Lakdawala, Sunil Dhansukhlal

HYPERFINE FREQUENCY IN MUONIC HELIUM

Yale University PH.D. 1982

PLEASE NOTE:

In all cases this material has been filmed in the best possible way from the available copy. Problems encountered with this document have been identified here with a check mark __✓__.

1. Glossy photographs or pages _____
2. Colored illustrations, paper or print _____
3. Photographs with dark background _____
4. Illustrations are poor copy _____
5. Pages with black marks, not original copy _____
6. Print shows through as there is text on both sides of page _____
7. Indistinct, broken or small print on several pages __✓__
8. Print exceeds margin requirements _____
9. Tightly bound copy with print lost in spine _____
10. Computer printout pages with indistinct print _____
11. Page(s) __________ lacking when material received, and not available from school or author.
12. Page(s) __________ seem to be missing in numbering only as text follows.
13. Two pages numbered __________. Text follows.
14. Curling and wrinkled pages _____
15. Other ______________________________

HYPERFINE FREQUENCY IN MUONIC HELIUM

A Dissertation

Presented to the Faculty of the Graduate School

of

Yale University

in Candidacy for the Degree of

Doctor of Philosophy

by

Sunil Dhansukhlal Lakdawala

May, 1982

HYPERFINE FREQUENCY IN MUONIC HELIUM

SUNIL DHANSUKHLAL LAKDAWALA

YALE UNIVERSITY

1982

Muonic Helium is an exotic atom consisting of ^4He (or ^3He) nucleus, a negative muon and an electron. It can be regarded as one-electron atom with an effective nucleus consisting of ^4He (or ^3He) nucleus and a muon. The hyperfine splitting in this atom is due to the spin-spin interaction between the electron and the effective nucleus. By making certain approximations, the hyperfine splitting of the muonic helium-four atom in its ground state is calculated in nonrelativistic perturbation theory. The result has been confirmed by experiments. A more accurate nonrelativistic number is calculated numerically in perturbation theory without any approximations. This is done by writing the summation over two-particle intermediate states as a convolution integral over the electron and the muon Green's functions. The one-particle Green's functions are expanded in Legendre series to facilitate integration over coordinate angles, and the radial Green's functions are expressed as products of Whittaker functions which are evaluated numerically. Adding the correction due to the anomalous magnetic moment of the electron and muon to the numerical result yields $\Delta\nu(^4He) = 4464.3 \pm 1.8$ MHz, which compares well with the experimental result: $\Delta\nu(^4He) = 4464.95 \pm 0.06$ MHz. The ground-state hyperfine splitting in the muonic helium-three atom is evaluated analytically by the same method. This requires a generalization to include the effect

of the magnetic moment of the ^{3}He nucleus. The nuclear spin and the muon spin are strongly coupled to form either a spin-zero or a spin-one effective nucleus. For the spin-one state, there is a subsplitting due to the interaction of the magnetic moment of the effective nucleus with the electron spin to form states with total angular momentum 1/2 or 3/2. The main interest is in this subsplitting, which should be measurable. The result for this subsplitting is $\Delta\nu(^3\text{He}) = 4164.9 \pm 3.0$ MHz. A semiempirical value for this subsplitting, based on the measured splitting in muonic ^{4}He, is $\Delta\nu(^3\text{He}) = 4166.5 \pm 0.4$ MHz.

ACKNOWLEDGMENTS

I believe that to earn the Ph.D. degree is not so much to solve a given problem as to learn how to think logically towards the solution of any such problem. I am deeply grateful to Professor Peter Mohr for helping me realize those broader goals. I am also thankful for his constanst encouragement and patience throughout the course of this research. I would also like to thank the other members of the Theory group for several useful discussions.

I thank Yale University and the National Science Foundation for their financial support, Professors Peter Parker and Horace Taft for the use of their computers, and James Brosious for drawing the figures which appear in the body of this work.

I am greatly indebted to Sara Batter and Bernice Kijewski for their extremely helpful nature. Finally, I would like to thank all my friends for making my stay at Yale a pleasant one.

TABLE OF CONTENTS

1. INTRODUCTION

Muonic ^{4}He is an exotic atom consisting of ^{4}He nucleus, a negative muon and an electron. It was first formed and detected by Souder et al in 1975.[1] Since the muon is about 200 times more massive than the electron, it is relatively close to the ^{4}He nucleus. Hence the atom may be regarded as an one-electron atom with an effective nucleus consisting of a ^{4}He nucleus and a negative muon.

The muon (or the effective nucleus) and the electron both have spin 1/2, and the combined system can form a singlet or triplet state. Since the muon and the electron are two different particles, their wave functions are not symmetrized (or antisymmetrized), in contrast to Rydberg states of the helium atom, for example. Hence the Coulomb interation does not remove the degeneracy of the singlet and triplet states. This degeneracy is removed by the spin-spin interaction. The energy difference is defined as the hyperfine splitting, $\Delta\nu$.

The ground-state hyperfine splitting was measured in a weak magnetic field at the Swiss Institute for Nuclear Research SIN,[2] and in a strong magnetic field at the Los Alamos Meson Physics Facility LAMPF.[3] In this thesis, perturbation theory is applied in a nonrelativistic calculation of the ground-state hyperfine splitting.[4] Various other theoretical studies of this atom have been made.[5-11] The Nonrelativistic expression for the ground-state hyperfine splitting has been evaluated by Huang and

Hughes using a variational method.[9] Drachman has evaluated the same expression by applying a Born-Oppenheimer approximation, i.e., treating muon as stationary with respect to the electron.[10] Drachman has also evaluated the same expression by transforming the Fermi contact term into a global operator.[11]

The possible generalizations of this study are as follows. The techniques developed in this thesis could be applied to other problems such as calculating the energy levels of Rydberg states of helium. The muonic Helium atom can serve as a solvable model for nuclear polarization effects. The approach employed here can be generalized to a relativistic calculation for muonic helium, and may eventually give a precise value for the frequency which can be compared with the experimental results for testing Q.E.D. effects.

The picture of an effective nucleus suggests a natural division of the Hamiltonian into a zero-order part and a perturbation. Successive orders in perturbation theory should give roughly a series in M_e/M_μ. In Chapter 2, the zero-order hyperfine splitting $\Delta\nu_0$ is calculated analyticaly with the zero-order wave function. This value contains some corrections to the Fermi value due to the finite size of the effective nucleus. Fermi value $\Delta\nu_F$ is the value of the hyperfine splitting when the effecive nucleus is taken as pointlike. In the same Chapter, the first order correction to the hyperfine splitting $\Delta\nu_1$ is calculated analytically with the first order correction to the wave function. This correction can be conveniently broken into two parts, $\Delta\nu_1^g$ and $\Delta\nu_1^e$. The first part $\Delta\nu_1^g$ is obtained by restricting the intermediate muon state to the ground state. It can be regarded as a correction due to the size of the effective nucleus. It can be analytically calculated as precisely as needed, as a series in M_e/M_μ. The leading term is of order (size of the effective nucleus)/ (Bohr radius of the electron) relative to the Fermi value, analogous to the well-known nuclear size corrections in deuterium,[12-13] hydrogen[14-16] and heavy atoms.[17-19]

Otten has applied the Bohr-Weisskopf formulation to calculate the corrections due to the finite size of this effective nucleus.[6] His value agrees well with the value obtained here.

The second part $\Delta\nu_1^e$ is obtained by restricting the intermediate muon states to excited states. It is associated with the excitation of the core, or equivalently the polarization of the effective nucleus. This correction, which is of order $(M_e/M_\mu)\Delta\nu_F$, is much larger than the analogous corrections in hydrogen or deuterium because the effective nucleus is weakly bound. The analytical calculation of $\Delta\nu_1^e$ is similar to the calculation of hyperfine structure for deuterium by Low[20] and for hydrogen by Drell and Sullivan.[21] The following two approximations are made to facilitate the calculation.

(I) The Intermediate electron states are replaced by free electron states.

(II) The electron ground-state wave function is replaced by its value at the origin. The errors due to the two approximations are estimated to be of order $(M_e/M_\mu)^2 \ln(M_\mu/M_e)$.

In Chapter 3, the wave function for the electron is calculated by numerically solving the Schrödinger equation with the effective potential due to the combined charge distribution of a point ^{4}He nucleus and ground-state muon. This wave function is used to calculate the hyperfine splitting. This is equivalent to calculating the effecive nucleus size corrections in all orders of perturbation theory. The difference between this result and $\Delta\nu_0 + \Delta\nu_1^g$ is numerically of order $(M_e/M_\mu)^2\Delta\nu_F$, as expected.

The excited muon intermediate state contribution was only calculated approximately by analytical methods. In Chapter 4 a numerical calculation of $\Delta\nu_1^e$ is described. The sum over the intermediate sates of both particles together with the energy denominator is written as a convolution integral over the electron and the muon Green's functions. The one-particle Green's functions are expanded in Legendre series to facilitate integration over coordinate angles, and the radial Green's functions are expressed as products of Whittaker functions which are calculated numerically. The numerical result has an error that is two orders of magnitude smaller than the error in the analytic result, and also sheds light on the validity of the approximations made in the analytical calculation.

In Chapter 5, the numerical calculation of the contribution of the mass-polarization term $\Delta\nu_1^m$ to the hyperfine splitting is given. The numerical methods are very similar to those described in the previous Chapter.

The accuracy of the total nonrelativistic result is limited by uncalculated higher order terms in the perturbation expansion. An order of magnitude estimate of the next term in the perturbation expansion is given in Chapter 6. It is of order $(M_e/M_\mu)^2 \ln(M_\mu/M_e)\Delta\nu_F$ or higher.

In Chapter 7, the quantum electrodynamic Hamiltonian of the system is written in the Furry bound-interaction picture.[22] The division of the Hamiltonian into the zero order part and the perturbation part is done in accordance with the effective nucleus picture. The hyperfine splitting in the nonrelativistic limit is obtained from certain Feynman graphs, by making a series of approximations. These Feynman graphs give back the nonrelativisic limit plus corrections estimated to be of order $\alpha^2\Delta\nu_F$.

In Chapter 8, the analytical method discussed in Chapter 2 is applied to evaluate the ground-state hyperfine splitting in muonic ^{3}He. This requires a generalization to include the effect of the spin of the ^{3}He nucleus. The nuclear spin and the muon spin are strongly coupled to form either a spin-zero or spin-one effective nucleus. For the spin-one state, there is a subsplitting due to the interaction of the effective nucleus spin and the electron spin to form states with total angular momentum 1/2 or 3/2. The main interest is in this smaller splitting, which should be measurable.[6,11,23,24] The comparision of theory and experiment could provide a test of our understanding of the structure of this unique atom.

In Chapter 9, the results are summarized and compared to experimental results[2,3] and other theoretical resuls.[9-11] There is good agreement.

2. ANALYTICAL CALCULATION OF THE HYPERFINE SPLITTING IN MUONIC ^{4}He

In this Chapter, perturbation theory is applied in a nonrelativistic calculation of the ground-state hyperfine splitting in muonic ^{4}He.

The structure of muonic helium is described, to a good approximation, by the nonrelaivistic Schrodinger equation (units in which $c=\hbar=1$ are employed here)

$$\left(-\frac{1}{2M_\mu}\nabla_\mu^2-\frac{1}{2M_e}\nabla_e^2-\frac{2\alpha}{x_\mu}-\frac{2\alpha}{x_e}-\frac{\bar{\nabla}_\mu\cdot\bar{\nabla}_e}{m_\alpha}\right)\psi(\bar{x}_\mu,\bar{x}_e)$$

$$=E\psi(\bar{x}_\mu,\bar{x}_e), \qquad (2.1)$$

where $\bar{x}_\mu$ and $\bar{x}_e$ are the position vectors of the muon and electron relative to the α particle, and $M_\mu = m_\mu m_\alpha/(m_\mu+m_\alpha)$ and $M_e = m_e m_\alpha/(m_e+m_\alpha)$ are the reduced masses of the muon and electron with respect to the α paricle, and $\bar{x}_{\mu e}=\bar{x}_\mu-\bar{x}_e$.

In the nonrelativistic limit of the Breit equation, the operator associated with the hyperfine splitting of the ground state is given by

$$\delta H = -\frac{8\pi}{3}\bar{\mu}_\mu\cdot\bar{\mu}_e\,\delta^3(\bar{x}_\mu-\bar{x}_e) \qquad (2.2)$$

where $\bar{\mu}_\mu = -g_\mu(m_e/m_\mu)\mu_o\bar{S}_\mu$ and $\bar{\mu}_e = -g_e\mu_o\bar{S}_e$ are the magnetic moment vectors of the muon and the elecron. The nonrelativistic wave function can be factorized into coordinate-space part $|\psi\rangle$ and spin-space part $|\chi\rangle$, i.e.

$$|\Psi\rangle = |\psi\rangle|\chi\rangle \tag{2.3}$$

The hyperfine splitting $\Delta\nu$, which is the difference between the hyperfine shifts of the ground-state levels with total angular momentum 0 and 1, is given by

$$\begin{aligned}\Delta\nu &= \langle\Psi|\delta H|\Psi\rangle_0 - \langle\Psi|\delta H|\Psi\rangle_1 \\ &= -\frac{2\pi}{3} g_\mu g_e \frac{\alpha}{m_\mu m_e} \langle\delta^3(\bar{x}_\mu - \bar{x}_e)\rangle \\ &\times \left[\langle\chi|\bar{s}_\mu\cdot\bar{s}_e|\chi\rangle_0 - \langle\chi|\bar{s}_\mu\cdot\bar{s}_e|\chi\rangle_1\right],\end{aligned} \tag{2.4}$$

where < > denotes the expectation value in coordinate space. With the aid of

$$\bar{s}_\mu\cdot\bar{s}_e = \frac{(\bar{s}_\mu+\bar{s}_e)^2 - \bar{s}_\mu^2 - \bar{s}_e^2}{2}, \tag{2.5}$$

one obtains

$$\langle\chi|\bar{s}_\mu\cdot\bar{s}_e|\chi\rangle_0 - \langle\chi|\bar{s}_\mu\cdot\bar{s}_e|\chi\rangle_1 = -1 \tag{2.6}$$

With approximate values for g_μ and g_e taken to be 2, we have

$$\Delta\nu = \frac{8\pi}{3}\frac{\alpha}{m_e m_\mu}\langle\delta^3(\bar{x}_\mu - \bar{x}_e)\rangle \tag{2.7}$$

To evaluate the expectation value in (2.7), we apply perturbation theory to the ground-state wave function. the effective nucleus picture as discussed in the Introduction suggests that in the lowest order, the muon sees the charge 2e while the electron sees the charge e because of the screening by the muon. Hence, the Hamiltonian is divided ino a zero-order part and perturbations,

$$H = H_0 + \delta V + \delta M \tag{2.8}$$

in which

$$H_0 = -\frac{1}{2M_\mu}\nabla_\mu^2 - \frac{1}{2M_e}\nabla_e^2 - \frac{2\alpha}{x_\mu} - \frac{\alpha}{x_e} \tag{2.9a}$$

$$\delta V(\bar{x}_\mu, \bar{x}_e) = \frac{\alpha}{x_{\mu e}} - \frac{\alpha}{x_e} \tag{2.9b}$$

$$\delta M = -\frac{1}{m_\alpha}\bar{\nabla}_\mu \cdot \bar{\nabla}_e \tag{2.9c}$$

The mass-polarizaion term is negligible to the accuracy considered here, and is discussed in Chapter 5. The zero-order wave function for the ground state is the product of normalized 1s hydrogenic wave functions (with Z=2 for the muon and Z=1 for the electron).

$$\psi_0(\bar{x}_\mu,\bar{x}_e) = \psi_{\mu 0}(\bar{x}_\mu)\psi_{e0}(\bar{x}_e)$$

$$= \frac{1}{\pi}(2\alpha^2 M_\mu M_e)^{3/2} e^{-2\alpha M_\mu x_\mu} e^{-\alpha M_e x_e} \qquad (2.10)$$

which has the sum of corresponding hydrogenic 1s state energies as its energy ($E_0 = E_{\mu 0}+E_{e0}$).

The zero-order hyperfine splitting is given by

$$\Delta\nu_0 = \frac{8\pi}{3}\frac{\alpha}{m_\mu m_e}\langle\psi_0|\delta^3(\bar{x}_\mu-\bar{x}_e)|\psi_0\rangle$$

$$= \frac{8\pi}{3}\frac{\alpha}{m_\mu m_e}\int d^3x_\mu\int d^3x_e\,\psi_0^\dagger(\bar{x}_\mu,\bar{x}_e)\,\delta^3(\bar{x}_\mu-\bar{x}_e)\psi_0(\bar{x}_\mu,\bar{x}_e)$$

$$= \left(1+\frac{M_e}{2M_\mu}\right)^{-3}\Delta\nu_F\ , \qquad (2.11)$$

where $\Delta\nu_F = 8\alpha(\alpha M_e)^3/(3m_\mu m_e)$ is the Fermi value, whose physical significance is discussed in the Introduction.

The first-order correction to the wave function is given by

$$\psi_1(\bar{x}_4,\bar{x}_3) = \int d^3x_2\int d^3x_1 \sum_{\substack{n,n'\\ \neq 0,0}} \frac{\psi_{\mu n}(\bar{x}_4)\psi_{en'}(\bar{x}_3)\psi^\dagger_{\mu n}(\bar{x}_2)\psi^\dagger_{en'}(\bar{x}_1)}{E_{\mu 0}+E_{e0}-E_{\mu n}-E_{en'}}$$

$$\times \ \delta V(\bar{x}_2,\bar{x}_1)\,\psi_0(\bar{x}_2,\bar{x}_1) \tag{2.12}$$

Note that in the above equation n and n' both can not be zero simultaneously. The first-order correction to the hyperfine splitting, $\Delta\nu_1$, due to the first-order correction to the wave function is

$$\Delta\nu_1 = \frac{8\pi\alpha}{3m_e m_\mu}\left[\langle\psi_0|\delta^3(\bar{x}_\mu-\bar{x}_e)|\psi_1\rangle + \langle\psi_1|\delta^3(\bar{x}_\mu-\bar{x}_e|\psi_0\rangle\right]$$

$$= \frac{16\pi\alpha}{3m_e m_\mu}\langle\psi_0|\delta^3(\bar{x}_\mu-\bar{x}_e)|\psi_1\rangle$$

$$= \frac{16\pi\alpha}{3m_e m_\mu}\int d^3x_4\int d^3x_3\,\psi_0^+(\bar{x}_4,\bar{x}_3)\,\delta^3(\bar{x}_4-\bar{x}_3)\,\psi_1(\bar{x}_4,\bar{x}_3)$$

$$= \frac{16\pi\alpha}{3m_e m_\mu}\int d^3x_3\int d^3x_2\int d^3x_1\sum_{\substack{n,n'\\ \neq 0,0}}\psi_0^+(\bar{x}_3,\bar{x}_3)$$

$$\times\,\frac{\psi_{\mu n}(\bar{x}_3)\psi_{en'}(\bar{x}_3)\psi_{\mu n}^+(\bar{x}_2)\psi_{en'}^+(\bar{x}_1)}{E_{\mu o}+E_{eo}-E_{\mu n}-E_{en'}}\,\delta V(\bar{x}_2,\bar{x}_1)\psi_0(\bar{x}_2,\bar{x}_1) \tag{2.13}$$

It is convenient to divide the sum over muon states in (2.13) into two parts $\Delta\nu_1 = \Delta\nu_1^g + \Delta\nu_1^e$, where $\Delta\nu_1^g$ is the contribution to $\Delta\nu_1$ from the term with n=0, i.e., where the intermediate muon state is the 1s state. The physical significance of this term is discussed in the Introduction. For this part, we have

$$\Delta\nu_1^g = \frac{16\pi\alpha}{3m_e m_\mu}\int d^3x_2\int d^3x_1\sum_{n\neq 0}\psi_{eo}^+(\bar{x}_2)\,\psi_{\mu o}^+(\bar{x}_2)\,\psi_{\mu o}(\bar{x}_2)$$

$$\times\,\frac{\psi_{en}(\bar{x}_2)\psi_{en}^+(\bar{x}_1)}{E_{eo}-E_{en}}\,V_\mu(\bar{x}_1)\,\psi_{eo}(\bar{x}_1) \tag{2.14}$$

with

$$V_\mu(\bar{x}) = \int d^3x_\mu \, \psi^\dagger_{\mu 0}(\bar{x}_\mu)\, \delta V(\bar{x}_\mu, \bar{x})\, \psi_{\mu 0}(\bar{x}_\mu)$$

$$= -\frac{\alpha}{x}(1+2\alpha M_\mu x)\, e^{-4\alpha M_\mu x} \tag{2.15}$$

Only s states contribute to the sum over n in (2.14), so we may replace the sum by the s state reduced Green's function for the electron.[25]

$$\sum_{n\neq 0} \frac{\psi_{ens}(\bar{x}_2)\psi^\dagger_{ens}(\bar{x}_1)}{E_{e0} - E_{ens}} = -\frac{\alpha M_e^2}{\pi} e^{-\alpha M_e(x_1+x_2)}$$

$$\times \left[\frac{1}{2\alpha M_e x_>} - \ln(2\alpha M_e x_>) + \frac{5}{2} - \gamma - \alpha M_e(x_1+x_2) \right.$$

$$\left. + \sum_{i=1}^{\infty} \frac{(2\alpha M_e x_<)^i}{i(i+1)!} \right], \tag{2.16}$$

where $x_> = \max(x_1, x_2)$, $x_< = \min(x_1, x_2)$, and $\gamma = 0.5772..$ is Euler's constant. Evaluation of Equation (2.14) yields

$$\Delta\nu_1^g = \Delta\nu_F \left\{ \frac{11}{16}\frac{M_e}{M_\mu} + \left(\frac{M_e}{M_\mu}\right)^2 \ln\left(\frac{M_\mu}{M_e}\right) - \frac{7}{64}\left(\frac{M_e}{M_\mu}\right)^2 \right.$$

$$\left. + O\left[\left(\frac{M_e}{M_\mu}\right)^3 \ln\left(\frac{M_\mu}{M_e}\right)\right] \right\} \tag{2.17}$$

Note that $\Delta\nu_1^g$ can be evaluated as precisely as desired, in as a series in (M_e/M_μ).

The part $\Delta\nu_1^e$ corresponding to excited muon intermediate states, i.e. $n\neq 0$ in (2.13), may be written as

$$\Delta\nu_1^e = -\frac{16\pi\alpha}{3m_\mu m_e}\int d^3x_3\int d^3x_2\int d^3x_1 \sum_{n\neq 0}\psi_{\mu o}^{+}(\bar{x}_3)\psi_{eo}^{+}(\bar{x}_3)\psi_{\mu n}(\bar{x}_3)$$
$$\times\ \psi_{\mu n}^{+}(\bar{x}_2)\, G_e(\bar{x}_3,\bar{x}_1, E_{\mu o}-E_{\mu n}+E_{eo})\frac{\alpha}{x_{21}}$$
$$\times\ \psi_{\mu o}(\bar{x}_2)\psi_{eo}(\bar{x}_1) \qquad (2.18)$$

where

$$G_e(\bar{x}_3,\bar{x}_1,z) = \sum_n \frac{\psi_{en}(\bar{x}_3)\psi_{en}^{+}(\bar{x}_1)}{E_{en}-z} \qquad (2.19)$$

is the electron Coulomb Green's function. In (2.18), there is no contribution from the term $-\alpha/x_1$ in $\delta v(\bar{x}_2,\bar{x}_1)$ due to the orthogonality of $\psi_{\mu n}(\bar{x}_2)$ and $\psi_{\mu o}(\bar{x}_2)$ for $n\neq 0$.

Two approximations are made to evaluate (2.18).

(I) The ground-state wave function for the electron is replaced by its value at the origin, i.e., $\psi_{eo}^{+}(\bar{x}_3)$ and $\psi_{eo}(\bar{x}_1)$ are replaced by $\psi_{eo}(0)$.

(II) The electron intermediate states are approximated by the free states. This is equivalent to replacing the electron Green's function by the free Green's function.

Physically these approximations are motivated by the following arguements. The hyperfine splitting is proportional to the spatial overlap integral of the muon wave function and the electron wave function. The important region of integration is of order $1/(\alpha M_\mu)$ because of the exponential factor in the muon wave function. The fact that ground-state electron wave function does not vary much from its value at the origin in this region is the motivation for approximation I. The fact that high momentum components of the electron intermediate states dominate in this region is the motivation for Approximation II.

In perticular, for justifying Approximation I, we have

$$\psi_{eo}(\bar{x}) = \psi_{eo}(o)e^{-\alpha M_e x}$$

$$= \psi_{eo}(o)[1-\alpha M_e x + \cdots\cdot] \tag{2.20}$$

Because of the associated exponential factor due to the ground-state wave function for the muon, the important values of x_3 are of order $1/(\alpha M_\mu)$. Hence

$$\psi_{eo}(\bar{x}_3) = \psi_{eo}(o)[1+ O(\frac{M_e}{M_\mu})] \tag{2.21}$$

Replacing $\psi_{eo}(\bar{x}_3)$ by $\psi_{eo}(0)$ introduces the error of order $\Delta\nu_F(M_e/M_\mu)^2$ in the calculation of $\Delta\nu_1^e$. The important values of x_1 are of order $1/[\alpha(M_e M_\mu)^{1/2}]$ due to the associated exponential factor from the free electron Green's function [see (2.24)], and hence

$$\psi_{eo}(\bar{x}_1) = \psi_{eo}(o)[1 + O(\frac{M_e}{M_\mu})^{1/2}] \tag{2.22}$$

introducing the error of nominal order $\Delta\nu_F(M_e/M_\mu)^{3/2}$ in the calculation of

$\Delta\nu_1^e$. The calculation carried out in the later part of this Chapter shows that the contribution of the second term of (2.20) for $x=x_1$ to $\Delta\nu_1^e$, is in fact of order $\Delta\nu_F(M_e/M_\mu)^2 \ln(M_\mu/M_e)$.

The justification for Approximation II is based on the equation satisfied by the electron Green's function

$$\left(-\frac{\nabla_3^2}{2M_e} - \frac{\alpha}{x_3} - z\right) G_e(\bar{x}_3, \bar{x}_1, z) = \delta^3(\bar{x}_3 - \bar{x}_1) \tag{2.23}$$

The value of interest for z is $E_{eo}+E_{\mu o}-E_{\mu n}$. In the calculation of $\Delta\nu_1^a$, replacing the Green's function by the free Green's function gives an error of order $\Delta\nu_F(M_e/M_\mu)^2 \ln(M_\mu/M_e)$, suggesting that the binding term $-\alpha/x_3$ in (2.23) plays a minor role. A similar error can be expected in the calculation of $\Delta\nu_1^e$. The calculation carried out in the later part of this Chapter indicates that the leading correction due to the second approximation is of order $\Delta\nu_F(M_e/M_\mu)^2 \ln(M_\mu/M_e)$. Comparision with the numerical result for $\Delta\nu_1^e$ suggests that the errors introduced in the analytical calculation due to these two approximations are of order $\Delta\nu_F(M_e/M_\mu)^2 \ln(M_\mu/M_e)$ (see Chapter 4).

