Nonperturbative numerical calculation of the fine and hyperfine structure of muonic hydrogen by Breit potential including the effects from the proton size

Hou-Rong Pang¹, Hai-Qing Zhou¹,² *

¹Department of Physics, Southeast University, Nanjing, 210094
²State Key Laboratory of Theoretical Physics, Institute of Theoretical Physics, Chinese Academy of Sciences, Beijing 100190, P. R. China

Abstract

By solving the two-body Schordinger equation in a very high precise nonperturbative numerical (NPnum) way, we reexamine the contributions of fine, hyperfine structure splittings of muonic hydrogen based on the Breit potential. The comparison of our results with those by the first order perturbative theory (¹stPT) in the literature shows, when the structure of proton is considered, the differences between the results by the ¹stPT and NPnum methods are small for the fine and hyperfine splitting of 2P state, while are about −0.009 meV and 0.08 meV for the F = 1 and total hyperfine splitting of 2S state of muonic hydrogen, respectively. These differences are larger than the current experimental precision and would be significant to be considered in the theoretical calculation.

PACS numbers: 31.30.jf, 36.10.Ee, 31.30.Gs, 32.10.Fn

Keywords: Breit potential, muonic hydrogen, finite size corrections, high accuracy

* Email: zhouhq@seu.edu.cn
I. INTRODUCTION

In 2010, a precision measurement \[1\] of the Lamb shift in muonic hydrogen by using pulsed laser spectroscopy was performed and gave \( E^{Ex}_{2P_{3/2}} - E^{Ex}_{2S_{1/2}} = 206.2949 \text{ meV} \). Combining this precise value with the theoretical calculation \[1\]

\[
E^{Th}_{2P_{3/2}} - E^{Th}_{2S_{1/2}} = 209.9779 - 5.2262r_p^2 + 0.0347r_p^3, \tag{1}
\]

the values of the proton radius is extracted as \( r_p = 0.84184 \text{ fm} \). In 2013, the further precise measurements of \( 2S - 2P \) transition frequencies of muonic hydrogen \[2\] gave the magnetic radius of proton \( r_M = 0.87 \text{ fm} \) and the charge radius \( r_E = 0.84087 \text{ fm} \) which are not significantly different from the value given by Ref. \[1\].

On the other hand, based on the hydrogen data or the ep scattering data, CODATA-2010 gave \( r_p \approx 0.878 \text{ fm} \) \[3\], which is much larger than the results by the muonic hydrogen’s Lamb-shift. And if this value of proton radius is used, the theoretical prediction for the Lambs shift of muonic hydrogen gives \[4\]

\[
E^{Th}_{2P_{3/2}} - E^{Th}_{2S_{1/2}} \big|_{r_p=0.878\text{fm}} = 205.9726 \text{ meV}, \tag{2}
\]

which deviates from the experimental Lamb shift of muonic hydrogen about 0.32 meV.

Many theoretical calculations \[5\], data analysis \[6\] and possible new mechanisms such as the three body physics \[7\], the new exotic particles interactions \[8\], the higher-order contribution of the finite size \[9\] etc., have been discussed to try to understand such discrepancy. And also new experiment of ep scattering is proposed in JLab \[10\]. Combining all these current analysis, briefly, the radius of proton is still not well understood.

For the muonic hydrogen, the energy transition of \( 2P_{3/2} \) and \( 2S_{1/2} \) usually are expressed as

\[
E^{Th}_{2P_{3/2}} - E^{Th}_{2S_{1/2}} = \Delta E_{Lamb}^{2S-2P} + \Delta E_{FS}^{2P} + \frac{3}{8}\Delta E_{HFS}^{2P_{3/2}} - \frac{1}{4}\Delta E_{HFS}^{2S}. \tag{3}
\]

