Three-body bound-state calculations by the Lagrange-mesh method: Selection of a coordinate system

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Four coordinate systems adapted to three-body problems, the relative, Jacobi, perimetric, and renormalized Hylleraas coordinates, are compared in bound-state Lagrange-mesh calculations. The convergence of the energy with respect to the Lagrange basis size and the filling rate of the Hamiltonian matrix are analyzed. Three kinds of potentials are considered: harmonic, Gaussian, and Coulomb-like potentials. When at most one interaction potential presents a singularity at the origin, Jacobi coordinates represent the best choice for three-body Lagrange-mesh calculations. When all three potentials contain $1/r$ singularities, Jacobi coordinates provide only a limited accuracy, and perimetric coordinates take over. In all cases, with a good choice of coordinates, the Lagrange-mesh method provides very good accuracies on the three-body ground-state energy with small numbers of mesh points.

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I. INTRODUCTION

Three-body bound states can be studied by different techniques. Some of them, such as Faddeev equations or the method of hyperspherical coordinates [1,2], are accurate but difficult to implement. Variational calculations are also much used. The variational methods require the evaluation of Hamiltonian matrix elements between trial wave functions. In particular the determination of the matrix elements of the interaction potentials may be difficult and time consuming when the expressions of these potentials and/or trial functions are complicated. From this point of view the Lagrange-mesh method is very interesting as it is simple to implement, whatever the potentials, and provides accurate results.

The Lagrange-mesh method is an approximate variational calculation which resembles a mesh calculation [3–6]. Its main advantages are its simplicity and accuracy. Its simplicity comes from the use of a basis of Lagrange functions, i.e., indefinitely differentiable and orthonormal functions which vanish at all points but one of an associated mesh, and of the Gauss quadrature corresponding to this mesh. In quantum mechanical problems, the potential matrix in the Lagrange basis becomes diagonal with the help of the Gauss approximation, and its diagonal terms are simply given by the potential evaluated at mesh points.

The Lagrange-mesh method provides accurate results for a number of bound-state and scattering calculations in atomic and nuclear physics [4,7–12]. However, this astonishing and yet unexplained accuracy [13] may drop in the presence of singularities [14]. This problem can be solved by a regularization technique if all singularities occur at the same point [4,5]. Of course, this is not the case in three-body problems. However, the singularities can sometimes be eliminated by a good choice of coordinate system [12].

Three-body systems can be studied with the help of different coordinate systems. In the context of the Lagrange-mesh method we can then wonder whether there exists an optimal choice of the coordinate system to analyze a three-body problem. We thus make a twofold comparison of some of them, based on (i) the convergence of the bound-state energy with the Lagrange basis size and (ii) the filling rate of the Hamiltonian matrix in this basis. The former may depend on the expression of the interaction potentials between the three particles and, in particular, on the presence of singularities in these potentials. The latter does not depend at all on the potentials. Indeed, as pointed out above, in the Lagrange basis the potentials take part only on the diagonal of the Hamiltonian matrix, thanks to the use of the Gauss approximation. So, in the Lagrange-mesh method, the number of nonzero elements in the Hamiltonian matrix is completely determined by the kinetic energy operator. Here we consider four coordinate systems which are the relative coordinates with respect to one of the particles, the Jacobi coordinates, the perimetric coordinates [15,16], and some combination of Hylleraas coordinates [17], which we call renormalized Hylleraas coordinates. The relative coordinates have already been partly associated to Lagrange meshes to study nuclear three-body systems [8,9], and the perimetric coordinates have recently been used in atomic and molecular three-body Lagrange-mesh calculations [12].

The four coordinate systems and the corresponding three-body Hamiltonians are developped in Sec. II. The Lagrange-mesh method and three-dimensional Lagrange bases are explained in detail in Sec. III. The comparison between the four coordinate systems in Lagrange-mesh calculations is made with different potentials in Sec. IV. Conclusions are given in Sec. V.

II. THREE-BODY HAMILTONIAN AND COORDINATE SYSTEMS

The Hamiltonian of a three-body system can be written as

$$H=\frac{p_1^2}{2m_1}+\frac{p_2^2}{2m_2}+\frac{p_3^2}{2m_3}+V_{13}(|\boldsymbol{r}_1-\boldsymbol{r}_3|)+V_{23}(|\boldsymbol{r}_2-\boldsymbol{r}_3|)+V_{12}(|\boldsymbol{r}_1-\boldsymbol{r}_2|), \tag{1}$$

where $\mathbf{r}_i$ is the coordinate of particle i, with mass m_i, and $\boldsymbol{p}_i$

is the associated momentum. We assume here that the potentials V_{ij} only depend on the distances between particles.

After the elimination of the center-of-mass motion, the Hamiltonian is reduced to an internal Hamiltonian $H_{\rm int}$ describing the relative motion of the three particles. This Hamiltonian $H_{\rm int}$ is the sum of an internal kinetic energy $T_{\rm int}$ and of the potential V

$$H_{\rm int}=T_{\rm int}+V, \tag{2}$$

with

$$V=V_{13}(|\mathbf{r}_1-\mathbf{r}_3|)+V_{23}(|\mathbf{r}_2-\mathbf{r}_3|)+V_{12}(|\mathbf{r}_1-\mathbf{r}_2|). \tag{3}$$

In the center-of-mass frame, a three-body system has six degrees of freedom. They can be represented by three variables describing the shape of the triangle defined by the three particles, and by three Euler angles giving the orientation of this triangle in space. In order to simplify the problem, we are here interested only in S states, which correspond to a zero total angular momentum. In this case the wave function describing the three-body system is independent of Euler angles, and only depends on the three internal coordinates. To represent these internal variables, we consider four different sets of coordinates: the relative, Jacobi, perimetric, and renormalized Hylleraas coordinates.

A. Relative coordinates

The relative coordinates are simply defined by

$$\boldsymbol{r}_{13}=\boldsymbol{r}_1-\boldsymbol{r}_3, \tag{4}$$

$$\boldsymbol{r}_{23}=\boldsymbol{r}_2-\boldsymbol{r}_3, \tag{5}$$

when the third particle is chosen as reference. We take as internal coordinates the following variables:

$$r_{13}=|\boldsymbol{r}_{13}|,$$

$$r_{23}=|\boldsymbol{r}_{23}|, \tag{6}$$

$$x=\frac{\boldsymbol{r}_{13}\cdot\boldsymbol{r}_{23}}{r_{13}r_{23}}.$$

They are formed by the two interparticle distances r_{13} and r_{23} defined on $[0,\infty[$ and by the cosine x of the angle between the two relative coordinates $\boldsymbol{r}_{13}$ and $\boldsymbol{r}_{23}$, x varying in the interval $[-1,1]$. The volume element associated to these variables is given by

$$dV=r_{13}^2r_{23}^2dr_{13}dr_{23}dx. \tag{7}$$

The matrix element of the internal kinetic energy $T_{\rm int}$ between two functions $F(r_{13},r_{23},x)$ and $G(r_{13},r_{23},x)$ can be written as