With these two approximations, i.e., replacing $\psi_{eo}^+(\bar{x}_3)$ and $\psi_{eo}(\bar{x}_1)$ by $\psi_{eo}(0)$, and replacing $G_e(\bar{x}_3, \bar{x}_1, E_{\mu o}+E_{eo}-E_{\mu n})$ by the free electron Green's function

$$G_e^0(\bar{x}_3, \bar{x}_1, E_{\mu o}-E_{\mu n}+E_{eo}) = \frac{M_e}{2\pi} \frac{e^{-b_n x_{31}}}{x_{31}} \tag{2.24}$$

in which $b_n = [2M_e(E_{\mu n}-E_{\mu o}-E_{eo})]^{1/2}$, $b_n>0$, we get

$$\Delta\nu_1^e = -\Delta\nu_F \frac{\alpha M_e}{2\pi} \int d^3x_3 \int d^3x_2 \int d^3x_1 \sum_{n\neq 0} \psi^{\dagger}_{\mu o}(\bar{x}_3)\psi_{\mu n}(\bar{x}_3)\psi^{\dagger}_{\mu n}(\bar{x}_2)$$

$$\times \frac{e^{-b_n x_{31}}}{x_{31}} \frac{1}{x_{21}} \psi_{\mu o}(\bar{x}_2) \qquad (2.25)$$

Integration over $\bar{x}_1$ yields

$$\int d^3x_1 \frac{e^{-b_n x_{31}}}{x_{31}x_{21}} = \frac{4\pi}{b_n^2}\frac{1}{x_{32}}(1-e^{-b_n x_{32}}) \qquad (2.26a)$$

$$= 4\pi\left(\frac{1}{b_n} - \frac{1}{2}x_{32} + \frac{1}{6}b_n x_{32}^2 - \frac{1}{24}b_n^2 x_{32}^3 + \cdots\right) \qquad (2.26b)$$

In view of the exponential falloff of the muon wave functions, the main contribution to (2.25) in the integration over $\bar{x}_2$ and $\bar{x}_3$ comes from the region in which x_2 and x_3 are of order $1/(\alpha M_\mu)$. The order of magnitudes $x_{32} \sim 1/(\alpha M_\mu)$ and $b_n \sim \alpha(M_e M_\mu)^{1/2}$, suggest that the series in (2.26) gives a series in increasing powers of $(M_e/M_\mu)^{1/2}$ for $\Delta\nu_1^e$. The leading term b_n^{-1} gives no contribution because of the orthogonality of the muon wave functions. In view of the completeness of the muon wave functions, we have

$$\sum_{n\neq 0} \psi_{\mu n}(\bar{x}_3)\psi^{\dagger}_{\mu n}(\bar{x}_2) = \delta^3(\bar{x}_3-\bar{x}_2) - \psi_{\mu o}(\bar{x}_3)\psi^{\dagger}_{\mu o}(\bar{x}_2) \qquad (2.27)$$

so the second term in (2.26b) yields

$$-\Delta\nu_F\, 2\alpha M_e \int d^3x_3 \int d^3x_2 |\psi_{\mu o}(\bar{x}_3)|^2 x_{32} |\psi_{\mu o}(\bar{x}_2)|^2$$

$$= -\Delta\nu_F \frac{35}{16}\frac{M_e}{M_\mu} \tag{2.28}$$

in (2.25). In the third term in the series in (2.26), E_{eo} is neglected in comparison to $E_{\mu n}-E_{\mu o}$ in b_n, and again because of orthogonality of the wave function in (2.25), we may replace $|\bar{x}_3-\bar{x}_2|^2$ by $-2\bar{x}_3\cdot\bar{x}_2$. Hence in (2.25) this term contributes

$$\Delta\nu_F \frac{4}{3}\alpha M_e \int d^3x_3 \int d^3x_2 \sum_n \psi^+_{\mu o}(\bar{x}_3)\,[2M_e(E_{\mu n}-E_{\mu o})]^{1/2}\,\bar{x}_3\,\psi_{\mu n}(\bar{x}_3)$$
$$\times\cdot\psi^+_{\mu n}(\bar{x}_2)\,\bar{x}_2\,\psi_{\mu o}(\bar{x}_2) = \Delta\nu_F \frac{2}{3}\left(\frac{M_e}{M_\mu}\right)^{3/2} S_{1/2} \tag{2.29}$$

where we define

$$S_p = \sum_n \left(\frac{E_{\mu n}-E_{\mu o}}{R_\mu}\right)^p |\langle\mu o|\frac{\bar{x}}{a_\mu}|\mu n\rangle|^2 \tag{2.30}$$

with $R_\mu=2\alpha^2 M_\mu$, $a_\mu=1/(2\alpha M_\mu)$, the effective Rydberg and Bohr radius for the muon. By neglecting E_{eo} compared to $E_{\mu n}-E_{\mu o}$ in b_n, the error involved is clearly of order $\Delta\nu_F(M_e/M_\mu)^{5/2}$, which can be neglected. For a simple estimate of $S_{1/2}$, note that the standard sum rules[26] $S_0=S_1=3$, together with $S_{1/2}\leq 1/2(S_0+S_1)$, give $S_{1/2}\leq 3$. A lower bound on $S_{1/2}$ is given by

$$S_{1/2} \geq \min_{n\neq 0}\left[\left(\frac{E_{\mu n}-E_{\mu o}}{R_\mu}\right)^{1/2}\right]\sum_{m\neq 0}|\langle\mu o|\frac{\bar{x}}{a_\mu}|\mu m\rangle|^2$$
$$= 3\left(\frac{3}{4}\right)^{1/2} \tag{2.31}$$

Hence $S_{1/2} = 2.8 \pm 0.2$. Contributions from all other terms in (2.26) are of order $\Delta\nu_F (M_e/M_\mu)^2$ or higher, and hence can be neglected.

Errors due to the first two approximations are estimated by replacing b_n by some average b, independent of n, and of order $\alpha(M_e M_\mu)^{1/2}$. This is based on the expectation that the order of magnitude of the remainder is given by the excited bound states of muon, and for excited bound states of muon, b_n is a slowly varying function of n.

Now

$$\psi_{e0}(\bar{x}_1) = \psi_{e0}(0)\,[1 - \alpha M_e x_1 + \cdots] \tag{2.32}$$

Hence the leading correction due to the first approximation is due to the second term on right hand side of (2.32), and is given by

$$\begin{aligned}\delta_1[\Delta\nu_1^e] = & -\frac{16\pi\alpha^2}{3m_\mu m_e}\int d^3x_3 \int d^3x_2 \int d^3x_1 \sum_{n\neq 0} \psi^\dagger_{\mu 0}(\bar{x}_3)\,\psi^\dagger_{e0}(\bar{x}_3) \\ & \times \psi_{\mu n}(\bar{x}_3)\,\psi^\dagger_{\mu n}(\bar{x}_2)\,G_e(\bar{x}_3,\bar{x}_1, E_{\mu 0} - E_{\mu n} + E_{e0})\left[\frac{1}{x_{21}} - \frac{1}{x_1}\right] \\ & \times \psi_{\mu 0}(\bar{x}_2)\,[-\alpha M_e x_1 \psi_{e0}(0)]\end{aligned} \tag{2.33}$$

To estimate (2.33), the same approximations are made, as described above and b_n is replaced by b. This gives

$$\delta_1[\Delta\nu_1^e] = \frac{\Delta\nu_F}{\pi}(\alpha M_e)^2 \int d^3x_3 \int d^3x_2 \int d^3x_1 \sum_{n\neq 0} \psi^\dagger_{\mu 0}(\bar{x}_3)\,\psi_{\mu 0}(\bar{x}_2)$$

$$\times \psi_{\mu n}(\bar{x}_3)\psi^+_{\mu n}(\bar{x}_2)\frac{e^{-bx_{13}}}{x_{13}}\left(\frac{1}{x_{12}}-\frac{1}{x_1}\right)x_1 \qquad (2.34)$$

Using (2.27)

$$\delta_1[\Delta\nu_1^e] = I_1 + I_2 \qquad (2.35)$$

where

$$I_1 = \frac{\Delta\nu_F}{\pi}(\alpha M_e)^2\int d^3x_3\int d^3x_2\int d^3x_1\,\psi^+_{\mu 0}(\bar{x}_3)\psi_{\mu 0}(\bar{x}_2)$$

$$\times\,\delta^3(\bar{x}_3-\bar{x}_2)\frac{e^{-bx_{13}}}{x_{13}}\left(\frac{1}{x_{12}}-\frac{1}{x_1}\right)x_1 \qquad (2.36)$$

$$I_2 = -\frac{\Delta\nu_F}{\pi}(\alpha M_e)^2\int d^3x_3\int d^3x_2\int d^3x_1\,|\psi_{\mu 0}(\bar{x}_3)|^2|\psi_{\mu 0}(\bar{x}_2)|^2$$

$$\times\,\frac{e^{-bx_{13}}}{x_{13}}\left(\frac{1}{x_{12}}-\frac{1}{x_1}\right)x_1 \qquad (2.37)$$

Now

$$\int d^3x_1\frac{e^{-bx_{12}}}{(x_{12})^2}x_1 = \frac{4\pi}{b^2}\left[1-\frac{1}{3}b^2x_2^2\ln(bx_2)+O(b^2x_2^2)\right] \qquad (2.38)$$

where the expansion in a power series of bx_2 is justified because $bx_2 \sim (M_e/M_\mu)^{1/2}$ as described previously. We have

$$\int d^3x_1\frac{e^{-bx_{12}}}{x_{12}} = \frac{4\pi}{b^2} \qquad (2.39)$$

Using (2.38) and (2.39),

$$I_1 = -\frac{4}{3}\Delta\nu_F(\alpha M_e)^2\int d^3x\,|\psi_{\mu 0}(\bar{x})|^2x^2\ln(bx)$$

$$+\,O\left[\Delta\nu_F\left(\frac{M_e}{M_\mu}\right)^2\right] \qquad (2.40)$$

Since b is of order $\alpha(M_eM_\mu)^{1/2}$,

$$I_1 = \frac{1}{2}\Delta\nu_F\left(\frac{M_e}{M_\mu}\right)^2\ln\left(\frac{M_\mu}{M_e}\right)+O\left[\Delta\nu_F\left(\frac{M_e}{M_\mu}\right)^2\right] \qquad (2.41)$$

To evaluate I_2, note that

$$\int d^3x_2 |\psi_{\mu 0}(\bar{x}_2)|^2 \left(\frac{1}{x_{12}} - \frac{1}{x_1}\right)$$
$$= -\frac{1}{x_1}(1+2\alpha M_\mu x_1) e^{-4\alpha M_\mu x_1} \qquad (2.42)$$

Hence important values of x_1 are of order $1/(\alpha M_\mu)$, thus giving

$$I_2 = O\left[\Delta\nu_F \left(\frac{M_e}{M_\mu}\right)^2\right] . \qquad (2.43)$$

From (2.41) and (2.43),

$$\delta_1[\Delta\nu_1^e] = \frac{1}{2}\Delta\nu_F \left(\frac{M_e}{M_\mu}\right)^2 \ln\left(\frac{M_\mu}{M_e}\right) + O\left[\Delta\nu_F\left(\frac{M_e}{M_\mu}\right)^2\right] \qquad (2.44)$$

The Green's function for the electron can be written as

$$G_e(\bar{x}_3,\bar{x}_1,z) = G_e^0(\bar{x}_3,\bar{x}_1,z) - \int d^3x_4 G_e^0(\bar{x}_3,\bar{x}_4,z) V(\bar{x}_4) G_e^0(\bar{x}_4,\bar{x}_1,z)$$
$$+ \cdots\cdot \qquad (2.45)$$

where

$$V(\bar{x}_4) = -\frac{\alpha}{x_4} \qquad (2.46)$$

Hence the leading term of the error due to the second approximation is from the second term on right hand side of (2.45), and is given by

$$\delta_2[\Delta\nu_1^e] = -\frac{16\pi\alpha}{3m_\mu m_e}\int d^3x_1 \int d^3x_2 \int d^3x_3 \int d^3x_4 \sum_{n\neq 0} \psi_{\mu 0}^+(\bar{x}_3)\psi_{e0}^+(\bar{x}_3)$$

$$\times \psi_{\mu n}(\bar{x}_3)\psi_{\mu n}(\bar{x}_2) G_e^0(\bar{x}_3,\bar{x}_4, E_{\mu 0}-E_{\mu n}+E_{e0}) \frac{\alpha}{x_4} G_e^0(\bar{x}_4,\bar{x}_1,E_{\mu 0}-E_{\mu n}+E_{e0})$$

$$\times \alpha\left(\frac{1}{x_{12}} - \frac{1}{x_1}\right)\psi_{\mu 0}(\bar{x}_2)\psi_{e0}(\bar{x}_1) \qquad (2.47)$$

To estimate (2.47), the same approximations are made as described above. This gives, with the aid of (2.27),

$$\delta_2[\Delta\nu_1^e] = I_{31} + I_{32} + I_4 \tag{2.48}$$

where

$$I_{31} = -\frac{\Delta\nu_F}{2\pi^2}(\alpha M_e)^2 \int d^3x_1 \int d^3x_2 \int d^3x_3 \int d^3x_4\, \psi^+_{\mu 0}(\bar{x}_3)\psi_{\mu 0}(\bar{x}_2)$$

$$\times \frac{e^{-bx_{34}}}{x_{34}} \frac{1}{x_4} \frac{e^{-bx_{41}}}{x_{41}} \frac{1}{x_{12}} \delta^3(\bar{x}_3-\bar{x}_2) \tag{2.49}$$

$$I_{32} = \frac{\Delta\nu_F}{2\pi^2}(\alpha M_e)^2 \int d^3x_1 \int d^3x_2 \int d^3x_3 \int d^3x_4\, \psi^+_{\mu 0}(\bar{x}_3)\psi_{\mu 0}(\bar{x}_2)$$

$$\times \frac{e^{-bx_{34}}}{x_{34}} \frac{1}{x_4} \frac{e^{-bx_{41}}}{x_{41}} \frac{1}{x_1} \delta^3(\bar{x}_3-\bar{x}_2) \tag{2.50}$$

$$I_4 = \frac{\Delta\nu_F}{2\pi^2}(\alpha M_e)^2 \int d^3x_1 \int d^3x_2 \int d^3x_3 \int d^3x_4\, |\psi_{\mu 0}(\bar{x}_3)|^2 |\psi_{\mu 0}(\bar{x}_2)|^2$$

$$\times \frac{e^{-bx_{34}}}{x_{34}} \frac{1}{x_4} \frac{e^{-bx_{41}}}{x_{41}} \left(\frac{1}{x_{12}} - \frac{1}{x_1}\right) \tag{2.51}$$

Integration over x can be carried out in (2.49) by using (2.26). Using the integral

$$\int d^3x_4 \frac{e^{-bx_{42}}}{(x_{42})^2} \frac{1}{x_4} = 4\pi\left[1-\gamma-\ln bx_2 - \sum_{n=1}^{\infty} \frac{(-bx_2)^n}{n(n+1)!}\right] \tag{2.52}$$

integration over $\bar{x}_4$ in (2.49) gives

$$\int d^3x_4 \frac{e^{-bx_{42}}}{x_{42}} \frac{1}{x_4} \left(\frac{1-e^{-bx_{42}}}{x_{42}}\right)$$

$$= 4\pi\left[\ln 2 - \frac{bx_2}{2} + O(b^2x_2^2)\right] \tag{2.53}$$

Using (2.53), we get

$$I_{31} = -8\ln 2\,\Delta\nu_F \frac{(\alpha M_e)^2}{b^2} + 3\Delta\nu_F \frac{\alpha M_e}{b}\frac{M_e}{M_\mu} + O\left[\Delta\nu_F\left(\frac{M_e}{M_\mu}\right)^2\right] \quad (2.54)$$

Integration over $\tilde{x}_1$ and $\tilde{x}_2$ in (2.50) carried out by using

$$\int d^3x_1 \frac{e^{-bx_{41}}}{x_{41}}\frac{1}{x_1} = \frac{4\pi}{b^2}\left(\frac{1-e^{-bx_4}}{x_4}\right) \quad (2.55)$$

and

$$\int d^3x_2\, e^{-ax_2}\frac{e^{-bx_{24}}}{x_{24}} = \frac{4\pi}{x_4}\left[\frac{2a(e^{-bx_4}-e^{-ax_4})}{(a^2-b^2)^2} - \frac{x_4 e^{-ax_4}}{a^2-b^2}\right] \quad (2.56)$$

where $a = 4\alpha M_\mu$ in (2.50). Using

$$\int_0^\infty \frac{dx}{x}(e^{-bx}-e^{-ax})(1-e^{-bx}) = \ln 2 - \frac{b}{a} + O\left(\frac{b^2}{a^2}\right) \quad (2.57)$$

we have

$$I_{32} = 8\ln 2\,\Delta\nu_F \frac{(\alpha M_e)^2}{b^2} - 3\Delta\nu_F \frac{\alpha M_e}{b}\frac{M_e}{M_\mu}$$
$$+ O\left[\Delta\nu_F\left(\frac{M_e}{M_\mu}\right)^2\right] \quad (2.58)$$

Integration over $\tilde{x}_2$ in (2.51) can be carried out with the aid of (2.42). From (2.56) and the integral

$$\int d^3x_1 \frac{e^{-ux_1}}{x_1}\frac{e^{-vx_{14}}}{x_{14}} = \frac{4\pi}{x_4}\left(\frac{e^{-vx_4}-e^{-ux_4}}{u^2-v^2}\right) \quad (2.59)$$

it follows that

$$I_4 = -\Delta\nu_F\left(\frac{M_e}{M_\mu}\right)^2\int_0^\infty \frac{dx}{x}(e^{-bx}-e^{-ax})(e^{-bx}-e^{-ax}) + O\left[\Delta\nu_F\left(\frac{M_e}{M_\mu}\right)^2\right]$$

$$= -\Delta\nu_F\left(\frac{M_e}{M_\mu}\right)^2\ln\frac{a}{b} + O\left[\Delta\nu_F\left(\frac{M_e}{M_\mu}\right)^2\right] \quad (2.60)$$

Since b is of order $\alpha(M_eM_\mu)^{1/2}$,

$$I_4 = -\frac{1}{2}\Delta\nu_F\left(\frac{M_e}{M_\mu}\right)^2 \ln\left(\frac{M_\mu}{M_e}\right) + O\left[\Delta\nu_F\left(\frac{M_e}{M_\mu}\right)^2\right] \qquad (2.61)$$

using (2.54), (2.58) and (2.61),

$$\delta_2[\Delta\nu_1^e] = -\frac{1}{2}\Delta\nu_F\left(\frac{M_e}{M_\mu}\right)^2 \ln\left(\frac{M_\mu}{M_e}\right) + O\left[\Delta\nu_F\left(\frac{M_e}{M_\mu}\right)^2\right] \qquad (2.62)$$

Equations (2.44) and (2.62) suggest that the errors, due to the approximations made in evaluation of $\Delta\nu_1^e$, are of order $\Delta\nu_F(M_e/M_\mu)^2 \ln(M_\mu/M_e)$ or higher. This is also consistent with the numerical calculation discussed in Chapter 4.

Summarizing,

$$\Delta\nu_1 = \Delta\nu_1^a + \Delta\nu_1^e$$

$$= \Delta\nu_F\left\{-\frac{3}{2}\frac{M_e}{M_\mu} + \frac{2}{3}S_{1/2}\left(\frac{M_e}{M_\mu}\right)^{3/2} + O\left[\left(\frac{M_e}{M_\mu}\right)^2 \ln\left(\frac{M_\mu}{M_e}\right)\right]\right\} \qquad (2.63)$$

and

$$\Delta\nu \simeq \Delta\nu_0 + \Delta\nu_1$$

$$= \Delta\nu_F\left\{1 - 3\frac{M_e}{M_\mu} + \frac{2}{3}S_{1/2}\left(\frac{M_e}{M_\mu}\right)^{3/2} + O\left[\left(\frac{M_e}{M_\mu}\right)^2 \ln\left(\frac{M_\mu}{M_e}\right)\right]\right\} \qquad (2.64)$$

3. NUMERICAL CALCULATION OF THE CORRECTION DUE TO THE FINITE SIZE OF THE EFFECTIVE NUCLEUS

In this Chapter, the wave function for the electron is calculated by numerically solving the Schrodinger equation with the effective potential due to the combined charge distribution of a point ^{4}He nucleus and ground-state muon. This wave function is used to calculate the hyperfine splitting. This is equivalent to calculating the effective nucleus size contribution in all orders of perturbation theory.

The electron experiences the effective potential due to the ^{4}He nucleus as well as the charge distribution of the muon (represented by the zero-order muon wave function). The effecive potential is given by

$$V_{eff}(x_e) = -\frac{2\alpha}{x_e} + \int d^3x_\mu |\psi_{\mu 0}(\bar{x}_\mu)|^2 \frac{\alpha}{x_{\mu e}}$$

$$= -\frac{\alpha}{x_e} + \delta V(x_e) \qquad (3.1)$$

where the zero-order ground-state wave function for the muon is

$$\psi_{\mu 0}(\bar{x}) = \frac{1}{\sqrt{\pi}}(2\alpha M_\mu)^{3/2} e^{-2\alpha M_\mu x} \qquad (3.2)$$

and

$$\delta V(x_e) = -\frac{\alpha}{x_e}(1+2\alpha M_\mu x_e) e^{-4\alpha M_\mu x_e} \qquad (3.3)$$

The ground-state wave function $\psi_e(\vec{x})$ depends only on the radial coordinate x, and hence F(x) defined by

$$F(x) = x\psi_e(x) \tag{3.4}$$

satisfies

$$\frac{d^2F}{dx^2} = 2M_e[V_{eff}(x) - E]F(x) \tag{3.5}$$

By using perturbaion theory to first order

$$E = -\frac{1}{2}M_e\alpha^2 + \int d^3x\,|\psi_{eo}(x)|^2\delta V(x) \tag{3.6}$$

where the zero-order ground-state wave function for the electron is given by

$$\psi_{eo}(x) = \frac{1}{\sqrt{\pi}}(\alpha M_e)^{3/2}e^{-\alpha M_e x} \tag{3.7}$$

substituting (3.3) and (3.7) in (3.6),

$$E = -\frac{1}{2}M_e\alpha^2\{1 + (\frac{M_e}{M_\mu})^2[1 + O(\frac{M_e}{M_\mu})]\} \tag{3.8}$$

With the aid of (2.7), the hyperfine splitting can be written as

$$\Delta\nu_g = \frac{8\pi\alpha}{3m_\mu m_e}\int d^3x\,|\psi_{\mu o}(x)|^2|\psi_e(x)|^2 \tag{3.9}$$

Since F(x) is not normalized, the right hand side of (3.9) has to include the normalization constant. Hence

$$\Delta\nu_g = \frac{8\pi\alpha}{3m_\mu m_e}\frac{\int_0^\infty dx\,|F(x)|^2|\psi_{\mu o}(x)|^2}{\int_0^\infty dx\,|F(x)|^2} \tag{3.10}$$

The function $F(x)$ is evaluated numerically with the value of E given by (3.8) as follows. The sum of the two power series

$$F(x+h) = F(x) + hF'(x) + \frac{h^2}{2!}F''(x) + \frac{h^3}{3!}F'''(x) + O(h^4) \tag{3.11}$$

and

$$F(x-h) = F(x) - hF'(x) + \frac{h^2}{2!}F''(x) - \frac{h^3}{3!}F'''(x) + O(h^4) \tag{3.12}$$

together with (3.5) yields

$$F(x+h) + F(x-h) = 2\{1 + M_e h^2 [V_{eff}(x) - E]\} F(x) + O(h^4) \tag{3.13}$$

Using this relation one can, in principle, go in either direction of x to find $F(x)$, if $F(x)$ is known for two neighbouring values of x. In this problem $F(x)$ is known in two regions. In the first region, defined by $\alpha M_\mu x \ll 1$, with the aid of (3.1) and (3.3), the effective potential is well approximated by

$$V_{eff}(x_e) \simeq -\frac{2\alpha}{x_e} \tag{3.14}$$

This result can also be obtained from the physical consideration that when the electron is very near the nucleus compared to the muon Bohr radius, the electron moves in the potential due to the nuclear charge of 2e. In this region $F(x)$ satisfies

$$\frac{d^2F}{dx^2} + \left[\frac{4\alpha M_e}{x} + 2EM_e\right]F = 0 \qquad (3.15)$$

The solution of (3.15) which is regular at origin, is obtained by a power-series expansion.

$$F(x) = M_e x\,[1 - 2\alpha M_e x + O(x^2)]$$

$$\simeq M_e x\, e^{-2\alpha M_e x} \qquad (3.16)$$

where the second term in (3.16) is independent of binding energy. In the second region, defined by $\alpha M_\mu x >> 1$, the effective potential is well approximated by

$$V_{eff}(x) \simeq -\frac{\alpha}{x_e} \qquad (3.17)$$

This result also can be seen from the physical consideration that when the electron is far from the nucleus compared to the muon Bohr radius, the electron moves in the potential due to the nuclear charge of e, because of the complete screening by the muon. In this region F(x) satisfies

$$\frac{d^2F}{dx^2} + \left[\frac{2\alpha M_e}{x} + 2EM_e\right]F = 0 \qquad (3.18)$$

and F should be square integrable in this region. The solution F for arbitrary E is given by

$$F(x) \propto W_{\nu,1/2}(2cM_e x) \qquad (3.19)$$

where W is the Whittaker function which is regular at infinity, $\nu = \alpha/c$ and $c=(-2E/M_e)^{1/2}$, c>0. The asymptotic expansion for W is given by

$$W_{\nu,1/2}(x) = e^{-x/2} x^{\nu}\left[1 + \frac{\nu(1-\nu)}{x} + O\left(\frac{1}{x^2}\right)\right] \qquad (3.20)$$

The value of $(1-\nu)$ is of order $(M_e/M_\mu)^2$, and c is of order α. Hence apart from normalization,

$$F(x) = (M_e x)^\nu e^{-cM_e x}\{1 + O[(\frac{M_e}{M_\mu})^2 \frac{1}{\alpha M_e x}]\} \qquad (3.21)$$

If one starts from the values of x in the region where $\alpha M_\mu x \ll 1$ ($\alpha M_\mu x \gg 1$), then the procedure of numerically evaluating F(x) with the aid of (3.16) and (3.21) for increasing (decreasing) values of x, is eventually unstable(see Appendix A). To avoid this problem, Equation (3.13) is used to calculate $F_1(x)$, in the direction of increasing x starting from x=0 with initial values given by (3.16). Also Equation (3.13) is used to calculate $F_2(x)$ in the direction of decreasing x starting from a large value of $x(=x_I)$, with initial values given by (3.21). The calculations are terminated at some intermediate x such that both functions are stable. This point $x(=x_M)$ is chosen to give the best match of the logarithmic derivatives of the functions. The function F(x) is given by

$$\begin{aligned} F(x) &= F_1(x), \qquad x < x_M \\ &= cF_2(x), \qquad x > x_M \end{aligned} \qquad (3.22)$$

where the constant $c = F_1(x_M)/F_2(x_M)$ provides the continuity of F(x) at x_M.

