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Hyperspherical harmonics approach to the trinucleon system with Reid soft core potential: Calculation of geometrical structure coefficients

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Abstract. We present the full set of equations for the solution of the trinucleon problem by the hyperspherical harmonics expansion (HHE) method where nucleons interact via the Reid soft core (RSC) potential. The coupling potential matrix elements are expressed in terms of geometrical structure coefficients (GSC) and potential multipoles (PM). Introduction of GSC greatly simplifies the calculation of the potential matrix and makes the numerical algorithm efficient. A method for calculating all the twelve independent sets of GSC needed, by using the completeness property of the Jacobi polynomials has been presented. A convenient sum rule for each set of GSC has also been derived and precision of the calculated GSC has been checked by the sum rule. Such calculations of GSC are efficient and fast, in view of the complexity of the HHE equations.

Keywords. Nuclear structure; few-body problem; hyperspherical harmonics expansion method; geometrical structure coefficients; Reid soft core potential.

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1. Introduction

The hyperspherical harmonics expansion (HHE) method is a powerful tool for the few body problem and has been in use for over two decades for the solution of the trinucleon problem, though with simple potentials only [1–6]. One of the most important and commonly used realistic two nucleon potentials is the Reid soft core (RSC) potential [7], where the interaction potential of a pair of nucleons depends on the isospin (t), spin (s) and total angular momentum (j) of the pair. This makes the potential rather inconvenient to use with the HHE method. Hence a complete solution of the trinucleon bound state with RSC potential by the HHE method has not been attempted during the last two decades, while sophisticated Faddeev calculations with the RSC potential have been reported by several authors [8–11] since the seventies. Since the HHE approach gives a clear physical picture of the few body system and its wave function, it is of interest to solve the trinucleon RSC problem by the HHE method also. This is in addition to the inherent interest in solving the extremely involved set of equations in this case. Furthermore, preliminary studies by Ghosh and Das [12] with simple potentials have indicated that the asymptotic behaviour of the wave function obtained by HHE method may not be reliable. However, the asymptotic wave function is strongly influenced by the model

potentials considered by them; none of the potentials had the required one pion exchange two nucleon potential tail. Thus to investigate this aspect properly and to compare the calculated asymptotic normalization constants with the experimental values it is essential to solve the HHE trinuclear equations with the RSC potential.

In the present work, we obtain the full set of HHE equations for the bound trinucleon system interacting via RSC potential. A straightforward numerical calculation of all the coupling potential matrix elements would be difficult and slow even in a powerful computer. We expand each component of the interaction potential $V(r_{12})$ for the (12) pair in a complete set of Jacobi polynomials and express the coupling potential matrix element as a sum of products of potential multipoles (PM) and geometrical structure coefficients (GSC), the latter being independent of the interaction but dependent on the state of the interacting nucleon pair. We have identified 12 independent sets of GSC needed for the full calculation. Each of these 12 sets of GSC has been calculated by linear inhomogeneous equation (LIE) method [13, 14] which utilizes the completeness property of the Jacobi polynomials. A convenient sum rule for each set of GSC has also been derived. Precision of the calculated GSC has been checked by comparing the appropriately weighted sum of calculated GSC with the sum rule. This method of calculation of the GSC is very fast compared to a straightforward numerical integration and high precision can be achieved easily, while numerical integrations become inaccurate for large k-values.

In § 2, we present the HHE equation for the trinucleon RSC problem, obtain all the components of RSC potential and identify 12 independent sets of coupling potential matrix elements (CPME). In § 3, each CPME is expressed in terms of the GSC and PM, and linear inhomogeneous equations have been set up to calculate the GSC. We present a comparison of the calculated and theoretical values of the sum rules for the GSC. To emphasize the speed of calculation and accuracy of the LIE method relative to those of the direct integration method, we compare the CPU time and precision in both cases.

2. HHE equations for the bound trinucleon system with RSC potential

The Jacobi coordinates for the three-body systems are

$$\mathbf{x} = \mathbf{r}_2 - \mathbf{r}_1$$
$$\mathbf{y} = \frac{2}{\sqrt{3}}\left[\mathbf{r}_3 - \frac{\mathbf{r}_1 + \mathbf{r}_2}{2}\right] \tag{1}$$

where $\mathbf{r}_i$ is the position of the ith nucleon. We define a hyperradius

$$r = (x^2 + y^2)^{1/2} \tag{2}$$

which is invariant under all permutations of particles and under three dimensional rotations. Five hyper angles (denoted collectively by Ω) consisting of the orientations of $\mathbf{x}$ and $\mathbf{y}$ (namely θ_x, ϕ_x and θ_y, ϕ_y respectively) and a fifth defined through

$$\phi = \tan^{-1}\left(\frac{y}{x}\right) \tag{3}$$

complete the full set of six hyperspherical coordinates. The wave function is expanded

in the complete set of hyperspherical harmonics [6] as

$$\psi_{JM_J}(\mathbf{x},\mathbf{y}) = \sum_{k\varepsilon TS} N(\varepsilon) r^{-5/2} u^{\varepsilon TS}_{2k+l}(r) \cdot [\Gamma_{TS}(\varepsilon^*) \otimes^{(\varepsilon)} B_{2k+l}(\Omega)]_{JM_J} \tag{4}$$

where $[\Gamma_{TS}(\varepsilon^*) \otimes^{(\varepsilon)} B_{2k+l}(\Omega)]_{JM_J}$ represents angular momentum coupling and

$$N(\varepsilon) = 1 \text{ for } S \text{ state},$$

$$= \frac{1}{\sqrt{2}} \quad \text{for } S'^{+},\ D^{+} \text{ and } D^{-} \text{ states},$$

$$= -\frac{1}{\sqrt{2}} \quad \text{for } S'^{-} \text{ state},$$

for the dominant symmetry components of the trinucleon wave function. $\Gamma_{TS}(\varepsilon)$ is the isospin-spin state of three particle system with total isospin T and total spin S and specified symmetry (ε) under exchange of particles,

$$\Gamma^{M_T M_S}_{TS}(\varepsilon) = \sum_{st} b^t_s(\varepsilon) |(s\tfrac{1}{2}) S M_S\rangle |(t\tfrac{1}{2}) T M_T\rangle \tag{5}$$

Here s, t are the spin and isospin of the (12) pair. The coefficients $b^t_s(\varepsilon)$ as well as the expression for the orthonormalized elements of the optimal subset $(\varepsilon)B^M_{2k+}(\Omega)$ are given by Ballot and Fabre [6].

