Nonvariational calculation of the hyperfine splitting and other properties of the ground state of the muonic helium atom

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The properties of the ground state of the muonic Helium atom $e\mu\ ^4He^{2+}$ have been calculated nonvariationally. The correlation function hyperspherical harmonic method utilizing a nonlinear parametrization of the correlation function has been used. Up to $N=561$ coupled second-order differential equations were taken into account. Although all parametrizations of the correlation function accelerate the convergence with respect to linear parametrizations by several orders of magnitude, an especially fast converging parametrization was found. All parametrizations make the observables converge to the same values in the limit of large N. The lowest-order hyperfine splitting obtained, 4454.206(3) MHz, has error margins smaller than the differences in the literature. One variational value is 0.023 MHz lower and another 0.013 MHz higher, after the adjustment for the different masses used. The expectation value of the distance between the electron and the muon also differs slightly from that in the literature, while the energy obtained was below the variational values. [S1050-2947(97)06311-7]

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I. INTRODUCTION

The muonic helium atom, which consists of an alpha particle, a negative muon, and an electron, is of great interest to atomic physicists for the following reasons:

(i) It is a pure atomic three-body system, which is quite unusual since all three particles are not identical, have very different masses, and no Pauli principle applies.

(ii) The atom is produced in the reaction of capture of the negative muon by the positive helium ion. It is one of the products in the process of muon catalyzed fusion, and its spectroscopic properties have to be therefore studied carefully to properly understand the fusion reactions.

(iii) The precise knowledge of the hyperfine splitting in this atom is especially important since it, together with the Zeeman effect, provides the most accurate and direct measurements of the muon magnetic momentum and of the electron-muon interaction constant.

In this work we concentrate on the computation of the lowest-order hyperfine splitting, which is given by (see Refs. [1,2] and references therein)

$$\nu_{\mathrm{HF}}=\frac{8}{3}\pi\alpha^2\frac{m_e}{m_\mu}\langle\delta(\mathbf{r}_{e\mu})\rangle,$$

representing an expectation value of the contact term of the spin-spin interaction obtained in the nonrelativistic reduction of the Breit equation; $\mathbf{r}_{e\mu}$ is the muon-electron separation and $\langle\delta(\mathbf{r}_{e\mu})\rangle$ is the expectation value calculated with the help of the spatial part of the wave function. In the Conclusion we will make a comparison of our result with the values in the literature that exibit rather large discrepancies [1–6]. The radiative and recoil corrections amount to about 10 MHz [1,2,4,5] such that the lowest-order value is $\nu_{\mathrm{HF}}\approx 4454.2$ MHz.

II. APPLICATION OF CFHHM TO MUONIC HELIUM

A. Construction of the correlation function

To calculate precisely the wave function and observables of the ground state of the muonic helium atom, we used the correlation function hyperspherical harmonic method (CFHHM) [7,8] in which the wave function is decomposed as $\Psi=e^f\phi$, where f is a correlation function and ϕ is a smooth function expandable in hyperspherical harmonics (HH). The Schrödinger equation is converted into an equation for ϕ with the non-Hermitian effective potential $\overline{W}$, which is a function of f. As a consequence, the eigenvalue obtained by solving the equation is not the true energy; $\langle H\rangle$ must be calculated for this purpose from Ψ.

For the total angular momentum zero, $\overline{W}$ and Ψ depend on the hyperradius ρ and on two hyperangles, a and λ [7].

The CFHHM system of differential equations is a system of coupled second-order differential equations in a single variable in the hyperspherical–harmonic basis, which 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 ρ_U is the maximum value of the hyperradius, is subdivided using the parameter T_z [8] in a sequence of subintervals of increasing length equal to zT_z. The parameter p_W is the maximum power p in the expansion of $\overline{W}$ into a series of terms ρ^p, $p=-1,0,\ldots,p_W$, with matrix coefficients.

We use the following general form of the correlation function f:

$$f=\sum_{i=1}^{3}\left[a_i+(b_i-a_i)e^{-r_i/(n_i\overline{r}_i)}\right]r_i, \tag{1}$$

where the spectator notation is used. The particles $\{1,2,3\}$ correspond to the electron (e), the muon (μ), and $^4He^{2+}$, respectively; e.g., r_3 denotes the distance be-

tween the electron and the muon. The b_i are the cusp parameters whose rounded values are $(-402.141, -1.999\,726, 0.995\,187)$. $\overline{r_i}$ is a constant approximately equal to the equilibrium distances of the particles in the ith pair. We used $\overline{r_1}=0.0037$ a.u., and $\overline{r_2}=\overline{r_3}=1.5$ a.u..

The form (1) takes all the cusp conditions exactly into account.

For the purpose of calculating the matrix elements of the expansion coefficients of $\overline{W}$ into a series of terms ρ^p, the form (1) is first expanded in a series in r_i^q, $i=1,2,3$, $q=0,1,\ldots,p_W+2$. In the part of the matrix elements calculated by quadrature, those terms are expressed as functions of (ρ,a,λ).

Two of the a_i can in principle be determined from asymptotic conditions in the breakup channels [9]. In the present case the electron tail is expected to be the most important. Because the heavy negative particle has charge -1, in our case the sum b_2+b_3 already has approximately the naively expected ''screening'' type value of -1. One would therefore expect that a linear f of the form (1) where $a_i=b_i$, $i=1,2,3$, would be a good first approximation. (Additionally, the muon mass lies in the correct range for b_3+b_1 to have approximately the correct value for the muon tail.)

However, it was first found that the linear f gives extremely slow convergent results (see Tables I and V). Second, it was found that the primary cause of the slow convergence is the divergence of e^f with the linear f at large distances between the electron and the muon. Therefore we attempted to construct several parametrizations of f with the least possible number of free parameters, each stressing one expectedly important aspect of f that would accelerate convergence. (All parametrizations eventually converge to the same limits, but the rate of convergence is of decisive importance.)

The parametrization A is defined by $a_1=b_1$, $a_2=b_2$ in Eq. (1):

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

This ansatz assumes the weak coupling of the electron and muon and only corrects the $e-\mu$ term, which would otherwise be non-negative. a_3 and n_3 are free parameters.