To calculate $F_1(x)$ starting from small x, one needs the values of F_1 at two neighbouring values of x. In the limit of x tending to zero, Equation (3.16) is exact. Hence the value of F_1 at the origin is zero.

To find F_1 at the neighbouring value of x=D, following method is used. For D=0.01 and for various values of h=0.1D,0.01D,0.001D, $F_1(h)$ is calculated by using (3.16) and then $F_1(2h)$, $F_1(3h)$,....$F_1(D)$ are calculated using (3.13). The various values of $F_1(D)$ for various h, agree very well with each other. For example, the values of $F_1(D)$ agree within 1 part in 10^{10} for the last two values of h. This gives an indication of the accuracy of the value for $F_1(D)$. Now $F_1(x)$ is calculated with the step size h=0.01 for $0 \leq x \leq 24$. Then with the step size h=0.1, $F_1(x)$ is calculated for $24 \leq x \leq x_M + h$, where $x_M=360$. For x>24,

$$\frac{\delta V(x)}{V_{eff}(x)} \lesssim 10^{-30} \tag{3.23}$$

and hence δV is neglected in (3.13) for those values of x. The derivative of F_1 at x_M is calculated by the symmetric difference formula

$$F_1'(x_M) = \frac{F_1(x_M+h) - F_1(x_M-h)}{2h} + O(h^2) \tag{3.24}$$

to evaluate the logarithmic derivative

$$L_1 = \frac{F_1'(x_M)}{F_1(x_M)} \tag{3.25}$$

For large x, $F_2(x_I)$ and $F_2(x_I-h)$ are obtained using (3.21), where $x_I=2400$, and h=0.1. The error in the value of $F_2(x_I)$ is about 2 PPM, and this error in the subsequent evaluation of $F_2(x)$ is expected to decrease because we are going in the stable direction. With those initial values and the step size h, $F_2(x)$ is integrated in the direction of decreasing x to the point x_M-h. The logarithmic derivative of $F_2(x)$ at x_M

$$L_2 = \frac{F_2'(x_M)}{F_2(x_M)} \tag{3.26}$$

matches L_1 within 2 PPM. Using F(x) at various x, $\int_0^\infty dx|F(x)|^2$ and $\int_0^\infty dx|F(x)|^2|\psi_{\mu 0}(x)|^2$ are calculated by the trapezoidal rule. Substitution of these integrals in (3.10) yields $\Delta\nu_8 = 4494.44$ MHz.

The calculation is repeated by reducing the mash-size(h) by a factor of two. The hyperfine frequency changes by 0.003 MHz. The calculation is also repeated with the values of E given by

$$E = -\tfrac{1}{2}M_e\alpha^2[1+0.95(\tfrac{M_e}{M_\mu})^2] \qquad (3.27)$$

and

$$E = -\tfrac{1}{2}M_e\alpha^2[1+1.05(\tfrac{M_e}{M_\mu})^2] \qquad (3.28)$$

The logarithmic derivatives match within 15 PPM, while the hyprfine frequency changes by 0.01 MHz. Hence the error in $\Delta\nu_8$ should be less than 0.01 MHz. The program is checked by solving the hydrogen problem, i.e. with

$$V_{eff}(x) = -\frac{\alpha}{x} \qquad (3.29)$$

and

$$E = -\tfrac{1}{2}M_e\alpha^2 \qquad (3.30)$$

The hyperfine splitting obtained is 4483.38 MHz, in exact agreement with the result obtained analytically.

Summarizing, $\Delta\nu_8 = 4499.44 \pm 0.01$ MHz. The quantity $\Delta\nu_0 + \Delta\nu_1^8$ (which takes into account the effective nucleus size contribution to the hyperfine splitting upto first order of perturbation theory), agrees numerically with $\Delta\nu_g$ (which takes into account the effective nucleus size contribution in all orders of perturbation theory) up to order $\Delta\nu_F(M_e/M_\mu)^2$, as expected.

4. NUMERICAL CALCULATION OF THE CORRECTION DUE TO THE EXCITATION OF THE EFFECTIVE NUCLEUS

The numerical calculation of $\Delta\nu_1^e$, the contribution to the hyperfine splitting in the first order of perturbation theory when the intermediate muon-states are excited states, is described in this Chapter. The correction $\Delta\nu_1^e$ can be physically interpreted as the contribution due to the excitation of the effective nucleus.

The correction $\Delta\nu_1^e$ is given by

$$\Delta\nu_1^e = \frac{16\pi\alpha}{3m_\mu m_e}\int d^3x_3\int d^3x_2\int d^3x_1 \sum_{\substack{n\neq 0\\ n'}} \psi_0^+(\bar{x}_3,\bar{x}_3)$$

$$\times \frac{\psi_{\mu n}(\bar{x}_3)\psi_{en'}(\bar{x}_3)\psi_{\mu n}^+(\bar{x}_2)\psi_{en'}^+(\bar{x}_1)}{E_{\mu 0}+E_{e0}-E_{\mu n}-E_{en'}}\,\delta V(\bar{x}_2,\bar{x}_1)\psi_0(\bar{x}_2,\bar{x}_1) \quad (4.1)$$

It is difficult to deal with the summation over all intermediate states numerically, particularly for the continuum. The summation over intermediate states along with the energy denominator can be replaced by Green's functions, which are easier to handle numerically. To achieve this, the energy denominator has to be written as a product of two terms, one containing only the electron intermediate energy levels and the other containing only the muon intermediate energy levels:

$$\frac{1}{a-b} = \frac{1}{2\pi i}\int_C \frac{dz}{(z-a)(z-b)} \tag{4.2}$$

where the contour C in the complex z plane can be chosen to be a straight line parallel to y-axis with 'a' on the left side of the contour and 'b' on the right side of the contour. With $a = E_{eo}-E_{en'}$ for any n' and $b = -E_{\mu o}+E_{\mu n}$ for any $n\neq 0$ in (4.2), we have[27]

$$\frac{1}{E_{\mu o}+E_{eo}-E_{\mu n}-E_{en'}}$$
$$= \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} dz \frac{1}{[z-(E_{eo}-E_{en'})][z-(E_{\mu n}-E_{\mu o})]} \tag{4.3}$$

where

$$0 < c < \frac{3}{2}\alpha^2 m_\mu \tag{4.4}$$

The Figure 1 shows the contour in the complex z plane with the bound states and continuum states for the electron and muon.

Equation (4.3) is true for any $n\neq 0$ and any n', and the right hand side of that equation gives zero for n=0 and any n'. Hence

$$\sum_{\substack{n\neq 0\\ n'}} \frac{\psi_{\mu n}(\bar{x}_3)\psi_{en'}(\bar{x}_3)\psi^{+}_{\mu n}(\bar{x}_2)\psi^{+}_{en'}(\bar{x}_1)}{E_{\mu o}+E_{eo}-E_{\mu n}-E_{en'}} = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} dz \sum_{n,n'}$$

$$\times \frac{\psi_{\mu n}(\bar{x}_3)\psi_{en'}(\bar{x}_3)\psi^{+}_{\mu n}(\bar{x}_2)\psi^{+}_{en'}(\bar{x}_1)}{[z-(E_{eo}-E_{en'})][z-(E_{\mu n}-E_{\mu o})]} \tag{4.4}$$

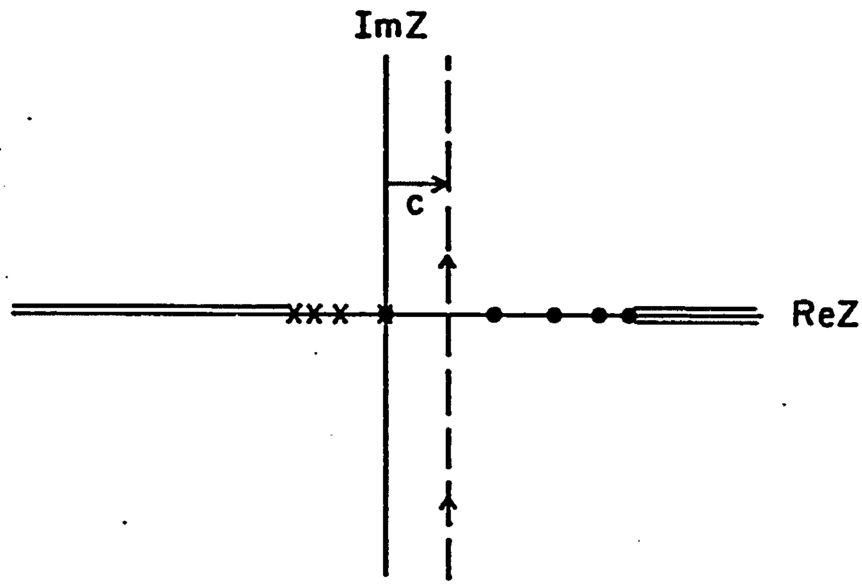

Figure 1 : The Contour in the complex z plane

• muon bound states

muon continuum states

× electron bound states

electron continuum states

From the definitions

$$\sum_{n'} \frac{\psi_{en'}(\bar{x}_3)\psi^{\dagger}_{en'}(\bar{x}_1)}{E_{en'} - (E_{eo} - z)} = G_e(\bar{x}_3, \bar{x}_1, E_{eo} - z) \qquad (4.5)$$

$$\sum_{n} \frac{\psi_{\mu n}(\bar{x}_3)\psi^{\dagger}_{\mu n}(\bar{x}_2)}{E_{\mu n} - (z + E_{\mu o})} = G_{\mu}(\bar{x}_3, \bar{x}_2, E_{\mu o} + z) \qquad (4.6)$$

where G_e and G_{μ} are the Coulomb Green's functions for the electron and the muon respectively, we have

$$\Delta\nu_1^e = \frac{i8\alpha^2}{3m_\mu m_e} \int d^3x_3 \int d^3x_2 \int d^3x_1 \int_{c-i\infty}^{c+i\infty} dz\, \psi_0^+(\bar{x}_3,\bar{x}_3)\psi_0(\bar{x}_2,\bar{x}_1)$$

$$\times\, G_e(\bar{x}_3,\bar{x}_1,E_{e0}-z)\, G_\mu(\bar{x}_3,\bar{x}_2,E_{\mu 0}+z)\left(\frac{1}{x_{12}}-\frac{1}{x_1}\right) \quad (4.7)$$

$$= \frac{i8\alpha^2}{3m_\mu m_e}\int_{c-i\infty}^{c+i\infty} dz\, h(z) \quad (4.8)$$

In equation (4.8) $h(z^*)=h^*(z)$, hence

$$\Delta\nu_1^e = \frac{i8\alpha^2}{3m_\mu m_e}\int_c^{c+i\infty} dz\,[h(z)+h(z^*)]$$

$$= \frac{i16\alpha^2}{3m_\mu m_e}\,\mathrm{Re}\Big[\int_c^{c+i\infty} dz\, h(z)\Big]$$

$$= -\frac{64\alpha^2 M_\mu}{3m_\mu m_e}\,\mathrm{Re}\Big[\int_0^1 \frac{dt}{t^3}\, h(z(t))\Big], \quad (4.9)$$

where

$$z(t) = 2\alpha^2 M_\mu\left[k + i\left(\frac{1}{t^2}-1\right)\right] \quad (4.10)$$

and $k=c/(2\alpha^2 M_\mu)$. In this calculation we have chosen k to be 0.306 so the Equation (4.4) is satisfied.

The Green's function can be expanded into angular and radial parts.

$$G_e(\bar{x}_3,\bar{x}_1,E_{e0}-z) = \sum_{\ell m} G_{e\ell}(x_3,x_1,E_{e0}-z)\,Y_{\ell m}(\hat{x}_1)\,Y^*_{\ell m}(\hat{x}_3) \quad (4.11)$$

$$G_\mu(\bar{x}_3,\bar{x}_2,E_{\mu 0}+z) = \sum_{\ell m} G_{\mu\ell}(x_3,x_2,E_{\mu 0}+z)\,Y_{\ell m}(\hat{x}_3)\,Y^*_{\ell m}(\hat{x}_2) \quad (4.12)$$

Also

$$\frac{1}{x_{12}} = \sum_{\ell''m''} \frac{4\pi}{2\ell''+1} Y_{\ell''m''}(\hat{x}_2) Y^*_{\ell''m''}(\hat{x}_1) \frac{(x'^{12}_<)^\ell}{(x'^{12}_>)^{\ell+1}} \tag{4.13}$$

where $x'^{12}_< = \min(x_1, x_2)$ and $x'^{12}_> = \max(x_1, x_2)$. The integration over the angular part can be easily carried out to get

$$\Delta\nu_1^e = -\frac{256\alpha^2\Delta\nu_F(\alpha M_\mu)^4}{\pi} \mathrm{Re}\Big\{ \int_0^1 \frac{dt}{t^3} \int_0^\infty dx_1 \int_0^\infty dx_2 \int_0^\infty dx_3 \, x_1^2 x_2^2 x_3^2$$

$$\times e^{-2\alpha M_\mu x_3} e^{-\alpha M_e x_3} e^{-2\alpha M_\mu x_2} e^{-\alpha M_e x_1}$$

$$\times \sum_\ell G_{e\ell}(x_3, x_1, E_{e0} - z) G_{\mu\ell}(x_3, x_2, E_{\mu 0} + z) \Big[\frac{(x'^{12}_<)^\ell}{(x'^{12}_>)^{\ell+1}} - \frac{1}{x_1}\delta_{\ell 0} \Big] \Big\} \tag{4.14}$$

As derived in Appendix B,

$$G_{e\ell}(x_2, x_1, z) = M_e^2 G_\ell(M_e x_2, M_e x_1, \frac{z}{M_e}) \tag{4.15}$$

$$G_{\mu\ell}(x_2, x_1, z) = 2M_\mu^2 G_\ell(2M_\mu x_2, 2M_\mu x_1, \frac{z}{4M_\mu}) \tag{4.16}$$

where radial part of the Coulomb Green's function G_ℓ, independent of mass and charge, satisfies

$$\Big[-\frac{1}{2x_2}\frac{d^2}{dx_2^2}x_2 + \frac{\ell(\ell+1)}{2x_2^2} - \frac{\alpha}{x_2} - z\Big] G_\ell(x_2, x_1, z)$$

$$= \frac{1}{x_1 x_2}\delta(x_1 - x_2) \tag{4.17}$$

The function G can be written as the product of the two Whittaker functions M and W.

$$G_\ell(x_2,x_1,z) = \frac{1}{cx_1x_2}\frac{\Gamma(1+\ell-\nu)}{\Gamma(2\ell+2)} M_{\nu,\ell+1/2}(2cx_<^{12}) \times W_{\nu,\ell+1/2}(2cx_>^{12}), \tag{4.18}$$

where $c = (-2z)^{1/2}$ such that $Re(c) > 0$, and $\nu = \alpha/c$. The functions M and W satisfy the following confluent hypergeometric equation[28]

$$\left[\frac{d^2}{dx^2} + \left(\frac{\frac{1}{4}-\beta^2}{x^2} + \frac{\nu}{x} - \frac{1}{4}\right)\right] \begin{matrix} W_{\nu,\beta}(x) \\ M_{\nu,\beta}(x) \end{matrix} = 0, \tag{4.19}$$

where M is regular at $x=0$ while W is regular as $x\to\infty$. The following integral representations for M and W are used for the purpose of numerical evaluation.[29]

$$M_{\nu,\ell+1/2}(z) = \frac{\Gamma(2\ell+2)}{\Gamma(1+\ell+\nu)\Gamma(1+\ell-\nu)} z^{\ell+1} \times \int_0^1 dt\, t^{\ell-\nu}(1-t)^{\ell+\nu} e^{-\frac{1}{2}(1-2t)z} \tag{4.20}$$

$$W_{\nu,\ell+1/2}(z) = \frac{1}{\Gamma(1+\ell-\nu)} z^{\ell} \int_0^\infty ds\, e^{-s} e^{-\frac{1}{2}z} \left(\frac{s}{z}\right)^{\ell-\nu} \left(1+\frac{s}{z}\right)^{\ell+\nu} \tag{4.21}$$

To evaluate M, the following integral has to be calculated.

$$I = \int_0^1 dx\, x^{\ell-\nu} (1-x)^{\ell+\nu} e^{zx} \tag{4.22}$$

For $0 \leq \mathrm{Re}(z) \leq 8$, I is evaluated by using the 12 point Gauss-Legendre quadrature formula.[30] For $8 < \mathrm{Re}(z) \leq 18$, the change of variable $y=x^2$ is made, and then the integral I is evaluated by the same 12 point formula. For $\mathrm{Re}(z) \geq 18$, the new variable $s=z(1-x)$ is introduced. Then

$$\begin{aligned} I &= \frac{e^z}{z} \int_0^z ds \left(\frac{s}{z}\right)^{\ell+\nu} \left(1-\frac{s}{z}\right)^{\ell-\nu} e^{-s} \\ &= \frac{e^z}{z} \int_0^{\infty e^{i\theta}} ds \left(\frac{s}{z}\right)^{\ell+\nu} \left(1-\frac{s}{z}\right)^{\ell-\nu} e^{-s} \\ &\quad - \frac{e^z}{z} \int_z^{\infty e^{i\theta}} ds \left(\frac{s}{z}\right)^{\ell+\nu} \left(1-\frac{s}{z}\right)^{\ell-\nu} e^{-s} \end{aligned} \tag{4.23}$$

where $\theta=\arg(z)$, and the integration contour is chosen to lie below the branch cut extending from z to $\infty e^{i\theta}$. For the relevant values of z, ν, l ($\mathrm{Re}(z)>18$, $l=5$, $\mathrm{Re}(\nu)<1.2$), the magnitude of the ratio of the second term to the first term in (4.23) is of order

$$\frac{\Gamma(2\ell+1)}{\Gamma(\ell+1+\nu)} |z|^{\nu-\ell} e^{-|z|} \tag{4.24}$$

Hence for the relevant values of z, ν, l, neglecting the second term in (4.23) introduces an error of less than 1 part in 10^5. Hence the integral I can be approximated by

$$I \simeq \frac{e^z}{z} \int_0^{\infty e^{i\theta}} ds \left(\frac{s}{z}\right)^{\ell+\nu} \left(1-\frac{s}{z}\right)^{\ell-\nu} e^{-s}$$

$$= \frac{e^z}{z} \int_0^\infty ds \left(\frac{s}{z}\right)^{\ell+\nu} \left(1 - \frac{s}{z}\right)^{\ell-\nu} e^{-s} \tag{4.25}$$

The integral given by (4.25) is calculated by the 10 point Gauss-Laguerre quadrature method.[30]

To evaluate W, the following integral has to be evaluated.

$$I = \int_0^\infty ds\, e^{-s} \left(\frac{s}{z}\right)^{\ell-\nu} \left(1 + \frac{s}{z}\right)^{\ell+\nu} \tag{4.26}$$

For $0<\mathrm{Re}(z)<0.35$, we use

$$I = \int_0^\infty ds\, e^{-s} \left(\frac{s}{z}\right)^{\ell-\nu} \left[\left(1+\frac{s}{z}\right)^{\ell+\nu} - 1 - (\ell+\nu)\frac{s}{z}\right] + \frac{\Gamma(\ell+1-\nu)}{z^{\ell-\nu}} + \frac{(\ell+\nu)\Gamma(\ell+2-\nu)}{z^{\ell+1-\nu}} \tag{4.27}$$

The first term can be written as

$$I_1 = I_{11} + I_{12} \tag{4.28}$$

where

$$I_{11} = \int_0^1 ds\, e^{-s} \left(\frac{s}{z}\right)^{\ell-\nu} \left[\left(1+\frac{s}{z}\right)^{\ell+\nu} - 1 - (\ell+\nu)\frac{s}{z}\right] \tag{4.29}$$

and is evaluated by using 10 point Gauss-Legendre quadrature formula, while

$$I_{12} = \int_1^\infty ds\, e^{-s} \left(\frac{s}{z}\right)^{\ell-\nu} \left[(1+\frac{s}{z})^{\ell+\nu} - 1 - (\ell+\nu)\frac{s}{z}\right]$$

$$= \int_0^\infty dt \frac{e^{-t}}{e} \left(\frac{t+1}{z}\right)^{\ell-\nu} \left[(1+\frac{t+1}{z})^{\ell+\nu} - 1 - (\ell+\nu)\frac{t+1}{z}\right] \qquad (4.30)$$

is evaluated by 10 point Gauss-Laguerre quadrature formula. For $Re(z) \geq 0.35$, we use

$$I = \int_0^\infty ds\, e^{-s} \left(\frac{s}{z}\right)^{\ell-\nu} \left[(1+\frac{s}{z})^{\ell+\nu} - 1 - (\ell+\nu)\frac{s}{z} - \frac{(\ell+\nu)(\ell+\nu-1)}{2}\left(\frac{s}{z}\right)^2\right]$$

$$+ \frac{\Gamma(\ell+1-\nu)}{z^{\ell-\nu}} + \frac{(\ell+\nu)\Gamma(\ell+2-\nu)}{z^{\ell+1-\nu}} + \frac{(\ell+\nu)(\ell+\nu-1)\Gamma(\ell+3-\nu)}{2\, z^{\ell+2-\nu}} \qquad (4.31)$$

The first term is evaluated by same methods discussed for the case where $Re(z)<0.35$. The 10 point integration for W gives a good result only for $Re(\nu)<1.2$. This restriction on ν is ensured by the choice of k in (4.10).

The recursion relation in l for $M_{\nu,\ell+1/2}(z)$ and $W_{\nu,\ell+1/2}(z)$ for fixed ν and z, can be derived from the integral representations. They are given as follows[31]

$$\frac{1}{\mathcal{H}_{\nu,\ell-1}(z)} = \left[\frac{(\ell+1)^2-\nu^2}{4(\ell+1)^2(2\ell+1)(2\ell+3)}\right]\mathcal{H}_{\nu,\ell}(z) + \frac{1}{z} - \frac{\nu}{2\ell(\ell+1)} \qquad (4.32a)$$

$$\mathcal{U}_{\nu,\ell}(z) = \frac{2\ell+1}{\ell(\ell+1-\nu)}\left[\frac{2\ell(\ell+1)}{z} - \nu\right] + \frac{(\ell+1)(\ell+\nu)}{\ell(\ell+1-\nu)\mathcal{U}_{\nu,\ell-1}(z)}, \qquad (4.33a)$$

where

$$\mathcal{H}_{\nu,\ell}(z) = \frac{M_{\nu,\ell+3/2}(z)}{M_{\nu,\ell+1/2}(z)} \tag{4.32b}$$

$$U_{\nu,\ell}(z) = \frac{W_{\nu,\ell+3/2}(z)}{W_{\nu,\ell+1/2}(z)} \,. \tag{4.33b}$$

For numerical stability, the recursion relation has to be employed in the direction of decreasing l for M and in the direction of increasing l for W. For a qualitative explanation, see Appendix D. To calculate $M_{\nu,\ell+1/2}(z)$ for $0 \leq l \leq L$(the choice of L is discussed later in this Chapter), a value for $r_{\nu,L}(z)$ is required. With the aid of (4.32) by downward recursion starting from

$$\ell = L_M = \mathrm{Max}\,[L, \mathrm{Re}(\tfrac{z}{2})] + 15 + \mathrm{Re}(\tfrac{z}{20}) \tag{4.34}$$

and the initial guess

$$\mathcal{H}_{\nu,L_M}(z) = z \tag{4.35}$$

the ratio $r_{\nu,L}(z)$ is obtained by downward recursion. To estimate the error involved, this ratio is calculated starting from various values of L_M. The agreement among those various values indicate that the error is less than 1 part in 10^5 for all ν and z. From Equation (4.32) and the value for $r_{\nu,L}(z)$, $r_{\nu,\ell}(z)$ is obtained for all $l \leq L$. The function $M_{\nu,\ell+1/2}(z)$ is calculated for l=5(the most convenient choice for numerical calculation), and then from the values of $r_{\nu,\ell}(z)$, the $M_{\nu,\ell+1/2}(z)$ are calculated for all $l \leq L$. To calculate W for $0 \leq l \leq L$, first $W_{\nu,\ell+1/2}(z)$ is evaluated for l=0 and l=1, and thus $u_{\nu,0}(z)$ can be calculated. Then from the relation (4.33), $u_{\nu,\ell}(z)$ and $W_{\nu,\ell+1/2}(z)$ are calculated for all $l \leq L$.

