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The Schrödinger equation for a spherical two-particle system in r_1, r_2, r_{12} variables

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Abstract

The two-particle Schrödinger eigenvalue equation in a spherical potential is considered. For an arbitrary total angular momentum L, its projection M and the parity π, the Hamiltonian and its eigenvalue problem is expressed in terms of r_1, r_2 and r_{12} only. The dependence on the remaining angles as well as on the angular momentum is reflected by the finite multi-dimensional structure of the eigenvalue equations.

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1. Introduction

The reduction of the helium eigenvalue problem for ${}^1S^e$ and ${}^3S^e$ to an equation which depends on the three triangle variables r_1, r_2 and r_{12} only, was given by Hylleraas nearly 80 years ago [1]. A year later, in 1930, Breit [2] extended this approach to P^o and P^e states[1]. Since then the equations of Hylleraas and Breit became a starting point for many approaches aimed at deriving very precise approximations to the wavefunctions describing the pertinent states of the helium atom [3–6]. Next, every 30 years consecutive generalizations to arbitrary values of L appeared: Bhatia and Temkin [7] in 1964 and Kalotas [8] in 1965 followed by Bottcher *et al* [9] in 1994. In the first two approaches the problem has been solved on the basis of Wigner $\mathcal{D}^{\mathcal{L}}_{\mathcal{M},\mathcal{K}}$ functions, while the third one utilizes the bipolar basis. In all these papers, the Schrödinger equation for a helium-like atom has been reduced to a finite system of equations depending on the triangle variables only for an arbitrary angular momentum L and parity π. Both Wigner and bipolar bases were recently applied by Korobov *et al* to a study on antiprotonic helium atom [10, 11] and on H_2^+, HD^+ molecular ions [12]. Similar ideas were

[1] In fact, Breit used r_1, r_2 and ϑ_{12}, but the relation $\cos\vartheta_{12} = (r_1^2 + r_2^2 - r_{12}^2)/(2r_1r_2)$ determines the mutual correspondence between Breit's coordinates and those of Hylleraas. In further discussions the specific choice of r_1, r_2 and r_{12} is not significant. In general, they can be replaced by any three equivalent variables.

also used by Jeziorski *et al* [13] in studies concerned with the completeness of the functional bases used in molecular structure calculations.

The reduction of the Schrödinger equation presented in this paper is performed in the bipolar basis. This basis was introduced, analyzed and applied by Schwartz [14] in 1961. Later, in 1967, King [15] gave its extensive analysis. In the present work the earlier results are generalized for the case of two, not necessarily identical, interacting particles confined in an external spherical potential. In this way the results are applicable to all kinds of exotic systems, such as, for example, to muonic, positronic or antiprotonic atoms [11, 16]. The bipolar expansion proved to be particularly useful to the description of antiprotonic atoms [11]. Besides, the resulting equations are simpler (the coupling terms are simpler than in [7, 8] and contain no complicated sums, in contrast to [9]). The reduction to the finite system of equations is based on the construction of a space which is invariant under the action of operators forming the Schrödinger Hamiltonian.

2. General considerations

Let us take a product of a radial function $f(r_1, r_2, r_{12})$ depending on the triangle variables and the angular function $\Omega_{l_1,l_2}(\hat{\boldsymbol{r}}_1, \hat{\boldsymbol{r}}_2)$ which is an eigenfunction of the angular momenta l_1 and l_2 of each particle. The way the angular variables $\hat{\boldsymbol{r}}_1$ and $\hat{\boldsymbol{r}}_2$ are defined is irrelevant for this discussion. In order to avoid any misunderstanding curly brackets are used to denote the range of actions of an operator. For example, $\{\hat{\boldsymbol{X}} f\}g$ means that $\hat{\boldsymbol{X}}$ acts on f only, where $\hat{\boldsymbol{X}}$ is an operator and f, g functions belonging to its domain. For simplicity, throughout this work, $i = 1, 2$ refers to a specific particle. A complementary index $\hat{\imath} = 1 + (i \bmod 2)$ has also been introduced.

As one can see,

$$\begin{aligned} \triangle_i\, f(r_1, r_2, r_{12})\Omega_{l_1,l_2}(\hat{\boldsymbol{r}}_1, \hat{\boldsymbol{r}}_2) &= \{\triangle_i f(r_1, r_2, r_{12})\}\Omega_{l_1,l_2}(\hat{\boldsymbol{r}}_1, \hat{\boldsymbol{r}}_2) \\ &\quad - f(r_1, r_2, r_{12})\frac{\hat{l}_i^2}{r_i^2}\Omega_{l_1,l_2}(\hat{\boldsymbol{r}}_1, \hat{\boldsymbol{r}}_2) \\ &\quad + \left\{(-2)\frac{r_{\hat{\imath}}}{r_i r_{12}}\frac{\partial f(r_1, r_2, r_{12})}{\partial r_{12}}\right\}\{\Lambda_i \Omega_{l_1,l_2}(\hat{\boldsymbol{r}}_1, \hat{\boldsymbol{r}}_2)\}, \end{aligned} \tag{1}$$

where $\triangle_i$ is the Laplace operator of the ith particle and

$$\begin{aligned} &\{\triangle_i f(r_1, r_2, r_{12})\} \\ &\quad \equiv \left(\frac{\partial^2}{\partial r_i^2} + \frac{2}{r_i}\frac{\partial}{\partial r_i} + \frac{\partial^2}{\partial r_{12}^2} + \frac{2}{r_{12}}\frac{\partial}{\partial r_{12}} + \frac{r_i^2 - r_{\hat{\imath}}^2 + r_{12}^2}{r_i r_{12}}\frac{\partial^2}{\partial r_i \partial r_{12}}\right) f(r_1, r_2, r_{12}). \end{aligned} \tag{2}$$

The angular operators Λ_i read

$$\begin{aligned} \Lambda_i &\equiv \frac{r_i}{r_{\hat{\imath}}}\sum_{a\in\{x,y,z\}} a_{\hat{\imath}}\frac{\partial}{\partial a_i} \\ &= \frac{1}{\cos\Theta_i}\sqrt{\frac{2\pi}{3}}\left[\left(Y_{-1}^1(\hat{\boldsymbol{r}}_{\hat{\imath}})\hat{l}_i^+ + Y_{+1}^1(\hat{\boldsymbol{r}}_{\hat{\imath}})\hat{l}_i^-\right) - \cos\vartheta_{12}\left(Y_{+1}^1(\hat{\boldsymbol{r}}_i)\hat{l}_i^- + Y_{-1}^1(\hat{\boldsymbol{r}}_i)\hat{l}_i^+\right)\right], \end{aligned} \tag{3}$$

where $\hat{l}_i^+, \hat{l}_i^-$ are the ladder operators for both particles, Y_m^l are spherical harmonics, $\cos\vartheta_{12} = \left(r_1^2 + r_2^2 - r_{12}^2\right)/(2r_1 r_2)$ and Θ_i are the polar angles of the particles [6]. Let us note that equation (1) is equivalent to equation (11.30) of reference [6].