In the literature, the contributions of the four terms are usually calculated by the perturbative theory. Using the quasipotential method in quantum electrodynamics \[11\], the contributions to the four terms can be expressed as \[1\, 12\, 14\]
\[
\begin{align*}
\Delta E_{2S-2P}^{2P} &= \Delta E_{\text{ovp}} + \Delta E_{KS} + \Delta E_{SE} + \Delta E_{QCD} - 5.2262 r_p^2 + 0.0347 r_p^3 \\
\Delta E_{2S}^{2P,\text{HFS}} &= \Delta E_{2P,\text{HFS}} + \Delta E_{2S,\text{AMM}}^{2P,\text{HFS}} + \Delta E_{2P,\text{other}}^{2S,\text{other}} \\
\Delta E_{2P_{3/2}}^{2P,\text{HFS}} &= \Delta E_{2P_{3/2},\text{HFS}} + \Delta E_{2P_{3/2},\text{AMM}}^{2P_{3/2},\text{AMM}} + \Delta E_{2P_{3/2},\text{other}}^{2P_{3/2},\text{other}} \\
\Delta E_{2P_{1/2}}^{2P,\text{F S}} &= \Delta E_{2P_{1/2},\text{F S}} + \Delta E_{2P_{1/2},\text{AMM}}^{2P_{1/2},\text{AMM}} + \Delta E_{2P_{1/2},\text{other}}^{2P_{1/2},\text{other}}
\end{align*}
\]

where \(\Delta E_{\text{ovp}}\) (205.0074 meV by the first order perturbative theory (1stPT) and 0.1509 meV by the second order perturbative theory), \(\Delta E_{KS}\) (1.5081 meV) and \(\Delta E_{SE}\) (−0.6677 meV) are the energy shifts due to the one-loop vacuum polarization, two-loop vacuum polarization and the sum of self-energy and muonic-vacuum polarization, correspondingly, \(\Delta E_{QED}\) (0.0586 meV) by the first order perturbative theory (1stPT) and 0.1509 meV by the second order perturbative theory).
meV) is the energy shift due to all further QED corrections, and the last two terms in $\Delta E^{2S-2P}_{\text{Lamb}}$ are relevant radius-dependent contributions, $\Delta E^{2S,B}_{\text{HFS}}$ (22.8054 meV), $\Delta E^{2P_{3/2},B}_{\text{HFS}}$ (3.392112 meV) and $\Delta E^{2P,B}_{\text{HFS}}$ (8.329150 meV) are the energy shifts due to the Breit potential without considering the proton size, $\Delta E^{2S,\text{AMM}}_{\text{HFS}}$ (0.0266 meV), $\Delta E^{2P_{3/2},\text{AMM}}_{\text{HFS}}$ (−0.00086 meV) and $\Delta E^{2P,\text{AMM}}_{\text{FS}}$ (0.017637 meV) are the corrections due to the anomalous magnetic moment of muon, $\Delta E^{2S,\text{other}}_{\text{HFS}}$, $\Delta E^{2P_{3/2},\text{other}}_{\text{HFS}}$ and $\Delta E^{2P,\text{other}}_{\text{FS}}$ are the other contributions.

Some of the above perturbative results have been checked by the nonperturbative numerical (NPnum) calculations, for example within the framework of the multiconfiguration Dirac-Fock (MCDF) method in [15] and shotting-like method using quad-precision Fortran in [16]. In this work, by using the Mathematica, we present another high precise NPnum calculations (much more precise than the quad-precision) on the energy shifts $E^{2S,B+\text{AMM}}_{\text{HFS}}$, $E^{2P_{3/2},B+\text{AMM}}_{\text{HFS}}$ and $E^{2P,B+\text{AMM}}_{\text{FS}}$ with considering the effects from the proton size. And as a comparison, also the calculation of $\delta E_{\text{ovp}}$ is presented.

\section{Formula and Numerical Method}

The One-loop Uehling potential and the general fine and hyperfine Breit potential including the effects from the proton size and the anomalous magnetic moment of muon can be expressed as [12, 17]

\begin{align*}
V_{\text{ovp}}(r) &= -\frac{\alpha^2}{\pi r} \int_1^\infty du e^{-2urm_e} \frac{u^2 - 1}{3u^4} \sqrt{(u^2 - 1)(2u^2 + 1)} \\
V_{\text{fs}}(r) &= \frac{\alpha}{2m_\mu^2} [(1 + 2\kappa_\mu) + \frac{2m_\mu}{m_p}(1 + \kappa_\mu)] \left( \frac{1}{r_3} + \frac{G_{fs}}{r^3} \right) \mathbf{L} \cdot \mathbf{S}_\mu \\
V_{\text{HFS}}^{\text{Swave}}(r) &= \frac{\alpha \mu_p \mu_\mu}{4r^3m_\mu m_p} \sigma_\mu \cdot \sigma_p \frac{m^3 r^3}{3} e^{-mr} \\
V_{\text{HFS}}^{\text{Pwave}}(r) &= \frac{\alpha \mu_p \mu_\mu}{4r^3m_\mu m_p} [(3\sigma_\mu \cdot \hat{r} \sigma_p \cdot \hat{r} (1 + h_1) - \sigma_\mu \cdot \sigma_p (1 + h_2)) \\
&\quad + 2\mathbf{L} \cdot \sigma_p (\frac{1 + h_3}{\mu_\mu} + \frac{m_\mu}{2m_p \mu_p \mu_\mu} h_4)]
\end{align*}