To evaluate the integrand of the integral over x_1, x_2, x_3 and t, the infinite sum over l has to be carried out. This sum is divided into two parts

$$\sum_{\ell=0}^{\infty} f(\ell) = \sum_{\ell=0}^{L} f(\ell) + \sum_{L+1}^{\infty} f(\ell) \tag{4.36}$$

The quantity L is initially chosen so that the Green's functions for electron and muon approach the asymptotic limit within 1% for l>L(note that this L is same as mentioned previously in this Chapter). For $l \gg |x|$,[32]

$$M_{\nu,\ell+1/2}(x) \sim x^{\ell+1} \tag{4.37}$$

$$W_{\nu,\ell+1/2}(x) \sim \frac{\Gamma(2\ell+1)}{\Gamma(\ell+1-\nu)} x^{-\ell} \tag{4.38}$$

Hence

$$G_\ell(x_1,x_2,z) \sim \frac{2}{2\ell+1} \frac{(x_<^{12})^\ell}{(x_>^{12})^{\ell+1}} \tag{4.39}$$

Using (4.15), (4.16) and the above equations, we find

$$G_{ee}(x_3, x_1, E_{eo}-z)\, G_{\mu\ell}(x_3, x_2, E_{\mu o}+z)\left[\frac{(x_<^{12})^\ell}{(x_>^{12})^{\ell+1}} - \frac{1}{x_1}\delta_{\ell,0}\right]$$

$$\sim \frac{a\,r^\ell}{(\ell+1/2)^2} \tag{4.40}$$

where

$$a = \frac{M_e M_\mu}{(x_>^{12})(x_>^{23})(x_>^{31})} \tag{4.41}$$

is independent of l, and

$$r = \frac{(x_<^{12})(x_<^{23})(x_<^{31})}{(x_>^{12})(x_>^{23})(x_>^{31})} \tag{4.42}$$

The asymptotic limit given by equation (4.40) is reached within 1% for all relevant values of x_1, x_2, x_3 and z, if one chooses

$$L = 10 + 2\cdot \mathrm{Max}\left\{\left|\, 4\left[-\tfrac{1}{2}M_\mu(E_{\mu o}+z)\right]^{1/2}\mathrm{Max}(x_2,x_3)\right|,\right.$$

$$\left.\left|\, 2\left[-2M_e(E_{eo}-z)\right]^{1/2}\mathrm{Max}(x_1,x_3)\right|\right\} \tag{4.43}$$

In the sum (L+1 to ∞) the function f is replaced by its asymptotic form in the large l limit. That sum is proportional to $\sum_{L+1}^{\infty} r^\ell/(l+1/2)^2$, and is approximated by

$$\sum_{L+1}^{\infty}\frac{r^\ell}{(\ell+1/2)^2} \simeq \int_{L+1/2}^{\infty} dy\,\frac{r^y}{(y+1/2)^2} = \frac{1}{\sqrt{r}}\frac{1}{L+1}E_2(x) \tag{4.44}$$

where

$$x = (L+1)\ln\frac{1}{r} , \tag{4.45}$$

$$E_n(x) = \int_1^\infty \frac{dt\, e^{-tx}}{t^n} . \tag{4.46}$$

For $x>10^{-10}$, $E_2(x)$ is calculated by the relation[29]

$$E_2(x) = e^{-x} - x E_1(x) \tag{4.47}$$

and $E_1(x)$ is evaluated by a library subroutine. The first sum from l=0 to L in (4.36) is evaluated without any approximation. Starting from l=0, after every ten terms of the sum, a check is made to determine whether the remaining sum over l is significant (i.e., more than 1 part in 10^4) compared to the partial sum $S(\mathcal{L})$ for $l \leq \mathcal{L}$. If the remainder is insignificant, the summation over l is terminated. For making the check, following method is used. It is assumed that

$$\sum_{\ell=\mathcal{L}+1}^{\infty} f(\ell) \simeq \sum_{\ell=\mathcal{L}+1}^{\infty} f_A(\ell) \tag{4.48}$$

where

$$f_A(\ell) = \frac{a r^\ell}{(\ell+1/2)^2} \tag{4.49}$$

It can be shown that

$$\sum_{\ell=\mathcal{L}+1}^{\infty} f_A(\ell) < (\mathcal{L}+1/2)\, f_A(\mathcal{L}) \qquad (4.50)$$

$$\sum_{\ell=\mathcal{L}+1}^{\infty} f_A(\ell) < \frac{f_A(\mathcal{L})}{1-\mathcal{R}} \qquad (4.51)$$

Hence if

$$\frac{\min\left[(\mathcal{L}+1/2)\, f_A(\mathcal{L}),\ \frac{f_A(\mathcal{L})}{1-\mathcal{R}}\right]}{S(\mathcal{L})} < 0.0001 \qquad (4.52)$$

then $\sum_{\ell=\mathcal{L}+1}^{\infty} f(1)$ is insignificant and the summation is terminated. Note that this termination, contrary to what one might expect, does not save any computer time. For the justification of the approximation given by (4.48), this calculation is checked against the calculation in which the sum is not terminated.

The integration over x_1, x_2, x_3 and z(or t) is carried out as follows. For large arguments of M and W, i.e., $|x| >> 1$,[32]

$$M_{\nu,\ell+1/2}(x) \sim e^{x/2}\, x^{-\nu}\, \frac{\Gamma(2\ell+2)}{\Gamma(\ell+1-\nu)} \qquad (4.53)$$

$$W_{\nu,\ell+1/2}(x) \sim e^{-x/2}\, x^{\nu} \qquad (4.54)$$

Hence the exponential factors of Green's functions are given by

$$G_{e\ell}(x_3, x_1, z) \propto e^{-\sqrt{-2M_e z}\,|x_3 - x_1|} \qquad (4.55)$$

$$G_{\mu\ell}(x_3,x_2,z) \propto e^{-\sqrt{-2M_\mu z}\,|x_3-x_2|} \tag{4.56}$$

Hence for large x_1, x_2, x_3, the integrand has peaks at $x_1=x_3$ and $x_2=x_3$. These peaks become more and more sharp for larger values of $|z|$, making the task of integration difficult. To deal with this feature, the integration region is divided into six regions defined by $x_1 \geq x_2 \geq x_3$, $x_1 \geq x_3 \geq x_2$ and so on. In each region the exponential behavior of the integrand is known for large arguments of the functions M and W. This peaked behavior is removed by a variable transformation. For example in the region given by $x_1 \geq x_2 \geq x_3$, define the variables y, r_1 and r_2 by $y=x_1$, $r_1=x_2/x_1$ and $r_2=x_3/x_2$. then

$$\int_0^\infty dx_1 x_1^2 \int_0^{x_1} dx_2 x_2^2 \int_0^{x_2} dx_3 x_3^2\, S'(x_1,x_2,x_3,z)$$

$$= \int_0^\infty dy\, y^8 \int_0^1 dr_1 r_1^5 \int_0^1 dr_2 r_2^2\, S'(y, r_1 y, r_1 r_2 y, z) \tag{4.57}$$

Integration over y, i.e.,

$$I = \int_0^\infty dy f''(y) \tag{4.58}$$

is carried out first. It is empirically verified that for large y the exponential behavior of $f''(y)$ is given by

$$f''(y) \propto e^{-Ay}, \tag{4.59}$$

where

$$A = \alpha M_e + \alpha(2M_\mu + M_e)r_1 r_2 + 2\alpha M_\mu r_1 + \mathrm{Re}\left[\sqrt{-2M_e(E_{e0} - z)}\,(1 - r_1 r_2)\right] + \mathrm{Re}\left[\sqrt{-2M_\mu(E_{\mu d} + z)}\,r_1(1 - r_2)\right] \tag{4.60}$$

This value of A is inferred from the exponential behavior of wave functions for electron and muon and exponential behavior of Green's functions. By the change of variable $y \to y' = Ay$, we have

$$I = \int_0^\infty \frac{dy'\, f''(\frac{y'}{A})}{A} , \tag{4.61}$$

where the exponential factor of $f''(y'/A)$ is $f''(y'/A) \propto e^{-y'}$ for large y'. The integral I is broken into two parts

$$I = \int_0^R \frac{dy'\, f''(\frac{y'}{A})}{A} + \int_R^\infty \frac{dy'\, g''(\frac{y'}{A})}{A}$$

$$= \frac{R}{A}\int_0^1 dx\, f''\left(\frac{Rx}{A}\right) + \frac{1}{A}\int_0^\infty dx\, g''\left(\frac{R+x}{A}\right) \tag{4.62}$$

A convenient value of R is found empirically to be 5. The first integral in (4.62) is evaluated by the 8 point Gauss-Legendre quadrature method, and the second integral in (4.62) is evaluated by the 8 point Gauss-Laguerre quadrature method. Once the integration over y is carried out, the integrand of the integral over r_1 and r_2 has peaks at $r_1 = 1$ and $r_2 = 1$. The peaks are roughly given by A^{-9}. For large $|z|$ this poses a formidable problem and is discussed subsequently in this Chapter. The 16 point Gauss-Legendre quadrature method is used to integrate over r_1

and r_2 (the 18 point formula is used for $t<0.1$). Integration over t is evaluated by the Gauss-Legendre quadrature method, using 4,6,..,16 points.

This completes the description of the method used in the calculation of $\Delta\nu_1^e$ except when $|z|$ is very large. For very large $|z|$ (corresponding to $t<0.05$), accurate evaluation of the integrand for the integral over t, becomes very difficult because of various factors. Firstly L is large for large $|z|$. Hence the calculation of M and W functions(for all $l\leq L$), requires a great deal of computer time and storage space. Secondly accurate integration over r_1 and r_2 is difficult because of the peaks at $r_1=1$ and $r_2=1$. Thirdly a significant contribution to $\Delta\nu_1^e$ comes from the region $0<t<0.05$ and hence the integrand has to be accurately evaluated in that region. To overcome this difficulty, an asymptotic expression for the integrand is used in this region. The exact integrand is given by

$$g(t) = -\frac{64\alpha^4 M_\mu}{3m_e m_\mu} \, \mathrm{Re}\left[\frac{h(z)}{t^3}\right] \tag{4.63}$$

so that

$$\Delta\nu_1^e = \int_0^1 dt\, g(t) \tag{4.64}$$

The function h in (4.63) is

$$h(z) = \int d^3x_1 \int d^3x_2 \int d^3x_3\, \psi_0^+(\bar{x}_3,\bar{x}_3)\,\psi_0(\bar{x}_2,\bar{x}_1)$$

$$\times\, G_e(\bar{x}_3,\bar{x}_1,E_{e0}-z)\,G_\mu(\bar{x}_3,\bar{x}_2,E_{\mu 0}+z)\left(\frac{1}{x_{12}}-\frac{1}{x_1}\right) \tag{4.65}$$

The asymptotic expression for F is obtained based on the following approximations.

(I) The Green's functions for electron and muon are replaced by the free Green's functions for electron and muon respectively. As discussed in Chapter 2 and shown in more detail in Appendix C, this is a good approximation for large $|z|$.

$$G_e(\bar{x}_3, \bar{x}_1, E_{e0} - z) \simeq G_e^0(\bar{x}_3, \bar{x}_1, E_{e0} - z)$$

$$= \frac{M_e}{2\pi} \frac{e^{-b_e x_{31}}}{x_{31}} \qquad (4.66)$$

$$G_\mu(\bar{x}_3, \bar{x}_2, E_{\mu 0} + z) \simeq G_\mu^0(\bar{x}_3, \bar{x}_2, E_{\mu 0} + z)$$

$$= \frac{M_\mu}{2\pi} \frac{e^{-b_\mu x_{32}}}{x_{32}} \qquad (4.67)$$

where $b_e = [-2M_e(E_{e0}-z)]^{1/2}$, $Re(b_e)>0$ and $b_\mu = [-2M_\mu(E_{\mu 0}+z)]^{1/2}$, $Re(b_\mu)>0$.

(II) Because of the exponential behavior of the Green's functions, the integrand has peaks at $\bar{x}_1=\bar{x}_3$ and $\bar{x}_2=\bar{x}_3$. Those peaks become very pronounced for large $|z|$. Hence, most of the contribution comes from $\bar{x}_1=\bar{x}_3$ and $\bar{x}_2=\bar{x}_3$. This suggests that evaluating the ground-state wave functions at the argument $\bar{x}_3$, i.e., $\psi_0(\bar{x}_2,\bar{x}_1) \rightarrow \psi_0(\bar{x}_3,\bar{x}_3)$, is a good approximation.

With these two approximations,

$$h(z) \simeq h_A(z) = \frac{M_e M_\mu}{4\pi^2} \int d^3x_3 \int d^3x_2 \int d^3x_1 \, |\psi_0(\bar{x}_3,\bar{x}_3)|^2 \left(\frac{1}{x_{12}} - \frac{1}{x_1}\right)$$

$$\times \frac{e^{-b_\mu x_{32}}}{x_{32}} \frac{e^{-b_e x_{31}}}{x_{31}} \qquad (4.68)$$

With the aid of (2.26a) we obtain

$$h_A(z) = \frac{4}{\pi}\frac{(\alpha M_e)^3 M_e M_\mu}{b_e b_\mu (b_e+b_\mu)}\left(1+\frac{M_e}{2M_\mu}\right)^{-3}$$

$$-\frac{4}{\pi}\frac{(2\alpha^2 M_\mu M_e)^3 M_e M_\mu (4s+b_e)}{b_e b_\mu^2 s^2 (2s+b_e)^2}, \qquad (4.69)$$

where $s=2\alpha M_\mu+\alpha M_e$. With the aid of (4.63) and (4.69), we have for higher $|z|$

$$g(t) \simeq g_A(t) = \mathrm{Re}\left[\frac{32\Delta\nu_F \alpha^3 M_e M_\mu^2}{\pi b_e b_\mu (b_e+b_\mu) t^3}\left(1+\frac{M_e}{2M_\mu}\right)^{-3}\right]$$

$$+\mathrm{Re}\left[\frac{256\Delta\nu_F \alpha^6 M_e M_\mu^5}{\pi b_e b_\mu^2 t^3}\;\frac{4s+b_e}{s^2(2s+b_e)^2}\right] \qquad (4.70)$$

From this derivation we expect that $g(t) \sim g_A(t)$ as $t \to 0$ and this is confirmed empirically. Hence for very small values of $t(t<0.05)$, $g(t)$ is approximated by $g_A(t)$ in the integration over t in (4.64).

The errors involved in the calculation are discussed in the following. The desired accuracy is about 1 part in 10^4, which corresponds to an error of 0.005 MHz in $\Delta\nu_1^e$. Care has been taken so that this accuracy is maintained at each stage of the calculation. For example, the integral representing $M_{\nu,\ell+1/2}(z)$ is calculated by employing a 6,8,10 or 12 point quadrature formula for l=5 and various values of ν and z which cover the range of these parameters. The convergence of the integral is better than 1 part in 10^4 for all values of ν and z. To ensure that the value for M converges to the right number, M is calculated by other methods, i.e., series expansion or asymptotic expansion. The two values agree within 1 part in 10^4 in all cases. Also, for some fixed ν and z, M is calculated for l=4,5,6. These values were compared by the recursion relation. Again the agreement is better than 1 part in 10^4. The value for Green's function is compared in asymptotic region($l \gg |x|$ or $l \ll |x|$) with the analytic value obtained by appropriate series expansion. The agreement within 1 part in 10^4 suggests that the errors made at each stage of calculation do not accumulate. Once the program is built up to calculate g(t), some of the parameters are changed one at a time. For example, the integral representing M is evaluated with 14 point quadrature instead of 12 point quadrature. The quantity L_M is calculated by

$$L_M = \mathrm{Max}\,[L, \mathrm{Re}(\tfrac{z}{2})] + 115 + \mathrm{Re}(\tfrac{z}{z_0}) \qquad (4.71)$$

instead of (4.34). Also

$$L = 10 + \mathrm{Max}\,\{\, |\, 4\,[-\tfrac{1}{2}M_\mu(E_{\mu 0}+z)]^{1/2}\,\mathrm{Max}\,(x_2, x_3)\,|\,,$$

$$|\, 2\,[-2M_e(E_{e0}-z)]^{1/2}\,\mathrm{Max}\,(x_1, x_3)\,|\,\} \qquad (4.72)$$

is used instead of (4.43). For each of these changes, g(t) is calculated for various t, and compared with the value obtained without the change in that parameter. The agreement is always better than 1 part in 10^4. For the final integration over t, (4.72) is used instead of (4.43) with no significant loss of accuracy, thus considerably saving computer-time and storage space. Also for the same reason, W is evaluated using only half as many points as discussed previously (one is interested in achieving a particular accuracy globally rather than achieving that particular accuracy locally).

For an estimate of the errors involved in the values of g(t) for $0.05 \leq t \leq 0.5$, g(t) is calculated numerically after making the same approximations as are made in obtaining the analytical expression $g_A(t)$. The approximate value thus obtained, $g'_A(t)$, is compared with the analytical value $g_A(t)$. The difference, $g'_A(t)-g\ (t)$, gives an errror estimate for the calculated value of g(t). This is so because g(t) and $g_A(t)$ have similar qualitative behavior, and in fact quantitatively they do not differ much (the fractional difference between g(t) and $g_A(t)$ is 20% at t=0.5 and 4% at t=0.1). In the region $0.1 \leq t \leq 0.5$, the error involved in g(t) is estimated (by the above mentioned method) to be less than 0.005 MHz. For t>0.5, the convergence at each stage in the calculation of g(t), is much better and hence the errors involved in g(t) are much less than 0.005 MHz. For $0.05 \leq t \leq 0.1$, estimated errors in g(t) increase as t decreases, and increase to about 0.035 MHz at t=0.05. However the error in the integrated result is much smaller. For $t<0.05$, g(t) is approximated by $g_A(t)$, and the difference $\Delta g(t)[=g(t)-g_A(t)]$ is estimated by the following method. The difference $\Delta g(t)$ is calculated for various t, in the range $0 \leq t \leq 0.12$ ($t_1=0, t_2 \simeq 0.05, t_3 \simeq 0.09, t_4 \simeq 0.12$). Then $\Delta g(t)$ is fitted to a third-order polynomial using the values of $\Delta g(t)$ at t_1, t_2, t_3 and t_4. This polynomial is used to obtain $\Delta g(t)$ at any other value of t in this range. For an estimation of the error, the upper (lower) limit of $g(t_1)$, $g(t_2)$, $g(t_3)$ and $g(t_4)$ are also fitted to similar polynomials to estimate the upper (lower) limit for the value g(t). Note that for $0.05 \leq t \leq 0.1$, the value for g(t) obtained in this way agrees well with the value calculated by direct integration. Even for $t<0.05$, the two values agree within the limits of the estimated error of each one.

Table (1) gives $\Delta\nu_1^e$ obtained by employing 4,6,...or 16 point quaduature method for integration over t. The estimated errors in $\Delta\nu_1^e$ for n=16 is 0.008 MHz, based on the weighted sum of the errors at the individual integration points in the integral over t. The difference between $\Delta\nu_1^e$ for N=16 and $\Delta\nu_1^e$ for N=14 is 0.0006 MHz, showing a good convergence. The quoted error of 0.008 MHz is larger because the individual errors were only consistently checked to one part in 10^4. Hence $\Delta\nu_1^e = -45.670 \pm 0.008$ MHz.

TABLE 1

N(no. of points)	$\Delta\nu_1^e$ (MHz)
4	-43.1346
6	-45.3567
8	-45.7640
10	-45.7172
12	-45.6796
14	-45.6708
16	-45.6702

Two additional consistency checks on the calculation have been made. (I) A differemt contour, corresponding to k=0.174, is used to evaluate

$\Delta\nu_1^e$. The result agrees within 1 part in 10^4 with the result obtained with the previous contour.

(II) The hyperfine splitting is numerically calculated with the same approximations as made in the analytical calculation of $\Delta\nu_1^e$ in Chapter 2. This result agrees well with the analytical result of Chapter 2.

5 NUMERICAL CALCULATION OF THE CORRECTION DUE TO MASS-POLARIZATION

In the preceeding discussion, the mass-polaization term $(-1/m_\alpha \bar{\nabla}_\mu \cdot \bar{\nabla}_e)$ in (2.9) has been neglected. In this Chapter we estimate the order of magniude of this term on the hyperfine splitting, $\Delta\nu_1^m$, and describe the numerical evaluation.

Replacing δV in (2.13) by the mass-polarization term and using

$$\bar{\nabla}_\mu \psi_{\mu o}(\bar{x}_2) = -2\alpha M_\mu \psi_{\mu o}(\bar{x}_2)\hat{x}_2 \tag{5.1}$$

$$\bar{\nabla}_e \psi_{eo}(\bar{x}_1) = -\alpha M_e \psi_{eo}(\bar{x}_1)\hat{x}_1 \tag{5.2}$$

we have,

$$\Delta\nu_1^m = -\frac{32\pi\alpha^3 M_\mu M_e}{3m_e m_\mu m_\alpha} \int d^3x_1 \int d^3x_2 \int d^3x_3 \psi_o^+(\bar{x}_3,\bar{x}_3)$$

$$\times \sum_{\substack{n,n' \\ \neq 0,0}} \frac{\psi_{\mu n}(\bar{x}_3)\psi_{en'}(\bar{x}_3)\psi_{\mu n}^+(\bar{x}_2)\psi_{en'}^+(\bar{x}_1)}{E_{\mu o}+E_{eo}-E_{\mu n}-E_{en'}}$$

$$\times \hat{x}_2\cdot\hat{x}_1 \psi_o(\bar{x}_2,\bar{x}_1) \tag{5.3}$$

We estimate the order of magnitude of $\Delta\nu_1^m$ with the same approximations as made in the analytical calculation of $\Delta\nu_1^e$. With those approximations, we have

$$\Delta\nu_1^m = -\frac{16\alpha^3 M_\mu M_e^2}{3 m_\mu m_e m_\alpha} \int d^3x_1 \int d^3x_2 \int d^3x_3 \sum_{n\neq 0} \psi_{\mu o}^+(\bar{x}_3)\psi_{eo}^+(0)$$

$$\times \frac{e^{-b_n x_{31}}}{x_{31}} \psi_{\mu n}(\bar{x}_3)\psi_{\mu n}^+(\bar{x}_2)\hat{x}_2\cdot\hat{x}_1$$

$$\times \psi_{\mu o}(\bar{x}_2)\psi_{eo}(0) \tag{5.4}$$

where $b_n = [-2M_e(E_{\mu o}-E_{\mu n}+E_{eo})]^{1/2}$, $b_n>0$. The term $n=0$ in (5.4) is excluded because in that case the integration over $\bar{x}_2$ gives zero. Integration over $\bar{x}_1$ can be carried out with the aid of

$$\int d^3x_1 \frac{e^{-b_n x_{31}}}{x_{31}} \hat{x}_1 \quad .$$

$$= 4\pi \bar{\nabla}_3 \frac{1}{x_3}\left[\frac{2}{b_n^4}(1-e^{-b_n x_3}) + \frac{x_3^2}{b_n^2}\right] \tag{5.5}$$

As discussed in Chapter 2, the major contribution to $\Delta\nu_1^m$ comes from the region where x_2, x_3 are of order $1/(\alpha M_\mu)$. Since b_n is of order $\alpha(M_e M_\mu)^{1/2}$, $b_n x_3$ is of order $(M_e/M_\mu)^{1/2}$. Hence the leading term in (5.5) [obtained by expanding the exponential on the right hand side of (5.5)] is $(8\pi/3)(x_3/b_n)\hat{x}_2\cdot\hat{x}_3$. With this leading term, the order of magnitude for $\Delta\nu_1^m$ is

$$\Delta\nu_1^m \sim \Delta\nu_F \frac{M_e}{m_\alpha}\sqrt{\frac{M_e}{M_\mu}} \sim 0.1 \text{ MHz}. \tag{5.6}$$

Hence neglecting the mass-polarization term is justified for the analytical calculation. However for the numerical calculation this has to be evaluated because the accuracy desired is about 0.005 MHz. With the same techniques as described in the numerical calculation of $\Delta\nu_1^e$, Equation (5.3) gives

$$\Delta\nu_1^m = -\frac{16 i \alpha^3 M_\mu M_e}{3 m_\mu m_e m_\alpha} \int d^3x_3 \int d^3x_2 \int d^3x_1 \psi_0^+(\vec{x}_2,\vec{x}_3)\, \psi_0(\vec{x}_2,\vec{x}_1)$$

$$\times \int_{c-i\infty}^{c+i\infty} dz\, G_e(\vec{x}_3,\vec{x}_1,E_{eo}-z)\, G_\mu(\vec{x}_3,\vec{x}_2,E_{\mu o}+z)\, \hat{x}_1\cdot\hat{x}_2 \tag{5.7}$$

where c is any real number satisfying (4.4). We have

$$\hat{x}_1\cdot\hat{x}_2 = \sum_{\ell m} \frac{4\pi}{2\ell+1}\, \delta_{\ell,1}\, Y^*_{\ell m}(\hat{x}_1)\, Y_{\ell m}(\hat{x}_2) \tag{5.8}$$

Expanding Green's functions into radial and angular parts and then carrying out angular integration, we get

$$\Delta\nu_1^m = \int_0^1 dt\, H(t) \tag{5.9}$$

where

$$H(t) = -\frac{512\alpha^2 \Delta\nu_F M_e (\alpha M_\mu)^5}{\pi m_\alpha} \mathrm{Re}\Big[\frac{1}{t^3} \int_0^\infty dx_1 x_1^2 \int_0^\infty dx_2 x_2^2$$

$$\times \int_0^\infty dx_3 x_3^2\, e^{-2\alpha M_\mu x_3}\, e^{-\alpha M_e x_3}\, e^{-2\alpha M_\mu x_2}\, e^{-\alpha M_e x_1}$$

$$\times G_{e1}(x_3,x_1,E_{eo}-z)\, G_{\mu 1}(x_3,x_2,E_{\mu o}+z) \Big] \tag{5.10}$$

$$Z = 2\alpha^2 M_\mu \left[K + i\left(\frac{1}{t^2} - 1\right) \right] \tag{5.11}$$

$$K = \frac{c}{2\alpha^2 M_\mu}. \tag{5.12}$$

In this calculation we choose the same value of k as of the previous Chapter, namely, k=0.306. Hence (4.4) is satisfied. The above equation is very similar to Equation (4.14), except that in in this case only the l=1 term contributes. The same numerical methods as described in the previous Chapter are employed to evaluate (4.14). For t>0.1, the integrations over r_1, r_2 and y (see previous Chapter) are carried out by 22 point, 8 point and 8 point quadrature methods respectively.

For high z (t<0.1), accurate integrations over r_1 and r_2 are difficult for reasons similar to those discussed in the previous Chapter. To overcome this problem, an approximate analytical formula for H(t) is derived as follows. With the aid of (5.7), H(t) can be written as

$$H(t) = \frac{128\alpha^5 M_\mu^2 M_e}{3m_\mu m_e m_\alpha t^3} \int d^3\bar{x}_1 \int d^3 x_2 \int d^3 x_3 \, \psi_0^+(\bar{x}_3, \bar{x}_3)\, \psi_0(\bar{x}_2, \bar{x}_1)\, \hat{x}_1 \cdot \hat{x}_2$$

$$\times \, \mathrm{Re}\left[G_e(\bar{x}_3, \bar{x}_1, E_{e0} - Z)\, G_\mu(\bar{x}_3, \bar{x}_2, E_{\mu 0} + Z) \right] \tag{5.13}$$

With the same approximations made in deriving (4.70),

$$H(t) \simeq H_A(t) = \frac{128\alpha^5 M_\mu^2 M_e}{3 m_\mu m_e m_\alpha t^3} \frac{M_e M_\mu}{4\pi^2} \int d^3x_1 \int d^3x_2 \int d^3x_3$$

$$\times |\psi_0(\bar{x}_3, \bar{x}_3)|^2 \hat{x}_2 \cdot \hat{x}_1 \, \mathrm{Re}\left[\frac{e^{-b_e x_{31}}}{x_{31}} \frac{e^{-b_\mu x_{32}}}{x_{32}} \right] \qquad (5.14)$$

where $b_e = [-2M_e(E_{e0}-z)]^{1/2}$, $\mathrm{Re}(b_e)>0$ and $b_\mu = [-2M_\mu(E_{\mu 0}+z)]$, $\mathrm{Re}(b_\mu)>0$. We first integrate over $\bar{x}_1$ and $\bar{x}_2$ by using (5.5). Then integrating over $\bar{x}_3$,

$$H_A(t) = \frac{4096 \, \Delta\nu_F (\alpha M_\mu)^6 (\alpha M_e) M_e}{\pi m_\alpha t^3} \frac{1}{b_e^4 b_\mu^4}$$

$$\times \left\{ \frac{b_e^2 b_\mu^2}{A_1^3} + b_e b_\mu \left(\frac{b_\mu}{A_2^2} + \frac{b_e}{A_3^2} \right) + 2A_1 \ln \frac{A_1 A_4}{A_2 A_3} \right.$$

$$\left. + \frac{1}{A_1} \left(2 b_e b_\mu \frac{A_1}{A_4} - \frac{b_\mu b_e^2}{A_3} - \frac{b_e b_\mu^2}{A_2} \right) \right\} , \qquad (5.15)$$

where

$$A_1 = 4\alpha M_\mu + 2\alpha M_e \qquad (5.16a)$$

$$A_2 = A_1 + b_e \qquad (5.16b)$$

$$A_3 = A_1 + b_\mu \qquad (5.16c)$$

$$A_4 = A_1 + b_e + b_\mu \qquad (5.16d)$$

For $t<0.1$, $H(t)$ is approximated by $H_A(t)$.

