Bound states with arbitrary angular momenta in nonrelativistic three-body systems

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The generalization of the highly accurate exponential variational expansion in the relative coordinates r_{32}, r_{31}, and r_{21} is presented for the computation of bound states with arbitrary values of the total angular momentum L and space parity π for three-body nonrelativistic systems with arbitrary particle masses. For all matrix elements explicit analytical formulas are presented which have relatively simple structures and contain L and π as parameters.

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I. INTRODUCTION

In the present work we consider the bound state spectra of three-body nonrelativistic systems consisting of three point particles. Let m_1, m_2, and m_3 be the masses of the first, second and third particles, respectively. When two of the masses are significantly greater than the third mass, e.g., $\min(m_1,m_2) \gg m_3$, the adiabatic approximation can be applied to reduce the initial problem to the one-body two-center problem [1]. Such a one-body problem can be solved, in principle, with very high accuracy [2] and, moreover, for the two-center Coulomb problem even the analytical solution can be found [2].

Recently, a number of highly accurate results have been published for Coulomb three-body systems with one infinite mass, e.g., for the He atom, H^-, Li^+, and other ions (see, e.g., [3–13]). These include calculations for the $S(L=0)$, $P(L=1)$, $D(L=2)$, and $F(L=3)$ bound states in such systems. However, in the general case when all three particle masses are comparable with each other the achieved progress is quite modest. All highly accurate numerical results for such three-body systems have been obtained only for the ground and lowest ''vibrationally'' ($\nu \leqslant 2$) and ''rotationally'' ($L \leqslant 1$) excited states. Only a few years ago the first highly accurate variational calculations were made for the ground states in muonic molecular ions with $L=2$ [14]. The further generalization for the calculation of the bound states with $L \geqslant 3$ presents a number of difficulties.

Briefly, our present goal is to propose a highly accurate variational expansion to compute the bound states in three-body systems with $L \geqslant 0$, where L is the total angular momentum. Actually, to solve this problem we need to find appropriate formulas for the matrix elements. Note, that such rotationally and vibrationally excited bound states can be found only in the three-body Coulomb systems. This means that the Coulomb three-body systems are the main interest for the present work. However, we do not wish to restrict our present study to the consideration of only Coulomb three-body systems, since the generalization of the proposed approach to non-Coulomb potentials is relatively simple.

Most highly accurate calculations for the bound states of the three-body systems are carried out in the so-called relative coordinates which are determined for the three-body system in the following way: Let $\mathbf{r}_1$, $\mathbf{r}_2$, and $\mathbf{r}_3$ be the position vectors of the first, second, and third particles, respectively. Instead of $\mathbf{r}_i$ $(i=1,2,3)$ let us introduce the three scalar relative coordinates r_{31}, r_{32}, and r_{21}, determined by the relations (see, e.g., [15])

$$r_{ij}=|\mathbf{r}_{ij}|=|\mathbf{r}_i-\mathbf{r}_j|, \tag{1}$$

where $i=1,2,3$; $j(\neq i)=1,2,3$, (ij) = (32), (31), (21), and $r_{ij}=r_{ji}$ [16]. These three, always non-negative, coordinates coincide with the interparticle distances, but they are not independent, since, e.g., $|r_{32}-r_{31}| \leqslant r_{21} \leqslant r_{32}+r_{31}$. However, there are the three so-called perimetric coordinates $u_i=\frac{1}{2}(r_{ij}+r_{ik}-r_{jk})$, where $i \neq j \neq k=1,2,3$, which are always non-negative and independent. It can be easily shown that $0 \leqslant u_i < +\infty$ for $i=1,2,3$ and $r_{ij}=u_i+u_j$, where $i \neq j=1,2,3$ [15]. In the present study we shall use the variational expansion in the relative coordinates.

To illustrate briefly the accuracy achieved in modern highly accurate calculations for the three-body systems (bound states) we note the following: By applying the variational expansions in the relative (r_{32}, r_{31}, and r_{21}) or perimetric (u_1, u_2, and u_3) coordinates the accuracy $\approx 1\times 10^{-10}$ or even $\approx 1\times 10^{-12}$ atomic units (a.u.) has been achieved in recent calculations of the ground and lowest excited bound $S(L=0)$, $P(L=1)$, $D(L=2)$, and $F(L=3)$ states [17] in the two-electron atoms and ions, i.e., for the three-body systems with one infinite mass (see, e.g., [3–10]). For the lowest bound excited states in the Ps^-, Mu^-, H^- ions, $pp\mu$, $dd\mu$, and other muonic molecular ions and for so-called exotic systems the best accuracy is also approximately $10^{-8}-10^{-12}$ a.u. (see, e.g., [18–24]). However, most of these results were obtained only for $S(L=0)-$ and $P(L=1)-$ states in such systems. The first variational results for the bound $D(L=2)$ states in the $dd\mu$, $tt\mu$, and $dt\mu$ ions were computed by our group [14] (see also [23]).

In all our earlier calculations the trial variational expression for the wave function Ψ_{LM} has the form [22–25]

$$\Psi_{LM}=\sum_{i=1}^{N} C_i \psi_{i,LM}=\sum_{i=1}^{N} \sum_{\ell_1=\epsilon}^{L} C_i \mathscr{Y}_{LM}^{\ell_1,\ell_2}(\mathbf{r}_{31},\mathbf{r}_{32}) \exp(-\alpha_i r_{32}-\beta_i r_{31}-\gamma_i r_{21}), \tag{2}$$

where $\ell_1+\ell_2=L+\epsilon$ and $\epsilon=0$ or 1. The first choice of ϵ corresponds to the natural space parity $\pi=(-1)^L$, [26] while the second choice represents states with the unnatural space parity $\pi=(-1)^{L+1}$. In Eq. (2) the coefficients C_i are the linear or variational parameters which are found by solving the secular problem. In all our previous highly accurate calculations the nonlinear parameters $\{\alpha_i,\beta_i,\gamma_i\}$ $(i=1,2,\ldots,N)$ have been generated in a quasirandom manner from the three real intervals, i.e., $\alpha_i\in[A_1,A_2]$, $\beta_i\in[B_1,B_2]$, $\gamma_i\in[G_1,G_2]$ (for more details see, e.g., [24]). Such a choice of the nonlinear parameters was used successfully for highly accurate calculations in many systems, including quite a few very complicated cases, e.g., the so-called weakly bound (or prethreshold) states, the nuclear three-body systems and many others. From our results for $D(L=2)$ states in muonic molecular ions it follows that a similar quasirandom procedure can be applied also to the case with $L\geqslant 3$. In Eq. (2) the functions $\mathscr{Y}_{LM}^{\ell_1,\ell_2}(\mathbf{r}_{31},\mathbf{r}_{32})$ are the so-called bipolar (or Schwartz [27]) harmonics. Their explicit form is

$$\begin{aligned}\mathscr{Y}_{LM}^{\ell_1,\ell_2}(\mathbf{r}_{31},\mathbf{r}_{32}) &= r_{31}^{\ell_1} r_{32}^{\ell_2}\mathscr{Y}_{LM}^{\ell_1,\ell_2}(\mathbf{n}_{31},\mathbf{n}_{32}) \\ &= r_{31}^{\ell_1} r_{32}^{\ell_2}\sum_{m_1,m_2} C^{LM}_{\ell_1 m_1,\ell_2 m_2} \\ &\quad\times Y_{\ell_1 m_1}(\mathbf{n}_{31}) Y_{\ell_2 m_2}(\mathbf{n}_{32}),\end{aligned} \tag{3}$$

where $\mathbf{n}_{ij}=\mathbf{r}_{ij}/r_{ij}$ and $C^{LM}_{\ell_1 m_1,\ell_2 m_2}$ are the Clebsch-Gordan coefficients and $Y_{\ell m}(\mathbf{n})$ are the usual spherical harmonics.

The exponential variational expansion, Eq. (2), was used previously to compute the bound states with $L=0$, 1, and 2 in the three-body systems with comparable masses (see, e.g., [23] and references therein). The related Hylleraas expansion was applied to the bound states in such systems with $L=0$ and $L=1$ (see, e.g., [18–21]). Moreover, the variational results for bound states with $L\geqslant 3$ for systems with three comparable masses, e.g., for the $tt\mu$ muonic molecular ion, cannot be found in the modern literature. In contrast with this the boundedness of the $tt\mu$ ion in this state was shown nonvariationally many years ago [28]. Likewise, at the present time the so-called mass threshold values for bound states with $L\geqslant 3$ cannot be determined numerically. Actually now, there is only an approximate formula [29] which predicts the threshold masses for the bound states with $L\geqslant 3$ in the symmetric Coulomb three-body systems. However, the accuracy of such predictions is often unknown. Another well known problem which can be solved in the near future is the determination of the resonance states with $L\geqslant 2$ in the muonic molecular ions and other exotic systems. Also, there are a number of other three-body problems for which the highly accurate determination of the energy levels and the appropriate wave functions for the bound states with $L\geqslant 3$ is needed for their solution.

