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COMPUTATION OF RAYNAL-REVAI COEFFICIENTS FOR THE HYPERSPHERICAL APPROACH TO A THREE-BODY SYSTEM

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The calculation of matrix elements of two-body interactions needed in the hyperspherical harmonics method for a three-body system is greatly simplified by expanding the bra- and ket-vector states in the hyperspherical harmonics basis states appropriate for the partition corresponding to the interacting pair. This involves the Raynal-Revai coefficients (RRC) which are the transformation coefficients between the hyperspherical harmonics bases corresponding to the two partitions. In this work, we present a fast algorithm for an accurate numerical computation of RRC. We have used this technique for two-electron atoms where the two-body interactons are purely Coulombic, and compared the results with the direct numerical integrations. Both the individual matrix element of the total interaction potential as well as the calculated binding energy agree within the computational error.

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1. Introduction

The hyperspherical harmonics expansion method is a powerful tool for the *ab initio* solution of the few-body Schrödinger equation, for a given set of potentials of interaction among constituent particles. The method has been used for bound states in atomic [1–4], nuclear [5–14] and particle physics [15–17]. Attempts have been made to use it also in scattering problems [18]. In this method, one introduces hyperspherical variables in terms of Jacobi coordinates, the i^{th} Jacobi coordinate being proportional to the separation vector of the $(i+1)^{\text{th}}$ particle from the centre of mass of the first i particles. In this way, the centre of mass motion is automatically separated and the relative motion of an N-particle system is described in terms of $(N-1)$ Jacobi vectors. Next, hyperspherical variables [19] are introduced

(Sect. 2) and the wave function is expanded in the complete set of hyperspherical harmonics (HH), which are the eigenfunction of the hyper-angular-momentum operator in $(3N-4)$ dimensions. Substitution of this expansion into the Schrödinger equation and projection on a particular set of hyperspherical harmonics leads to a set of coupled differential equations. Solution of this set of equations, subject to appropriate boundary conditions for a bound system, gives the binding energy and the wave function of the system. The method is *ab initio* and essentially exact (i.e., the precision of the results depend only on the extent of truncation of the expansion basis). The method also provides a clear physical picture of the system in terms of the configuration space wave function [5]. One of the most difficult computational aspects of this method is the calculation of the coupling matrix elements. We will see in the next section that the calculation of the matrix elements of the interaction between the first two particles (numbered 1 and 2) is straightforward, while that between any other pair is very cumbersome, because the corresponding separation vector becomes a linear combination of more than one Jacobi coordinate, and the calculation procedure is not unique, since we can number the particles in any one of the $N!$ ways. Each choice will lead to an equivalent set of $(N-1)$ Jacobi vectors, and a corresponding equivalent set of hyperspherical coordinates. It can be shown that the hyperradius, which is the invariant global length in $3(N-1)$ dimensions, is the same for all choices. The hyperangles form a set of $(3N-4)$ angle variables. These are constituted by $2(N-1)$ polar angles of the $(N-1)$ Jacobi vectors and $(N-2)$ angles defined in terms of the relative lengths of the Jacobi vectors. The hyperangles depend on the particular partition chosen. Consequently, HH also depend on the partition. Each complete set of HH corresponding to a given partition span the same $(3N-4)$ dimensional angular hyperspace. Hence, a given HH of a particular set can be expanded in the complete set of HH corresponding to any other partition, there being a unitary transformation between such sets of basis vectors. In calculating the matrix element of $V(r_{ij})$, the interaction potential of the (ij) pair, it is then convenient to expand the chosen HH in the set of HH corresponding to the partition in which $\vec{r}_{ij}$ is proportional to the first Jacobi vector. To do this, we need the transformation coefficients, called Raynal-Revai coefficients (RRC), from one choice of partition to another. Raynal and Revai [20] obtained an expression for these coefficients for a three-body system consisting of particles of arbitrary masses. In this communication, we present a computational algorithm for the calculation of these coefficients which can be used in any three-body calculation. We have checked the calculation of these coefficients by computing the matrix elements needed in two-electron atoms and compared them, as well as the binding energy, with direct numerical integration of the matrix elements.

