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Four-body perimetric coordinates

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Abstract

The new approach to the analysis of four-body systems and computation of various four-body integrals is proposed. The approach is based on the use of six perimetric coordinates which can be introduced for an arbitrary four-body system. The proper (i.e. non-conflicting) definition of the four-body perimetric coordinates is given for an arbitrary four-body system. It is shown that these six internal perimetric coordinates describe all possible configurations in an arbitrary four-body system and can be used to simplify computations of many four-body integrals written in the relative coordinates r_{12}, r_{13}, r_{23}, r_{14}, r_{24} and r_{34}. In addition to this, a number of new, very effective procedures for variational computation of different four-body systems can now be developed.

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1. Introduction

In this study, we consider the problem which has a principal value for the physics of four-body systems. The solution of this problem will mean a revolutionary turn for the future analytical considerations and for highly accurate computations of many four-body (quantum) systems. Note that the current progress achieved in theoretical studies of four-body systems is very modest in comparison to the three-body case. The main problem here is related to very inefficient approaches which are used to compute various four-body integrals. Below, we propose another approach based on the use of four-body perimetric coordinates. The four-body perimetric coordinates introduced in this study have a number of advantages in actual computations. In particular, the use of four-body perimetric coordinates must simplify numerical and analytical calculations of various four-body integrals written in relative coordinates. Also, an extensive development of highly accurate numerical methods for four-body systems will become possible and actual.

Below, we introduce the six four-body perimetric coordinates which are independent and always positive. The use of these perimetric coordinates allows one to transform currently used, very complicated procedure for four-body computations into a process which is only slightly more complicated than analogous computations for three-body systems. In the case of three-body systems, the use of three truly independent perimetric coordinates u_1, u_2 and u_3 instead of relative coordinates r_{12}, r_{13}, r_{23} drastically simplifies all problems related to the three-body integral computations (see below). For the first time numerous advantages of the three-body perimetric coordinates have been noticed by C L Pekeris [1] who was a geophysicist at that time. Later, he used the three-body perimetric coordinates in a number of studies of the helium atom and helium-like ions (see, e.g., [2] and references therein).

For an arbitrary three-body system the perimetric coordinates are introduced in the following way

$$u_1 = \frac{1}{2}(r_{12} + r_{13} - r_{23}), \qquad u_2 = \frac{1}{2}(r_{12} + r_{23} - r_{13}), \qquad u_3 = \frac{1}{2}(r_{13} + r_{23} - r_{12}), \tag{1}$$

where $r_{ij} \equiv r_{ji} = |\mathbf{r}_i - \mathbf{r}_j|$ $(i \neq j = (1, 2, 3))$ are the three interparticle distances (scalars). The variables r_{ij} are also called by the relative coordinates (= interparticle separations), emphasizing the principal difference between them and Cartesian coordinates $\mathbf{r}_i$ of the three particles, where $i = (1, 2, 3)$. Note that the relative coordinates r_{32}, r_{31}, r_{21} and, therefore, perimetric coordinates u_1, u_2, u_3 are translationally and rotationally invariant. Furthermore, the three perimetric coordinates u_1, u_2, u_3 are truly independent and each of them changes from 0 to $+\infty$. The relations of perimetric coordinates with the relative coordinates are also linear and simple:

$$r_{12} = u_1 + u_2, \qquad r_{13} = u_1 + u_3, \qquad r_{23} = u_2 + u_3. \tag{2}$$

It is interesting to note that the surface $\mathcal{S}$ of the triangle formed by the three particles (123) written in perimetric coordinates takes a very simple form:

$$\mathcal{S} = \sqrt{(u_1 + u_2 + u_3)u_1u_2u_3}. \tag{3}$$

However, the real importance of perimetric coordinates and their numerous advantages for computations and analytical considerations of various three-body systems can be understood by applying these coordinates to many different problems.

In general, the four-body perimetric coordinates cannot be defined in the same way as for the three-body systems. The definition of the four-body perimetric coordinates is based on a number of facts from the geometry of polyhedrons, rather than from elementary geometry of plane triangles. In a number of earlier works we have discussed an approach which can be used to introduce the six independent perimetric coordinates for an arbitrary four-body system. At that time, however, it was not clear how to deal with additional troubles arising in this process. Now, all problems have been solved and our main goal in this work is to introduce the six independent perimetric coordinates explicitly. Our present analysis starts from the discussion of the three-body case. Then we consider the definition and computations of the different basic four-body integrals. In section 4, the six independent four-body perimetric coordinates are introduced. In section 5, the basic four-body integral I_4 is computed with the use of the six four-body perimetric coordinates. Concluding remarks can be found in the final section. The appendix contains a brief review of the closely related Hylleraas method developed for the four-body atomic systems.

2. Three-body systems

In this section, we illustrate how by using the three-body perimetric coordinates u_1, u_2 and u_3 instead of relative coordinates r_{32}, r_{31} and r_{21} one can simplify numerical/analytical computation of various three-body integrals. Our main interest, however, is related to those three-body integrals which are needed to solve the bound state three-body problems. In general, such integrals can be reduced to one of the following forms

$$\begin{aligned} I_3 &= \int_0^\infty \exp(-a_1 r_{32})\,\mathrm{d}r_{32} \int_0^\infty \exp(-a_2 r_{31})\,\mathrm{d}r_{31} \int_{|r_{31}-r_{32}|}^{r_{31}+r_{32}} F(r_{32}, r_{31}, r_{21}) \exp(-a_3 r_{21})\,\mathrm{d}r_{21} \\ &= \iiint \mathrm{d}r_{32}\,\mathrm{d}r_{31}\,\mathrm{d}r_{21} F(r_{32}, r_{31}, r_{21}) \exp(-a_1 r_{32} - a_2 r_{31} - a_3 r_{21}) \\ &= \frac{1}{8\pi^2} \iiint \mathrm{d}^3\mathbf{r}_{32}\,\mathrm{d}^3\mathbf{r}_{31} F(r_{32}, r_{31}, r_{21}) \exp(-a_1 r_{32} - a_2 r_{31} - a_3 r_{21}) \end{aligned} \tag{4}$$

where $F(x, y, z)$ is a regular/analytical function of the x, y and z variables.