Let $\mathcal{O}$ be the space spanned by eigenfunctions $\Omega_{l_1,l_2}(\hat{\boldsymbol{r}}_1, \hat{\boldsymbol{r}}_2)$ with $l_1, l_2 = 0, 1, 2, \ldots$ and $\mathcal{O}_{L,M,\pi}$ its subspace spanned by

$$\Omega^{L,M}_{l_1,l_2}(\hat{\boldsymbol{r}}_1, \hat{\boldsymbol{r}}_2) = (-1)^{l_1+l_2+M}\sqrt{2L+1}\sum_{m_1,m_2}\begin{pmatrix} l_1 & l_2 & L \\ m_1 & m_2 & -M\end{pmatrix} Y^{l_1}_{m_1}(\hat{\boldsymbol{r}}_1) Y^{l_2}_{m_2}(\hat{\boldsymbol{r}}_2), \tag{4}$$

corresponding to a specific pair L, M and parity $\pi = (-1)^{l_1+l_2}$. By the construction, the closure $\overline{\mathcal{O}}$ of $\mathcal{O}$ is complete on the spheres defined by $\hat{\boldsymbol{r}}_1, \hat{\boldsymbol{r}}_2$ while $\overline{\mathcal{O}}_{L,M,\pi}$ is its complete L, M, π adapted subspace. As demonstrated by King [15], every element of $\overline{\mathcal{O}}_{L,M,\pi}$ can be expanded in terms of

$$Q^{L,M}_{l,l_1,l_2} \equiv P_l(\cos\vartheta_{12})\Omega^{L,M}_{l_1,l_2}(\hat{\boldsymbol{r}}_1, \hat{\boldsymbol{r}}_2), \tag{5}$$

where the values l_1, l_2 are restricted by the condition $l_1 + l_2 = L$ for the natural parity $\pi = (-1)^L$ and by $l_1 + l_2 = L + 1$ for the unnatural parity $\pi = (-1)^{L+1}$, and P_l, $l = 0, 1, 2, \ldots$ are the Legendre polynomials. In equation (5) $d = L+1$ functions $\Omega^{L,M}_{l_1,L-l_1}$, $l_1 = 0, 1, \ldots, L$ in the case of the natural parity $\pi = (-1)^L$ and $d = L$ functions $\Omega^{L,M}_{l_1,L-l_1+1}$, $l_1 = 1, \ldots, L$ in the case of the unnatural parity $\pi = (-1)^{L+1}$ are referred to as the *generator functions*.

The one-particle Laplace operators commute with $\hat{L}^2$ and $\hat{L}_z$. Therefore the operators Λ_1, Λ_2 also commute with $\hat{L}^2$ and $\hat{L}_z$. Consequently, the completeness of $\overline{\mathcal{O}}_{L,M,\pi}$ implies that the rhs of equation (1) can be expressed as

$$\triangle_i f(r_1, r_2, r_{12})\Omega^{L,M}_{l_1,l_2}(\hat{\boldsymbol{r}}_1, \hat{\boldsymbol{r}}_2) = \sum_{\tilde{l}_1=d_0}^{L}\left\{\hat{\boldsymbol{X}}^{\tilde{l}_i l_i}_i f(r_1, r_2, r_{12})\right\}\Omega^{L,M}_{\tilde{l}_1,\tilde{l}_2}(\hat{\boldsymbol{r}}_1, \hat{\boldsymbol{r}}_2), \tag{6}$$

where the operators $\hat{\boldsymbol{X}}^{\tilde{l}_1,l_1}_1, \hat{\boldsymbol{X}}^{\tilde{l}_2,l_2}_2$ depend on the triangle variables only and act on the radial function f and

$$d_0 = L + 1 - d = \begin{cases} 0, & \text{if} \quad d = L + 1, \\ 1, & \text{if} \quad d = L. \end{cases}$$

The first particle angular momentum quantum number $\tilde{l}_1$ is chosen as the summation index in expansion (6) for both values of i but, for the convenience, quantum numbers $\tilde{l}_2 = d - \tilde{l}_1$ and $l_2 = d - l_1$ have been used as labels in the operator $\hat{\boldsymbol{X}}^{\tilde{l}_2,l_2}_2$. One can also see that

$$\hat{\boldsymbol{X}}^{\tilde{l},l}_2(r_1, r_2, r_{12}) = \hat{\boldsymbol{X}}^{\tilde{l},l}_1(r_2, r_1, r_{12}), \tag{7}$$

where $d_0 \leqslant l, \tilde{l} \leqslant L$.

On the other hand, any eigenfunction of a two-particle Schrödinger Hamiltonian can be expanded in the same manner

$$\Psi(\boldsymbol{r}_1, \boldsymbol{r}_2) = \sum_{l_1=d_0}^{L}\Phi_{l_1}(r_1, r_2, r_{12})\Omega^{L,M}_{l_1,l_2}(\hat{\boldsymbol{r}}_1, \hat{\boldsymbol{r}}_2). \tag{8}$$

If expansion (8) is inserted into the Schrödinger equation

$$\left[\frac{1}{2m_1}\hat{\boldsymbol{p}}_1^2 + \frac{1}{2m_2}\hat{\boldsymbol{p}}_2^2 + V - E\right]\Psi = 0, \tag{9}$$

where $V \equiv V(r_1, r_2, r_{12})$ depends on the triangle variables only, then the application of equation (6) to the operators $\hat{\boldsymbol{p}}_1^2 = -\triangle_1$ and $\hat{\boldsymbol{p}}_1^2 = -\triangle_2$ implies

$$\sum_{\tilde{l}_1=d_0}^{L}\left\{\sum_{l_1=d_0}^{L}\hat{\boldsymbol{A}}^{\tilde{l}_1,l_1}_1\Phi_{l_1}\right\}\Omega^{L,M}_{\tilde{l}_1,\tilde{l}_2} = 0, \tag{10}$$

where

$$\hat{\boldsymbol{A}}^{\tilde{l}_1,l_1} = \frac{(-1)}{2m_1}\hat{\boldsymbol{X}}_1^{\tilde{l}_1,l_1} + \frac{(-1)}{2m_2}\hat{\boldsymbol{X}}_2^{\tilde{l}_2,l_2} + \delta_{\tilde{l}_1,l_1}(V - E). \tag{11}$$

As demonstrated by King [15], the set of generator functions $\Omega^{L,M}_{\tilde{l}_1,\tilde{l}_2}(\hat{\boldsymbol{r}}_1, \hat{\boldsymbol{r}}_2)$ in equation (10) uniquely corresponds to the set of Wigner's functions $\mathcal{D}^{\mathcal{L}}_{\mathcal{M},\mathcal{K}}$ which depend on the three Euler angles only. Then, the generator functions $\Omega^{L,M}_{\tilde{l}_1,\tilde{l}_2}$ form a set of linearly independent functions of the angular variables. A two-particle function can be expressed as a linear combination of the generator functions with coefficients dependent on the triangle variables r_1, r_2, r_{12} only. Consequently, the curly brackets in expansion (10) are equal to zero. Thus, we have obtained a system of $d = L + 1$ or $d = L$ coupled equations in the triangle variables

$$\sum_{l_1=d_0}^{L}\left(\frac{(-1)}{2m_1}\hat{\boldsymbol{X}}_1^{\tilde{l}_1,l_1} + \frac{(-1)}{2m_2}\hat{\boldsymbol{X}}_2^{\tilde{l}_2,l_2}\right)\Phi_{l_1} + (V - E)\Phi_{\tilde{l}_1} = 0. \tag{12}$$

Each of these equations, indexed by $\tilde{l}_1$ and depending only on the triangle variables, is the expansion coefficient of initial Schrödinger equation (9), associated with the angular generator function $\Omega^{L,M}_{\tilde{l}_1,\tilde{l}_2}(\hat{\boldsymbol{r}}_1, \hat{\boldsymbol{r}}_2)$.