It should be mentioned that a method which can be used, in principle, to determine a bound state with arbitrary L in the relative coordinates r_{31}, r_{32}, and r_{21} was proposed by Bhatia and Temkin [30,31]. In [30,31] the integration over the three angular variables (actually the Euler angles of the system [16]) had been made before the integration over the three radial variables (relative coordinates). Such a semiseparation of the angular and radial variables was very fruitful and has been used in all recent works related to this problem. To compute the bound states with $L\geqslant 1$ they proposed to use the matrix elements of finite rotations [i.e., the $D^{L,\pm}_{M,K}(\varphi,\Theta,\psi)$ functions of three Euler angles for the three-body system] as the angular parts of the wave functions [30,31].

At about the same time Schwartz [27] proposed the use of the bipolar harmonics $\mathscr{Y}_{LM}^{\ell_1,\ell_2}(\mathbf{r}_{31},\mathbf{r}_{32})$, Eq. (3). Calais and Löwdin [32] calculated the overlap matrix element for the functions with the bipolar harmonics. However, closed formulas for all matrix elements in the case of the two-electron problem were obtained by Drake [33]. Efros [34] applied only bipolar harmonics of special kinds such as $\mathscr{Y}_{LM}^{\ell_1,L-\ell_1}(\mathbf{r}_{31},\mathbf{r}_{32})$ and $\mathscr{Y}_{LM}^{\ell_1,L-\ell_1+1}(\mathbf{r}_{31},\mathbf{r}_{32})$. This enabled him to achieve a significant simplification in comparison with [33]. However, final closed formulas for the matrix elements were not given [34].

Our present goal is to generalize the highly accurate exponential variational expansion, Eq. (2), in the relative coordinates r_{31}, r_{32}, and r_{21} to the case of bound states of three-body systems with arbitrary values of the angular momentum L and space parity π. To do this, the following variational ansatz is used:

$$\begin{aligned}\Psi_{LM} &= \sum_{i=1}^{N} C_i\psi_{i,LM} \\ &= \sum_{i=1}^{N} C_i\mathscr{Y}_{LM}^{\ell_1,\ell_2}(\mathbf{r}_{31},\mathbf{r}_{32})\phi_i(r_{32},r_{31},r_{21}),\end{aligned} \tag{4}$$

where the coefficients C_i are the linear (variational) parameters and the ''angular functions'' $\mathscr{Y}_{LM}^{\ell_1,\ell_2}(\mathbf{r}_{31},\mathbf{r}_{32})$ are Schwartz's bipolar harmonics. In the present work we apply the same relation between the superscripts ℓ_1 and ℓ_2 as mentioned above [34], namely, $\ell_2=L-\ell_1+\epsilon$, where $\epsilon=0$ for states with the space parity $\pi=(-1)^L$ (natural parity) and $\epsilon=1$ for states with the space parity $\pi=(-1)^{L+1}$ (unnatural parity). In Eq. (4) we suppose that the value ℓ_1 and, therefore the value $\ell_2(\ell_2=L+\epsilon-\ell_1)$ are determined from the index number of the basis function i by use of the relation $\ell_1=\mathrm{mod}(i,L+1)$, where the notation $\mathrm{mod}(a,b)$ stands for the remainder of the integer division a/b. This relation has been used in our previous works related with $P(L=1)$ and $D(L=2)$ bound states (see [23]).

The radial basis functions in Eq. (4), $\{\phi_i(r_{32},r_{31},r_{21})\}$, depend only on the three radial variables r_{31}, r_{32}, and r_{21}. They can be chosen in various forms. The three following sets of radial basis functions are well known and widely used in various applications: the so-called exponential expansion in the relative coordinates

$$\phi_i(r_{32},r_{31},r_{21})=\exp(-\alpha_i r_{32}-\beta_i r_{31}-\gamma_i r_{21}), \tag{5}$$

the Hylleraas expansion

$$\phi_i(r_{32},r_{31},r_{21})=r_{32}^{n_{1,i}} r_{31}^{n_{2,i}} r_{21}^{n_{3,i}}\exp(-\alpha r_{32}-\beta r_{31}-\gamma r_{21}), \tag{6}$$

where the constants α, β, and γ do not depend upon i, and the variational expansion in three-dimensional gaussoids in the relative coordinates

$$\phi_i(r_{32},r_{31},r_{21})=\exp(-\alpha_i r_{32}^2-\beta_i r_{31}^2-\gamma_i r_{21}^2). \quad (7)$$

The exponential variational expansion, Eq. (4), with the radial basis functions in the form of Eq. (5), has been used successfully in various atomic, ionic, muonic molecules, and nuclear three-body bound states calculations (see, e.g., [22–25,29,35,36]). The Hylleraas expansion, Eq. (6), was applied to the cases of the He-like atoms and ions, exotic systems and muonic molecules (see, e.g., [10–13,18–21,37]). The three-dimensional gaussoids expansion, Eq. (7), is of specific interest [38], since it can be easy generalized to the $\mathcal{N}$-body nonrelativistic system [39]. The main reason is that the appropriate analytical formulas for the matrix elements contain $\mathcal{N}$ as a parameter [39]. At the present time these formulas have been applied to find lower and upper energy estimates for the bound S states ($L=0$) in various three-, four-, and five-body systems (see, e.g., [40,41]). However, the successful generalization of the last approach to bound states with $L\geqslant 1$ has not been developed.

The approach proposed in the present work was initially used for the variational exponential expansion, Eq. (2). However, later we understood that it is possible to write all formulas for the matrix elements in the form which can be easily changed to the general case of Eq. (4) with the different radial basis functions ϕ_i from Eqs. (5)–(7). Briefly, we can say that the method presented here can be used for highly accurate calculations of bound states in three-body nonrelativistic systems with arbitrary values of the angular momentum L and space parity π.

II. GENERAL STRUCTURE OF THE MATRIX ELEMENTS

As is well known the solution of the Schrödinger equation $(H-E)\Phi=0$ may be reduced to the equivalent variational problem, i.e., to minimize the energy functional

$$E=\frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle}=\frac{\langle\Psi|T|\Psi\rangle+\langle\Psi|V|\Psi\rangle}{\langle\Psi|\Psi\rangle}. \quad (8)$$

Here and below $H=T+V$ is the Hamiltonian, T is the kinetic energy, and V is the potential energy. The variational problem, Eq. (8), can be rewritten in the form of the following eigenvalue problem:

$$\sum_{n'=1}^{N}(H_{n,n'}-ES_{n,n'})C_{n'}=\sum_{n'=1}^{N}(T_{n,n'}+V_{n,n'}-ES_{n,n'})C_{n'}=0, \quad (9)$$

where $n=1,2,\ldots,N$, and N is the number of basis functions used. The appropriate matrix elements $S_{n,n'}$, $V_{n,n'}$, and $T_{n,n'}$ are

$$S_{n,n'}=\langle\psi_{n,LM}|S|\psi_{n',LM}\rangle,$$
$$V_{n,n'}=\langle\psi_{n,LM}|V|\psi_{n',LM}\rangle, \quad (10)$$
$$T_{n,n'}=\langle\psi_{n,LM}|T|\psi_{n',LM}\rangle.$$

Each of these matrix elements can be presented in the general form in terms of the basis functions given in Eq. (2),

$$A_{n,n'}=\langle\psi_{n,LM}|A|\psi_{n',LM}\rangle=\int d\tau\mathscr{Y}_{LM}^{\ell_1,\ell_2}(\mathbf{r}_{31},\mathbf{r}_{32})\exp(-\alpha_n r_{32}-\beta_n r_{31}-\gamma_n r_{21})$$
$$\times A\mathscr{Y}_{LM}^{\ell_1',\ell_2'}(\mathbf{r}_{31},\mathbf{r}_{32})\exp(-\alpha_{n'} r_{32}-\beta_{n'} r_{31}-\gamma_{n'} r_{21}), \quad (11)$$

where A is the generalized notation for an operator which depends on the three scalar relative coordinates r_{31}, r_{32}, and r_{21} as well as on the three angular variables. We choose the Euler angles $\Omega=(\varphi,\Theta,\psi)$ as the three independent angular variables. In the present study our choice of the three Euler angles $\Omega=(\varphi,\Theta,\psi)$ coincides with that in previous works [22,34]. These angles determine the orientation of the coordinate system rigidly related with the triangle formed by the three particles, relative to the outside space. In this case the elementary volume $d\tau$ takes the form (more details can be found in [33,34])

$$d\tau=r_{32}r_{31}r_{21}dr_{32}dr_{31}dr_{21}d\Omega, \quad (12)$$

where the elementary angular volume $d\Omega$ is

$$d\Omega=\sin\Theta d\Theta d\psi d\phi. \quad (13)$$

Now, it can be shown that the integration over the angular variables (φ,Θ,ψ) can be separated from the integration over the three radial (r_{32},r_{31},r_{21}) ones but not vice versa. This means that by integrating Eq. (10) first over the angular variables (φ,Θ,ψ) we obtain an expression which depends upon only the three scalar radial variables r_{32},r_{31},r_{21}. Moreover, this expression is a polynomial in these three relative coordinates. Then this polynomial must be integrated over these radial variables r_{32}, r_{31}, and r_{21}.

