Accuracy of three-body wave functions obtained with the correlation-function hyperspherical-harmonic method

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The local convergence and accuracy of wave functions obtained by direct solution of the Schrödinger equation with the help of the correlation-function hyperspherical-harmonic method are analyzed for ground and excited states of the helium atom and for the ground state of the positronium negative ion. The inclusion of the cusp conditions into the correlation function is shown to be of crucial importance, not only near the coalescence points, but also away from them. The proper inclusion of all cusps yields for the ground state of the helium atom the local wave-function accuracy of about 10^{-7} for different interparticle distances. The omission of one of the cusps in the excited helium atom reduces the wave-function precision to 10^{-2} near the corresponding coalescence point and to 10^{-4}–10^{-5} away from it.

The problem of finding exact solutions of the few-body Schrödinger equation is one of long standing, but the situation is still far from being satisfactory. Only very sophisticated variational calculations[1,2] can match the precision of nine decimal places for the energy that is reached in experiments with two-electron atoms.

We still do not know, therefore, the correct analytical structure of three-body wave functions, since inclusion or omission of logarithmic terms, suggested in Ref. 1, or negative powers of interparticle distances, suggested in Ref. 2, has negligible effect on the value of the variational energy. A variational function coincides with the precise one only on the average, and could wildly or even infinitely deviate from it locally. The local discrepancies could lead to wrong estimates of expectation values of different operators which have significant contributions from the regions of the configuration space where the deviations occur. The possibility of the direct precise solution of the few-body Schrödinger equation is thus important not only for understanding of the analytical structure of the wave function, but for proper estimate of relativistic, QED, and hyperfine effects, as well as positron annihilation in the positronium negative ion, parity violation in atoms, fusion and sticking probabilities in muon-catalyzed fusion, etc.

The Green's-function Monte Carlo method, which was used for the estimate of the ground-state energy and sticking probabilities in μdt catalyzed fusion,[3] does not have these limitations, but its extension to the excited mesomolecular states, which are expected to be the most important in the fusion process, is difficult due to the fact that any, however small, admixture of the ground state in the importance function will eventually dominate the numerical simulation.

In view of the difficulties of the above-mentioned approaches, the correlation-function hyperspherical-harmonic (CFHH) method[4–9] was recently introduced by the present authors, which, in principle, can generate accurate ground- and excited-state wave functions for all interparticle distances, including coalescence points, for three-body atomic and molecular systems. To date the accuracy of the CFHH method in the calculation of expectation values of different operators, including the Hamiltonian, has been verified for systems with different mass ratios, i.e., for systems consisting of one heavy and two light particles,[4–6] of one light and two heavy particles,[9] and of particles of equal masses.[7] It has been shown that direct solution of the Schrödinger equation by the CFHH method for bound three-body atomic systems yields precision comparable to that obtained by elaborate variational calculations. For example, for maximum global momentum $K_m = 48$, up to nine significant figure precision has been obtained for the energy of the helium atom[4–6] and seven significant figures for the positronium ion[7] $e^- e^- e^+$ (also denoted Ps^-). The values of wave functions taken at a few representative interparticle distances and different expectation values for these systems have shown about six and five significant figure precision, respectively.

The purpose of this paper is to complete our study of an accuracy of the CFHH method for the ground-state wave functions, started in Ref. 6, and to extend it also to excited states for which direct estimates of the convergence of wave functions were not previously obtained. In order to properly estimate the accuracy of the method, we systematically analyzed here not only convergence trends of wave functions themselves at many different interparticle distances, but also calculate the local deviation at the same points

$$\Delta = \frac{H\psi}{E\psi} - 1 \tag{1}$$

and an expectation value of its absolute value

$$\langle|\Delta|\rangle=\left\langle\left|\frac{H\psi}{E\psi}-1\right|\right\rangle . \tag{2}$$

These two quantities were shown to be extremely sensitive measures of the local and overall goodness of the wave function, respectively, and could be used therefore for proper judging of accuracy of any method of solving the Schrödinger equation. For a true eigenfunction ψ both Δ and $\langle\Delta\rangle$ are equal strictly to zero. However, Δ becomes infinite at any of the singularities if they are not properly included in the calculated wave function, even when the wave function itself displays very smooth behavior, as shown by Bartlett *et al.*[10,11] many years ago.

In the CFHH method[4-9] one writes the wave function as a product of two factors

$$\psi=\chi\phi , \tag{3}$$

where χ is the "correlation function" and ϕ is expanded in the usual hyperspherical-harmonic (HH) functions. If the correlation function χ is chosen to describe the singular features of ψ (like cusps), the convergence of the HH expansion for ϕ should be rapid. The solution for ϕ proceeds as in the usual HH method, except the potential V is replaced by an effective velocity-dependent potential V':

$$V'=V-\frac{1}{2}\frac{\nabla^2\chi}{\chi}-(\nabla\ln\chi)\nabla , \tag{4}$$

where ∇ is the six-dimensional gradient operator. For systems of two identical particles a correlation function $\chi=\exp(f)$ of the simple spatially symmetric form has been normally employed:

$$f=-\gamma(r_{13}+r_{23})-\delta r_{12} , \tag{5}$$

where particle 3 is the unlike mass and parameters γ and δ are chosen to describe cusps or other physical features of the wave function.[4-9]

Two obvious choices for these parameters are used in calculations presented in this paper. The first one is based on requirements of absence of Coulomb singularities in the equation for function f [cusp parametrization,[4-9] for which $\gamma=MZ/(M+1)$ and $\delta=-0.5$]. Clearly, the cusp parametrization is expected to work best for small systems, and therefore was used in our calculations of the ground-state helium atom, since electrons there are close to the nucleus and to each other. An alternative description could be given by the uncorrelated cusp parametrization for which $\gamma=MZ/(M+1)$ and $\delta=0$. This choice takes care of the singularity of interaction between the nucleus and the electron, which are attracted and therefore closer to each other, but neglects those between two electrons which are more distantly located due to their repulsion. Such parametrizations could be most appropriate for loosely bound and clustered systems, such as the positronium ion Ps^- or excited $2\,^1S$ state of the helium atom He*. These systems are adequately represented, respectively, as a positronium or He^+ core with an extra loosely bound and nearly uncorrelated electron.