Schrödinger equation (9), reduced to the system of coupled equations (12), can be written as a homogeneous multicomponent matrix-operator equation

$$\left[\frac{(-1)}{2m_1}\hat{\mathbb{D}}_1 + \frac{(-1)}{2m_2}\hat{\mathbb{D}}_2 + (V - E)\mathbb{I}_d\right]\Phi_L = \mathbf{0}_d, \tag{13}$$

where

$$\hat{\mathbb{D}}_1 \equiv \left[\hat{\boldsymbol{X}}_1^{\tilde{l}_1,l_1}\right]_{d_0\leqslant\tilde{l}_1,l_1\leqslant L},$$

$$\hat{\mathbb{D}}_2 \equiv \left[\hat{\boldsymbol{X}}_2^{\tilde{l}_2=d-\tilde{l}_1,l_2=d-l_1}\right]_{d_0\leqslant\tilde{l}_1,l_1\leqslant L}$$

are matrix operators representing the Laplace operators of both particles, $\mathbb{I}_d$ is the identity matrix of dimension d,

$$\Phi_L \equiv [\Phi_{d_0}, \Phi_{d_0+1}, \ldots, \Phi_L]^T$$

is a d-component column, representative of the wavefunction, and $\mathbf{0}_d$ is the column of zeros.

In the following two sections the exact expressions for $\Lambda_1, \Lambda_2, \hat{\boldsymbol{X}}_1^{\tilde{l}_1,l_1}, \hat{\boldsymbol{X}}_2^{\tilde{l}_2,l_2}$ and, thus, Schrödinger equation (12) in the triangle variables for any state of given L, M and π are derived.

3. The case of a state of given L, M and $\pi = (-1)^L$

For a state corresponding to given L, M and $\pi = (-1)^L$ the set of generator functions (4) is determined by the values of $l_1 = 0, 1, 2, \ldots, L$ and $l_2 = L - l_1$. When we act on a chosen generator $\Omega^{L,M}_{l_1,l_2}$ with the angular operators Λ_1 and Λ_2 (3) then for both particles, after arduous calculations, we get

$$\Lambda_1\Omega^{L,M}_{l_1,l_2} = \sqrt{\frac{(L - l_2)(2l_1 + 1)(L - l_1 + 1)}{(2l_2 + 3)}}\Omega^{L,M}_{l_1-1,l_2+1} - l_1\cos\vartheta_{12}\Omega^{L,M}_{l_1,l_2}, \tag{14}$$

$$\Lambda_2\Omega^{L,M}_{l_1,l_2} = \sqrt{\frac{(L - l_1)(2l_2 + 1)(L - l_2 + 1)}{(2l_1 + 3)}}\Omega^{L,M}_{l_1+1,l_2-1} - l_2\cos\vartheta_{12}\Omega^{L,M}_{l_1,l_2}, \tag{15}$$

and

$$\triangle_1 f(r_1, r_2, r_{12})\Omega^{L,M}_{l_1,l_2} = \left\{\hat{\boldsymbol{X}}^{l_1,l_1}_1 f(r_1, r_2, r_{12})\right\}\Omega^{L,M}_{l_1 l_2} + \left\{\hat{\boldsymbol{X}}^{l_1-1,l_1}_1 f(r_1, r_2, r_{12})\right\}\Omega^{L,M}_{l_1-1,l_2+1}, \quad (16)$$

$$\triangle_2 f(r_1, r_2, r_{12})\Omega^{L,M}_{l_1,l_2} = \left\{\hat{\boldsymbol{X}}^{l_2,l_2}_2 f(r_1, r_2, r_{12})\right\}\Omega^{L,M}_{l_1 l_2} + \left\{\hat{\boldsymbol{X}}^{l_2-1,l_2}_2 f(r_1, r_2, r_{12})\right\}\Omega^{L,M}_{l_1+1,l_2-1}. \quad (17)$$

As we can see, in this case expansion (6) contains only two non-zero operators. The first corresponds to $0 \leqslant l_i \leqslant L$:

$$\hat{\boldsymbol{X}}^{l_i,l_i}_i = \frac{\partial^2}{\partial r_i^2} + \frac{2}{r_i}\frac{\partial}{\partial r_i} + \frac{\partial^2}{\partial r_{12}^2} + \frac{(2+l_i)r_i^2 + l_i\left(r_{\hat{\imath}}^2 - r_{12}^2\right)}{r_i^2 r_{12}}\frac{\partial}{\partial r_{12}} + \frac{r_i^2 - r_{\hat{\imath}}^2 + r_{12}^2}{r_i r_{12}}\frac{\partial^2}{\partial r_i \partial r_{12}} - \frac{l_i(l_i+1)}{r_i^2}, \quad (18)$$

and the second one to $1 \leqslant l_i \leqslant L$:

$$\hat{\boldsymbol{X}}^{l_i-1,l_i}_i = \frac{-2r_{\hat{\imath}}}{r_i r_{12}}\sqrt{\frac{(L-l_{\hat{\imath}})(2l_i+1)(L-l_i+1)}{(2l_{\hat{\imath}}+3)}}\frac{\partial}{\partial r_{12}}. \quad (19)$$

The operators Λ_1, Λ_2, $\hat{\boldsymbol{X}}^{l_1-1,l_1}_1$ and $\hat{\boldsymbol{X}}^{l_2-1,l_2}_2$ depend on l_1, l_2 indices only. However, for the sake of further generalizations, it is convenient to insert an auxiliary index L, which in this case is equal to $l_1 + l_2$. Let us note that for a given value of the total angular momentum L and the parity π the coefficients in expansions (14), (15) and, in consequence, the operators $\hat{\boldsymbol{X}}^{\tilde{l}_1,l_1}_1$, $\hat{\boldsymbol{X}}^{\tilde{l}_2,l_2}_2$ and equation (12) are independent of M.

In this case Schrödinger equation (9) with the wavefunction of form (8) reduces to a system of $(L+1)$ coupled equations

$$\begin{aligned}
&\frac{(-1)}{2m_1}\left(\hat{\boldsymbol{X}}^{0,0}_1\Phi_0 + \hat{\boldsymbol{X}}^{0,1}_1\Phi_1\right) + \frac{(-1)}{2m_2}\left(\hat{\boldsymbol{X}}^{L,L}_2\Phi_0\right) = (E-V)\Phi_0,\\
&\frac{(-1)}{2m_1}\left(\hat{\boldsymbol{X}}^{l_1,l_1}_1\Phi_{l_1} + \hat{\boldsymbol{X}}^{l_1,l_1+1}_1\Phi_{l_1+1}\right) + \frac{(-1)}{2m_2}\left(\hat{\boldsymbol{X}}^{l_2,l_2}_2\Phi_{l_1} + \hat{\boldsymbol{X}}^{l_2,l_2+1}_2\Phi_{l_1-1}\right) = (E-V)\Phi_{l_1},\\
&\frac{(-1)}{2m_1}\left(\hat{\boldsymbol{X}}^{L,L}_1\Phi_L\right) + \frac{(-1)}{2m_2}\left(\hat{\boldsymbol{X}}^{0,0}_2\Phi_L + \hat{\boldsymbol{X}}^{0,1}_2\Phi_{L-1}\right) = (E-V)\Phi_L,
\end{aligned} \quad (20)$$

where $l_1 = 1, 2, \ldots, L-1$. In order to construct the energy functional necessary for an application of the variational method, the equations should be multiplied, respectively, by the generator functions $\Omega^{L,M}_{0,L}$, $\Omega^{L,M}_{l_1,l_2}$, $\Omega^{L,M}_{L,0}$, summed together and integrated over the angular variables with trial function (8).

