# Nonvariational calculation of the hyperfine splitting and other properties of the ground state of the muonic $^3$He atom

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The properties of the ground state of the muonic helium atom $e\mu\ ^3\mathrm{He}^{2+}$ have been calculated nonvariationally, using the correlation function hyperspherical harmonic method utilizing a nonlinear parametrization of the correlation function. The parametrization is similar to the one used in an earlier paper for $e\mu\ ^4\mathrm{He}^{2+}$ but the differences in the convergence were found to be important for the choice of optimal parameters. The parametrization is especially suited to accelerate the convergence of singular operators. As a result, the obtained expectation values of the $\delta(\mathbf{r}_k)$ operators have error margins smaller than the differences in the literature. The lowest-order hyperfine splitting, which depends on the fine structure constant and on the magnetic moment of the $^3\mathrm{He}^{2+}$ nucleus, is compared with values in the literature. [S1050-2947(98)11106-X]

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This paper, which deals with the system $e\mu\ ^3\mathrm{He}^{2+}$, is a continuation of Ref. [1], which deals with the system $e\mu\ ^4\mathrm{He}^{2+}$. In this work the main objective is the computation of the lowest-order hyperfine splitting, which is given by the equation [2]

TABLE I. Eigenvalues and expectation values of the Hamiltonian for the parametrization $A$ ($a_3=-5$, $n_3=0.5$), $(z_U, p_W, T_z)=(700, 100, 0.05)$, and mass set I [6]. The matrix elements were calculated using the same parameters as in Ref. [1]. The subseries with $K_m/2$ even and odd are displayed separately in the first and second parts of the table. The third part displays the final values obtained from the convergence of the interpolated values, as well as final values corresponding to additional parametrizations. The fourth part compares values for the mass set II.

| $K_m$ | $-E$ | $-\langle H\rangle$ |
|---|---|---|
| 48 | 399.042412541 | 399.042 336 819 |
| 52 | 399.042400861 | 399.042 336 819 |
| 56 | 399.042388694 | 399.042 336 830 |
| 50 | 399.042259133 | 399.042 336 810 |
| 54 | 399.042272833 | 399.042 336 810 |
| CFHHM | | 399.042 336 830 24[a] |
| | | 399.042 336 809 27[a,b] |
| | | 399.042 336 793 32[a,c] |
| Ref. [6] | | 399.042 336 832 8585 |
| CFHHM | | 399.048 293 0499[d] |
| Ref. [2] | | 399.048 222 312 2257[e,f] |
| Ref. [6] | | 399.048 295 018 0752[e,g] |

[a]The lowest noninterpolated value is taken.
[b]$a_3=-4$, $n_3=0.5$, $z_U=700$.
[c]$a_3=-4$, $n_3=0.7$, $z_U=900$.
[d]Mass set II.
[e]Masses as in set II except $m_{^3\mathrm{He}}=3.016\,029\,70$ a.m.u.
[f]$m_\mu$ actually 105.65946 MeV (see erratum, Ref. [12]).
[g]Refs. [6,2] agree well if using the same $m_\mu$, see Ref. [6].

$$\nu_{\mathrm{HF}}=\nu_{\mathrm{HF}}^{(e\mu)}+\nu_{\mathrm{HF}}^{(e)},$$

where

$$\nu_{\mathrm{HF}}^{(e\mu)}=2\pi\alpha^2\frac{m_e}{m_\mu}\langle\delta(\mathbf{r}_{e\text{-}\mu})\rangle=\omega^{(e\mu)}\langle\delta(\mathbf{r}_{e\text{-}\mu})\rangle,$$

$$\nu_{\mathrm{HF}}^{(e)}=2\pi\alpha^2\mu_n\langle\delta(\mathbf{r}_{^3\mathrm{He}\text{-}e})\rangle=\omega^{(e)}\langle\delta(\mathbf{r}_{^3\mathrm{He}\text{-}e})\rangle,$$

$\mu_n$ being the magnetic moment of the $^3\mathrm{He}^{2+}$ nucleus. $r_{e\text{-}\mu}$ ($r_{^3\mathrm{He}\text{-}e}$) is the electron-muon (electron-nucleus) separation, respectively, and $\langle\delta(\mathbf{r}_{e\text{-}\mu})\rangle$ ($\langle\delta(\mathbf{r}_{^3\mathrm{He}\text{-}e})\rangle$) are the corresponding expectation values calculated with the help of the spatial part of the wave function. We compare our results with the values in the literature, which exhibit rather large discrepancies [2–6]. For this reason, we did not include the recoil, relativistic, and radiative corrections, and consequently the comparison with experiment (cf. Ref. [2]).