The results of calculations are presented in Tables I–VII. In order to estimate the influence of the inclusion of all cusp conditions, the extended system He* is calculated in both cusp and uncorrelated cusp parametrizations. The resulting energies E and expectation values of the Hamiltonian $\langle H\rangle$ (which in our approach are not automatically equal to each other[4]) are presented in Table I. One can see that for higher $K_m\geq 32$ the values of $\langle H\rangle$ in both parametrizations are approximately equally good, so the quality of the wave function is of decisive importance in choosing the proper parametrization. Tables II, III, and V show that the inclusion of all the proper cusp conditions in the calculation of the helium atom gives an extremely good wave function accurate (in case of the ground state) up to 10^{-7} near the coalescence points. Table II shows that such accuracy for the ground-state wave function holds in fact over nearly the whole range of values of the interparticle distances, including the asymptotic ones. This is not true, however, for the excited-state wave function, displayed in Table III, due to the fact that the inclusion of the repulsive electron-electron cusp, represented by a growing exponential, tends to distort the description of the asymptotic behavior of the wave function, which results in inferior convergence of the wave function at larger distances. On the other hand, a failure in cases of the excited helium state and of the negative positronium ion to include even the least important cusp condition, corresponding to the two repelling electrons generally located far from each other, leads to the wave functions (displayed in Tables IV and VI) which are much less accurate not only near the coalescence points ($\sim 10^{-2}$) but also away from them ($\sim 10^{-4}$–10^{-5}). This shows up most dramatically in the huge values of local relative deviation Δ near the coalescence point $r_{12}=0$. Away from the coalescence points Δ, though reasonably small, does not yet in some cases display the convergent behavior. The inclusion of the electron-electron cusp condition for the excited helium atom, as can be seen from the comparison of Tables III and IV), immediately reduces the value of Δ at the coalescence points by 5–6 orders of magnitude. (Even a more

TABLE I. Eigenvalues E and expectation values of the Hamiltonian $\langle H\rangle$ (a.u.) for the excited helium atom. The numbers in the first and second lines of each entry are calculated in the uncorrelated cusp and cusp parametrizations, respectively.

K_m	$-E$	K_m	$-E$	$-\langle H\rangle$
0	1.586 5273	24	2.145 921 28	2.145 972 60
	1.752 2815		2.145 072 77	2.145 951 11
4	1.775 7997	32	2.145 953 75	2.145 973 44
	1.923 7454		2.145 732 78	2.145 971 02
8	2.140 2364	40	2.145 965 21	2.145 973 76
	2.075 2848		2.145 899 43	2.145 973 54
12	2.145 8083	48	2.145 969 76	2.145 973 85
	2.155 6280		2.145 948 36	2.145 973 77
16	2.145 8095	exact		2.145 974 05
	2.141 6743			
20	2.146 0331			
	2.147 9710			

TABLE II. Ground-state helium wave function ψ (a.u.) and the local relative deviation Δ (%) at different interparticle distances r_{13}, r_{23}, and r_{12}, in the units of their corresponding expectation values (Ref. 5) $\langle r_{13}\rangle=\langle r_{23}\rangle=0.929\,472\,341$ and $\langle r_{12}\rangle=1.422\,070\,455$ a.u. The three consecutive numbers in each column correspond to the maximum global angular momenta $K_m=32$, 40, and 48. The value of the normalization integral $\langle\psi|\psi\rangle$ is $8.068\,527\times10^{-4}$ for all K_m. The values marked zero in the table were actually calculated at distances equal to $10^{-6}\langle r_{ij}\rangle$. The numbers in brackets represent powers of 10.