In Sect. 2, we discuss the fundamentals of the hyperspherical harmonics expansion method and the transformation coefficients between two sets of HH belonging to two different partitions. In Sect. 3, we discuss the numerical algorithm and in Sect. 4, we use the calculated RRC for the ground states of some two-electron atoms and compare them with the results in which matrix elements were obtained in a straightforward manner, paying attention to the total computation time involved in each process.

2. *Hyperspherical harmonics expansion method*

To study the structure of a three-particle system by the hyperspherical harmonics expansion (HHE) method, we label the particles by "i", "j" and "k", having masses m_i, m_j, m_k, respectively, as shown in Fig. 1. For such a system consisting of three unequal-mass particles having spatial coordinates $\vec{r}_i$, $\vec{r}_j$ and $\vec{r}_k$, the relative motion is described by the Jacobi coordinates in partition "i" defined by [3]:

$$\begin{aligned}
\vec{x}_i &= \left[\frac{m_j m_k M}{m_i(m_j+m_k)^2}\right]^{1/4} (\vec{r}_j - \vec{r}_k)\,, \\
\vec{y}_i &= \left[\frac{m_i(m_j+m_k)^2}{m_j m_k M}\right]^{\frac{1}{4}} \left(\vec{r}_i - \frac{m_j\vec{r}_j + m_k\vec{r}_k}{m_j+m_k}\right)\,, \\
\vec{R} &= (m_i\vec{r}_i + m_j\vec{r}_j + m_k\vec{r}_k)/M\,,
\end{aligned} \tag{1}$$

where $M = m_i + m_j + m_k$. The sign of $\vec{x}_i$ is fixed by the condition that (i, j, k) should form a cyclic permutation of (1, 2, 3).

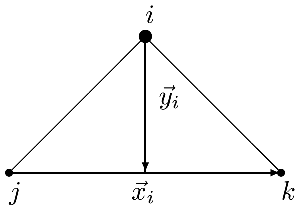

Fig. 1. Choices of the Jacobi coordinates for the partition "i".

The set of Jacobi coordinates represented by Eqs. (1) corresponds to the partition in which the particle labelled "i" is called the spectator and particles labelled "j" and "k" form the interacting pair. It is so named, since the calculation of matrix element of $V(\vec{r}_{jk})$ in terms of these set of Jacobi coordinates is straightforward. We can likewise define two other sets of Jacobi coordinates by cyclically permuting $i \to j \to k \to i$ twice, which correspond to the partitions labelled "j" and "k", respectively.

In terms of the Jacobi coordinates, Eqs.(1), the three-body Schrödinger equation immediately separates into the centre of mass motion (which is uninteresting) and the relative motion described by

$$\left[-\frac{\hbar^2}{2\mu}(\nabla^2_{x_i} + \nabla^2_{y_i}) + V_{jk}(\vec{x}_i) + V_{ki}(\vec{x}_i, \vec{y}_i) + V_{ij}(\vec{x}_i, \vec{y}_i) - E\right] \Psi(\vec{x}_i, \vec{y}_i) = 0\,, \tag{2}$$

where $\mu = \sqrt{m_i m_j m_k / M}$ is an effective mass parameter. One next introduces the hyperspherical variables defined by [3, 4]

$$\begin{aligned}
x_i &= \rho\cos\phi_i\,, \\
y_i &= \rho\sin\phi_i\,,
\end{aligned} \tag{3}$$

where $\rho = \sqrt{x_i^2 + y_i^2}$ is invariant under three-dimensional rotations and independent of the partition (this can be seen from Eq. (13) below). Hence, ρ is invariant under permutations of the particle indices.

