol{k},\lambda)}{\sqrt{2\omega_k V}}\left(c^\dagger_{\boldsymbol{k},\lambda}e^{-ikx} + c_{\boldsymbol{k},\lambda}e^{ikx}\right) \tag{5.1}$$

where we define $kx \equiv \omega_k t - \boldsymbol{k}\cdot\boldsymbol{r}$, and $\boldsymbol{\epsilon}(\boldsymbol{k},\lambda)$ denotes the polarization vector of photon. Here, one sees that the energy of photon appears in the denominator as $\frac{1}{\sqrt{2\omega_k}}$ and this clearly indicates that zero energy photon does not exist. Thus, the infra-red divergence, if at all exists, should be originated from this energy denominator. This means that the ultra-violet divergence should be physically meaningful while the infra-red divergence is not due to a physical consequence. Therefore, there is no way that the two divergences can be physically canceled out with each other whatever one makes any manipulations.

Finally we note that there exists no logarithmic divergence in the vertex corrections due to the massive weak vector bosons any more since the new correct propagator of the weak vector boson gives a finite value of the vertex correction to the fermion-weak boson vertex [15]. This strongly suggests that the perturbative scheme itself is quite sound, except the photon case in which the vertex correction is still logarithmically divergent. This must be partly due to the fact that the Feynman propagator of photon ($D^{\mu\nu}(k) = -\frac{g^{\mu\nu}}{k^2 - i\varepsilon}$) is not a correct one as is well-known [5, 15]. Even though this gives a correct scattering amplitude for the fermion fermion scattering process, this can be justified only when the corresponding fermions are on the mass shell. Therefore, it is clear that this propagator should not be applied to the evaluation of the loop diagrams since, in this case, fermions are not on the mass shell. In this sense, there is no reason that the vertex correction so far evaluated should be a correct one. Since the theory of the Lamb shifts by Bethe is closely connected to the self-energy of electron, one should reconsider the theoretical aspect of the Lamb shifts from the fundamental point of view.

VI. CONCLUSIONS

We have presented a careful calculation of the Lamb shifts energy in muonium, and discuss a fundamental question concerning the theoretical aspect of the Lamb shifts energy. Even though the interpretation of the Lamb shifts energy is considered to be well established for a long time, it is quite important to examine the theory of Lamb shifts since Bethe's calculation contains the logarithmic divergence. Here, we carefully calculate the center of mass effect which is very normal and standard. In some sense, it is hard to find any reasons why people overlooked this important effect. However, it is also understandable since Barker and Glover claimed that there should be no effect from the proton recoil corrections on the Lamb shifts energy.

The center of mass effect is simple, but there has been no solid calculation of the center of mass effect on the Lamb shifts energy in muonium where the effect becomes significant. Even though we cannot treat it in terms of the Dirac equation as a two body problem, the calculation with the proper non-relativistic reduction has no ambiguity, and therefore the effects we evaluate are very reliable indeed.

Now, what should we do next for the Lamb shifts energy ? Unfortunately, we do not find any good candidates for the mechanism of the Lamb shifts energy for the moment except that the Feynman propagator of photon cannot be applied to the diagrams which contain any loops such as self-energy of fermions or vertex corrections [15].

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