We include the factor $N(\varepsilon)$ to accommodate factors ρ_{TS} of their equation (III.41) and a factor $1/\sqrt{2}$ in their equation (III.44). Note that the isospin-spin wave-function $\Gamma_{TS}(\varepsilon^*)$ must have a symmetry complementary (ε^*) to that of the spatial wave function ${}^{(\varepsilon)}B_{2k+l}(\Omega)$, so that ψ_{JM_J} is totally antisymmetric. The quantity l is zero for potentials which are central in nature and 2 for the tensor potential.

The ground state of the trinucleon has dominant contribution from a space totally symmetric $S(L=0)$ state, mixed symmetry $S'(L=0)$ and $D(L=2)$ states. The components of S' and D whose spatial parts are even (odd) under P_{12} are denoted by $S'^{+}(S'^{-})$ and $D^{+}(D^{-})$, respectively. Each symmetry component of the total wave function is characterized by specified values of T and S and symmetry (ε) of the spatial part under particle exchange ($\varepsilon = 0$ for space totally symmetric and $+(-)$ for symmetric (antisymmetric) under P_{12}).

Substitution of (4) into the Schrödinger equation and projection on a particular symmetry component leads to a set of coupled differential eigenvalue (CDE) equations:

$$\left\{-\frac{\hbar^2}{m}\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{(2k+l+2)^2 - 1/4}{r^2}\right] - E\right\} u^{TS}_{2k+l}(r) + \sum_{k'\varepsilon'T'S'l'} N(\varepsilon) N(\varepsilon')$$

$$\times \left\langle [\Gamma_{TS}(\varepsilon^*) \otimes^{\varepsilon} B_{2k+l}(\Omega)]_{JM_J} \middle| \sum_{i>j} V(r_{ij}) \middle| [\Gamma_{TS}(\varepsilon') \otimes^{\varepsilon'} B_{2k'+l'}(\Omega)]_{JM_J} \right\rangle$$

$$u^{\varepsilon' T' S'}_{2k'+l'}(r) = 0 \tag{6}$$

In (6), $V(r_{ij})$ represents the interaction potential of the (ij) pair. Due to the complete antisymmetry of the full wave function, $\langle \Sigma_{i>j} V(r_{ij}) \rangle$ can be replaced by three times $\langle V(r_{12}) \rangle$. For the RSC potential $V(r_{12})$ depends on the isospin (t), spin (s) and total angular momentum (j) of the interacting (12) pair. To facilitate the calculation, we

express $[\Gamma_{TS}(\varepsilon^*)\otimes^{(\varepsilon)}B_{2k+l}(\Omega)]_{JM_J}$ in the j–j coupling scheme

$$[\Gamma_{TS}(\varepsilon^*)\otimes^{(\varepsilon)}B_{2k+l}(\Omega)]^{TM_T}_{JM_J} = {}^{(\varepsilon)}C_{2k+l}$$
$$\times \sum_{l_1,l_2,s,t} {}^{(\varepsilon)}F^{l_2l_1}_{2k+l}(\varphi)\,{}^{(2)}P^{l_2l_1}_{2k+l}(\phi)\,b^t_s(\varepsilon^*)|(t\tfrac{1}{2})\,TM_T\rangle|(l_1l_2)l;(s\tfrac{1}{2})S;JM_J\rangle$$
$$= {}^{(\varepsilon)}C_{2k+l} \sum_{l_1,l_2,s,t} {}^{(\varepsilon)}F^{l_2l_1}_{2k+l}(\varphi)\,{}^{(2)}P^{l_2l_1}_{2k+l}(\phi)\,b^t_s(\varepsilon^*)|(t\tfrac{1}{2})\,TM_T\rangle$$
$$\times \sum_{j_1,j_2} \begin{bmatrix} l_1 & l_2 & l \\ s & 1/2 & S \\ j_1 & j_2 & J \end{bmatrix} |(l_1 s)j_1,(l_2\tfrac{1}{2})j_2;JM_J\rangle \tag{7}$$

where the square array on the right side represents a 9-j symbol and other quantities have the same meaning as in [6].

2.1 *Reid soft core potential*

The RSC potential depends on the (tsj_1) of the interacting pair and only $j_1 \leqslant 2$ contribute where $\mathbf{j}_1 = \mathbf{l}_1 + \mathbf{s}, \mathbf{l}_1$ being the orbital angular momentum of (12) pair. Whenever only a single value of l_1 is allowed (by angular momentum selection and antisymmetry of the pair), the interaction is central (V_c). This is the case for $(tsj_1) = (001), (012), (100), (102), (110)$ and (111) corresponding to ${}^1P_1$, ${}^3D_2$, ${}^1S_0$, ${}^1D_2$, ${}^3P_0$ and ${}^3P_1$, respectively. On the other hand when more than one l_1 value contribute to the same (tsj_1), the interaction is a sum of central (V_c), spin orbit (V_{LS}) and tensor (V_T) terms. This happens for $(tsj_1) = (011)$ and (112) corresponding to $({}^3S_1 - {}^3D_1)$ and $({}^3P_2 - {}^3F_2)$, respectively.

The complete coupling matrix in (6) has contributions from S, S' and D components of the trinucleon ground state (the corresponding hyperradial wave functions are denoted by $u^{S,1/2,1/2}_{2k}(r)$, $u^{S',1/2,1/2}_{2k}(r)$ and $u^{D,1/2,3/2}_{2k+2}(r)$ respectively) and therefore has 9 sub-matrix blocks. Because of the symmetry of the full coupling matrix one has to calculate only (say) the upper triangular part. Each component of the RSC potential contributes to one or more of the sub-matrix blocks depending on the (tsj_1) values and the particular matrix element will have contribution from only one or two allowed l_1-values. In the following we enumerate the contribution of each of the component of the RSC potential. We will abbreviate the coupling matrix element of (6) for each component of RSC by $\langle \sigma,k|\, V^{(tsj_1)}|\sigma',k'\rangle$ where σ stands for $S,(S')^+,(S')^-,D^+$ and D^-.

(i) $\qquad V^{({}^1P_1)}, \quad (tsj_1) = (001).$

Since $V_{{}^1P_1}(r_{12})$ is central, it does not couple S and D trinucleon states. Furthermore $l_1 = 1$ (odd), hence only two $(S')^-$ states are coupled. Since $s = 0$, D states (which require $s = 1$) do not contribute. Substitution of these restricted values to (7) gives

$$\langle (S')^-,k|\, V^{({}^1P_1)}|(S')^-,k'\rangle = \tfrac{1}{4}({}^-)C_{2k}\,{}^-)C_{2k'}\,({}^-)F^{1,1}_{2k}(\varphi)\,({}^-)F^{1,1}_{2k'}(\varphi)$$
$$\times \langle {}^{(2)}P^{1,1}_{2k}|\, V^{(001)}_c(r_{12})|{}^{(2)}P^{1,1}_{2k'}\rangle \tag{8}$$

where

$$\langle {}^{(2)}P^{l_2l_1}_L|\, V^{(tsj_1)}(r_{12})|{}^{(2)}P^{l'_2l'_1}_{L'}\rangle$$
$$= \int_0^{\pi/2} {}^{(2)}P^{l_2l_1}_L(\phi)\; V^{(tsj_1)}(r\cos\phi)\,{}^{(2)}P^{l'_2l'_1}_{L'}(\phi)\sin^2\phi\cos^2\phi\,\mathrm{d}\phi \tag{9}$$

(ii) $V^{(^3D_2)}$, $(tsj_1) = (012)$.