where

\begin{align*}
G_{fs} &= -(1 + \frac{\kappa_p}{(1 - k^2)^2}) e^{-mr} (1 + mr) - (1 + \frac{\kappa_p}{1 - k^2}) \frac{m^2}{2} r^2 e^{-mr} \\
&\quad + (1 - k^2)^2 e^{-mkr} (1 + mkr)
\end{align*}
\[
\begin{array}{|c|c|c|c|}
\hline
2S_{1/2}^{F=0} & -3 & -3 & 0 \\
\hline
2S_{1/2}^{F=1} & 1 & 1 & 0 \\
\hline
2P_{1/2}^{F=0} & -3 & 1 & -4 \\
\hline
2P_{1/2}^{F=1} & 1 & -\frac{1}{3} & \frac{4}{3} \\
\hline
2P_{3/2}^{F=2} & \frac{3}{5} & 1 & 2 \\
\hline
2P_{3/2}^{F=1} & -1 & -\frac{5}{3} & -\frac{10}{3} \\
\hline
\end{array}
\]

TABLE I: The contributions of the spin related operators to 2S and 2P states.

\[
h_1 = -e^{-mr}(1 + mr) - \frac{m^2r^2}{2}e^{-mr} - \frac{m^3r^3}{6}e^{-mr}
\]

\[
h_2 = -e^{-mr}(1 + mr) - \frac{m^2r^2}{2}e^{-mr} - \frac{m^3r^3}{2}e^{-mr}
\]

\[
h_3 = -e^{-mr}(1 + mr) - \frac{m^2r^2}{2}e^{-mr}
\]

\[
h_4 = (1 + 2\kappa_p)(1 + h_3) + \frac{\kappa_p}{(1 - k^2)^2}e^{-mr}(1 + mr) + \frac{\kappa_p}{1 - k^2} \frac{m^2r^2}{2}e^{-mr} - \frac{\kappa_p}{(1 - k^2)^2}e^{-mk}\]

with \(\alpha\) the fine-structure constant, \(\mu_p\) and \(\mu_\mu\) the anomalous magnetic moments of proton and muon, \(m\) the parameter in the electromagnetic form factors of proton which can be related with proton size as \(r_p^2 = \frac{12}{m^2}\), \(k = 2m_p/m\), \(m_e\), \(m_\mu\) and \(m_p\) the masses of electron, muon and proton. It should be pointed out that to include the effects from the proton size in the above Breit potential, the electromagnetic form factors of proton have been taken approximately as the special one as [17]. The contributions of spin related operators in the Breit potential to the 2S and 2P states are listed in Tab. I.

When the effects from the proton size are neglected in the above effective potentials (taking \(m \to \infty\)), the energy shifts by \(1^{st}\)PT reproduce the same \(E_{HFS}^{2S,B+AMM}\), \(E_{HFS}^{2P_{3/2},B+AMM}\) and \(E_{FS}^{2P,B+AMM}\) with those used in the literatures [13, 14]. The corrections from the proton structure in the above Breit potential is corresponding to replace the zero momentum transfer approximation by including the full \(q^2\) dependence of the electromagnetic form factors of
proton in the one photon exchange Feynman diagram. This is different with the corrections due to the proton structure discussed in [13, 14]. Since in this work our focus is on the difference between the results by 1stPT and NPnum calculation, we do not discuss the detail of the different treatments of the effects from the proton size.