$$\begin{aligned}\langle F|T_{\rm int}|G\rangle=&\int_0^\infty\int_0^\infty\int_{-1}^1 dr_{13}dr_{23}dx r_{13}r_{23}F(r_{13},r_{23},x)\\&\times\Bigg[-\frac{1}{2\mu_{13}}\partial_{r_{13}}^2-\frac{1}{2\mu_{23}}\partial_{r_{23}}^2-\left(\frac{1}{2\mu_{13}r_{13}^2}\right.\\&\left.+\frac{1}{2\mu_{23}r_{23}^2}\right)[(1-x^2)\partial_x^2-2x\partial_x]\\&-\frac{1}{m_3}\Bigg\{x\partial_{r_{13}}\partial_{r_{23}}+[(1-x^2)\partial_x-x]\\&\times\left(\frac{1}{r_{13}}\partial_{r_{23}}+\frac{1}{r_{23}}\partial_{r_{13}}\right)+\frac{1}{r_{13}r_{23}}[x+(3x^2-1)\partial_x\\&-x(1-x^2)\partial_x^2]\Bigg\}\Bigg]r_{13}r_{23}G(r_{13},r_{23},x),\end{aligned} \tag{8}$$

with $\hbar=1$. The term depending on m_3 is called the mass polarization term in atomic physics. The functions F and G are assumed to vanish when r_{13} or r_{23} tends towards infinity. In Eq. (8) we have switched the factor $r_{13}r_{23}$, coming from the volume element (7), and the derivative operators, so we can introduce this factor in the definition of the functions F and G. In relative coordinates, the potential V becomes

$$V=V_{13}(r_{13})+V_{23}(r_{23})+V_{12}(\sqrt{r_{13}^2+r_{23}^2-2r_{13}r_{23}x}). \tag{9}$$

B. Jacobi coordinates

Jacobi coordinates are similar to relative coordinates, and are often used to study many-body problems. For a three-body system, with the third particle as reference, they are given by

$$\mathbf{r}=\mathbf{r}_2-\mathbf{r}_1,$$

$$\boldsymbol{R}=\mathbf{r}_3-\frac{1}{m_1+m_2}(m_1\mathbf{r}_1+m_2\mathbf{r}_2), \tag{10}$$

and depend on the masses of particles 1 and 2.

As for the relative coordinates, we choose to represent the three internal degrees of freedom, the two distances r and R, and the cosine x of the angle between the Jacobi coordinates $\mathbf{r}$ and $\boldsymbol{R}$. The volume element is similar to Eq. (7), i.e.,

$$dV=r^2R^2drdRdx. \tag{11}$$

The matrix element of the internal kinetic energy in Jacobi coordinates is

$$\begin{aligned}\langle F|T_{\rm int}|G\rangle=&\int_0^\infty\int_0^\infty\int_{-1}^1 drdRdxrRF(r,R,x)\\&\times\Bigg\{-\frac{1}{2\mu_{12}}\partial_r^2-\frac{1}{2\mu_{123}}\partial_R^2-\left(\frac{1}{2\mu_{12}r^2}+\frac{1}{2\mu_{123}R^2}\right)\\&\times[(1-x^2)\partial_x^2-2x\partial_x]\Bigg\}rRG(r,R,x),\end{aligned} \tag{12}$$

where $\mu_{12}=m_1m_2/(m_1+m_2)$ and $\mu_{123}=m_3(m_1+m_2)/(m_1+m_2+m_3)$ are reduced masses, and the interaction potential becomes

$$V=V_{13}\left(\sqrt{R^2+\frac{m_2^2}{(m_1+m_2)^2}r^2+\frac{2m_2}{m_1+m_2}rRx}\right)+V_{23}\left(\sqrt{R^2+\frac{m_1^2}{(m_1+m_2)^2}r^2-\frac{2m_1}{m_1+m_2}rRx}\right)+V_{12}(r). \tag{13}$$

The simplification of the kinetic term with respect to the relative coordinates (there is no more a mass polarization term) goes together with a more complicated expression for the potential.

C. Perimetric coordinates

The perimetric coordinates [15,16] are defined as linear combinations of interparticle distances r_{ij}

$$x=r_{12}-r_{23}+r_{13},\qquad y=r_{12}+r_{23}-r_{13},\qquad z=-r_{12}+r_{23}+r_{13}. \tag{14}$$

All three take values on $[0,\infty[$. The volume element associated to these coordinates is

$$dV=(x+y)(x+z)(y+z)dxdydz. \tag{15}$$

The matrix element of the internal kinetic energy between two functions $F(x,y,z)$ and $G(x,y,z)$, which tend to zero when x, y or z goes to infinity, can be written in the symmetric form

$$\langle F|T_{\rm int}|G\rangle=\int_0^\infty\int_0^\infty\int_0^\infty dxdydz\times\sum_{\mu,\nu}(\partial_\mu F)(x,y,z)A_{\mu\nu}(x,y,z)(\partial_\mu G)(x,y,z), \tag{16}$$

where μ and ν represent the perimetric coordinates x, y, and z. The coefficients A_{xx} and A_{xy} can be written as

$$A_{xx}=2\left(\frac{x(y+z)(x+y+z)}{m_1}+\frac{xz(z+x)}{m_2}+\frac{xy(x+y)}{m_3}\right), \tag{17}$$

$$A_{xy}=A_{yx}=-2\frac{xy(x+y)}{m_3}. \tag{18}$$

The other $A_{\mu\nu}$ coefficients are obtained from A_{xx} and A_{xy} by cyclic permutations of perimetric coordinates x, y, and z and simultaneously of masses m_1, m_2, and m_3. The potential is expressed as

$$V=V_{13}\left(\frac{x+z}{2}\right)+V_{23}\left(\frac{y+z}{2}\right)+V_{12}\left(\frac{x+y}{2}\right). \tag{19}$$

D. Renormalized Hylleraas coordinates

The Hylleraas coordinates have been introduced to study the helium atom [17]. As the perimetric coordinates, they take the form of linear combinations of interparticle distances

$$s=r_{13}+r_{23},\qquad t=r_{13}-r_{23},\qquad u=r_{12}. \tag{20}$$

The s variable is defined on $[0,\infty[$, and the conditions on the three interparticle distances give $0\leqslant u\leqslant s$ and $-u\leqslant t\leqslant u$. The definition domains of these three variables are then interdependent. The renormalized Hylleraas coordinates are introduced in order to have three variables whose domains of variation are independent. They are given by

$$x=t/u,\qquad y=u/s,\qquad z=s. \tag{21}$$

These new coordinates x, y, and z are defined on the intervals $[-1,1]$, $[0,1]$, and $[0,\infty[$, respectively. The associated volume element can be written as

$$dV=y^2z^5(1-x^2y^2)dxdydz. \tag{22}$$

Chuluunbaatar, Puzynin, and Vinitsky [18] have recently used these coordinates to determine the ground-state energies of several two-electron atomic systems. With these renormalized Hylleraas coordinates, the matrix element of the internal kinetic energy between two functions $F(x,y,z)$ and $G(x,y,z)$ can be written in the symmetric form

$$\langle F|T_{\rm int}|G\rangle=\int_{-1}^1\int_0^1\int_0^\infty dxdydz\times\sum_{\mu,\nu}(\partial_\mu F)(x,y,z)B_{\mu\nu}(x,y,z)(\partial_\nu G)(x,y,z), \tag{23}$$

where μ and ν represent the renormalized Hylleraas coordinates x, y, and z. The coefficients $B_{\mu\nu}$ are given by

$$B_{xx}=z^3(1-x^2)\left(\frac{(1-xy)^2}{2m_1}+\frac{(1+xy)^2}{2m_2}+\frac{2y^2}{m_3}\right), \tag{24}$$

$$B_{yy}=y^2z^3(1-y^2)\left(\frac{(1-xy)^2}{2m_1}+\frac{(1+xy)^2}{2m_2}+\frac{2y^2}{m_3}\right), \tag{25}$$

$$B_{zz}=y^2z^5\left[\left(\frac{1}{2m_1}+\frac{1}{2m_2}\right)(1-x^2y^2)+\frac{2(1-y^2)}{m_3}\right], \tag{26}$$

$$B_{xy}=B_{yx}=0, \tag{27}$$

$$B_{xz}=B_{zx}=yz^4(1-x^2)\left(\frac{1-xy}{2m_1}-\frac{1+xy}{2m_2}\right), \tag{28}$$

$$B_{yz}=B_{zy}=y^2z^4(1-y^2)\left(\frac{x(1-xy)}{2m_1}-\frac{x(1+xy)}{2m_2}-\frac{2y}{m_3}\right). \tag{29}$$