For an estimate of the errors involved in the values of $H(t)$ for t

near 0.1, the same procedure, as described in the previous Chapter, is used. The error in the value of H(t) at t=0.1, is thus estimated to be 0.00001 MHz. Again for the same reasons as described in the previous Chapter, the errors in the values of H(t) for t>0.1, should be less than 0.00001 MHz. The difference between $H_A(t)$ and the calculated value of H(t) at t=0.1 is 0.002 MHz. This difference decreases as t decreases. Hence approximating H(t) by $H_A(t)$ in the region t<0.1, introduces an error which is smaller than 0.0002 MHz.

The quantity $\Delta\nu_1^m$ is evaluated by integrating over t with a 4,6 or 8 point quadrature method. The results are shown in Table 2. The estimated error in $\Delta\nu_1^m$ for N=8 is less than 0.0002 MHz. Hence $\Delta\nu_1^m$= 0.0785±0.0002 MHz.

TABLE 2

N(no. of points)	$\Delta\nu_1^m$ (MHz)
4	0.07887
6	0.07853
8	0.07852

6. ESTIMATE OF HIGHER ORDER NONRELATIVISTIC CORRECTIONS

In this Chapter we estimate the order of magnitude of the second-order correction $\Delta\nu_2$ to the hyperfine splitting, due to the second-order correction to the wave function.

The ground-state eigenvector of the Hamiltonian H, given by Equation (2.8), is

$$|\psi\rangle = |\psi_0\rangle + |\psi_1\rangle + |\psi_2\rangle + \cdots \quad (6.1)$$

where $|\psi_0\rangle$ is the eigenvector of the zero-order Hamiltonian, and $|\psi_1\rangle$ and $|\psi_2\rangle$ are the first-order and second-order corrections respectively. The magnitude of the hyperfine splitting is given by[see Equation (2.7)]

$$\Delta\nu = \Delta\nu_0 + \Delta\nu_1 + \Delta\nu_2 + \cdots = \langle\psi|\Delta H|\psi\rangle \quad (6.2)$$

where

$$\Delta H = \frac{8\pi\alpha}{3m_\mu m_e}\delta^3(\vec{x}_\mu - \vec{x}_e) \quad (6.3)$$

From (6.1) and (6.2), the second-order correction to the hyperfine splitting is given by

$$\Delta\nu_2 = \langle\psi_1|\Delta H|\psi_1\rangle + 2\,\mathrm{Re}\,\langle\psi_0|\Delta H|\psi_2\rangle \tag{6.4}$$

Now let $|n,n'\rangle$ be the eigenvector of the zero-order Hamiltonian with the eigenvalue $E_{\mu n}+E_{en'}$, i.e.,

$$\langle\bar{x}_\mu,\bar{x}_e|n,n'\rangle = \psi_{\mu n}(\bar{x}_\mu)\psi_{en'}(\bar{x}_e) \tag{6.5}$$

With this notation,

$$|\psi_0\rangle = |0,0'\rangle \tag{6.6}$$

$$|\psi_1\rangle = \sum_{\substack{n,n'\\ \neq 0,0}} \frac{|n,n'\rangle\langle n,n'|\delta V|0,0'\rangle}{E_{\mu 0}+E_{e0}-E_{\mu n}-E_{en'}} \tag{6.7}$$

$$|\psi_2\rangle = \sum_{m,m'} C_{m,m'}\,|m,m'\rangle \tag{6.8}$$

where

$$C_{0,0} = -\sum_{\substack{n,n'\\ \neq 0,0}} \frac{1}{2}\,\frac{|\langle n,n'|\delta V|0,0'\rangle|^2}{(E_{\mu 0}+E_{e0}-E_{\mu n}-E_{en'})^2} \tag{6.9}$$

and for $m,m' \neq 0,0$

$$C_{m,m'} = -\frac{\langle m,m'|\delta V|0,0'\rangle\langle 0,0'|\delta V|0,0'\rangle}{(E_{\mu 0}+E_{e0}-E_{\mu m}-E_{em'})^2}$$

$$+\sum_{\substack{n,n'\\ \neq 0,0}} \frac{\langle m,m'|\delta V|n,n'\rangle\langle n,n'|\delta V|0,0'\rangle}{(E_{\mu 0}+E_{e0}-E_{\mu n}-E_{en'})(E_{\mu 0}+E_{e0}-E_{\mu m}-E_{em'})} \tag{6.10}$$

We estimate the order of magnitude of $\Delta\nu_2$ with the same approximations as used for the analytical calculation of $\Delta\nu_1^a$. One expects that those approximations give the leading order correctly. The contribution to $\Delta\nu_2$ due to the first term in (6.4) can be written as

$$\langle\psi_1|\Delta H|\psi_1\rangle = \sum_{\substack{n,n' \\ \neq 0,0}} \sum_{\substack{m,m' \\ \neq 0,0}} \frac{\langle 0,0'|\delta V|m,m'\rangle\langle m,m'|\Delta H|n,n'\rangle\langle n,n'|\delta V|0,0\rangle}{(E_{\mu 0}+E_{e0}-E_{\mu m}-E_{em'})(E_{\mu 0}+E_{e0}-E_{\mu n}-E_{en'})}$$

$$= \frac{8\pi\alpha^3}{3m_\mu m_e} \sum_{\substack{n,n' \\ \neq 0,0}} \sum_{\substack{m,m' \\ \neq 0,0}} \int d^3x_1 \int d^3x_2 \int d^3x_3 \int d^3x_4 \int d^3x_5 \, \psi^+_{\mu 0}(\bar{x}_1)\psi^+_{e0}(\bar{x}_2)$$

$$\times \left(\frac{1}{x_{12}} - \frac{1}{x_1}\right) \frac{\psi_{\mu m}(\bar{x}_1)\psi_{em'}(\bar{x}_2)\psi^+_{\mu m}(\bar{x}_3)\psi^+_{em'}(\bar{x}_3)}{E_{\mu 0}+E_{e0}-E_{\mu m}-E_{em'}}$$

$$\times \frac{\psi_{\mu n}(\bar{x}_3)\psi_{en'}(\bar{x}_3)\psi^+_{\mu n}(\bar{x}_4)\psi^+_{en'}(\bar{x}_5)}{E_{\mu 0}+E_{e0}-E_{\mu n}-E_{en'}} \left(\frac{1}{x_{45}} - \frac{1}{x_5}\right)$$

$$\times \psi_{\mu 0}(\bar{x}_4)\psi_{e0}(\bar{x}_5) \tag{6.11}$$

With the above mentioned approximations and neglecting numerical factors

$$\langle\psi_1|\Delta H|\psi_1\rangle \sim \Delta\nu_F (\alpha M_e)^2 \sum_m \sum_n \int d^3x_1 \int d^3x_2 \int d^3x_3 \int d^3x_4 \int d^3x_5$$

$$\times \psi^+_{\mu 0}(\bar{x}_1)\psi_{\mu m}(\bar{x}_1)\psi^+_{\mu m}(\bar{x}_3)\psi_{\mu n}(\bar{x}_3)\psi^+_{\mu n}(\bar{x}_4)\psi_{\mu 0}(\bar{x}_4)$$

$$\times \frac{e^{-b_m x_{23}}}{x_{23}} \left(\frac{1}{x_{12}} - \frac{1}{x_2}\right) \frac{e^{-b_n x_{35}}}{x_{35}} \left(\frac{1}{x_{45}} - \frac{1}{x_5}\right) \tag{6.12}$$

where $b_n = [2M_e(E_{\mu n}-E_{\mu 0}-E_{e0})]^{1/2}$, $b_n>0$. Integration over $\bar{x}_2$ and $\bar{x}_5$ can be carried out with the aid of (2.26a) to give

$$\langle\psi_1|\Delta H|\psi_1\rangle \sim \Delta\nu_F(\alpha M_e)^2 \sum_m \sum_n \int d^3x_1 \int d^3x_3 \int d^3x_4\, \psi^+_{\mu 0}(\bar{x}_1)$$

$$\times\, \psi_{\mu m}(\bar{x}_1)\psi^+_{\mu m}(\bar{x}_3)\psi_{\mu n}(\bar{x}_3)\psi^+_{\mu n}(\bar{x}_4)\psi_{\mu 0}(\bar{x}_4)\,\frac{1}{b_m^2}\,\frac{1}{b_n^2}$$

$$\times\left(\frac{1-e^{-b_m x_{13}}}{x_{13}} - \frac{1-e^{-b_m x_3}}{x_3}\right)\left(\frac{1-e^{-b_n x_{34}}}{x_{34}} - \frac{1-e^{-b_n x_3}}{x_3}\right) \quad (6.13)$$

The important contributions come from the region where x_1, x_3 and x_4 are of order $1/(\alpha M_\mu)$, while $b_m(b_n)$ is of order $\alpha(M_e M_\mu)^{1/2}$ for $m\neq 0(n\neq 0)$ and of order αM_e for $m=0(n=0)$. Hence we expect that the leading term is given by the lowest power of $b_m x(b_n x)$.

$$\langle\psi_1|\Delta H|\psi_1\rangle \sim \Delta\nu_F(\alpha M_e)^2 \sum_m \sum_n \int d^3x_1 \int d^3x_3 \int d^3x_4\, \psi^+_{\mu 0}(\bar{x}_1)\psi_{\mu m}(\bar{x}_1)$$

$$\times\, \psi^+_{\mu m}(\bar{x}_3)\psi_{\mu n}(\bar{x}_3)\psi^+_{\mu n}(\bar{x}_4)\psi_{\mu 0}(\bar{x}_4)\,(x_{13}-x_3)(x_{34}-x_3) \quad (6.14)$$

By completeness of the muon wave functions,

$$\langle\psi_1|\Delta H|\psi_1\rangle \sim \Delta\nu_F(\alpha M_e)^2 \int d^3x\, x^2\, \psi^+_{\mu 0}(\bar{x})\psi_{\mu 0}(\bar{x})$$

$$\sim \Delta\nu_F\left(\frac{M_e}{M_\mu}\right)^2 \quad (6.15)$$

The contribution to $\Delta\nu_2$ due to the second term in (6.4) can be written as

$$2\,\mathrm{Re}\,\langle\psi_0|\Delta H|\psi_2\rangle = 2\,\mathrm{Re}\,\Big\{ C_{0,0}\langle 0,0|\Delta H|0,0\rangle$$

$$-\sum_{\substack{m,m'\\ \neq 0,0}} \frac{\langle 0,0|\Delta H|m,m'\rangle\langle m,m'|\delta V|0,0'\rangle\langle 0,0'|\delta V|0,0'\rangle}{(E_{\mu 0}+E_{e0}-E_{\mu m}-E_{em'})^2}$$

$$+\sum_{\substack{m,m'\\ \neq 0,0}}\sum_{\substack{n,n'\\ \neq 0,0}} \frac{\langle 0,0'|\Delta H|m,m'\rangle\langle m,m'|\delta V|n,n'\rangle\langle n,n'|\delta V|0,0'\rangle}{(E_{\mu 0}+E_{e0}-E_{\mu m}-E_{em'})(E_{\mu 0}+E_{e0}-E_{\mu n}-E_{en'})} \qquad (6.16)$$

First two terms in (6.16) are estimated by the same method described for estimating (6.11). In this calculation we make the approximation

$$\sum_{n'} \frac{\psi_{en'}(\bar{x})\psi^{+}_{en'}(\bar{y})}{(E_{en'}-z)^2} = \frac{\partial}{\partial z}\sum_{n'} \frac{\psi_{en'}(\bar{x})\psi^{+}_{en'}(\bar{y})}{E_{en'}-z}$$

$$= \frac{\partial}{\partial z} G_e(\bar{x},\bar{y},z)$$

$$\simeq \frac{M_e}{2\pi}\frac{\partial}{\partial z}\frac{e^{-b_n|\bar{x}-\bar{y}|}}{|\bar{x}-\bar{y}|} \qquad (6.17)$$

where $b_n = (-2M_e z)^{1/2}$, $b_n>0$. First two terms are estimated to be of order $\Delta\nu_F(M_e/M_\mu)^2$. Third term is Re(T), where

$$T = 2\sum_{\substack{m,m'\\ \neq 0,0}}\sum_{\substack{n,n'\\ \neq 0,0}} \frac{\langle 0,0'|\Delta H|m,m'\rangle\langle m,m'|\delta V|n,n'\rangle\langle n,n'|\delta V|0,0'\rangle}{(E_{\mu 0}+E_{e0}-E_{\mu m}-E_{em'})(E_{\mu 0}+E_{e0}-E_{\mu n}-E_{en'})}$$

$$= \frac{16\pi\alpha^3}{3m_\mu m_e}\sum_{\substack{m,m'\\ \neq 0,0}}\sum_{\substack{n,n'\\ \neq 0,0}} \int d^3x_1\int d^3x_2\int d^3x_3\int d^3x_4\int d^3x_5\,\psi^{+}_{\mu 0}(\bar{x}_1)\psi^{+}_{e0}(\bar{x}_1)$$

$$\times \frac{\psi_{\mu m}(\bar{x}_1)\psi^{+}_{\mu m}(\bar{x}_2)\psi_{em'}(\bar{x}_1)\psi^{+}_{em'}(\bar{x}_3)}{(E_{\mu 0}+E_{e0}-E_{\mu m}-E_{em'})}\left(\frac{1}{x_{23}}-\frac{1}{x_3}\right)$$

$$\times \frac{\psi_{\mu n}(\bar{x}_2)\psi_{en'}(\bar{x}_3)\psi^{+}_{\mu n}(\bar{x}_4)\psi^{+}_{en'}(\bar{x}_5)}{E_{\mu o}+E_{eo}-E_{\mu n}-E_{en'}}\left(\frac{1}{x_{45}}-\frac{1}{x_5}\right)$$

$$\times \; \psi_{\mu o}(\bar{x}_4)\psi_{eo}(\bar{x}_5) \tag{6.18}$$

We make the approximations stated above, and carry out the integration over $\bar{x}_5$ with the aid of (2.26a), with the result

$$T \simeq \frac{2\Delta\nu_F(\alpha M_e)^2}{\pi}\sum_m\sum_n \int d^3x_1\int d^3x_2\int d^3x_3\int d^3x_4\, \psi^{+}_{\mu o}(\bar{x}_1)\psi_{\mu m}(\bar{x}_1)$$

$$\times \psi^{+}_{\mu m}(\bar{x}_2)\psi_{\mu n}(\bar{x}_2)\psi^{+}_{\mu n}(\bar{x}_4)\psi_{\mu o}(\bar{x}_4)\frac{e^{-b_m x_{13}}}{x_{13}}\left(\frac{1}{x_{23}}-\frac{1}{x_3}\right)$$

$$\times \frac{1}{b_n^2}\left(\frac{1-e^{-b_n x_{34}}}{x_{34}} - \frac{1-e^{-b_n x_3}}{x_3}\right) \tag{6.19}$$

The major contributions in (6.19) come from the region where x_1, x_2, x_4 are of order $1/(\alpha M_\mu)$. Let us assume that the major contributions come from the region where $b_n x_3 < 1$ (this assumption is justified later in this Chapter). Therefore $\exp(-b_n x_{34})$ and $\exp(-b_n x_3)$ in (6.19) can be expanded in power series to obtain a leading term. The leading term is independent of b_n. Hence using the completeness of the muon wave functions,

$$T \simeq \frac{\Delta\nu_F(\alpha M_e)^2}{\pi}\sum_m \int d^3x_1\int d^3x_2\int d^3x_3\, \psi^{+}_{\mu o}(\bar{x}_1)\psi_{\mu m}(\bar{x}_1)\psi^{+}_{\mu m}(\bar{x}_2)$$

$$\times \psi_{\mu o}(\bar{x}_2)\frac{e^{-b_m x_{13}}}{x_{13}}\left(\frac{1}{x_{23}}-\frac{1}{x_3}\right)(x_3-x_{23}) \tag{6.20}$$

The term T can be conveniently broken into two parts: T_1, corresponding to m=0, and T_2, corresponding to $m \neq 0$ in (6.20) For $m \neq 0$, b_m is replaced by an average b, independent of m, and of order $\alpha(M_e M_\mu)^{1/2}$. The second term T_2 is further divided into two parts, T_{21} and T_{22}, by using (2.27). Hence,

$$T = T_1 + T_{21} + T_{22} \tag{6.21}$$

$$T_1 = \frac{\Delta\nu_F(\alpha M_e)^2}{\pi} \int d^3x_1 \int d^3x_2 \int d^3x_3 |\psi_{\mu 0}(\bar{x}_1)|^2 |\psi_{\mu 0}(\bar{x}_2)|^2$$

$$\times \frac{e^{-b_0 x_{13}}}{x_{13}} \left(\frac{1}{x_{23}} - \frac{1}{x_3}\right)(x_3 - x_{23}) \tag{6.22}$$

$$T_{21} = \frac{\Delta\nu_F(\alpha M_e)^2}{\pi} \int d^3x_1 \int d^3x_2 \int d^3x_3 \psi^+_{\mu 0}(\bar{x}_1)\, \delta^3(\bar{x}_1 - \bar{x}_2)$$

$$\times \psi_{\mu 0}(\bar{x}_2) \frac{e^{-b x_{13}}}{x_{13}} \left(\frac{1}{x_{23}} - \frac{1}{x_3}\right)(x_3 - x_{23}) \tag{6.23}$$

$$T_{22} = -\frac{\Delta\nu_F(\alpha M_e)^2}{\pi} \int d^3x_1 \int d^3x_2 \int d^3x_3 |\psi_{\mu 0}(\bar{x}_1)|^2 |\psi_{\mu 0}(\bar{x}_2)|^2$$

$$\times \frac{e^{-b x_{13}}}{x_{13}} \left(\frac{1}{x_{23}} - \frac{1}{x_3}\right)(x_3 - x_{23}) \tag{6.24}$$

With the aid of integral

$$\int d^3x_3 \frac{e^{-b x_{13}}}{x_{13}} \left(\frac{1}{x_{13}} - \frac{1}{x_3}\right)(x_3 - x_{13})$$

$$= -\frac{4\pi}{3} x_1^2 \ln(b x_1) + O(x_1^2), \tag{6.25}$$

we obtain

$$T_{21} = -\frac{4\Delta\nu_F(\alpha M_e)^2}{3}\int d^3x_1 |\psi_{\mu o}(\vec{x}_1)|^2 x_1^2 \ln(bx_1)$$

$$+ O\left[\Delta\nu_F\left(\frac{M_e}{M_\mu}\right)^2\right]$$

$$= -\Delta\nu_F\left(\frac{M_e}{M_\mu}\right)^2 \ln\left(\frac{b}{\alpha M_\mu}\right) + O\left[\Delta\nu_F\left(\frac{M_e}{M_\mu}\right)^2\right] \tag{6.26}$$

Since b is of order $\alpha(M_e M_\mu)^{1/2}$,

$$T_{21} = \frac{\Delta\nu_F}{2}\left(\frac{M_e}{M_\mu}\right)^2 \ln\left(\frac{M_\mu}{M_e}\right) + O\left[\Delta\nu_F\left(\frac{M_e}{M_\mu}\right)^2\right] \tag{6.27}$$

To evaluate T_{22}, following integrals are used:

$$\int d^3x_1 |\psi_{\mu o}(\vec{x}_1)|^2 \frac{e^{-bx_{13}}}{x_{13}}$$

$$= \frac{a^3}{2x_3}\left[\frac{2a(e^{-bx_3} - e^{-ax_3})}{(a^2-b^2)^2} - \frac{x_3 e^{-ax_3}}{a^2-b^2}\right] \tag{6.28}$$

where $a=4\alpha M_\mu$

$$\int d^3x_2 |\psi_{\mu o}(\vec{x}_2)|^2 \frac{x_3}{x_{23}}$$

$$= \frac{a^3}{2}\left[\frac{2}{a^3}(1-e^{-ax_3}) - \frac{x_3 e^{-ax_3}}{a^2}\right] \tag{6.29}$$

$$\int d^3x_2 |\psi_{\mu o}(\vec{x}_2)|^2 \frac{x_{23}}{x_3}$$

$$= \frac{a^3}{2x_3^2}\left[\frac{2x_3^2}{a^3} + \frac{8}{a^5}(1-e^{-ax_3}) - \frac{2x_3 e^{-ax_3}}{a^2}\right] \tag{6.30}$$

From (6.29) and (6.30),

$$\int d^3x_2 |\psi_{\mu 0}(\bar{x}_2)|^2 \left(\frac{1}{x_{23}} - \frac{1}{x_3}\right)(x_3 - x_{23})$$

$$\simeq \frac{4}{x_3^2 a^2}(1 - e^{-ax_3}) \qquad (6.31)$$

where the terms neglected on right—hand side give contribution of order $\Delta\nu_F(M_e/M_\mu)^2$ to T_{22}. From (6.28) and (6.31),

$$T_{22} = -\Delta\nu_F\left(\frac{M_e}{M_\mu}\right)^2 \int_0^\infty \frac{dx}{x}(e^{-bx} - e^{-ax})(1 - e^{-ax}) + O[\Delta\nu_F(\tfrac{M_e}{M_\mu})^2]$$

$$= -\Delta\nu_F\left(\frac{M_e}{M_\mu}\right)^2 \ln\frac{a}{b} + O[\Delta\nu_F(\tfrac{M_e}{M_\mu})^2] \qquad (6.32a)$$

$$= -\frac{\Delta\nu_F}{2}\left(\frac{M_e}{M_\mu}\right)^2 \ln\left(\frac{M_\mu}{M_e}\right) + O[\Delta\nu_F(\tfrac{M_e}{M_\mu})^2] \qquad (6.32b)$$

Now T_1 is same as T_{22}, except for the sign and the fact that b_0 appears instead of b. Since $b_0 = \alpha M_e$, with the aid of (6.32a), we have

$$T_1 = \Delta\nu_F\left(\frac{M_e}{M_\mu}\right)^2 \ln\left(\frac{M_\mu}{M_e}\right) + O[\Delta\nu_F(\tfrac{M_e}{M_\mu})^2] \qquad (6.33)$$

Hence

$$T \simeq \Delta\nu_F\left(\frac{M_e}{M_\mu}\right)^2 \ln\left(\frac{M_\mu}{M_e}\right) + O[\Delta\nu_F(\tfrac{M_e}{M_\mu})^2] \qquad (6.34)$$

This result is obtained with the assumption that the major contribution in (6.19) comes from the region where $b_n x_3 < 1$. To justify that assumption, consider the region $x_3 \gtrsim 1/b_n$. In this region

$$\frac{1}{b_n^2}\left(\frac{1-e^{-b_n x_{34}}}{x_{34}} - \frac{1-e^{-b_n x_3}}{x_3}\right)$$

$$\simeq \frac{1}{b_n^2 x_3}\left[O(b_n x_4) + O\left(\frac{x_4}{x_3}\right)\right] \tag{6.35}$$

$$\frac{1}{x_{23}} - \frac{1}{x_3} \simeq \frac{x_2}{x_3^2} \tag{6.36}$$

Hence the contribution from this region to T is

$$T' \sim \Delta\nu_F\left(\frac{M_e}{M_\mu}\right)^2 \int_{1/b_n}^{\infty} dx_3 \left[O\left(\frac{1}{b_n x_3^2}\right) + O\left(\frac{1}{b_n^2 x_3^3}\right)\right]$$

$$\sim O\left[\Delta\nu_F\left(\frac{M_e}{M_\mu}\right)^2\right] \tag{6.37}$$

which is smaller than (6.34), and can be neglected. with the aid of (6.15) and (6.34),

$$\Delta\nu_2 \simeq \Delta\nu_F\left(\frac{M_e}{M_\mu}\right)^2 \ln\left(\frac{M_\mu}{M_e}\right) + O\left[\Delta\nu_F\left(\frac{M_e}{M_\mu}\right)^2\right] \tag{6.38}$$

Summarizing, the second order correction to the hyperfine splitting is estimated to be of order $\Delta\nu_F(M_e/M_\mu)^2 \ln(M_\mu/M_e)$.

7. ESTIMATE OF RELATIVISTIC CORRECTONS

In this Chapter, the quantum electrodynamic Hamiltonian of the system is written in the Furry bound-interaction picture.[22] The division of the Hamiltonian into the zero order part and the perturbation part is done in accordance with the effective nucleus picture. The hyperfine splitting in the nonrelativistic limit is obtained from certain Feynman graphs, by making a series of approximations. These Feynman graphs give back the nonrelativistic limit plus corrections estimated to be of order $\alpha^2 \Delta\nu_F$ or higher.