First consider the case when the operator A in Eq. (11) does not contain any differential operator. In this case the appropriate angular integral takes the form

$$W^{L}_{\ell_1,\ell_2;\ell'_1,\ell'_2}(r_{32},r_{31},r_{21})=\int_{\Omega} d\Omega\, \mathscr{Y}^{\ell_1,\ell_2}_{LM}(\mathbf{r}_{31},\mathbf{r}_{32})\mathscr{Y}^{\ell'_1,\ell'_2}_{LM}(\mathbf{r}_{31},\mathbf{r}_{32}), \tag{14}$$

where the notation $\int_\Omega$ designates the integration over the three angular variables (φ,Θ,ψ) (i.e., over the Euler angles of the three-body system). An explicit expression for $W^{L}_{\ell_1,\ell_2;\ell'_1,\ell'_2}(r_{32},r_{31},r_{21})$ was found by Drake [33],

$$W^{L}_{\ell_1,\ell_2;\ell'_1,\ell'_2}(r_{32},r_{31},r_{21})=\frac{1}{2}(-1)^L r_{31}^{\ell_1+\ell'_1} r_{32}^{\ell_2+\ell'_2}\sqrt{(2\ell_1+1)(2\ell'_1+1)(2\ell_2+1)(2\ell'_2+1)}$$
$$\times\sum_{\lambda=\lambda_{min}}^{\lambda_{max}}(-1)^{\lambda}(2\lambda+1)\begin{pmatrix}\ell_1 & \ell'_1 & \lambda\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}\ell_2 & \ell'_2 & \lambda\\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix}\ell'_1 & \ell'_2 & L\\ \ell_2 & \ell_1 & \lambda\end{Bmatrix}P_{\lambda}(x), \tag{15}$$

where $x=\mathbf{r}_{31}\cdot\mathbf{r}_{32}/r_{31}r_{32}$. The notation $\binom{abc}{000}$ denotes the Wigner 3-j symbol with $m_1=0,m_2=0,m_3=0$ [42]. $\{{abc \atop def}\}$ is the 6-j symbol [42]. In Eq. (15) the $P_\lambda(x)$ are the Legendre polynomials. Since

$$x=\frac{\mathbf{r}_{31}\cdot\mathbf{r}_{32}}{r_{31}r_{32}}=\frac{r_{31}^2+r_{32}^2-r_{21}^2}{2r_{31}r_{32}} \tag{16}$$

and $P_\lambda(x)=\Sigma_{n=0}^{\lambda}b_{n,\lambda}x^n$, we transform this expression to the form

$$W^{L}_{\ell_1,\ell_2;\ell'_1,\ell'_2}(r_{32},r_{31},r_{21})=\frac{1}{2}(-1)^L\sqrt{(2\ell_1+1)(2\ell'_1+1)(2\ell_2+1)(2\ell'_2+1)}$$
$$\times\sum_{\lambda=\lambda_{min}}^{\lambda_{max}}(-1)^{\lambda}(2\lambda+1)\begin{pmatrix}\ell_1 & \ell'_1 & \lambda\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}\ell_2 & \ell'_2 & \lambda\\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix}\ell'_1 & \ell'_2 & L\\ \ell_2 & \ell_1 & \lambda\end{Bmatrix}$$
$$\times\sum_{n=0}^{\lambda}\frac{b_{n,\lambda}}{2^n}\left\{\sum_{k=0}^{n}C_n^k\left[\sum_{m=0}^{k}C_k^m(-1)^m r_{32}^{2k-2m-n+\ell_2+\ell'_2}r_{31}^{n-2k+\ell_1+\ell'_1}r_{21}^{2m}\right]\right\}, \tag{17}$$

where the C_n^k are the binominal coefficients, i.e., $C_n^k=n!/(n-k)!k!$. Note that the coefficients $b_{n,\lambda}$ can be easily found from the recursion relation (see, e.g., [43])

$$P_\lambda(x)=\frac{(2\lambda-1)xP_{\lambda-1}(x)-(\lambda-1)P_{\lambda-2}(x)}{\lambda} \tag{18}$$

with the initial conditions $P_0(x)=1$ and $P_1(x)=x$. Otherwise, these coefficients $b_{n,\lambda}$ can be obtained from the well known formula for the Legendre polynomials [43]

$$P_\lambda(x)=\frac{1}{2^\lambda}\sum_{k=0}^{\left[\frac{\lambda}{2}\right]}\frac{(-1)^k(2\lambda-2k)!}{k!(\lambda-k)!(\lambda-2k)!}x^{\lambda-2k} \tag{19}$$

where $[\cdots]$ denotes the integer part of a number. Thus we have shown that the angular integral $W^{L}_{\ell_1,\ell_2;\ell'_1,\ell'_2}(r_{32},r_{31},r_{21})$ is a polynomial in the three radial variables r_{32}, r_{31}, and r_{21}.

Note that, since $\ell_1+\ell_2=L+\epsilon$ and $\ell'_1+\ell'_2=L+\epsilon$ we can reduce the total number of independent indexes to be four for each angular integral, i.e., $W^{L}_{\ell_1,\ell_2;\ell'_1,\ell'_2}(r_{32},r_{31},r_{21})=W^{L,\epsilon}_{\ell_1,\ell'_1}(r_{32},r_{31},r_{21})$. Then Eq. (14) takes another form

$$W^{L,\epsilon}_{\ell_1,\ell'_1}(r_{32},r_{31},r_{21})=\frac{1}{2}(-1)^L\sqrt{(2\ell_1+1)(2\ell'_1+1)(2\ell_2+1)(2\ell'_2+1)}$$
$$\times\sum_{\lambda=\lambda_{min}}^{\lambda_{max}}(-1)^{\lambda}(2\lambda+1)\begin{pmatrix}\ell_1 & \ell'_1 & \lambda\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}\ell_2 & \ell'_2 & \lambda\\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix}\ell'_1 & \ell'_2 & L\\ \ell_2 & \ell_1 & \lambda\end{Bmatrix}$$
$$\times\sum_{n=0}^{\lambda}\frac{b_{n,\lambda}}{2^n}\left\{\sum_{k=0}^{n}C_n^k\left[\sum_{m=0}^{k}C_k^m(-1)^m r_{32}^{2k-2m-n+L+\epsilon}r_{31}^{n-2k+L+\epsilon}r_{21}^{2m}\right]\right\}, \tag{20}$$

where $\ell_2=L+\epsilon-\ell_1$ and $\ell'_2=L+\epsilon-\ell'_1$.

To simplify our formulas further we introduce the operator $B^{L,\epsilon}_{\ell_1,\ell'_1}$ by the following relation:

$$W^{L,\epsilon}_{\ell_1,\ell_1'}(r_{32},r_{31},r_{21})=\frac{1}{2}(-1)^L\sqrt{(2\ell_1+1)(2\ell_1'+1)(2\ell_2+1)(2\ell_2'+1)}$$
$$\times\sum_{\lambda=\lambda_{min}}^{\lambda_{max}}(-1)^\lambda(2\lambda+1)\begin{pmatrix}\ell_1 & \ell_1' & \lambda\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}\ell_2 & \ell_2' & \lambda\\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix}\ell_1' & \ell_2' & L\\ \ell_2 & \ell_1 & \lambda\end{Bmatrix}$$
$$\times\sum_{n=0}^{\lambda}\frac{b_{n,\lambda}}{2^n}\left\{\sum_{k=0}^{n}C_n^k\left[\sum_{m=0}^{k}C_k^m(-1)^m\delta_{n_1,2k-2m-n+L+\epsilon}\delta_{n_2,n-2k+L+\epsilon}\delta_{n_3,m}\right]\right\}r_{32}^{n_1}r_{31}^{n_2}r_{21}^{n_3}$$
$$=B^{L,\epsilon}_{\ell_1,\ell_1'}r_{32}^{n_1}r_{31}^{n_2}r_{21}^{n_3}. \tag{21}$$

It should be noted that (1) the operator $B^{L,\epsilon}_{\ell_1,\ell_1'}$ does not depend on the radial variables and (2) this operator contains the total angular momentum L and space parity π (or ϵ) as parameters. It can be shown that in the case when the operator A contains differential operators on the radial variables r_{32}, r_{31}, and r_{21} the angular matrix element $W^{L,\epsilon}_{\ell_1,\ell_1'}(r_{32},r_{31},r_{21})$ is exactly the same as described above in Eqs. (20) and (21). The difference appears only when this operator A contains differential operators on the angular variables. In this case the respective matrix elements are represented as the sum of a few different members, which contain the polynomial $W^{L,\epsilon}_{\ell_1,\ell_1'}(r_{32},r_{31},r_{21})$ as well as the two additional polynomials (see below) $W^{L,\epsilon}_{\ell_1,\ell_1'+1}(r_{32},r_{31},r_{21})$ and $W^{L,\epsilon}_{\ell_1,\ell_1'-1}(r_{32},r_{31},r_{21})$. The explicit expressions can be easily found from the general formulas Eqs. (17), (20), and (21) given above. It should be mentioned that the differential operators on the angular variables [and, therefore, the polynomials $W^{L,\epsilon}_{\ell_1,\ell_1'+1}(r_{32},r_{31},r_{21})$ and $W^{L,\epsilon}_{\ell_1,\ell_1'-1}(r_{32},r_{31},r_{21})$] are found only in the kinetic energy.