The spherical polar angles (θ_{x_i}, ϕ_{x_i}) and (θ_{y_i}, ϕ_{y_i}) of $\vec{x}_i$ and $\vec{y}_i$, together with the angle ϕ_i constitute the set of five hyperangles and is denoted by

$$\Omega_i \quad \rightarrow \quad \{\phi_i, \theta_{x_i}, \phi_{x_i}, \theta_{y_i}, \phi_{y_i}\}\,. \tag{4}$$

The hyperangles Ω_i are obviously dependent on the partition. The set of six variables (ρ, Ω_i) form the hyperspherical variables. In terms of these variables, the Schrödinger equation becomes

$$\left[-\frac{\hbar^2}{2\mu}\left\{\frac{1}{\rho^5}\frac{\partial}{\partial\rho}(\rho^5\frac{\partial}{\partial\rho}) - \frac{\hat{\mathcal{K}}^2(\Omega_i)}{\rho^2}\right\} + V(\rho,\Omega_i) - E\right]\Psi(\rho,\Omega_i) \;=\; 0\,, \tag{5}$$

where $V(\rho, \Omega_i) = V_{jk} + V_{ki} + V_{ij}$ is the total interaction potential, and $\hat{K}^2(\Omega_i)$ is the square of hyper-angular-momentum operator given by [19]

$$\hat{\mathcal{K}}^2(\Omega_i) \;=\; -\frac{\partial^2}{\partial{\phi_i}^2} - 4\cot\phi_i\frac{\partial}{\partial\phi_i} + \frac{1}{\cos^2\phi_i}\hat{l}^2(\hat{x_i}) + \frac{1}{\sin^2\phi_i}\hat{l}^2(\hat{y_i})\,. \tag{6}$$

Here $\hat{l}^2(\hat{x_i})$ and $\hat{l}^2(\hat{y_i})$ are the squares of ordinary orbital angular momenta associated with $\vec{x}_i$ and $\vec{y}_i$ motions. The operator $\hat{K}^2(\Omega_i)$ satisfies the eigenvalue equation [19]

$$\hat{\mathcal{K}}^2(\Omega_i)\mathcal{Y}_{K\alpha_i}(\Omega_i) \;=\; K(K+4)\mathcal{Y}_{K\alpha_i}(\Omega_i)\,. \tag{7}$$

The normalized eigenfunctions, called the hyperspherical harmonics (HH) having specified total orbital angular momentum of the system (L) and its projection (M), are given by [19]

$$\begin{aligned}\mathcal{Y}_{k\alpha_i}(\Omega_i) \;&\equiv\; \mathcal{Y}_{Kl_{x_i}l_{y_i}LM}(\phi_i, \theta_{x_i}, \phi_{x_i}, \theta_{y_i}, \phi_{y_i})\\ &=\; N_K^{l_{x_i}l_{y_i}}(\cos\phi_i)^{l_{x_i}}(\sin\phi_i)^{l_{y_i}}P_{n_i}^{l_{y_i}+\frac{1}{2},\,l_{x_i}+\frac{1}{2}}(\cos 2\phi_i)\\ &\quad\;\left[Y_{l_{x_i}m_{x_i}}(\theta_{x_i}\phi_{x_i})Y_{l_{y_i}m_{y_i}}(\theta_{y_i}\phi_{y_i})\right]_{LM}\\ &\equiv\; {}^{(2)}P_K^{l_{x_i}l_{y_i}}(\phi_i)\left[Y_{l_{x_i}m_{x_i}}(\theta_{x_i}\phi_{x_i})Y_{l_{y_i}m_{y_i}}(\theta_{y_i}\phi_{y_i})\right]_{LM}\,,\end{aligned} \tag{8}$$

where $\alpha_i \equiv \{l_{x_i}, l_{y_i}, L, M\}$ is a short-hand notation, $[\,]_{LM}$ indicates the angular momentum coupling, $P_n^{\alpha,\beta}$ is a Jacobi polynomial and

$$N_K^{l_{x_i}l_{y_i}} = \left[\frac{2n_i!(K+2)(n_i+l_{x_i}+l_{y_i}+1)!}{\Gamma(n_i+l_{x_i}+\frac{3}{2})\Gamma(n_i+l_{y_i}+\frac{3}{2})}\right]^{\frac{1}{2}}\,, \tag{9}$$

$n_i = (K - l_{x_i} - l_{y_i})/2$ being a non-negative integer. The quantity K is the hyperangular-momentum quantum number (not a good quantum number of the three-body system) and is the degree of the homogeneous harmonic polynomials $\rho^K \mathcal{Y}_{K\alpha_i}(\Omega_i)$ in the Cartesian components of $\vec{x}_i$ and $\vec{y}_i$.