It can be easily seen that the above system of equations corresponds to a very simple tridiagonal $d \times d$ matrix operator ($d = L+1$) of the multi-component Schrödinger equation (13). The operator $\hat{\mathbb{D}}_1$ consists of the diagonal elements $\hat{\boldsymbol{X}}^{l_1,l_1}_1$ and of the upper diagonal elements $\hat{\boldsymbol{X}}^{l_1,l_1+1}_1$. Similarly the operator $\hat{\mathbb{D}}_2$ consists of the diagonal elements $\hat{\boldsymbol{X}}^{d-l_1,d-l_1}_2$ and of the lower diagonal elements $\hat{\boldsymbol{X}}^{d-l_1,d-(l_1-1)}_2$ placed in the operator matrix at the positions (l_1, l_1-1).

4. The case of a state of given L, M and $\pi = (-1)^{L+1}$

This is the complementary case to the previous one—it has the unnatural parity, $\pi = (-1)^{L+1}$. Now the set of generator functions (4) is determined by the values of $l_1 = 1, 2, \ldots, L$ and

$l_2 = L + 1 - l_1$. The results of the action of the angular operators Λ_1, Λ_2 (3) on the generator functions $\Omega^{L,M}_{l_1,l_2}$ are given by the same formulae as before (14), (15), but now with $L = l_1 + l_2 - 1$. Similarly, the action of the Laplace operators $\triangle_1$, $\triangle_2$ can be expressed by the same expansions (16), (17) with the same expansion operators $\hat{\boldsymbol{X}}_1^{l_1,l_1}$, $\hat{\boldsymbol{X}}_2^{l_2,l_2}$ (18), where $1 \leqslant l_1, l_2 \leqslant L$; and the same operators $\hat{\boldsymbol{X}}_1^{l_1-1,l_1}$, $\hat{\boldsymbol{X}}_2^{l_2-1,l_2}$ (19), where $2 \leqslant l_1, l_2 \leqslant L$.

Schrödinger equation (9) transforms to the following system of L equations:

$$
\begin{aligned}
&\frac{(-1)}{2m_1}\left(\hat{\boldsymbol{X}}_1^{1,1}\Phi_1 + \hat{\boldsymbol{X}}_1^{1,2}\Phi_2\right) + \frac{(-1)}{2m_2}\left(\hat{\boldsymbol{X}}_2^{L,L}\Phi_1\right) = (E - V)\Phi_1,\\
&\frac{(-1)}{2m_1}\left(\hat{\boldsymbol{X}}_1^{l_1,l_1}\Phi_{l_1} + \hat{\boldsymbol{X}}_1^{l_1,l_1+1}\Phi_{l_1+1}\right) + \frac{(-1)}{2m_2}\left(\hat{\boldsymbol{X}}_2^{l_2,l_2}\Phi_{l_1} + \hat{\boldsymbol{X}}_2^{l_2,l_2+1}\Phi_{l_1-1}\right) = (E - V)\Phi_{l_1},\\
&\frac{(-1)}{2m_1}\left(\hat{\boldsymbol{X}}_1^{L,L}\Phi_L\right) + \frac{(-1)}{2m_2}\left(\hat{\boldsymbol{X}}_2^{1,1}\Phi_L + \hat{\boldsymbol{X}}_2^{1,2}\Phi_{L-1}\right) = (E - V)\Phi_L,
\end{aligned}
\tag{21}
$$

where $2 \leqslant l_1 \leqslant L - 1$. The energy functional may be obtained by multiplying the above equations by the generators $\Omega^{L,M}_{1,L}$, $\Omega^{L,M}_{l_1,l_2}$, $\Omega^{L,M}_{L,1}$, summed together and integrated over the angular variables with the trial function (8). Similarly to the previous case the above system of equations forms a tridiagonal $d \times d$ matrix operator (now with $d = L$) of the Schrödinger multi-component equation (13) with the same structure of the operators $\hat{\mathbb{D}}_1$ and $\hat{\mathbb{D}}_2$ as before.

5. Explicit forms of some equations

In this section we present the explicit expressions for the two-particle Schrödinger equations in the triangle variables for the states corresponding to the most important lowest values of the total angular momentum. Due to the independence of the resulting equations on M, in generator functions $\Omega^{L,M}_{l_1,l_2}$ with $L = 0, 1, 2$ we introduced the shorthand notation, respectively $\Omega^S_{l_1,l_2}$, $\Omega^P_{l_1,l_2}$, $\Omega^D_{l_1,l_2}$.

5.1. The equation for S^e states

The equation for this symmetry was obtained by Hylleraas [1]. The parity is even with $L = l_1 + l_2 = 0$ and thus $l_1 = l_2 = 0$. The problem reduces to one scalar equation ($d = L + 1 = 1$) with one constant generator function $\Omega^S_{00} \equiv 1/(4\pi)$. Then, the wavefunction takes the form

$$
\Psi^S_e(\boldsymbol{r}_1, \boldsymbol{r}_2) = \Phi^S_{00}(r_1, r_2, r_{12})\, \Omega^S_{00}. \tag{22}
$$

The angular momentum operator in (1) acts on a constant Ω^S_{00} so that the corresponding terms vanish (see table 1). Thus, Schrödinger equation (9) reduces to

$$
\left[\frac{(-1)}{2m_1}\hat{\boldsymbol{X}}_1^{00} + \frac{(-1)}{2m_2}\hat{\boldsymbol{X}}_2^{00} + V - E\right]\Phi^S_{00}(r_1, r_2, r_{12}) = 0, \tag{23}
$$

where the Laplace operators of both particles are reduced to $\hat{\boldsymbol{X}}_1^{00}$, $\hat{\boldsymbol{X}}_2^{00}$. Their explicit forms are determined by equation (2), linked by relation (7) and are given in table 2. In the case of identical particles, the radial function Φ^S_{00} has to be either symmetric or antisymmetric with respect to the interchange of r_1 and r_2.

Table 1. The action of the angular operators Λ_1, Λ_2 on some generator functions Ω.

State	L	π	Ω	$\Lambda_1\Omega$	$\Lambda_2\Omega$
S^e	0	+1	Ω^S_{00}	0	0
P^e	1	+1	Ω^P_{11}	$-\cos\vartheta_{12}\Omega^P_{11}$	$-\cos\vartheta_{12}\Omega^P_{11}$
P^o	1	−1	Ω^P_{01}	0	$\Omega^P_{10} - \cos\vartheta_{12}\Omega^P_{01}$
			Ω^P_{10}	$\Omega^P_{01} - \cos\vartheta_{12}\Omega^P_{10}$	0
D^o	2	−1	Ω^D_{12}	$-\cos\vartheta_{12}\Omega^D_{12}$	$\Omega^D_{21} - 2\cos\vartheta_{12}\Omega^D_{12}$
			Ω^D_{21}	$\Omega^D_{12} - 2\cos\vartheta_{12}\Omega^D_{21}$	$-\cos\vartheta_{12}\Omega^D_{21}$
D^e	2	+1	Ω^D_{02}	0	$\sqrt{\frac{10}{3}}\Omega^D_{11} - 2\cos\vartheta_{12}\Omega^D_{02}$
			Ω^D_{20}	$\sqrt{\frac{10}{3}}\Omega^D_{11} - 2\cos\vartheta_{12}\Omega^D_{20}$	0
			Ω^D_{11}	$\sqrt{\frac{6}{5}}\Omega^D_{02} - \cos\vartheta_{12}\Omega^D_{11}$	$\sqrt{\frac{6}{5}}\Omega^D_{20} - \cos\vartheta_{12}\Omega^D_{11}$

Table 2. Explicit forms of the non-zero operators $\hat{\boldsymbol{X}}_1^{\bar{l}_1,l_1}$ for S, P, D states; $\hat{\boldsymbol{X}}_2^{\bar{l}_1,l_1}$ are given by equation (7).