In our numerical calculation, we use the shooting method to find out the energy spectrum by solving the reduced Schrödinger equations for $u(r)$ directly, with $u(r) = R(r)r$, $\psi(r) = R(r)Y(\theta, \phi)$ and $\psi(r)$ the wave function. In the detail, for muonic hydrogen we take approximately $u(r = 0) \approx u(r = 10^{-50} fm)$ and $u(r = \infty) \approx u(r = 10^6 fm)$ to simulate the behaviors of wave function at the boundary. We keep 200 digits of the numbers in the calculation and take the PrecisionGoal of NDSolve in Mathematica as 15, respectively. By these approximations, as a check we reproduce the energy spectrum of muonic hydrogen under the Coulomb potential with the precision better than $10^{-10}$ meV. Since the numerical calculation is based on the shooting method, the precision is not sensitive on the form of the potentials or the solutions, this is different with the basis expansion method or variational methods usually used, and ensures our numerical calculation reliable for the other potentials.

III. NUMERICAL RESULT

In Tab. II and III we present the results by the 1stPT and NPnum calculation including the effects from the proton size in the Breit potential. The corresponding results without considering the proton size by 1stPT and from the one-loop Uehling potential are also presented for comparison.

From the last two columns of Tab. II we see the results by 1stPT and NPnum calculations give about 0.15088 meV difference for $V_{ovp}$. Actually the second order perturbative calculation of $V_{ovp}$ gives the contribution about 0.1509 meV [12], so the combination of the first and second order perturbative calculation of $V_{ovp}$ is almost same with our NPnum calculation. When including the effects from the proton size and taking $r_p = 0.83112$ fm, 0.84184 fm, 0.878 fm as examples, the differences between the 1stPT and precise NPnum calculations are about $3 \times 10^{-4}$ and $2 \times 10^{-5}$ meV for the fine and hyperfine splitting of $2P$ states, respectively, and also these two splittings are almost independent on the proton size in the region $r_p \in [8.2, 9.0]$ fm. From the Tab. III we see the derivations of the 1stPT and NPnum calculation are about $-0.009$ and $0.02$ meV for the hyperfine splitting of $2S$ state.
TABLE II: Energy shifts of different potentials using perturbative and precise numerical calculations in meV where $1^{st}$PT and NPnum denote the first order perturbative and precise nonperturbative numerical calculation, respectively. The typical proton size $r_p = 0, 0.83112, 0.84184, 0.87800 \, fm$ are taken as examples for comparison. The results by $1^{st}$PT are same with those in \[12, 13\].

| $r_p (fm)$ | $\Delta E_{FS}^{2S}(F=1)$ | $\Delta E_{FS}^{2S}(F=0)$ | $\Delta E_{FS}^{2S}(F=0)/\Delta E_{FS}^{2S}(F=1)$ | $\Delta E_{FS}^{2S}$ |
|-------------|-----------------|-----------------|-----------------|-----------------|
| 0           | 5.70798         | 17.12394        | 3               | 22.83192        |
| 0.83112     | 5.67921         | 5.66943         | 17.03762        | 22.71683        |
| 0.84184     | 5.67884         | 5.66918         | 17.03651        | 22.71535        |
| 0.87800     | 5.67759         | 5.66832         | 17.03277        | 22.71036        |

TABLE III: Energy shifts of different potentials using perturbative and precise numerical calculations in meV. The notations are same with Tab. II. The results by $1^{st}$PT are same with those in \[14\].

$\Delta E_{HFS}^{2S}(F = 1)$ and $\frac{1}{4}\Delta E_{HFS}^{2S}$, respectively, which should not be omitted comparing with the precision of current experiments. We want to emphasize that by the NPnum calculation, the ratios $\frac{\Delta E_{HFS}^{2S}(F=0)}{\Delta E_{HFS}^{2S}(F=1)}$ are not strictly equal to 3 as predicted by the $1^{st}$PT, but are about 3.02 as showed in Tab. II and the absolute difference between $\Delta E_{HFS}^{2S}(F = 1)$ and $\frac{1}{4}\Delta E_{HFS}^{2S}$ are large. Such a discrepancy means the relation $\Delta E_{HFS}^{2S}(F = 1) = \frac{1}{4}\Delta E_{HFS}^{2S}$ is not suitable to be used as usual. To show the results in a more direct way, we use the polynomial of $r_p$ to fit the numerical results of $\Delta E_{HFS}^{2S}(F = 1)$ in the region $r_p \in [8.2, 9.0] \, fm$ by taking one point every 0.001 fm and the results are expressed as

\[
\begin{align*}
\Delta E_{HFS}^{2S}(F = 1, \text{NPnum}) &= 5.68008 - 0.00261343 r_p - 0.0122699 r_p^2 \, \text{meV} \\
\Delta E_{HFS}^{2S}(F = 1, \text{1st PT}) &= 5.70793 - 0.0346149 r_p + 0.0000613066 r_p^2 \, \text{meV}
\end{align*}
\]
with the residual mean square of the fitting as small as about $10^{-11}$ meV$^2$.