Once again potential is central, $s = 1$, $l_1 = 2$. Couplings are possible between S and S, S and $(S')^+$, $(S')^+$ and $(S')^+$ and D^+ and D^+ states. These are given by (the numerical factors originate from 9-j symbols)

$$\langle S,k|\, V^{^3D_2}|S,k'\rangle = 0{\cdot}16767917^{(0)}C_{2k}{}^{(0)}C_{2k'}{}^{(0)}F^{2,2}_{2k}(\varphi)^{(0)}F^{2,2}_{2k'}(\varphi) \times \langle {}^{(2)}P^{2,2}_{2k}|\, V_c^{(012)}(r_{12})|{}^{(2)}P^{2,2}_{2k'}\rangle \tag{10}$$

$$\langle S,k|\, V_c^{^3D_2}|(S')^+,k'\rangle = -0{\cdot}11856708^{(0)}C_{2k}{}^{(+)}C_{2k'}{}^{(0)}F^{2,2}_{2k}(\varphi)^{(+)}F^{2,2}_{2k'}(\varphi) \times \langle {}^{(2)}P^{2,2}_{2k}|\, V_c^{(012)}(r_{12})|{}^{(2)}P^{2,2}_{2k'}\rangle \tag{11}$$

$$\langle (S')^+,k|\, V_c^{^3D_2}|(S')^+,k'\rangle = 0{\cdot}083839587^{(+)}C_{2k}{}^{(+)}C_{2k'}{}^{(+)}F^{2,2}_{2k}(\varphi)^{(+)}F^{2,2}_{2k'}(\varphi) \times \langle {}^{(2)}P^{2,2}_{2k}|\, V_c^{(012)}(r_{12})|{}^{(2)}P^{2,2}_{2k'}\rangle \tag{12}$$

$$\langle D^+,k|\, V_c^{^3D_2}|D^+,k'\rangle = 0{\cdot}41666655^{(D^+)}C_{2k+2}{}^{(D^+)}C_{2k'+2} \times {}^{(+)}F^{2,2}_{2k+2}(\varphi)^{(+)}F^{2,2}_{2k'+2}(\varphi)\langle {}^{(2)}P^{2,2}_{2k+2}|\, V_c^{(012)}(r_{12})|{}^{(2)}P^{2,2}_{2k'+2}\rangle \tag{13}$$

(iii) $V^{(^1S_0)}$, $(tsj_1) = (100)$.

Potential is central with $l_1 = 0$, $s = 0$, $j_1 = 0$. Hence couplings occur in the (S,S), $(S,(S')^+)$ and $(S')^+$, $(S')^+$ blocks:

$$\langle S,k|\, V^{^1S_0}|S,k'\rangle = 1/2^{(0)}C_{2k}{}^{(0)}C_{2k'}{}^{(0)}F^{0,0}_{2k}(\varphi)^{(0)}F^{0,0}_{2k'}(\varphi) \times \langle {}^{(2)}P^{0,0}_{2k}|\, V_c^{(100)}(r_{12}|{}^{(2)}P^{0,0}_{2k'}\rangle \tag{14}$$

$$\langle S,k|\, V^{^1S_0}|(S')^+,k'\rangle = \frac{1}{2\sqrt{2}}{}^{(0)}C_{2k}{}^{(+)}C_{2k'}{}^{(0)}F^{0,0}_{2k}(\varphi)^{(+)}F^{0,0}_{2k'}(\varphi) \times \langle {}^{(2)}P^{0,0}_{2k}(\phi)|\, V_c^{(100)}(r_{12})|{}^{(2)}P^{0,0}_{2k'}(\phi)\rangle \tag{15}$$

$$\langle (S')^+,k|\, V^{^1S_0}|(S')^+,k'\rangle = \tfrac{1}{4}{}^{(+)}C_{2k}{}^{(+)}C_{2k'}{}^{(+)}F^{0,0}_{2k}(\varphi)^{(+)}F^{0,0}_{2k'}(\varphi) \times \langle {}^{(2)}P^{0,0}_{2k}|\, V_c^{(100)}(r_{12})|{}^{(2)}P^{0,0}_{2k'}\rangle \tag{16}$$

(iv) $V^{(^1D_2)}$ $(tsj_1) = (102)$.

Potential is central with $l_1 = 2$, $s = 0$, $j_1 = 2$. Couplings are possible in the (S,S), $(S,(S')^+)$, $(S')^+$, $(S')^+$) blocks, there are no contribution to the (D,D) blocks since $s = 0$.

$$\langle S,k|\, V^{^1D_2}|S,k'\rangle = 1/2^{(0)}C_{2k}{}^{(0)}C_{2k'}{}^{(0)}F^{2,2}_{2k}(\varphi)^{(0)}F^{2,2}_{2k'}(\varphi) \times \langle {}^{(2)}P^{2,2}_{2k}|\, V_c^{(102)}(r_{12})|{}^{(2)}P^{2,2}_{2k'}\rangle \tag{17}$$

$$\langle S,k|\, V_c^{^1D_2}(r_{12})|(S')^+,k'\rangle = \frac{1}{2\sqrt{2}}{}^{(0)}C_{2k}{}^{(+)}C_{2k'}{}^{(0)}F^{2,2}_{2k}(\varphi)^{(+)}F^{2,2}_{2k'}(\varphi) \times \langle {}^{(2)}P^{2,2}_{2k}|\, V_c^{(102)}(r_{12})|{}^{(2)}P^{2,2}_{2k'}\rangle \tag{18}$$

$$\langle (S')^+,k|\, V^{^1D_2}|(S')^+,k'\rangle = \tfrac{1}{4}{}^{(+)}C_{2k}{}^{(+)}C_{2k'}{}^{(+)}F^{2,2}_{2k}(\varphi)^{(+)}F^{2,2}_{2k'}(\varphi) \times \langle {}^{(2)}P^{2,2}_{2k}|\, V_c^{(102)}(r_{12})|{}^{(2)}P^{2,2}_{2k'}\rangle \tag{19}$$

