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Highly accurate evaluation of the few-body auxiliary functions and four-body integrals

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Abstract

Analytical formulae suitable for numerical calculations of the second- and third-order auxiliary functions $A_2(k, m, a, b)$ and $A_3(k, \ell, m, a, b, c)$ are presented. These formulae can directly be used in highly accurate calculations of the $A_2(k, m, a, b)$ and $A_3(k, \ell, m, a, b, c)$ functions. In turn, the highly accurate auxiliary functions of the second and third order are used to compute various four-body integrals, fourth-order auxiliary functions $A_4(k, \ell, m, n, a, b, c, d)$ and so-called general four-body integrals. The $A_2(k, m, a, b)$ and $A_3(k, \ell, m, a, b, c)$ functions can be used to solve a large number of four-, five- and many-body problems from atomic, nuclear and molecular physics.

1. Introduction

In this communication we discuss the problem of highly accurate computations of the few-body auxiliary functions which play a very important role in many few-body problems of atomic, molecular and nuclear physics. Originally, the few-body auxiliary functions were introduced to solve the atomic four-body problems by James and Coolidge [1]. In fact, the computation of the bound states in various few-electron atomic systems is reduced to the calculation of these auxiliary functions. The explicit forms of such functions of the lowest orders are (see e.g. [2–4] and references therein)

$$A_1(k, a) \equiv A(k, a) = \int_0^{+\infty} x^k \exp(-ax)\, \mathrm{d}x = \frac{k!}{a^{k+1}} \tag{1}$$

$$A_2(k, m, a, b) \equiv V(k, m, a, b) = \int_0^{+\infty} x^k \exp(-ax)\, \mathrm{d}x \int_x^{+\infty} y^m \exp(-by)\, \mathrm{d}y \tag{2}$$

$$A_3(k, \ell, m, a, b, c) \equiv W(k, \ell, m, a, b, c)$$
$$= \int_0^{+\infty} x^k \exp(-ax)\, \mathrm{d}x \int_x^{+\infty} y^\ell \exp(-by)\, \mathrm{d}y \int_y^{+\infty} z^m \exp(-cz)\, \mathrm{d}z \tag{3}$$

where all values k, ℓ, m are integers. The first integer parameter k is always non-negative, while m (in the A_2 and A_3 functions) can be positive, equal to zero or negative. The three parameters a, b, c are real positive numbers. The three auxiliary functions A_1, A_2 and A_3 are sufficient to solve a number of actual four-body problems. For five-, six- and many-body problems one has to use the auxiliary functions A_n with index n greater than 3. The auxiliary functions with index greater than 3 can be determined in an analogous manner (see e.g. [5] and below). Note that in this study the auxiliary functions of the order n (where $n = 1, 2, 3, \ldots$) are designated by the notation A_n. In the literature, (see e.g. [1–3]), the notation A, V and W stands for the auxiliary functions of the first, second and third orders, i.e. for the A_1, A_2 and A_3 functions.

Presently, we restrict ourselves to the case of four-body systems, i.e. to the three auxiliary functions A_1, A_2, A_3 of the lowest orders. Our first goal is to derive some simple and numerically stable formulae and recurrence relations for these functions which can be directly used in numerical calculations. Note that the first recurrence relations for the $A_2(k, m, a, b)$ and $A_3(k, \ell, m, a, b, c)$ functions were produced by James and Coolidge [1]. However, later [2] (see also [3]) it was shown that such recurrence relations are not numerically stable for negative m. In this study we develop an approach which allows one to compute the $A_2(k, m, a, b)$ and $A_3(k, \ell, m, a, b, c)$ auxiliary functions for arbitrary values of their arguments to very high (in principle, unlimited) numerical accuracy. All our formulae are tested in actual computations. Moreover, by using the formulae derived by Perkins [6] we also computed highly accurate numerical values for a number of actual four-body integrals. In section 4 we discuss some new applications for the $A_2(k, m, a, b)$ and $A_3(k, \ell, m, a, b, c)$ auxiliary functions.