The Hamiltonian density $\mathcal{H}$, in the interaction picture, can be devided into a zero-order part $\mathcal{H}_0$ and a perturbation $\delta\mathcal{H}_I$, where

$$\mathcal{H}_0(x) = \overline{\Psi}_e(x)(-i\vec{\gamma}\cdot\vec{\nabla} + m_e)\Psi_e(x)$$

$$+ \overline{\Psi}_\mu(x)(-i\vec{\gamma}\cdot\vec{\nabla} + m_\mu)\Psi_\mu(x) \qquad (7.1)$$

$$\delta\mathcal{H}_I(x) = -\frac{e}{2}[\overline{\Psi}_e(x)\gamma^\nu, \Psi_e(x)](A_\nu(x) + A_\nu^{(e)}(x))$$

$$-\frac{e}{2}[\overline{\Psi}_\mu(x)\gamma^\nu, \Psi_\mu(x)](A_\nu(x) + A_\nu^{(\mu)}(x)) \qquad (7.2)$$

In (7.2), $A_\nu(x)$ is the vector potential for the quantized radiation field. The external potentials are given by

$$A_\nu^{(e)}(x) = A_\nu^{(\mu)}(x) = \frac{2e}{4\pi|\vec{x}|} \qquad (7.3)$$

Consider the equation of motion of the state vector in the interaction picture

$$i\frac{\partial}{\partial t}|\Psi(t)\rangle = \int d^3x\, \delta\mathcal{H}_I(x)|\Psi(t)\rangle \qquad (7.4)$$

We now make the following unitary transformation on $|\Psi(t)\rangle$ to transform to the Furry picture

$$|\Psi^F(t)\rangle = V^{-1}|\Psi(t)\rangle \qquad (7.5)$$

where V(t) satisfies

$$i\frac{\partial}{\partial t}V(t) = -\int d^3x \Big\{ \frac{e}{2}[\overline{\Psi}_e(x)\gamma^\nu, \Psi_e(x)]\Big(A_\nu^{(e)}(x) - \frac{e}{4\pi|\vec{x}|}\Big)$$

$$+ \frac{e}{2}[\overline{\Psi}_\mu(x)\gamma^\nu, \Psi_\mu(x)]\big(A_\nu^{(\mu)}(x)\big)\Big\} V(t) \qquad (7.6)$$

From the above equation, we get

$$i\frac{\partial}{\partial t}|\Psi^F(t)\rangle = \int d^3x \Big\{ -\frac{e}{2}[\overline{\Psi}_e^F(x)\gamma^\nu, \Psi_e^F(x)]\Big(A_\nu(x) + \frac{e}{4\pi|\vec{x}|}\Big)^F$$

$$-\frac{e}{2}[\overline{\Psi}_\mu^F(x)\gamma^\nu, \Psi_\mu(x)]\big(A_\nu(x)\big)^F \Big\} |\Psi_F(t)\rangle \qquad (7.7)$$

where

$$\Psi_e^F(x) = V^{-1}(t)\Psi_e(x)V(t)$$

$$\Psi_\mu^F(x) = V^{-1}(t)\Psi_\mu(x)V(t)$$

$$\left(A_\nu(x) + \frac{e}{4\pi|\vec{x}|}\right)^F = V^{-1}(t)\left(A_\nu(x) + \frac{e}{4\pi|\vec{x}|}\right)V(t) = A_\nu(x) + \frac{e}{4\pi|\vec{x}|}$$

$$(A_\nu(x))^F = V^{-1}(t)A_\nu(x)V(t) = A_\nu(x) \qquad (7.8)$$

With the aid of (7.5), (7.6), (7.7) and the equations

$$\frac{\partial}{\partial t}\Psi_e(x) = (-\gamma^0\vec{\gamma}\cdot\vec{\nabla} - i\gamma^0 m_e)\Psi_e(x) \qquad (7.9)$$

$$\frac{\partial}{\partial t}\Psi_\mu(x) = (-\gamma^0\vec{\gamma}\cdot\vec{\nabla} - i\gamma^0 m_\mu)\Psi_\mu(x) \qquad (7.10)$$

the fields $\Psi_e^F(x)$ and $\Psi_\mu^F(x)$ satisfy

$$(i\gamma^\nu\partial_\nu - m_e)\Psi_e^F(x) = e\gamma^\nu\left(A_\nu^{(e)}(x) - \frac{e}{4\pi|\vec{x}|}\right)\Psi_e^F(x) \qquad (7.11)$$

$$(i\gamma^\nu\partial_\nu - m_\mu)\Psi_\mu^F(x) = e\gamma^\nu A_\nu^{(\mu)}(x)\Psi_\mu^F(x) \qquad (7.12)$$

By comparing (7.4) and (7.7), we have

$$\delta\mathcal{H}_I^F(x) = \delta\mathcal{H}_R^F(x) + \delta\mathcal{H}_v^F(x) \qquad (7.13)$$

where the radiation term is

$$\delta\mathcal{H}_R^F(x) = -\frac{e}{2}[\overline{\Psi}_e^F(x)\gamma^\nu, \Psi_e^F(x)]\,A_\nu(x)$$

$$- \frac{e}{2} [\bar{\Psi}^F_\mu(x)\gamma^\nu, \Psi^F_\mu(x)] A_\nu(x) \tag{7.14}$$

and the potential term is

$$\delta\mathcal{H}^F_v(x) = -\frac{\alpha}{2|\vec{x}|} [\bar{\Psi}^F_e(x)\gamma^0, \Psi^F_e(x)] \tag{7.15}$$

The superscript 'F' will be omitted for the rest of the Chapter. Let $\{\Phi_n(x)\}$ be the nonoperator solutions of Equation (7.11) or (7.12), where n specifies the quantum number of the state. The operators $\Psi(x)$ can be expanded in terms of the $\Phi_n(x)$, i.e.,

$$\Psi_\mu(x) = \sum_{n,E+} b_{\mu n}\Phi_{\mu n}(x) + \sum_{n,E-} d^*_{\mu n}\Phi_{\mu n}(x) \tag{7.16}$$

$$\Psi_e(x) = \sum_{n,E+} b_{en}\Phi_{en}(x) + \sum_{n,E-} d^*_{en}\Phi_{en}(x) \tag{7.17}$$

where the first summation extends over positive energy solutions, and the second summation extends over negative energy solutions. The operator $b_{en}(b_{\mu n})$ is the destruction operator for an electron (a negative muon) in the state n, and $d^*_{en}(d^*_{\mu n})$ is the creation operator for a positron (a positive muon) in the state n.

The zero-order ground state vector for muonic helium is given by

$$|a\rangle = \sum_{u,v} C(u,v)\, b^*_{\mu u}\, b^*_{ev} |0\rangle \tag{7.18}$$

where $b^{*}_{ev}(b^{*}_{\mu u})$ is a creation operator for the electron(muon) in the ground state with the z-component of the spin to be v(u). The Clebsch-Gordan coefficients c are chosen to give the total angular momentum F=0 or 1.

$$C(u,v) = \langle \tfrac{1}{2} u \, \tfrac{1}{2} v | \tfrac{1}{2} \, \tfrac{1}{2} \, F \, M_F \rangle \tag{7.19}$$

The level shift is

$$\Delta E_a = \lim_{\substack{\delta \to 0 \\ \lambda \to 1}} \frac{1}{2} i\delta\lambda \frac{\frac{\partial}{\partial\lambda} \langle S_\delta \rangle_c}{\langle S_\delta \rangle_c}$$

$$= \Delta E_a^{(1)} + \Delta E_a^{(2)} + \cdots \tag{7.20}$$

where the subscript c implies that only the connected graphs are taken, $\Delta E_a^{(n)}$ is of order e^n and

$$\langle S_\delta \rangle = \langle a | S_\delta | a \rangle \tag{7.21}$$

The adiabatic S-matrix, S_δ, is

$$S_\delta = 1 + \lambda S_\delta^{(1)} + \lambda^2 S_\delta^{(2)} + \cdots$$

$$= 1 - \lambda i \int d^4x \, T[\mathcal{H}_I(x)] \, e^{-\delta|t|}$$

$$- \frac{\lambda^2}{2} \iint d^4x_1 d^4x_2 T[\mathcal{H}_I(x_1) \mathcal{H}_I(x_2)] e^{-\delta|t_1|} e^{-\delta|t_2|}$$

$$+ \cdots \tag{7.22}$$

where T denotes the time-ordered product. For the Feynman graphs in

Figure 2,

$$\Delta E_{a}^{(2)} = i \lim_{\delta\to 0} \delta \left(\langle S_{\delta}^{(2)} \rangle_{R} + \tfrac{1}{2} \langle S_{\delta}^{(1)} \rangle_{V} \right) \tag{7.23}$$

$$\Delta E_{a}^{(4)} = 2i \lim_{\delta\to 0} \delta \Big(\langle S_{\delta}^{(4)} \rangle_{R} - \tfrac{1}{2} \langle S_{\delta}^{(2)} \rangle_{R}^{2} + \tfrac{3}{4} \langle S_{\delta}^{(3)} \rangle_{RV}$$

$$- \tfrac{3}{4} \langle S_{\delta}^{(1)} \rangle_{V} \langle S_{\delta}^{(2)} \rangle_{R} - \tfrac{1}{4} \langle S_{\delta}^{(1)} \rangle_{V}^{2} + \tfrac{1}{2} \langle S_{\delta}^{(2)} \rangle_{V} \Big) \tag{7.24}$$

$$\Delta E_{a}^{(2n-1)} = 0 \ , \ n = 1, 2, \dots \tag{7.25}$$

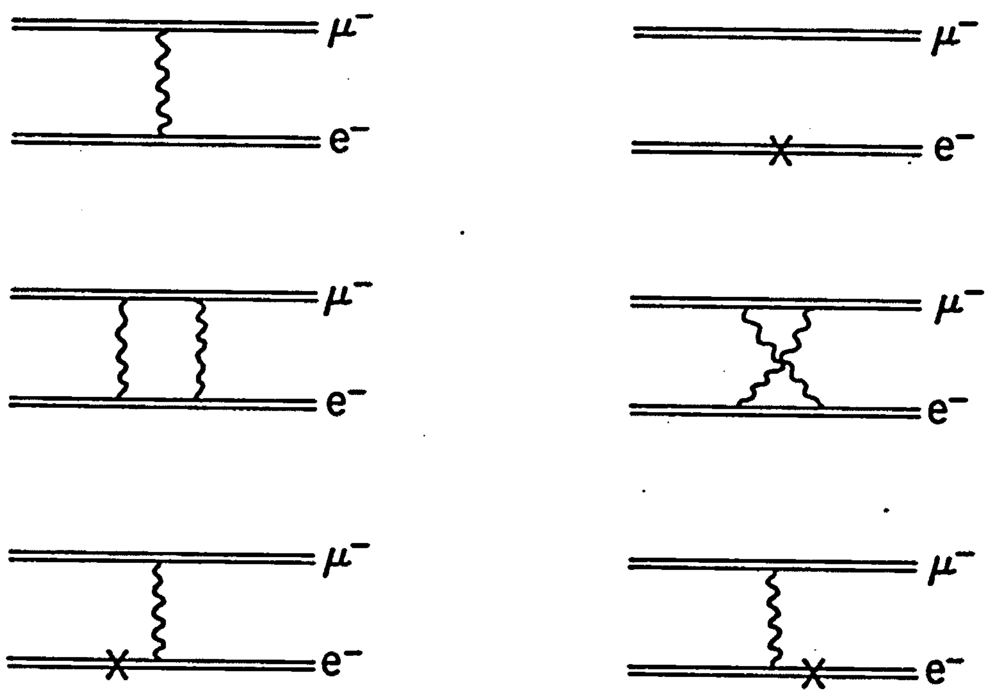

Figure 2 : Feynman graphs corresponding to one-photon and two-photon exchange.

The subscripts R or V indicate that the contribution to S_{δ} arises from the radiation term $\delta\mathcal{H}_R$ or the potential term $\delta\mathcal{H}_V$ respectively, and the subscript RV indicates the cross term of $\delta\mathcal{H}_R$ and $\delta\mathcal{H}_V$. The second term on the right hand side of (7.23) and the last two terms on the right hand side of (7.24) do not contribute to the hyperfine splitting. With the notation

$$\langle 0|T[A^{\nu_2}(x_2)A^{\nu_1}(x_1)]|0\rangle = g^{\nu_2\nu_1}D_F(x_2,x_1)$$

$$= -g^{\nu_2\nu_1}\frac{i}{(2\pi)^4}\int d^4k\,\frac{e^{-ik(x_2-x_1)}}{k^2+i\epsilon}\,, \tag{7.26}$$

$$S_e^F(x_2,x_1) = \sum_{n>0}\Phi_{en}(x_2)\overline{\Phi}_{en}(x_1)\,,\quad x_{20}>x_{10}$$

$$= -\sum_{n<0}\Phi_{en}(\bar{x}_2)\overline{\Phi}_{en}(x_1)\,,\quad x_{20}<x_{10}$$

$$= \frac{1}{2\pi i}\int_{-\infty}^{\infty}dz\sum_n\frac{\Phi_{en}(\bar{x}_2)\overline{\Phi}_{en}(\bar{x}_1)}{E_{en}(1-i\theta)-z}\,e^{-iz(t_2-t_1)}\,, \tag{7.27}$$

where θ is arbitrarily small positive number and

$$\Phi_{en}(x) = \Phi_{en}(\bar{x})\,e^{-iE_{en}t} \tag{7.28}$$

and a similar expression for $S_\mu^F(x_2,x_1)$, one can obtain in the limit of small δ

$$\langle S_\delta^{(1)}\rangle_V = -\frac{2i\alpha}{\delta}\int d^3x\,\overline{\Phi}_{e0}(\bar{x})\,\gamma^0\,\frac{1}{x}\,\Phi_{e0}(\bar{x}) \tag{7.29}$$

$$\langle S_\delta^{(2)}\rangle_R = \sum_{\substack{u v\\ u' v'}} C^*(u',v')\,C(u,v)\int d^4x_2\int d^4x_1\,e^{-\delta(|t_2|+|t_1|)}\,e^2$$

$$\times\,\overline{\Phi}_{\mu u'}(x_2)\,\gamma_{\nu_2}\,\Phi_{\mu u}(x_2)\,\overline{\Phi}_{e v'}(x_1)\,\gamma_{\nu_1}\,\Phi_{e v}(x_1)$$

$$\times\, g^{\nu_2\nu_1} D_F(x_2-x_1) \tag{7.30}$$

$$= -\frac{i\alpha}{\delta} \sum_{\substack{u v \\ u' v'}} c^*(u',v')\, c(u,v) \int d^3x_2 \int d^3x_1\, \bar{\Phi}_{\mu u'}(\bar{x}_2)\gamma_\nu \Phi_{\mu u}(\bar{x}_2)$$

$$\times\, \bar{\Phi}_{ev'}(\bar{x}_1)\gamma^\nu \Phi_{ev}(\bar{x}_1)\, \frac{1}{x_{21}} \tag{7.31}$$

$$\langle S_\delta^{(3)}\rangle' = \langle S_\delta^{(3)}\rangle_{RV} - \langle S_\delta^{(2)}\rangle_R \langle S_\delta^{(1)}\rangle_V$$

$$= 4\pi i\alpha^2 \sum_{\substack{u v \\ u' v'}} c^*(u',v')\, c(u,v) \int d^4x_3 \int d^4x_2 \int d^4x_1\, e^{-\delta(|t_3|+|t_2|+|t_1|)}$$

$$\times\, \bar{\Phi}_{\mu u'}(x_3)\gamma_{\nu_3}\Phi_{\mu u}(x_3) \{ \bar{\Phi}_{ev'}(x_2)\gamma_{\nu_2} S_e^F(x_2,x_1)\gamma_0 \Phi_{ev}(x_1)$$

$$+\, \bar{\Phi}_{ev'}(x_1)\gamma_0 S_e^F(x_1,x_2)\gamma_{\nu_2}\Phi_{ev}(x_2)\}\, g^{\nu_2\nu_3} D_F(x_3-x_2)\, \frac{1}{x_1}$$

$$-\, \langle S_\delta^{(2)}\rangle_R \langle S_\delta^{(1)}\rangle_V \tag{7.32}$$

$$= \frac{4\alpha i}{3\delta} \sum_{\substack{u v \\ u' v'}} c^*(u',v')\, c(u,v) \int d^3x_3 \int d^3x_2 \int d^3x_1\, \bar{\Phi}_{\mu u'}(\bar{x}_3)\gamma_\nu \Phi_{\mu u}(\bar{x}_3)$$

$$\times\, \frac{1}{x_{32}}\, \bar{\Phi}_{ev'}(\bar{x}_2)\gamma^\nu \sum_{n\neq 0} \frac{\Phi_{en}(\bar{x}_2)\,\bar{\Phi}_{en}(\bar{x}_1)}{\epsilon_{e0}-\epsilon_{en}}\, \frac{\gamma^0}{x_1}\Phi_{e0}(\bar{x}_1) \tag{7.33}$$

and

$$\langle S_\delta^{(4)}\rangle' = \langle S_\delta^{(4)}\rangle_R - \tfrac{1}{2}\langle S_\delta^{(2)}\rangle_R^2$$

$$= (4\pi\alpha)^2 \int d^4x_1 \int d^4x_2 \int d^4x_3 \int d^4x_4\, e^{-\delta(|t_1|+|t_2|+|t_3|+|t_4|)}$$

$$\times \sum_{\substack{u,\upsilon\\u',\upsilon'}} c^*(u',\upsilon')\, c(u,\upsilon)\, \bar{\Phi}_{\mu u'}(x_4)\gamma_{\nu_4} S_\mu^F(x_4,x_3)\gamma_{\nu_3}\Phi_{\mu u}(x_3)$$

$$\times \bar{\Phi}_{e\upsilon'}(x_2)\gamma_{\nu_2} S_e^F(x_2,x_1)\gamma_{\nu_1}\Phi_{e\upsilon}(x_1) \quad [g^{\nu_4\nu_2} g^{\nu_3\nu_1}$$

$$\times D_F(x_4-x_2)D_F(x_3-x_1) + g^{\nu_4\nu_1} g^{\nu_3\nu_2} D_F(x_4-x_1)D_F(x_3-x_2)]$$

$$- \tfrac{1}{2}\langle S_\delta^{(2)}\rangle_R^2 \tag{7.34}$$

$$= \frac{\alpha^2}{4\pi\delta} \sum_{\substack{u\upsilon\\u'\upsilon'}} c^*(u',\upsilon')\, c(u,\upsilon) \int d^3x_4 \int d^3x_3 \int d^3x_2 \int d^3x_1$$

$$\times \Big[\sum_{\substack{n,n'\\ \neq 0,0}} \bar{\Phi}_{\mu u'}(\bar{x}_4)\gamma_\nu \Phi_{\mu n}(\bar{x}_4)\bar{\Phi}_{\mu n}(\bar{x}_3)\gamma_{\nu'}\Phi_{\mu u}(\bar{x}_3)\bar{\Phi}_{e\upsilon'}(\bar{x}_2)\gamma^\nu \Phi_{en'}(\bar{x}_2)$$

$$\times \bar{\Phi}_{en'}(\bar{x}_1)\gamma^{\nu'}\Phi_{e\upsilon}(\bar{x}_1)\, \frac{1}{x_{42}x_{31}} \int_{-\infty}^{\infty} dz\, \frac{e^{ix_{42}\sqrt{z^2+i\epsilon_1}}\, e^{ix_{31}\sqrt{z^2+i\epsilon_2}}}{[z+\epsilon_{\mu 0}-\epsilon_{\mu n}(1-i\theta)][\epsilon_{e0}-\epsilon_{en'}(1-i\theta)-z]}$$

$$+ \sum_{n,n'} \bar{\Phi}_{\mu u'}(\bar{x}_4)\gamma_\nu \Phi_{\mu n}(\bar{x}_4)\bar{\Phi}_{\mu n}(\bar{x}_3)\gamma_{\nu'}\Phi_{\mu u}(\bar{x}_3)$$

$$\times \bar{\Phi}_{e\upsilon'}(\bar{x}_2)\gamma^{\nu'}\Phi_{en'}(\bar{x}_2)\bar{\Phi}_{en'}(\bar{x}_1)\gamma^{\nu}\Phi_{e\upsilon}(\bar{x}_1)\, \frac{1}{x_{41}x_{32}}$$

$$\times \int_{-\infty}^{\infty} dz\, \frac{e^{ix_{41}\sqrt{z^2+i\epsilon_1}}\, e^{ix_{32}\sqrt{z^2+i\epsilon_2}}}{[z+\epsilon_{\mu 0}-\epsilon_{\mu n}(1-i\theta)][z+\epsilon_{e0}-\epsilon_{en}(1-i\theta)]} \tag{7.35}$$

For the nonrelativistic limit of the hyperfine splitting, the muon wave function for any state is written in the Pauli approximation, i.e.,

$$\bar{\Phi}_{\mu n}(\bar{x}) \simeq \begin{pmatrix} \phi_{\mu n}(\bar{x}) \\ \frac{1}{2m_\mu}\bar{\sigma}\cdot\bar{p}_\mu \phi_{\mu n}(\bar{x}) \end{pmatrix} \tag{7.36}$$

where $\phi_{\mu n}(\bar{x})$ is the Pauli-Schrödinger wave function. The electron ground-state wave function is also treated in Pauli approximation.

One can show that in the nonrelativistic limit,

$$\int d^3x\, \bar{\Phi}_n^+(\bar{x})\alpha_i f(\bar{x})\bar{\Phi}_m(\bar{x})$$

$$\simeq \frac{1}{2m}\int d^3x\, \phi_n^+(\bar{x})[\sigma_i f(\bar{x})\bar{\sigma}\cdot\bar{p} + \bar{\sigma}\cdot\bar{p}\sigma_i f(\bar{x})]\phi_m(\bar{x})$$

$$\rightarrow -\frac{i}{2m}\int d^3x\, \phi_n^+(\bar{x})\bar{\sigma}\cdot[\bar{\nabla}f(\bar{x})]\sigma_i\phi_m(\bar{x}) \tag{7.37}$$

where latin indices run from 1,2,3. Only the parts effecting hyperfine splitting are retained in (7.37). Also, in the nonrelativistic limit,

$$\int d^3x_1 \int d^3x_2\, \bar{\Phi}_n^+(\bar{x}_2) f(\bar{x}_1,\bar{x}_2)\alpha_i\bar{\Phi}_m(\bar{x}_1)$$

$$\simeq \frac{i}{2m}\int d^3x_1\int d^3x_2\, \phi_n^+(\bar{x}_2)[\sigma_i\bar{\sigma}\cdot(\bar{\nabla}_1 f) - \bar{\sigma}\cdot(\bar{\nabla}_2 f)\sigma_i]\phi_m(\bar{x}_1) \tag{7.38}$$

For the nonrelativistic limit of (7.31) for $\nu \neq 0$, we have

$$\langle S_\delta^{(2)}\rangle_R(\nu\neq 0) = \frac{i\alpha}{\delta}\sum_{\substack{u\upsilon\\u'\upsilon'}} c^*(u',\upsilon')\,c(u,\upsilon)\int d^3x_2\int d^3x_1$$

$$\times\,\bar{\Phi}^+_{\mu u'}(\bar{x}_2)\,\bar{\Phi}^+_{e\upsilon'}(\bar{x}_1)\,\alpha_i^{(e)}\alpha_i^{(\mu)}\frac{1}{x_{21}}\,\bar{\Phi}_{e\upsilon}(\bar{x}_1)\,\bar{\Phi}_{\mu u}(\bar{x}_2) \tag{7.39}$$

$$\rightarrow -\frac{i\alpha}{\delta}\frac{1}{4m_\mu m_e}\sum_{\substack{u\upsilon\\u'\upsilon'}} c^*(u',\upsilon')\,c(u,\upsilon)\int d^3x_2\int d^3x_1\,\phi^+_{\mu u'}(\bar{x}_2)\,\phi^+_{e\upsilon'}(\bar{x}_1)$$

$$\times\,\sigma_k^{(\mu)}\sigma_i^{(\mu)}\sigma_j^{(e)}\sigma_i^{(e)}\left(\nabla_{2k}\nabla_{ij}\frac{1}{x_{12}}\right)\phi_{e\upsilon}(\bar{x}_1)\,\phi_{\mu u}(\bar{x}_2) \tag{7.40}$$

Because of the spherical symmetry of the wave functions, we have

$$\left(\nabla_{2k}\nabla_{ij}\frac{1}{x_{12}}\right)\rightarrow -\frac{1}{3}\left(\nabla_1^2\frac{1}{x_{12}}\right)\delta_{jk} = \frac{4\pi}{3}\,\delta^3(\bar{x}_1-\bar{x}_2)\,\delta_{jk} \tag{7.41}$$

Hence

$$\langle S_\delta^{(2)}\rangle_R(\nu\neq 0)\rightarrow -\frac{i\alpha\pi}{\delta\cdot 3m_\mu m_e}\sum_{\substack{u\upsilon\\u'\upsilon'}} c^*(u',\upsilon')\,c(u,\upsilon)\int d^3x_2\int d^3x_1$$

$$\times\,\phi^+_{\mu u'}(\bar{x}_2)\,\phi^+_{e\upsilon'}(\bar{x}_1)\,\bar{\sigma}^{(\mu)}\cdot\sigma^{(e)}\,\sigma^{(\mu)}\cdot\bar{\sigma}^{(e)}\,\delta^3(\bar{x}_1-\bar{x}_2)\,\phi_{e\upsilon}(\bar{x}_1)\,\phi_{\mu u}(\bar{x}_2) \tag{7.42}$$

Now decomposing the Pauli wave function into a Schrödinger wave function and a spin part,

$$\phi(\bar{x}) = \psi(\bar{x})\cdot\chi \tag{7.43}$$

and noting that

$$\bar{\sigma}^{(\mu)} \cdot \bar{\sigma}^{(e)} \chi_{\text{singlet}} = -3\chi_{\text{singlet}} \tag{7.44}$$

$$\bar{\sigma}^{(\mu)} \cdot \bar{\sigma}^{(e)} \chi_{\text{triplet}} = \chi_{\text{triplet}} , \tag{7.45}$$

the splitting due to (7.42) between the singlet and triplet is given by

$$\Delta[\langle S_{\delta}^{(2)}\rangle(\nu\neq 0)] \to -\frac{i}{\delta}\frac{8\pi\alpha}{3m_{\mu}m_{e}}\int d^3x_2\int d^3x_1$$

$$\times\, \psi^{+}_{\mu o}(\bar{x}_2)\,\psi^{+}_{eo}(\bar{x}_1)\,\delta^3(\bar{x}_1-\bar{x}_2)\,\psi_{\mu o}(\bar{x}_2)\,\psi_{eo}(\bar{x}_1) \tag{7.46}$$

Consider the term $\nu=0$ in (7.31). Since γ_0 is diagonal, and the upper components of the wave functions have no σ matrices, the contribution to the hyperfine splitting in the nonrelativistic limit is due to the lower components. Hence compared to (7.42), this term has an additional factor of $(\bar{p}_e/m_e)(\bar{p}_{\mu}/m_{\mu})$. For the ground state wave function, $\bar{p}_e$ is of order (αm_e) and $\bar{p}_{\mu}$ is of order (αm_{μ}). Thus the contribution to the hyperfine splitting due to this term is α^2 times smaller than (7.46).

$$\Delta[\langle S_{\delta}^{(2)}\rangle_R(\nu=0)] \to O\{\alpha^2\Delta[\langle S_{\delta}^{(2)}\rangle_R(\nu\neq 0)]\} \tag{7.47}$$

From (7.47) and (7.23), we have

$$\Delta[\Delta E_{a}^{(2)}] = \frac{8\pi\alpha}{3m_{\mu}m_{e}}\int d^3x_2\int d^3x_1\,\psi^{+}_{\mu o}(\bar{x}_2)\,\psi^{+}_{eo}(\bar{x}_1)$$

$$\times\ \delta^3(\bar{x}_1-\bar{x}_2)\,\psi_{\mu 0}(\bar{x}_2)\,\psi_{e0}(\bar{x}_1)\,[1+O(\alpha^2)] \qquad (7.48)$$