Expressed in these coordinates, the potential becomes

$$V=V_{13}\left(\frac{z(1+xy)}{2}\right)+V_{23}\left(\frac{z(1-xy)}{2}\right)+V_{12}(yz). \tag{30}$$

III. LAGRANGE-MESH METHOD

A one-dimensional Lagrange mesh is formed of N mesh points x_i spread over the interval (a,b) and associated with an orthonormal set of N indefinitely derivable functions $\mathcal{F}_i^N(x)$ [3–5]. At mesh points, these functions satisfy the Lagrange conditions

$$\mathcal{F}_i^N(x_{i'})=\lambda_i^{-1/2}\delta_{ii'}, \tag{31}$$

i.e., the Lagrange functions $\mathcal{F}_i^N$ vanish at all mesh points but one. The x_i and λ_i are connected with a Gauss quadrature formula

$$\int_a^b g(x)dx\approx\sum_{i=1}^{N}\lambda_i g(x_i). \tag{32}$$

The Lagrange functions are used as basis functions in a variational calculation. The potential matrix elements in this basis are given by

$$V_{ij}=\int_a^b \mathcal{F}_i^N(x)V(x)\mathcal{F}_j^N(x)dx\approx V(x_i)\delta_{ij}, \tag{33}$$

with the help of the Gauss approximation and Eq. (31). The potential matrix is then both simple to obtain and diagonal.

To study S states of three-body systems, we use three-dimensional Lagrange functions F_{ijk} expressed in one of the four coordinate systems described previously

$$F_{ijk}(c_1,c_2,c_3)=N_{ijk}^{-1/2}\mathcal{F}_{1i}^{N_1}(c_1/h_1)\mathcal{F}_{2j}^{N_2}(c_2/h_2)\mathcal{F}_{3k}^{N_3}(c_3/h_3), \tag{34}$$

where $\mathcal{F}_{pl}^N$ $(p=1,2,3)$ is a one-dimensional Lagrange function, and c_1, c_2, and c_3 represent the three internal coordinates, described by Lagrange meshes with N_1, N_2, and N_3 points respectively; h_1, h_2, and h_3 are scale factors which can be introduced in the case of infinite intervals in order to adjust the position of the mesh points. The Lagrange functions $\mathcal{F}_{1i}^{N_1}$, $\mathcal{F}_{2j}^{N_2}$, and $\mathcal{F}_{3k}^{N_3}$ may be based on different kinds of mesh, i.e., corresponding to different intervals (see below). The Lagrange functions F_{ijk} satisfy the Lagrange conditions with respect to the three-dimensional mesh

$$F_{ijk}(h_1x_{1i'},h_2x_{2j'},h_3x_{3k'})=N_{ijk}^{-1/2}(\lambda_{1i}\lambda_{2j}\lambda_{3k})^{-1/2}\delta_{ii'}\delta_{jj'}\delta_{kk'}, \tag{35}$$

where x_{pi} and λ_{pi} are, respectively, the mesh points and weights associated to the c_p coordinate. As for the $\mathcal{F}_{pl}^N$ Lagrange functions, the x_{1i}, x_{2i}, and x_{3i} points do not correspond necessarily to the same kind of Lagrange mesh. With the normalization factor N_{ijk}, the Lagrange basis functions F_{ijk} are orthonormal at the Gauss approximation with respect to the associated volume element $dV=J(c_1,c_2,c_3)dc_1dc_2dc_3$

$$\int\int\int dc_1dc_2dc_3J(c_1,c_2,c_3)F_{ijk}(c_1,c_2,c_3)\times F_{i'j'k'}(c_1,c_2,c_3)\approx\delta_{ii'}\delta_{jj'}\delta_{kk'}. \tag{36}$$

With Eq. (35), this induces

$$N_{ijk}=h_1h_2h_3J(c_{1i},c_{2j},c_{3k}), \tag{37}$$

i.e., the normalization factor is equal to the Jacobian J evaluated at the three-dimensional mesh points.

These three-dimensional Lagrange functions F_{ijk} are used as a basis for a variational calculation to determine the ground-state energy of the three-body system. The trial wave function can be written as

$$\Psi=\sum_{i=1}^{N_1}\sum_{j=1}^{N_2}\sum_{k=1}^{N_3}C_{ijk}F_{ijk}=\sum_{I=1}^{N_T}C_IF_I, \tag{38}$$

where the C_{ijk} coefficients play the role of linear variational parameters, and I represent the three indexes (ijk). The scale factors h_1, h_2, and h_3 in Eq. (34) may be treated as nonlinear parameters, but usually the binding energy is not very sensitive to the precise values of these factors. The total number of basis functions N_T is equal to $N_1N_2N_3$. The Schrödinger equation takes finally the form of an eigenvalue problem of size N_T

$$\sum_{I'=1}^{N_T}H_{II'}C_{I'}=EC_I, \tag{39}$$

where $H_{II'}$ is the Hamiltonian matrix element between Lagrange basis functions. In the right-hand side of the equation, we have used the orthonormality at the Gauss approximation of the Lagrange basis functions.

We can now analyze the form of the three-dimensional Lagrange functions in each coordinate system described in the previous section. The Lagrange meshes used are chosen by looking at the domains of definition of the variables. The four coordinate sets considered here introduce only three different domains. They are the semi-infinite interval $[0,\infty[$, and the two finite intervals $[-1,1]$ and $[0,1]$. To variables de-

fined on $[0,\infty[$ we associate a Laguerre mesh, i.e., a Lagrange mesh based on the Laguerre polynomials [12]. The N mesh points r_i are given by the N zeros of the Laguerre polynomial $L_N(r)$ of degree N

$$L_N(r_i)=0, \tag{40}$$

and the associated Gauss-Laguerre weights [19] are noted λ_i^r. The corresponding Lagrange functions can be written as

$$f_i^N(r)=(-1)^i r_i^{1/2}\frac{L_N(r)}{r-r_i}e^{-r/2}. \tag{41}$$

The distribution of the mesh points over the $[0,\infty[$ interval is controled by the scale factor h. For the variables defined on the $[-1,1]$ and $[0,1]$ intervals, we choose Lagrange meshes based on Legendre and shifted Legendre polynomials respectively. The Legendre mesh [3] is formed by N points x_i corresponding to the N zeros of the Legendre polynomial $P_N(x)$ of degree N

$$P_N(x_i)=0, \tag{42}$$

and the associated Gauss-Legendre weights λ_i^x [19]. The Lagrange-Legendre functions are given by

$$g_i^N(x)=(-1)^{i+N}\sqrt{\frac{1-x_i^2}{2}}\frac{P_N(x)}{x-x_i}. \tag{43}$$

The shifted Legendre mesh is obtained by shifting the Legendre mesh to the interval $[0,1]$ [10]. The N mesh points y_i are defined by $y_i=(1+x_i)/2$, and the corresponding weights are $\lambda_i^y=\lambda_i^x/2$. The Lagrange functions for this mesh can be written as

$$q_i^N(y)=(-1)^{i+N}\sqrt{y_i(1-y_i)}\,\frac{P_N(2y-1)}{y-y_i}. \tag{44}$$

As the points of these two meshes are already distributed in the correct interval, no scale factor is required. We will now exemplify the above expressions in the case of the four coordinate systems of the previous section.