(v) $V^{(^3P_0)}(tsj_1) = (110).$

This is a central potential with $l_1 = 1$, $s = 1$, and $j_1 = 0$. Hence coupling is possible in the $((S')^-, (S')^-)$ and (D^-, D^-) blocks:

$$\langle (S')^-, k| V^{^3P_0}|(S')^-, k'\rangle = \tfrac{1}{36}{}^{(-)}C_{2k}{}^{(-)}C_{2k'}{}^{(-)}F^{1,1}_{2k}(\varphi){}^{(-)}F^{1,1}_{2k'}(\varphi)$$
$$\times \langle {}^{(2)}P^{1,1}_{2k}| V_c^{(110)}(r_{12})|{}^{(2)}P^{1,1}_{2k'}\rangle \tag{20}$$

$$\langle D^-, k| V^3P_0|D^-, k'\rangle = \tfrac{1}{3}{}^{(D^-)}C_{2k+2}{}^{(D^-)}C_{2k'+2}{}^{(-)}F^{1,1}_{2k+2}(\varphi){}^{(-)}F^{1,1}_{2k'+2}(\varphi)$$
$$\times \langle {}^{(2)}P^{1,1}_{2k+2}| V_c^{(110)}(r_{12})|{}^{(2)}P^{1,1}_{2k'+2}\rangle \tag{21}$$

(vi) $V^{(^3P_1)}(tsj_1) = (111).$

Once again the potential is purely central with $l_1 = 1$, $s = 1$, $j_1 = 1$. Hence contributions occur in the $(S')^-$, $(S')^-$ and (D^-, D^-) blocks only

$$\langle (S')^-, k| V^{^3P_1}|(S')^-, k^-\rangle = \tfrac{1}{12}{}^{(-)}C_{2k}{}^{(-)}C_{2k'}{}^{(-)}F^{1,1}_{2k}(\varphi){}^{(-)}F^{1,1}_{2k'}(\varphi)$$
$$\times \langle {}^{(2)}P^{1,1}_{2k}| V_c^{(111)}(r_{12})|{}^{(2)}P^{1,1}_{2k'}\rangle \tag{22}$$

$$\langle D^-, k| V^{^3P_1}|D^-, k'\rangle = \tfrac{1}{4}{}^{(D^-)}C_{2k+2}{}^{(D^-)}C_{2k'+2}{}^{(-)}F^{1,1}_{2k+2}(\varphi){}^{(-)}F^{1,1}_{2k'+2}(\varphi)$$
$$\times \langle {}^{(2)}P^{1,1}_{2k+2}| V_c^{(111)}(r_{12})|{}^{(2)}P^{1,1}_{2k+2}\rangle \tag{23}$$

(vii) $V^{(^3S_1 - {}^3D_1)} \quad (tsj_1) = (011).$

In this case

$$V^{(^3S_1 - {}^3D_1)}(r_{12}) = V_c^{(011)}(r_{12}) + V_{LS}^{(011)}(r_{12})\mathbf{l}_1\cdot\mathbf{s} + V_T^{(011)}(r_{12})S_{12} \tag{24}$$

where S_{12} is the standard tensor operator; and $s = 1$, $j_1 = 1$ with $l_1 = 0$ or 2. The central and LS terms contribute to the (S, S), $(S, (S')^+; (S')^+$, $(S')^+)$ and (D^+, D^+) blocks. Note that the LS term contributes only if $l_1 \neq 0$.

The expression for the coupling matrix elements are given below

$$\langle S, k| V_c^{(^3S_1 - {}^3D_1)} + V_{LS}^{(^3S_1 - {}^3D_1)}|S, k'\rangle = \tfrac{1}{2}{}^{(0)}C_{2k}{}^{(0)}C_{2k'}[{}^{(0)}F^{0,0}_{2k}(\varphi){}^{(0)}F^{0,0}_{2k'}(\varphi)$$
$$\times \langle {}^{(2)}P^{0,0}_{2k}| V_c^{(011)}(r_{12})|{}^{(2)}P^{0,0}_{2k'}\rangle + \tfrac{1}{5}{}^{(0)}F^{2,2}_{2k}(\varphi){}^{(0)}F^{2,2}_{2k'}(\varphi)$$
$$\times \langle {}^{(2)}P^{2,2}_{2k}|(V_c^{(011)}(r_{12}) - 3V_{LS}^{(011)}(r_{12}))|{}^{(2)}P^{2,2}_{2k'}\rangle] \tag{25}$$

$$\langle S, k| V_c^{(^3S_1 - {}^3D_1)} + V_{LS}^{(^3S_1 - {}^3D_1)}|(S')^+, k'\rangle = -\frac{1}{2\sqrt{2}}{}^{(0)}C_{2k}{}^{(+)}C_{2k'}$$
$$\times [{}^{(0)}F^{0,0}_{2k}(\varphi){}^{(+)}F^{0,0}_{2k'}(\varphi)\langle {}^{(2)}P^{0,0}_{2k}| V_c^{(011)}(r_{12})|{}^{(2)}P^{0,0}_{2k'}\rangle$$
$$+ \tfrac{1}{5}{}^{(0)}F^{2,2}_{2k}(\varphi){}^{(+)}F^{2,2}_{2k'}(\varphi)\langle {}^{(2)}P^{2,2}_{2k}|(V_c^{(011)}(r_{12}) - 3V_{LS}^{(011)}(r_{12}))|{}^{(2)}P^{2,2}_{2k'}\rangle] \tag{26}$$

$$\langle (S')^+, k| V_c^{(^3S_1 - {}^3D_1)} + V_{LS}^{(^3S_1 - {}^3D_1)}|(S')^+, k'\rangle =$$
$$\tfrac{1}{4}{}^{(+)}C_{2k}{}^{(+)}C_{2k'}[{}^{(+)}F^{0,0}_{2k}(\varphi){}^{(+)}F^{0,0}_{2k'}(\varphi)\langle {}^{(2)}P^{0,0}_{2k}| V_c^{(011)}(r_{12})|{}^{(2)}P^{0,0}_{2k'}\rangle$$
$$+ \tfrac{1}{5}{}^{(+)}F^{2,2}_{2k}(\varphi){}^{(+)}F^{2,2}_{2k'}(\varphi)\langle {}^{(2)}P^{2,2}_{2k}|(V_c^{(011)}(r_{12}) - 3V_{LS}^{(011)}(r_{12}))|{}^{(2)}P^{2,2}_{2k'}\rangle] \tag{27}$$