From the computational standpoint, the aim of this paper is to check the applicability of the optimal parametrization of the CFHHM correlation function for the system $e\mu\ ^4\mathrm{He}^{2+}$ on a system with a different mass of one of the particles.

We used the correlation function hyperspherical harmonic method (CFHHM) [7,8]. The wave function is decomposed

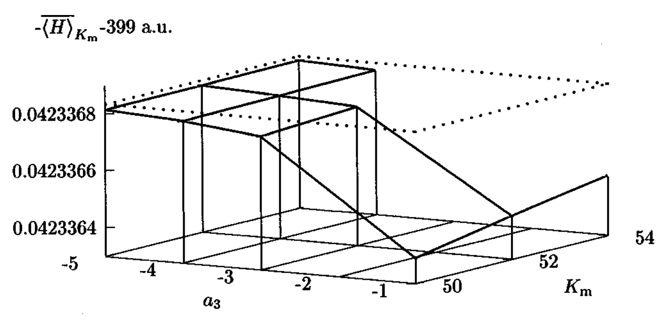


FIG. 1. Convergence of $\overline{-\langle H\rangle_{K_m}}-399$ a.u. with $K_m$ and $a_3$ for the parametrization $A$ with $n_3=0.5$; $z_U=700$. Masses of Ref. [6] are used. The dotted rectangle is the value from Ref. [6].

 

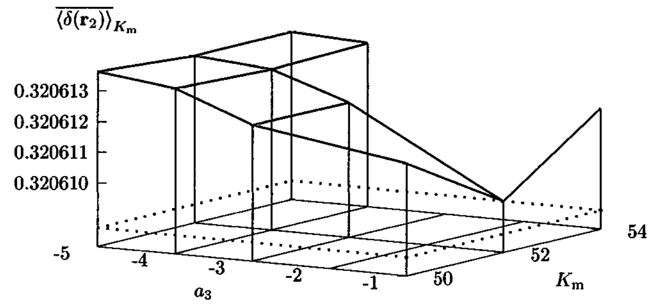


FIG. 2. As in Fig. 1, but showing the values of $\overline{\langle\delta(\mathbf{r}_2)\rangle}_{K_m}$ (a.u.). Values of $\overline{\langle\delta(\mathbf{r}_2)\rangle}_{K_m}$ for $a_3=-6$ and $K_m=34-40$ indicate divergence from the plateau in the figure.

as $\Psi=e^f\phi$, where $f$ is the correlation function and $\phi$ is a smooth function expandable in hyperspherical harmonics. The nonlinear parametrization of $f$ denoted by ''$A$'' is of the form [1]:

$$f=b_1r_1+b_2r_2+[a_3+(b_3-a_3)e^{-r_3/(n_3\overline{r_3})}]r_3.$$

The particles {1,2,3} correspond to $\{e,\mu,{}^3\mathrm{He}^{2+}\}$; in the odd-man-out notation $r_{e\text{-}\mu}=r_3$, $r_{^3\mathrm{He}\text{-}e}=r_2$. $b_i$ are the precise values of the cusp parameters [$\approx(-398.5,-2.000,0.9952)$ for the masses of Ref. [6]]. $\overline{r_1}=0.0037$ a.u., $\overline{r_2}=\overline{r_3}=1.5$ a.u. are constants equal to average particle pair distances. The same values as in Ref. [1] were used, although in the present case $\overline{r_1}$ is about 0.0038 a.u., so $n_3$ will tend to be proportionally larger. (In practice such minor changes have negligible effects.)

Parametrization $A$ employs the weak coupling of the electron and muon and regularizes the $e$-$\mu$ term, which in the cusp parametrization ($a_3=b_3$) would be non-negative and cause slow convergence [1,8].

$a_3$ and $n_3$ are free parameters. To find their optimal values, an extended region of parameter space including the values of Ref. [1] was investigated.

Due to the non-Hermitian property [9] of the effective potential $\overline{W}$ appearing in the equation for $\phi$, the expectation value $\langle H\rangle$ represents the energy value.