For the first term of (7.35), we assume that the important contribution comes from z of order $\alpha^2 m_\mu$ and x_{ij} of order $1/(\alpha m_\mu)$. These assumptions are motivated by the fact that the integrand of the integral over z is largest when z is of order $\alpha^2 m_\mu$, and in nonrelativistic problem x_{ij} do scale as $1/(\alpha m_\mu)$. With these assumptions, $zx_{ij}\sim\alpha$, and therefore in the first term of (14.2),

$$e^{ix_{ij}\sqrt{z^2+i\epsilon}} \simeq 1\,. \qquad (7.49)$$

For the second term of (14.2), the important contribution comes from z of order m_e, and hence the contribution, expected to be $\alpha^2(m_\mu/m_e)$ times that of the first term, is neglected. Hence making the above mentioned approximation and integrating over z, we find

$$\langle S_8^{(4)}\rangle' \to -\frac{i\alpha^2}{2\delta}\sum_{\substack{u\vartheta\\ u'\vartheta'}} C^*(u',\vartheta')\,C(u,\vartheta)\int d^3x_1\int d^3x_2\int d^3x_3\int d^3x_4 \sum_{\substack{\epsilon_{\mu n}>0\\ \epsilon_{en'}>0\\ n,n'\neq 0,0}}$$

$$\times\ \bar{\Phi}_{\mu u'}(\bar{x}_4)\,\bar{\Phi}_{e\vartheta'}(\bar{x}_2)\,\gamma^{(\mu)}_\nu\,\gamma^{(e)\nu}\,\frac{1}{x_{42}}\,\frac{\Phi_{\mu n}(\bar{x}_4)\,\Phi_{en'}(\bar{x}_2)\,\bar{\Phi}_{\mu n}(\bar{x}_3)\,\bar{\Phi}_{en'}(\bar{x}_1)}{\epsilon_{e0}+\epsilon_{\mu 0}-\epsilon_{en'}-\epsilon_{\mu n}}$$

$$\times\ \gamma^{(\mu)}_{\nu'}\,\gamma^{(e)\nu'}\,\frac{1}{x_{31}}\,\Phi_{\mu u}(\bar{x}_3)\,\Phi_{e\vartheta}(\bar{x}_1) \qquad (7.50)$$

Consider the sum of the terms with $\nu=0, \nu'\neq 0$ and $\nu\neq 0, \nu'=0$

$$\langle S_S^{(4)}\rangle'(\nu\nu'=0) \rightarrow \frac{i\alpha^2}{8}\sum_{\substack{u\upsilon\\u'\upsilon'}} C^*(u',\upsilon')C(u,\upsilon)\int d^3x_1\int d^3x_2\int d^3x_3\int d^3x_4$$

$$\times\,\Phi^+_{\mu u'}(\bar{x}_4)\Phi^+_{e\upsilon'}(\bar{x}_2)\frac{1}{x_{42}}\,\frac{\Phi_{\mu n}(\bar{x}_4)\Phi_{en'}(\bar{x}_2)\Phi^+_{\mu n}(\bar{x}_3)\Phi^+_{en'}(\bar{x}_1)}{\epsilon_{eo}+\epsilon_{\mu o}-\epsilon_{en'}-\epsilon_{\mu n}}$$

$$\times\,\alpha_i^{(\mu)}\alpha_i^{(e)}\frac{1}{x_{31}}\Phi_{\mu u}(\bar{x}_3)\Phi_{e\upsilon}(\bar{x}_1) \tag{7.51}$$

If we replace all wave functions (including intermediate electron states) by the Pauli approximation, and the energy differences by the nonrelativistic energy differences, we can reproduce the nonrelativistic result. However we treat the intermediate electron states relativistically to examine the validity of the Pauli approximation in that case. As in the nonrelativistic case, the electron intermediate states are approximated by the free states. Thus

$$\sum_{\epsilon_{en'}>0}\frac{\Phi_{en'}(\bar{x}_2)\Phi^+_{en'}(\bar{x}_1)}{\epsilon_{eo}+\epsilon_{\mu o}-\epsilon_{en'}-\epsilon_{\mu n}} \simeq \sum_{\epsilon_{en'}}\frac{\Phi_{en'}(\bar{x}_2)\Phi^+_{en'}(\bar{x}_1)}{\epsilon_{eo}+\epsilon_{\mu o}-\epsilon_{en'}-\epsilon_{\mu n}}$$

$$\simeq -\left[\bar{p}_2\cdot\bar{\alpha}_e+\beta_e m_e+\epsilon_{\mu o}+\epsilon_{eo}-\epsilon_{\mu n}\right]\frac{e^{-c_n x_{12}}}{4\pi x_{12}}$$

$$\simeq -\left[\bar{p}_2\cdot\bar{\alpha}_e+\beta_e m_e-\frac{\alpha}{x_2}+\epsilon_{\mu o}+\epsilon_{eo}-\epsilon_{\mu n}\right]\frac{e^{-c_n x_{12}}}{4\pi x_{12}} \tag{7.52}$$

where $c_n = [m_e^2-(\epsilon_{\mu o}-\epsilon_{\mu n}+\epsilon_{eo})\ ]$, $Re(c_n)>0$, and where $\bar{p}_2$ only acts on $\exp(-cx_{12})/x_{12}$. The binding term $-\alpha/x_2$ can be added because it is of order $\alpha^2 m_e$, while the leading term is of order m_e. Now

$$\bar{\Phi}^{+}_{ev}(\bar{x}_2)\frac{1}{x_{42}}(\bar{P}_2\cdot\bar{\alpha}_e+\beta_e m_e-\frac{\alpha}{x_2}+\epsilon_{\mu o}-\epsilon_{\mu n}+\epsilon_{eo})$$

$$=\bar{\Phi}^{+}_{ev}(\bar{x}_2)(\epsilon_{\mu o}-\epsilon_{\mu n}+2\epsilon_{eo})\frac{1}{x_{42}}+\bar{\Phi}^{+}_{ev}(\bar{x}_2)i(\bar{\nabla}_2\frac{1}{x_{42}})\cdot\bar{\alpha}_e \quad (7.53)$$

With the aid of (7.52) and (7.53),

$$\langle S_S^{(4)}\rangle'(vv'=0)\rightarrow-\frac{i\alpha^2}{4\pi\delta}\sum_{\substack{uv\\u'v'}}c^*(u',v')\,c(u,v)\int d^3x_1\int d^3x_2\int d^3x_3\int d^3x_4$$

$$\times\sum_{\epsilon_{\mu n}>0}\Big[\bar{\Phi}^{+}_{\mu u'}(\bar{x}_4)\bar{\Phi}^{+}_{ev'}(\bar{x}_2)\frac{1}{x_{42}}\,\bar{\Phi}_{\mu n}(\bar{x}_4)(\epsilon_{\mu o}-\epsilon_{\mu n}+2\epsilon_{eo})\frac{e^{-c_n x_{12}}}{x_{12}}$$

$$\times\,\bar{\Phi}^{+}_{\mu n}(\bar{x}_3)\,\frac{\bar{\alpha}^{(\mu)}\cdot\bar{\alpha}^{(e)}}{x_{31}}\,\bar{\Phi}_{\mu u}(\bar{x}_3)\bar{\Phi}_{ev}(\bar{x}_1)$$

$$+\,\bar{\Phi}^{+}_{\mu u'}(\bar{x}_4)\bar{\Phi}^{+}_{ev'}(\bar{x}_2)\,i(\bar{\nabla}_2\frac{1}{x_{42}})\cdot\bar{\alpha}^{(e)}\,\bar{\Phi}_{\mu n}(\bar{x}_4)\bar{\Phi}^{+}_{\mu n}(\bar{x}_3)\frac{e^{-c_n x_{12}}}{x_{12}}$$

$$\times\,\frac{\bar{\alpha}^{(\mu)}\cdot\bar{\alpha}^{(e)}}{x_{31}}\,\bar{\Phi}_{\mu u}(\bar{x}_3)\bar{\Phi}_{ev}(\bar{x}_1)\Big] \quad (7.54)$$

All the wave functions in (7.51) are approximated with the aid of (7.36). With the repeated application of (7.37) and (7.38), we have in the nonrelativistic limit

$$\bar{\Phi}^{+}_{ev'}(\bar{x}_2)\bar{\Phi}^{+}_{\mu n}(\bar{x}_3)f(x_{42})g(x_{12})h(x_{31})\,\bar{\alpha}^{(\mu)}\cdot\bar{\alpha}^{(e)}\,\bar{\Phi}_{\mu u}(\bar{x}_3)\bar{\Phi}_{ev}(\bar{x}_1)$$

$$\rightarrow\frac{1}{4m_e m_\mu}\phi^{+}_{ev'}(\bar{x}_2)\phi^{+}_{\mu n}(\bar{x}_3)\sigma_i^{(\mu)}\sigma_j^{(\mu)}\sigma_j^{(e)}\sigma_k^{(e)}$$

$$\times\{f(x_{42})g(x_{12})\,[\nabla_{1k}\nabla_{3i}h(x_{31})]+[\nabla_{2k}f(x_{42})]g(x_{12})$$

$$\times\,[\nabla_{3i}h(x_{31})]\}\,\phi_{\mu u}(\bar{x}_3)\,\phi_{ev}(\bar{x}_1) \quad (7.55)$$

where only the terms contributing to hyperfine structure are retained. With the aid of (7.55),

$$\bar{\Phi}^{+}_{\mu u'}(\bar{x}_4)\bar{\Phi}_{\mu n}(\bar{x}_4)\bar{\Phi}^{+}_{ev}(\bar{x}_2)\bar{\Phi}^{+}_{\mu n}(\bar{x}_3)\frac{1}{x_{42}}\,2\epsilon_{eo}\,\frac{e^{-c_n x_{12}}}{x_{12}}$$

$$\times\frac{\bar{\alpha}^{(\mu)}\cdot\bar{\alpha}^{(e)}}{x_{31}}\,\bar{\Phi}_{\mu u}(\bar{x}_3)\bar{\Phi}_{ev}(\bar{x}_1)$$

$$\longrightarrow\frac{\epsilon_{eo}}{2m_\mu m_e}\,\phi^{+}_{\mu u'}(\bar{x}_4)\phi_{\mu n}(\bar{x}_4)\phi^{+}_{ev'}(\bar{x}_2)\phi^{+}_{\mu n}(\bar{x}_3)\,\sigma_j^{(e)}\sigma_k^{(e)}$$

$$\times\sigma_i^{(\mu)}\sigma_j^{(\mu)}\left[\frac{1}{x_{42}}\frac{e^{-c_n x_{12}}}{x_{12}}\left(\nabla_{1k}\nabla_{3i}\frac{1}{x_{31}}\right)+\left(\nabla_{2k}\frac{1}{x_{42}}\right)\frac{e^{-c_n x_{12}}}{x_{12}}\right.$$

$$\left.\times\left(\nabla_{3i}\frac{1}{x_{31}}\right)\right]\phi_{\mu u}(\bar{x}_3)\phi_{ev}(\bar{x}_1) \qquad (7.56)$$

The analogous term with $\epsilon_{\mu o}-\epsilon_{\mu n}$ is neglected, since

$$\frac{\epsilon_{\mu o}-\epsilon_{\mu n}}{2\epsilon_{eo}}\sim\frac{\alpha^2 m_\mu}{m_e} \qquad (7.57)$$

Also,

$$\bar{\Phi}^{+}_{\mu u'}(\bar{x}_4)\bar{\Phi}^{+}_{ev}(\bar{x}_2)\,i\left(\bar{\nabla}_2\frac{1}{x_{42}}\right)\cdot\bar{\alpha}^{(e)}\,\bar{\Phi}_{\mu n}(\bar{x}_4)\bar{\Phi}^{+}_{\mu n}(\bar{x}_3)\,\frac{e^{-c_n x_{12}}}{x_{12}}$$

$$\times\frac{\bar{\alpha}^{(\mu)}\cdot\bar{\alpha}^{(e)}}{x_{31}}\,\bar{\Phi}_{\mu u}(\bar{x}_3)\bar{\Phi}_{ev}(\bar{x}_1)$$

$$\longrightarrow-\frac{1}{2m_\mu}\,\phi^{+}_{\mu u'}(\bar{x}_4)\phi_{\mu n}(\bar{x}_4)\phi^{+}_{ev}(\bar{x}_2)\phi^{+}_{\mu n}(\bar{x}_3)\sigma_j^{(e)}\sigma_k^{(e)}$$

$$\times\sigma_i^{(\mu)}\sigma_j^{(\mu)}\left(\nabla_{2k}\frac{1}{x_{42}}\right)\frac{e^{-c_n x_{12}}}{x_{12}}\left(\nabla_{3i}\frac{1}{x_{13}}\right)\phi_{ev}(\bar{x}_1)\phi_{\mu u}(\bar{x}_3) \qquad (7.58)$$

Now

$$\epsilon_{eo} = m_e + O(\alpha^2 m_e) \simeq m_e \qquad (7.59)$$

Hence the hyperfine splitting between the singlet and the triplet is given by

$$\Delta[\langle S_6^{(4)}\rangle'(\nu\nu'=0)] \simeq \frac{i}{6}\frac{8\pi\alpha^2}{3m_\mu m_e}\sum_n \int d^3x_1 \int d^3x_2 \int d^3x_3 \int d^3x_4$$

$$\times\ \psi^+_{\mu o}(\bar{x}_4)\psi^+_{eo}(\bar{x}_2)\frac{1}{x_{42}}\psi_{\mu n}(\bar{x}_4)\frac{m_e}{2\pi}\frac{e^{-C_n x_{12}}}{x_{12}}\psi^+_{\mu n}(\bar{x}_3)$$

$$\times\ \delta^3(\bar{x}_1-\bar{x}_3)\psi_{\mu o}(\bar{x}_3)\psi_{eo}(\bar{x}_1) \qquad (7.60)$$

The contribution from (7.50) in the case where $\nu\neq 0, \nu'\neq 0$ and $\nu=\nu'=0$ is estimated to be α times smaller than (7.60). This is so because an additional $\bar{\alpha}^{(\mu)}$ effects an additional cross term between the upper and lower components of the muon wave function. Hence there is an additional factor of $\bar{p}_\mu/m_\mu$, and $|\bar{p}_\mu| \sim \alpha m_\mu$. Therefore

$$\Delta[\langle S_6^{(4)}\rangle'] \simeq \Delta[\langle S_6^{(4)}\rangle'(\nu\nu'=0)] \qquad (7.61)$$

By employing the same method, we find

$$\Delta[\tfrac{3}{4}\langle S_6^{(3)}\rangle'] = -\frac{i}{6}\frac{8\pi\alpha^2}{3m_\mu m_e}\sum_n \int d^3x_1 \int d^3x_2 \int d^3x_3 \int d^3x_4$$

$$\times\ \psi^+_{\mu o}(\bar{x}_4)\psi^+_{eo}(\bar{x}_2)\frac{1}{x_2}\psi_{\mu n}(\bar{x}_4)\frac{m_e}{2\pi}\frac{e^{-C_n x_{12}}}{x_{12}}\psi^+_{\mu n}(\bar{x}_3)$$

$$\times\ \delta^3(\bar{x}_1-\bar{x}_3)\,\psi_{\mu o}(\bar{x}_3)\,\psi_{eo}(\bar{x}_1) \tag{7.62}$$

Now

$$c_n = \sqrt{m_e^2-(\epsilon_{\mu o}-\epsilon_{\mu n}+\epsilon_{eo})^2}$$

$$\simeq \sqrt{-2m_e(E_{\mu o}-E_{\mu n}-E_{eo})} \tag{7.63}$$

where E denotes nonrelativistic energy. Hence the factor $m_e \exp(-cx_{12})/(2\pi x_{12})$ can be approximated by the free nonrelativistic Green's function for the electron $G_e^0(\bar{x}_1,\bar{x}_2,E_{\mu o}-E_{\mu n}+E_{eo})$. Hence the hyperfine splitting due to the fourth order correction in E_a is given by

$$\Delta[\Delta E_a^{(4)}] \simeq -\frac{16\pi\alpha^2}{3m_\mu m_e}\sum_n \int d^3x_1\int d^3x_2\int d^3x_3\int d^3x_4\,\psi^+_{\mu o}(\bar{x}_4)\psi^+_{eo}(\bar{x}_2)$$

$$\times\left(\frac{1}{x_{42}}-\frac{1}{x_2}\right)\psi_{\mu n}(\bar{x}_4)\,\psi^+_{\mu n}(\bar{x}_3)\,G_e^0(\bar{x}_1,\bar{x}_2,E_{\mu o}-E_{\mu n}+E_{eo})$$

$$\times\ \delta^3(\bar{x}_1-\bar{x}_3)\,\psi_{\mu o}(\bar{x}_3)\,\psi_{eo}(\bar{x}_1) \tag{7.64}$$

Examination of (7.48) and (7.64) indicates that the hyperfine splitting is same as the nonrelativistic result of Chapter 2 with the electron intermediate states replaced by free states. The errors due to the approximations, are estimated to be of nominal order $\alpha^2\Delta\nu_F$.

8. ANALYTICAL CALCULATION OF THE HYPERFINE SPLITTING IN MUONIC ^{3}He

In this Chapter, the analytical method discussed in Chapter 2 is applied to evaluate the ground-state hyperfine splitting in muonic ^{3}He.

In analogy with Equation (2.1), the Schrodinger equation for muonic ^{3}He is

$$\left(-\frac{\nabla_\mu^2}{2M_\mu}-\frac{\nabla_e^2}{2M_e}-\frac{2\alpha}{x_\mu}-\frac{2\alpha}{x_e}+\frac{\alpha}{x_{\mu e}}-\frac{\vec{\nabla}_\mu\cdot\vec{\nabla}_e}{m_N}\right)\psi(\vec{x}_\mu,\vec{x}_e)$$

$$= E\psi(\vec{x}_\mu,\vec{x}_e) \qquad (8.1)$$

where $\vec{x}_\mu$ and $\vec{x}_e$ are the position vectors of the muon and the electron relative to the nucleus, and where $M_\mu = m_\mu m_N/(m_\mu+m_N)$ and $M_e = m_e m_N/(m_e+m_N)$ are the reduced masses of the muon and the elecron with respect to the nunleus, and m_N is the mass of the nucleus. The mass-polarization term $-\vec{\nabla}_\mu\cdot\vec{\nabla}_e/m_N$ is negligible to the accuracy considered here.

The hyperfine interaction in the ground state, which is a generalization of Equation (2.2), is given by

$$\delta H = -\frac{8\pi}{3}\vec{\mu}_N\cdot\vec{\mu}_\mu\,\delta^3(\vec{x}_\mu) - \frac{8\pi}{3}\vec{\mu}_\mu\cdot\vec{\mu}_e\,\delta^3(\vec{x}_\mu-\vec{x}_e)$$

$$- \frac{8\pi}{3} \bar{\mu}_e \cdot \bar{\mu}_N \, \delta^3(\bar{x}_e) \tag{8.2}$$

where $\bar{\mu}_e = -g_e e/(2m_e)\bar{s}_e$, $\bar{\mu}_\mu = -g_\mu e/(2m_\mu)\bar{s}_\mu$ and $\bar{\mu}_N = -g_N e/(2m_p)\bar{I}_N$ are the magnetic vectors of the electron, the muon, and the nucleus, respectively, and where m_p is the proton mass. The nonrelativistic ground-state wave function factorizes into a product of coordinate-space and spin-space parts, so the level shift can be written as the spin-space expectation value of the operator

$$\delta H_s = -a \bar{I}_N \cdot \bar{s}_\mu - b \bar{s}_\mu \cdot \bar{s}_e - c \bar{s}_e \cdot \bar{I}_N \tag{8.3}$$

where

$$a = \frac{2\pi\alpha}{3} \frac{g_N g_\mu}{m_p m_\mu} \langle \delta^3(\bar{x}_\mu) \rangle \tag{8.4}$$

$$b = \frac{2\pi\alpha}{3} \frac{g_\mu g_e}{m_\mu m_e} \langle \delta^3(\bar{x}_\mu - \bar{x}_e) \rangle \tag{8.5}$$

$$c = \frac{2\pi\alpha}{3} \frac{g_e g_N}{m_e m_p} \langle \delta^3(\bar{x}_e) \rangle \tag{8.6}$$

and where $\langle\ \rangle$ denotes the expectation value in coordinate space. The leading contribution to b in powers of (M_e/M_μ) is calculated in Chapter 2. The leading contribution to a and c are calculated in this Chapter.

To evaluate the coordinate-space expectation value in (8.4) and (8.6), perturbation theory is applied with the division

$$H = H_o + \delta V \tag{8.7}$$

in which

$$H_o = -\frac{\nabla_\mu^2}{2M_\mu} - \frac{\nabla_e^2}{2M_e} - \frac{2\alpha}{x_\mu} - \frac{\alpha}{x_e} \tag{8.8}$$

$$\delta V = \frac{\alpha}{x_{\mu e}} - \frac{\alpha}{x_e} \tag{8.9}$$

similar to equations (2.8) and (2.9).

The zero-order wave function for the ground state is given by Equation (2.10). Thus, the zero-order contribution to the expectation values in (8.4) and (8.6) are

$$a^{(0)} = \frac{2\pi\alpha}{3}\frac{g_N g_\mu}{m_p m_\mu}\int d^3x_\mu \int d^3x_e \, \psi_o^+(\bar{x}_\mu, \bar{x}_e)\, \delta^3(\bar{x}_\mu)\, \psi_o(\bar{x}_\mu, \bar{x}_e)$$

$$= \frac{16\alpha(\alpha M_\mu)^3}{3 m_p m_\mu} g_N g_\mu \tag{8.10}$$

$$c^{(0)} = \frac{2\pi\alpha}{3}\frac{g_e g_N}{m_e m_p}\int d^3x_\mu \int d^3x_e \, \psi_o^+(\bar{x}_\mu, \bar{x}_e)\, \delta^3(\bar{x}_e)\, \psi_o(\bar{x}_\mu, \bar{x}_e)$$

$$= \Delta\nu_F \frac{g_e g_N}{4}\frac{m_\mu}{m_p} \tag{8.11}$$

with the Fermi value $\Delta\nu_F = (8/3)\alpha/(m_e m_\mu)(\alpha M_e)^3$.

The first-order correction to the wave function is given by Equation (2.12). The first-order correction in a is

$$a^{(1)} = \frac{4\pi\alpha}{3}\,\frac{g_N g_\mu}{m_p m_\mu}\int d^3x_\mu \int d^3x_e\, \Psi_0^+(\bar{x}_\mu,\bar{x}_e)\,\delta^3(\bar{x}_\mu)$$

$$\times\ \Psi_1(\bar{x}_\mu,\bar{x}_e) \qquad (8.12)$$

Substitution of (2.12) in (8.12) yields non-zero terms only for $n' = 0$ because of the orthogonality of the electron wave functions. Thus

$$a^{(1)} = \frac{4\pi\alpha}{3}\,\frac{g_N g_\mu}{m_p m_\mu}\int d^3x\ \psi_{\mu 0}^+(0)\sum_{n\neq 0}\frac{\psi_{\mu n}(0)\,\psi_{\mu n}^+(\bar{x})}{E_{\mu 0}-E_{\mu n}}$$

$$\times\ V_e(x)\,\psi_{\mu 0}(\bar{x}) \qquad (8.13)$$

where

$$V_e(x) = \int d^3x_e\, \psi_{e0}^+(\bar{x}_e)\,\delta V(\bar{x},\bar{x}_e)\,\psi_{e0}(\bar{x}_e)$$

$$= -\frac{\alpha}{x}\left[\alpha M_e x - 1 + (\alpha M_e x + 1)\, e^{-2\alpha M_e x}\right] \qquad (8.14)$$

Only s-states contribute to the sum over n in (8.13), so the sum may be replaced by the s-state reduced Green's function for the muon,[25] with one coordinate set equal to zero.

$$\sum_{n\neq 0}\frac{\psi_{\mu ns}(0)\,\psi_{\mu ns}^+(\bar{x})}{E_{\mu 0}-E_{\mu ns}} = -\frac{2\alpha M_\mu^2}{\pi}\, e^{-2\alpha M_\mu x}$$

$$\times\left[\frac{1}{4\alpha M_\mu x} - \ln(4\alpha M_\mu x) + \frac{5}{2} - \gamma - 2\alpha M_\mu x\right] \qquad (8.15)$$

where $\gamma=0.5772\ldots$ is Euler's constant. Evaluation of (8.13) with the aid of (8.14) and (8.15) yields a result of order $(M_e/M_\mu)^3\, a^{(0)}$ for $a^{(1)}$, which is negligible to the accuracy considered here. The term $a^{(1)}$ may be regarded as the correction to the muon density at the origin due to the perturbation of the muon wave function by the electron. Only the fraction of order $(M_e/M_\mu)^3$, of the electron charge distribution inside the muon Bohr radius is effective in modifying this density. The quantity $c^{(1)}$ is

$$c^{(1)} = \frac{4\pi\alpha}{3}\,\frac{g_e g_N}{m_e m_p}\int d^3x_\mu \int d^3x_e\, \psi_0^+(\bar{x}_\mu,\bar{x}_e)$$

$$\times\, \delta^3(\bar{x}_e)\,\psi_1(\bar{x}_\mu,\bar{x}_e) \qquad (8.16)$$

Because of the orthogonality of the muon wave functions, only the n=0 term in (2.12) survives upon substitution in (8.16). Hence,

$$c^{(1)} = \frac{4\pi\alpha}{3}\,\frac{g_e g_N}{m_e m_p}\int d^3x\, \psi_{eo}^+(0)\sum_{n\neq 0}\frac{\psi_{en}(0)\,\psi_{en}^+(\bar{x})}{E_{eo}-E_{en}}$$

$$\times\, V_\mu(x)\,\psi_{eo}(\bar{x}) \qquad (8.17)$$

where

$$V_\mu(x) = \int d^3x_\mu\, \psi_{\mu o}^+(\bar{x}_\mu)\,\delta V(\bar{x}_\mu,\bar{x})\,\psi_{\mu o}(\bar{x}_\mu)$$

$$= -\frac{\alpha}{x}(1+2\alpha M_\mu x)\,e^{-4\alpha M_\mu x} \qquad (8.18)$$

Only s-states contribute to the sum over n in (8.17), so once again the s-state reduced Green's function may be employed, which is given by

$$\sum_{n\neq 0} \frac{\psi_{ens}(0)\psi^{+}_{ens}(\bar{x})}{E_{eo} - E_{ens}} = -\frac{\alpha M_e^2}{\pi} e^{-\alpha M_e x}$$

$$\times \left[\frac{1}{2\alpha M_e x} - \ln(2\alpha M_e x) + \frac{5}{2} - \gamma - \alpha M_e x\right] \qquad (8.19)$$

Substitution of (8.18) and (8.19) in (8.17) yields

$$c^{(1)} = \Delta\nu_F \frac{g_e g_N}{4} \frac{m_\mu}{m_p} \left\{ \frac{3}{2}\frac{M_e}{M_\mu} + \left(\frac{M_e}{M_\mu}\right)^2 \ln\frac{M_\mu}{M_e} \right.$$

$$\left. + \left(\ln 2 + \frac{1}{4}\right)\left(\frac{M_e}{M_\mu}\right)^2 + O\left[\left(\frac{M_e}{M_\mu}\right)^3 \ln\frac{M_\mu}{M_e}\right] \right\} \qquad (8.20)$$

An alternate derivation of the leading term in (8.20) is obtained by applying Zeemach's formula to take into account the effect of the finite charge distribution of the effective nucleus on the electron-nucleus hyperfine interaction.[15] The fractional correction in c is given by

$$\frac{\Delta c}{c^{(0)}} = -\frac{2\langle r\rangle_{em}}{a_0} \qquad (8.21)$$

where $a_o = 1/(\alpha M_e)$ is the Bohr radius of the electron, and where

$$\langle r\rangle_{em} = \int d^3r\, r \int d^3s\, \rho_e(\bar{r}-\bar{s})\,\rho_m(\bar{s}) \qquad (8.22)$$

The quantities ρ_e and ρ_m are electric and magnetic distribution factors respectively, of the effective nucleus, which are normalized to unity. For this problem

$$\rho_e(\bar{r}) = 2\delta^3(\bar{r}) - |\psi_{\mu o}(\bar{r})|^2$$

$$= 2\delta^3(\bar{r}) - \frac{(2\alpha M_\mu)^3}{\pi} e^{-4\alpha M_\mu r} \qquad (8.23)$$

$$\rho_m(\bar{r}) = \delta^3(\bar{r}) \; . \qquad (8.24)$$

Substituting (8.23) and (8.24) in (8.22) yields

$$\langle r \rangle_{em} = -\frac{3}{4\alpha M_\mu} \qquad (8.25)$$

which upon substitution in (8.21) yields

$$\Delta C = \Delta\nu_F \frac{g_e g_N}{4} \frac{m_\mu}{m_p} \cdot \frac{3}{2} \frac{M_e}{M_\mu} \qquad (8.26)$$

which is the leading term of (8.20).

