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The Muonic Helium Atom in CFHHM

R. Krivec[1], V.B. Mandelzweig[2]

[1] Department of Theoretical Physics, J. Stefan Institute, PO Box 3000, 1001 Ljubljana, Slovenia

[2] Racah Institute of Physics, Hebrew University, Jerusalem 91904, Israel

Abstract. The properties of the ground states of the muonic Helium atoms $e\mu\,{}^4\mathrm{He}^{2+}$ and $e\mu\,{}^3\mathrm{He}^{2+}$ have been calculated nonvariationally. In particular, the hyperfine splitting has been evaluated, including all relativistic and other corrections. The obtained theoretical precision is much larger than the discrepancies resulting from different versions of expressions for corrections, implying that the latter have to be reexamined before further comparison is possible.

To obtain precisely the wave function Ψ in both singular and nonsingular regions, we used the correlation function hyperspherical harmonic method (CFHHM), separating $\Psi = e^f\phi$ where e^f contains the cusps and the factor ϕ is expanded in the hyperspherical harmonic (HH) basis up to the maximum global angular momentum K_m, containing $N = (K_\mathrm{m}/2+1)(K_\mathrm{m}/2+2)/2$ functions.

Due to the two-scale nature of the muonic Helium the main difficulty was to find a nonlinear correlation function f [1] yielding stable results for a range of parameters: in the odd-man-out notation, $f = \sum_{i=1}^{3}\left[a_i + (b_i - a_i)e^{-r_i/(n_i\overline{r_i})}\right]r_i$,

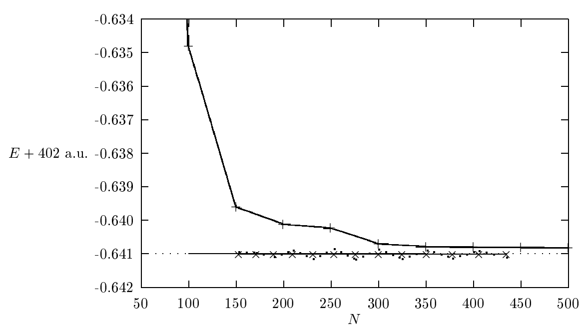

Figure 1. Convergence of $e\mu\,{}^4\mathrm{He}^{2+}$ ground state energy with basis size N for CFHHM [2] ("×": $\langle H\rangle$; "...": eigenvalue) and stochastic variational method (SVM) ("+")

Table 1. Comparison of HFS values for the ground state of muonic ^{4}He atom (MHz). The lowest order HFS is [5] $\nu_{\rm HF} = (8/3)\pi\alpha^2(m_e/m_\mu)\langle\delta(\mathbf{r}_{e-\mu})\rangle$. Corrections are given as $\nu = \nu_{\rm HF} f_{\rm corr} = \nu_{\rm HF} + \nu_{\rm corr}$. CFHHM $\langle\delta(\mathbf{r}_{e-\mu})\rangle$ values are from ref. [2]

Source	$\langle\delta(\mathbf{r}_{e-\mu})\rangle$	$\nu_{\rm HF}$	ν	$f_{\rm corr}$	$\nu_{\rm corr}$
Exp. [13]			4464.95(6)		
Exp. [14]			4465.004(29)		
Chen [6]		4454.181(1)	4464.907(1)	1.0024081	10.726[a]
CFHHM		4454.204(3)	4464.930(3)	1.0024081	10.726[b]
CFHHM	.3137622(2)	4454.206(3)	4464.982(3)	1.0024193	10.776[c]
CFHHM	.3137622(2)	4454.207(3)	4464.**983**(3)	1.0024193	10.776[d]
Smith [4]	.3137630(1)		4464.559(1)		[e]
	.3137630(1)	4454.226(1)			[f]
CFHHM	.3137621(2)	4454.213(3)			[g]
CFHHM	.3137621(2)	4454.213(3)	4464.**989**(3)	1.0024193	10.776[h]
CFHHM	.3137621(2)	4454.213(3)	4464.939(3)	1.0024081	10.726[i]
Ref. [15]			4464.8		

[a] $f_{\rm corr}$ derived from ref. [6]. Correct recoil (0.8004 MHz) is used (see [15, 6])

[b] Masses and α from ref. [6]

[c] $f_{\rm corr}$ via formulas of ref. [5], but the recoil correction by refs. [6, 15] (0.800 MHz). Masses: refs. [11, 5]; α: ref. [2] (differs from Huang's); $\nu_{\rm HF}$ by CFHHM

[d] As [c], but using Huang's value of α [5]. This multiplies $\nu_{\rm HF}$ of [c] by 1.00000011

[e] $\langle\delta(\mathbf{r}_{e-\mu})\rangle$ of ref. [4] times 14229.08 (ref. [4], containing all corrections?)