The parametrization B is defined by $a_1=b_1$, $a_3=0$:

$$f=b_1r_1+[a_2+(b_2-a_2)e^{-r_2/(n_2\overline{r_2})}]r_2+b_3e^{-r_3/(n_3\overline{r_3})}r_3.$$

This form attempts to control, with the single parameter a_2, the electron tail of the form $\approx e^{a_2s_1}$ where s_1 is the distance between the electron and the center of mass of the μ-$^4He^{2+}$ system.

The parametrization C is defined by $a_1=b_1$, $a_2=0$:

$$f=b_1r_1+b_2e^{-r_2/(n_2\overline{r_2})}r_2+[a_3+(b_3-a_3)e^{-r_3/(n_3\overline{r_3})}]r_3.$$

This controls the electron tail with a_3 instead of a_2 (parametrization B), but also removes asymptotically the linear term a_2r_2, which is a somewhat arbitrary proposition.

To find the optimal parameters of f, it is not necessary to perform a time-consuming variational procedure [8]. A few values of the free parameters need to be tested only, at fairly small K_m.

TABLE I. Eigenvalues and expectation values of the Hamiltonian for the parametrization A ($a_3=-4$, $n_3=0.5$), using $(z_U,p_W,T_z)=(700, 100, 0.05)$ and $(n_{\rm sub},n_G)=(1, 64)$ (see Secs. I, III B). The subseries with $K_m/2$ even and odd are displayed separately. The final result for $n_3=0.7$, which is more optimal for $\langle H\rangle$, is also shown. For comparison the results with the linear (cusp) correlation function [$a_i=b_i$ in Eq. (1)] are shown in the last part of the table for $K_m/2$ even.

K_m	$-E$	$-\langle H\rangle$
32	402.640 950 660	402.641 015 359
36	402.641 096 568	402.641 015 351
40	402.641 149 784	402.641 015 337
44	402.641 158 391	402.641 015 339
48	402.641 146 896	402.641 015 345
52	402.641 127 811	402.641 015 348
56	402.641 107 328	402.641 015 352
34	402.640 974 478	402.641 015 359
38	402.640 887 229	402.641 015 345
42	402.640 863 367	402.641 015 342
46	402.640 869 013	402.641 015 339
50	402.640 886 882	402.641 015 344
54	402.640 908 323	402.641 015 350
	($n_3=0.5$)	402.641 0153(1)[a]
	($n_3=0.7$)	402.641 01534(1)[b]
Ref. [4]		402.641 0153
32	402.627 61	402.637 27
40	402.662 85	402.640 63
48	402.670 40	402.639 24
56	402.667 78	402.638 90
64	402.661 91	402.639 36

[a]The main contribution to the error is due to the plateau smoothness estimated as $\partial\langle H\rangle(z_q)/\partial z_q$ (see Sec. III B).
[b]Error estimated from $K_m\leqslant 52$ calculations (see Fig. 4).

B. Convergence of the expectation values

In some systems the CFHHM basis exhibits a twofold convergence of the expectation values of some operators with respect to K_m. In the present case, the expectation values converge smoothly in two subsequences determined by whether $K_m/2$ is even or odd. The subsequences approach the limit from different sides. This is the case for the eigenvalue E and for all operators except $\langle H\rangle$. $\langle H\rangle$ values in both subsequences are essentially the same (Fig. 4).

Another example are the $(2p)^2$ helium resonances [10] where there are subsequences determined by whether $K_m/8$ is even or odd.

The described pattern of twofold convergence offers a way of accelerating the convergence. We take the expectation values $\langle O\rangle_{K_m}$ of an operator O for three successive values of K_m and calculate the arithmetic mean of the linearly interpolated subsequences:

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

$\overline{\langle O\rangle}_{K_m}$ typically converges much faster than $\langle O\rangle_{K_m}$.

C. Numerical considerations

Compared to calculations of systems with comparable masses, the upper value of the hyperradius in the present system had to be increased by a factor of 6–8. This is because the electron and the muon define very different ''natural'' scales via their very different binding energies to ^{4}He.

The larger value of z_U necessitated a careful consideration of the permissible values of z_U and p_W. Too large z makes the expansion of $\overline{W}$ meaningless because the large intermediate z^p terms in the alternating-sign summation cause loss of precision in the sum. Also, at large p the coefficients have less significant digits.

The terms of $\overline{W}$ that are quadratic in f have to be calculated by numerical quadrature, while all other terms are calculated algebraically [7]. The quadrature is done as follows. The interval of the variable a is divided into $[0,\pi/2-d_a]$ and $[\pi/2-d_a,\pi/2]$. The interval of the variable λ is divided into $[0,s_2-d_\lambda]$, $[s_2-d_\lambda,s_2]$, $[s_2,s_2+d_\lambda]$, $[s_2+d_\lambda, s_3-d_\lambda]$, $[s_3-d_\lambda,s_3]$, $[s_3,s_3+d_\lambda]$, $[s_3+d_\lambda,s_1-d_\lambda]$, $[s_1-d_\lambda,s_1]$, $[s_1,s_1+d_\lambda]$, and $[s_1+d_\lambda,2\pi]$. Here s_i are the points where, at $a=\pi/2$, $r_i=0$. The integrands are finite at $r_i=0$ because f cancels the Coulomb terms in $\overline{W}$ but $\partial r_i/\partial a$ and $\partial r_i/\partial\lambda$ entering the numerically calculated part of $\overline{W}$ are discontinuous; the weight factor $\sin 2a$ makes the integrand continuous but complicated close to $r_i=0$.

d_a and d_λ are small numbers (smaller than 0.1 and 0.03), which make the quadrature grid dense in the vicinity of singularities. The two a intervals are divided into $n^{(a)}_{\mathrm{sub},r}$ and $n^{(a)}_{\mathrm{sub},s}$ equal subintervals, respectively. The λ intervals are subdivided into $n^{(\lambda)}_{\mathrm{sub},r}$ or $n^{(\lambda)}_{\mathrm{sub},s}$ subintervals, depending on whether they include one of s_i points. Since different subdivisions are rarely taken, we use the simple notation $n^{(a)}_{\mathrm{sub}}$, $n^{(\lambda)}_{\mathrm{sub}}$, or even n_{sub} in the case equal subdivisions were taken in all variables and intervals. The same Gaussian order n_G is taken in all a,λ subintervals.