2. Computational formulae for the second- and third-order auxiliary functions

Let us present the formulae for the second- and third-order auxiliary functions $A_2(k, m, a, b)$ and $A_3(k, \ell, m, a, b, c)$. In general, the second-order auxiliary functions $A_2(k, m, a, b)$ are needed in actual four-body calculations for $k \geqslant 0$ and $k+m \geqslant -1$. For the third-order auxiliary functions $A_3(k, \ell, m, a, b, c)$ the three inequalities $k \geqslant 0$, $\ell \geqslant 0$ and $k + \ell + m \geqslant -1$ must be obeyed [6]. To present the analytical formulae for the second- and third-order auxiliary functions $A_2(k, m, a, b)$ and $A_3(k, \ell, m, a, b, c)$ it is convenient to consider the three following cases. In the first case the parameter m is positive in both the functions $A_2(k, m, a, b)$ and $A_3(k, \ell, m, a, b, c)$. In the second case $m = 0$, while in the third case the parameter m is negative, i.e. $m < 0$. The formulae for the $A_2(k, m, a, b)$ and $A_3(k, \ell, m, a, b, c)$ functions are different in each of these cases.

In the first case, i.e. for positive m, we can write [4]

$$A_2(k, m, a, b) = \sum_{m_1=0}^{m} C_m^{m_1} A_1(m_1, b) A_1(k + m - m_1, a + b), \tag{4}$$

where $A_1(m, c) = \frac{m!}{c^{m+1}}$ is as defined in equation (1), and C_n^m are the binomial coefficients, i.e.

$$C_n^m = \frac{n!}{m!(n-m)!}$$

where $0! = 1$, $C_0^0 = 1$ and $C_m^m = 1$. Analogously, for the $A_3(k, \ell, m, a, b, c)$ function one finds

$$A_3(k, \ell, m, a, b, c) = \sum_{m'=0}^{m} C_m^{m'} A_1(c, m') A_2(k, \ell + m - m', a + b + c, b + c). \tag{5}$$

These formulae can be used in computations of the second- and third-order auxiliary functions $A_2(k, m, a, b)$ and $A_3(k, \ell, m, a, b, c)$ in the case of positive values of m.

In fact, very similar relations can be found for the few-body auxiliary wavefunctions of arbitrary order n. For instance, for the five-body auxiliary function $A_4(k, \ell, m, n, a, b, c, d)$ one finds the following formula:

$$A_4(k, \ell, m, n, a, b, c, d) = \sum_{n_1=0}^{n} C_n^{n_1} A_1(n_1, d) \times A_3(k, \ell, m + n - n_1, a + b + c + d, b + c + d, c + d), \qquad (6)$$

where n is non-negative. This formula can be directly used in computations of the five-body auxiliary functions in the cases when all integer parameters are non-negative. The five-body auxiliary functions are of paramount importance in the bound-state and scattering calculations of various five-body systems, e.g. the beryllium atom and beryllium-like ions.

In the second case, when $m = 0$, we have [4]

$$A_2(k, 0, a, b) = \frac{1}{b}\frac{k!}{(a+b)^{k+1}} = \frac{A_1(k, a+b)}{b}, \qquad (7)$$

where k is an arbitrary (non-negative) integer. In the case when $k = 0$, $m = -1$, the expression for the $A_2(k, m, a, b)$ function takes the form

$$A_2(0, -1, a, b) = \frac{1}{a}\ln\left(\frac{a+b}{b}\right). \qquad (8)$$

Analogously, for the $A_3(k, \ell, m = 0, a, b, c)$ auxiliary function one finds

$$A_3(k, \ell, 0, a, b, c) = \frac{A_2(a, b + c; k, \ell)}{c}. \qquad (9)$$

By using equation (3) one can simplify this expression even further, since k and ℓ are non-negative in this case. If $\ell + m = 0$, then the appropriate expression for the $A_3(k, \ell, m, a, b, c)$ function takes the form

$$A_3(k, \ell, m, a, b, c) = \frac{A_1(a + b + c; k)}{(b + c)c}. \qquad (10)$$

The third case, when $m < 0$, is of great interest in applications. In this case we can write [4]