A. Relative coordinates

In the case of relative coordinates, the three variables describing the internal degrees of freedom are the two distances r_{13} and r_{23}, and the angular coordinate x. To the coordinate r_{13} is associated a Laguerre mesh of N_1 points r_{1i} and the scale factor h_1. The Laguerre mesh for the r_{23} coordinate includes N_2 points r_{2j}, and the scale factor is h_2. The x variable is described by a Legendre mesh of N_x points x_k.

The three-dimensional Lagrange basis functions take then the form

$$F_{ijk}(r_{13},r_{23},x)=(h_1h_2)^{-1/2}\tilde{f}_i^{N_1}(r_{13}/h_1)\tilde{f}_j^{N_2}(r_{23}/h_2)g_k^{N_x}(x). \tag{45}$$

The $\tilde{f}_i^N(r)$ functions are the so-called regularized Lagrange functions [9,13]. They are obtained by multiplying the Lagrange-Laguerre functions $f_i^N(r)$ (41) by the factor r/r_i coming from the volume element (7). Because of this choice the normalization factor N_{ijk} is simply equal to h_1h_2.

The expression of the matrix element of the internal kinetic energy between two three-dimensional Lagrange basis functions (45) is given in the Appendix. It is clear from Eq. (A1) that the mass polarization term is the most important source of nonzero elements in the matrix. The total number $\mathcal{N}$ of nonzero elements in the Hamiltonian matrix is equal to

$$\mathcal{N}=N_1N_2N_x[(N_1+N_2)(N_x-1)+N_1N_2-N_x+1]. \tag{46}$$

The potential matrix elements are easily obtained at the Gauss approximation

$$\begin{aligned}\langle F_{ijk}|V|F_{i'j'k'}\rangle\approx&[V_{13}(h_1r_{1i})+V_{23}(h_2r_{2j})\\&+V_{12}(\sqrt{h_1^2r_{1i}^2+h_2^2r_{2j}^2-2h_1h_2r_{1i}r_{2j}x_k})]\\&\times\delta_{ii'}\delta_{jj'}\delta_{kk'},\end{aligned} \tag{47}$$

and the associated matrix is purely diagonal.

B. Jacobi coordinates

As in the case of relative coordinates, we associate to the r and R coordinates two Laguerre meshes of N_r and N_R points (r_i and R_j), with the scale factors h_r and h_R, respectively. The Legendre mesh for the x coordinate contains N_x points x_k.

The three-dimensional Lagrange functions can be written as

$$F_{ijk}(r,R,x)=(h_rh_R)^{-1/2}\tilde{f}_i^{N_r}(r/h_r)\tilde{f}_j^{N_R}(R/h_R)g_k^{N_x}(x). \tag{48}$$

As before we use the regularized Lagrange-Laguerre functions $\tilde{f}_i^N(r)$ with the regularization factor coming from the volume element (11). The normalization factor N_{ijk} is similar to the relative coordinate's one, and is equal to h_rh_R.

The matrix elements of the internal kinetic energy between basis functions (48) can be deduced from expression (A1) by changing the reduced masses. The total number $\mathcal{N}$ of nonzero elements in the Hamiltonian matrix is

$$\mathcal{N}=N_rN_RN_x(N_r+N_R+N_x-2). \tag{49}$$

With the same basis size, the number $\mathcal{N}$ for Jacobi coordinates is much smaller than for relative coordinates because there is no mass polarization term in the kinetic energy expression.

At the Gauss approximation, the potential matrix is diagonal and its nonzero elements are given by

$$\langle F_{ijk}|V|F_{i'j'k'}\rangle \approx \left[V_{13}\left(\sqrt{h_R^2 R_j^2 + \frac{m_2^2}{(m_1+m_2)^2} h_r^2 r_i^2 + \frac{2m_2}{m_1+m_2} h_r r_i h_R R_j x_k} \right) + V_{23}\left(\sqrt{h_R^2 R_j^2 + \frac{m_1^2}{(m_1+m_2)^2} h_r^2 r_i^2 - \frac{2m_1}{m_1+m_2} h_r r_i h_R R_j x_k} \right) + V_{12}(h_r r_i) \right] \delta_{ii'} \delta_{jj'} \delta_{kk'} . \quad (50)$$

As said before, the mathematical expression of the potential is more complicated than in relative coordinates, but it is not a problem as we only need its evaluation at mesh points.

C. Perimetric coordinates

The three Laguerre meshes associated to the perimetric variables x, y, and z contain N_x, N_y, and N_z points, which are noted x_i, y_j, and z_k respectively. Their distribution on $[0,\infty[$ is adjusted with the scale factors h_x, h_y, and h_z.

The three-dimensional Lagrange functions are in this case

$$F_{ijk}(x,y,z) = N_{ijk}^{-1/2} f_i^{N_x}(x/h_x) f_j^{N_y}(y/h_y) f_k^{N_z}(z/h_z). \quad (51)$$

With Eq. (15) the normalization factor N_{ijk} is equal to

$$N_{ijk} = (h_x x_i + h_y y_j)(h_x x_i + h_z z_k)(h_y y_j + h_z z_k). \quad (52)$$

The evaluation at the Gauss approximation of the matrix elements of the internal kinetic energy between two Lagrange functions (51) is illustrated in the Appendix for one term of the sum in Eq. (16). A full expression can be found in Ref. [12]. The total number $\mathcal{N}$ of nonzero elements in the Hamiltonian matrix is given by

$$\mathcal{N} = N_x N_y N_z [(N_x + N_y)(N_z - 1) + N_x N_y - N_z + 1]. \quad (53)$$

The potential matrix elements can be written as

$$\langle F_{ijk}|V|F_{i'j'k'}\rangle \approx \left[V_{13}\left(\frac{h_x x_i + h_z z_k}{2} \right) + V_{23}\left(\frac{h_y y_j + h_z z_k}{2} \right) + V_{12}\left(\frac{h_x x_i + h_y y_j}{2} \right) \right] \delta_{ii'} \delta_{jj'} \delta_{kk'} . \quad (54)$$

D. Renormalized Hylleraas coordinates

As the three renormalized Hylleraas coordinates are defined on different intervals, we use three different Lagrange meshes. To the z coordinate we associate a Laguerre mesh of N_z points z_k, and the scale factor h_z. The Legendre and shifted Legendre meshes associated to the x and y variables contain N_x and N_y points, respectively, whose notation is x_i and y_j.

The three-dimensional Lagrange functions take the following form:

$$F_{ijk}(x,y,z) = N_{ijk}^{-1/2} g_i^{N_x}(x) q_j^{N_y}(y) f_k^{N_z}(z/h_z). \quad (55)$$

With Eq. (22) the normalization factor N_{ijk} is given by

$$N_{ijk} = h_z^6 y_j^2 z_k^5 (1 - x_i^2 y_j^2). \quad (56)$$

The matrix elements of the internal kinetic energy in this Lagrange basis can be obtained at the Gauss approximation just as in the case of perimetric coordinates, which is illustrated in the Appendix. The choice of the symmetric expression (23) ensures the hermiticity of the Hamiltonian matrix when we evaluate it with the Gauss quadrature rule. The total number $\mathcal{N}$ of nonzero elements in the Hamiltonian matrix can be expressed as

$$\mathcal{N} = N_x N_y N_z^2 (N_x + N_y - 1). \quad (57)$$

The potential matrix elements are always simply given by

$$\langle F_{ijk}|V|F_{i'j'k'}\rangle \approx \left[V_{13}\left(\frac{h_z z_k (1 + x_i y_j)}{2} \right) + V_{23}\left(\frac{h_z z_k (1 - x_i y_j)}{2} \right) + V_{12}(h_z y_j z_k) \right] \delta_{ii'} \delta_{jj'} \delta_{kk'} , \quad (58)$$

at the Gauss approximation.