The corresponding parameters of the quadrature for the expectation values are denoted with primes.

Because the main problem to be overcome in this calculation, besides the construction of an appropriate correlation function, was the accuracy of the numerical quadrature used in part of the matrix elements of $\overline{W}$, we would like to point out that the solution of this problem had to preserve the great efficiency of the calculations of the quadratures. For example, at $K_m = 64$ and $p_W = 100$, one has to calculate $(64/2+1)^2\times 102\times 2 = 222\,156$ two-dimensional integrals of products of Jacobi polynomials and complex functions of $r_i(a,\lambda)$. Using 8-byte arithmetic and recurrence relations for Jacobi polynomials, we need only 1300 sec on a 300-Mflop machine for the integrals at $n_{\mathrm{sub}} = 8$, $n_{\mathrm{G}} = 16$ (10×2 subregions giving a 1280×256 grid). At $K_m = 56$, $n_{\mathrm{sub}} = 4$ we calculate 171 564 integrals in 275 sec using double precision arithmetic, and in 71 000 sec using quadruple precision arithmetic. In the latter case, this is still only 0.4 sec per integral, and we decided to keep the method also for quadruple precision instead of going to Romberg–type schemes. (The complete matrix elements calculation time increases by a lesser factor of 40, due to the unchanged angular momentum coupling algebra part.)

The solution of the Schrödinger equations was performed in the usual (8-byte, double) precision arithmetic; thus the two-scale nature of the physical system was reflected only in the need for more precise quadrature in the matrix elements, and for a larger z_U; all other parameters like T_z and p_W were found to be as in other, more ordinary systems such as He atom or positronium negative ion.

III. RESULTS

A. Initial estimates of the CFHHM parameters

From first tests it was deduced that we can attempt to fix the intrinsic parameters so as to give $\overline{\nu_{\mathrm{HF}}}$ to about $\delta = 0.03$ MHz accuracy without improving the precision of the matrix elements. These tests served to obtain the convergence patterns of the expectation values and to identify possible other necessary improvements in accuracy.

The best results for parametrization A were obtained with $a_3 = -4$, despite the fact that in that case the sum $b_2 + a_3 \approx -6$ does not correspond to the expected form of the asymptotics of the wave function when the electron is removed from the μ-$^4\mathrm{He}^{2+}$ subsystem. A similar effect was observed in Ref. [11] in a variational calculation (behavior of the parameters α and β), where it was impossible to fix the behavior of the electron tail (see also [4]). The explanation of this effect may have to do with the short-range behavior of f, as follows.

Generally it turns out that n_3 should be as small as possible, with the lower limit constrained by the numerical stability of the sum of the power series for f at the largest hyperradius. The smallness of n_3 indicates that the nonlinear term in f should decay as fast as possible. A large absolute value of a_3 then assures the fast decay of the $O(r_3^2)$ term in f.

The results with parametrization B did show the effect that a_2 tended to be much smaller than expected (-4, as in parametrization A), which is similar to the behavior in Ref. [11], but it shows that the idea that f should be modeled after the variational results for the optimum exponents is misleading.

In addition, we tested several parametrizations that take into account the ''cutoff'' effect that the solution ϕ has, for small coupled systems, asymptotics that can differ appreciably from those of $\Psi = e^f\phi$ (see Refs. [8,12]). This entails a self-consistent determination of the parameters a_i so as to give the correct asymptotics of Ψ in the first approximation, usually at $K_m = 0$ [13]. For the cases tested, the imposition of asymptotic constraints on f was found to be of little relevance, and we could not find parametrizations as good as A in this way.

We can summarize the above observations on the choice of the optimal f in the same way as suggested in the CFHHM calculation of the properties of the μdt system [12], namely, that it is not necessary to impose the proper asymptotic behavior on Ψ itself. It is sufficient to impose it on the correlation factor e^f, which is straightforward and eliminates the self-consistent determination of a_i. The only exception to this rule so far has been the positronium negative ion [9], although even in this case the a_i determination

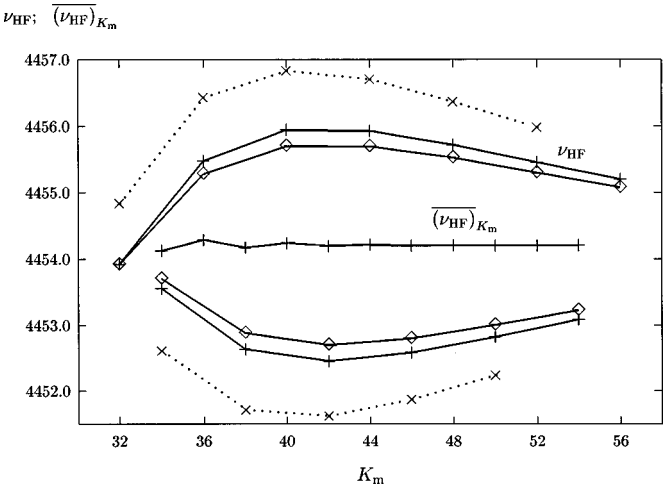

FIG. 1. Convergence of $\nu_{\rm HF}$ and $\overline{(\nu_{\rm HF})}_{K_m}$ with K_m for the parametrization A (see Sec. II A), using the masses of Refs. [1,11], α of Ref. [15], and $a_3=-4$. ''+'' denotes the curves with $n_3=0.5$. The curve denoted by $\diamond$ has the same value of n_3, but includes the global correction, while the curve denoted by $\times$ corresponds to $n_3=0.7$.

was far from intractable because only 1 significant digit in a_i is required.

The averaged expectation values $\overline{\langle O\rangle}_{K_m}$ were convergent and stable as functions of K_m for $K_m=50-60$, which are not much larger than the K_m needed in simpler systems. (A calculation at $K_m=50$ takes three times less CPU time than at $K_m=64$.)