$$A_2(k, m, a, b) = \frac{A_1(k + m + 1, a + b)}{k + 1}\, {}_2F_1\left(1, k + m + 2; k + 2; \frac{a}{a + b}\right),$$

where ${}_2F_1(\alpha, \beta; \gamma; z)$ is the Gaussian hypergeometric function

$${}_2F_1(\alpha, \beta; \gamma; z) = 1 + \sum_{n=1} \frac{(\alpha)_n(\beta)_n}{(\gamma)_n n!} z^n \qquad (11)$$

and $(\alpha)_0 = 1, (\alpha)_1 = \alpha, \ldots, (\alpha)_n = \alpha(\alpha + 1)\cdots(\alpha + n - 1) = \frac{\Gamma(\alpha+n)}{\Gamma(\alpha)}$, where $\Gamma(x)$ is the usual gamma function and n is always a positive integer; $(1)_n = n!$ in this notation. In fact, in the present case we always have $0 < z < 1$ and $k + m + 2 < k + 2$.

The analogous expression for the A_3 auxiliary function takes the form [4]

$$A_3(k, \ell, m, \alpha, \beta, \gamma) = A_1(k + \ell + m + 2, \alpha + \beta + \gamma) \sum_{n=0} \frac{(k + \ell + m + 3)_n}{(k + 1)_{n+1}} \times \left(\frac{\alpha}{\alpha + \beta + \gamma}\right)^n D^m_{k+\ell+n+3}\left(\frac{\alpha + \beta}{\alpha + \beta + \gamma}\right) \qquad (12)$$

where the coefficients $D^m_K(y)$ are

$$D_K^m(y) = \frac{{}_2F_1(1, K+m; K; y)}{K-1} \tag{13}$$

where $m < 0$, $K \geqslant 2$, $K + m \geqslant 0$, $K + m < K$ and $0 \leqslant y < 1$ always. Note that all formulae for the A_2 and A_3 auxiliary functions contain only the hypergeometric functions of special kind, i.e. the ${}_2F_1(1, a; c; z)$ functions, where also $a < c$ and $z < 1$. This simplifies drastically the numerical calculations of such functions. Furthermore, by using equation (12) in actual computations of the $A_3(k, \ell, m, \alpha, \beta, \gamma)$ functions one needs to compute only the first hypergeometric function ${}_2F_1(1, a; c; z)$. All other hypergeometric functions ${}_2F_1(1, a+n; c+n; z)$ needed in equation (12) can easily be obtained from ${}_2F_1(1, a; c; z)$ by using the following relation for hypergeometric functions (see e.g. [7, 8]):

$${}_2F_1(1, a, c; z) = 1 + \left(\frac{a}{c}\right) z \; {}_2F_1(1, a+1; c+1; z). \tag{14}$$

In fact, this relation follows directly from the definition of the ${}_2F_1(1, a; c; z)$ hypergeometric function, equation (11). In the present case, we also have $a < c$.

All presented formulae for the $A_2(k, m, a, b)$ and $A_3(k, \ell, m, a, b, c)$ auxiliary functions have been extensively tested in numerical computations. The numerical results of such computational tests can be found in tables 1 and 2. Table 1 contains the numerical values of the auxiliary functions $A_2(k, m, a, b)$ and $A_3(k, \ell, m, a, b, c)$ determined for different values of the variables. Note that all our present calculations are performed using high-precision arithmetic [9, 10]. The arithmetic accuracy is equivalent to 116–320 decimal digits. In particular, to compute the $A_2(k, m, a, b)$ and $A_3(k, \ell, m, a, b, c)$ functions presented in table 1 we used multi-precision variables with 280–320 decimal digits. However, due to the presence of a few infinite series the overall accuracy of our computations can be evaluated as ≈144 decimal digits. In fact, such an accuracy can easily be increased to ≈1000 decimal digits for each computed auxiliary function. The original versions of tables 1–3 included 116 decimal digits. These tables can be obtained from the authors. However, the versions presented here contain only 65, 52 and 70 decimal digits, respectively, for each computed function (or integral). Note also that in our previous studies we successfully used the extended arithmetic accuracy to solve a number of three-body problems (see e.g. [11] and references therein).