In turn, each of these integrals can be approximated by the finite sums of the following power-type integrals $J_3(a_1, a_2, a_3; n_1, n_2, n_3)$

$$J_3 = \int_0^\infty r_{32}^{n_1} \exp(-a_1 r_{32})\,\mathrm{d}r_{32} \int_0^\infty r_{31}^{n_2} \exp(-a_2 r_{31})\,\mathrm{d}r_{31} \int_{|r_{31}-r_{32}|}^{r_{31}+r_{32}} r_{21}^{n_3} \exp(-a_3 r_{21})\,\mathrm{d}r_{21}. \tag{5}$$

The direct analytical computation of this and other similar integrals is a quite complicated problem. However, by introducing the three perimetric coordinates $u_1 = \frac{1}{2}(r_{31} + r_{21} - r_{32})$, $u_2 = \frac{1}{2}(r_{32} + r_{21} - r_{31})$, $u_3 = \frac{1}{2}(r_{32} + r_{31} - r_{21})$ one may significantly simplify this problem. In fact, the integral $J_3(a_1, a_2, a_3; n_1, n_2, n_3)$ is easily computed with the use of the following formula

$$\begin{aligned} J_3 = 2 \int_0^\infty\int_0^\infty\int_0^\infty & (u_1 + u_2)^{n_3} (u_1 + u_3)^{n_2} (u_2 + u_3)^{n_1} \exp(-(a_2 + a_3) u_1) \\ & \times \exp(-(a_1 + a_3) u_2) \exp(-(a_1 + a_2) u_3)\,\mathrm{d}u_1\,\mathrm{d}u_2\,\mathrm{d}u_3 \\ & = 2 \sum_{k_1=0}^{n_1} \sum_{k_2=0}^{n_2} \sum_{k_3=0}^{n_3} C_{n_1}^{k_1} C_{n_2}^{k_2} C_{n_3}^{k_3} \frac{m_3! m_2! m_1!}{(a_1 + a_2)^{m_3+1} (a_1 + a_3)^{m_2+1} (a_2 + a_3)^{m_1+1}} \end{aligned} \tag{6}$$

where $C_n^k = \frac{n!}{k!(n-k)!}$ are the binomial coefficients, $m_1 = k_1 + k_2$, $m_2 = n_3 - k_3$ and $m_3 = n_1 - k_1 + n_2 - k_2$ (all these values are non-negative) and $a_i + a_j > 0$ for $i \neq j = 1, 2, 3$. In fact, the analytical computation of the J_3 integral in perimetric coordinates is reduced to the three independent Laplace transformations of the power-type expressions. The considered J_3 example shows an obvious advantage of perimetric coordinates for analytical and numerical computation of the regular three-body integrals. In actual applications, the perimetric three-body coordinates provide some other important advantages. For instance, only perimetric coordinates are appropriate for developing very fast and effective algorithms for optimization of the nonlinear parameters in trial wavefunctions [3]. Due to this and other similar reasons, recently all our trial wavefunctions for arbitrary three-body systems have been written explicitly in the perimetric coordinates u_1, u_2 and u_3.

The formula, equation (6), explicitly solves the problem of calculation of an arbitrary three-body (regular) integral, equation (5). An alternative approach is based on the use of explicit formula for the integral, equation (5), with zero powers of all relative coordinates, i.e.

$$\begin{aligned} J_3 &= \int_0^\infty \exp(-a_1 r_{32})\,\mathrm{d}r_{32} \int_0^\infty \exp(-a_2 r_{31})\,\mathrm{d}r_{31} \int_{|r_{31}-r_{32}|}^{r_{31}+r_{32}} \exp(-a_3 r_{21})\,\mathrm{d}r_{21} \\ &= \frac{2}{(a + b)(a + c)(b + c)} = J_3(a, b, c; 0, 0, 0) \end{aligned} \tag{7}$$

which is also easily computed in perimetric coordinates. Then the right-hand side of this formula must be differentiated as many times as needed to produce the required powers of all relative coordinates. The explicit relation is

$$J_3(a, b, c; k, l, m) = (-1)^{k+l+m} \frac{\partial^{k+l+m} J_3(a, b, c; 0, 0, 0)}{\partial^k a \partial^l b \partial^m c}. \tag{8}$$

The use of this formula is another way to compute all regular three-body integrals needed in actual computations.

3. Four-body systems

In contrast with the three-body case there are a number of different four-body integrals which can be considered as the basic four-body integrals and each can be used to develop the highly accurate procedure. In this section, we consider a few examples of such integrals. In the following sections, we shall show that the use of four-body perimetric coordinates simplifies the analysis and numerical computation of an arbitrary four-body integral. We begin with the consideration of the basic four-body integral $I_4(a_{12}, a_{13}, a_{14}, a_{23}, a_{24}, a_{34})$ written in the form

$$I_4(a_{12}, a_{13}, a_{23}, a_{14}, a_{24}, a_{34}) = \int\!\!\int\!\!\int\!\!\int\!\!\int\!\!\int \mathrm{d}r_{12}\,\mathrm{d}r_{13}\,\mathrm{d}r_{23}\,\mathrm{d}r_{14}\,\mathrm{d}r_{24}\,\mathrm{d}r_{34} \times \exp(-a_{12}r_{12} - a_{13}r_{13} - a_{23}r_{23} - a_{14}r_{14} - a_{24}r_{24} - a_{34}r_{34}) \quad (9)$$

where $a_{12}, a_{13}, a_{23}, a_{14}, a_{24}$ and a_{34} are the nonlinear parameters. The analytical and numerical computation of this integral is almost impossible, since twenty four additional inequalities must always be obeyed for the six relative coordinates. For instance, for the r_{23} and r_{24} coordinates one finds

$$\min(|r_{13} - r_{12}|, |r_{34} - r_{24}|) \leqslant r_{23} \leqslant \max(r_{13} + r_{12}, r_{34} + r_{24}) \quad (10)$$

$$\min(|r_{12} - r_{14}|, |r_{23} - r_{34}|) \leqslant r_{24} \leqslant \max(r_{12} + r_{14}, r_{23} + r_{34}) \quad (11)$$

i.e. four inequalities for each of the r_{23} and r_{24} coordinates. There are also sixteen more similar inequalities for four other relative coordinates r_{12}, r_{13}, r_{14} and r_{34}. All these inequalities are related to each other and this transforms computation of the I_4 integral, equation (9), into an extremely complex task. This problem has not been solved in earlier four-body studies.