The diagonal operators
$\hat{\boldsymbol{X}}_1^{00} = \hat{\boldsymbol{Y}} + \frac{2}{r_{12}}\frac{\partial}{\partial r_{12}}$, $\quad\hat{\boldsymbol{X}}_1^{11} = \hat{\boldsymbol{Y}} + \frac{3r_1^2+r_2^2-r_{12}^2}{r_1^2 r_{12}}\frac{\partial}{\partial r_{12}}$,
$\hat{\boldsymbol{X}}_1^{22} = \hat{\boldsymbol{Y}} + \frac{4r_1^2+2r_2^2-2r_{12}^2}{r_1^2 r_{12}}\frac{\partial}{\partial r_{12}}$,
where $\hat{\boldsymbol{Y}} = \frac{\partial^2}{\partial r_1^2} + \frac{2}{r_1}\frac{\partial}{\partial r_1} + \frac{\partial^2}{\partial r_{12}^2} + \frac{r_{12}^2+r_1^2-r_2^2}{r_1 r_{12}}\frac{\partial^2}{\partial r_1 \partial r_{12}}$.
The off-diagonal operators
For P^o states $L = l_1 + l_2 = 1$ and D^o states $L = l_1 + l_2 - 1 = 2$:
$\hat{\boldsymbol{X}}_1^{01} = \hat{\boldsymbol{X}}_1^{12} = -2\frac{r_2}{r_1 r_{12}}\frac{\partial}{\partial r_{12}}$,
For D^e states $L = l_1 + l_2 = 2$:
$\hat{\boldsymbol{X}}_1^{01} = -2\sqrt{\frac{6}{5}}\frac{r_2}{r_1 r_{12}}\frac{\partial}{\partial r_{12}}$, $\quad\hat{\boldsymbol{X}}_1^{12} = -2\sqrt{\frac{10}{3}}\frac{r_2}{r_1 r_{12}}\frac{\partial}{\partial r_{12}}$.

5.2. *The equation for P^e states*

This is the case considered by Breit [2] ($L = 1$, even parity). It can be identified by $L = l_1 + l_2 - 1$, $l_1 = l_2 = 1$ and $d = L = 1$. Then, in this case we have one antisymmetric generator function Ω^P_{11}.

For Ω^P_{11} the angular operator (3) (see table 1 for details) leads to the following expression:

$$\triangle_i \Phi^P_{11}(r_1, r_2, r_{12})\Omega^P_{11} = \left\{\hat{\boldsymbol{X}}_i^{11}\, \Phi^P_{11}(r_1, r_2, r_{12})\right\}\Omega^P_{11},$$

where $\hat{\boldsymbol{X}}_1^{11}$, $\hat{\boldsymbol{X}}_2^{11}$ are given in table 2. Schrödinger equation (9) takes the same form as in the previous case:

$$\left[\frac{(-1)}{2m_1}\hat{\boldsymbol{X}}_1^{11} + \frac{(-1)}{2m_2}\hat{\boldsymbol{X}}_2^{11} + V - E\right]\Phi^P_{11}(r_1, r_2, r_{12}) = 0. \tag{24}$$

The wavefunction is given by

$$\Psi^P_e(\boldsymbol{r}_1, \boldsymbol{r}_2) = \Phi^P_{11}(r_1, r_2, r_{12})\, \Omega^P_{11}, \tag{25}$$

where for identical particles the radial part Φ_{11}^P has to be either symmetric or antisymmetric in r_1, r_2.

5.3. The equation for P^o states

This is the second case considered by Breit [2] ($L = 1$, odd parity). The values l_1 and l_2 are confined by $L = l_1 + l_2 = 1$. There are two generator functions in this case ($d = L + 1 = 2$): Ω_{01}^P and Ω_{10}^P, for $l_1 = 0, l_2 = 1$ and for $l_1 = 1, l_2 = 0$, respectively. Each of them is neither symmetric nor antisymmetric. The relation between them

$$\Omega_{10}^P(\hat{\boldsymbol{r}}_1, \hat{\boldsymbol{r}}_2) = \Omega_{01}^P(\hat{\boldsymbol{r}}_2, \hat{\boldsymbol{r}}_1), \tag{26}$$

is independent of M. The wavefunction for any P^o state can be written in the form

$$\Psi_o^P = \Phi_{01}^P(r_1, r_2, r_{12})\, \Omega_{01}^P + \Phi_{10}^P(r_1, r_2, r_{12})\, \Omega_{10}^P. \tag{27}$$

For both generators the angular operators Λ_1, Λ_2 (3) are given in table 1 and

$$\Delta_1\left(\Phi_{01}^P\, \Omega_{01}^P\right) = \left\{\hat{\boldsymbol{X}}_1^{00}\Phi_{01}^P\right\}\Omega_{01}^P,$$

$$\Delta_1\left(\Phi_{10}^P\, \Omega_{10}^P\right) = \left\{\hat{\boldsymbol{X}}_1^{11}\Phi_{10}^P\right\}\Omega_{10}^P + \left\{\hat{\boldsymbol{X}}_1^{01}\Phi_{10}^P\right\}\Omega_{01}^P.$$

Similarly for the second particle

$$\Delta_2\left(\Phi_{10}^P\, \Omega_{10}^P\right) = \left\{\hat{\boldsymbol{X}}_2^{00}\Phi_{10}^P\right\}\Omega_{10}^P,$$

$$\Delta_2\left(\Phi_{01}^P\, \Omega_{01}^P\right) = \left\{\hat{\boldsymbol{X}}_2^{11}\Phi_{01}^P\right\}\Omega_{01}^P + \left\{\hat{\boldsymbol{X}}_2^{01}\Phi_{01}^P\right\}\Omega_{10}^P,$$

where the operators $\hat{\boldsymbol{X}}_i^{00}, \hat{\boldsymbol{X}}_i^{11}, \hat{\boldsymbol{X}}_i^{01}$ are given in table 2. Schrödinger equation (9) transforms to the following pair of coupled equations:

$$\begin{aligned}
&\left(\frac{(-1)}{2m_1}\hat{\boldsymbol{X}}_1^{00} + \frac{(-1)}{2m_2}\hat{\boldsymbol{X}}_2^{11} + V - E\right)\Phi_{01}^P + \frac{(-1)}{2m_1}\hat{\boldsymbol{X}}_1^{01}\Phi_{10}^P = 0,\\
&\frac{(-1)}{2m_2}\hat{\boldsymbol{X}}_2^{01}\Phi_{01}^P + \left(\frac{(-1)}{2m_1}\hat{\boldsymbol{X}}_1^{11} + \frac{(-1)}{2m_2}\hat{\boldsymbol{X}}_2^{00} + V - E\right)\Phi_{10}^P = 0,
\end{aligned} \tag{28}$$

where the first equation is associated with Ω_{01}^P and the second one with Ω_{10}^P. For identical particles, due to (26), the symmetric or antisymmetric wavefunction can be obtained if the radial functions, Φ_{01}^P and Φ_{10}^P, are linked by the relation