After including the difference of $\Delta E_{HF S}^2(F = 1)$ by our estimation, the theoretical energy shift Eq. (1) is changed as

$$E_{2p_{3/2}}^{Th} - E_{2s_{1/2}}^{Th} = 209.9869 - 5.2262r_p^2 + 0.0347r_p^3$$ \hspace{2cm} (7)$$

and if $r_p$ is taken as 0.878fm, then the modified $E_{2p_{3/2}}^{Th} - E_{2s_{1/2}}^{Th}$ is estimated as 205.9816 meV, which deviates from the experimental results about 0.31 meV. This means after using the precise NPnum calculation of $\Delta E_{HF S}^2(F = 1)$, the discrepancy of the measurement of the proton sized is reduced about 3%, while if we take the $\frac{1}{4}\Delta E_{HF S}^2$ as input then the energy shift Eq. (1) is changed as

$$E_{2p_{3/2}}^{Th} - E_{2s_{1/2}}^{Th} = 209.9579 - 5.2262r_p^2 + 0.0347r_p^3$$ \hspace{2cm} (8)$$

and if $r_p$ is taken as 0.878fm, then $E_{2p_{3/2}}^{Th} - E_{2s_{1/2}}^{Th}$ is estimated as 205.9526 meV, which deviates from the experimental results about 0.34 meV. We see the discrepancy will be intensified about 7%. The full results show we should be careful to deal with the splitting beyond the $1^{st}$ PT and should replace $\frac{1}{4}\Delta E_{HF S}^2$ by $\Delta E_{HF S}^2(F = 1)$ in our calculation.

According to Tab. I and Fig. I we also have

$$E_{2p_{3/2}}^{F = 1} - E_{2s_{1/2}}^{F = 0} = \Delta E_{HF S} - \frac{5}{8}\Delta E_{2p_{3/2}}^{2S} + \Delta E_{F S} + \frac{3}{4}\Delta E_{HF S}^2.$$ \hspace{2cm} (9)$$

and

$$\Delta E = (E_{2p_{3/2}}^{F = 1} - E_{2s_{1/2}}^{F = 0}) - (E_{2p_{3/2}}^{F = 2} - E_{2s_{1/2}}^{F = 1}) = \Delta E_{HF S} - \Delta E_{HF S}^{2p_{1/2}}.$$ \hspace{2cm} (10)$$

We note that $\Delta E$ depends on $\Delta E_{HF S}^2$ instead of $\Delta E_{HF S}^2(F = 1)$ appeared in $E_{2p_{3/2}}^{F = 2} - E_{2s_{1/2}}^{F = 1}$, so for $\Delta E$ the NPnum calculation gives relative larger corrections. We present the results of $\Delta E$ from the Breit potential by the two methods in Tab. IV. With the different proton radius as input, the differences of $\Delta E$ are about $10^{-3} \sim 10^{-2}$ meV. At present, the $E_{2p_{3/2}}^{F = 2} - E_{2s_{1/2}}^{F = 1}$ and $E_{2p_{3/2}}^{F = 1} - E_{2s_{1/2}}^{F = 0}$ transition frequency in muonic hydrogen have been both measured with very high accuracy \textsuperscript{2}, the experimental value of $\Delta E$ is about 19.56 meV. Our numerical results are different from the experimental value since we have not considered the other corrections beside Breit potential. However, our calculation implies the precise NPnum calculation is needed.
\[ \Delta E (\text{meV}) \]

| \( r_p (\text{fm}) \) | \( \Delta E (\text{meV}) \) |
|-----------------|-----------------|
| \( 0 \)        | 19.44070        |
| \( 0.83112 \)   | 19.32562        |
| \( 0.84184 \)   | 19.32414        |
| \( 0.87800 \)   | 19.31915        |