In actual applications, the unknown basic four-body integral I_4 is replaced by another four-body integral $\mathcal{I}_4(a_{12}, a_{13}, a_{23}, a_{14}, a_{24}, a_{34})$ defined in [4]

$$\mathcal{I}_4(a_{12}, a_{13}, a_{23}, a_{14}, a_{24}, a_{34}) = \int\!\!\int\!\!\int \frac{\mathrm{d}^3\mathbf{r}_{14}\,\mathrm{d}^3\mathbf{r}_{24}\,\mathrm{d}^3\mathbf{r}_{34}}{r_{12}r_{13}r_{14}r_{23}r_{24}r_{34}} \exp(-a_{12}r_{12} - a_{13}r_{13} - a_{23}r_{23}) \times \exp(-a_{14}r_{14} - a_{24}r_{24} - a_{34}r_{34}) \quad (12)$$

where $a_{12}, a_{13}, a_{23}, a_{14}, a_{24}$ and a_{34} are the nonlinear parameters. The integral $\mathcal{I}_4$ can be computed analytically and numerically with the use of some currently developed methods (see, e.g., [4, 5]). A few examples of the $\mathcal{I}_4$ integrals computed numerically with the use of our method [5] (parameters a_{23}, a_{24} and a_{34} are small in comparison a_{12}, a_{13} and a_{14}) can be found in table 1. In general, each of the basic integrals determines the corresponding metric in the six-dimensional space of four-body functions. Moreover, each of these integrals can be used to develop a separate, highly accurate, numerical method for four-body computations.

Note that in contrast with the three-body case, the basic four-body integrals I_4 and $\mathcal{I}_4$ belong to the two different classes of four-body integrals. Indeed, the reduction of the $\mathcal{I}_4$ integral to the form of the I_4 integral produces the following expression

$$\mathcal{I}_4 = 16\pi^2 \int\!\!\int\!\!\int\!\!\int\!\!\int\!\!\int \frac{\mathrm{d}r_{12}\,\mathrm{d}r_{13}\,\mathrm{d}r_{14}\,\mathrm{d}r_{23}\,\mathrm{d}r_{24}\,\mathrm{d}r_{34}}{\left[\left(r_{34}^2 - r_{12}^2\right)\left(r_{24}^2 - r_{31}^2\right)\left(r_{14}^2 - r_{23}^2\right) - S(r_{ij})\right]^{\frac{1}{2}}} \times \exp(-a_{12}r_{12} - a_{13}r_{13} - a_{23}r_{23} - a_{14}r_{14} - a_{24}r_{24} - a_{34}r_{34}) \quad (13)$$

Table 1. The basic four-body integrals $\mathcal{I}_4(a_{12}, a_{13}, a_{23}, a_{14}, a_{24}, a_{34})$ and $\mathcal{J}_4(K, L, M, n_1, n_2, n_3, \alpha, \beta, \gamma)$ determined for different values of the parameters. In all $\mathcal{J}_4$ integrals in this table $\alpha = 2.55$, $\beta = 3.33$ and $\gamma = 2.19$.

a_{12}	a_{13}	a_{23}	a_{14}	a_{24}	a_{24}	$\mathcal{I}_4(a_{12}, a_{13}, a_{23}, a_{14}, a_{24}, a_{34})$
1.45	2.11	0.073	2.34	0.051	0.028	53.485 524 063 312 394 377 914 75
2.45	1.83	0.037	2.85	0.028	0.028	31.735 887 493 889 782 020 519 46
3.45	2.83	0.057	3.15	0.048	0.061	13.241 947 762 748 636 706 061 20
4.45	3.83	0.077	3.25	0.058	0.081	7.262 555 920 538 248 299 302 260
n_1	n_2	n_3	K	L	M	$\mathcal{J}_4(K, L, M, n_1, n_2, n_3, \alpha, \beta, \gamma)$
2	1	1	3	3	3	$1.060\,253\,575\,329\,366\,412\,291\,388\,165\,8060 \times 10^{2}$
2	1	1	5	5	5	$1.954\,630\,466\,219\,216\,718\,952\,347\,577\,6488 \times 10^{6}$
2	1	1	7	7	7	$1.694\,354\,329\,196\,115\,014\,113\,261\,665\,7577 \times 10^{11}$
0	1	1	0	1	1	$6.148\,992\,526\,558\,168\,137\,734\,507\,505\,0335 \times 10^{-3}$
1	0	2	3	0	−1	$6.414\,013\,396\,200\,065\,232\,059\,221\,183\,9672 \times 10^{-2}$

where the function $S(r_{ij})$ is

$$S(r_{ij}) = r_{14}^2 r_{24}^2 r_{34}^2 + r_{14}^2 r_{12}^2 r_{13}^2 + r_{24}^2 r_{23}^2 r_{12}^2 + r_{34}^2 r_{13}^2 r_{23}^2 + r_{14}^2 r_{23}^2 \times \left(r_{14}^2 + r_{23}^2 - r_{24}^2 - r_{34}^2 - r_{12}^2 - r_{13}^2\right) + r_{24}^2 r_{13}^2 \left(-r_{14}^2 + r_{24}^2 - r_{34}^2 - r_{12}^2 - r_{23}^2 + r_{13}^2\right) + r_{34}^2 r_{12}^2 \left(-r_{14}^2 - r_{24}^2 + r_{34}^2 + r_{12}^2 - r_{23}^2 - r_{13}^2\right). \tag{14}$$

Now, it is easy to see that the partial derivatives of the I_4 integral equation (9) upon the nonlinear parameters $a_{12}, a_{13}, a_{23}, a_{14}, a_{24}$ and a_{34} will never coincide with either the $\mathcal{I}_4$ integral equation (13), or with one of its partial derivatives. This means that the I_4 and $\mathcal{I}_4$ integrals belong to the two different families of six-dimensional (i.e. four-body) integrals. Further analysis shows that such a difference between I_4 and $\mathcal{I}_4$ integrals cannot be eliminated by using various substitutions and/or transformations of radial variables. Note that in the three-body case, the corresponding I_3 and $\mathcal{I}_3$ integrals are essentially identical. Another type of the important four-body integrals is considered in the appendix.

The four-body integral $I_4(a_{12}, a_{13}, a_{23}, a_{14}, a_{24}, a_{34})$ has a number of advantages in actual computations. For instance, the closed analytical form for this integral allows one to compute analytically all derivatives of the fifth and sixth orders which are needed in real variational computations. Furthermore, the finite-term form of these derivatives can be used to track all possible singularities, i.e. those values of the nonlinear parameters $a_{12}, a_{13}, a_{23}, a_{14}, a_{24}, a_{34}$ at which the integral I_4 and/or its derivatives are singular. In actual computations singularity usually means the rapid loss of numerical precision. For the $\mathcal{I}_4(a_{12}, a_{13}, a_{23}, a_{14}, a_{24}, a_{34})$ integral, equation (12), and for the $\mathcal{J}_4$ integral from the appendix such a separation of singularities is impossible.