r_{13}	r_{23}	r_{12}	ψ	Δ	r_{13}	r_{23}	r_{12}	ψ	Δ
0.0	0.0	0.0	6.099 432 910[−2]	0.412	1.0	1.0	1.0	2.859 228 718[−3]	0.002
			6.099 431 812[−2]	−0.211				2.859 227 732[−3]	0.005
			6.099 431 705[−2]	0.473				2.859 228 115[−3]	0.003
0.25	0.25	0.0	2.485 126 200[−2]	2.040	1.5	0.25	1.0	4.899 098 600[−3]	0.045
			2.485 130 244[−2]	1.647				4.899 111 928[−3]	0.012
			2.485 132 315[−2]	1.382				4.899 117 194[−3]	−0.006
0.25	0.25	0.25	2.856 250 722[−2]	−0.013	1.5	0.5	1.0	3.100 052 838[−3]	−0.008
			2.856 250 051[−2]	−0.006				3.100 049 825[−3]	0.002
			2.856 249 975[−2]	−0.005				3.100 050 881[−3]	−0.004
0.5	0.25	0.25	1.866 329 611[−2]	−0.003	1.5	1.0	0.5	1.081 333 596[−3]	0.011
			1.866 329 145[−2]	0.025				1.081 335 887[−3]	−0.002
			1.866 329 813[−2]	−0.029				1.081 336 390[−3]	−0.010
0.5	0.5	0.0	1.037 909 881[−2]	2.166	1.5	1.0	1.0	1.267 833 925[−3]	−0.011
			1.037 917 238[−2]	1.754				1.267 833 310[−3]	−0.010
			1.037 920 688[−2]	1.474				1.267 832 374[−3]	−0.002
0.5	0.5	0.25	1.199 624 536[−2]	0.057	1.5	1.0	1.5	1.422 608 388[−3]	−0.019
			1.199 625 652[−2]	0.016				1.422 603 885[−3]	0.002
			1.199 625 617[−2]	0.024				1.422 602 745[−3]	0.014
0.5	0.5	0.5	1.329 645 285[−2]	−0.007	1.5	1.5	0.0	3.457 218 125[−4]	2.584
			1.329 644 858[−2]	−0.001				3.457 457 922[−4]	2.111
			1.329 644 817[−2]	−0.002				3.457 570 701[−4]	1.786
1.0	0.25	0.5	9.242 905 573[−3]	0.147	1.5	1.5	0.25	4.031 247 668[−4]	−0.111
			9.242 986 764[−3]	−0.083				4.031 109 749[−4]	0.131
			9.242 980 196[−3]	−0.026				4.031 115 181[−4]	0.127
1.0	0.5	0.5	5.840 423 361[−3]	−0.003	1.5	1.5	0.5	4.535 748 851[−4]	−0.082
			5.840 422 246[−3]	0.015				4.535 691 152[−4]	0.008
			5.840 427 312[−3]	−0.017				4.535 678 750[−4]	0.038
1.0	1.0	0.0	1.870 552 685[−3]	2.367	1.5	1.5	1.0	5.395 148 621[−4]	0.046
			1.870 608 273[−3]	1.922				5.395 199 929[−4]	−0.007
			1.870 634 308[−3]	1.618				5.395 196 550[−4]	−0.002
1.0	1.0	0.25	2.174 282 408[−3]	0.172	1.5	1.5	1.5	6.113 661 550[−4]	0.009
			2.174 310 638[−3]	−0.009				6.113 662 520[−4]	0.011
			2.174 314 085[−3]	−0.038				6.113 667 192[−4]	0.006
1.0	1.0	0.5	2.432 549 115[−3]	0.043	2.0	0.5	1.0	1.485 704 606[−3]	0.040
			2.432 558 258[−3]	0.001				1.485 724 921[−3]	−0.037
			2.432 556 829[−3]	0.016				1.485 723 578[−3]	−0.003
2.0	0.5	1.5	1.613 896 863[−3]	−0.070	2.0	2.0	2.0	1.302 852 680[−4]	0.017
			1.613 872 273[−3]	0.021				1.302 854 914[−4]	0.019
			1.613 871 507[−3]	0.013				1.302 857 923[−4]	0.011
2.0	1.0	1.0	5.891 266 529[−4]	−0.003	4.0	1.0	2.0	4.144 591 397[−5]	−0.046
			5.891 269 508[−4]	0.007				4.144 613 741[−5]	−0.009
			5.891 279 279[−4]	−0.007				4.144 596 221[−5]	0.016
2.0	1.0	1.5	6.554 470 342[−4]	−0.010	4.0	1.5	2.0	1.623 453 732[−5]	−0.038
			6.554 461 506[−4]	−0.005				1.623 419 942[−5]	0.018
			6.554 457 689[−4]	−0.001				1.623 431 773[−5]	0.001
2.0	1.5	0.5	2.031 936 703[−4]	0.021	4.0	2.0	1.5	5.927 249 390[−6]	−0.060
			2.031 948 347[−4]	0.0005				5.926 994 260[−6]	0.034
			2.031 949 671[−4]	−0.0001				5.927 155 888[−6]	−0.021
2.0	1.5	1.0	2.408 889 961[−4]	−0.038	4.0	2.0	2.0	6.405 748 910[−6]	−0.004
			2.408 860 041[−4]	0.026				6.405 784 389[−6]	0.004
			2.408 872 792[−4]	−0.006				6.405 820 175[−6]	−0.002
2.0	1.5	1.5	2.728 023 496[−4]	0.026	4.0	4.0	0.0	8.871 882 723[−8]	3.341
			2.728 038 825[−4]	0.008				8.876 892 727[−8]	2.763
			2.728 042 903[−4]	−0.001				8.879 270 256[−8]	2.364
2.0	1.5	2.0	3.005 757 523[−4]	0.010	4.0	4.0	0.25	1.042 123 924[−7]	−0.727
			3.005 762 023[−4]	0.003				1.042 119 083[−7]	−0.833
			3.005 767 736[−4]	−0.014				1.042 026 225[−7]	−0.772

TABLE II. (*Continued*).

r_{13}	r_{23}	r_{12}	ψ	Δ	r_{13}	r_{23}	r_{12}	ψ	Δ
2.0	2.0	0.0	6.493 186 410[−5]	2.766	4.0	4.0	0.5	1.187 755 550[−7]	−0.910
			6.494 014 137[−5]	2.268				1.187 041 843[−7]	−0.341
			6.494 404 641[−5]	1.925				1.186 759 862[−7]	0.014
2.0	2.0	0.25	7.588 085 214[−5]	−0.629	4.0	4.0	1.0	1.453 903 728[−7]	0.312
			7.587 271 769[−5]	−0.231				1.454 467 201[−7]	−0.046
			7.586 939 744[−5]	0.015				1.454 503 300[−7]	−0.103
2.0	2.0	0.5	8.569 591 026[−5]	0.200	4.0	4.0	1.5	1.696 674 107[−7]	−0.161
			8.570 131 609[−5]	−0.027				1.696 238 658[−7]	0.103
			8.570 180 347[−5]	−0.061				1.696 417 465[−7]	−0.033
2.0	2.0	1.0	1.028 487 740[−4]	0.042	4.0	4.0	2.0	1.916 603 804[−7]	0.081
			1.028 505 601[−4]	−0.014				1.916 838 496[−7]	−0.040
			1.028 500 593[−4]	0.014				1.916 760 334[−7]	0.024
2.0	2.0	1.5	1.174 899 074[−4]	−0.031	4.0	4.0	4.0	2.640 290 949[−7]	0.080
			1.174 884 698[−4]	0.014				2.640 415 403[−7]	0.085
			1.174 885 673[−4]	0.015				2.640 530 317[−7]	0.051