$$\Phi_{10}^P(r_1, r_2, r_{12}) = \pm\Phi_{01}^P(r_2, r_1, r_{12}). \tag{29}$$

In the case of a symmetric or antisymmetric wavefunction the symmetrized form of equation (28) may be more convenient. To this end let us transform the generator functions Ω_{01}^P, Ω_{10}^P as follows (cf [15]):

$$\Omega^A \equiv \tfrac{1}{\sqrt{2}}\left(\Omega_{01}^P - \Omega_{10}^P\right), \tag{30}$$

$$\Omega^S \equiv \tfrac{1}{\sqrt{2}}\left(\Omega_{01}^P + \Omega_{10}^P\right), \tag{31}$$

where Ω^A is antisymmetric and Ω^S is symmetric. Then, the symmetric or antisymmetric wavefunction, Ψ_+^P or Ψ_-^P respectively, is

$$\Psi_\pm^P = \Phi_\pm^P\Omega^S + \Phi_\mp^P\Omega^A, \tag{32}$$

when Φ_+^P is symmetric and Φ_-^P is antisymmetric radial function. The pair of equations (28) in the new representation reads:

$$\left(\frac{(-1)}{2m_1}\hat{\boldsymbol{T}}_1^{S+} + \frac{(-1)}{2m_2}\hat{\boldsymbol{T}}_2^{S+} + V - E\right)\Phi_+^P + \left(\frac{(-1)}{2m_2}\hat{\boldsymbol{T}}_2^{A+} - \frac{(-1)}{2m_1}\hat{\boldsymbol{T}}_1^{A+}\right)\Phi_-^P = 0,$$
$$\left(\frac{(-1)}{2m_2}\hat{\boldsymbol{T}}_2^{A-} - \frac{(-1)}{2m_1}\hat{\boldsymbol{T}}_1^{A-}\right)\Phi_+^P + \left(\frac{(-1)}{2m_1}\hat{\boldsymbol{T}}_1^{S-} + \frac{(-1)}{2m_2}\hat{\boldsymbol{T}}_2^{S-} + V - E\right)\Phi_-^P = 0, \tag{33}$$

where

$$\hat{\boldsymbol{T}}_i^{S\pm} \equiv \tfrac{1}{2}\big(\hat{\boldsymbol{X}}_i^{00} + \hat{\boldsymbol{X}}_i^{11} \pm \hat{\boldsymbol{X}}_i^{01}\big), \qquad \hat{\boldsymbol{T}}_i^{A\pm} \equiv \tfrac{1}{2}\big(-\hat{\boldsymbol{X}}_i^{00} + \hat{\boldsymbol{X}}_i^{11} \pm \hat{\boldsymbol{X}}_i^{01}\big),$$

or, in the explicit form,

$$\hat{\boldsymbol{T}}_i^{S\pm} = \frac{\partial^2}{\partial r_i^2} + \frac{2}{r_i}\frac{\partial}{\partial r_i} + \frac{\partial^2}{\partial r_{12}^2} + \left[\frac{2}{r_{12}} + \frac{(r_1 \mp r_2)^2 - r_{12}^2}{2r_i^2 r_{12}}\right]\frac{\partial}{\partial r_{12}} + \frac{r_{12}^2 + r_i^2 - r_{\hat{i}}^2}{r_i r_{12}}\frac{\partial^2}{\partial r_i \partial r_{12}} - \frac{1}{r_i^2},$$
$$\hat{\boldsymbol{T}}_i^{A\pm} = \frac{-1}{r_i^2}\left[1 + \frac{r_{12}^2 - (r_1 \mp r_2)^2}{2r_{12}}\frac{\partial}{\partial r_{12}}\right].$$

The first equation (33) is the radial coefficient associated with Ω^S and the second one is associated with Ω^A. Thus, solutions of equations (33) give symmetric, Φ_+^P, and antisymmetric, Φ_-^P, coefficients of the symmetric wavefunction Ψ_+^P (27). In the case of the antisymmetric wavefunction Ψ_-^P, the coefficients Φ_+^P and Φ_-^P should be interchanged in equations (33).

5.4. *The equation for D^o states*

This is the case with two generators ($d = L = 2$) for which $l_1 = 1, l_2 = 2$ and $l_1 = 2, l_2 = 1$. The wavefunction can be expressed as

$$\Psi_o^D = \Phi_{12}^D(r_1, r_2, r_{12})\Omega_{12}^D + \Phi_{21}^D(r_1, r_2, r_{12})\Omega_{21}^D, \tag{34}$$

where the generator functions Ω_{21}^D, Ω_{12}^D are linked by the relation

$$\Omega_{21}^D(\hat{\boldsymbol{r}}_1, \hat{\boldsymbol{r}}_2) = -\Omega_{12}^D(\hat{\boldsymbol{r}}_2, \hat{\boldsymbol{r}}_1). \tag{35}$$

The angular operators Λ_1 and Λ_2 (3) are given in table 1. For the first particle

$$\triangle_1\Phi_{12}^D\Omega_{12}^D = \big\{\hat{\boldsymbol{X}}_1^{11}\Phi_{12}^D\big\}\Omega_{12}^D,$$
$$\triangle_1\Phi_{21}^D\Omega_{21}^D = \big\{\hat{\boldsymbol{X}}_1^{22}\Phi_{21}^D\big\}\Omega_{21}^D + \big\{\hat{\boldsymbol{X}}_1^{12}\Phi_{21}^D\big\}\Omega_{12}^D,$$

and for the second particle

$$\triangle_2\Phi_{21}^D\Omega_{21}^D = \big\{\hat{\boldsymbol{X}}_2^{11}\Phi_{21}^D\big\}\Omega_{21}^D,$$
$$\triangle_2\Phi_{12}^D\Omega_{12}^D = \big\{\hat{\boldsymbol{X}}_2^{22}\Phi_{12}^D\big\}\Omega_{12}^D + \big\{\hat{\boldsymbol{X}}_2^{12}\Phi_{12}^D\big\}\Omega_{21}^D.$$

The explicit forms of $\hat{\boldsymbol{X}}_i^{11}$, $\hat{\boldsymbol{X}}_i^{22}$ and $\hat{\boldsymbol{X}}_i^{12}$ are given in table 2. The Schrödinger equation reduces to the pair of equations

$$\left(\frac{(-1)}{2m_1}\hat{\boldsymbol{X}}_1^{11} + \frac{(-1)}{2m_2}\hat{\boldsymbol{X}}_2^{22} + V - E\right)\Phi_{12}^D + \frac{(-1)}{2m_1}\hat{\boldsymbol{X}}_1^{12}\Phi_{21}^D = 0,$$
$$\frac{(-1)}{2m_2}\hat{\boldsymbol{X}}_2^{12}\Phi_{12}^D + \left(\frac{(-1)}{2m_1}\hat{\boldsymbol{X}}_1^{22} + \frac{(-1)}{2m_2}\hat{\boldsymbol{X}}_2^{11} + V - E\right)\Phi_{21}^D = 0, \tag{36}$$

where the first/second equation results from the coefficient associated with $\Omega_{12}^D/\Omega_{21}^D$.