IV. APPLICATIONS

In the case of the Lagrange-mesh method we must solve the eigenvalue problem (39). The determination of the ground-state energy requires the search for the smallest eigenvalue of the Hamiltonian matrix. This is done here by using the Davidson algorithm as developed by Stathopoulos and Fisher [20].

We consider three types of potentials: harmonic oscillator, Gaussian, and Coulomb-like potentials. For simplicity we choose here the same expression for the three potentials V_{ij} $(i \neq j = 1,2,3)$ and unit masses for the three particles $(m_i = 1)$. This induces the symmetry of the three-body system with respect to the exchange of the three particles.

In Tables I–III are indicated the errors ϵ obtained on the ground-state energy of the three-body problem with the four coordinate systems for each type of potentials. These errors are defined by

$$\epsilon = E - E_{\text{ref}}, \quad (59)$$

where E is the energy value obtained by our Lagrange-mesh calculations and E_{ref} is a reference value for the ground-state energy. The results in the three tables illustrate the conver-

TABLE I. Errors ϵ on the ground-state energy of a three-body system with harmonic potentials (60), obtained with the Lagrange-mesh method. The exact ground-state energy is equal to 3. N_T is the Lagrange basis size and $\mathcal{N}$ is the number of nonzero elements of the Hamiltonian matrix in the Lagrange basis.

Coordinates	N_1	N_2	N_3	h_1	h_2	h_3	N_T	ϵ	$\mathcal{N}$
Relative	7	7	4	0.2	0.2		196	1×10^{-3}	17 248
	11	11	7	0.2	0.2		847	1×10^{-6}	209 209
	14	14	10	0.2	0.2		1960	3×10^{-8}	860 440
Jacobi	5	5	1	0.4	0.4		25	-2×10^{-3}	225
	10	10	1	0.2	0.2		100	-2×10^{-6}	1900
	12	12	1	0.2	0.2		144	4×10^{-9}	3312
Perimetric	5	5	5	0.4	0.4	0.4	125	-2×10^{-3}	7625
	9	9	9	0.4	0.4	0.4	729	-4×10^{-6}	158 193
	12	12	12	0.4	0.4	0.4	1728	1×10^{-8}	686 016
Renormalized	8	8	8			0.3	512	-4×10^{-3}	61 440
Hylleraas	8	8	14			0.3	896	-8×10^{-7}	188 160
	10	10	18			0.3	1800	-6×10^{-9}	615 600

gence of the ground-state energy with respect to the Lagrange-basis size. For each coordinate system three calculations are done which correspond to the minimum Lagrange basis size required to obtain accuracies of about 10^{-3}, 10^{-6}, and 10^{-8}, respectively.

The numbers of mesh points N_1, N_2, and N_3 correspond to the numbers N_1, N_2, and N_x for relative coordinates, N_r, N_R, and N_x for Jacobi coordinates, and N_x, N_y, and N_z for perimetric and renormalized Hylleraas coordinates. The scale factors associated to the meshes of N_1, N_2, and N_3 points are represented by h_1, h_2, and h_3, respectively. They are roughly optimized to minimize the error on the energy. Because of the symmetry of the problem, we take $N_1=N_2$ and $h_1=h_2$ in the case of relative coordinates $N_r=N_R$ and $h_r=h_R$ in the case of Jacobi coordinates, and $N_x=N_y=N_z$ and $h_x=h_y=h_z$ in the case of perimetric coordinates. The number N_T represents the Lagrange basis size, which is equal to $N_1N_2N_3$. The total number $\mathcal{N}$ of nonzero elements of the Hamiltonian matrix is indicated in the last column for each coordinate system.

The Lagrange-mesh method is an approximate variational calculation. The use of the Gauss approximation induces that errors ϵ may be negative, and the results do not represent an upper bound to the exact energy value. So we cannot determine the best result by searching the minimum value. Usually we estimate the accuracy of the results by increasing the basis size and by slightly varying the scale factors.

A. Harmonic potentials

In order to analyze the convergence of Lagrange-mesh calculations according to the coordinate system used, we first consider harmonic potentials. The three interparticle potentials V_{ij} are defined as

$$V_{ij}(r_{ij})=\frac{r_{ij}^2}{6}. \tag{60}$$

TABLE II. Errors ϵ on the ground-state energy of a three-body system with Gaussian potentials (61), obtained with the Lagrange-mesh method. The reference energy is equal to $-0.704\,924\,422\,104$. N_T is the Lagrange basis size, and $\mathcal{N}$ is the number of nonzero elements of the Hamiltonian matrix in the Lagrange basis.

Coordinates	N_1	N_2	N_3	h_1	h_2	h_3	N_T	ϵ	$\mathcal{N}$
Relative	8	8	6	0.2	0.2		384	3×10^{-3}	53 376
	12	12	14	0.2	0.2		2016	-2×10^{-6}	893 088
	20	20	22	0.2	0.2		9600	-2×10^{-8}	10 727 200
Jacobi	6	6	4	0.2	0.2		144	4×10^{-3}	2016
	12	12	8	0.2	0.2		1152	4×10^{-6}	34 560
	16	16	12	0.2	0.2		3072	4×10^{-8}	129 024
Perimetric	4	4	4	0.5	0.5	0.5	64	1×10^{-3}	2368
	8	8	8	0.4	0.4	0.4	512	-4×10^{-6}	86 528
	12	12	12	0.4	0.4	0.4	1728	1×10^{-8}	686 016
Renormalized	6	8	10			0.3	480	-1×10^{-3}	62 400
Hylleraas	10	12	16			0.3	1920	-1×10^{-6}	645 120
	10	12	20			0.3	2400	-4×10^{-8}	1008 000

TABLE III. Errors ϵ on the ground-state energy of a three-body system with Coulomb-like potentials (62), obtained with the Lagrange-mesh method. The reference energy for this state is $E=-1.071\,779\,372\,992$. N_T is the Lagrange basis size and $\mathcal{N}$ is the number of nonzero elements of the Hamiltonian matrix in the Lagrange basis.

Coordinates	N_1	N_2	N_3	h_1	h_2	h_3	N_T	ϵ	$\mathcal{N}$
Relative	14	14	14	0.4	0.4		2744	-3×10^{-3}	1 500 968
	20	20	20	0.2	0.2		8000	7×10^{-4}	9 128 000
	26	26	26	0.2	0.2		17 576	6×10^{-4}	34 290 776
Jacobi	14	14	14	0.8	0.8		2744	-3×10^{-3}	109 760
	20	20	20	0.8	0.8		8000	2×10^{-4}	464 000
	26	26	26	1.0	1.0		17 576	-1×10^{-4}	1 335 776
Perimetric	3	3	3	0.9	0.9	0.9	27	9×10^{-7}	513
	6	6	6	0.8	0.8	0.8	216	5×10^{-9}	19 656
Renormalized	2	4	6			0.7	48	-2×10^{-3}	1440
Hylleraas	4	6	8			0.7	192	-4×10^{-6}	13 824
	6	8	10			0.7	480	-1×10^{-8}	62 400

With these potentials, the ground-state energy of the three-body system can be determined exactly, and is equal to 3. Indeed the searched energy E is the one associated to the internal Hamiltonian of the system, and can be deduced as the total energy E_{tot} of the three-body system minus the energy $E_{\mathrm{c.m.}}$ of the center of mass. The total energy E_{tot} is equal to $\frac{9}{2}$. As the center of mass is also characterized by an harmonic potential, its ground-state energy $E_{\mathrm{c.m.}}$ is given by $\frac{3}{2}$. We then use $E_{\mathrm{ref}}=3$.