In conclusion let us determine the so-called basic radial integral

$$F(n_1,n_2,n_3;X_{ij}^{(1)},X_{ij}^{(2)},X_{ij}^{(3)})=\int\int\int dr_{32}dr_{31}dr_{21}r_{32}^{n_1}r_{31}^{n_2}r_{21}^{n_3}\exp(-X_{ij}^{(1)}r_{32}-X_{ij}^{(2)}r_{31}-X_{ij}^{(3)}r_{21}), \tag{22}$$

where $X_{ij}^{(k)}$ $(k=1,2,3)$ are real numbers. By introducing the three perimetric coordinates u_1,u_2,u_3 [24] we find the following analytical expression for this integral:

$$F(n_1,n_2,n_3;X_{ij}^{(1)},X_{ij}^{(2)},X_{ij}^{(3)})=\sum_{k_1=0}^{n_1}\sum_{k_2=0}^{n_2}\sum_{k_3=0}^{n_3}C_{n_1}^{k_1}C_{n_2}^{k_2}C_{n_3}^{k_3}\frac{m_1!m_2!m_3!}{(X_{ij}^{(1)}+X_{ij}^{(2)})^{m_3+1}(X_{ij}^{(1)}+X_{ij}^{(3)})^{m_2+1}(X_{ij}^{(2)}+X_{ij}^{(3)})^{m_1+1}}, \tag{23}$$

where $m_1=k_1+k_2$, $m_2=k_1+n_2-k_3$, and $m_3=n_1+n_2-k_1-k_2$. The function $F(n_1,n_2,n_3;X_{ij}^{(1)},X_{ij}^{(2)},X_{ij}^{(3)})$ determined in the last equations plays a very important role in the further development.

III. MATRIX ELEMENTS OF THE OVERLAP MATRIX AND THE POTENTIAL

In this section explicit expressions for the matrix elements of the overlap matrix $\mathbf{S}_{ij}$ and the potential energy matrix $\mathbf{V}_{ij}$ are derived. First, consider the overlap matrix $\mathbf{S}_{ij}$. The explicit expression for the appropriate integral is

$$\mathbf{S}_{ij}=\langle\psi_{i,LM}|\psi_{j,LM}\rangle=\int\int\int\int_\Omega d\Omega dr_{32}dr_{31}dr_{21}r_{32}r_{31}r_{21}\mathscr{Y}_{LM}^{\ell_1,\ell_2}(\mathbf{r}_{31},\mathbf{r}_{32})\mathscr{Y}_{LM}^{\ell_1',\ell_2'}(\mathbf{r}_{31},\mathbf{r}_{32})\exp[-(\alpha_i+\alpha_j)r_{32}-(\beta_i+\beta_j)r_{31}$$
$$-(\gamma_i+\gamma_j)r_{21}]. \tag{24}$$

After the integration over the angular variables this expression takes the form

$$\mathbf{S}_{ij}=\langle\psi_{i,LM}|\psi_{j,LM}\rangle=\int\int\int dr_{32}dr_{31}dr_{21}r_{32}r_{31}r_{21}W^{L,\epsilon}_{\ell_1,\ell_1'}(r_{32},r_{31},r_{21})\exp(-X_{ij}^{(1)}r_{32}-X_{ij}^{(2)}r_{31}-X_{ij}^{(3)}r_{21}), \tag{25}$$

where $X_{ij}^{(1)}=\alpha_i+\alpha_j$, $X_{ij}^{(2)}=\beta_i+\beta_j$, and $X_{ij}^{(3)}=\gamma_i+\gamma_j$. By applying the operator $B^{L,\epsilon}_{\ell_1,\ell_1'}$ determined above in Eq. (21) we can rewrite this expression in the form

$$\mathbf{S}_{ij}=B^{L,\epsilon}_{\ell_1,\ell_1'}S_{ij}=B^{L}_{\ell_1,\ell_1'}F(n_1+1,n_2+1,n_3+1;X_{ij}^{(1)},X_{ij}^{(2)},X_{ij}^{(3)}). \tag{26}$$

We shall call the matrix element $\mathbf{S}_{ij}$ in the left side of this equation as the complete matrix element, while the S_{ij} matrix element in the right-hand side of this equation can be called as the elementary matrix element. The elementary matrix element for the overlap matrix has the form

$$S_{ij}=F(n_1+1,n_2+1,n_3+1;X_{ij}^{(1)},X_{ij}^{(2)},X_{ij}^{(3)}), \tag{27}$$

where the function F (the basic radial integral) has been determined in Eq. (22). In Eqs. (25)–(27) and everywhere below $X_{ij}^{(1)}=\alpha_i+\alpha_j$, $X_{ij}^{(2)}=\beta_i+\beta_j$, and $X_{ij}^{(3)}=\gamma_i+\gamma_j$.

Now consider the matrix elements of the potential energy. According to our assumption made above the potential energy in the general case is represented as a sum of the three scalar interaction potentials, i.e.,

$$V=V_{32}(r_{32})+V_{31}(r_{31})+V_{21}(r_{21}). \tag{28}$$

Therefore, the potential energy matrix element $\mathbf{V}_{ij}$ takes the form

$$\mathbf{V}_{ij}=B^{L,\epsilon}_{\ell_1,\ell'_1}V_{ij}=B^{L}_{\ell_1,\ell'_1}\{[V_{32}(r_{32})]_{ij}+[V_{31}(r_{31})]_{ij}+[V_{21}(r_{21})]_{ij}\}. \tag{29}$$

In the case of the Coulomb potential where $V=\Sigma_{(nk)}q_nq_kr_{nk}^{-1}$ [where $(nk)=(21)$, (31), and (32)] the appropriate elementary matrix element V_{ij} is

$$\begin{aligned}V_{ij}=&q_3q_2F(n_1,n_2+1,n_3+1;X_{ij}^{(1)},X_{ij}^{(2)},X_{ij}^{(3)})+q_3q_1F(n_1+1,n_2,n_3+1;X_{ij}^{(1)},X_{ij}^{(2)},X_{ij}^{(3)})\\&+q_2q_1F(n_1+1,n_2+1,n_3;X_{ij}^{(1)},X_{ij}^{(2)},X_{ij}^{(3)}).\end{aligned} \tag{30}$$

In the case of an exponential potential $V=\Sigma_{(nk)}A_{nk}\exp(-\alpha_{nk}r_{nk})$ the elementary matrix element V_{ij} has the form

$$\begin{aligned}V_{ij}=&A_{32}F(n_1+1,n_2+1,n_3+1;X_{ij}^{(1)}+\alpha_{32},X_{ij}^{(2)},X_{ij}^{(3)})+A_{31}F(n_1+1,n_2+1,n_3+1;X_{ij}^{(1)},X_{ij}^{(2)}+\alpha_{31},X_{ij}^{(3)})\\&+A_{21}F(n_1+1,n_2+1,n_3+1;X_{ij}^{(1)},X_{ij}^{(2)},X_{ij}^{(3)}+\alpha_{21}),\end{aligned} \tag{31}$$

where the notation $X_{ij}^{(q)}$ has been introduced above. For a Yukawa-type potential $V=\Sigma_{(nk)}A_{nk}\exp(-\alpha_{nk}r_{nk})r_{nk}^{-1}$ the expression for V_{ij} can be written as

$$\begin{aligned}V_{ij}=&A_{32}F(n_1,n_2+1,n_3+1;X_{ij}^{(1)}+\alpha_{32},X_{ij}^{(2)},X_{ij}^{(3)})+A_{31}F(n_1+1,n_2,n_3+1;X_{ij}^{(1)},X_{ij}^{(2)}+\alpha_{31},X_{ij}^{(3)})\\&+A_{21}F(n_1+1,n_2+1,n_3;X_{ij}^{(1)},X_{ij}^{(2)},X_{ij}^{(3)}+\alpha_{21}).\end{aligned} \tag{32}$$

In the same manner it is easy to produce similar formulas for potentials which are represented as the sum of gaussoids, harmonic oscillator potentials, spherical potential holes, etc. Here, we do not wish to discuss these problems and obtain now formulas for the matrix elements of the kinetic energy.