In the HHE method, $\Psi(\rho, \Omega_i)$ is expanded in the complete set of HH associated with a given partition (say partition "i"):

$$\Psi(\rho, \Omega_i) = \sum_{k\alpha_i} \frac{U_{k\alpha_i}(\rho)}{\rho^{5/2}} \mathcal{Y}_{k\alpha_i}(\Omega_i)\,. \tag{10}$$

The factor $\rho^{-5/2}$ is included to remove the first derivative with respect to ρ in Eq. (5). Substitution of Eq. (10) in Eq. (5), the use of Eq. (7) and the orthonormality of HH, give a set of coupled differential equations (CDE) in ρ

$$\begin{aligned} &\left[-\frac{\hbar^2}{2\mu}\left(\frac{\mathrm{d}^2}{\mathrm{d}\rho^2}\right) - \frac{\mathcal{L}_K(\mathcal{L}_K+1)}{\rho^2}) - E\right] U_{K\alpha_i}(\rho) \\ + \quad &\textstyle\sum_{K'\alpha_i{}'} < K\alpha_i \mid V(\rho,\Omega_i) \mid K'\alpha_i{}' > U_{K'\alpha_i{}'}(\rho) \;=\; 0\,, \end{aligned} \tag{11}$$

where $\mathcal{L}_K = K + 3/2$ and

$$< K\alpha_i | V | K', \alpha_i{}' > = \int \mathcal{Y}^*_{K\alpha_i}(\Omega_i) V(\rho, \Omega_i) \mathcal{Y}_{K'\alpha_i{}'}(\Omega_i) d\Omega_i\,. \tag{12}$$

Evaluation of the matrix elements of the type $<\mathcal{Y}_{K\alpha_i}(\Omega_i)|V_{jk}(x_i)|\mathcal{Y}_{K'\alpha_i{}'}(\Omega_i)>$ (for the central potentials) is straightforward, while for matrix elements of the type $<\mathcal{Y}_{K\alpha_i}(\Omega_i)|V_{ki}(x_j)|\mathcal{Y}_{K'\alpha_i{}'}(\Omega_i)>$ or $<\mathcal{Y}_{K\alpha_i}(\Omega_i)|V_{ij}(x_k)|\mathcal{Y}_{K'\alpha_i{}'}(\Omega_i)>$, calculations become very complicated even for central potentials, since x_j or x_k depend on the polar angles $\hat{x_i}$ and $\hat{y_i}$. Using Eq. (1), we express $\vec{x}_k$ and $\vec{y}_k$ in terms of $\vec{x}_i$ and $\vec{y}_i$ [20]

$$\begin{aligned} \vec{x}_k &= -\cos\zeta_{ki}\;\vec{x}_i + \sin\zeta_{ki}\;\vec{y}_i\,, \\ \vec{y}_k &= -\sin\zeta_{ki}\;\vec{x}_i - \cos\zeta_{ki}\;\vec{y}_i\,, \end{aligned} \tag{13}$$

where $\zeta_{ki} = \tan^{-1}\{(-1)^P \sqrt{Mm_j/(m_i m_k)}\}$, P being even (odd) if (kij) is an even (odd) permutation of the triad (1 2 3).