$$\langle D^+,k|V_c^{(^3S_1-{}^3D_1)}+V_{LS}^{(^3S_1-{}^3D_1)}|D^+,k'\rangle=\tfrac{1}{2}{}^{(D^+)}C_{2k+2}{}^{(D^+)}C_{2k'+2}$$
$$\times[{}^{(+)}F^{2,0}_{2k+2}(\varphi){}^{(+)}F^{2,0}_{2k'+2}(\varphi)\langle{}^{(2)}P^{2,0}_{2k+2}|V_c^{(011)}(r_{12})|{}^{(2)}P^{2,0}_{2k'+2}\rangle$$
$$+{}^{(+)}F^{0,2}_{2k+2}(\varphi){}^{(+)}F^{0,2}_{2k'+2}(\varphi)\langle{}^{(2)}P^{0,2}_{2k+2}|(V_c^{(011)}(r_{12})$$
$$-3V_{LS}^{(011)}(r_{12}))|{}^{(2)}P^{0,2}_{2k'+2}\rangle+\tfrac{1}{2}{}^{(+)}F^{2,2}_{2k+2}(\varphi){}^{(+)}F^{2,2}_{2k'+2}(\varphi)$$
$$\times\langle{}^{(2)}P^{2,2}_{2k+2}|(V_c^{(011)}(r_{12})-3V_{LS}^{(011)}(r_{12}))|{}^{(2)}P^{2,2}_{2k'+2}\rangle]. \tag{28}$$

The tensor term contributes to the (S,D^+), $((S')^+,D^+)$ and (D^+,D^+) blocks:

$$\langle S,k|V_T^{(^3S_1-{}^3D_1)}|D^+,k'\rangle=-{}^{(0)}C_{2k}{}^{(D^+)}C_{2k'+2}[\sqrt{2}{}^{(0)}F^{0,0}_{2k}(\varphi){}^{(+)}F^{0,2}_{2k'+2}(\varphi)$$
$$\times\langle{}^{(2)}P^{0,0}_{2k}|V_T^{(011)}(r_{12})|{}^{(2)}P^{0,2}_{2k'+2}\rangle+0{\cdot}6324554{}^{(0)}F^{2,2}_{2k}(\varphi){}^{(+)}F^{2,0}_{2k'+2}(\varphi)$$
$$\times\langle{}^{(2)}P^{2,2}_{2k}|V_T^{(011)}(r_{12})|{}^{(2)}P^{2,0}_{2k'+2}\rangle+0{\cdot}3162277{}^{(0)}F^{2,2}_{2k}(\varphi){}^{(+)}F^{2,2}_{2k'+2}(\varphi)$$
$$\times\langle{}^{(2)}P^{2,2}_{2k}|V_T^{(011)}(r_{12})|{}^{(2)}P^{2,2}_{2k'+2}\rangle] \tag{29}$$

$$\langle(S')^+,k'|V_T^{(^3S_1-{}^3D_1)}|D^+,k'\rangle={}^{(+)}C_{2k}{}^{(+)}C_{2k'+2}[{}^{(+)}F^{0,0}_{2k}(\varphi){}^{(+)}F^{0,2}_{2k'+2}(\varphi)$$
$$\times\langle{}^{(2)}P^{0,0}_{2k}|V_T^{(011)}(r_{12})|{}^{(2)}P^{0,2}_{2k'+2}\rangle+0{\cdot}4472135{}^{(+)}F^{2,2}_{2k}(\varphi){}^{(+)}F^{2,0}_{2k'+2}(\varphi)$$
$$\times\langle{}^{(2)}P^{2,2}_{2k}|V_T^{(011)}(r_{12})|{}^{(2)}P^{2,0}_{2k'+2}\rangle+0{\cdot}2236067{}^{(+)}F^{2,2}_{2k}(\varphi){}^{(+)}F^{2,2}_{2k'+2}(\varphi)$$
$$\times\langle{}^{(2)}P^{2,2}_{2k}|V_T^{(011)}(r_{12})|{}^{(2)}P^{2,2}_{2k'+2}\rangle] \tag{30}$$

$$\langle D^+,k|V_T^{(^3S_1-{}^3D_1)}|D^+,k'\rangle=-{}^{(D^+)}C_{2k+2}{}^{(D^+)}C_{2k'+2}$$
$$\times[{}^{(+)}F^{2,2}_{2k+2}(\varphi){}^{(+)}F^{2,0}_{2k'+2}(\varphi)\langle{}^{(2)}P^{2,2}_{2k+2}|V_T^{(011)}(r_{12})|{}^{(2)}P^{2,0}_{2k'+2}\rangle$$
$$+{}^{(+)}F^{0,2}_{2k+2}(\varphi){}^{(+)}F^{0,2}_{2k'+2}(\varphi)\langle{}^{(2)}P^{0,2}_{2k+2}|V_T^{(011)}(r_{12})|{}^{(2)}P^{0,2}_{2k'+2}\rangle$$
$$+{}^{(+)}F^{2,0}_{2k+2}(\varphi){}^{(+)}F^{2,2}_{2k'+2}(\varphi)\langle{}^{(2)}P^{2,0}_{2k+2}|V_T^{(011)}(r_{12})|{}^{(2)}P^{2,2}_{2k'+2}\rangle$$
$$+0{\cdot}8451542{}^{(+)}F^{2,2}_{2k+2}(\varphi){}^{(+)}F^{2,2}_{2k'+2}(\varphi)$$
$$\times\langle{}^{(2)}P^{2,2}_{2k+2}|V_T^{(011)}(r_{12})|{}^{(2)}P^{2,2}_{2k'+2}\rangle] \tag{31}$$

(viii) $V^{(^3P_2-{}^3F_2)}\ (tsj_1)=(112)$.

In this case $s=1$, $j_1=2$ and $l_1=1$ or 3. The interaction potential is again a sum of central, LS and tensor terms:

$$V^{(^3P_2-{}^3F_2)}(r_{12})=V_c^{(112)}(r_{12})+V_{LS}^{(112)}(r_{12})\mathbf{l}_1\cdot\mathbf{s}+V_T^{(112)}(r_{12})S_{12}. \tag{32}$$