The four-body perimetric coordinates defined in the following sections allows one to compute the basic four-body integral $I_4(a_{12}, a_{13}, a_{23}, a_{14}, a_{24}, a_{34})$. However, these coordinates are also very useful for many other purposes, including analytical/numerical computation of many different four-body integrals. Moreover, the four-body perimetric coordinates can be used to analyse and predict all problems related to the convergence of various four-body integrals, including the basic four-body integrals $\mathcal{I}_4$. The principal point here is a possibility of using the negative values for some nonlinear parameters $a_{12}, a_{13}, a_{23}, a_{14}, a_{24}$ and a_{34}. In many cases the negative parameters may accelerate the overall convergence of the whole procedure. On the other hand, they also produce various instability problems, when the overall numerical accuracy of the method is lost rapidly. By using four-body perimetric coordinates one can find all essential numerical restrictions of the values of nonlinear parameters $a_{12}, a_{13}, a_{23}, a_{14}, a_{24}$ and a_{34}. Some of such restrictions for the nonlinear parameters are obtained and discussed in section 5.

4. Four-body perimetric coordinates

Our present approach is based on the introduction of the six independent perimetric coordinates. These six coordinates will be used later instead of the six relative coordinates $r_{12}, r_{13}, r_{23}, r_{14}, r_{24}$ and r_{34}. Here and everywhere below $r_{ij} \equiv r_{ji}$ are the relative coordinates between the two particles i and j, i.e. $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$, where $\mathbf{r}_i$ are the Cartesian coordinates of the particles $i \neq j = 1, 2, 3, 4$. The six independent perimetric coordinates for an arbitrary four-body system are introduced in the following way. First, note that, in the general case, the six interparticle vectors $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j = -\mathbf{r}_{ji}$ (where $i \neq j = (1, 2, 3, 4)$) form a tetrahedron. Such a tetrahedron has four vertices, six edges ($\mathbf{r}_{ij}$) and four faces. The four particles are assumed to be placed in each of the four vertices. The corresponding faces of this tetrahedron can be designated as $(123) = U$, $(124) = T$, $(134) = W$ and $(234) = S$. The six edges coincide with the corresponding relative coordinates $r_{12}, r_{13}, r_{23}, r_{14}, r_{24}$ and r_{34}.

Now, for the triangles at each of the faces one can introduce three perimetric coordinates. Let us designate those coordinates as u_1, u_2, u_3 (for the $U = (123)$ triangle), t_1, t_2, t_3 (for the $T = (124)$ triangle), w_1, w_2, w_3 (for the $W = (134)$ triangle) and s_1, s_2, s_3 (for the $S = (234)$ triangle). The perimetric coordinates defined for each triangle are simply (linearly) related to the relative coordinates, e.g., for the U triangle: $u_1 = \frac{1}{2}(r_{12}+r_{13}-r_{23})$, $u_2 = \frac{1}{2}(r_{12}+r_{23}-r_{13})$ and $u_3 = \frac{1}{2}(r_{13}+r_{23}-r_{12})$. Analogous relations for other three triangles T, W, S are

$$\begin{aligned}
&t_1 = \tfrac{1}{2}(r_{12}+r_{14}-r_{24}), && t_2 = \tfrac{1}{2}(r_{12}+r_{24}-r_{14}), && t_3 = \tfrac{1}{2}(r_{24}+r_{14}-r_{12}),\\
&s_1 = \tfrac{1}{2}(r_{34}+r_{24}-r_{23}), && s_2 = \tfrac{1}{2}(r_{23}+r_{24}-r_{34}), && s_3 = \tfrac{1}{2}(r_{34}+r_{23}-r_{24}),\\
&w_1 = \tfrac{1}{2}(r_{13}+r_{14}-r_{34}), && w_2 = \tfrac{1}{2}(r_{14}+r_{34}-r_{13}), && w_3 = \tfrac{1}{2}(r_{34}+r_{13}-r_{14}).
\end{aligned} \tag{15}$$

All these coordinates are positive, since the corresponding triangle conditions $|r_{ik} - r_{jk}| \leqslant r_{ij} \leqslant r_{ik} + r_{jk}$ are obeyed for each relative coordinate r_{ij}.

The 12 inverse relations take the form

$$\begin{aligned}
&u_1+u_2 = r_{12}, && t_1+t_2 = r_{12}, && s_2+s_3 = r_{23}, && w_1+w_3 = r_{13},\\
&u_1+u_3 = r_{13}, && t_3+t_1 = r_{14}, && s_2+s_1 = r_{24}, && w_2+w_3 = r_{34},\\
&u_2+u_3 = r_{23}, && t_3+t_2 = r_{24}, && s_3+s_1 = r_{34}, && w_2+w_1 = r_{14}.
\end{aligned} \tag{16}$$

As follows from these equations there are the six additional constrains for the 12 perimetric coordinates. The number of constrains equals to the number of edges in the tetrahedron and also equals to the number of relative coordinates. These conditions take the form

$$\begin{aligned}
&u_1+u_2 = r_{12} = t_1+t_2, && u_1+u_3 = r_{13} = w_1+w_3, && u_2+u_3 = r_{23} = s_2+s_3,\\
&t_1+t_3 = r_{14} = w_1+w_2, && t_2+t_3 = r_{24} = s_1+s_2, && w_2+w_3 = r_{34} = s_1+s_3.
\end{aligned} \tag{17}$$

By using these six constrains one can exclude six (of original twelve) perimetric coordinates. The six remaining perimetric coordinates can be considered as the four-body perimetric coordinates, or independent perimetric coordinates at the tetrahedron surface. In fact, there are a few possible and different ways to choose these six independent perimetric coordinates. Below, we shall choose them in the following way. Three of these perimetric coordinates coincide with the u_1, u_2, u_3 perimetric coordinates in the U triangle. It is clear that such a choice provides a uniform correspondence with the limiting (or degenerate) three-body case. Each of these three additional perimetric coordinates is chosen from different triangles at the tetrahedron surface, i.e. from the T, W or S triangles, respectively. In fact, below we shall choose the t_3, w_3 and s_3 coordinates. By using these coordinates one can find the explicit expressions for the six remaining perimetric coordinates:

$$\begin{aligned} w_1 &= u_1 + u_3 - w_3, \qquad & s_1 &= t_3 + w_3 - u_3, \qquad & t_1 &= u_1 + s_3 - w_3, \\ w_2 &= t_3 + s_3 - u_3, \qquad & s_2 &= u_2 + u_3 - s_3, \qquad & t_2 &= u_2 + w_3 - s_3. \end{aligned} \tag{18}$$

All these values must be positive. This produces, in principle, six additional inequalities:

$$\begin{aligned} w_3 &\leqslant u_1 + u_3, \qquad & u_3 &\leqslant t_3 + w_3, \qquad & w_3 &\leqslant u_1 + s_3 \\ u_3 &\leqslant t_3 + s_3, \qquad & s_3 &\leqslant u_2 + u_3, \qquad & s_3 &\leqslant u_2 + w_3. \end{aligned} \tag{19}$$

Now, it is straightforward to check that the following equations

$$\begin{aligned} w_1 + w_3 &= u_1 + u_3 = r_{13}, \qquad & t_1 + t_2 &= u_1 + u_2 = r_{12}, \qquad & s_2 + s_3 &= u_2 + u_3 = r_{23} \\ t_3 + t_1 &= w_2 + w_1 = r_{14}, \qquad & t_3 + t_2 &= s_1 + s_2 = r_{24}, \qquad & s_1 + s_3 &= w_2 + w_3 = r_{34} \end{aligned} \tag{20}$$

are always obeyed. This can be considered as the first test for our approach.