The results of Table I illustrate fairly well the very good precision of the Lagrange-mesh method as, for the four coordinate systems considered here, we obtain errors on the three-body ground-state energy better than 10^{-6} with only about 1000 Lagrange basis functions. The fastest convergence with respect to the basis size is obtained with Jacobi coordinates. This comes from the very little number of Legendre mesh points N_x ($N_x=1$) required. With N_r and N_R fixed, an increase of N_x does not improve the energy value. This is peculiar to the choice of harmonic potentials. Indeed, in spite of the dependence of the V_{ij} potentials on the x coordinate, the sum (50) of the three potentials is independent of x. Furthermore, the ground-state wave function, which can be written as the product of Gaussian functions, is independent of the x variable. This induces that a Legendre mesh containing one point (and thus one Lagrange function) is enough to represent this coordinate. The number of nonzero elements of the Hamiltonian matrix is also strongly reduced with respect to the other coordinate systems, only partly thanks to the choice $N_x=1$.

The use of relative coordinates requires bigger Lagrange bases. Here also the harmonic potential is a particular case which is not characteristic of the use of relative coordinates on Lagrange meshes. Indeed, even if, unlike the case of Jacobi coordinates, the potential depends on the x angular variable, its dependence is purely linear for the harmonic potential. This induces that the integral over x in potential matrix elements is exactly evaluated with the N_x points Gauss-Legendre quadrature rule. Indeed, the N_x points Gauss-Legendre approximation is exact when the integrand is a polynomial of order at most $2N_x-1$, which is the case for the harmonic potential as the polynomial degree of Lagrange-Legendre functions (43) is N_x-1. This property accelerates the convergence of calculations with respect to the x dependence of the wave function. The number N_x of mesh points must be chosen bigger than one because, unlike the case of Jacobi coordinates, the ground-state wave function of the three-body system depends on the x variable when it is expressed in relative coordinates. Regarding the number $\mathcal{N}$ of nonzero elements in the Hamiltonian matrix, it is clearly much larger with relative coordinates, because of the mass polarization term.

In the perimetric coordinates case, unlike the three others coordinates systems, the three particles are treated symmetrically, which induces a similar convergence with respect to the three numbers of Laguerre mesh points N_x, N_y, and N_z, when the masses of the three bodies are equal. When the basis size is fixed, the accuracy on the energy is better than for relative and renormalized Hylleraas coordinates. The filling of the Hamiltonian matrix is comparable to relative and renormalized Hylleraas coordinates for low accuracy, but is reduced with respect to relative coordinates when the searched accuracy increases.

In the case of renormalized Hylleraas coordinates, the convergence with respect to the basis size N_T is slower than for the other three coordinate systems, when N_T is smaller than 1000. For example, an error of order 10^{-3} on the energy requires about 500 Lagrange basis functions, while for the three other coordinate systems the same accuracy is already reached with less than 200 Lagrange functions. With $N_T=1800$, the accuracy on the energy is similar to that of relative and perimetric coordinates with about the same basis size, and the filling rate $\mathcal{N}$ is about the same as for perimetric coordinates. Renormalized Hylleraas coordinates require a number N_z of mesh points larger than the numbers N_x and N_y. This property is also valid for the other coordinate systems: numbers of mesh points associated to variables defined on the $[0,\infty[$ interval generally have to be chosen larger than those corresponding to finite intervals.

B. Gaussian potentials

As the harmonic potentials (60) represent a special case for Jacobi and relative coordinates, we now consider Gaussian potentials in order to define the general characteristics of these two coordinate systems in Lagrange-mesh calculations. The Gaussian potentials are chosen as

$$V_{ij} = -2e^{-0.5r_{ij}^2}. \tag{61}$$

Unlike for harmonic potentials, the ground-state energy of the three-body system with the potentials (61) cannot be determined analytically. However Lagrange-mesh calculations with large basis sizes (typically about 10 000 Lagrange functions in perimetric coordinates) provide the estimate $E_{\mathrm{ref}} = -0.704\,924\,422\,104$, which we use as reference value.

In Table II we present the errors (59) on the ground-state energy of the three-body system obtained by Lagrange-mesh calculations with the four coordinate systems. If we are only interested in the convergence of the energy with respect to the Lagrange basis size, we note that perimetric coordinates are the optimal choice, as they provide the best accuracy for a fixed basis size. For example, with only 1728 Lagrange basis functions, the accuracy is about 10^{-8}. The same order of accuracy requires about 2400 functions with renormalized Hylleraas coordinates and about 3000 functions with Jacobi coordinates. With relative coordinates, the convergence of the energy is much slower than in the harmonic potentials case. Indeed an accuracy of 2×10^{-8} requires about 9600 Lagrange basis functions, and in particular more Lagrange-mesh points for the x angular coordinate. The example of Gaussian potentials is more representative of basis sizes required in Lagrange-mesh calculations with relative coordinates than the harmonic one.

If we take into account the filling of the Hamiltonian matrix, Jacobi coordinates become the best choice, because the number of nonzero elements of the matrix is much smaller in this case than with the other three coordinate systems. Perimetric coordinates are the second choice, with about ten times more nonzero elements in the matrix for the same accuracy, even if the basis size is smaller. As relative coordinates require the largest bases, their filling rate is also the largest for a chosen accuracy. So this coordinate system seems to be the less efficient one to study three-body problems with the Lagrange-mesh method, when the forces are purely central.

C. Coulomb-like potentials

Until now we have considered only regular potentials, i.e., without singular points. This characteristic of the potentials is very important in Lagrange-mesh calculations. Indeed in the presence of singularities in the potentials the accuracy of the Lagrange-mesh method may drop drastically [14]. In order to analyze this problem for three-body systems, we consider the example of three attractive Coulomb-like potentials

$$V_{ij} = -1/r_{ij}\,. \tag{62}$$

This example does not correspond to a realistic problem, as there exists no physical three-body system in which the three Coulomb interactions are attractive. Nevertheless this example is suitable to study the problem of singularities in the potentials. It has also the advantage that the three particles can be treated symmetrically. The reference value of the ground-state energy of the three-body system is determined by Lagrange-mesh calculations with about 14 000 functions in perimetric coordinates, and is equal to $E_{\mathrm{ref}} = -1.071\,779\,372\,992$. The results for this energy obtained with the four coordinate systems and Lagrange meshes are given in Table III.

As said before, a regularization technique has been developed which can solve the problem of singularities when they occur at the same point [4]. This is obvously not the case in three-body problems as shown by potentials (62). In the case of relative coordinates, we deduce from Eqs. (7) and (9) that singularities at the origin in the V_{13} and V_{23} potentials are automatically regularized by the $r_{13}^2 r_{23}^2$ factor from the volume element. However, the singularity in the V_{12} potential is not regularized by this factor. Furthermore, it cannot be regularized easily with relative coordinates. Lagrange-mesh calculations with relative coordinates as presented here provide good results only if the potential V_{12} is perfectly regular, i.e., without singularity. This is illustrated by the results obtained with the potentials (62) in Table III. The error on the energy value stays higher than 10^{-4}, even if we use more than 15 000 Lagrange basis functions. This limitation of accuracy is entirely due to the singularity at the origin in the V_{12} potential, as shown by the previous examples.