The central and LS terms contribute to the coupling between $((S')^-,(S')^-)$ and (D^-,D^-):

$$\langle(S')^-,k|V^{(^3P_2-{}^3F_2)}|(S')^-,k'\rangle=\tfrac{1}{2}{}^{(-)}C_{2k}{}^{(-)}C_{2k'}[\tfrac{5}{18}{}^{(-)}F^{1,1}_{2k}(\varphi){}^{(-)}F^{1,1}_{2k'}(\varphi)$$
$$\langle{}^{(2)}P^{1,1}_{2k}|(V_c^{(112)}(r_{12})+V_{LS}^{(112)}(r_{12}))|{}^{(2)}P^{1,1}_{2k'}\rangle+0{\cdot}1190473{}^{(-)}F^{3,3}_{2k}(\varphi)$$
$$\times{}^{(-)}F^{3,3}_{2k'}(\varphi)\langle{}^{(2)}P^{3,3}_{2k}|(V_c^{(112)}(r_{12})-4V_{LS}^{(112)}(r_{12}))|{}^{(2)}P^{3,3}_{2k'}\rangle] \tag{33}$$

$$\langle D^-,k|V^{(^3P_2-{}^3F_2)}|D^-,k'\rangle={}^{(D^-)}C_{2k+2}{}^{(D^-)}C_{2k'+2}$$
$$\times[\tfrac{1}{60}{}^{(-)}F^{1,1}_{2k+2}(\varphi){}^{(-)}F^{1,1}_{2k'+2}(\varphi)\langle{}^{(2)}P^{1,1}_{2k+2}|(V_c^{(112)}(r_{12})$$
$$+V_{LS}^{(112)}(r_{12}))|{}^{(2)}P^{1,1}_{2k'+2}\rangle+0{\cdot}9{}^{(-)}F^{3,1}_{2k+2}(\varphi){}^{(-)}F^{3,1}_{2k'+2}(\varphi)$$

$$\times \langle {}^{(2)}P^{3,1}_{2k+2}|(V_c^{(112)}(r_{12}) + V_{LS}^{(112)}(r_{12}))|{}^{(2)}P^{3,1}_{2k'+2}\rangle$$
$$+ 0{\cdot}9\,{}^{(-)}F^{1,3}_{2k+2}(\varphi)\,{}^{(-)}F^{1,3}_{2k'+2}(\varphi)\langle {}^{(2)}P^{1,3}_{2k+2}|(V_c^{(112)}(r_{12})$$
$$- 4V_{LS}^{(112)}(r_{12}))|{}^{(2)}P^{1,3}_{2k'+2}\rangle + \tfrac{4}{15}\,{}^{(-)}F^{3,3}_{2k+2}(\varphi)\,{}^{(-)}F^{3,3}_{2k'+2}(\varphi)$$
$$\times \langle {}^{(2)}P^{3,3}_{2k+2}|(V_c^{(112)}(r_{12}) - 4V_{LS}^{(112)}(r_{12}))|{}^{(2)}P^{3,3}_{2k'+2}\rangle]. \tag{34}$$

The tensor part of $V^{(^3P_2-{}^3F_2)}$ component contributes to the couplings $((S')^-, D^-)$ and (D^-, D^-)

$$\langle (S')^-, k|V_T^{(^3P_2-{}^3F_2)}|D^-, k'\rangle = \tfrac{1}{2}\,{}^{(-)}C_{2k}\,{}^{(D^-)}C_{2k'+2}$$
$$\times [0{\cdot}0384898\,{}^{(-)}F^{1,1}_{2k}(\varphi)\,{}^{(-)}F^{1,1}_{2k'+2}(\varphi)\langle {}^{(2)}P^{1,1}_{2k}|V_T^{(112)}(r_{12})|{}^{(2)}P^{1,1}_{2k'+2}\rangle$$
$$+ 2{\cdot}078460964\,{}^{(-)}F^{1,1}_{2k}(\varphi)\,{}^{(-)}F^{1,3}_{2k'+2}(\varphi)\langle {}^{(2)}P^{1,1}_{2k}|V_T^{(112)}(r_{12})|{}^{(2)}P^{1,3}_{2k'+2}\rangle$$
$$+ 1{\cdot}360672082\,{}^{(-)}F^{3,3}_{2k}(\varphi)\,{}^{(-)}F^{3,1}_{2k'+2}(\varphi)\langle {}^{(2)}P^{3,3}_{2k}|V_T^{(112)}(r_{12})|{}^{(2)}P^{3,1}_{2k'+2}\rangle$$
$$+ 0{\cdot}4031599\,{}^{(-)}F^{3,3}_{2k}(\varphi)\,{}^{(-)}F^{3,3}_{2k'+2}(\varphi)\langle {}^{(2)}P^{3,3}_{2k}|V_T^{(112)}(r_{12})|{}^{(2)}P^{3,3}_{2k'+2}\rangle] \tag{35}$$

$$\langle D^-, k|V^{(^3P_2-{}^3F_2)}|D^-, k'\rangle = -\tfrac{1}{2}\,{}^{(D^-)}C_{2k+2}\,{}^{(D^-)}C_{2k'+2}[\tfrac{1}{75}\,{}^{(-)}F^{1,1}_{2k+2}(\varphi)$$
$$\times {}^{(-)}F^{1,1}_{2k'+2}(\varphi)\langle {}^{(2)}P^{1,1}_{2k+2}|V_T^{(112)}(r_{12})|{}^{(2)}P^{1,1}_{2k'+2}\rangle + 0{\cdot}72\,{}^{(-)}F^{1,1}_{2k+2}(\varphi)$$
$$\times {}^{(-)}F^{1,3}_{2k'+2}(\varphi)\langle {}^{(2)}P^{1,1}_{2k+2}|V_T^{(112)}(r_{12})|{}^{(2)}P^{1,3}_{2k'+2}\rangle$$
$$+ 0{\cdot}72\,{}^{(-)}F^{3,1}_{2k+2}(\varphi)\,{}^{(-)}F^{3,1}_{2k'+2}(\varphi)\langle {}^{(2)}P^{3,1}_{2k+2}|V_T^{(1\cdot12)}|{}^{(2)}P^{3,1}_{2k'+2}\rangle$$
$$+ 2{\cdot}88\,{}^{(-)}F^{3,1}_{2k+2}(\varphi)\,{}^{(-)}F^{3,3}_{2k'+2}(\varphi)\langle {}^{(2)}P^{3,1}_{2k+2}|V_T^{(122)}(r_{12})|{}^{(2)}P^{3,3}_{2k'+2}\rangle$$
$$+ 2{\cdot}88\,{}^{(-)}F^{1,3}_{2k+2}(\varphi)\,{}^{(-)}F^{1,3}_{2k'+2}(\varphi)\langle {}^{(2)}P^{1,3}_{2k+2}|V_T^{(112)}(r_{12})|{}^{(2)}P^{1,3}_{2k'+2}\rangle$$
$$+ 0{\cdot}72\,{}^{(-)}F^{1,3}_{2k+2}(\varphi)\,{}^{(-)}F^{1,1}_{2k'+2}(\varphi)\langle {}^{(2)}P^{1,3}_{2k+2}|V_T^{(112)}(r_{12})|{}^{(2)}P^{1,1}_{2k'+2}\rangle$$
$$+ 2{\cdot}88\,{}^{(-)}F^{3,3}_{2k+2}(\varphi)\,{}^{(-)}F^{3,1}_{2k'+2}(\varphi)\langle {}^{(2)}P^{3,3}_{2k+2}|V_T^{(112)}(r_{12})|{}^{(2)}P^{3,1}_{2k'+2}\rangle$$
$$+ 0{\cdot}85332621\,{}^{(-)}F^{3,3}_{2k+2}(\varphi)\,{}^{(-)}F^{3,3}_{2k'+2}(\varphi)\langle {}^{(2)}P^{3,3}_{2k+2}|V_T^{(112)}(r_{12})|{}^{(2)}P^{3,3}_{2k'+2}\rangle] \tag{36}$$

The expression of matrix elements given in equations (8) and (10)–(36) can be grouped together for each of the blocks of the full potential matrix. Note that both $(S')^{\pm}$ and $D^{\pm}$ should be grouped into the corresponding block involving S' or D respectively.