Diagonalization of δH_s in (8.3) yields the eigenvalues

$$\lambda_{1,2} = \frac{a+b+c}{4} \pm \frac{1}{2}(a^2+b^2+c^2-ab-bc-ca)^{1/2} \qquad (8.27)$$

$$\lambda_3 = -\frac{a+b+c}{4} \tag{8.28}$$

Both λ_1 and λ_2 are doubly degenerate, and λ_3 is quadruply degenerate, corresponding to angular momentum 1/2 and 3/2, respectively. In the present case, a>>b and a>>c, so λ_1 and λ_2 are well approximated by

$$\lambda_1 = \frac{3a}{4} + \cdots \tag{8.29}$$

$$\lambda_2 = -\frac{a}{4} + \frac{b+c}{2} + \cdots \tag{8.30}$$

where the omitted terms are higher order in b/a or c/a. The smaller splitting is given by

$$\begin{aligned} \Delta\nu &= \lambda_2 - \lambda_3 \\ &= \frac{3}{4}(b+c) \end{aligned} \tag{8.31}$$

to lowest order in b/a and c/a.

9. SUMMARY

The results are summarized in this Chapter. The corrections due to the anomalous magnetic moments of the electron and muon are added to the nonrelativistic results and comparisons are made with other theoretical as well as experimental findings.

The nonrelativistic results for muonic ^{4}He are based on constants $R_\infty = 3.289842\times10^9$ MHz, $\alpha^{-1} = 137.0360$, $m_\mu/m_e = 206.7686$ and $m_\alpha/m_e = 7294$. The zero-order hyperfine splitting $\Delta\nu_0$ is

$$\Delta\nu_0 = \Delta\nu_F\,(1+\frac{m_e}{2M_\mu})^{-3} = 4483.38\ \text{MHz}. \qquad (9.1)$$

The first-order hyperfine splitting when the intermediate muon states are restricted to the ground state, $\Delta\nu_1^g$, is

$$\Delta\nu_1^g = \Delta\nu_F\Big[\frac{11}{16}\frac{m_e}{M_\mu} + \Big(\frac{m_e}{M_\mu}\Big)^2 \ln\frac{M_\mu}{m_e} - \frac{7}{64}\Big(\frac{m_e}{M_\mu}\Big)^2$$
$$+\,O\Big(\Big(\frac{m_e}{M_\mu}\Big)^3 \ln\Big(\frac{M_\mu}{m_e}\Big)\Big)\Big] = 16.02\ \text{MHz}. \qquad (9.2)$$

The first-order hyperfine splitting when the intermediate muon states are restricted to the excited states, $\Delta\nu_1^e$, is

$$\Delta\nu_1^e = \Delta\nu_F \left\{ -\frac{35}{16}\frac{M_e}{M_\mu} + \frac{2}{3}S_{1/2}\left(\frac{M_e}{M_\mu}\right)^{3/2} + O\left[\left(\frac{M_e}{M_\mu}\right)^2 \ln\frac{M_\mu}{M_e}\right] \right\}$$

$$= -46.2 \pm 1.2 \text{ MHz.} \qquad (9.3)$$

where $S_{1/2} = 2.8 \pm 0.2$ and the Fermi value is

$$\Delta\nu_F = \frac{8}{3}\frac{\alpha}{m_\mu m_e}(\alpha M_e)^3 = 4516.91 \text{ MHz.} \qquad (9.4)$$

The numerical results for $\Delta\nu_1^e$ and the contribution to the first-order hyperfine splitting $\Delta\nu_1^m$ due to mass-polarization term are

$$\Delta\nu_1^e\,(\text{num}) = -45.67 \text{ MHz}, \qquad (9.5)$$

$$\Delta\nu_1^m\,(\text{num}) = 0.08 \text{ MHz.} \qquad (9.6)$$

The second-order hyperfine splitting is of order $\Delta\nu_F(M_e/M_\mu)^2 \ln(M_\mu/M_e)$. Hence the analytical result for the hyperfine splitting is

$$\Delta\nu = \Delta\nu_0 + \Delta\nu_1^g + \Delta\nu_1^e + \cdots$$

$$= \Delta\nu_F \left\{ 1 - 3\frac{M_e}{M_\mu} + \frac{2}{3}S_{1/2}\left(\frac{M_e}{M_\mu}\right)^{3/2} + O\left[\left(\frac{M_e}{M_\mu}\right)^2 \ln\frac{M_\mu}{M_e}\right] \right\}$$

$$= 4452.5 \pm 2.4 \text{ MHz.} \qquad (9.7)$$

while the numerical result is

$$\Delta\nu\,(\mathrm{num}) = \Delta\nu_0 + \Delta\nu_1^g + \Delta\nu_1^e\,(\mathrm{num}) + \Delta\nu_1^m\,(\mathrm{num})$$

$$+ O\left[\Delta\nu_F\left(\frac{M_e}{M_\mu}\right)^2 \ln\frac{M_\mu}{M_e}\right] = 4453.8 \pm 1.2\ \mathrm{MHz}. \tag{9.8}$$

A variational calculation of Huang and Hughes gives 4455.2 ± 1.0 MHz.[9] Drachman's calculation using a Born-Oppenheimer approximation reproduces the two leading terms of $\Delta\nu$ and yields 4450 MHz,[10] while a later calculation in which first Fermi contact term is rewritten as a global operator, yields 4450 MHz.[11] Clearly all the results are in good agreement with the one obtained in this thesis.

The main correction to the nonrelativistic result is due to the lowest order anomalous magnetic moments of the electron and muon. The corrected g-factors for the electron and muon are

$$g_e \simeq g_\mu \simeq 2\left(1 + \frac{\alpha}{2\pi}\right). \tag{9.9}$$

These factors shift the hyperfine freqency by $\Delta\nu_F\alpha/\pi$ = 10.5 MHz. Higher order self-energy and vacuum-polarization corrections can be roughly approximated by the hydrogenic value,[33] and are of order $\alpha^2\Delta\nu_F$. These corrections are discussed elsewhere,[8-9] but they are smaller than the current uncertainty in the nonrelativistic result. Also other relativistic corrections may contribute terms of order $\alpha^2\Delta\nu_F$. Hence the corrections amount to 10.5 ± 0.6 MHz. Hence the corrected analytical and numerical values are given by

$$\Delta\nu = 4463.0 \pm 3.0 \text{ MHz}, \qquad (9.10)$$

$$\Delta\nu(\text{num}) = 4464.3 \pm 1.8 \text{ MHz}. \qquad (9.11a)$$

If the second-order hyperfine splitting [given by Equation (6.38)] is added to (9.11a), we get

$$\Delta\nu(\text{num}) = 4464.9 \text{ MHz}. \qquad (9.11b)$$

The results are in good agreement with the result of the experiment at SIN : 4464.95(6) MHz[2], and with the preliminary experimental result at LAHPF : 4464.99(4) MHz.[3]

The hyperfine splitting in muonic ^{3}He is given by

$$\Delta\nu(^3\text{He}) = \frac{3}{4}(b+c) + O\left(\frac{b}{a}\right) + O\left(\frac{c}{a}\right)$$

$$= 4164.9 \pm 3.0 \text{ MHz}, \qquad (9.12)$$

where the values for a,b and c in the two lowest orders of perturbation theory are

$$a = \frac{16}{3}\alpha(\alpha M_\mu)^3 \frac{g_N g_\mu}{m_p m_\mu} = 3.3 \times 10^8 \text{ MHz} \qquad (9.13)$$

$$b = \Delta\nu_F \frac{g_e g_\mu}{4}\left[1 - 3\frac{M_e}{M_\mu} + \frac{2}{3} S_{1/2}\left(\frac{M_e}{M_\mu}\right)^{3/2}\right]$$

$$= 4461.7 \text{ MHz} \qquad (9.14)$$

$$C = \Delta\nu_F \frac{g_e g_N}{4} \frac{m_\mu}{m_p} \left[1 + \frac{3}{2}\frac{M_e}{M_\mu}\right]$$

$$= 1091.5 \text{ MHz}, \tag{9.15}$$

based on the constants $m_p/m_e = 1836.15$, $m_N/m_p = 2.993$, $g_N = 4.25525$, $g_e \simeq g_\mu \simeq 2[1+\alpha/(2\pi)]$, and other constants given earlier in this Chapter. The corrections due to the anomalous magnetic moments of the electron and muon are accounted for in g-factors of the electron and muon. The uncertainty in the hyperfine splitting arises mainly from the uncertainty in b, which is similar to the uncertainty for muonic ^{4}He. To the accuracy considered here, $\Delta\nu(^4\text{He}) = b(^4\text{He})$, where the difference, $b(^4\text{He})-b(^3\text{He}) = 1.2$ MHz, is due to the difference in the reduced masses. Hence employing the experimental value,[2] $\Delta\nu(^4\text{He}) = 4465.0$ MHz, a semiempirical estimate for the muonic ^{3}He hyperfine splitting is:

$$\Delta\nu(^3\text{He}) = \frac{3}{4}\left[b(^3\text{He}) + C\right]$$

$$= \frac{3}{4}\left[\Delta\nu(^4\text{He}) + C + b(^3\text{He}) - b(^4\text{He})\right]$$

$$= 4166.5 \pm 0.4 \text{ MHz}. \tag{9.16}$$

Drachman has calculated this quantity by rewriting the Fermi contact term as a global operator and evaluating it with the wave function given by (2.10).[11] His value is 4163 MHz.

APPENDIX A

The question of stability in calculating the numerical solution of (3.5) for $E<0$ with the use of the recursion relation (3.13) is discussed in this Appendix.

The asymptotic behavior of the wave function satisfying (3.5) is given by Equations (3.16) and (3.21). Our interest is in solving (3.13) with the exact eigenvalue E_n. But due to roundoff errors and the inexact knowledge of E_n, we solve (3.13) with $E \neq E_n$. The general solution of (3.13) with $E \neq E_n$ can be spanned by any pair $A(x), B(x)$ of linearly independent solutions. We are interested in the special case where the asymptotic behavior of $A(x)$ is given by Equations (3.16) and (3.21):

$$A(x) \propto M_e x, \qquad \alpha M_\mu x \ll 1 \tag{A.1}$$

$$A(x) \propto (M_e x)^\nu e^{-\sqrt{-2EM_e}\, x}, \quad \alpha M_\mu x \gg 1 \tag{A.2}$$

where $\nu = [-\alpha^2 M_e/(2E)]^{1/2}$. For small x ($\alpha M_\mu x \ll 1$), any solution that is linearly independent of $A(x)$ diverges at the origin. Hence $|A(x)/B(x)|$ is an increasing function of x, and therefore as explained in Appendix D, the procedure of calculating $A(x)$ recursively in the direction of increasing x is stable. For large x ($\alpha M_\mu x \gg 1$), any solution that is linearly independent of $A(x)$ diverges at infinity. Hence $|A(x)/B(x)|$ is a decreasing function of x, and therefore as explained in Appendix D, the procedure of calculating $A(x)$ recursively in the direction of decreasing x is stable. Thus we calculate $A(x)$ recursively starting from small x going in the direction of increasing x, and starting from large x going in the direction of decreasing x (and match the functions in between).

APPENDIX B

In this Appendix, the scaling properties of the Coulomb Green's function are derived.

The Coulomb Green's function satisfies

$$\left(-\frac{\nabla_2^2}{2m} - \frac{Z\alpha}{x_2} - E\right) G(\bar{x}_2,\bar{x}_1,E) = \delta^3(\bar{x}_2-\bar{x}_1) \tag{B.1}$$

With the change of variables $y_2=mZx_2$, $y_1=mZx_1$, $\nabla_2^2 \to (mZ)^2\nabla_2^2$ and we obtain

$$\left(-\frac{\nabla_2^2}{2} - \frac{\alpha}{y_2} - \frac{E}{mZ^2}\right)\frac{1}{m^2 Z}\, G\left(\frac{\bar{y}_2}{mZ},\frac{\bar{y}_1}{mZ},E\right) = \delta^3(\bar{y}_2-\bar{y}_1) \tag{B.2}$$

comparing it with

$$\left(-\frac{\nabla_2^2}{2} - \frac{\alpha}{y_2} - E'\right) H(\bar{y}_2,\bar{y}_1,E') = \delta^3(\bar{y}_2-\bar{y}_1) \tag{B.3}$$

where H is independent of m and Z, we obtain

$$G(\bar{x}_2,\bar{x}_1,E) = m^2 Z\, H\left(mZ\bar{x}_2, mZ\bar{x}_1, \frac{E}{mZ^2}\right) \tag{B.4}$$

If G and H are expanded into angular and radial parts

$$G(\bar{x}_2,\bar{x}_1,E) = \sum_{\ell m} G_\ell(x_2,x_1,E)\, Y_{\ell m}(\hat{x}_2)\, Y^*_{\ell m}(\hat{x}_1) \tag{B.5}$$

$$H(\bar{x}_2, \bar{x}_1, E) = \sum_{\ell m} H_\ell(x_2, x_1, E) Y_{\ell m}(\hat{x}_2) Y^*_{\ell m}(\hat{x}_1) \tag{B.6}$$

then

$$G_\ell(x_2, x_1, E) = m^2 Z H_\ell(mZx_2, mZx_1, \frac{E}{mZ^2}) \tag{B.7}$$

APPENDIX C

In this Appendix, it is shown that the relative errors involved in making the approximations in (4.65) in deriving the analytical asymptotic formula for large z, tend to zero as z tends to infinity.

We first make approximation I in (4.65), i.e., we replace the Green's functions for the electron and muon by the corresponding free green's functions given by (4.66) and (4.67). Then we show that the relative error involved in making approximation II, namely evaluating all ground-state wave functions at $\bar{x}_1=\bar{x}_2=\bar{x}_3$, tends to zero as z tends to infinity. Then we make approximation II in (4.65), and show that the relative error involved in making approximation I tends to zero as z tends to infinity.

With approximation I, h(z) in (4.65) becomes

$$h(z) \simeq \frac{M_e M_\mu}{4\pi^2} \int d^3x_3 \int d^3x_2 \int d^3x_1 \, \psi_0^+(\bar{x}_3, \bar{x}_3)\, \psi_0(\bar{x}_2, \bar{x}_1)$$

$$\times \frac{e^{-b_\mu x_{32}}}{x_{32}} \frac{e^{-b_e x_{31}}}{x_{31}} \frac{1}{x_{21}}$$

$$- \frac{M_e M_\mu}{4\pi^2} \int d^3x_3 \int d^3x_2 \int d^3x_1 \, \psi_0^+(\bar{x}_3, \bar{x}_3)\, \psi_0(\bar{x}_2, \bar{x}_1)$$

$$\times \frac{e^{-b_\mu x_{32}}}{x_{32}} \frac{e^{-b_e x_{31}}}{x_{31}} \frac{1}{x_1} \qquad (C.1)$$

Let $h_1(z)$ be the first term of (C.1). By expanding $\psi_0(\bar{x}_2,\bar{x}_1)$ around $\bar{x}_3$

$$\psi_0(\bar{x}_2,\bar{x}_1) = \psi_0(\bar{x}_3,\bar{x}_3) + (\bar{x}_2-\bar{x}_3)\cdot\bar{\nabla}_2\psi_0(\bar{x}_2,\bar{x}_3)|_{\bar{x}_2=\bar{x}_3}$$

$$+ (\bar{x}_1-\bar{x}_3)\cdot\bar{\nabla}_1\psi_0(\bar{x}_3,\bar{x}_1)|_{\bar{x}_1=\bar{x}_3} + \cdots \qquad (C.2)$$

and then integrating explicitly the terms exhibited in (C.2),

$$h_1(z) = \frac{M_e M_\mu}{4\pi^2}\int d^3x_3\int d^3x_2\int d^3x_1\,|\psi_0(\bar{x}_3,\bar{x}_3)|^2\,\frac{e^{-b_\mu x_{32}}e^{-b_e x_{31}}}{x_{32}x_{31}x_{12}}$$

$$\times\left[1+O\left(\frac{\alpha M_e}{b_e}\right)+O\left(\frac{\alpha M_\mu}{b_\mu}\right)\right]$$

$$\rightarrow \frac{M_e M_\mu}{4\pi^2}\int d^3x_3\int d^3x_2\int d^3x_1\,|\psi_0(\bar{x}_3,\bar{x}_3)|^2\,\frac{e^{-b_\mu x_{32}}e^{-b_e x_{31}}}{x_{32}x_{31}x_{12}}$$

$$= \frac{A}{b_e b_\mu(b_e+b_\mu)} \qquad (C.3)$$

as $z\rightarrow\infty$, where A is independent of z. Thus we have shown that the relative error involved in making approximation II in the first term of (C.1) tends to zero as z tends to infinity. The same is true for the second term of (C.1).

With approximation II, h(z) in (4.65) can be written as

$$h(z) \simeq \int d^3x_3\int d^3x_2\int d^3x_1\,|\psi_0(\bar{x}_3,\bar{x}_3)|^2\,G_e(\bar{x}_3,\bar{x}_1,E_{e0}-z)$$

$$\times\, G_\mu(\bar{x}_3,\bar{x}_2,E_{\mu0}+z)\,\frac{1}{x_{12}}$$

$$- \int d^3x_3 \int d^3x_2 \int d^3x_1 |\psi_0(\bar{x}_3,\bar{x}_3)|^2 G_e(\bar{x}_3,\bar{x}_1,E_{e0}-z)$$

$$\times G_\mu(\bar{x}_3,\bar{x}_2,E_{\mu 0}+z)\frac{1}{x_1} \qquad (C.4)$$

Let $g_1(z)$ be the first term of (C.4). Expanding the green's functions in terms of the free Green's functions with the aid of (2.45), we obtain

$$g_1(z) = \int d^3x_3 \int d^3x_2 \int d^3x_1 |\psi_0(\bar{x}_3,\bar{x}_3)|^2 G_e^0(\bar{x}_3,\bar{x}_1,E_{e0}-z)$$

$$\times G_\mu^0(\bar{x}_3,\bar{x}_2,E_{\mu 0}+z)\frac{1}{x_{12}}$$

$$+ \int d^3x_4 \int d^3x_3 \int d^3x_2 \int d^3x_1 |\psi_0(\bar{x}_3,\bar{x}_3)|^2 G_e^0(\bar{x}_3,\bar{x}_4,E_{e0}-z)\frac{\alpha}{x_4}$$

$$\times G_e^0(\bar{x}_4,\bar{x}_1,E_{e0}-z) G_\mu^0(\bar{x}_3,\bar{x}_2,E_{\mu 0}+z)\frac{1}{x_{12}}$$

$$+ \int d^3x_4 \int d^3x_3 \int d^3x_2 \int d^3x_1 |\psi_0(\bar{x}_3,\bar{x}_3)|^2 G_e^0(\bar{x}_3,\bar{x}_2,E_{e0}-z)$$

$$\times G_\mu^0(\bar{x}_3,\bar{x}_4,E_{\mu 0}+z)\frac{2\alpha}{x_4} G_\mu^0(\bar{x}_4,\bar{x}_2,E_{\mu 0}+z)\frac{1}{x_{12}} + \cdots \qquad (C.5)$$

The first term in (C.5), $g_{11}(z)$, is same as (C.3). The second term in (C.5), $g_{12}(z)$, is evaluated with the aid of (2.26a) and the relation

$$\int d^3x_4 \frac{e^{-bx_{34}}}{(x_{34})^2\, x_4} = \int_b^\infty ds \int d^3x_4 \frac{e^{-sx_{34}}}{x_{34}x_4} \qquad (C.6)$$

The leading contribution of the second term is

$$g_{12}(z) \simeq \frac{B}{b_e b_\mu (b_e+b_\mu)[(b_e+b_\mu)^2 - b_e^2]} , \tag{C.7}$$

where B is independent of z. In the limit $z \to \infty$, $|g_{12}(z)/g_{11}(z)| \to 0$. Similarly the relative contribution of the third term in (C.5) tends to zero as $z \to \infty$. Thus we have shown that the relative error involved in making approximation I in the first term of (C.4), tends to zero as z tends to infinity. The same result can be shown for the second term of (C.4).

APPENDIX D

In this Appendix, we explain in a qualitative way why in some cases one has to use the recursion relation in a particular direction for numerical stability.[34]

Consider a three term recurrence relation of the form

$$y(\ell+2) + a_\ell y(\ell+1) + b_\ell y(\ell) = 0 , \qquad (D.1)$$

where $b_\ell \neq 0$. The general solution can be spanned by any pair u(l),v(l) of linearly independent solutions. We are interested in the special case where such a pair has the property

$$\lim_{\ell \to \infty} \left| \frac{u(\ell)}{v(\ell)} \right| = 0 . \qquad (D.2)$$

Serious problems then arise if one attempts to compute u(l) with (D.1) for increasing l. To see this, consider y(l) to be the computed value of u(l). If we generate y(l) using only approximate values $y(0) \neq u(0)$, $y(1) \neq u(1)$ (due to rounding, for example), but recurring with infinite precision, the computed solution y(l), in general, will be linearly independent of u(l), i.e.,

$$y(\ell) = cu(\ell) + dv(\ell), \quad d \neq 0. \tag{D.3}$$

Hence in the limit $l \to \infty$,

$$\left| \frac{y(\ell) - u(\ell)}{u(\ell)} \right| \to \infty \tag{D.4}$$

Thus the relative error of y(l), the intended approximation to u(l), becomes arbitrarily large. On other hand, consider the computation of v(l) for increasing l. Let the computed value of v(l) be z(l). Then the relative error in z(l), the intended approximation to v(l), tends to zero as l tends to infinity. Thus the procedure of evaluating v(l) recursively in the direction of increasing l is stable, while the procedure of evaluating u(l) recursively in the direction of increasing l is not stable. By similar arguments, if |u(l)/v(l)| increases as l decreases, the procedure of evaluating v(l) recursively in the direction of decreasing l is not stable while the procedure of evaluating u(l) recursively in the direction of decreasing l is stable.

REFERENCES

1. P. A. Souder, D. E. Casperson, T. W. Crane, V. W. Hughes, D. C. Lu, H. Orth, H. W. Reist, M. H. Yam, and G. zu Putlitz, Phys. Rev. Lett. 34, 1417 (1975).
2. H. Orth, K. P. Arnold, P. O. Egan, M. Gladisch, W. Jacobs, J. Vetter, W. Wahl, M. Wigand, V. W. Hughes, and G. zu Putlitz, Phys. Rev. Lett. 45, 1483 (1980).
3. C. K. Gardner, W. Beer, P. Bolton, B. Dichter, P. O. Egan, V. W. Hughes, D. C. Lu, F. G. Mariam, P. A. Souder, H. Orth, G. zu Putlitz, and J. Vetter, Bull. Am. Phys. Soc. 25, 19 (1980).
4. S. D. Lakdawala and P. J. Mohr, Phys. Rev. A 22, 1572 (1980).
5. V. W. Hughes and S. Penman, Bull. Am. Phys. Soc. 4, 80 (1959).
6. E. W. Otten, Z. Phys. 225, 393 (1969).
7. K.-N. Huang, Ph.D. thesis, Yale University, 1974 (unpublished).
8. E. Borie, Z. Phys. A 291, 107 (1979).
9. K.-N. Huang and V. W. Hughes, Phys. Rev. A 20, 706 (1979): 21, 1071 (1980).
10. R. J. Drachman, Phys. Rev. A 22, 1751 (1980).
11. R. J. Drachman, J. Phys. B:At. Mol. Phys. 14, 2733 (1981).
12. J. E. Nafe, E. B. Nelson, and I. I. Rabi, Phys. Rev.71, 914 (1947).
13. A. Bohr, Phys. Rev. 73, 1109 (1948).
14. G. E. Brown and G. B. Arfken, Phys. Rev. 76, 1305 (1949).
15. A. C. Zemach, Phys. Rev. 104, 1771 (1956).
16. H. Grotch and D. R. Yennie, Rev. Mod. Phys. 41, 350 (1969).
17. E. Rosenthal and G. Breit, Phys. Rev. 41, 459 (1932).

18. M. F. Crawford and A. L. Schawlow, Phys. Rev. 76, 1310 (1949).

19. A. Bohr and V. W. Weisskopf, Phys. Rev. 77, 94 (1950).

20. F. Low, Phys. Rev. 77, 361 (1950).

21. s. D. Drell and J. D. Sullivan, Phys. Rev. 154, 1477 (1967).

22. S. S. Schweber, An Introduction to Relativistic Quantum Field Theory (Harper and Row, New York, 1962).

23. S. D. Lakdawala and P. J. Mohr, Phys. Rev. A 24, 2224 (1981).

24. K.-N. Huang and V. W. Hughes, Bull. Am. Phys. Soc. 26, 547 (1981).

25. H. F. Hameka J. Chem. Phys. 47, 2728 (1967): 48, 4810 (1968).

26. H. A. Bethe and E. E. Salpeter, Quantum Mechanics of One- and Two-Electron Atoms (Springer, Berlin, 1957).

27. A similar identity is used by M. O'Carroll and J. Schuser, Phys. Rev. Lett. 21, 1143 (1968).

28. E. T. Whittaker and G. N. Watson, A Course of Modern Analysis (Cambridge University Press, 1920).

29. M. Abramowitz and I. A. Stegun, Handbook of Mathematical Functions (Dover, New York, 1970).

30. A. H. Stroud and D. Secrest, Gaussian Quadrature Formulas (Prentice-Hall, Englewood Cliffs, NJ, 1966).

31. H. Buchholz, The Confluent Hypergeometric Function (Springer-Verlag, New York, 1969).

32. W. Magnus, F. Oberhettinger, and R. P. Soni, Formulas and Theorems for the Special Functions of Mathematical Physics (Springer-Verlag, New York, 1966).

33. For a review of the analogous effects in hydrogen, see B. E. Lautrup, A. Peterman, and E. de Rafael, Phys. Rep. 3, 193 (1972).

34. W. Gautschi, SIAM REV. 9, 24 (1967).