IV. MATRIX ELEMENTS OF THE KINETIC ENERGY

The kinetic energy operator $\mathbf{T}$ for an arbitrary three-body system in Cartesian coordinates is

$$\mathbf{T}=-\frac{1}{2m_1}\boldsymbol{\nabla}_1^2-\frac{1}{2m_2}\boldsymbol{\nabla}_2^2-\frac{1}{2m_3}\boldsymbol{\nabla}_3^2, \tag{33}$$

where m_1, m_2, and m_3 are the particle masses. In the relative coordinates r_{31}, r_{32}, and r_{21} the operator $\mathbf{T}$ has the form [44]

$$\begin{aligned}\mathbf{T}=&-\frac{1}{2\mu_{32}}\boldsymbol{\nabla}_{32}^2-\frac{1}{2\mu_{31}}\boldsymbol{\nabla}_{31}^2-\frac{1}{2\mu_{21}}\boldsymbol{\nabla}_{21}^2-\frac{1}{m_3}\boldsymbol{\nabla}_{32}\cdot\boldsymbol{\nabla}_{31}\\&-\frac{1}{m_2}\boldsymbol{\nabla}_{32}\cdot\boldsymbol{\nabla}_{12}-\frac{1}{m_1}\boldsymbol{\nabla}_{21}\boldsymbol{\nabla}\cdot_{31},\end{aligned} \tag{34}$$

where $\mu_{kn}^{-1}=m_k^{-1}+m_n^{-1}$, $k=1,2,3$, and $n(\neq k)=1,2,3$. By introducing the definitions $\mathbf{T}_{kn}=-1/2\mu_{kn}\boldsymbol{\nabla}_{kn}^2$, and $\mathbf{T}_{kn,kn'}=-1/m_k\boldsymbol{\nabla}_{kn}\cdot\boldsymbol{\nabla}_{kn'}$ we write the kinetic energy operator $\mathbf{T}$ in the form

$$\mathbf{T}=\mathbf{T}_{32}+\mathbf{T}_{31}+\mathbf{T}_{21}+\mathbf{T}_{32,31}+\mathbf{T}_{32,12}+\mathbf{T}_{31,21}. \tag{35}$$

As is well known the gradient operator $\boldsymbol{\nabla}$ can be written as a sum of its normal and planar components [45]

$$\begin{aligned}\boldsymbol{\nabla}_{kn}=&\mathbf{n}_{kn}\frac{\partial}{\partial r_{kn}}+\frac{1}{r_{kn}}\boldsymbol{\nabla}_{\Omega_{kn}}\\=&\mathbf{n}_{kn}\frac{\partial}{\partial r_{kn}}-\imath\cdot\frac{1}{r_{kn}}[\mathbf{n}_{kn}\times\mathbf{L}_{kn}(\Omega_{kn})],\end{aligned} \tag{36}$$

where $\mathbf{n}_{kn}=\mathbf{r}_{kn}/r_{kn}$, and for the normal and planar components the following equality

$$\mathbf{n}_{kn}\cdot\boldsymbol{\nabla}_{\Omega_{kn}}=\mathbf{n}_{kn}\cdot[\mathbf{n}_{kn}\times\mathbf{L}_{kn}(\Omega_{kn})]=0 \tag{37}$$

holds. In this section (as well as above) we assume that the metric in the relative coordinates r_{32}, r_{31}, and r_{21} is determined by the following scalar product

$$\langle \phi_1(r_{32},r_{31},r_{21})|\phi_2(r_{32},r_{31},r_{21})\rangle = \int\int\int \phi_1(r_{32},r_{31},r_{21})\phi_2(r_{32},r_{31},r_{21}) \times r_{32}r_{31}r_{21}dr_{32}dr_{31}dr_{21}. \quad (38)$$

In terms of this metric we can rewrite the formula for the gradient operator ∇_{kn} in the relative coordinates to the form [45]

$$\nabla_{kn}=\mathbf{r}_{kn}p_{kn}+\frac{1}{r_{kn}}\nabla_{\Omega_{kn}}, \quad (39)$$

where the p_{kn} operator is the so-called quasimomentum operator in the relative coordinates

$$p_{kn}=\frac{1}{r_{kn}}\frac{\partial}{\partial r_{kn}}. \quad (40)$$

It is easy to show that the operator $(-\imath)\cdot p_{kn}$ is a self-adjoint operator in terms of the metric defined above. According to this definition the expression for the ∇^2_{kn} operator takes the form

$$\nabla^2_{kn}=p_{kn}r^2_{kn}p_{kn}+\frac{1}{r^2_{kn}}\nabla^2_{\Omega_{kn}}=\frac{\partial^2}{\partial r^2_{kn}}+\frac{2}{r_{kn}}\frac{\partial}{\partial r_{kn}}+\frac{1}{r^2_{kn}}\nabla^2_{\Omega_{kn}}. \quad (41)$$

It is well known (see, e.g., [34]) that

$$\nabla^2_{kn}\mathscr{Y}^{\ell_1,\ell_2}_{LM}(\mathbf{r}_{31},\mathbf{r}_{32})=0 \quad (42)$$

for (kn) = (32), (31), and (21). This means that the equality

$$\nabla^2_{kn}[\mathscr{Y}^{\ell_1,\ell_2}_{LM}(\mathbf{r}_{31},\mathbf{r}_{32})\phi(r_{32},r_{31},r_{21})]=2[\nabla_{kn}\mathscr{Y}^{\ell_1,\ell_2}_{LM}(\mathbf{r}_{31},\mathbf{r}_{32})]\cdot[\nabla_{kn}\phi(r_{32},r_{31},r_{21})] + \mathscr{Y}^{\ell_1,\ell_2}_{LM}(\mathbf{r}_{31},\mathbf{r}_{32})[\nabla^2_{kn}\phi(r_{32},r_{31},r_{21})] \quad (43)$$

must be obeyed for an arbitrary scalar function $\phi(r_{32},r_{31},r_{21})$ of the three relative coordinates. Likewise, for an arbitrary scalar function ϕ of the three scalar variables r_{32}, r_{31}, and r_{21} the following equation

$$\nabla^m_{\Omega_{kn}}\phi(r_{32},r_{31},r_{21})=0 \quad (44)$$

holds for $m=1,2,3,\ldots$ and $(kn)=(32),(31),(21)$. Therefore, the previous equation can be rewritten in the form

$$\nabla^2_{kn}[\mathscr{Y}^{\ell_1,\ell_2}_{LM}(\mathbf{r}_{31},\mathbf{r}_{32})\phi(r_{32},r_{31},r_{21})]=2\left(\frac{\partial}{\partial r_{kn}}\mathscr{Y}^{\ell_1,\ell_2}_{LM}(\mathbf{r}_{31},\mathbf{r}_{32})\right)\left(\frac{\partial}{\partial r_{kn}}\phi(r_{32},r_{31},r_{21})\right) + \mathscr{Y}^{\ell_1,\ell_2}_{LM}(\mathbf{r}_{31},\mathbf{r}_{32})\left[\left(\frac{\partial^2}{\partial r^2_{kn}}+\frac{2}{r_{kn}}\frac{\partial}{\partial r_{kn}}\right)\phi(r_{32},r_{31},r_{21})\right]. \quad (45)$$

Now, by applying the last equations we easily find analytical expressions for the $\mathbf{T}_{kn}=-1/2\mu_{kn}\nabla^2_{kn}$ matrix elements. These formulas can be also written in the form

$$[\mathbf{T}_{kn}]_{ij}=B^{L,\epsilon}_{\ell_1,\ell_1'}[T_{kn}]_{ij}, \quad (46)$$

where $(ij)=(32),(31),(21)$ and the appropriate elementary matrix elements $[T_{32}]_{ij}$, $[T_{31}]_{ij}$, and $[T_{21}]_{ij}$ are

$$[T_{32}]_{ij}=-\frac{1}{2\mu_{32}}\alpha_j^2S_{ij}+\frac{\ell_2+1}{\mu_{32}}\alpha_j\left\langle\psi_{i,LM}\left|\frac{1}{r_{32}}\right|\psi_{j,LM}\right\rangle = -\frac{1}{2\mu_{32}}\alpha_j^2F(n_1+1,n_2+1,n_3+1;X^{(1)}_{ij},X^{(2)}_{ij},X^{(3)}_{ij})+\frac{\ell_2+1}{\mu_{32}}\alpha_jF(n_1+1,n_2+1,n_3;X^{(1)}_{ij},X^{(2)}_{ij},X^{(3)}_{ij}), \quad (47)$$