TABLE III. Same as in Table II, but for the excited $2\,^1S$ normalized helium wave function for the cusp parametrization. The values of r_{13}, r_{23}, and r_{12} are given in units of the corresponding expectation values (Ref. 5): $\langle r_{13}\rangle = \langle r_{23}\rangle = 2.973\,0707$, $\langle r_{12}\rangle = 5.269\,7209$ a.u. The numbers in brackets represent powers of 10.

r_{13}	r_{23}	r_{12}	ψ	Δ	r_{13}	r_{23}	r_{12}	ψ	Δ
0.0	0.0	0.0	0.660 181 420	−0.1808	1.0	1.0	1.0	−3.942 093 86[−4]	0.3050
			0.658 858 052	−0.1503				−3.935 253 41[−4]	−0.1762
			0.658 422 916	−0.0109				−3.932 341 17[−4]	0.0329
0.25	0.25	0.0	3.187 474 27[−2]	4.179	1.5	0.5	1.0	−2.748 559 09[−3]	−0.0960
			3.181 332 96[−2]	3.401				−2.744 526 13[−3]	−0.0098
			3.179 320 15[−2]	2.864				−2.743 169 81[−3]	0.0283
0.25	0.25	0.25	4.701 868 50[−2]	−0.0164	1.5	1.0	0.5	−1.259 657 05[−4]	−0.0281
			4.692 709 63[−2]	−0.0380				−1.257 781 29[−4]	0.0032
			4.689 672 64[−2]	−0.0120				−1.257 171 86[−4]	−0.0059
0.5	0.25	0.25	3.327 235 33[−3]	−0.0253	1.5	1.0	1.0	−1.517 816 19[−4]	−0.0185
			3.322 818 36[−3]	0.0440				−1.515 529 04[−4]	0.0009
			3.321 337 56[−3]	−0.0015				−1.514 762 84[−4]	0.0059
0.5	0.5	0.0	−7.258 783 39[−4]	−11.98	1.5	1.5	0.0	−5.467 392 15[−6]	0.3867
			−7.236 632 95[−4]	−9.738				−5.459 849 62[−6]	0.3666
			−7.229 165 96[−4]	−8.205				−5.457 409 18[−6]	0.3366
0.5	0.5	0.25	−1.079 283 75[−3]	−0.1518	1.5	1.5	0.25	−8.561 247 14[−6]	0.6704
			−1.076 201 00[−3]	0.0753				−8.550 435 64[−6]	0.7545
			−1.075 219 27[−3]	−0.0031				−8.550 527 69[−6]	0.1450
0.5	0.5	0.5	−1.268 172 96[−3]	0.0703	1.5	1.5	0.5	−1.093 195 55[−5]	−0.3471
			−1.264 516 01[−3]	−0.1123				−1.090 911 89[−5]	0.3169
			−1.263 305 38[−3]	−0.0111				−1.090 776 63[−5]	−0.1696
1.0	0.25	0.5	−1.355 128 66[−2]	0.0634	1.5	1.5	1.0	−1.435 521 12[−5]	−0.5830
			−1.352 522 63[−2]	0.0204				−1.432 473 94[−5]	−0.1033
			−1.351 661 00[−2]	−0.0010				−1.431 480 63[−5]	0.1314
1.0	0.5	0.5	−3.161 166 30[−3]	−0.0006	1.5	1.5	1.5	−1.672 031 09[−5]	1.453
			−3.154 999 07[−3]	0.0108				−1.673 584 80[−5]	0.7001
			−3.152 949 35[−3]	−0.0072				−1.671 467 57[−5]	0.1658
1.0	1.0	0.0	−1.582 422 15[−4]	0.3238	2.0	0.25	1.0	−7.542 141 61[−3]	0.0249
			−1.579 382 04[−4]	0.2967				−7.540 125 59[−3]	0.0445
			−1.578 387 63[−4]	0.2670				−7.539 395 58[−3]	0.0287
1.0	1.0	0.25	−2.450 659 55[−4]	0.0324	2.0	0.5	1.0	−1.697 297 47[−3]	0.0906
			−2.446 179 08[−4]	0.2662				−1.696 841 91[−3]	0.0508
			−2.444 324 75[−4]	0.0575				−1.696 701 03[−3]	0.0040
1.0	1.0	0.5	−3.077 953 56[−4]	−0.2232	2.0	1.0	1.0	−8.599 268 98[−5]	0.0012
			−3.071 418 59[−4]	−0.0844				−8.596 243 96[−5]	−0.0273
			−3.069 532 94[−4]	−0.0135				−8.594 719 43[−5]	−0.0072

TABLE III. (*Continued*).