The arithmetic mean reduces the error of the method by two orders of magnitude. The degree of convergence of $\overline{\langle O\rangle}_{K_m}$ was the same in the test calculation and in the final accurate calculation. Because of this, as can be seen from Figs. 1–3 depicting the final results, a higher-order interpolation is not necessary. It was only necessary to ensure that the accuracy of the separate $\langle O\rangle_{K_m}$ values matched the degree of convergence of $\overline{\langle O\rangle}_{K_m}$.

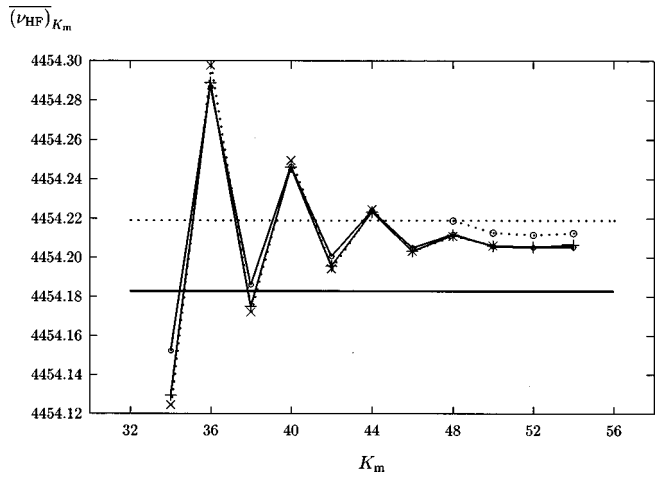

FIG. 2. As in Fig. 1, but showing the $\overline{(\nu_{\rm HF})}_{K_m}$ values only. The curve denoted by $\bigcirc$ presents the CFHHM values using the masses of Ref. [6] and α of Ref. [15] (see Sec. III C). The solid horizontal line is obtained from the value of Ref. [5] by adding 0.002 MHz (see Sec. IV). The dotted horizontal line is obtained by adding the difference (0.013 MHz) between Ref. [6] and CFHHM when using the same masses (see Sec. IV), to the CFHHM value (denoted by ''+'').

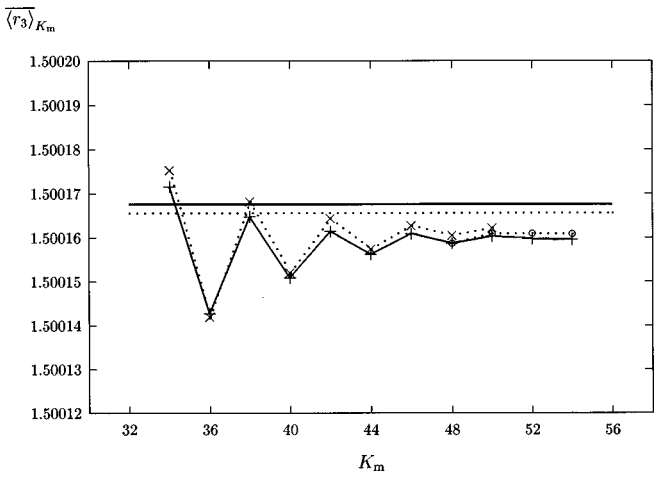

FIG. 3. As in Fig. 2, but for $\overline{\langle r_3\rangle}_{K_m}$. The solid and dotted horizontal lines are obtained from the values of Refs. [4] and [6], respectively, by adjusting for the mass differences (see Table IV and Sec. IV) (adding and subtracting 0.000 001 a.u., respectively).

In particular, $\overline{(\nu_{\rm HF})}_{K_m}$ is stable to within 0.002 MHz, which by far exceeds the absolute error of the individual points in the test calculation, and shows the accuracy we ought to strive for in the improved calculation.

The dependence on n_3 was tested to be rather large for the $K_m/2$ odd and even values separately, but smaller for $\overline{\langle O\rangle}_{K_m}$, so we need not be concerned with n_3 at this level of accuracy except to the extent it is constrained by the numerical convergence.

In the present work it was also considered desirable to test the stability of the numerical algorithm at larger systems of equations; we calculated several cases with up to 561 equations ($K_m=64$) with linear and nonlinear f and found no evidence of numerical instability.

We deduced that the most critical parameters were the following: (a) *quadrature in matrix elements*: $n_{\rm sub}, n_G, d_a$,

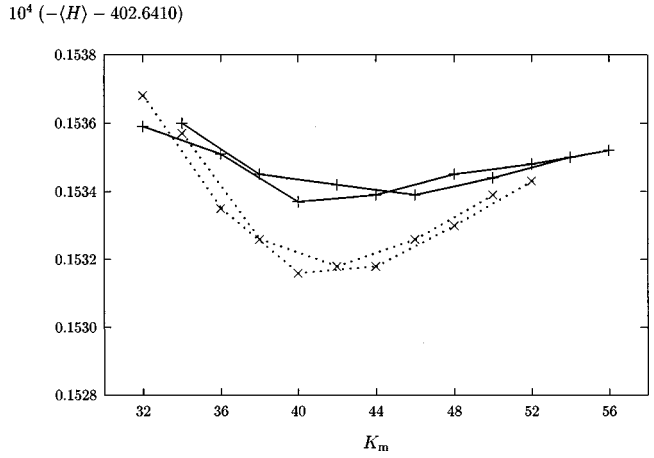

FIG. 4. Convergence of $\langle r_3\rangle$ as function of K_m, separately for $K_m/2$ even and odd. Labels are as in Fig. 1. The error due to plateau smoothness for $n_3=0.5$ is about 0.001 units on the ordinate while for $n_3=0.7$ it is negligible (see Sec. III B).

TABLE II. As in Table I, but expectation values of functions of $\mathbf{r}_1=\mathbf{r}_{\mu\text{-He}}$ for $n_3=0.5$. The third part of the table shows the CFHHM interpolated values. The last part of the table compares the CFHHM interpolated values using the masses of Ref. [6] with the values of Ref. [6]. The numbers in parentheses are last digit uncertainties defined as the differences of the interpolated values at $K_m=52$ and 54, showing the convergence but not the final error estimates (see Secs. III C and IV).