$$[T_{31}]_{ij}=-\frac{1}{2\mu_{31}}\beta_j^2S_{ij}+\frac{\ell_1+1}{\mu_{31}}\beta_j\left\langle\psi_{i,LM}\left|\frac{1}{r_{31}}\right|\psi_{j,LM}\right\rangle = -\frac{1}{2\mu_{31}}\beta_j^2F(n_1+1,n_2+1,n_3+1;X^{(1)}_{ij},X^{(2)}_{ij},X^{(3)}_{ij})+\frac{\ell_1+1}{\mu_{31}}\beta_jF(n_1+1,n_2,n_3+1;X^{(1)}_{ij},X^{(2)}_{ij},X^{(3)}_{ij}), \quad (48)$$

$$[T_{21}]_{ij}=-\frac{1}{2\mu_{21}}\gamma_j^2 S_{ij}+\frac{1}{\mu_{21}}\gamma_j\left\langle \psi_{i,LM}\left|\frac{1}{r_{21}}\right|\psi_{j,LM}\right\rangle$$
$$=-\frac{1}{2\mu_{21}}\gamma_j^2 F(n_1+1,n_2+1,n_3+1;X_{ij}^{(1)},X_{ij}^{(2)},X_{ij}^{(3)})+\frac{1}{\mu_{21}}\gamma_j F(n_1,n_2+1,n_3+1;X_{ij}^{(1)},X_{ij}^{(2)},X_{ij}^{(3)}), \tag{49}$$

where S_{ij} is the respective elementary matrix element for the overlap matrix Eq. (27). Note, also that the matrix elements $\langle\psi_{i,LM}|1/r_{kn}|\psi_{j,LM}\rangle$, [$(kn)$ = (32), (31), and (21)] include the appropriate elementary matrix element of the Coulomb potential energy.

Now, consider the three remaining matrix elements in the kinetic energy $[\mathbf{T}_{31,32}]_{ij}$, $[\mathbf{T}_{21,31}]_{ij}$, and $[\mathbf{T}_{32,12}]_{ij}$. To derive analytical formulas for the matrix element $[\mathbf{T}_{31,32}]_{ij}$ we use the well known relation [34]

$$\boldsymbol{\nabla}_{31}\cdot\boldsymbol{\nabla}_{32}[\mathscr{Y}_{LM}^{\ell_1,\ell_2}(\mathbf{r}_{31},\mathbf{r}_{32})]=0. \tag{50}$$

This relation holds, since $\ell_1+\ell_2=L+\epsilon$. Therefore, in the appropriate matrix element we find

$$\boldsymbol{\nabla}_{31}\cdot\boldsymbol{\nabla}_{32}[\mathscr{Y}_{LM}^{\ell_1,\ell_2}(\mathbf{r}_{31},\mathbf{r}_{32})\phi(r_{32},r_{31},r_{21})]=[\boldsymbol{\nabla}_{31}\mathscr{Y}_{LM}^{\ell_1,\ell_2}(\mathbf{r}_{31},\mathbf{r}_{32})\cdot\boldsymbol{\nabla}_{32}\phi(r_{32},r_{31},r_{21})]+[\boldsymbol{\nabla}_{32}\mathscr{Y}_{LM}^{\ell_1,\ell_2}(\mathbf{r}_{31},\mathbf{r}_{32})]$$
$$\times[\boldsymbol{\nabla}_{31}\phi(r_{32},r_{31},r_{21})]+\mathscr{Y}_{LM}^{\ell_1,\ell_2}(\mathbf{r}_{31},\mathbf{r}_{32})\boldsymbol{\nabla}_{31}\cdot\boldsymbol{\nabla}_{32}[\phi(r_{32},r_{31},r_{21})]$$
$$=[\mathbf{r}_{32}\cdot\boldsymbol{\nabla}_{31}\mathscr{Y}_{LM}^{\ell_1,\ell_2}(\mathbf{r}_{31},\mathbf{r}_{32})]\left(\frac{1}{r_{32}}\frac{\partial}{\partial r_{32}}\phi(r_{32},r_{31},r_{21})\right)$$
$$+[\mathbf{r}_{31}\cdot\boldsymbol{\nabla}_{32}\mathscr{Y}_{LM}^{\ell_1,\ell_2}(\mathbf{r}_{31},\mathbf{r}_{32})]\left(\frac{1}{r_{31}}\frac{\partial}{\partial r_{31}}\phi(r_{32},r_{31},r_{21})\right)$$
$$+\mathscr{Y}_{LM}^{\ell_1,\ell_2}(\mathbf{r}_{31},\mathbf{r}_{32})\frac{\mathbf{r}_{31}\cdot\mathbf{r}_{32}}{r_{31}r_{32}}\left(\frac{\partial^2}{\partial r_{31}\partial r_{32}}\phi(r_{32},r_{31},r_{21})\right). \tag{51}$$

To simplify this expression we apply the two following relations (see, e.g., [34]):

$$\mathbf{r}_{31}\cdot\boldsymbol{\nabla}_{32}\mathscr{Y}_{LM}^{\ell_1,\ell_2}(\mathbf{r}_{31},\mathbf{r}_{32})=A(\ell_2,\ell_1)\mathscr{Y}_{LM}^{\ell_1+1,\ell_2-1}(\mathbf{r}_{31},\mathbf{r}_{32}), \tag{52}$$

$$\mathbf{r}_{32}\cdot\boldsymbol{\nabla}_{31}\mathscr{Y}_{LM}^{\ell_1,\ell_2}(\mathbf{r}_{31},\mathbf{r}_{32})=A(\ell_1,\ell_2)\mathscr{Y}_{LM}^{\ell_1-1,\ell_2+1}(\mathbf{r}_{31},\mathbf{r}_{32}), \tag{53}$$

where the factor $A(\ell_1,\ell_2)$ equals

$$A(\ell_1,\ell_2)=\sqrt{\frac{(\ell_1-\epsilon)(\ell_2+1-\epsilon)(2\ell_1+1)}{(2\ell_2+3)}}. \tag{54}$$

Thus we find for $\boldsymbol{\nabla}_{31}\cdot\boldsymbol{\nabla}_{32}[\mathscr{Y}_{LM}^{\ell_1,\ell_2}(\mathbf{r}_{31},\mathbf{r}_{32})\phi(r_{32},r_{31},r_{21})]$ the following expression:

$$\boldsymbol{\nabla}_{31}\cdot\boldsymbol{\nabla}_{32}[\mathscr{Y}_{LM}^{\ell_1,\ell_2}(\mathbf{r}_{31},\mathbf{r}_{32})\phi(r_{32},r_{31},r_{21})]=A(\ell_1,\ell_2)\mathscr{Y}_{LM}^{\ell_1-1,\ell_2+1}(\mathbf{r}_{31},\mathbf{r}_{32})\left(\frac{1}{r_{32}}\frac{\partial}{\partial r_{32}}\phi(r_{32},r_{31},r_{21})\right)$$
$$+A(\ell_2,\ell_1)\mathscr{Y}_{LM}^{\ell_1+1,\ell_2-1}(\mathbf{r}_{31},\mathbf{r}_{32})\left(\frac{1}{r_{31}}\frac{\partial}{\partial r_{31}}\phi(r_{32},r_{31},r_{21})\right)$$
$$+\mathscr{Y}_{LM}^{\ell_1,\ell_2}(\mathbf{r}_{31},\mathbf{r}_{32})\frac{r_{31}^2+r_{32}^2-r_{21}^2}{2r_{31}r_{32}}\left(\frac{\partial^2}{\partial r_{31}\partial r_{32}}\phi(r_{32},r_{31},r_{21})\right). \tag{55}$$

Finally, the expression for the $[\mathbf{T}_{31,32}]_{ij}$ matrix element takes the form

$$[\mathbf{T}_{31,32}]_{ij}=\frac{\alpha_j}{m_3}B^{L,\epsilon}_{\ell_1,\ell_1'-1}A(\ell_1',\ell_2')F(n_1,n_2+1,n_3+1;X_{ij}^{(1)},X_{ij}^{(2)},X_{ij}^{(3)})+\frac{\beta_j}{m_3}B^{L,\epsilon}_{\ell_1,\ell_1'+1}A(\ell_2',\ell_1')F(n_1+1,n_2,n_3$$
$$+1;X_{ij}^{(1)},X_{ij}^{(2)},X_{ij}^{(3)})-\frac{\alpha_j\beta_j}{2m_3}B^{L,\epsilon}_{\ell_1,\ell_1'}[F(n_1,n_2+2,n_3+1;X_{ij}^{(1)},X_{ij}^{(2)},X_{ij}^{(3)})+F(n_1+2,n_2,n_3+1;X_{ij}^{(1)},X_{ij}^{(2)},X_{ij}^{(3)})$$
$$-F(n_1,n_2,n_3+3;X_{ij}^{(1)},X_{ij}^{(2)},X_{ij}^{(3)})]. \tag{56}$$