r_{13}	r_{23}	r_{12}	ψ	Δ	r_{13}	r_{23}	r_{12}	ψ	Δ
2.0	1.0	1.5	−9.314 167 92[−5]	0.1469	4.0	1.5	1.5	−3.529 349 12[−7]	0.1452
			−9.312 959 65[−5]	−0.0334				−3.576 875 27[−7]	−0.0919
			−9.311 381 58[−5]	−0.0323				−3.593 811 20[−7]	0.0356
2.0	1.5	0.5	−3.750 780 47[−6]	0.0441	4.0	1.5	2.0	−3.654 247 82[−7]	0.2770
			−3.749 135 71[−6]	−0.0080				−3.706 293 61[−7]	−0.0053
			−3.748 390 09[−6]	−0.0064				−3.726 167 42[−7]	−0.0831
2.0	1.5	1.0	−4.607 592 39[−6]	0.2427	4.0	2.0	1.5	−1.767 581 91[−8]	0.1507
			−4.607 615 26[−6]	−0.1529				−1.791 232 94[−8]	−0.1157
			−4.605 931 16[−6]	0.0042				−1.798 322 72[−8]	0.0709
2.0	1.5	1.5	−5.226 217 72[−6]	0.1877	4.0	2.0	2.0	−1.855 148 57[−8]	0.0444
			−5.221 224 34[−6]	0.1123				−1.880 692 61[−8]	−0.1576
			−5.220 183 48[−6]	0.1669				−1.888 759 55[−8]	−0.0246
2.0	2.0	0.0	−1.538 171 42[−7]	0.0833	4.0	4.0	0.0	−5.989 975 33[−14]	1.950
			−1.537 359 14[−7]	0.1398				−6.037 879 51[−14]	−1.595
			−1.537 103 38[−7]	0.1584				−6.055 218 34[−14]	−1.347
2.0	2.0	0.25	−2.432 184 65[−7]	−1.771	4.0	4.0	0.25	−9.912 061 37[−14]	−9.920
			−2.423 552 49[−7]	0.2049				−9.838 639 42[−14]	−7.373
			−2.422 061 83[−7]	0.8110				−9.770 829 91[−14]	−5.375
2.0	2.0	0.5	−3.122 580 34[−7]	0.0732	4.0	4.0	0.5	−1.255 418 17[−13]	−2.898
			−3.123 274 03[−7]	−0.7080				−1.245 001 98[−13]	−1.366
			−3.119 102 44[−7]	0.1351				−1.249 411 20[−13]	2.541
2.0	2.0	1.0	−4.169 477 21[−7]	−1.147	4.0	4.0	1.0	−1.740 462 56[−13]	−0.8581
			−4.155 125 90[−7]	0.4331				−1.754 308 97[−13]	−4.117
			−4.156 650 56[−7]	−0.0897				−1.721 202 04[−13]	0.8531
2.0	2.0	1.5	−4.888 702 52[−7]	2.106	4.0	4.0	1.5	−1.900 276 72[−13]	11.28
			−4.898 806 69[−7]	1.020				−2.122 564 89[−13]	−2.275
			−4.902 681 39[−7]	0.4479				−2.085 082 59[−13]	−0.4664
2.0	2.0	2.0	−5.409 686 84[−7]	6.730	4.0	4.0	2.0	−2.721 283 51[−13]	−25.24
			−5.507 054 35[−7]	2.969				−2.287 738 60[−13]	11.11
			−5.475 206 28[−7]	0.7181				−2.379 691 44[−13]	−2.416
4.0	0.5	2.0	−1.411 301 96[−4]	0.1298	4.0	4.0	4.0	4.350 761 85[−12]	−183.1
			−1.432 143 16[−4]	0.1266				−1.840 481 05[−12]	−166.3
			−1.440 382 95[−4]	0.0551				2.275 326 08[−15]	−26 724.0
4.0	1.0	2.0	−7.189 067 17[−6]	0.2073					
			−7.290 419 79[−6]	0.1130					
			−7.331 429 11[−6]	0.0034					

TABLE IV. Same as in Table III, but for the uncorrelated cusp parametrization.

r_{13}	r_{23}	r_{12}	ψ	Δ	r_{13}	r_{23}	r_{12}	ψ	Δ
0.0	0.0	0.0	0.658 143 901	−3.596[+5]	1.0	1.0	1.0	−3.931 301 975[−4]	−0.169
			0.658 153 576	3.044[+5]				−3.930 670 278[−4]	0.122
			0.658 155 906	−1.427[+5]				−3.930 913 118[−4]	−0.066
0.25	0.25	0.0	3.263 367 526[−2]	−8.842[+6]	1.5	0.5	1.0	−2.742 432 147[−3]	−0.027
			3.247 609 822[−2]	−8.842[+6]				−2.742 373 679[−3]	−0.001
			3.236 758 773[−2]	−8.842[+6]				−2.742 341 526[−3]	0.027
0.25	0.25	0.25	4.687 933 475[−2]	−1.015	1.5	1.0	0.5	−1.257 089 543[−4]	−0.275
			4.687 716 367[−2]	0.815				−1.256 624 651[−4]	0.202
			4.687 859 674[−2]	−0.404				−1.256 860 540[−4]	−0.143
0.5	0.25	0.25	3.320 015 713[−3]	0.551	1.5	1.0	1.0	−1.514 296 456[−4]	0.013
			3.320 513 753[−3]	−1.160				−1.514 302 284[−4]	0.003
			3.320 362 495[−3]	−0.488				−1.514 301 635[−4]	−0.005

TABLE IV. (*Continued*).