Thus, for an arbitrary four-body problem instead of the six relative (or interparticle) coordinates $r_{12}, r_{13}, r_{23}, r_{14}, r_{24}$ and r_{34} one can introduce the six independent perimetric coordinates u_1, u_2, u_3, t_3, s_3 and w_3

$$\begin{aligned} u_1 &= \tfrac{1}{2}(r_{12} + r_{13} - r_{23}), \qquad & u_2 &= \tfrac{1}{2}(r_{12} + r_{23} - r_{13}), \qquad & u_3 &= \tfrac{1}{2}(r_{13} + r_{23} - r_{12}) \\ t_3 &= \tfrac{1}{2}(r_{14} + r_{24} - r_{12}), \qquad & s_3 &= \tfrac{1}{2}(r_{34} + r_{23} - r_{24}), \qquad & w_3 &= \tfrac{1}{2}(r_{34} + r_{13} - r_{14}). \end{aligned} \tag{21}$$

The corresponding inverse relations are

$$\begin{aligned} r_{12} &= u_1 + u_2, \qquad & r_{13} &= u_1 + u_3, \qquad & r_{23} &= u_2 + u_3, \\ r_{14} &= u_1 + s_3 + t_3 - w_3, \qquad & r_{24} &= u_2 + t_3 + w_3 - s_3, \qquad & r_{34} &= t_3 + s_3 + w_3 - u_3. \end{aligned} \tag{22}$$

From these definitions of the six perimetric coordinates u_1, u_2, u_3, t_3, s_3 and w_3 we may assume that only these six variables are needed to consider an arbitrary four-body problem. The six variables $s_1, s_2, t_1, t_2, w_1, w_2$ mentioned above can be considered as some supplementary values which can be ignored in further analysis. However, all six inequalities, equation (19), must be obeyed in any case.

Note also that from equation (22) and from the condition $r_{i4} \geqslant 0$ for $i = 1, 2, 3$, one finds the following inequalities:

$$w_3 \leqslant u_1 + s_3 + t_3, \qquad s_3 \leqslant u_2 + t_3 + w_3, \qquad u_3 \leqslant t_3 + s_3 + w_3. \tag{23}$$

It should be mentioned, however, that these three inequalities (as well as all twenty-four original inequalities, equations (10), (11), etc) are automatically obeyed, if the six conditions, equation (19), hold for the six perimetric coordinates u_1, u_2, u_3, t_3, w_3 and s_3, and each of these coordinates is positive.

To conclude this section we need to show that any operator originally written in the relative coordinates can be re-written in the four-body perimetric coordinates u_1, u_2, u_3, t_3, w_3 and s_3. In fact, if such an operator is an analytical functions of interparticle coordinates $r_{12}, r_{13}, r_{23}, r_{14}, r_{24}$ and r_{34}, then their expressions given by equation (22) must be used. Such a substitution essentially solves the problem in this case. For differential operators of the first order, the corresponding relations take the form

$$\frac{\partial}{\partial r_{12}} = \frac{\partial}{\partial u_1} + \frac{\partial}{\partial u_2}, \qquad \frac{\partial}{\partial r_{13}} = \frac{\partial}{\partial u_1} + \frac{\partial}{\partial u_3}, \qquad \frac{\partial}{\partial r_{23}} = \frac{\partial}{\partial u_2} + \frac{\partial}{\partial u_3},$$
$$\frac{\partial}{\partial r_{14}} = \frac{\partial}{\partial u_1} + \frac{\partial}{\partial s_3} + \frac{\partial}{\partial t_3} - \frac{\partial}{\partial w_3}, \qquad \frac{\partial}{\partial r_{24}} = \frac{\partial}{\partial u_2} + \frac{\partial}{\partial t_3} + \frac{\partial}{\partial w_3} - \frac{\partial}{\partial s_3},$$
$$\frac{\partial}{\partial r_{34}} = \frac{\partial}{\partial t_3} + \frac{\partial}{\partial s_3} + \frac{\partial}{\partial w_3} - \frac{\partial}{\partial u_3}.$$

The differential operators of higher order can be obtained as the powers of these expressions.

5. Computation of the basic four-body integral I_4

Thus, in the previous section we have shown that the following six coordinates

$$\begin{aligned} u_1 &= \tfrac{1}{2}(r_{13}+r_{12}-r_{23}), & u_2 &= \tfrac{1}{2}(r_{12}+r_{23}-r_{13}), & u_3 &= \tfrac{1}{2}(r_{23}+r_{13}-r_{12}), \\ s_3 &= \tfrac{1}{2}(r_{34}+r_{23}-r_{24}), & t_3 &= \tfrac{1}{2}(r_{24}+r_{14}-r_{12}), & w_3 &= \tfrac{1}{2}(r_{34}+r_{13}-r_{14}) \end{aligned} \tag{24}$$

are independent, positive and can be considered as the six perimetric coordinates defined at the surface of tetrahedron which represents an arbitrary four-body systems. The inverse relations take the form

$$\begin{aligned} r_{12} &= u_1+u_2, & r_{13} &= u_1+u_3, & r_{23} &= u_2+u_3 \\ r_{14} &= u_1+s_3+t_3-w_3, & r_{24} &= u_2+w_3+t_3-s_3, & r_{34} &= t_3+w_3+s_3-u_3. \end{aligned} \tag{25}$$

The six inequalities, equation (19), must be always obeyed for these six perimetric coordinates. It follows from here that the three relative coordinates r_{i4} ($i = 1, 2, 3$) defined by equation (25) are non-negative.