[f] $\langle\delta(\mathbf{r}_{e-\mu})\rangle$ of ref. [4] times 14196.1472 (masses of ref. [4], our α value)

[g] CFHHM $\langle\delta(\mathbf{r}_{e-\mu})\rangle$, using masses of ref. [4] (α not quoted), times 14196.1472, as in [f]

[h] As in [g], but $f_{\rm corr} = 1.0024193$ (not sensitive to masses of refs. [11, 5] or [4])

[i] As in [h], but using $f_{\rm corr}$ of ref. [6]

where particles $\{1,2,3\}$ correspond to the electron, the muon and He^{2+}; e.g., r_3 is the distance between the electron and the muon. b_i are the cusp factors; the constants $\overline{r_i}$ represent the equilibrium distances of the particles in the i–th pair: $\overline{r_1} = 0.0037$ a.u., $\overline{r_2} = \overline{r_3} = 1.5$ a.u.. The optimized values of the free parameters are $a_3 = -4$, $n_3 = 0.5$ in both $e\mu\,^4\mathrm{He}^{2+}$ and $e\mu\,^3\mathrm{He}^{2+}$ [2, 3].

The acceleration of convergence with respect to the linear cusp f ($a_i = b_i$) is as follows: at $K_{\rm m} = 56$ the error of energy is less than 1×10^{-7} a.u. instead of 0.002 a.u.; the error of $\nu_{\rm HF}$ is reduced from 440 MHz to 1 MHz.

Interpolating the doubly-convergent expectation values of operators as functions of $K_{\rm m}$ decreases the errors by additional 2–3 orders of magnitude.

With $N = 435$ we obtain the ground state energy -402.64101534 a.u., which is lower than most variational values, but may depend slightly on the roundoff errors in mass value manipulations. The rate of convergence is faster than in the SVM method (Fig. 1).

Table 2. Lowest order and total HFS of the ground state of $e\mu\,{}^3\mathrm{He}^{2+}$ (MHz). $\nu_{\mathrm{HF}} = \omega^{(e\mu)}\langle\delta(\mathbf{r}_{e-\mu})\rangle + \omega^{(e)}\langle\delta(\mathbf{r}_{{}^3\mathrm{He}-e})\rangle$

Source	$\nu_{\mathrm{HF}}^{(e\mu)}$	$\nu_{\mathrm{HF}}^{(e)}$	ν_{HF}	ν
Exp. (see [9])				4166.3(2)
CFHHM [3]	3339.830(3)	817.861(1)	4157.691(3)	4166.571(3)[a]
CFHHM [3]	3339.82(1)	817.859(5)	4157.68(1)	4166.56(1)[b]
Ref. [4]	3347.585	767.2	4166.34	[c,d]
	3339.837(1)	817.849(0)	4157.685(1)	[e]
Ref. [7]			4164.9(3.0)	[f]
Ref. [8]	3339.78(5)	817.85(5)	4157.623	[g]
Ref. [6]	3339.8037(5)	817.8558(5)	4157.659(1)	4166.620(1)[h]
Ref. [9]	3339.8037	817.8558	4157.6595	4166.540(5)[i]

[a] Mass set I (ref. [4]). Error estimate based on $n_3 = 0.5, 0.7$; $a_3 = -4, -5$. $\alpha = 1/137.0359895$, other constants from ref. [8], see below. $\omega^{(e\mu)}$, $\omega^{(e)}$: 10647.110, 2550.926 MHz/a.u.. The correction factors of ref. [9] are used (see [i])

[b] As [a], but mass set II (close to [8]) and a less precise calculation. $\omega^{(e\mu)}$, $\omega^{(e)}$: see [g]

[c] $\omega^{(e\mu)}$, $\omega^{(e)}$ quoted [4]: 10671.81, 0.2393 MHz/a.u. (see also ref. [10])

[d] Quoted $\langle\delta(\mathbf{r}_k)\rangle$, $\omega^{(e\mu)}$, $\omega^{(e)}$ lead to 4114.801 MHz

[e] $\langle\delta(\mathbf{r}_k)\rangle$ of ref. [4], $\omega^{(e\mu)}$, $\omega^{(e)}$ of the present work. Errors inferred from [4]

[f] $m_\mu = 206.7686$ a.u., 1 a.u. $= 6.579684 \times 10^9$ MHz, $\alpha = 1/137.0360$, etc.