r_{13}	r_{23}	r_{12}	ψ	Δ	r_{13}	r_{23}	r_{12}	ψ	Δ
0.5	0.5	0.0	−7.606 344 964[−4]	−8.842[+6]	1.5	1.5	0.0	−6.298 999 850[−6]	−8.843[+6]
			−7.536 696 294[−4]	−8.842[+6]				−6.148 591 366[−6]	−8.843[+6]
			−7.488 432 870[−4]	−8.842[+6]				−6.043 570 969[−6]	−8.843[+6]
0.5	0.5	0.25	−1.074 502 894[−3]	1.135	1.5	1.5	0.25	−8.548 785 920[−6]	−1.025
			−1.074 749 950[−3]	−0.586				−8.563 976 481[−6]	−2.469
			−1.074 655 393[−3]	0.161				−8.553 935 418[−6]	−0.785
0.5	0.5	0.5	−1.262 793 669[−3]	−0.487	1.5	1.5	0.5	−1.089 683 796[−5]	0.375
			−1.262 624 956[−3]	0.333				−1.090 787 883[−5]	−0.480
			−1.262 667 306[−3]	−0.190				−1.090 074 311[−5]	0.391
1.0	0.25	0.5	−1.351 047 238[−2]	0.121	1.5	1.5	1.0	−1.430 889 595[−5]	0.152
			−1.351 094 068[−2]	0.093				−1.431 100 141[−5]	0.054
			−1.351 124 941[−2]	0.022				−1.431 214 170[−5]	−0.064
1.0	0.5	0.5	−3.151 586 911[−3]	0.067	1.5	1.5	1.5	−1.671 438 075[−5]	−0.102
			−3.151 821 826[−3]	−0.148				−1.671 070 883[−5]	0.062
			−3.151 742 303[−3]	−0.066				−1.671 192 228[−5]	−0.039
1.0	1.0	0.0	−1.742 995 912[−4]	−8.843[+6]	2.0	0.25	1.0	−7.538 395 563[−3]	−0.033
			−1.713 059 202[−4]	−8.843[+6]				−7.538 703 769[−3]	−0.012
			−1.692 296 710[−4]	−8.843[+6]				−7.538 744 316[−3]	0.008
1.0	1.0	0.25	−2.444 129 479[−4]	−0.251	2.0	0.5	1.0	−1.696 476 074[−3]	0.021
			−2.441 764 608[−4]	1.664				−1.696 510 923[−3]	0.011
			−2.443 503 331[−4]	−0.424				−1.696 536 222[−3]	0.002
1.0	1.0	0.5	−3.067 480 932[−4]	0.444	2.0	1.0	1.0	−8.593 578 691[−5]	0.010
			−3.068 630 298[−4]	−0.228				−8.593 933 710[−5]	−0.026
			−3.068 247 442[−4]	0.062				−8.593 767 941[−5]	−0.013
2.0	1.0	1.5	−9.310 161 232[−5]	0.021	4.0	1.5	1.5	−3.606 879 961[−7]	−0.001
			−9.310 274 758[−5]	−0.012				−3.606 562 997[−7]	−0.0002
			−9.310 170 639[−5]	−0.010				−3.606 520 782[−7]	−0.0008
2.0	1.5	0.5	−3.746 071 315[−6]	0.302	4.0	1.5	2.0	−3.739 565 979[−7]	−0.0003
			−3.747 430 444[−6]	0.075				−3.739 125 144[−7]	0.0002
			−3.748 673 455[−6]	−0.246				−3.739 019 564[−7]	−0.001
2.0	1.5	1.0	−4.606 034 205[−6]	−0.084	4.0	2.0	1.5	−1.804 710 816[−8]	−0.0003
			−4.604 904 387[−6]	0.069				−1.804 594 397[−8]	−0.0003
			−4.605 266 673[−6]	0.005				−1.804 532 122[−8]	−0.0001
2.0	1.5	1.5	−5.220 415 866[−6]	0.003	4.0	2.0	2.0	−1.895 064 214[−8]	−0.001
			−5.220 426 649[−6]	−0.019				−1.894 866 110[−8]	−0.0007
			−5.220 379 825[−6]	−0.028				−1.894 794 477[−8]	−0.002
2.0	2.0	0.0	−1.847 759 868[−7]	−8.843[+6]	4.0	4.0	0.0	−8.258 062 436[−14]	−8.843[+6]
			−1.793 408 379[−7]	−8.843[+6]				−7.935 449 799[−14]	−8.843[+6]
			−1.755 099 511[−7]	−8.843[+6]				−7.685 301 512[−14]	−8.843[+6]
2.0	2.0	0.25	−2.403 340 852[−7]	3.703	4.0	4.0	0.25	−9.556 158 974[−14]	4.772
			−2.419 019 839[−7]	0.290				−9.507 141 379[−14]	5.991
			−2.426 753 649[−7]	−2.042				−9.505 956 606[−14]	6.267
2.0	2.0	0.5	−3.120 625 907[−7]	−0.059	4.0	4.0	0.5	−1.243 738 585[−13]	2.304
			−3.115 877 507[−7]	0.717				−1.259 895 938[−13]	0.247
			−3.119 500 433[−7]	−0.170				−1.266 554 932[−13]	−0.841
2.0	2.0	1.0	−4.154 168 589[−7]	0.194	4.0	4.0	1.0	−1.730 795 553[−13]	0.424
			−4.156 516 602[−7]	−0.082				−1.729 428 647[−13]	0.552
			−4.155 727 738[−7]	0.029				−1.733 703 558[−13]	0.045
2.0	2.0	1.5	−4.905 773 793[−7]	−0.079	4.0	4.0	1.5	−2.093 237 419[−13]	0.138
			−4.905 178 619[−7]	−0.063				−2.092 760 334[−13]	0.207
			−4.904 861 757[−7]	−0.042				−2.093 838 732[−13]	0.099
2.0	2.0	2.0	−5.480 879 177[−7]	−0.077	4.0	4.0	2.0	−2.379 052 225[−13]	0.283
			−5.479 296 973[−7]	0.041				−2.382 800 061[−13]	0.059
			−5.479 719 293[−7]	−0.029				−2.382 581 931[−13]	0.073
4.0	0.5	2.0	−1.446 576 726[−4]	−0.013	4.0	4.0	4.0	−3.148 682 722[−13]	−0.169
			−1.446 541 526[−4]	−0.007				−3.145 210 851[−13]	−0.049
			−1.446 520 806[−4]	0.0001				−3.144 943 551[−13]	−0.055
4.0	1.0	2.0	−7.361 354 234[−6]	0.002					
			−7.360 698 977[−6]	−0.001					
			−7.360 490 534[−6]	−0.0002					