3. Geometrical structure coefficients

All the individual terms of the form

$$\langle {}^{(2)}P^{l_2 l_1}_{2k}|V^{(tsj_1)}(r_{12})|{}^{(2)}P^{l'_2 l'_1}_{2k'}\rangle$$

with various combinations of l_2, l_1, l'_2 and l'_1 appearing in equations (8)–(36) can be classified into twelve types, eight of which are symmetric with respect to k and k'. Table 1 shows this classification, together with the subblocks where each type contributes. The general matrix element can be expressed as

$$\langle {}^{(2)}P^{l_2 l_1}_{2k}|V^{(tsj_1)}(r_{12})|{}^{(2)}P^{l'_2 l'_1}_{2k'}\rangle = N^{l_2 l_1}_{2k} N^{l'_2 l'_1}_{2k'} 2^{-(l_1+l'_1+l_2+l'_2+6)/2}$$
$$\times \int_{-1}^{+1} P_n^{l_1+1/2, l_2+1/2}(x)\, V^{(tsj_1)}\left(r\sqrt{\frac{1+x}{2}}\right) P_{n'}^{l'_1+1/2, l'_2+1/2}(x)$$
$$\times (1-x)^{(l_1+l'_1+1)/2}(1+x)^{(l_2+l'_2+1)/2}\mathrm{d}x \tag{37}$$

Table 1. Classification of matrix elements of the form $\langle {}^{(2)}P^{l_2 l_1}_{2k} | V^{(tsj_1)} | {}^{(2)}P^{l'_2 l'_1}_{2k'} \rangle$.

l_2	l_1	l'_2	l'_1	Symmetric or not	Appearing in sub-block	Reference equation No.
0	0	0	0	Yes	$(S,S),(S,S'),(S',S')$	14, 15, 16, 25, 26, 27
2	2	2	2	Yes	$(S,S),(S,S'),(S,D),(S',S'),$ $(S',D),(D,D)$	10, 11, 12, 13, 17, 18, 19, 25, 26, 27, 28, 29, 30, 31
1	1	1	1	Yes	$(S',S'),(S',D),(D,D)$	8, 20, 21, 22, 23, 33, 34, 35, 36
3	3	3	3	Yes	$(S',S'),(S',D),(D,D)$	33, 34, 35, 36
2	0	2	0	Yes	(D,D)	28
0	2	0	2	Yes	D,D	28, 31
3	1	3	1	Yes	(D,D)	34, 36
1	3	1	3	Yes	(D,D)	34, 36
0	2	0	0	No	$(S,D),(S',D)$	29, 30
2	0	2	2	No	$(S,D),(S',D),(D,D)$	31, 30, 29
1	1	1	3	No	$(S',D),(D,D)$	35, 36
3	1	3	3	No	$(S',D),(D,D)$	35, 36

where $P_n^{\alpha,\beta}(x)$ is the Jacobi polynomial and $n=(2k-l_1-l_2)/2$, $n'=(2k'-l'_1-l'_2)/2$. The normalization factor $N^{l_2 l_1}_{2k}$ is given by Ballot and Fabre [6].

In order to evaluate the integral in (37) we expand $V^{(tsj_1)}(r[(1+x)/2]^{1/2})$ is the complete set $\{P_{n''}^{1/2\,1/2}(x)\}$ over the interval $(-1,1)$ of x (for a fixed value of r)

$$V^{(tsj_1)}\left(r\sqrt{\frac{1+x}{2}}\right)=\sum_{n''} v_{n''}^{(tsj_1)}(r)P_{n''}^{1/2\,1/2}(x). \tag{38}$$

Using the orthonormality of Jacobi polynomials, the potential multipole is given by

$$v_n^{(tsj_1)}(r)=\frac{1}{h_n^{1/2\,1/2}}\int_{-1}^{+1} V^{(tsj_1)}\left(r\sqrt{\frac{1+x}{2}}\right)P_n^{1/2\,1/2}(x)(1-x^2)^{1/2}\,dx \tag{39}$$

where $h_n^{\alpha,\beta}$ is the norm of the Jacobi polynomial. Substituting the expression for $V^{(tsj_1)}(r[(1+x)/2]^{1/2})$ of (38) in (37), we have

$$\langle {}^{(2)}P^{l_2 l_1}_{2k} | V^{(tsj_1)}(r_{12}) | {}^{(2)}P^{l'_2 l'_1}_{2k'} \rangle = N^{l_2 l_1}_{2k} N^{l'_2 l'_1}_{2k'} 2^{-(l_1+l_2+l'_1+l'_2+6)/2}$$
$$\times \sum_{n''=n_{\min}}^{n_{\max}} v_{n''}^{(tsj_1)}(r)\langle l_1, l_2, n | n'' | l'_1, l'_2, n' \rangle \tag{40}$$

where

$$\langle l_1, l_2, n | n'' | l'_1, l'_2, n' \rangle = \int_{-1}^{+1} P_n^{l_1+1/2, l_2+1/2}(x) P_{n''}^{1/2\,1/2}(x) P_{n'}^{l'_1+1/2, l'_2+1/2}(x)$$
$$\times (1-x)^{(l_1+l'_1+1)/2}(1+x)^{(l_2+l'_1+1)/2}\,dx \tag{41}$$

is the effective geometrical structure coefficients (GSC) for the particular type of matrix elements. Since $P_n^{\alpha,\beta}(x)$ is a polynomial of degree n, one can see from equation (41), using the orthonormality of Jacobi Polynomials, that the GSC vanishes unless n'' satisfies $n_{\max} \leqslant n'' \leqslant n_{\min}$. The values of $n_{\max}$ and $n_{\min}$ depend on l_1, l'_1, l_2 and l'_2 and have been presented in table 2 for each of the 12 types of GSC. Since the GSC is zero for n'' outside this range, the right side of (40) involves a finite sum, making the evaluation practical.

Table 2. Limits of the sum in equations (40) and (42).