The case of Jacobi coordinates is even more unfavorable because the r^2R^2 factor from the volume element (11) only allows the regularization of singularities in the V_{12} potential. Indeed, the r_{13} and r_{23} distances take a relatively complicated form when expressed in Jacobi coordinates (13), and singularities at the origin in the V_{13} and V_{23} potentials cannot be regularized easily. The use of Jacobi coordinates in Lagrange-mesh calculations then requires strictly regular V_{13} and V_{23} potentials. In the example presented in Table III, we obtain results similar to those of relative coordinates, i.e., the error on the ground-state energy is higher than 10^{-4}, even when the Lagrange basis size is increased beyond 15 000 functions. In the case of Jacobi coordinates, the loss of accuracy is due to singularities in both V_{13} and V_{23} potentials.

On the other hand the renormalized Hylleraas and perimetric coordinate systems are perfectly adapted to $1/r$ singularities in potentials. Indeed, in these two cases the volume element (22) or (15) regularizes automatically this kind of singularity at the origin in the three potentials (30) or (19). In the case of Coulomb-like potentials (62), the convergence of the energy is as good as for regular potentials. The error on the ground-state energy is already approximately 10^{-8} with less than 500 Lagrange functions, both for renormalized Hylleraas and perimetric coordinates. These two coordinate systems are then well adapted to study three-body atomic and molecular systems, where the particles interact via the Coulomb force [12].

V. CONCLUSIONS

The Lagrange-mesh method is very efficient to study the ground-state of three-body quantum mechanical problems. It

is very simple as the potential matrix is purely diagonal and easily evaluated, and its accuracy is comparable to that of a variational calculation. We have made a comparison of four coordinate systems in order to determine if there is an optimal choice for a three-body treatment by the Lagrange-mesh method. As the accuracy of the method may depend on the expressions of the interaction potentials, and more particularly on the presence of singularities, we chose different types of potentials.

The analysis of the convergence of the bound-state energy with the Lagrange basis size and of the filling of the Hamiltonian matrix allows us to classify the four coordinate systems for Lagrange-mesh calculations. One advantage of the method is that the filling rate is independent of the potential expression, because the potential matrix is diagonal in the Lagrange basis, thanks to the use of the Gauss approximation.

The results obtained for three kinds of potentials show us that Jacobi coordinates represent the optimal choice for three-body Lagrange-mesh calculations, if and only if two of the three interparticle interactions are nonsingular. Indeed, the number of nonzero matrix elements is much smaller in this case than with the other three coordinate systems, and Jacobi coordinates provide a very good accuracy on the energy with a fixed basis size unless more than one interaction potential present a singularity at the origin. The problem comes from the fact that only the singularity at the origin in one potential can be eliminated by the regularization technique of Ref. [4] when we use Jacobi coordinates. If only one potential has no singularity, the accuracy obtained with Jacobi coordinates is limited, and the relative coordinate system can take over. The Lagrange basis sizes required for a fixed accuracy, and the corresponding numbers of nonzero matrix elements are in this case much bigger. When the three potentials present some singularity at the origin, both Jacobi and relative coordinates are ruled out. In the case of $1/r$ singularities, perimetric coordinates become ideal for Lagrange-mesh calculations because all $1/r$ singularities are automatically regularized by the corresponding volume element. This property is also true for renormalized Hylleraas coordinates, but perimetric ones provide better accuracies at fixed basis size, the filling of the Hamiltonian matrix being of the same magnitude in these two coordinate systems.

The results presented in this work only concern *S*-state calculations of three-body problems. The case of bound states corresponding to a nonzero total orbital momentum requires a complementary study. In particular this case introduces a singularity in the Hamiltonian via the centrifugal term. As the method provides good results for three-body bound states, it would be interesting to extend it to the analysis of resonances. This could be done, for example, by using the complex-scaling method [21,22].

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APPENDIX

The matrix elements of the internal kinetic energy between two Lagrange functions (45) in relative coordinates can be written as

$$\begin{aligned}\langle F_{ijk}|T_{\rm int}|F_{i'j'k'}\rangle \approx & \frac{1}{2\mu_{13}h_1^2}(\lambda_i^{r_1})^{1/2}\tilde{f}_{i'}^{N_1'}(r_{1i})\delta_{jj'}\delta_{kk'}+\frac{1}{2\mu_{23}h_2^2}(\lambda_j^{r_2})^{1/2}\tilde{f}_{j'}^{N_2'}(r_{2j})\delta_{ii'}\delta_{kk'}+\delta_{ii'}\delta_{jj'}\left(\frac{1}{2\mu_{13}h_1^2r_{1i}^2}+\frac{1}{2\mu_{23}h_2^2r_{2j}^2}\right)\\ &\times(\lambda_k^x)^{1/2}[2x_k g_{k'}^{N_x'}(x_k)-(1-x_k^2)g_{k'}^{N_x''}(x_k)]-\frac{1}{m_3h_1h_2}\Bigg\{(\lambda_k^x)^{1/2}(1-x_k^2)g_{k'}^{N_x'}(x_k)(1-\delta_{kk'})\\ &\times\left(\frac{p_{jj'}^{N_2}}{r_{1i}}\delta_{ii'}+\frac{p_{ii'}^{N_1}}{r_{2j}}\delta_{jj'}\right)+x_k\delta_{kk'}p_{ii'}^{N_1}p_{jj'}^{N_2}+\frac{\delta_{ii'}\delta_{jj'}}{r_{1i}r_{2j}}[x_k\delta_{kk'}+(\lambda_k^x)^{1/2}(3x_k^2-1)g_{k'}^{N_x'}(x_k)\\ &-(\lambda_k^x)^{1/2}x_k(1-x_k^2)g_{k'}^{N_x''}(x_k)]\Bigg\},\end{aligned}\tag{A1}$$

at the Gauss approximation, where λ_i^r and λ_k^x are the weights of the Gauss-Laguerre and Gauss-Legendre quadratures, respectively. The prime notations for the functions $\tilde{f}_i^N(r)$ and $g_k^N(x)$ correspond to the derivatives with respect to the variables r and x, respectively. The $p_{ii'}^N$ terms represent the matrix elements of the one-body operator d/dr. The Gauss-Laguerre approximation is not only inexact for these terms, but it also gives rise to a nonantisymmetric expression for $p_{ii'}^N$, which induces the nonHermiticity of the corresponding Hamiltonian matrix. To solve this problem, we antisymmetrized the expression obtained at the Gauss approximation, which gives

$$p^N_{ii'}=\frac{1}{2}[(\lambda^r_i)^{1/2}\tilde{f}^{N'}_{i'}(r_i)-(\lambda^r_{i'})^{1/2}\tilde{f}^{N'}_i(r_{i'})]. \quad \text{(A2)}$$