TABLE V. Values of the normalized wave functions (a.u.) for ground (He) and excited (He*) states of the helium atom at zero distance between one of the electrons and the nucleus ($r_{13}\equiv 0$) for different interparticle distances $r_{23}\equiv r_{12}$ (a.u.). The Ψ and Δ (%) displayed in the first and second columns for the excited helium are calculated in uncorrelated cusp and cusp parametrizations, respectively. The numbers in brackets represent powers of 10.

	He		He*		He*	
r_{13}	ψ	Δ	ψ	Δ	ψ	Δ
0.25	1.476 907 667	0.672	0.448 514 143	5.079	0.449 905 410	0.699
	1.476 907 606	0.544	0.448 522 684	4.136	0.449 004 555	0.570
	1.476 907 806	0.457	0.448 525 163	3.486	0.448 708 324	0.479
0.5	1.017 707 174	0.464	0.298 516 692	2.360	0.299 442 059	0.233
	1.017 707 750	0.355	0.298 523 694	1.886	0.298 844 795	0.164
	1.017 708 171	0.281	0.298 525 883	1.562	0.298 648 302	0.115
1.0	0.486 157 075	0.049	0.113 520 592	0.357	0.113 866 559	−0.735
	0.486 158 016	−0.029	0.113 524 239	0.188	0.113 644 931	−0.686
	0.486 158 499	−0.083	0.113 525 393	0.075	0.113 571 403	−0.654
1.5	0.234 018 303	−0.317	1.807 898 331[−2]	−1.851	1.812 431 80[−2]	−3.176
	0.234 019 012	−0.374	1.807 972 363[−2]	−1.716	1.809 615 46[−2]	−2.721
	0.234 019 326	−0.412	1.808 075 049[−2]	−3.022	1.808 648 57[−2]	−2.416
2.0	0.113 418 896	0.822	−3.002 386 246[−2]	1.886	−3.012 771 99[−2]	1.838
	0.113 419 373	0.778	−3.002 513 825[−2]	1.675	−3.006 073 60[−2]	1.638
	0.113 419 535	0.751	−3.002 559 589[−2]	1.543	−3.003 885 19[−2]	1.506
4.0	6.588 016 599[−3]	−6.151	−5.731 974 258[−2]	−8.343	−5.746 294 39[−2]	−8.364
	6.588 391 102[−3]	−6.184	−5.732 212 502[−2]	−8.361	−5.737 369 79[−2]	−8.394
	6.588 471 703[−3]	−6.200	−5.732 303 780[−2]	−8.374	−5.734 328 19[−2]	−8.409
8.0	2.531 439 281[−5]	−5.833	−1.549 909 779[−2]	−8.430	−1.541 839 86[−2]	−8.265
	2.538 174 720[−5]	−6.039	−1.549 858 427[−2]	−8.431	−1.547 111 16[−2]	−8.351
	2.540 188 434	−6.128	−1.549 846 704[−2]	−8.431	−1.548 829 35[−2]	−8.391

dramatic effect occurs in the case of the positronium ion, where the values of Δ at the triple and different double coalescence points reduce from values 9.52×10^{6} and 3.82×10^{8} of Table VI to values around 0.3 and 10–20, respectively, that is, by more than 7 orders of magnitude.)

The expectation values of the absolute value of $|\Delta|$ presented in Table VII show the influence of the proper inclusion of cusp conditions on the overall goodness of the calculated wave function. One can see that though the inclusion of all cusp conditions produces wave functions which are much better near the coalescence points and at small and medium interparticle distances, the distortion of the asymptotic behavior of the wave function due to inclusion of the electron-electron cusp make values of $\langle|\Delta|\rangle$ for cusp and uncorrelated cusp parametrizations comparable in the case of the excited Helium atom. For the positronium ion the average value of $|\Delta|$ is even much larger for the cusp parametrization, due to the fact that the correlation function with cusp parameters gives a completely inadequate description of this rather extended system at the large distances.

The Kato cusp conditions, in the case of two particles of equal masses, specify that γ and δ defined as the logarithmic derivatives $\gamma=(1/\psi)(d\psi/dr_{13})$ and $\delta=(1/\psi)(d\psi/dr_{12})$ for the exact wave function should be $MZ/(M+1)$ and -0.5 when the derivatives are taken strictly at $r_{13}=0$ and $r_{12}=0$, respectively. (In that case they are also strictly independent of other interparticle distances.) Since in our case the exact wave function is given by Eq. (3) where the function ϕ is smooth, its derivatives strictly at the corresponding coalescence points will be equal, however, to the correlation parameters γ and δ of the correlation function χ, given by Eq. (5). Near the coalescence points, however, the hyperspherical harmonic expansion is expected to be able to reproduce the cusp behavior even if the chosen correlation parameters are different from those given above and the better the more hyperspherical harmonic functions are taken into account. In order to understand how closely this behavior is mimicked very near the coalescence points and how it changes with K_m in the case of the excited helium atom and the positron negative ion, we calculated the logarithmic derivative $\delta=(1/\psi)(d\psi/dr_{12})$ at zero interparticle distance r_{12} (actual numerical differentiation was performed at $r_{12}=10^{-6}$ a.u.). The results for uncorrelated cusp parametrization, where the correlation parameters δ of the correlation function χ was chosen to be 0, are -0.5011, -0.5002, and -0.4999 for $K_m=32$, 40, and 48 in the case of the excited helium atom and -0.4994 for $K_m=32$ in the case of the positronium ion, which shows that indeed the hyperspherical-harmonic expansion is able to reproduce cusp structure reasonably well if only a large enough number of hyperspherical-harmonic functions is taken into account.