Type of GSC	l_1	l'_1	l_2	l'_2	n_{max}	n_{min}
1	0	0	0	0	$n+n'$	$\|n-n'\|$
2	2	2	2	2	$n+n'+4$	$\|n-n'\|$
3	1	1	1	1	$n+n'+2$	$\|n-n'\|$
4	3	3	3	3	$n+n'+6$	$\|n-n'\|$
5	0	0	2	2	$n+n'+2$	$\|n-n'\|$
6	2	2	0	0	$n+n'+2$	$\|n-n'\|$
7	1	1	3	3	$n+n'+4$	$\|n-n'\|$
8	3	3	1	1	$n+n'+4$	$\|n-n'\|$
9	0	2	0	0	$n+n'+2$	$\mathrm{Max}(n'-n+1, n-n'-3, 0)$
10	0	2	2	2	$n+n'+4$	$\mathrm{Max}(n'-n+1, n-n'-3, 0)$
11	1	3	1	1	$n+n'+4$	$\mathrm{Max}(n'-n+1, n-n'-3, 0)$
12	1	3	3	3	$n+n'+6$	$\mathrm{Max}(n'-n+1, n-n'-3, 0)$

To evaluate the GSC, equation (41), we adopt the linear inhomogenous equation method of Das and De [13]. Multiplying both sides of (41) by $P_{n''}^{1/2\,1/2}(y)/h_{n''}^{1/2\,1/2}$, summing over n'' and using the completeness property of Jacobi polynomials [14] we get

$$\sum_{n''=n_{min}}^{n_{max}} \langle l_1 l_2 n | n'' | l'_1 l'_2 n' \rangle P_{n''}^{1/2\,1/2}(y)/h_{n''}^{1/2\,1/2}$$
$$= P_n^{l_1+1/2, l_2+1/2}(y) P_{n'}^{l'_1+1/2, l'_2+1/2}(y)(1-y)^{(l_1+l'_1)/2}(1+y)^{(l_1+l'_1)/2}. \tag{42}$$

Choosing suitable values of y in the interval $[-1, 1]$, (42) becomes a set of linear inhomogeneous equations for the unknown GSC and can be solved easily. This method is very convenient, fast and accurate compared to other direct numerical integration of the GSC using (41). An added advantage is that all the GSC of a given type for fixed values of n and n' are calculated by solving (42) once only. In table 3, we present a comparison of the CPU time taken to compute all the GSC needed for retaining up to 12 partial waves in each of S, S' and D states by the LIE method and the numerical integration of (41). In this table, we also include the total number of GSC needed in each category. To check the precision of the computed GSC we obtain a sum rule from (42) by setting $y = 1$

$$\sum_{n''} \langle l_1 l_2 n | n'' | l'_1 l'_2 n' \rangle P_{n''}^{1/2\,1/2}(1)/h_{n''}^{1/2\,1/2}$$
$$= \delta_{l_1 0}\delta_{l'_1 0} P_n^{l_1+1/2, l_2+1/2}(1) P_{n'}^{l'_1+1/2, l'_2+1/2}(1) 2^{(l_1+l'_1)/2}. \tag{43}$$

The difference of the left and right sides of (43), when calculated GSC's are used in the left side, is a measure of the precision of the calculated GSC. In table 3 we present the sum of the difference of the left and right sides of (43) for all the n, n' values needed for retaining up to 12 partial waves in each of S, S' and D states. This quantity has been referred to as 'precision' in table 3 and corresponds to the sum total error for all the GSC needed for a particular type. Calculations have been done on a HP 1000/A 700 computer in double precision. One can see from table 3 that the LIE method is about 12–15 times faster than the direct integration and has a much higher

Table 3. Comparison of calculated GSC by LIE and integral method.

Type of GSC	Total number of GSC	Precision		CPU time in sec.	
		LIE method	Integral method	LIE method	Integral method
1	819	$-5{\cdot}22933 \times 10^{-5}$	1·346990	51	847
2	1183	$2{\cdot}37601 \times 10^{-9}$	$5{\cdot}33280 \times 10^{-3}$	93	1309
3	1001	$-7{\cdot}67389 \times 10^{-10}$	$-7{\cdot}55730 \times 10^{-2}$	69	1064
4	1365	$-2{\cdot}08299 \times 10^{-7}$	$-2{\cdot}49955 \times 10^{-4}$	123	1511
5	1001	$-2{\cdot}09175 \times 10^{-4}$	6·83987	69	1052
6	1001	$7{\cdot}96798 \times 10^{-10}$	0·55940	69	1050
7	1183	$4{\cdot}45465 \times 10^{-10}$	−0·37517	93	1278
8	1183	$4{\cdot}34017 \times 10^{-8}$	$-2{\cdot}58487 \times 10^{-2}$	94	1285
9	1951	$6{\cdot}63154 \times 10^{-10}$	0·99517	127	2000
10	2289	$-5{\cdot}05207 \times 10^{-9}$	$8{\cdot}04270 \times 10^{-4}$	172	2427
11	2289	$1{\cdot}32246 \times 10^{-8}$	$-4{\cdot}46983 \times 10^{-2}$	172	2455
12	2627	$5{\cdot}63261 \times 10^{-8}$	$-7{\cdot}00406 \times 10^{-5}$	228	2858

precision than the latter. It is worth noting that $V^{(ts j_1)}(r[(1+x)/2]^{1/2})$ could be expanded in the complete set $\{P_{n''}^{\alpha,\beta}(x)\}$ with α, β arbitrary. The choice of the complete set $\{P_{n''(x)}^{1/2,1/2}\}$ in (38) is particularly convenient. For this choice, the calculation of the potential multipoles becomes easier. Furthermore the selection rules of the GSC (table 2) becomes simpler.

4. Summary and conclusion

In the present work, we have set up the equation for solving the trinucleon problem with RSC potential by the hyperspherical harmonics method. Introduction of potential multipoles and GSC make the calculation of the potential matrix feasible well within the realm of small-sized computers, which otherwise would be an enormously large numerical calculation. Choice of the set $\{P_n^{1/2,1/2}(x)\}$ as the expansion basis of the potential gives rise to the minimum number of convenient sets of GSC, required for the problem. Finally evaluation of the GSC by the LIE method is very fast and accurate. Even if the calculation of PM is done by numerical integration, the evaluation of the potential matrix will not be too slow if one uses the calculated GSC. Note that the GSC can be calculated once only and stored on disk, which can be read during the calculation of the potential matrix. The authors are presently working on an efficient scheme to evaluate the PM by calculating only a few of them by numerical integration.

In conclusion, we believe that the present procedure will lead to a relatively simple and accurate computer code for this problem. The estimated memory and CPU time requirements are well within the capacity of a PC 486 machine. As a first step towards this goal, we have been able to calculate all the GSC necessary with a high precision.

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