3. Calculation of the four-body integrals

The second- and third-order auxiliary functions A_2 and A_3 are of paramount importance, since these functions allow one to compute the so-called four-body integrals [6]

$$\mathcal{I}(K, L, M, n_1, n_2, n_3, \alpha, \beta, \gamma) = \frac{1}{(4\pi)^3} \iiint r_{14}^K r_{24}^L r_{34}^M r_{12}^{n_3} r_{13}^{n_2} r_{23}^{n_1} \times \exp(-\alpha r_{14} - \beta r_{24} - \gamma r_{34}) \, \mathrm{d}^3\boldsymbol{r}_{14} \, \mathrm{d}^3\boldsymbol{r}_{24} \, \mathrm{d}^3\boldsymbol{r}_{34}, \tag{15}$$

where K, L, M, n_1, n_2, n_3 are integer numbers, while α, β, γ are three real (positive) numbers. In actual computations the r_{23}, r_{13} and r_{12} variables are expressed in terms of 'radial' coordinates r_{14}, r_{24}, r_{34} and three Legendre polynomials which depend on the three angular variables [6]. After the integration over angular variables, one finds the final expression which is the infinite sum (in some cases, the finite sum) of the auxiliary functions [6]. The explicit expression for the integral, equation (15), takes the form [6]

$$\mathcal{I}(K, L, M, \lambda, \mu, \nu, \alpha, \beta, \gamma) = \sum_{q=0}^{\infty} \frac{1}{(2q+1)^2} \sum_{i=0}^{\lambda_a} P_{\lambda,q,i} \sum_{j=0}^{\mu_a} P_{\mu,q,j} \sum_{k=0}^{\nu_a} P_{\nu,q,k} \times [A_3(K+2+2q+2j+2k, L+2+2i+\nu-2k, M+2-2q+\lambda-2i$$

$$+ \mu - 2j; \alpha, \beta, \gamma) + A_3(K + 2 + 2q + 2j + 2k, M + 2 + 2i + \mu - 2j, L + 2 - 2q + \lambda - 2i + \nu - 2k; \alpha, \gamma, \beta) + A_3(L + 2 + 2q + 2i + 2k, K + 2 + 2j + \nu - 2k, M + 2 - 2q + \lambda - 2i + \mu - 2j; \beta, \alpha, \gamma) + A_3(L + 2 + 2q + 2i + 2k, M + 2 + \lambda - 2i + 2j, K + 2 - 2q + \mu - 2j + \nu - 2k; \beta, \gamma, \alpha) + A_3(M + 2 + 2q + 2i + 2j, K + 2 + \mu - 2j + 2k, L + 2 - 2q + \lambda - 2i + \nu - 2k; \gamma, \alpha, \beta) + A_3(M + 2 + 2q + 2i + 2j, L + 2 + \lambda - 2i + 2k, K + 2 - 2q + \mu - 2j + \nu - 2k; \gamma, \beta, \alpha)] \quad (16)$$

where $\lambda_a = [\frac{(\lambda+1)}{2}]$, $\mu_a = [\frac{(\mu+1)}{2}]$, $\nu_a = [\frac{(\nu+1)}{2}]$ and $[x]$ denotes the integral part of x. Also, in this equation $P_{\nu,q,k}$ are the so-called Perkins coefficients [6]

$$P_{\nu,q,k} = \frac{2q+1}{\nu+2} C_{\nu+2}^{2k+1} \prod_{t=0}^{N_{q,\nu}} \frac{(2k+2t-\nu)}{(2k+2q-2t+1)}, \quad (17)$$

where $N_{q,\nu} = \min((q-1), [\frac{(\nu+1)}{2}])$ and C_n^m are the binomial coefficients. As follows from this formula the computation of the four-body integrals is a very complex problem. Indeed, in the general case, such a four-body integral, equation (16), includes a significant number of terms (e.g., many thousands of terms). An additional problem is the relatively slow convergence of the Perkins formula, equation (16), for some four-body integrals. Briefly, the highly accurate evaluation of the four-body integrals $\mathcal{I}(K, L, M, n_1, n_2, n_3, \alpha, \beta, \gamma)$ is a very serious test for any approach which is proposed for computation of the auxiliary functions A_2 and A_3 of the second and third order.