K_m	$\langle r_1^{-2}\rangle\times10^{-3}$	$\langle r_1^{-1}\rangle$	$\langle\delta(\mathbf{r}_1)\rangle\times10^{-6}$	$\langle r_1\rangle\times10^{3}$	$\langle r_1^2\rangle\times10^{6}$
32	323.440 4104	402.142 9759	20.700 7107	3.730 0345	18.550 8797
36	323.440 6124	402.143 1071	20.700 7278	3.730 0333	18.550 8680
40	323.440 7040	402.143 1640	20.700 7359	3.730 0328	18.550 8635
44	323.440 7319	402.143 1792	20.700 7386	3.730 0327	18.550 8626
48	323.440 7248	402.143 1725	20.700 7383	3.730 0328	18.550 8635
52	323.440 7001	402.143 1554	20.700 7364	3.730 0329	18.550 8651
56	323.440 6682	402.143 1345	20.700 7337	3.730 0331	18.550 8669
34	323.440 3964	402.142 9739	20.700 7086	3.730 0344	18.550 8785
38	323.440 2588	402.142 8864	20.700 6967	3.730 0352	18.550 8859
42	323.440 2051	402.142 8545	20.700 6918	3.730 0354	18.550 8881
46	323.440 1985	402.142 8529	20.700 6909	3.730 0354	18.550 8879
50	323.440 2169	402.142 8666	20.700 6923	3.730 0352	18.550 8864
54	323.440 2469	402.142 8867	20.700 6947	3.730 0351	18.550 8846
	323.440 4655(5)	402.143 0158(2)	20.700 71488(5)	3.730 034042(1)	18.550 875307(5)
	323.434 4296(5)	402.139 2635(2)	20.700 13542(6)	3.730 068847(3)	18.551 221503(5)[a]
Ref. [6]		402.137 30303	20.700 1373610	3.730 069345	18.551 22347

[a]CFHHM values computed using masses from Ref. [6] (see Sec. III C).

d_λ; the irregular dependence on these indicates insufficient precision arithmetic; (b) K_m; (c) *density of the z points (parameter T_z)*; (d) a_3,n_3.

B. Optimization of the CFHHM parameters

Using quadruple-precision quadrature, we immediately reduced the quadrature error of ν_{HF} to the 0.002-MHz level. The individual integrals became converging to some 14 significant digits in contrast to the double-precision calculation where it was impossible to stabilize them to more than about 10 significant digits. This enabled the matrix elements to be accurate enough even at large z and large powers (about 100). We found that the results converge enough at $(d_a,d_\lambda)=(0.05,0.015)$, respectively. These values are smaller by a factor of 2 than those used in other systems. Still smaller values neither improve results nor cause instability.

TABLE III. As in Tables I and II, but expectation values of functions of $\mathbf{r}_2=\mathbf{r}_{\text{He-}e}$.

K_m	$\langle r_2^{-2}\rangle$	$\langle r_2^{-1}\rangle$	$\langle\delta(\mathbf{r}_2)\rangle$	$\langle r_2\rangle$	$\langle r_2^2\rangle$
32	1.999 7424	0.999 8616	0.320 6137	1.500 2496	3.001 0103
36	2.000 3544	1.000 0437	0.320 7256	1.499 9412	2.999 7741
40	2.000 5438	1.000 1025	0.320 7590	1.499 8353	2.999 3382
44	2.000 5424	1.000 1044	0.320 7575	1.499 8273	2.999 3056
48	2.000 4649	1.000 0832	0.320 7424	1.499 8586	2.999 4211
52	2.000 3639	1.000 0543	0.320 7234	1.499 9051	2.999 6054
56	2.000 2645	1.000 0254	0.320 7049	1.499 9529	2.999 7970
34	1.999 6482	0.999 8496	0.320 5874	1.500 2358	3.000 9195
38	1.999 2788	0.999 7382	0.320 5207	1.500 4295	3.001 7076
42	1.999 1984	0.999 7119	0.320 5073	1.500 4798	3.001 9159
46	1.999 2420	0.999 7228	0.320 5165	1.500 4671	3.001 8790
50	1.999 3323	0.999 7483	0.320 5338	1.500 4270	3.001 7207
54	1.999 4324	0.999 7773	0.320 5526	1.500 3783	3.001 5176
	1.999 8733(1)	0.999 90858(2)	0.320 63337(7)	1.500 1536(2)	3.000609(3)
	1.999 8726(1)	0.999 9083308(4)	0.320 63327(6)	1.500 1550(1)	3.000621(2)[a]
Ref. [6]		0.999 9057442	0.320 62688	1.500 160720	3.000 655964

[a]See footnote of Table II.

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

K_m	$\langle r_3^{-2}\rangle$	$\langle r_3^{-1}\rangle$	$\langle\delta(\mathbf{r}_3)\rangle$	$\langle r_3\rangle$	$\langle r_3^2\rangle$
32	1.999 1899	0.999 8471	0.313 7421	1.500 2556	3.00 10279
36	1.999 8018	1.000 0292	0.313 8520	1.499 9471	2.999 7917
40	1.999 9912	1.000 0879	0.313 8849	1.499 8412	2.999 3558
44	1.999 9898	1.000 0899	0.313 8836	1.499 8333	2.999 3232
48	1.999 9123	1.000 0686	0.313 8689	1.499 8645	2.999 4387
52	1.999 8113	1.000 0398	0.313 8503	1.499 9110	2.999 6230
56	1.999 7119	1.000 0108	0.313 8322	1.499 9588	2.999 8147
34	1.999 0958	0.999 8351	0.313 7166	1.500 2417	3.000 9371
38	1.998 7266	0.999 7237	0.313 6516	1.500 4354	3.001 7252
42	1.998 6462	0.999 6974	0.313 6387	1.500 4857	3.001 9335
46	1.998 6898	0.999 7083	0.313 6478	1.500 4730	3.001 8966
50	1.998 7801	0.999 7338	0.313 6648	1.500 4329	3.001 7383
54	1.998 8801	0.999 7628	0.313 6832	1.500 3842	3.001 5352
	1.999 3209(1)	0.999 894 06(2)	0.313 76223(8)	1.500 1596(2)	3.000 627(3)
	1.999 3202(1)	0.999 893 8168(5)	0.313 762 07(7)	1.500 1608(1)	3.000 639(2)[a]
Ref. [6]		0.999 891 2309	0.313 7630	1.500 166625	3.000 673563
Ref. [4]				1.500 166572	

[a]See footnote of Table II.