In the case of identical particles, the symmetric or antisymmetric wavefunctions (34) are obtained when

$$\Phi_{21}^{D}(r_1, r_2, r_{12}) = \mp\Phi_{12}^{D}(r_2, r_1, r_{12}). \tag{37}$$

We can also transform equation (36) to the symmetrized form, where antisymmetric Ω^A and symmetric Ω^S angular functions are defined as

$$\Omega^A \equiv \tfrac{1}{\sqrt{2}}\left(\Omega_{12}^{D} + \Omega_{21}^{D}\right), \tag{38}$$

$$\Omega^S \equiv \tfrac{1}{\sqrt{2}}\left(\Omega_{12}^{D} - \Omega_{21}^{D}\right). \tag{39}$$

The symmetric wavefunction, Ψ_+^D, or antisymmetric one, Ψ_-^D, reads

$$\Psi_\pm^D = \Phi_\pm^D \Omega^S + \Phi_\mp^D \Omega^A, \tag{40}$$

when Φ_+^D is symmetric and Φ_-^D is antisymmetric radial function. In the case of a symmetric wavefunction, Ψ_+^D, equations (36) transform to the symmetrized form

$$\begin{aligned}
&\left(\frac{(-1)}{2m_1}\hat{\boldsymbol{T}}_1^{S-} + \frac{(-1)}{2m_2}\hat{\boldsymbol{T}}_2^{S-} + V - E\right)\Phi_+^D + \left(\frac{(-1)}{2m_1}\hat{\boldsymbol{T}}_1^{A+} - \frac{(-1)}{2m_2}\hat{\boldsymbol{T}}_2^{A+}\right)\Phi_-^D = 0,\\
&\left(\frac{(-1)}{2m_1}\hat{\boldsymbol{T}}_1^{A-} - \frac{(-1)}{2m_2}\hat{\boldsymbol{T}}_2^{A-}\right)\Phi_+^D + \left(\frac{(-1)}{2m_1}\hat{\boldsymbol{T}}_1^{S+} + \frac{(-1)}{2m_2}\hat{\boldsymbol{T}}_2^{S+} + V - E\right)\Phi_-^D = 0,
\end{aligned} \tag{41}$$

where

$$\hat{\boldsymbol{T}}_i^{S\pm} = \tfrac{1}{2}\left(\hat{\boldsymbol{X}}_i^{11} + \hat{\boldsymbol{X}}_i^{22} \pm \hat{\boldsymbol{X}}_i^{12}\right),$$

$$\hat{\boldsymbol{T}}_i^{A\pm} = \tfrac{1}{2}\left(\hat{\boldsymbol{X}}_i^{11} - \hat{\boldsymbol{X}}_i^{22} \pm \hat{\boldsymbol{X}}_i^{12}\right).$$

In the explicit form

$$\hat{\boldsymbol{T}}_i^{S\pm} = \frac{\partial^2}{\partial r_i^2} + \frac{2}{r_i}\frac{\partial}{\partial r_i} + \frac{\partial^2}{\partial r_{12}^2} + \frac{7r_i^2 + 3r_{\hat{i}}^2 \mp 2r_1r_2 - 3r_{12}^2}{2r_i^2 r_{12}}\frac{\partial}{\partial r_{12}} + \frac{r_i^2 - r_{\hat{i}}^2 + r_{12}^2}{r_i r_{12}}\frac{\partial^2}{\partial r_i \partial r_{12}} - \frac{4}{r_i^2},$$

$$\hat{\boldsymbol{T}}_i^{A\pm} = \frac{1}{r_i^2}\left[2 + \frac{r_{12}^2 - (r_1 \pm r_2)^2}{2r_{12}}\frac{\partial}{\partial r_{12}}\right].$$

In the case of an antisymmetric wavefunction, Ψ_-^D, in the pair of equations (41) the radial functions Φ_+^D, Φ_-^D are interchanged. Let us note that the first equation (41) is associated with the expansion coefficient Ω^S and the second one with Ω^A.

5.5. The equation for D^e states

This is the even parity $L = 2$ state. There are three $(d = L + 1 = 3)$ generator functions Ω_{02}^D, Ω_{20}^D and Ω_{11}^D determined by $l_1 = 0, l_2 = 2$; $l_1 = 2, l_2 = 0$; and $l_1 = l_2 = 1$, respectively. The wavefunction may be expressed as

$$\Psi_e^D = \Phi_{02}^D(r_1, r_2, r_{12})\Omega_{02}^D + \Phi_{20}^D(r_1, r_2, r_{12})\Omega_{20}^D + \Phi_{11}^D(r_1, r_2, r_{12})\Omega_{11}^D \tag{42}$$

and the generator functions fulfil the symmetry identities:

$$\Omega_{20}^D(\hat{\boldsymbol{r}}_1, \hat{\boldsymbol{r}}_2) = \Omega_{02}^D(\hat{\boldsymbol{r}}_2, \hat{\boldsymbol{r}}_1), \tag{43}$$

$$\Omega_{11}^D(\hat{\boldsymbol{r}}_1, \hat{\boldsymbol{r}}_2) = \Omega_{11}^D(\hat{\boldsymbol{r}}_2, \hat{\boldsymbol{r}}_1). \tag{44}$$

Then for Ψ_e^D symmetric Φ_{11}^D has to be symmetric and

$$\Phi_{20}^D(r_1, r_2, r_{12}) = +\Phi_{02}^D(r_2, r_1, r_{12}).$$

In the case of Ψ_e^D antisymmetric Φ_{11}^D must be antisymmetric and

$$\Phi_{20}^D(r_1, r_2, r_{12}) = -\Phi_{02}^D(r_2, r_1, r_{12}).$$

The following relations may be easily obtained:

$$\begin{aligned}
\triangle_1 \Phi_{02}^D \Omega_{02}^D &= \{\hat{\boldsymbol{X}}_1^{00} \Phi_{02}^D\} \Omega_{02}^D, \\
\triangle_1 \Phi_{20}^D \Omega_{20}^D &= \{\hat{\boldsymbol{X}}_1^{22} \Phi_{20}^D\} \Omega_{20}^D + \{\hat{\boldsymbol{X}}_1^{12} \Phi_{20}^D\} \Omega_{11}^D, \\
\triangle_1 \Phi_{11}^D \Omega_{11}^D &= \{\hat{\boldsymbol{X}}_1^{11} \Phi_{11}^D\} \Omega_{11}^D + \{\hat{\boldsymbol{X}}_1^{01} \Phi_{11}^D\} \Omega_{02}^D, \\
\triangle_2 \Phi_{20}^D \Omega_{20}^D &= \{\hat{\boldsymbol{X}}_2^{00} \Phi_{20}^D\} \Omega_{20}^D, \\
\triangle_2 \Phi_{02}^D \Omega_{02}^D &= \{\hat{\boldsymbol{X}}_2^{22} \Phi_{02}^D\} \Omega_{02}^D + \{\hat{\boldsymbol{X}}_2^{12} \Phi_{02}^D\} \Omega_{11}^D, \\
\triangle_2 \Phi_{11}^D \Omega_{11}^D &= \{\hat{\boldsymbol{X}}_2^{11} \Phi_{11}^D\} \Omega_{11}^D + \{\hat{\boldsymbol{X}}_2^{01} \Phi_{11}^D\} \Omega_{20}^D.
\end{aligned}$$