In general, by using this formula one can determine, in principle, an arbitrary four-body integral. In particular, the values for some of such integrals can be found in table 2. Note that the numerical values for some integrals presented in table 2 coincide very well with the corresponding values determined in [2, 4, 12]. However, our table 2 contains significantly more stable decimal digits for each of these integrals. Originally, we wanted to determine these integrals with the maximal numerical accuracy. However, there are complications related to the slow convergence of the Perkins expression equation (16) for some four-body integrals. Finally, for some integrals in table 2 the total number of stable decimal digits is significantly less than 116 decimal digits. In general, the number of stable digits has been determined from a series of computations with different $q_{\max}$ in equation (16). The total number of terms in equation (16) ($q_{\max}$) has been increased in each case by 50%. The stable decimal digits for each of the considered four-body integrals in table 2 have been determined by comparing the results of such calculations. To illustrate the very slow convergence for the first integral in table 2, note that the term $W(q)$ with $q = 11\,500\,000$ is only $\approx$1.439 times smaller than the analogous term $W(q)$ with $q = 10\,500\,000$. The numerical value of the term $W(q = 10\,500\,000)$ is $\approx 5.078\,409\,535 \times 10^{-30}$. This gives us a principal limit ($\approx$25–27 decimal digits) for the Perkins formula in computations of the first integral in table 2. In general, such a limit does not depend upon the arithmetic accuracy used in calculations. Note also that the use of extended numerical precision allows us to perform a detailed study of the convergence of the computed four-body integrals in many special cases.

4. Applications of the second- and third-order auxiliary functions

As we mentioned above, the known second- and third-order auxiliary functions are extensively used to compute the four-body integrals equation (15). In turn, such integrals are used to solve

Table 1. Auxiliary functions $A_2(k, \ell, a, b)$ and $A_3(k, \ell, m, a, b, c)$ for different values of the parameters. In all computed functions $a = 2.5$, $b = 1.5$ and $c = 0.5$.

A_i	k	ℓ	m	Numerical value
A_2	15	−15	—	4.228 083 237 938 250 191 111 722 202 130 691 025 107 170 436 126 187 965 228 482 0594 × 10^{-3}
A_3	15	1	−15	7.290 423 272 533 868 050 520 045 492 477 171 882 362 047 505 446 511 566 123 033 3988 × 10^{-5}
A_2	25	−25	—	2.523 306 501 378 914 401 482 418 541 875 744 439 720 756 403 103 887 411 743 277 7781 × 10^{-3}
A_3	25	1	−25	2.510 183 716 900 327 672 817 691 423 202 591 203 581 174 302 536 339 662 050 197 6426 × 10^{-3}
A_2	45	−45	—	1.396 319 599 076 715 073 443 187 582 267 031 763 213 997 166 954 820 721 701 218 4925 × 10^{-3}
A_3	45	1	−45	7.513 832 286 771 623 487 662 938 295 645 777 112 840 073 150 955 226 986 952 438 4354 × 10^{-6}
A_2	75	−75	—	8.360 500 462 109 605 225 728 901 553 228 727 895 268 311 534 773 478 887 681 782 1626 × 10^{-4}
A_3	75	1	−75	2.663 259 162 143 116 509 318 287 937 525 880 454 953 229 745 471 841 454 827 263 7811 × 10^{-6}
A_2	95	−95	—	6.595 960 813 759 855 922 192 138 074 389 325 540 702 679 379 139 037 451 630 230 1305 × 10^{-4}
A_3	95	1	−95	1.651 750 386 528 926 265 880 302 983 343 666 157 525 513 086 714 135 382 692 955 0458 × 10^{-6}