In this section, we apply the four-body perimetric coordinates to analytical computation of the basic four-body integral $I_4 = I_4(a_{12}, a_{13}, a_{23}, a_{14}, a_{24}, a_{34})$, equation (9). First, let us transform the following linear combination of the relative coordinates by using the four-body perimetric coordinates:

$$\begin{aligned} L &= a_{12}r_{12}+a_{13}r_{13}+a_{23}r_{23}+a_{14}r_{14}+a_{24}r_{24}+a_{34}r_{34} \\ &= (a_{12}+a_{13}+a_{14})u_1+(a_{12}+a_{23}+a_{24})u_2+(a_{13}+a_{23}-a_{34})u_3 \\ &\quad +(a_{14}+a_{24}+a_{34})t_3+(a_{14}-a_{24}+a_{34})s_3+(-a_{14}+a_{24}+a_{34})w_3 \\ &= Au_1+Bu_2+Cu_3+Dt_3+Es_3+Fw_3. \end{aligned} \tag{26}$$

This linear form is included into the basic four-body integral I_4, equation (9), as the exponential factor $I_4 \sim \exp(-L)$. Various powers of different relative coordinates, e.g., r_{13}^n and/or r_{24}^k can be written in the four-body perimetric coordinates with the use of formulae from equation (25). For instance, for the r_{13}^n and r_{24}^k powers one finds ($n > 0$ and $k > 0$)

$$r_{13}^n = (u_1+u_3)^n = \sum_{m=0}^{n} C_n^m u_1^m u_3^{(n-m)} \tag{27}$$

$$\begin{aligned} r_{24}^k &= (u_2+w_3+t_3-s_3)^k = \sum_{m_1=0}^{k} C_k^{m_1}(w_3+t_3-s_3)^{m_1} u_2^{k-m_1} \\ &= \sum_{m_1=0}^{k}\sum_{m_2=0}^{m_1} C_k^{m_1} C_{m_1}^{m_2}(t_3-s_3)^{m_2} w_3^{m_1-m_2} u_2^{k-m_1} \\ &= \sum_{m_1=0}^{k}\sum_{m_2=0}^{m_1}\sum_{m_3=0}^{m_2} (-1)^{m_3} C_k^{m_1} C_{m_1}^{m_2} C_{m_2}^{m_3} s^{m_3} t_3^{m_2-m_3} w_3^{m_1-m_2} w_3^{m_1-m_2} u_2^{k-m_1}. \end{aligned} \tag{28}$$

These formulae allow one to construct different variational expansions of the unknown four-body wavefunctions written in perimetric coordinates.

Note also that from equation (31) one can obtain the six following restrictions for the nonlinear parameters $a_{12}, a_{13}, a_{23}, a_{14}, a_{24}, a_{34}$ which are used in the $\mathcal{I}_4$ integral computation. Indeed, since each of the four-body perimetric coordinates is non-negative and the $\mathcal{I}_4$ integral contains the same exponential factor $\sim\exp(-L)$, then from equation (31) we have

$$A = a_{12} + a_{13} + a_{14} \geqslant 0, \qquad B = a_{12} + a_{23} + a_{24} \geqslant 0, \qquad C = a_{13} + a_{23} - a_{34} \geqslant 0$$
$$D = a_{14} + a_{24} + a_{34} \geqslant 0, \qquad E = a_{14} - a_{24} + a_{34} \geqslant 0, \qquad F = -a_{14} + a_{24} + a_{34} \geqslant 0. \tag{29}$$

In computations with N basis functions, these conditions must be checked for each basis function. As follows from equation (29) often it is not sufficient to choose only positive nonlinear parameters, since the corresponding four-body integrals $\mathcal{I}_4$ may still be divergent. The divergence of one four-body (basic) integral in one matrix element (e.g., of 10 000 matrix elements) means numerical collapse of the whole procedure.

The Jacobian of the $(r_{12}, r_{13}, r_{23}, r_{14}, r_{24}, r_{34}) \rightarrow (u_1, u_2, u_3, t_3, s_3, w_3)$ transformation is

$$\det\left[\frac{\partial(r_{12}, r_{13}, r_{23}, r_{14}, r_{24}, r_{34})}{\partial(u_1, u_2, u_3, t_3, s_3, w_3)}\right] = 8. \tag{30}$$

Note that the corresponding Jacobian in the three-body case equals 2 (see, the factor in front of the right-hand side of equation (6)). Thus, the basic four-body integral, equation (9), in the relative variables can now be written in the form

$$\begin{aligned}
I_4(a_{12}, a_{13}, a_{23}, a_{14}, a_{24}, a_{34}) = {} & \iiiint\!\!\iint \mathrm{d}r_{12}\,\mathrm{d}r_{13}\,\mathrm{d}r_{23}\,\mathrm{d}r_{14}\,\mathrm{d}r_{24}\,\mathrm{d}r_{34} \\
& \times \exp(-a_{12}r_{12} - a_{13}r_{13} - a_{23}r_{23} - a_{14}r_{14} - a_{24}r_{24} - a_{34}r_{34}) \\
= {} & 8\int_0^{+\infty}\int_0^{+\infty}\int_{a_3}^{+\infty}\int_{b_1}^{+\infty}\int_{b_2}^{u_2+u_3}\int_{b_3}^{B_3} \exp(-L)\,\mathrm{d}u_1\,\mathrm{d}u_2\,\mathrm{d}u_3\,\mathrm{d}t_3\,\mathrm{d}s_3\,\mathrm{d}w_3 \\
= {} & 8\int_0^{+\infty} \exp[-(a_{12} + a_{13} + a_{14})u_1]\,\mathrm{d}u_1 \int_0^{+\infty} \exp[-(a_{12} + a_{23} + a_{24})u_2]\,\mathrm{d}u_2 \\
& \times \int_{a_3}^{+\infty} \exp[-(a_{13} + a_{23} - a_{34})u_3]\,\mathrm{d}u_3 \int_{b_1}^{+\infty} \exp[-(a_{14} + a_{24} + a_{34})t_3]\,\mathrm{d}t_3 \\
& \times \int_{b_2}^{B_2} \exp[-(a_{14} - a_{24} + a_{34})s_3]\,\mathrm{d}s_3 \int_{b_3}^{B_3} \exp[-(-a_{14} + a_{24} + a_{34})w_3]\,\mathrm{d}w_3
\end{aligned} \tag{31}$$

where the six remaining lower and upper limits a_3, b_1, b_2, b_3 and B_2, B_3 may also depend upon the perimetric coordinates included in the following integrals; e.g., the lower limit b_1 limit can depend upon the three perimetric coordinates u_1, u_2 and u_3.

Thus, the remaining question is to determine the limits for the perimetric coordinates used in various four-body integrals, including the basic four-body integral I_4, equation (31). Those inequalities can be written in the form

$$\begin{aligned}
&\max(0; u_3 - t_3) \leqslant s_3 \leqslant u_2 + u_3 \\
&\max(0; u_3 - t_3; s_3 - u_2) \leqslant w_3 \leqslant \min(u_1 + u_3; u_1 + s_3).
\end{aligned} \tag{32}$$

Here and below, we shall consider the perimetric coordinates u_1, u_2, u_3 and t_3 as the main (or leading) variables, while the s_3 and w_3 perimetric coordinates are assumed to be the two supplement variables. Also, we shall assume that the first integration is taken over the w_3 coordinate, while the integration integration is performed over the s_3 coordinate. The arising expression is the uniform function of the leading perimetric coordinates u_1, u_2, u_3 and t_3 only. At the last step this expression must be integrated over these four coordinates.