To calculate the $[\mathbf{T}_{31,21}]_{ij}$ matrix element ($[\mathbf{T}_{31,21}]_{ij}=-1/m_1\boldsymbol{\nabla}_{31}\cdot\boldsymbol{\nabla}_{21}$) we transform the expression for $\boldsymbol{\nabla}_{31}\cdot\boldsymbol{\nabla}_{21}[\mathscr{Y}_{LM}^{\ell_1,\ell_2}(\mathbf{r}_{31},\mathbf{r}_{32})\phi(r_{32},r_{31},r_{21})]$ in an analogous manner and find

$$\begin{aligned}\boldsymbol{\nabla}_{31}\cdot\boldsymbol{\nabla}_{21}[\mathscr{Y}_{LM}^{\ell_1,\ell_2}(\mathbf{r}_{31},\mathbf{r}_{32})\phi(r_{32},r_{31},r_{21})]&=[\boldsymbol{\nabla}_{31}\mathscr{Y}_{LM}^{\ell_1,\ell_2}(\mathbf{r}_{31},\mathbf{r}_{32})\cdot\boldsymbol{\nabla}_{21}\phi(r_{32},r_{31},r_{21})]\\&\quad+\mathscr{Y}_{LM}^{\ell_1,\ell_2}(\mathbf{r}_{31},\mathbf{r}_{32})\boldsymbol{\nabla}_{31}\cdot\boldsymbol{\nabla}_{21}[\phi(r_{32},r_{31},r_{21})]\\&=[\mathbf{r}_{21}\cdot\boldsymbol{\nabla}_{31}\mathscr{Y}_{LM}^{\ell_1,\ell_2}(\mathbf{r}_{31},\mathbf{r}_{32})]\left(\frac{1}{r_{21}}\frac{\partial}{\partial r_{21}}\phi(r_{32},r_{31},r_{21})\right)\\&\quad+\mathscr{Y}_{LM}^{\ell_1,\ell_2}(\mathbf{r}_{31},\mathbf{r}_{32})\frac{\mathbf{r}_{31}\cdot\mathbf{r}_{21}}{r_{31}r_{21}}\left(\frac{\partial^2}{\partial r_{31}\partial r_{21}}\phi(r_{32},r_{31},r_{21})\right).\end{aligned}\tag{57}$$

Since $\mathbf{r}_{21}=\mathbf{r}_{31}-\mathbf{r}_{32}$ and

$$\mathbf{r}_{31}\cdot\boldsymbol{\nabla}_{31}\mathscr{Y}_{LM}^{\ell_1,\ell_2}(\mathbf{r}_{31},\mathbf{r}_{32})=\ell_1\mathscr{Y}_{LM}^{\ell_1,\ell_2}(\mathbf{r}_{31},\mathbf{r}_{32}),\tag{58}$$

$$\mathbf{r}_{32}\cdot\boldsymbol{\nabla}_{32}\mathscr{Y}_{LM}^{\ell_1,\ell_2}(\mathbf{r}_{31},\mathbf{r}_{32})=\ell_2\mathscr{Y}_{LM}^{\ell_1,\ell_2}(\mathbf{r}_{31},\mathbf{r}_{32}),\tag{59}$$

we find the following formula

$$\begin{aligned}\boldsymbol{\nabla}_{31}\cdot\boldsymbol{\nabla}_{21}[\mathscr{Y}_{LM}^{\ell_1,\ell_2}(\mathbf{r}_{31},\mathbf{r}_{32})\phi(r_{32},r_{31},r_{21})]&=-A(\ell_1,\ell_2)\mathscr{Y}_{LM}^{\ell_1-1,\ell_2+1}(\mathbf{r}_{31},\mathbf{r}_{32})\left(\frac{1}{r_{21}}\frac{\partial}{\partial r_{21}}\phi(r_{32},r_{31},r_{21})\right)\\&\quad+\ell_1\mathscr{Y}_{LM}^{\ell_1,\ell_2}(\mathbf{r}_{31},\mathbf{r}_{32})\left(\frac{1}{r_{21}}\frac{\partial}{\partial r_{21}}\phi(r_{32},r_{31},r_{21})\right)\\&\quad+\mathscr{Y}_{LM}^{\ell_1,\ell_2}(\mathbf{r}_{31},\mathbf{r}_{32})\frac{r_{31}^2+r_{21}^2-r_{32}^2}{2r_{31}r_{21}}\left(\frac{\partial^2}{\partial r_{31}\partial r_{21}}\phi(r_{32},r_{31},r_{21})\right).\end{aligned}\tag{60}$$

The analogous expression for $\boldsymbol{\nabla}_{32}\cdot\boldsymbol{\nabla}_{12}[\mathscr{Y}_{LM}^{\ell_1,\ell_2}(\mathbf{r}_{31},\mathbf{r}_{32})\phi(r_{32},r_{31},r_{21})]$ can be found in a very similar form (all intermediate details have been omitted, since they are exactly the same as given above):

$$\begin{aligned}\boldsymbol{\nabla}_{32}\cdot\boldsymbol{\nabla}_{12}[\mathscr{Y}_{LM}^{\ell_1,\ell_2}(\mathbf{r}_{31},\mathbf{r}_{32})\phi(r_{32},r_{31},r_{21})]&=-A(\ell_2,\ell_1)\mathscr{Y}_{LM}^{\ell_1+1,\ell_2-1}(\mathbf{r}_{31},\mathbf{r}_{32})\left(\frac{1}{r_{21}}\frac{\partial}{\partial r_{21}}\phi(r_{32},r_{31},r_{21})\right)\\&\quad+\ell_2\mathscr{Y}_{LM}^{\ell_1,\ell_2}(\mathbf{r}_{31},\mathbf{r}_{32})\left(\frac{1}{r_{21}}\frac{\partial}{\partial r_{21}}\phi(r_{32},r_{31},r_{21})\right)\\&\quad+\mathscr{Y}_{LM}^{\ell_1,\ell_2}(\mathbf{r}_{31},\mathbf{r}_{32})\frac{r_{32}^2+r_{21}^2-r_{31}^2}{2r_{32}r_{21}}\left(\frac{\partial^2}{\partial r_{32}\partial r_{21}}\phi(r_{32},r_{31},r_{21})\right).\end{aligned}\tag{61}$$

Now, for the $[\mathbf{T}_{31,21}]_{ij}$ and $[\mathbf{T}_{32,12}]_{ij}$ matrix elements we obtain the expressions

$$\begin{aligned}[\mathbf{T}_{31,21}]_{ij}&=-\frac{\gamma_j}{m_1}B^{L,\epsilon}_{\ell_1,\ell_1'-1}A(\ell_1',\ell_2')F(n_1+1,n_2+1,n_3;X_{ij}^{(1)},X_{ij}^{(2)},X_{ij}^{(3)})+\frac{\gamma_j}{m_1}B^{L,\epsilon}_{\ell_1,\ell_1'}\ell_1'F(n_1+1,n_2+2,n_3;X_{ij}^{(1)},X_{ij}^{(2)},X_{ij}^{(3)})\\&\quad-\frac{\beta_j\gamma_j}{2m_1}B^{L,\epsilon}_{\ell_1,\ell_1'}[F(n_1+2,n_2+1,n_3;X_{ij}^{(1)},X_{ij}^{(2)},X_{ij}^{(3)})+F(n_1+1,n_2,n_3+2;X_{ij}^{(1)},X_{ij}^{(2)},X_{ij}^{(3)})\\&\quad-F(n_1+3,n_2,n_3;X_{ij}^{(1)},X_{ij}^{(2)},X_{ij}^{(3)})],\end{aligned}\tag{62}$$

$$\begin{aligned}[\mathbf{T}_{32,12}]_{ij}&=-\frac{\gamma_j}{m_2}B^{L,\epsilon}_{\ell_1,\ell_1'+1}A(\ell_2',\ell_1')F(n_1+1,n_2+1,n_3;X_{ij}^{(1)},X_{ij}^{(2)},X_{ij}^{(3)})+\frac{\gamma_j}{m_2}B^{L,\epsilon}_{\ell_1,\ell_1'}\ell_2'F(n_1+1,n_2+1,n_3;X_{ij}^{(1)},X_{ij}^{(2)},X_{ij}^{(3)})\\&\quad-\frac{\alpha_j\gamma_j}{2m_2}B^{L,\epsilon}_{\ell_1,\ell_1'}[F(n_1+2,n_2+1,n_3;X_{ij}^{(1)},X_{ij}^{(2)},X_{ij}^{(3)})+F(n_1,n_2+1,n_3+2;X_{ij}^{(1)},X_{ij}^{(2)},X_{ij}^{(3)})\\&\quad-F(n_1,n_2+3,n_3;X_{ij}^{(1)},X_{ij}^{(2)},X_{ij}^{(3)})].\end{aligned}\tag{63}$$

Now by applying these analytical formulas for the matrix elements given in Secs. II–IV we can calculate all matrix elements which are needed to solve the eigenvalue problem, Eq. (9). These formulas contain the total angular momentum L and the space parity π (or ϵ) as parameters. Thus, now it is possible to determine the bound states with arbitrary L and π in the nonrelativistic three-body systems which consist of three point particles with masses m_1, m_2, and m_3 and where the interaction potential can be written as a sum of two-body central and scalar potentials. It should be mentioned here that the given formulas can be used directly only for nonsymmetrical systems. Their modification to the case of the symmetrical systems is considered in the next section.