Summing up, we have shown that proper inclusion of all cusps dramatically increases the quality of the wave function at small and medium interparticle distances. For the ground state of the helium atom it yields local wave-function accuracy of about 10^{-7} at all interparticle distances. The omission of even the least important of the cusps in the case of the excited helium atom reduces the wave-function precision to 10^{-2} near the corresponding coalescence point and to 10^{-4}–10^{-5} away from it.

The results displayed in Tables I–VII clearly illustrate the utility of the CFHH method for direct calculation of

TABLE VI. Absolute values $|\Delta|$ of the local relative deviation (%) for $K_m=32$ for the positronium negative ion Ps^- in the uncorrelated cusp parametrization. Interparticle distances r_{13}, r_{23}, and r_{12} are in the units of the corresponding expectation values (Ref. 7): $\langle r_{13}\rangle=\langle r_{23}\rangle=5.488\,352$, $\langle r_{12}\rangle=8.546\,111$ a.u. The numbers in brackets represent powers of 10.

r_{13}	r_{23}	r_{12}	Δ	r_{13}	r_{23}	r_{12}	Δ
0.0	0.0	0.0	9.52[+6]	1.5	2.0	1.0	0.53
				1.5	2.0	1.5	1.01
0.25	0.25	0.0	3.82[+8]	1.5	2.0	2.0	3.51
0.25	0.25	0.25	2.17	1.5	4.0	1.5	0.21
0.25	0.5	0.25	1.22				
0.25	1.0	0.5	1.60	2.0	2.0	0.0	3.82[+8]
0.25	1.5	1.0	0.86	2.0	2.0	0.25	8.75
				2.0	2.0	0.5	0.88
0.5	0.5	0.0	3.82[+8]	2.0	2.0	1.0	0.67
0.5	0.5	0.25	3.86	2.0	2.0	1.5	0.79
0.5	0.5	0.5	0.95	2.0	2.0	2.0	0.63
0.5	1.0	0.5	0.43	2.0	4.0	1.5	0.07
0.5	1.5	1.0	0.03	2.0	4.0	2.0	0.04
0.5	2.0	1.0	0.58	2.0	8.0	4.0	0.03
0.5	2.0	1.5	1.25				
				4.0	4.0	0.0	3.82[+8]
1.0	1.0	0.0	3.82[+8]	4.0	4.0	0.25	20.17
1.0	1.0	0.25	2.64	4.0	4.0	0.5	3.01
1.0	1.0	0.5	1.53	4.0	4.0	1.0	0.26
1.0	1.0	1.0	0.55	4.0	4.0	1.5	0.20
1.0	1.5	0.5	0.52	4.0	4.0	2.0	0.44
1.0	1.5	1.0	0.53	4.0	4.0	4.0	2.53
1.0	1.5	1.5	2.17	4.0	8.0	4.0	0.003
1.0	2.0	1.0	0.15				
1.0	2.0	1.5	1.15	8.0	8.0	0.0	3.82[+8]
1.0	4.0	2.0	0.20	8.0	8.0	0.25	7.17
				8.0	8.0	0.5	8.71
1.5	1.5	0.0	3.82[+8]	8.0	8.0	1.0	1.10
1.5	1.5	0.25	1.53	8.0	8.0	1.5	0.32
1.5	1.5	0.5	1.47	8.0	8.0	2.0	0.09
1.5	1.5	1.0	0.82	8.0	8.0	4.0	0.91
1.5	1.5	1.5	0.53	8.0	8.0	8.0	68.5
1.5	2.0	0.5	1.51				

three-body wave functions since even without proper inclusion of the cusps local and overall quality of the wave functions is reasonably good for most points. The results displayed in Table VII show, however, the necessity of calculations with the more sophisticated correlation factors χ than the one given in Eq. (3) and used in the present calculations, since this correlation factor does not allow simultaneous incorporation of the singular and cluster structure.

For example, the correlation factor

$$\chi=\exp\left[-\sum_{i,j}(\alpha_{ij}+\beta_{ij}e^{-\gamma_{ij}r_{ij}^2})r_{ij}-\eta(r_{12}-R)^2e^{-\sigma r_{12}^2}\right], \tag{6}$$

suggested in Ref. 8, allows incorporation of both an asymptotic and cusp behavior of all three particles and simultaneously takes care of the tendency of two heavy particles to stay at a fixed distance R. It will ensure, therefore, very precise estimates of wave functions for all interparticle distances. The incorporation of such a correlation factor, however, demands essential changes in the present computer program and will be a subject of future calculations.

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TABLE VII. The expectation value $\langle|\Delta|\rangle$ (%) of absolute values of the relative deviation Δ for the ground and excited states of the helium atom and for the ground state of the positronium negative ion Ps^-. The numbers in the first and second lines of each entry for He^* and Ps^- are calculated in the uncorrelated cusp and cusp parametrizations, respectively.

K_m	He	He^*	Ps^-
32	0.0411	0.112	1.086
		0.211	364.0
40	0.0266	0.079	
		0.112	
48	0.0146	0.067	
		0.070	

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