Table 2. The basic four-body integral $\mathcal{I}(K, L, M, n_1, n_2, n_3, \alpha, \beta, \gamma)$ for different values of the parameters.

n_1	n_2	n_3	K	L	M	α	β	γ	$\mathcal{I}(K, L, M, n_1, n_2, n_3, \alpha, \beta, \gamma)$
0	0	0	−1	−1	−1	1.0	1.0	1.0	$3.447\,454\,259\,102\,525\,282\,937\,825 \times 10^{-1}$
0	0	0	−1	1	1	5.72	4.26	4.26	$6.906\,703\,593\,715\,354\,492\,629\,929\,163\,935\,775\,938\,987\,669\,903 \times 10^{-6}$
2	1	1	1	1	1	5.72	4.26	4.26	$3.395\,169\,394\,317\,930\,656\,174\,909\,681\,618\,605\,910\,453\,514\,463\,306\,301 \times 10^{-6}$
2	1	1	3	3	3	5.72	5.72	2.80	$1.030\,576\,811\,924\,965\,924\,374\,053\,550\,355\,904\,820\,524\,037\,650\,028\,308 \times 10^{-3}$
2	1	1	5	5	5	4.26	4.26	5.72	$1.979\,899\,031\,622\,284\,051\,751\,347\,216\,420\,991\,555\,877\,686\,199\,038\,181 \times 10^{-1}$
2	1	1	7	7	7	4.26	4.26	5.72	$5.008\,185\,838\,842\,137\,912\,103\,637\,394\,424\,245\,664\,497\,660\,106\,255\,086 \times 10^{+2}$
2	1	1	9	9	9	4.26	4.26	5.72	$4.345\,217\,386\,756\,292\,095\,872\,515\,956\,645\,580\,774\,689\,638\,256\,975\,456 \times 10^{+6}$
0	1	1	0	1	1	5.72	4.26	4.26	$4.336\,035\,040\,316\,289\,664\,448\,861\,480\,298\,613\,299\,987\,706\,147\,567\,394 \times 10^{-6}$
1	0	2	3	0	−1	2.80	4.26	5.72	$1.874\,028\,781\,856\,777\,749\,613\,231\,112\,042\,473\,707\,034\,713\,052\,464\,583 \times 10^{-5}$
2	1	0	1	−1	2	2.80	4.26	5.72	$8.442\,262\,663\,550\,442\,461\,583\,781\,028\,684\,196\,055\,178\,544\,029\,642\,788 \times 10^{-5}$
2	0	0	0	0	−1	2.80	5.72	5.72	$1.084\,350\,608\,446\,545\,938\,045\,123\,023\,977\,286\,688\,389\,421\,356\,930\,173 \times 10^{-5}$
0	0	2	−1	2	0	5.72	5.72	2.80	$7.742\,394\,164\,415\,103\,633\,345\,515\,703\,506\,814\,058\,213\,827\,820\,978\,968 \times 10^{-6}$
0	2	1	−1	2	0	2.80	4.26	5.72	$1.687\,954\,486\,696\,245\,522\,170\,427\,839\,101\,213\,771\,666\,483\,600\,681\,273 \times 10^{-5}$
0	0	2	0	0	0	5.72	5.72	2.80	$1.592\,593\,370\,562\,798\,895\,675\,276\,567\,151\,748\,792\,138\,356\,234\,953\,056 \times 10^{-5}$

a number of four-body problems. Note, however, that all applications of equation (15) are restricted to the one-centre systems, i.e. to the four-body systems in which an infinitely heavy (i.e. central) particle exists. Such systems include the lithium atom, various lithium-like ions, positronium hydride HPs ($^{\infty}H^{+}e^{-}e^{-}e^{+}$) and a few other similar systems. In order to consider the four-body systems with arbitrary masses one needs the general four-body integrals which are significantly more complicated than integrals defined by equation (15). The general four-body integral has the form