The explicit forms of operators $\hat{\boldsymbol{X}}_i^{00}, \hat{\boldsymbol{X}}_i^{11}, \hat{\boldsymbol{X}}_i^{22}, \hat{\boldsymbol{X}}_i^{01}, \hat{\boldsymbol{X}}_i^{12}$, as well as Λ_1, Λ_2 are given in tables 1 and 2. Finally, the Schrödinger equation reduces to three coupled equations:

$$\begin{aligned}
&\left(\frac{(-1)}{2m_1}\hat{\boldsymbol{X}}_1^{00} + \frac{(-1)}{2m_2}\hat{\boldsymbol{X}}_2^{22} + V - E\right)\Phi_{02}^D + \frac{(-1)}{2m_1}\hat{\boldsymbol{X}}_1^{01}\Phi_{11}^D = 0, \\
&\frac{(-1)}{2m_2}\hat{\boldsymbol{X}}_2^{12}\Phi_{02}^D + \left(\frac{(-1)}{2m_1}\hat{\boldsymbol{X}}_1^{11} + \frac{(-1)}{2m_2}\hat{\boldsymbol{X}}_2^{11} + V - E\right)\Phi_{11}^D + \frac{(-1)}{2m_1}\hat{\boldsymbol{X}}_1^{12}\Phi_{20}^D = 0, \\
&\frac{(-1)}{2m_2}\hat{\boldsymbol{X}}_2^{01}\Phi_{11}^D + \left(\frac{(-1)}{2m_1}\hat{\boldsymbol{X}}_1^{22} + \frac{(-1)}{2m_2}\hat{\boldsymbol{X}}_2^{00} + V - E\right)\Phi_{20}^D = 0,
\end{aligned} \tag{45}$$

where the first equation is associated with Ω_{02}^D, the second one with Ω_{20}^D and the third one with Ω_{11}^D.

In order to derive the symmetric form of equations (45) it is convenient to introduce a new basis of the generator functions

$$\Omega^A \equiv \tfrac{1}{\sqrt{2}}\left(\Omega^{02} - \Omega^{20}\right), \tag{46}$$

$$\Omega^S \equiv \tfrac{1}{\sqrt{2}}\left(\Omega^{02} + \Omega^{20}\right), \tag{47}$$

$$\Omega^{11} \equiv \Omega^{11}, \tag{48}$$

where Ω^A is antisymmetric and Ω^S, Ω^{11} are symmetric. If we introduce

$$\Psi_\pm^D = \Phi_\pm^D \Omega^S + \Phi_\mp^D \Omega^A + \Phi_{11}^D \Omega^{11}, \tag{49}$$

then for Φ_+^D symmetric and Φ_-^D antisymmetric, Ψ_+^D is symmetric when Φ_{11}^D is symmetric, and Ψ_-^D is antisymmetric when Φ_{11}^D is antisymmetric. Finally, we obtain the symmetrized form of equations (45)

$$\begin{aligned}
&\left[\frac{(-1)}{2m_1}\hat{\boldsymbol{T}}_1^S + \frac{(-1)}{2m_2}\hat{\boldsymbol{T}}_2^S + (V - E)\right]\Phi_+^D + \left[\frac{(-1)}{2m_1}\hat{\boldsymbol{T}}_1^A - \frac{(-1)}{2m_2}\hat{\boldsymbol{T}}_2^A\right]\Phi_-^D \\
&\quad + \frac{1}{\sqrt{2}}\left(\frac{(-1)}{2m_1}\hat{\boldsymbol{X}}_1^{01} + \frac{(-1)}{2m_2}\hat{\boldsymbol{X}}_2^{01}\right)\Phi_{11}^D = 0,
\end{aligned}$$

$$
\begin{aligned}
&\left[\frac{(-1)}{2m_1}\hat{\boldsymbol{T}}_1^A - \frac{(-1)}{2m_2}\hat{\boldsymbol{T}}_2^A\right]\Phi_+^D + \left[\frac{(-1)}{2m_1}\hat{\boldsymbol{T}}_1^S + \frac{(-1)}{2m_2}\hat{\boldsymbol{T}}_2^S + (V-E)\right]\Phi_-^D \\
&\qquad + \frac{1}{\sqrt{2}}\left(\frac{(-1)}{2m_1}\hat{\boldsymbol{X}}_1^{01} - \frac{(-1)}{2m_2}\hat{\boldsymbol{X}}_2^{01}\right)\Phi_{11}^D = 0, \\
&\frac{1}{\sqrt{2}}\left(\frac{(-1)}{2m_1}\hat{\boldsymbol{X}}_1^{12} + \frac{(-1)}{2m_2}\hat{\boldsymbol{X}}_2^{12}\right)\Phi_+^D + \frac{1}{\sqrt{2}}\left(\frac{(-1)}{2m_2}\hat{\boldsymbol{X}}_2^{12} - \frac{(-1)}{2m_1}\hat{\boldsymbol{X}}_1^{12}\right)\Phi_-^D \\
&\qquad + \left(\frac{(-1)}{2m_1}\hat{\boldsymbol{X}}_1^{11} + \frac{(-1)}{2m_2}\hat{\boldsymbol{X}}_2^{11} + (V-E)\right)\Phi_{11}^D = 0,
\end{aligned}
\tag{50}
$$

where

$$\hat{\boldsymbol{T}}_i^S = \tfrac{1}{2}\left(\hat{\boldsymbol{X}}_i^{00} + \hat{\boldsymbol{X}}_i^{22}\right), \qquad \hat{\boldsymbol{T}}_i^A = \tfrac{1}{2}\left(\hat{\boldsymbol{X}}_i^{00} - \hat{\boldsymbol{X}}_i^{22}\right).$$

In explicit form:

$$
\begin{aligned}
\hat{\boldsymbol{T}}_i^S &= \frac{\partial^2}{\partial r_i^2} + \frac{2}{r_i}\frac{\partial}{\partial r_i} + \frac{\partial^2}{\partial r_{12}^2} + \frac{3r_i^2 + r_{\hat{i}}^2 - r_{12}^2}{r_i^2 r_{12}}\frac{\partial}{\partial r_{12}} + \frac{r_i^2 - r_{\hat{i}}^2 + r_{12}^2}{r_i r_{12}}\frac{\partial^2}{\partial r_i \partial r_{12}} - \frac{3}{r_i^2}, \\
\hat{\boldsymbol{T}}_i^A &= \frac{1}{r_i^2}\left[3 + \frac{r_{12}^2 - r_1^2 - r_2^2}{r_{12}}\frac{\partial}{\partial r_{12}}\right].
\end{aligned}
$$

The first equation (50) is associated with Ω^S, the second one with Ω^A and the third one with Ω^{11}. With symmetric Φ_+^D and antisymmetric Φ_-^D, equations (50) determine a symmetric wavefunction Ψ_+^D if Φ_{11}^D is symmetric. If Φ_{11}^D is antisymmetric and functions Φ_+^D, Φ_-^D in equations (50) are interchanged then the resulting wavefunction, Ψ_-^D, is antisymmetric.

6. Final remarks

A simple form of the Schrödinger equation reduced to the triangle variables in a general case of two interacting particles confined in an external spherical potential. All equations are expressed in a simple, explicit form. The resulting formalism may be helpful in the extension of both theoretical and computational approaches developed for helium-like atoms (see e.g. [3–6]) to arbitrary two-particle spherically symmetric systems. It can be especially useful in non-variational approaches where the explicit form of the differential equations has to be known (e.g. in the iterative methods of solving Schödinger equation developed by Nakatsuji *et al* [17–19]). Apart from a straightforward application the obtained results for a determination of the relativistic corrections containing $\boldsymbol{p}^4$ terms, one can extend the equations for the description of three particle systems by including the mass-polarization term proportional to $\nabla_1\nabla_2$.

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