The results deviate from the initial results (Sec. III A) by about 0.02 MHz, showing that the test calculation accuracy estimate δ was correct.

An important result is that the precision obtained by $n_{\text{sub}}\times n_G = 1\times 64$ was equivalent to 4×32 and 16×16, which means a fourfold CPU time reduction in each case. High-order Gaussian quadrature with no subdivisions is therefore much more efficient than lower-order quadrature with more subdivisions at the same value of $n_{\text{sub}}\times n_G$.

To estimate the accuracy, we calculated the expectation values at $K_m=32$ for a set of values of n_{sub}, n_G, p_W, z_U, and T_z, and observed the global upper and lower limits of values on this set of results, taking into account only those results where all parameters lie in sufficiently narrow convergence regions. This is justified because we have finite regions of convergence in all parameters and a large enough set of results to be able to rely on mutual cancellations of some errors.

The convergence was confirmed by testing the critical parameters at $K_m=40$. Furthermore, these parameters were tested again at $n_3=0.7$ and for different a_3 at $n_3=0.5$. For example, z_U had to be taken different (700 for $n_3=0.5$, 900 for $n_3=0.7$). Except where explicitly noted, the following descriptions apply to $n_3=0.5$; in general the parameter dependence is appreciably smaller for $n_3=0.7$.

(i) $n_{\text{sub}}\times n_G$: among 4×16, 2×32, and 4×32, 1×64, at $K_m=32$, the latter was apparently the best, the dependence on the Gaussian density in the last three cases being within 0.0002 MHz. The smallest difference between cases $(z_U,p_W)=(700,92)$ and (800,100) is at 1×64. At $K_m=48$, the difference between the cases 4×32 and 1×64 [at $(T_z,z_U,p_W)=(0.05,700,100)$] is 0.0002 MHz.

(ii) T_z: the dependence on T_z is about 0.002 MHz in the range $0.01-0.1$. We took 0.05 for the final runs. The dependence on T_z for $T_z=0.03-0.1$ is 0.003 MHz for $(z_U,p_W)=(700,100)$, and 0.0015 MHz for (700,92). This indicates $p_W=100$ is a good choice. At $K_m=48$ the values of ν_{HF} were 4455.7202 and 4455.7208 MHz for $T_z=0.1$ and 0.05, respectively.

(iii) z_U: at $K_m=48$, $(T_z,p_W)=(0.05,100)$, the difference between the values for $z_U=700$ and 800 is 0.0005 MHz; $\langle H\rangle$ is higher at $z_U=800$ than at 700 by 1×10^{-8}, indicating that 800 is slightly too large and in the instability region.

(iv) p_W: for $p_W=84-120$, ν_{HF} decreases until $p_W=92$, then increases and starts to decrease, or stabilizes, at $p_W=96-100$; at larger values the oscillations cease and instability sets in at $z_U=700-800$. There is therefore just enough accuracy to sum the power series for $\overline{W}$ in a stable manner at large z. The above oscillations due to p_W are well within the 0.002 MHz range.

(v) $n'_{\text{sub}}\times n'_G$: we used 4×16 throughout. At $K_m=40$, the use of 8×16 increases ν_{HF} by 0.0004 MHz.

(vi) n_3: $\overline{\langle\delta(\mathbf{r}_k)\rangle}_{K_m}$ and $\overline{\langle r_k\rangle}_{K_m}$, $k=2,3$, and related observables have extrema at $a_3=-4$, while for $k=1$ they depend negligibly on a_3; $\overline{\langle\delta(\mathbf{r}_3)\rangle}_{50}=0.313\,7615,0.313\,7622,0.313\,7620$ a.u., and $\overline{\langle r_3\rangle}_{50}=1.500\,165,1.500\,160,1.500\,169$ a.u. at $n_3=0.5$ and $a_3=-3,-4,-5$ respectively.

(vii) *Plateaus*: the expectation values as functions of the upper z limit of integration, $\langle O\rangle(z_q)$, where $z_q\leqslant z_U$, may exhibit plateaus [8] at $z=z_p\leqslant z_U$, because the tail of the wave function may be inaccurate enough at very large z to affect the integrals. In the present calculation several test calculations with nonoptimal parameters exhibited plateaus in several expectation values with $z_p<z_U$. In all final runs displayed in the tables, $z_p=z_U$, and the error was deduced from $\partial\langle O\rangle(z_q)/\partial z_q$ at $z=z_U$. Except for $\langle H\rangle$ this error was found to be negligible.

TABLE V. As in Table I, but the hyperfine splitting in lowest order, $\nu_{\rm HF}$ and $(\nu_{\rm HF})_{\rm GC}$, for $n_3=0.5$, obtained as $\nu_{\rm HF}=14196.1209\langle\delta(\mathbf{r}_3)\rangle$. For comparison the results using the linear (cusp) correlation function are shown in the last part of the Table for $K_m/2$ even. For comparison the works where corrections or the factor $[1+1/(m_{\rm He}+m_\mu)]^{-3}$ are not included in their multiplicative factors are quoted.

K_m	$\nu_{\rm HF}$	$(\nu_{\rm HF})_{\rm GC}$[a]
32	4453.921	4453.920
36	4455.480	4455.280
40	4455.948	4455.700
44	4455.929	4455.696
48	4455.721	4455.523
52	4455.457	4455.298
56	4455.200	4455.077
34	4453.558	4453.704
38	4452.636	4452.883
42	4452.453	4452.703
46	4452.581	4452.800
50	4452.823	4453.001
54	4453.085	4453.223
	4454.206(3)	4454.206(3)[b]
Ref. [4]	4454.14(5)	
Ref. [5]	4454.181(1)	
Ref. [1]	4455.2(1.0)	
Ref. [6]	4454.226[c]	
Ref. [2]	4452.5	
Ref. [3]	4452.9[d]	
32	4844.177	
40	4217.573	
48	4023.569	
56	4013.421	
64	4081.879	

[a]Global correction included (see Sec. III B).