V. CASE OF IDENTICAL PARTICLES

Consider now the case when the three-body system contains two identical particles. Without loss of generality suppose that the first and second particles in the considered symmetric three-body system are the identical ones. Therefore, the relation $\hat{P}_{21}\Phi_{LM}=\Phi_{LM}$ must be obeyed for the exact wave function. Here $\hat{P}_{21}$ is the permutation operator (particles 1 and 2), i.e., $\hat{P}_{21}^2=1$. This means that the exact wave function Φ_{LM} is an eigenfunction for the operator $\hat{t}_{21}=1/\sqrt{2}(1\pm\hat{P}_{21})$ with eigenvalue 0 or 1, since $\hat{t}_{21}^2=\hat{t}_{21}$. Therefore, the trial variational function for a symmetric system Ψ_{LM} must be also found in the form

$$\Psi_{LM}=\hat{t}_{21}\psi_{LM}=\frac{1}{\sqrt{2}}(1\pm\hat{P}_{21})\psi_{LM}, \tag{64}$$

where the function ψ_{LM} is the nonsymmetrical coordinate function written in the form of Eq. (4). Let A be a fully symmetric operator, i.e., it does not change when the $\hat{P}_{21}$ permutation is applied, i.e., $A\hat{P}_{21}=\hat{P}_{21}A$. Then in this case we can write the formula for the (ij) matrix elements of A

$$\langle\Psi_{LM,i}|A|\Psi_{LM,j}\rangle=\langle\psi_{LM,i}|A|\psi_{LM,j}\rangle\pm\langle\hat{P}_{21}\psi_{LM,i}|A|\psi_{LM,j}\rangle, \tag{65}$$

where the symmetric and nonsymmetric trial functions Ψ_{LM} and ψ_{LM} are represented in the forms

$$|\Psi_{LM}\rangle=\sum_{i=1}^{N}C_i|\Psi_{LM,i}\rangle=\frac{1}{\sqrt{2}}\sum_{i=1}^{N}C_i(1\pm\hat{P}_{21})|\psi_{LM,i}\rangle;$$

$$|\psi_{LM}\rangle=\sum_{i=1}^{N}c_i|\psi_{LM,i}\rangle, \tag{66}$$

respectively. The first matrix element is calculated in the same manner as for nonsymmetric systems. Indeed, we write for the first matrix element in the right-hand side of Eq. (65)

$$\begin{aligned}&\langle\psi_{LM,i}|A|\psi_{LM,j}\rangle\\&\quad=\langle\alpha_i,\beta_i,\gamma_i,\ell_1(i),\ell_2(i);L,M,\epsilon|A|L,M,\epsilon;\\&\qquad\ell_1(j),\ell_2(j),\alpha_j,\beta_j,\gamma_j\rangle.\end{aligned} \tag{67}$$

Actually, in this equation the values of $\ell_1(j),\ell_2(j),\alpha_j,\beta_j,\gamma_j$ and $\ell_1(i),\ell_2(i),\alpha_i,\beta_i,\gamma_i$ are the so-called entrance parameters to compute this matrix element. The values of L,M,ϵ can be called as the outside parameters.

To calculate the second term we use the following relation for the $\mathscr{Y}_{LM}^{\ell_2,\ell_1}(\mathbf{r}_{31},\mathbf{r}_{32})$ functions

$$\hat{P}_{21}\mathscr{Y}_{LM}^{\ell_1,\ell_2}(\mathbf{r}_{31},\mathbf{r}_{32})=(-1)^{\epsilon}\mathscr{Y}_{LM}^{\ell_2,\ell_1}(\mathbf{r}_{31},\mathbf{r}_{32}), \tag{68}$$

where $\epsilon=0$ or 1, and the relation for the exponentials of the relative coordinates

$$\begin{aligned}&\hat{P}_{21}\exp(-\alpha_i r_{32}-\beta_i r_{31}-\gamma_i r_{21})\\&\quad=\exp(-\beta_i r_{32}-\alpha_i r_{31}-\gamma_i r_{21}).\end{aligned} \tag{69}$$

Finally, we have for the second term in the right-hand side of Eq. (65),

$$\begin{aligned}\langle\hat{P}_{21}\psi_{LM,i}|A|\psi_{LM,j}\rangle=(-1)^{\epsilon}\langle&\beta_i,\alpha_i,\gamma_i,\ell_2(i),\ell_1(i);\\&L,M,\epsilon|A|L,M,\epsilon;\ell_1(j),\ell_2(j),\\&\alpha_j,\beta_j,\gamma_j\rangle;\end{aligned} \tag{70}$$

in other words to compute the second term in Eq. (65) we need to permute only the four entrance parameters and repeat the procedure as for the nonsymmetrical matrix element. Thus, we can calculate all matrix elements which are needed to solve the appropriate eigenvalue problem for an arbitrary symmetric three-body nonrelativistic system with arbitrary values of L and π (or ϵ). The more complicated case when all three particles are identical requires separate consideration. However, such a situation seems to be actual only in some nuclear three-body problems.

VI. CASE OF THE ADIABATIC THREE-BODY SYSTEMS

The case mentioned above when two of the masses are significantly greater than the third mass (the so-called adiabatic systems) requires a separate investigation. Without loss of generality we suppose that $m_1\approx m_2\gg m_3$ and that the interaction potential between i and j particles is a Coulomb potential, i.e., $V_{ij}(r_{ij})=q_jq_i/r_{ij}$. Moreover, the variational expansions, Eqs. (2) and (4), have a very slow rate of convergence only when $q_2q_1>0$. Actually, this means [46] that the variational expansion Eq. (4) cannot be applied for highly accurate calculations in three-body systems such as $\mu^+\mu^+e^-$ and H_2^+ (the so-called adiabatic systems). This problem was studied in our work [46] and briefly the result can be formulated as follows. To compute with high accuracy the bound states in three-body systems, including adiabatic systems, we proposed [46] to use the so-called universal variational three-body expansion, which takes the form

$$\begin{aligned}\Psi_{LM}&=\sum_{i=1}^{N}C_i\psi_{i,LM}\\&=\sum_{i=1}^{N}\sum_{\ell=\epsilon}^{L}C_i\mathscr{Y}_{LM}^{\ell_1,\ell_2}(\mathbf{r}_{31},\mathbf{r}_{32})\\&\quad\times\exp(-\alpha_i r_{32}-\beta_i r_{31}-\gamma_i r_{21})\\&\quad\times\exp(\imath\delta_i r_{32}+\imath e_i r_{31}+\imath f_i r_{21}),\end{aligned} \tag{71}$$

where the C_i $(i=1,2,\ldots,N)$ are the linear (variational) parameters, which can be found by solving the secular equation. The real exponents $\{\alpha_i,\beta_i,\gamma_i,\delta_i,e_i,f_i\}$, where $i=1,2,\ldots,N$, are the nonlinear parameters which are generated in a quasirandom manner from the six real intervals. The angular functions $\mathscr{Y}_{LM}^{\ell_1,\ell_2}(\mathbf{r}_{31},\mathbf{r}_{32})$ are the bipolar harmonics.

It has been shown that this universal variational expansion can be applied successfully [in contrast with the expansion (2)] to compute the bound state spectra in arbitrary three-body nonrelativistic systems (for more details and numerical results see [46]), including the mentioned adiabatic systems. However, it is clear that all formulas for the matrix elements presented above hold for the universal variational expansion, Eq. (71), as well, i.e., when complex nonlinear parameters are used.

VII. CONCLUSION

A variational procedure is proposed to carry out highly accurate variational calculations for the all of the bound states in a three-body nonrelativistic system with arbitrary masses. In the present work we considered only the case when the interaction potential is represented as the sum of two-body central and scalar interaction potentials. The generalization to more general interaction potentials can be made in an analogous way. The presented formulas for all matrix elements contain the total angular momenta L and the space parity π (or ϵ) as parameters. This means that a bound state with arbitrary values of L and π in the nonrelativistic three-body systems can be calculated in terms of this highly accurate approach. It should be mentioned that these formulas include also the case of unnatural space parity. The presented method is relatively simple and logically closed. It can be used also for other radial basis functions in the relative coordinates r_{32}, r_{32}, and r_{21}. We hope that this approach will motivate further computational activities for bound states with arbitrary L and π for the various three-body systems.

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[17] A bound state of a nonrelativistic three-body system can be designated by a few conservative quantum numbers. When the interaction potential in such a system is represented as a sum of two-body central and scalar potentials we can choose as the conservative quantum numbers the following: the angular momentum L, its z component M, space parity π, and probably a few additional conservative quantum numbers.
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