$$I_4(K, L, M, n_1, n_2, n_3, a_{12}, a_{13}, a_{23}, a_{14}, a_{24}, a_{34}) = \frac{1}{(4\pi)^3} \iiint r_{14}^{K} r_{24}^{L} r_{34}^{M} r_{12}^{n_3} r_{13}^{n_2} r_{23}^{n_1} \exp(-a_{12}r_{12} - a_{13}r_{13} - a_{23}r_{23} - a_{14}r_{14} - a_{24}r_{24} - a_{34}r_{34}) \, d^3\boldsymbol{r}_{14} \, d^3\boldsymbol{r}_{24} \, d^3\boldsymbol{r}_{34}, \tag{18}$$

where the parameters $a_{12}, a_{13}, a_{23}, a_{14}, a_{24}$ and a_{34} are the six real and always positive numbers.

In general, the computation of the four-body integral, equation (18), is a very complex problem by itself. However, if the three parameters a_{12}, a_{13} and a_{23} are relatively small, then the integral I_4 can be reduced to a sum of four-body integrals from equation (15). The explicit expression takes the form

$$I_4(K, L, M, n_1, n_2, n_3, a_{12}, a_{13}, a_{23}, a_{14}, a_{24}, a_{34}) = \sum_{N_1=0}^{p_1} \sum_{N_2=0}^{p_2} \sum_{N_3=0}^{p_3} \frac{a_{23}^{N_1}}{N_1!} \frac{a_{13}^{N_2}}{N_2!} \frac{a_{12}^{N_3}}{N_3!} \times \mathcal{I}(K, L, M, n_1 + N_1, n_2 + N_2, n_3 + N_3, a_{14}, a_{24}, a_{34}) \tag{19}$$

where $\mathcal{I}(K, L, M, n_1 + N_1, n_2 + N_2, n_3 + N_3, a_{14}, a_{24}, a_{34})$ is the integral from equation (15). Note that, in general, the sum in the last equation is infinite. However, for relatively small values of the a_{12}, a_{13} and a_{23} parameters (e.g. if each of them <0.1) its approximations by finite sums converge rapidly. Finally, the formula, equation (19), can be used in actual computation of various four-body systems with arbitrary masses, e.g., for the positronium molecule Ps_2 and bi-muonic molecule $dt\mu\mu$ [15]. Note that Fromm and Hill [13] (see also [14]) proposed the direct method which can be used to compute the general four-body integral I_4, equation (19). By using formula (19), we calculated the four-body integral I_4 for $K = 3, L = 2, M = 1, n_1 = 1, n_2 = 2, n_3 = 0, a_{12} = 0.1, a_{13} = 0.085, a_{23} = 0.097, a_{14} = 2.5, a_{24} = 2$ and $a_{34} = 1.5$. The numerical value of this integral computed with $n_1 = n_2 = n_3 = 10$ is $\approx 1.189\,335\,704\,424 \times 10^2$. The analogous result for $n_1 = n_2 = n_3 = 11$ is $1.189\,335\,705\,494 \times 10^2$, while for $n_1 = n_2 = n_3 = 12$ we have $1.189\,335\,705\,595 \times 10^2$. Thus, formula (19) allows one to determine the approximate numerical value of the considered four-body integral I_4. Currently, we are trying to develop the new, efficient and optimal approach for highly accurate calculations of the general four-body integrals. The numerical results for a number of four-body systems will be published elsewhere.

Note also, that our present approach can also be generalized to the case of five-body systems, e.g. to the beryllium atom and beryllium-like ions. For the five-body systems the auxiliary functions of the fourth order $A_4(k, \ell, m, n, a, b, c, d)$ play a central role. In a large number of cases the function A_4 can be computed by using the auxiliary functions A_2 and A_3 defined above. In particular, in table 3 some numerical values of the A_4 functions are presented. These values have been computed for different values of the k, ℓ, m and n parameters. All computations have been performed with overall arithmetic accuracy $\approx$144 decimal digits. In table 3 only 70 digits per result are presented. The computation of the $A_4(k, \ell, m, n, a, b, c, d)$ functions contains no difficulties. However, in table 3 we restricted to the case when $n \geqslant 0$. The case of negative n is extremely complex and requires a separate consideration. The explicit expression for the $A_4(k, \ell, m, n, a, b, c, d)$ function in the case of negative n is