[b]Error estimate includes the $n_3=0.7$, $a_3=0.5$, and the $n_3=0.5$, $a_3=-3,-4,-5$ calculations.

[c]Converted from $\langle\delta(\mathbf{r}_3)\rangle$ using our value of α (Sec. III C).

[d]Approximate value obtained from the quoted total value by subtracting 10 MHz (see Sec. I).

(viii) *Behavior of* $\langle H\rangle$: $\langle H\rangle$ starts to decrease at $K_m=44$, showing that the variational property [8], depending on both the quadrature parameters and K_m, is setting in as required. At $K_m=32$, $(z_U,p_W)=(800,96)$ is no longer sufficient for $\langle H\rangle$: the value $-402.641\,015\,15$ a.u. is higher than $-402.641\,015\,36$ a.u. at $(z_U,p_W)=(800,100)$; this in turn agrees with $(z_U,p_W)=(700,100)$ so that $z_U=700$ is sufficient. The plateau error is 1×10^{-7} a.u. for $n_3=0.5$ and 3×10^{-10} a.u. for $n_3=0.7$. Therefore in the $n_3=0.5$ case the main error comes from the plateau flatness. This signifies that our f, which was optimized for $\nu_{\rm HF}$ is not optimal for $\langle H\rangle$. In Fig. 4, the $n_3=0.5$ curves have much larger errors than the $n_3=0.7$ ones.

(ix) *Global correction*: for the first time in CFHHM we have calculated the global correction to the delta function operator [14]

$$(\nu_{\rm HF})_{\rm GC}=\nu_{\rm HF}+\frac{m_{e\mu}}{\pi}\left(\langle H\rangle\langle r_3^{-1}\rangle-\left\langle\frac{H}{r_3}\right\rangle\right),$$

where $m_{e\mu}$ is the reduced mass of the electron and muon. The correction term becomes negligible at $K_m=48$, which is, interestingly, at the start of the convergence region (see Fig. 2). If this were not so, the validity of the application of the correction formula, in view of the non-Hermiticity of the effective Hamiltonian in CFHHM, should be questioned.

The largest contribution to the quoted errors of expectation values other than $\langle H\rangle$ comes from the behavior in the parameter space of (a_3,n_3).

C. Dependence on fundamental constants

The tests were performed at $n_3=0.5$, $a_3=-4$ except where noted.

For the sake of comparison, we use the following values for the particle masses [1,11]: $m_e=0.511\,0034$ MeV, $m_\mu=105.659\,48$ MeV (206.768 64 a.u.), and $m_{^4{\rm He}}=4.002\,603\times931.5016$ MeV. In Ref. [4], $m_\mu=105.659\,46$ (206.768 60 a.u.) is used, and the energy for the former set of masses [1,11] is calculated and compared to.

The effect of the small change in the muon mass is as follows: if we use the smaller muon mass from Ref. [4] (and presumably Ref. [5]), the eigenvalue E and $\langle H\rangle$ increase by 7×10^{-5} a.u., while $\nu_{\rm HF}$ increases by 0.0014, 0.00015, and 0.0014 MHz at $K_m=32$, 38, and 40, respectively. $\langle r_3\rangle$ decreases by about 1×10^{-6} on average at $K_m=32$, 38, and 40.

We use $\alpha=1/137.035\,9895$ [15], and employ the conversion factor $\frac{8}{3}\pi\alpha^2m_e/m_\mu=14196.1209$ MHz/a.u. The sensitivity to the value of α is as follows: if α of Ref. [4] is used, one gets the smaller factor 14196.1105 MHz/a.u., which would reduce the value of our $\nu_{\rm HF}$ by 0.003 MHz.

The ^{4}He mass used in Refs. [1,4,11] and presumably in Ref. [5], as well as in our work, is the atom mass; see also the discussion in Ref. [6]. In Ref. [6], a comparative calculation using the Ref. [4] masses instead of their own $^4{\rm He}^{2+}$ mass (7294.2996 a.u.) is presented. Also, the muon mass in Ref. [6] (206.768262 a.u.) differs appreciably from our usage.

To make a comparison of our values of observables with the values of Ref. [6], we first tested $\partial\nu_{\rm HF}/\partial m_{^4{\rm He}}$ by subtracting 2 a.u. from our $m_{^4{\rm He}}$ and found it to be positive as expected: $\nu_{\rm HF}$ decreased by 0.0009 MHz at $K_m=32$ and by 0.004 MHz at $K_m=34$. Since $\partial\nu_{\rm HF}/\partial m_\mu$ according to the above is negative as expected, the effects of Ref. [6] masses as compared to ours were expected to partially cancel out, which is what happened.

Our final value of $\langle\delta(\mathbf{r}_3)\rangle$ is 0.313 7622(2) a.u., where the error estimate takes into account the results of the $n_3=0.7$, $a_3=-4$ calculation (see Tables IV and V) as well as the $n_3=0.5$, $a_3=-3,-4,-5$ calculations (see Sec. III B). Ref. [6] quotes 0.313 7630 a.u. (implying the error 0.001 MHz in $\nu_{\rm HF}$). The only fundamental constants affecting the difference between these two values are $m_{^4{\rm He}}$ and m_μ.

We recomputed our observables with the masses of Ref. [6]. This mass change makes $\langle\delta(\mathbf{r}_3)\rangle$ smaller by about 1 on the last quoted digit: 0.313 7621(2) a.u. (Table IV; error

estimate taken from the calculation using our masses), moving our value further away from that of Ref. [6].

The effect of these mass differences on $\nu_{\rm HF}$ is as follows: the muon mass of Ref. [6] together with our value of α gives the multiplication factor of 14 196.1472 MHz/a.u. Multiplying by the $\langle \delta(\mathbf{r}_3)\rangle$ of Ref. [6], this gives 4454.226 MHz. We in turn obtain, using the same values of fundamental constants, $14\,196.1472\times 0.313\,7621(2)$ MHz$=4454.213(3)$ MHz.