The CFHHM system of differential equations is truncated at a maximum value $K_m$ of the global angular momentum $K=0,2,4,\ldots,K_m$ [8]. The hyperradial interval $[0,z_U]$, where $z_U=2\sqrt{2E}\rho_U$, $E$ is the eigenvalue, and $\rho_U$ is the maximum value of the hyperradius, is subdivided using the

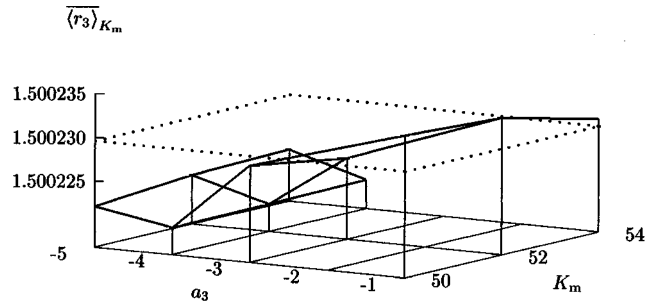


FIG. 4. As in Fig. 1, but showing the values of $\overline{\langle r_3\rangle}_{K_m}$ (a.u.).

parameter $T_z$ [8] in a sequence of subintervals $[z_i,z_{i+1}]$ of increasing length equal to $z_iT_z$. The matrix $\overline{W}$ is expanded in powers $\rho^p$, $p=-1,0,\ldots,p_W$.

The expectation values of operators except $\langle H\rangle$ converge in two subsequences determined by whether $K_m/2$ is even or odd [1], approaching the limit from different sides. The interpolated sequence $\overline{\langle\mathcal{O}\rangle}_{K_m}$ converges about two orders of magnitude faster [1]:

$$\overline{\langle\mathcal{O}\rangle}_{K_m}=\frac{1}{2}\left[\langle\mathcal{O}\rangle_{K_m}+\frac{1}{2}(\langle\mathcal{O}\rangle_{K_m-2}+\langle\mathcal{O}\rangle_{K_m+2})\right].$$

We use the following two sets of mass values:

(i) Set I: the set of Ref. [6]: $m_\mu=206.768262$ a.u., $m_{^3\mathrm{He}}=5495.8852$ a.u. (ion mass).

(ii) Set II: $m_e=0.5110034$ MeV (1 a.u.), $m_\mu=105.65948$ MeV (206.76864 . . . a.u.), 1 a.m.u. $=931.5016$ MeV [10,11], together with the $^3$He atomic mass $m_{^3\mathrm{He}}=3.01602930\times931.5016=5497.88145\ldots$ MeV.

(Note: Refs. [2,12] list the following values: $m_\mu=105.65948$ MeV; $m_{^3\mathrm{He}}=3.0160297\times931.5016$ MeV. It seems that the value of $m_\mu$ corrected to 105.65946 MeV in the erratum of [12] applies also to Ref. [2]; see Refs. [6,13].)

To calculate $\nu_{\mathrm{HF}}$ (Table V), $\alpha=1/137.035\,9895$ [14] and $\mu_n=0.001\,158\,73\mu_{\mathrm{B}}$ [2] are used.

If the $^3\mathrm{He}^{2+}$ mass is increased by $4\times10^{-7}$ a.u. and the muon mass is decreased by $4\times10^{-5}$ a.u., the energy is higher by $7\times10^{-5}$ a.u. (Table I). As was shown in Ref. [1], this is entirely due to the muon mass change.

Our value of $\langle H\rangle$ for mass set I differs from the variational value [6] by $0.3\times10^{-8}$ a.u. (Fig. 1, Table I), which may be due to different manipulations of the mass values.

The dependence of $\nu_{\mathrm{HF}}$ on the precise value of the $^3\mathrm{He}^{2+}$ ion mass is small, but may become significant if one uses the atom mass instead of the ion mass: in Ref. [1] it is estimated

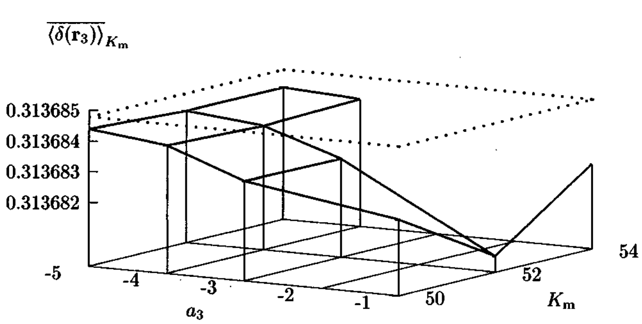


FIG. 3. As in Fig. 1, but showing the values of $\overline{\langle\delta(\mathbf{r}_3)\rangle}_{K_m}$ (a.u.).