The inequalities, equation (32), separate the six-dimensional space of four-body perimetric coordinates into a number of different regions/areas. Let us consider the structure of such a separation in detail. First, note that there are the two following possibilities: (a) $u_3 \geqslant t_3$ and (b) $u_3 \leqslant t_3$. In case (a) we have

$$u_3 - t_3 \leqslant s_3 \leqslant u_2 + u_3, \qquad \max(u_3 - t_3; s_3 - u_2) \leqslant w_3 \leqslant \min(u_1 + u_3; u_1 + s_3) \tag{33}$$

while in case (b)

$$0 \leqslant s_3 \leqslant u_2 + u_3, \qquad \max(0; s_3 - u_2) \leqslant w_3 \leqslant \min(u_1 + u_3; u_1 + s_3). \tag{34}$$

Below, we restrict ourselves to case (b) (case (a) can be considered analogously). Now, there are the two following subcases: (b.1) $s_3 \leqslant u_3$ and (b.2) $s_3 \geqslant u_3$. In subcase (b.1), one finds

$$0 \leqslant s_3 \leqslant u_3, \qquad \max(0; s_3 - u_2) \leqslant w_3 \leqslant u_1 + s_3. \tag{35}$$

Here, again we have the two following subcases: (b.1.1) $s_3 \leqslant u_2$ and (b.1.2) $s_3 \geqslant u_2$. In the second subcase, one finds

$$u_2 \leqslant s_3 \leqslant u_3, \qquad s_3 - u_2 \leqslant w_3 \leqslant u_1 + s_3. \tag{36}$$

These inequalities and one additional inequality $u_3 \leqslant t_3$ mentioned earlier determine the corresponding limits in the six-dimensional integral, equation (31). In this case the integral I_4 takes the form

$$\begin{aligned} I_4 = 8 \int_0^\infty & \exp[-(a_{12} + a_{13} + a_{14})u_1]\,\mathrm{d}u_1 \int_0^\infty \exp[-(a_{12} + a_{23} + a_{24})u_2]\,\mathrm{d}u_2 \\ & \times \int_{u_2}^\infty \exp[-(a_{13} + a_{23} - a_{34})u_3]\,\mathrm{d}u_3 \int_{u_3}^\infty \exp[-(a_{14} + a_{24} + a_{34})t_3]\,\mathrm{d}t_3 \\ & \times \int_{u_2}^{u_3} \exp[-(a_{14} - a_{24} + a_{34})s_3]\,\mathrm{d}s_3 \int_{s_3 - u_2}^{u_1 + s_3} \exp[-(-a_{14} + a_{24} + a_{34})w_3]\,\mathrm{d}w_3. \end{aligned} \tag{37}$$

The complete computation of these integrals is straightforward (but laborious) with the use of the following formula:

$$\int_a^b \exp(-\gamma x)\,\mathrm{d}x = \frac{1}{\gamma}[\exp(-\gamma a) - \exp(-\gamma b)]. \tag{38}$$

The computation of the integral in equation (37) produces the following expression

$$\begin{aligned} I_4 = \frac{8}{F(E+F)D(C+D+E+F)(C+D)} & \left[\frac{C-D}{(A+F)B} + \frac{C+D}{(B-F)A} \right. \\ & + \frac{C+D+E+F}{(A+F)(B+E+F)} - \frac{C+D+E+F}{A(B+E)} - \frac{E+F}{(A+F)(B+C+D+E+F)} \\ & \left. + \frac{E+F}{A(B+C+D+E)} \right] \end{aligned} \tag{39}$$

where A, B, C, D, E and F are defined in equation (29). In general, to compute the integral $I_4(a_{12}, a_{13}, a_{23}, a_{14}, a_{24}, a_{34})$ one needs to consider at least eight different areas of the original six-dimensional space. However, in each of these cases, the analytical computations of the basic four-body integral $I_4(a_{12}, a_{13}, a_{23}, a_{14}, a_{24}, a_{34})$ can be easily performed by using various platforms for analytical computations such as MAPLE[1]. The arising analytical expression for the basic four-body integral $I_4(a_{12}, a_{13}, a_{23}, a_{14}, a_{24}, a_{34})$ has a relatively simple structure, but contains a large number of terms. Note only that the correct final expression must be symmetric, i.e. it does not change its form, if some of the vertices/faces in the tetrahedron are

[1] The MAPLE package is the product of Waterloo Maple Inc., Waterloo, Ontario, Canada (http://www.maplesoft.com).

interchanged ($i \leftrightarrow j$, where $i \neq j = (1, 2, 3, 4)$). In the future, we hope to use this symmetry to simplify the analytical computations of the four-body integral $I_4(a_{12}, a_{13}, a_{23}, a_{14}, a_{24}, a_{34})$, equation (9).

In fact, after performing the analytical computations of the basic four-body integral $I_4(a_{12}, a_{13}, a_{23}, a_{14}, a_{24}, a_{34})$, equation (9), we have found that some other types of the four-body integrals can also be considered as the basic integrals for four-body bound state computations. For instance, in equation (37) instead of exponents upon s_3 and w_3 one may use the corresponding power-type or cosine-type functions. The four-body integrals will converge in such cases also, since the variables s_3 and w_3 vary between the finite limits. This allows one to construct a number of very flexible variational expansions (not only exponential expansion) in the four-body perimetric coordinates. It is interesting to note that, if we replace, e.g., each of the cosine-functions of the s_3 and w_3 variables by unity, then we can approximate an arbitrary four-body function (which depends upon the six variables) by using the four non-compact four-body variables (u_1, u_2, u_3 and t_3) only. This remarkable fact was first noticed and used by Hylleraas and Ore [6].

6. Conclusion

Thus, we have shown that six four-body perimetric coordinates do exist and can be determined as described above. These six perimetric coordinates u_1, u_2, u_3, s_3, t_3 and w_3 are independent and always positive. Furthermore, these six coordinates are uniformly related to the corresponding relative (or interparticle) coordinates $r_{ij} = r_{ji} = |\mathbf{r}_i - \mathbf{r}_j|$, where $i \neq j = (1, 2, 3, 4)$. It is important to note that all such relations (and corresponding inverse relations) take a linear form. This produces a significant number of advantages in numerical/analytical computations of various four-body integrals which are needed in bound-state problems. In fact, now the computation of any four-body integral can be performed in layers, i.e. by integrating all six perimetric coordinates one-by-one. This is impossible to achieve in the case of relative coordinates, where one has to consider 24 additional inequalities/constrains. In general, the four-body perimetric coordinates also have a great potential in applications to many other four-body problems, including photodetachment and scattering problems. It is also shown that the four-body perimetric coordinates are closely related to the geometry of tetrahedrons.