Table 3. Auxiliary functions $A_4(k, \ell, m, n, a, b, c, d)$ for different values of the integer parameters[a].

k	ℓ	m	n	Numerical value
5	3	2	1	$1.245\,110\,095\,492\,153\,249\,730\,734\,449\,238\,268\,397\,623\,474\,139\,814\,680\,995\,248\,324\,190\,059\,658 \times 10^{-6}$
5	4	3	2	$8.445\,360\,731\,572\,993\,471\,694\,832\,370\,457\,608\,972\,635\,740\,260\,570\,154\,718\,196\,057\,415\,365\,046 \times 10^{-6}$
4	5	6	0	$1.840\,702\,649\,607\,480\,594\,727\,261\,356\,815\,580\,326\,395\,795\,691\,340\,738\,791\,813\,536\,857\,695\,593 \times 10^{-5}$
4	5	6	1	$7.270\,131\,916\,899\,149\,342\,088\,849\,176\,223\,471\,042\,631\,264\,035\,501\,300\,404\,667\,326\,385\,552\,796 \times 10^{-5}$
1	1	1	1	$1.354\,537\,650\,128\,772\,875\,247\,558\,415\,286\,147\,778\,561\,653\,732\,713\,410\,228\,731\,225\,934\,772\,0763 \times 10^{-4}$
2	2	2	2	$5.855\,355\,178\,392\,992\,583\,927\,238\,170\,166\,193\,923\,772\,769\,202\,869\,168\,901\,945\,104\,577\,994\,3715 \times 10^{-5}$

[a] The real parameters for the computed $A_4(k, \ell, m, n, a, b, c, d)$ function are $a = 2.5$, $b = 1.5$, $c = 1.0$ and $d = 0.5$ in all cases.

$$A_4(k, \ell, m, n, a, b, c, d) = \frac{k!\ell!}{(a+b+c+d)^{k+\ell+m+n+4}} \sum_{p=0}^{\infty} C^{\ell}_{k+\ell+1+p} \left(\frac{a}{a+b+c+d} \right)^p$$
$$\times \sum_{q=0}^{\infty} \frac{(k+\ell+m+n+3+p+q)!}{(k+\ell+2+p+q)!} \left(\frac{a+b}{a+b+c+d} \right)^q \frac{1}{(k+\ell+m+3+p+q)}$$
$$\times {}_2F_1\left(1, k+\ell+m+n+p+q+4; k+\ell+m+p+q+3; \frac{a+b+c}{a+b+c+d}\right). \quad (20)$$

This formula has two small parameters and can be directly used in highly accurate calculations of various five-body systems. Note, however, that for five-body systems the formula which represents the expansion of the corresponding five-body integral in terms of the auxiliary functions $A_4(k, \ell, m, n, a, b, c, d)$ has not been produced yet. Moreover, for five-body systems one finds an additional and very serious problem which complicates computations of the five-body integrals: as follows from the Euler theorem, there are 10 interparticle (or relative) coordinates for an arbitrary five-body system, but only nine of them are truly independent (see, e.g., discussion in [15]).

5. Conclusion

Thus, in this study we have presented a few relatively simple analytical formulae for the auxiliary functions of the second and third order $A_2(k, m, a, b)$ and $A_3(k, \ell, m, a, b, c)$. The formulae can directly be used in numerical computations, since they are stable and easy to program. Moreover, the accuracy of such calculations for the four-body systems can now be made arbitrarily high. This study essentially marks the final step in the development of highly accurate procedures for the four-body integral, which are based on the Perkins formula, equation (16). The developed approach eliminates a number of computational restrictions which were crucial in earlier studies (see e.g. [2, 4, 12]). Furthermore, it opens a new chapter in highly accurate computations of four-body systems. We also discuss some new applications for the auxiliary functions of the second and third orders. In particular, it is shown that these functions can be used in the computations of five- and many-body systems. Another application of the auxiliary functions of the second and third orders is related to the calculation of the general four-body integrals, equation (19).

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