Expression (A1) depends on the first and second derivatives of the Lagrange-Laguerre and Lagrange-Legendre functions [Eqs. (41) and (43)] evaluated at the corresponding mesh points. The first derivative of the regularized Lagrange-Laguerre functions $\tilde{f}^N_i(r)$ evaluated at mesh points are given by

$$\tilde{f}^{N'}_i(r_i)=\frac{(\lambda^r_i)^{-1/2}}{2r_i} \quad \text{(A3)}$$

and

$$\tilde{f}^{N'}_i(r_{i'})=(-1)^{i+i'}\frac{(\lambda^r_{i'})^{-1/2}}{r_{i'}-r_i}\sqrt{\frac{r_{i'}}{r_i}}, \quad \text{(A4)}$$

for $i\neq i'$. Their second derivative at mesh points can be found in Ref. [9]. The first and second derivative of the Lagrange-Legendre functions $g^N_k(x)$ can be written as

$$g^{N'}_k(x_k)=(\lambda^x_k)^{-1/2}\frac{x_k}{1-x_k^2}, \quad \text{(A5)}$$

$$g^{N''}_k(x_k)=(\lambda^x_k)^{-1/2}\frac{(N^2+N+6)x_k^2-N^2-N+2}{3(1-x_k^2)^2}, \quad \text{(A6)}$$

and

$$g^{N'}_k(x_{k'})=(-1)^{k+k'}\frac{(\lambda^x_{k'})^{-1/2}}{x_{k'}-x_k}\sqrt{\frac{1-x_k^2}{1-x_{k'}^2}}, \quad \text{(A7)}$$

$$g^{N''}_k(x_{k'})=2(-1)^{k+k'}(\lambda^x_{k'})^{-1/2}\frac{2x_{k'}^2-x_kx_{k'}-1}{(1-x_{k'}^2)(x_{k'}-x_k)^2}\times\sqrt{\frac{1-x_k^2}{1-x_{k'}^2}}, \quad \text{(A8)}$$

for $k\neq k'$.

In the case of perimetric and renormalized Hylleraas coordinates, we have to evaluate integrals of the following form:

$$\mathcal{I}_{\mu\nu}=\int\int\int dxdydz[\partial_\mu F(x,y,z)]D_{\mu\nu}(x,y,z)\times[\partial_\nu G(x,y,z)], \quad \text{(A9)}$$

where μ and ν represent one of the x, y, and z coordinates, and the $D_{\mu\nu}$ coefficients are the $A_{\mu\nu}$ [Eq. (18)] or $B_{\mu\nu}$ [Eq. (29)] coefficients in perimetric and renormalized Hylleraas coordinates, respectively. When the functions F and G are three-dimensional Lagrange functions (34), the use of the Gauss approximation and of the Lagrange conditions (35) provides simple expressions for the $\mathcal{I}_{\mu\nu}$ integrals. For example, the $\mathcal{I}_{xx}$ and $\mathcal{I}_{xy}$ integrals can be written as

$$\mathcal{I}_{xx}=\int\int\int dxdydz[\partial_xF_{ijk}(x,y,z)]D_{xx}(x,y,z)\times[\partial_xF_{i'j'k'}(x,y,z)]\approx\delta_{jj'}\delta_{kk'}(N_{ijk}N_{i'j'k'})^{-1/2}\frac{h_yh_z}{h_x}\times\sum_{m=1}^{N_x}\lambda^x_mD_{xx}(h_xx_m,h_yy_j,h_zz_k)\mathcal{F}^{N_{x'}}_{1i}(x_m)\mathcal{F}^{N_{x'}}_{1i'}(x_m), \quad \text{(A10)}$$

$$\mathcal{I}_{xy}=\int\int\int dxdydz[\partial_xF_{ijk}(x,y,z)]D_{xx}(x,y,z)\times[\partial_yF_{i'j'k'}(x,y,z)]bf\approx\delta_{kk'}(N_{ijk}N_{i'j'k'})^{-1/2}h_z\times D_{xy}(h_xx_{i'},h_yy_j,h_zz_k)\times(\lambda^x_{i'})^{1/2}\mathcal{F}^{N_{x'}}_{1i}(x_{i'})(\lambda^y_j)^{1/2}\mathcal{F}^{N_{y'}}_{2j'}(y_j), \quad \text{(A11)}$$

where x_i, y_j, and z_k are the mesh points associated to the x, y, and z coordinates, and λ^x_i, λ^y_j, and λ^z_k are the corresponding weights. In the case of renormalized Hylleraas coordinates, the scale factors h_x and h_y have to be replaced by 1 in Eqs. (A10) and (A11). The expressions of $\mathcal{I}_{\mu\nu}$ only require the determination of the first derivative of the one-dimensional Lagrange functions $\mathcal{F}^N_{li}$ evaluated at the associated mesh points. The expressions of these derivatives for the Lagrange-Legendre functions g_k are given above [Eqs. (A5) and (A7)]. The case of the Lagrange-Laguerre functions f_i [Eq. (41)] is developed in Ref. [12]. The first derivative of the shifted Lagrange-Legendre functions q^N_i [Eq. (44)] evaluated at mesh points is

$$q^{N'}_i(y_i)=(\lambda^y_i)^{-1/2}\frac{2y_i-1}{2y_i(1-y_i)} \quad \text{(A12)}$$

and

$$q^{N'}_i(y_{i'})=(-1)^{i+i'}\frac{(\lambda^y_{i'})^{-1/2}}{y_{i'}-y_i}\sqrt{\frac{y_i(1-y_i)}{y_{i'}(1-y_{i'})}}, \quad \text{(A13)}$$

for $i'\neq i$.

[1] W. Glöcke, *The Quantum Mechanical Few-body Problem* (Springer, Berlin, 1983).

[2] M.V. Zhukov, B.V. Danilin, D.V. Fedorov, J.M. Bang, I.J. Thompson, and J.S. Vaagen, Phys. Rep. **231**, 87 (1990).

[3] D. Baye and P.-H. Heenen, J. Phys. A **19**, 2041 (1986).
[4] M. Vincke, L. Malegat, and D. Baye, J. Phys. B **26**, 811 (1993).
[5] D. Baye, J. Phys. B **28**, 4399 (1995).
[6] D. Baye and M. Vincke, Phys. Rev. E **59**, 7195 (1999).
[7] D. Baye and M. Vincke, J. Phys. B **24**, 3551 (1991).
[8] D. Baye, M. Kruglanski, and M. Vincke, Nucl. Phys. **A573**, 431 (1994).
[9] D. Baye, Nucl. Phys. **A627**, 305 (1997).
[10] D. Baye, M. Hesse, J-M. Sparenberg, and M. Vincke, J. Phys. B **31**, 3439 (1998).
[11] M. Hesse, J-M. Sparenberg, F. Van Raemdonck, and D. Baye, Nucl. Phys. **A640**, 37 (1998).
[12] M. Hesse and D. Baye, J. Phys. B **32**, 5605 (1999); **34**, 1425 (2001).
[13] D. Baye, M. Hesse, and M. Vincke, Phys. Rev. E **65**, 026701 (2002).
[14] M. Godefroid, J. Liévin, and P-H. Heenen, J. Phys. B **22**, 3119 (1989).
[15] C.L. Pekeris, Phys. Rev. **112**, 1649 (1958).
[16] Z. Zhen, Phys. Rev. A **41**, 87 (1990).
[17] H.A. Bethe and E.E. Salpeter, *Quantum Mechanics of One-and Two-electron Atoms* (Springer, Berlin, 1957).
[18] O. Chuluunbaatar, I.V. Puzynin, and S.I. Vinitsky, J. Phys. B **34**, L425 (2001).
[19] M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions* (Dover, New York, 1970).
[20] A. Stathopoulos and C.F. Fisher, Comput. Phys. Commun. **79**, 268 (1994).
[21] R. Yaris, J. Bendler, R.A. Lovett, C.M. Bender, and P.A. Fedders, Phys. Rev. A **18**, 1816 (1978).
[22] Y.K. Ho, Phys. Rep. **99**, 1 (1983).