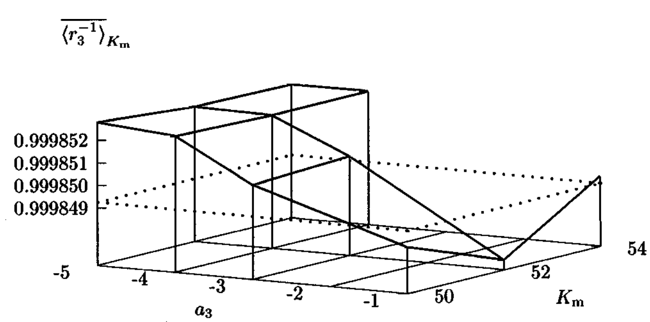


FIG. 5. As in Fig. 1, but showing the values of $\overline{\langle r_3^{-1}\rangle}_{K_m}$ (a.u.).

TABLE II. As in Table I, but expectation values of functions of $\mathbf{r}_1=\mathbf{r}_{\mu\text{-}^3\mathrm{He}}$. The numbers in parentheses are uncertainties defined as the differences of the interpolated values for the last two values of $K_m$. They show the degree of convergence for fixed $n_3$, $a_3$ but not the final error estimates. The values for the mass set II are calculated for the nonoptimal choice $a_3=-4$, $n_3=0.7$ where the $K_m$ dependence is stronger.

| $K_m$ | $\langle r_1^{-2}\rangle$ (units of $10^{-3}$) | $\langle r_1^{-1}\rangle$ | $\langle \delta(\mathbf{r}_1)\rangle$ (units of $10^{-6}$) | $\langle r_1\rangle$ (units of $10^3$) | $\langle r_1^2\rangle$ (units of $10^6$) |
|---|---|---|---|---|---|
| 48 | 317.677 7433 | 398.544 4227 | 20.149 9523 | 3.763 7138 | 18.887 3927 |
| 52 | 317.677 7256 | 398.544 4107 | 20.149 9509 | 3.763 7139 | 18.887 3937 |
| 56 | 317.677 7042 | 398.544 3969 | 20.149 9491 | 3.763 7140 | 18.887 3949 |
| 50 | 317.677 4165 | 398.544 2294 | 20.149 9222 | 3.763 7153 | 18.887 4068 |
| 54 | 317.677 4376 | 398.544 2434 | 20.149 9239 | 3.763 7152 | 18.887 4056 |
| CFHHM | 317.677 5763(1) | 398.544 323 60(5) | 20.149 936 96(2) | 3.763 714 575(2) | 18.887 399 95(2) |
| Ref. [6] | | 398.542 397 61 | 20.149 938 8565 | 3.763 715 066 | 18.887 401 85 |
| CFHHM | 317.687 070(4) | 398.550 279(2) | 20.150 8403(3) | 3.763 658 34(2) | 18.886 835 5(2)[a] |
| Ref. [2] | | | | 3.763 659 486 41[b] | |

[a]CFHHM values computed using mass set II.
[b]See footnotes e,f of Table I.

TABLE III. As in Table II, but expectation values of functions of $\mathbf{r}_2=\mathbf{r}_{^3\mathrm{He}\text{-}e}$.

| $K_m$ | $\langle r_2^{-2}\rangle$ | $\langle r_2^{-1}\rangle$ | $\langle \delta(\mathbf{r}_2)\rangle$ | $\langle r_2\rangle$ | $\langle r_2^2\rangle$ |
|---|---|---|---|---|---|
| 48 | 2.000 1188 | 0.999 9839 | 0.320 6909 | 1.500 0286 | 3.000 1192 |
| 52 | 2.000 0457 | 0.999 9635 | 0.320 6768 | 1.500 0611 | 3.000 2524 |
| 56 | 1.999 9762 | 0.999 9439 | 0.320 6635 | 1.500 0912 | 3.000 3656 |
| 50 | 1.999 3392 | 0.999 7610 | 0.320 5434 | 1.500 3874 | 3.001 5428 |
| 54 | 1.999 4076 | 0.999 7801 | 0.320 5566 | 1.500 3588 | 3.001 4407 |
| CFHHM | 1.999 7093(3) | 0.999 8669(1) | 0.320 613 38(2) | 1.500 2175(4) | 3.000 875(3) |
| Ref. [6] | | 0.999 863 851 | 0.320 608 57 | 1.500 223 659 | 3.000 907 793 |
| CFHHM | 1.999 71(1) | 0.999 866(3) | 0.320 613(2) | 1.500 220(5) | 3.000 89(2)[a] |
| Ref. [2][b] | | | 0.320 6116(2)[c] | 1.500 223 567 91 | |