In fact, the six four-body perimetric coordinates do not have all properties known for the three-body perimetric coordinates. In particular, six additional constrains (= inequalities) must be obeyed for the four-body perimetric coordinates. These six inequalities produce some problems during various operations with the four-body perimetric coordinates. Nevertheless, this work opens a new avenue in studying of the four-body systems with arbitrary particles masses, types of interactions between the particles, particle symmetries, etc. The procedure developed in this study can be applied to many actual systems, including lithium atoms and lithium-like ions, various exotic systems (e.g., bi-positronium molecule Ps_2 ($e^+e^-e^+e^-$), HPs system ($H^+e^-e^+e^-$), bi-muonic molecules $dt\mu\mu$, $tt\mu\mu$, etc), nuclear and hypernuclear systems (e.g., α particle and ${}^4_\Lambda$ He).

The perimetric four-body coordinates are very convenient to obtain and study the conditions for convergence of various four-body integrals written in relative coordinates. In particular, such 'convergence' conditions for the nonlinear parameters in an arbitrary exponential integral are written in the form of equation (29). As mentioned above the four-body integral $I_4(a_{12}, a_{13}, a_{23}, a_{14}, a_{24}, a_{34})$ defined in above (see, equation (9)) has a number of advantages in actual computations in comparison to the $\mathcal{I}_4$ integral, equation (12), and integral $\mathcal{J}_4$ mentioned in the appendix. In particular, the tracking of singularities is very easy for the $I_4(a_{12}, a_{13}, a_{23}, a_{14}, a_{24}, a_{34})$ integral and its partial derivatives in respect to the nonlinear parameters $a_{12}, a_{13}, a_{23}, a_{14}, a_{24}$ and a_{34}.

Also note that our present method can be generalized to define nine independent perimetric coordinates for an arbitrary five-body system. In general, there are ten interparticle distances in arbitrary five-body system $\left(C_5^2 = 10\right)$, but only nine such coordinates are independent. This produces a difficult problem to exclude one unnecessary coordinate. For the exponential five-body expansion explicitly written in the relative coordinates $r_{12}, r_{13}, \ldots, r_{35}, r_{45}$ such a problem is extremely difficult. On the other hand, only nine five-body perimetric coordinates can be introduced for an arbitrary five-body system, i.e. here we do not need to exclude any unnecessary coordinate. Indeed, the two tetrahedrons (1234) and (1235) which are placed at one common face (e.g., (123)) have only 9 (nine) edges. These nine edges correspond to the nine independent relative coordinates $r_{12}, r_{13}, r_{23}, r_{14}, r_{24}, r_{34}, r_{15}, r_{25}, r_{35}$ and only these coordinates are used to form the nine independent five-body perimetric coordinates. The relative coordinate r_{45} does not appear in the following formulae at all. Very likely that the introduction of the five-body perimetric coordinates has many other advantages, but this is the goal for the future studies. Note only that the current progress in studying of the five-body systems is very modest in comparison even to the four-body case.

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Appendix.

For atomic (=one-centre) four-body systems, there is another method which is essentially based on the original Hylleraas expansion for the three-body systems. In the case of the four-body atom/ion the corresponding variational expansion takes the form

$$\Psi = \mathcal{A}\left\{\left[\sum_{i=1}^{N} C_i \cdot r_{23}^{n_{1,i}} \cdot r_{13}^{n_{2,i}} \cdot r_{12}^{n_{3,i}} \cdot r_{14}^{m_{1,i}} \cdot r_{24}^{m_{2,i}} \cdot r_{34}^{m_{3,i}}\right] \cdot \exp(-\alpha \cdot r_{14} - \beta \cdot r_{24} - \gamma \cdot r_{34})\right\}$$
$$= \mathcal{A}\left\{\left[\sum_{i=1}^{N} C_i \cdot p_i(r_{12}, r_{13}, r_{23}, r_{14}, r_{24}, r_{34})\right] \cdot \exp(-\alpha \cdot r_{14} - \beta \cdot r_{24} - \gamma \cdot r_{34})\right\} \qquad \text{(A.1)}$$

where all $n_{k,i}$ and $m_{l,i}$ are non-negative integer numbers, and α, β and γ are the only three nonlinear parameters. Here r_{i4} are the electron–nucleus relative coordinates, while r_{ij} are the three electron–electron coordinates ($i \neq j = (1, 2, 3)$). The operator $\mathcal{A}$ is the corresponding (anti-)symmertizator, i.e. the operator which produces the trial wavefunction of the correct permutation symmetry.

The computation of matrix elements in this basis is reduced to the problem of analytical/numerical computation of the following auxiliary four-body integrals

$$\mathcal{J}_4(K, L, M, n_1, n_2, n_3, \alpha, \beta, \gamma) = \iiint r_{14}^{K+2} r_{24}^{L+2} r_{34}^{M+2} r_{12}^{n_3} r_{13}^{n_2} r_{23}^{n_1}$$
$$\times \exp(-\alpha r_{14} - \beta r_{24} - \gamma r_{34})\, dr_{14}\, dr_{24}\, dr_{34} \qquad \text{(A.2)}$$

where K, L, M, n_1, n_2, n_3 are integer numbers, while α, β, γ are three real (positive) numbers. Numerical computation of these integrals is a routine procedure well described in the literature (see, e.g., [5, 7–10] and references therein). Some of the auxiliary integrals $\mathcal{J}_4$ computed numerically can also be found in table 1.

Finally, it was found that the variational method based on the variational expansion, equation (A.1), provides a sufficient numerical accuracy for some atomic (i.e. one-centre) Coulomb systems. However, despite numerous claims made in the modern literature, for an arbitrary four-body systems, including Coulomb systems with arbitrary particle masses this method is not accurate. For instance, for the bi-positronium Ps_2 it fails to provide even relatively accurate results. Moreover, in the case of Ps_2 and for many other four-body systems the construction of trial wavefunctions in the form equation (A.1) with the correct permutation symmetry is a very complicated problem. The reason for this is quite clear, since electron–electron correlations are considered in equation (A.1) as perturbations. For some systems, e.g., for the Be^+ ion the perturbation series converges quite fast, while for other systems (e.g., for the bi-positronium Ps_2) such series converge very slow. In general, any method developed for highly accurate computations of arbitrary four-body systems can be based only on the use of four-body integrals such as I_4 and $\mathcal{I}_4$ discussed in the main text.

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