We also note that while our value of $\langle \delta(\mathbf{r}_3)\rangle$ using the masses of Ref. [6] is 9×10^{-7} a.u. smaller than in Ref. [6], our value of $\langle \delta(\mathbf{r}_2)\rangle$ is 6×10^{-6} a.u. *larger* than in Ref. [6]. This is an order of magnitude larger discrepancy than the effect of masses. In fact, if we use the masses of Ref. [6] *both* $\langle \delta(\mathbf{r}_2)\rangle$ and $\langle \delta(\mathbf{r}_3)\rangle$ decrease by about the same small amount of the order of 1×10^{-7} a.u. with respect to values obtained using our masses (Tables III, IV), keeping the difference $\langle \delta(\mathbf{r}_2)\rangle-\langle \delta(\mathbf{r}_3)\rangle$ unaffected.

Using the masses of Ref. [6] we get $\langle H\rangle=-402.637\,263\,01$ a.u., which is slightly higher than $-402.637\,263\,035\cdots$ of Ref. [6]; however, due to the large sensitivity to the muon mass (see above), it is possible that this is due to the way various derived quantities are calculated from masses.

The comparison of our observables and those of Ref. [6] using the same masses is given in Tables II–IV.

IV. CONCLUSION

The tables in Refs. [4,5] show that although the errors of $\nu_{\rm HF}$ quoted are derived from a comparison of results using different variational bases, the individual bases make $\nu_{\rm HF}$ converge to different values. This is not the case in CFHHM.

We deduce our final value of $\nu_{\rm HF}$ as 4454.206(3) MHz (Fig. 2, Table V).

To make an accurate comparison with Refs. [5,6], we recalculated the values of observables for several K_m in the convergence region using the constants from Refs. [5,6]. This comparison is given in Tables II–IV.

Using the muon mass as well as α from Ref. [4] (and presumably Ref. [5]) decreases our $\nu_{\rm HF}$ result by about 0.002 MHz, to give 4454.204(3) MHz as compared with the value 4454.181(1) MHz of Ref. [5].

Using the masses of Ref. [6] and our value of α, we obtain 4454.213(3) MHz as compared with 4454.226 MHz of Ref. [6].

This indicates that the value of Ref. [5] is 0.023(4) MHz too small while the value of Ref. [6] is 0.013(4) MHz too large, and that our values are more precise than the differences between the different variational calculations, although the quoted accuracy is approximately the same in all cases. These discrepancies are displayed in Fig. 2, where the full and dashed lines are obtained by shifting our final value by -0.023 and 0.013 MHz, respectively.

In particular we note that 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. [6] than in our work, while the effect of different masses and our computational error for these operators are both of the order of 2×10^{-7} a.u.

Our value of $\langle r_3\rangle$ [1.500160(5) a.u., i.e., the value of Table IV with the K_m, n_3 and a_3 dependence taken into account, see Fig. 3 and Sec. III B] should be compared with the value of Ref. [4] adjusted by about $+0.000\,001$ a.u. (which gives 1.500 1676 a.u., see Table IV) because of the muon mass difference. Likewise, our $\langle r_3\rangle$ value should be compared with the value of Ref. [6] decreased by 0.000 001 a.u. (giving about 1.500 1656 a.u.) because of mass differences (see Table IV). These discrepancies are displayed in Fig. 3.

It had been shown [8,16] that the CFHHM expectation value $\langle H\rangle$ satisfies a variational property in K_m, certain intrinsic parameters, and the quadrature parameters. Therefore it gives an upper bound to the true energy, which is an important aspect of CFHHM. According to Fig. 4 and Sec. III B, the CFHHM energy ($\langle H\rangle$) is lower than $-402.641\,015\,34$ a.u.; this could obviously be improved by calculating more values for $n_3=0.7$, which, however, was not our objective. Our ground-state energy is lower than in most recent variational calculations [4], although the last decimal places may be affected by the way the derived quantities are calculated from masses in various methods. On the other hand, the CFHHM value has a stable dependence on K_m.

The direction of the changes in E and $\langle H\rangle$ using the corresponding sets of fundamental constants agrees with the direction of changes between Refs. [4] and [11].

With respect to the linear parametrization of the correlation function, the best nonlinear parametrization decreases the errors of the CFHHM expectation values by several orders of magnitude. We define these errors as the absolute differences between the values for a given K_m and the limiting value. At $K_m=64$, $|\delta E|$ is reduced from 0.02 to 0.000 06 a.u., $|\delta\langle H\rangle|$ from 0.002 to 3×10^{-7} a.u., and $|\delta\nu_{\rm HF}|$ from 370 to 0.6 MHz. The $\overline{\langle O\rangle}_{K_m}$ values have two orders of magnitude smaller errors than the $\langle O\rangle_{K_m}$ values (except for $\langle H\rangle$).

The interpolation procedure is also more reliable than extrapolation employed in earlier works (Refs. [7,10]).

In the present system, more work was involved in finding the proper parametrization of the correlation function than in obtaining the final numerical results. This reflects the need to find a general algorithm for parametrizing the correlation function. On the other hand, the constructed correlation function reduced the errors of observables by $3-4$ orders of magnitude with respect to the linear (pure cusp) correlation function, which is an extreme case. We have established again [9] that the most important aspect of the correlation function for a well-correlated system is the elimination of the fast increase of e^f in the vicinity of the coalescence points, as the particle separation increases.

We calculated the global correction to delta-function-type operators in CFHHM. We have shown that in fact its calculation is unnecessary, as it becomes negligible even before final convergence is reached.

We found the electron tail parameters behave similarly to those in Ref. [11] for all parametrizations, but in CFHHM, this can be interpreted in the best parametrization to simply be the consequence of e^f trying to fall off as fast as possible. This makes it easier for the HH expansion to describe the fine details of the wave function because e^f with f of Eq. (1) containing at the most 6 free parameters, of which only 2 are

used in parametrization A, is a rather crude approximation to the true wave function in this two-scale system.

Summing up, one can state that CFHHM has proved successful in obtaining good convergent values of all observables. Our numerical error estimates are based on experience in different systems calculated by the CFHHM earlier [9,10,12,13,17–25] as well as on the fact that in the CFHHM due to its mathematically known convergence properties [7,8] it is easy to distinguish possible numerical instabilities from convergence patterns.

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