[a]See footnote a of Table II.
[b]See footnote b of Table II.
[c]Calculated from the published $\nu_{\mathrm{HF}}^{(e)}$.

TABLE IV. As in Table II, but expectation values of functions of $\mathbf{r}_3=\mathbf{r}_{e-\mu}$.

| $K_m$ | $\langle r_3^{-2}\rangle$ | $\langle r_3^{-1}\rangle$ | $\langle \delta(\mathbf{r}_3)\rangle$ | $\langle r_3\rangle$ | $\langle r_3^2\rangle$ |
|---|---|---|---|---|---|
| 48 | 1.999 5591 | 0.999 9693 | 0.313 7600 | 1.500 0346 | 3.000 1368 |
| 52 | 1.999 4861 | 0.999 9489 | 0.313 7463 | 1.500 0670 | 3.000 2700 |
| 56 | 1.999 4166 | 0.999 9293 | 0.313 7333 | 1.500 0971 | 3.000 3832 |
| 50 | 1.998 7799 | 0.999 7464 | 0.313 6157 | 1.500 3934 | 3.001 5604 |
| 54 | 1.998 8482 | 0.999 7655 | 0.313 6286 | 1.500 3647 | 3.001 4583 |
| CFHHM | 1.999 150(1) | 0.999 8523(1) | 0.313 684 212(4) | 1.500 223 4(4) | 3.000 892(2) |
| Ref. [6] | | 0.999 849 2590 | 0.313 6848 | 1.500 229 562 | 3.000 925 384 |
| CFHHM | 1.999 15(1) | 0.999 852(2) | 0.313 684(1) | 1.500 225(4) | 3.000 91(2)[a] |
| Ref. [2][b] | | | 0.313 682 45(5)[c] | 1.500 229 470 75 | |

[a]See footnote a of Table II.
[b]See footnote b of Table II.
[c]Calculated from the published $\nu_{\mathrm{HF}}^{(e\mu)}$.

TABLE V. Comparison of the values of the lowest order hyperfine splitting in the literature. Different values of fundamental constants are used.

| $K_m$ | $\nu_{\mathrm{HF}}^{(e\mu)}$ | $\nu_{\mathrm{HF}}^{(e)}$ | $\nu_{\mathrm{HF}}$ |
|---|---|---|---|
| Present work | 3339.830(3) | 817.861(1) | 4157.691(3)[a] |
| Ref. [6] | 3347.585 | 767.2 | 4166.34[b,c] |
| | 3339.837(1) | 817.849(0) | 4157.685(1)[d] |
| Ref. [3] | | | 4164.9(3.0)[e] |
| Ref. [2] | 3339.78(5) | 817.85(5) | 4157.623[f] |
| Ref. [4] | 3339.8037(5) | 817.8558(5) | 4157.659(1)[f] |
| Ref. [5] | 3339.8037 | 817.8558 | 4157.6595[f] |

[a]Mass set I. Error estimate based on $n_3=0.5$, 0.7; $a_3=-4,-5$. $\alpha=1/137.035\,9895$, other constants from Ref. [2], see below. $\omega^{(e\mu)}$, $\omega^{(e)}$: 10647.110, 2550.926 MHz/a.u.

[b]$\omega^{(e\mu)}$, $\omega^{(e)}$ quoted [6]: 10671.81, 0.2393 MHz/a.u. (see also Ref. [15]).

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

[d]$\langle\delta(\mathbf{r}_k)\rangle$ of Ref. [6], $\omega^{(e\mu)}$, $\omega^{(e)}$ of the present work. Errors inferred from the number of digits quoted for $\langle\delta(\mathbf{r}_k)\rangle$.