TABLE IV: The difference of \( 2S - 2P \) transition energy \( \Delta E \) of muonic hydrogen in meV with different radius of proton as input. The notations are same with Tab. II.

| \( r_p (\text{fm}) \) | \( E^{1S}_{\text{HFS}} (\text{kHz}) \) | \( E^{2S}_{\text{HFS}} (\text{kHz}) \) |
|-----------------|-----------------|-----------------|
| \( 0 \)        | 1420478.8       | 177559.8        |
| \( 0.83112 \)   | 1420440.1       | 1425769.6      |
| \( 0.84184 \)   | 1420439.6       | 1425700.8      |
| \( 0.87800 \)   | 1420438.0       | 1425481.1      |

TABLE V: Frequencies in kHz of hyperfine splitting \( E^{1S}_{\text{HFS}} \) and \( E^{2S}_{\text{HFS}} \) in hydrogen.

Since the obvious difference exists between the \( 1\text{st} \) PT and precise NPnum calculations of the hyperfine splitting of muonic hydrogen’s \( 2S \) state, we also present the similar comparison of the \( ep \) system in Tab. VII where the results show the calculation for the hyperfine splitting of \( S \) state in \( ep \) system by the \( 1\text{st} \) PT is also not good enough. Different with \( 1\text{st} \) PT, the results by the precise NPnum method are more sensitive on the proton size.

In a summary, by using shotting method in Mathematica we give a very high precise NPnum calculation for the energy shifts of the Breit potential including the effects from the proton size. Our results show that when taking into account the proton structure, the precise NPnum calculations give very small corrections to the hyperfine splitting of \( 2P_{3/2} \) and fine structure of \( 2P \) states, but give about \(-0.009 \text{ meV} \) and \(0.08 \text{ meV} \) differences for the hyperfine splitting \( \Delta E^{2S}_{\text{HFS}}(F = 1) \) and \( \Delta E^{2S}_{\text{HFS}} \) of muonic hydrogen with those usually used in the literatures by \( 1\text{st} \) PT. The similar properties are also found in the hydrogen case.
IV. ACKNOWLEDGMENTS

This work is supported by the National Sciences Foundations of China under Grant No. 11375044 and in part by the Fundamental Research Funds for the Central Universities under Grant No. 2242014R30012.

[1] Pohl R, et al., Nature 466, 213 (2010).
[2] Aldo Antognini, et al., Science 339, 417 (2013).
[3] Mohr P J, Taylor B N, Newell D B, Rev. Mod. Phys. 84, 1527 (2012).
[4] Sarely G. Karshenboim, Phys. Rep. 422, 1 (2005).
[5] E. Borie, Annals of Physics 327, 733 (2012).
[6] C. Adamuscin, S. Dubnicka, and A. Z. Dubnickova, Prog. Part. Nucl. Phys. 67, 479 (2012); I. Sick, Prog. Part. Nucl. Phys. 67, 473 (2012).
[7] Jean-Philippe Karr, Laurent Hilico, Phys. Rev. Lett. 109, 103401 (2012).
[8] Vernon Barger, Cheng-Wei Chiang, Wai-Yee Keung, Danny Marfatia, Phys. Rev. Lett. 106, 153001 (2011).
[9] Sarely G. Karshenboim, Phys. Rev. D 90, 053012 (2014).
[10] Ashot Gasparian, EPJ Web Conf. 73, 07006 (2014).
[11] R. N. Faustov, A. P. Martynenko, Teor. Math. Phys. 64, 765 (1985); R. N. Faustov, A. P. Martynenko, JETP 88, 672 (1999).
[12] U. D. Jentschura, Annals. Phys. 326, 500 (2011).
[13] A. P. Martynenko, Phys. Rev. A 71, 022506 (2005).
[14] A. P. Martynenko, Phys. Atomic Nuclei. 71, 125 (2008).
[15] P. Indelicato, Phys. Rev. A 87, 022501 (2013).
[16] J. D. Carroll, A. W. Thomas, J. Rafelski, G. A. Miller, Phys. Rev. A 84, 012506 (2011).
[17] N.G.Kelkar, F. Garcia Daza, M. Nowakowski, Nucl. Phys. B 864, 382(2012).