[g] Masses as in set II (m_μ, a.m.u.: ref. [11]), except $m_{{}^3\mathrm{He}} = 3.01602970$ a.m.u.; $m_\mu = 105.65946$ MeV (Erratum, ref. [12]); $\alpha = 1/137.03604$, 1 a.u. $= 6.57968413 \times 10^9$ MHz, $\mu_{\mathrm{n}} = 0.00115873\mu_{\mathrm{B}}$, $\omega^{(e\mu)}$, $\omega^{(e)}$: 10647.085, 2550.924 MHz/a.u.

[h] As in [f]. Correction factors are 1.002408, 1.001123

[i] As in [f]. Correction factors are 1.002408, 1.001025 (different from ref. [6])

The f described enabled us to obtain expectation values of singular operators better than in the literature. In particular the difference $\langle\delta(\mathbf{r}_2)\rangle - \langle\delta(\mathbf{r}_3)\rangle$ is smaller by about 6×10^{-6} a.u. in ref. [4] than in our work, while the effects of mass choice and of our computational error on $\langle\delta(\mathbf{r}_2)\rangle$, $\langle\delta(\mathbf{r}_3)\rangle$ are both smaller, i.e., of the order of 2×10^{-7} a.u. [2].

Tables 1 and 2 and Fig. 2 show the discrepancies in the values of the lowest-order hyperfine splitting (HFS) as well as the correction factors in the literature. The CFHHM values using Huang et al. [5] values for the corrections, except their recoil term which is claimed to be wrong [6] (see Table 1), agree with the more recent $e\mu\,{}^4\mathrm{He}^{2+}$ experiment. If the more recent Chen et al. [6] values of corrections are used, the CFHHM values agree only with the less precise experiment. Overall, the CFHHM values agree better with experiment than any other in the literature, in particular by Chen et al. [6]. The agreement in the $e\mu\,{}^3\mathrm{He}^{2+}$ case is less good but the same trend towards smaller values when using masses and corrections according to ref. [6] is observed.

The theoretical errors are larger than the dependence on fundamental constants but much smaller than the discrepancies between results using different

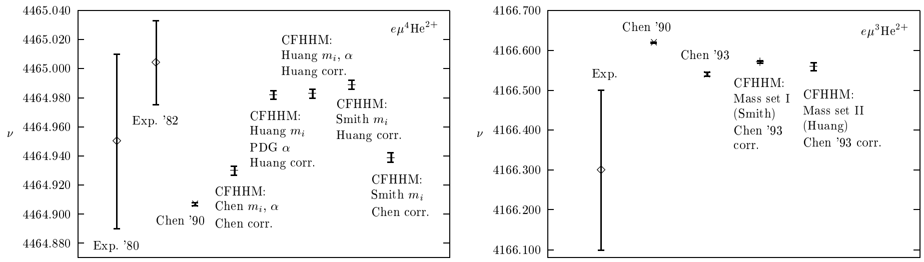

Figure 2. Comparison of theoretical and experimental results for muonic ^{4}He and ^{3}He; from Tables 1 and 2, respectively

expressions for correction terms. We conclude that the corrections need to be reevaluated before further comparison with experiment will be possible.

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References

1. M.I. Haftel, R. Krivec, V.B. Mandelzweig: J. Comp. Phys. **123**, 149 (1996)
2. R. Krivec, V.B. Mandelzweig: Phys. Rev. **A56**, 3614 (1997)
3. R. Krivec, V.B. Mandelzweig: Phys. Rev. **A57**, 4976 (1998)
4. V.H. Smith, A.M. Frolov: J. Phys. B: At. Mol. Phys. **28**, 1357 (1995)
5. K.-N. Huang, V.W. Hughes: Phys. Rev. **A20**, 706 (1979); Phys. Rev. **A21**, 1071 (1980)
6. M.-K. Chen: J. Phys. B: At. Mol. Phys. **23**, 4041 (1990)
7. S.D. Lakdawala, P.J. Mohr: Phys. Rev. **A24**, 2224 (1981)
8. M.-K. Chen, C.-S. Hsue: J. Phys. B: At. Mol. Phys. **22**, 3951 (1989)
9. M.-K. Chen: J. Phys. B: At. Mol. Phys. **26**, 2263 (1993)
10. R.J. Drachman: J. Phys. B: At. Mol. Phys. **16**, L749 (1983)
11. K.-N. Huang: Phys. Rev. **A15**, 1832 (1977)
12. M.-K. Chen, C.-S. Hsue: Phys. Rev. **A40**, 5520 (1989); Phys. Rev. **A42**, 1830E (1990)
13. H. Orth et al.: Phys. Rev. Lett. **45**, 1483 (1980)
14. C.J. Gardner et al.: Phys. Rev. Lett. **48**, 1168 (1982)
15. M.Ya. Amusia, M.Ju. Kuchiev, V.L. Yakhontov: Yad. Fiz. **47**, 877 (1988)