[e]$m_\mu=206.7686$ a.u., 1 a.u. $=6.579684\times10^9$ MHz, $\alpha=1/137.0360$, etc.

[f]See footnotes e,f of Table I; $\alpha=1/137.03604$, 1 a.u. $=6.579\,684\,13\times10^9$ MHz, $\mu_n=0.001\,158\,73\mu_{\mathrm{B}}$, $\omega^{(e\mu)}$, $\omega^{(e)}$: 10647.085, 2550.924 MHz/a.u.

that increasing the ion mass by 2 a.u. (mass set II versus set I) increases $\langle\delta(\mathbf{r}_3)\rangle$ by $3\times10^{-7}$ a.u., which changes the hyperfine splitting by several times 0.001 MHz. In contrast, the muon mass difference between sets I and II (0.0004 a.u.) should decrease the $\langle\delta(\mathbf{r}_2)\rangle$, $\langle\delta(\mathbf{r}_3)\rangle$ values by $5\times10^{-7}$ a.u. [1]. This cancellation is seen in the CFHHM values (Tables III and IV).

For the two variational calculations, Refs. [6] (mass set I) and [2] (close to mass set II), such cancellation is not apparent as they differ by $3\times10^{-6}$ a.u. in both $\langle\delta(\mathbf{r}_2)\rangle$ and $\langle\delta(\mathbf{r}_3)\rangle$. Interestingly, $\langle\delta(\mathbf{r}_2)\rangle$ and $\langle\delta(\mathbf{r}_3)\rangle$ deviate in opposite directions: $\langle\delta(\mathbf{r}_2)\rangle-\langle\delta(\mathbf{r}_3)\rangle=0.006\,9292$ a.u. in the present work and in Ref. [2], but equals 0.006 9238 a.u. in Ref. [6] (see Figs. 2 and 3). The discrepancy of $5\times10^{-6}$ a.u. is an order of magnitude larger than the quoted accuracy of observables in Ref. [6]. Moreover, we found [1] that Ref. [6] deviates the same way in $e\mu\ ^4\mathrm{He}^{2+}$.

The above results indicate that the optimized parametrization $A$ is slightly more adapted to singular operators than to nonsingular ones. This is corroborated by the convergence of $\overline{\langle r_3\rangle}_{K_m}$ (Fig. 4) and $\overline{\langle r_3^{-1}\rangle}_{K_m}$ (Fig. 5), the relative error being smaller in the latter case.

The main difference in the optimized parametrization with respect to the $e\mu\ ^4\mathrm{He}^{2+}$ case [1] is the value of $a_3=-5$ ($-4$ in $e\mu\ ^4\mathrm{He}^{2+}$); $n_3$ remained the same.

The final values of $\langle\delta(\mathbf{r}_2)\rangle=0.320\,6134(3)$ a.u. and $\langle\delta(\mathbf{r}_3)\rangle=0.313\,6842(3)$ a.u. were obtained using the parameter ranges $n_3=0.5,\ 0.7$; $z_U=700-900$; $a_3=-4,-5$; $K_m=48$–56. The parameter dependence is strongest for $a_3$, then for $K_m$, and the weakest between $(n_3,z_U)=(0.7,900)$ and $(0.5,700)$. $\langle\delta(\mathbf{r}_2)\rangle$ and $\langle\delta(\mathbf{r}_3)\rangle$ change by an amount of the order of $1\times10^{-8}$ a.u. between $(n_3,z_U)=(0.7,900)$ and $(0.5,700)$, at $a_3=-4$. As the results for the mass set II were calculated using nonoptimal values of $a_3$, $n_3$, the final errors lie between the $K_m$ dependencies for mass sets I and II listed in Tables II–IV.

As in Ref. [1], the global correction term [15] proved to be negligible, affecting $\overline{\langle\delta(\mathbf{r}_2)\rangle}_{K_m}$ and $\overline{\langle\delta(\mathbf{r}_3)\rangle}_{K_m}$ by less than $1\times10^{-7}$ a.u. at $K_m=54$.

Our final error of the hyperfine splitting is 0.003 MHz, while its value depends on additional fundamental constants ($\alpha$ and $\mu_n$). In Table V we show that the differences in the constants used make direct comparisons of the results in the literature impossible. In fact, the results depend on assumed values of $\alpha$ and $\mu_n$ more than they do on the computational accuracy.

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