Then for an arbitrary shape of the central potential and nonvanishing L, most of the five-dimensional integrals have to be done numerically. This makes the calculation slow and inaccurate. However, calculation of the latter matrix elements can be greatly simplified using the following tricks. We first note that each of the complete sets of HH functions $\{\mathcal{Y}_{K\alpha_i}(\Omega_i)\}$, $\{\mathcal{Y}_{K\alpha_j}(\Omega_j)\}$ or $\{\mathcal{Y}_{K\alpha_k}(\Omega_k)\}$ span the five-dimensional angular hyperspace. Hence, a particular member of a given set, say $\mathcal{Y}_{K\alpha_i}(\Omega_i)$, can be expanded in the complete set of $\{\mathcal{Y}_{K\alpha_j}(\Omega_j)\}$ through a unitary transformation:

$$\mathcal{Y}_{K\alpha_i}(\Omega_i) \;=\; \sum_{\alpha_j} < \alpha_j \mid \alpha_i >_{KL} \mathcal{Y}_{K\alpha_j}(\Omega_j)\,. \tag{14}$$

Note that K, L, M are conserved for Eq. (14); furthermore there is the rotational degeneracy with respect to the quantum number M for spin independent forces. Hence,

$$< \alpha_j \mid \alpha_i >_{KL} = < l_{x_j} l_{y_j} \mid l_{x_i} l_{y_i} >_{KL} \ . \tag{15}$$

Equation (14) can then be rewritten as [20]

$$\mathcal{Y}_{K\alpha_i}(\Omega_i) = \sum_{l_{x_j} l_{y_j}} < l_{x_j} l_{y_j} \mid l_{x_i} l_{y_i} >_{KL} \mathcal{Y}_{K\alpha_j}(\Omega_j) \,. \tag{16}$$

These coefficients are indepenent of M due to the overall rotational degeneracy. The coefficients (15) are called Raynal-Revai coefficients (RRC). Using them, the matrix element of a central interaction V_{ki} becomes

$$\begin{aligned} < \mathcal{Y}_{K\alpha_i}(\Omega_i) \mid V_{ki}(x_j) \mid \mathcal{Y}_{K'\alpha_i'}(\Omega_i) > &= \textstyle\sum_{l_{x_j}' l_{y_j}' l_{x_j} l_{y_j}} < l_{x_j} l_{y_j} \mid l_{x_i} l_{y_i} >^{*}_{KL} \\ &\times < l_{x_j}' l_{y_j}' \mid l_{x_i}' l_{y_i}' >_{K'L} < \mathcal{Y}_{K\alpha_j}(\Omega_j) \mid V_{ki}(x_j) \mid \mathcal{Y}_{K'\alpha_j'}(\Omega_j) > \ . \end{aligned} \tag{17}$$

The matrix element on the right side of Eq. (17) is of the same form as the matrix element of V_{jk} in the partition "i" and can be obtained in a simple manner. Thus evaluating the RRC's involved in Eq. (17), one can calculate the matrix element of V_{ki} easily. Similar treatment can be applied for the calculation of the matrix element of V_{ij}.

The explicit expression for RRC is given in Ref. [20]

$$\begin{aligned} < l_{x_j} l_{y_j} \mid l_{x_i} l_{y_i} >_{KL} = \frac{\pi}{4} \left[C^{n_j}_{l_{x_j}, l_{y_j}} C^{n_i}_{l_{x_i}, l_{y_i}} \right]^{1/2} \sum_{\lambda_1 \lambda_2 \lambda_3 \lambda_4} (\mathrm{i})^{\lambda_2 + \lambda_4 + l_{y_i} - l_{y_j}} (-1)^{\lambda_1 + \lambda 2} \\ \times f(\lambda_1 \lambda_3; l_{x_i}) f(\lambda_4 \lambda_2; l_{y_i}) f(\lambda_1 \lambda_4; l_{x_j}) f(\lambda_3 \lambda_2; l_{y_j}) \begin{pmatrix} \lambda_1 & \lambda_3 & l_{x_i} \\ \lambda_4 & \lambda_2 & l_{y_i} \\ l_{x_j} & l_{y_j} & L \end{pmatrix} \\ \times \textstyle\sum_{\mu\nu} (-1)^{\mu} C^{\mu}_{\lambda_3 \lambda_4} C^{\nu}_{\lambda_1 \lambda 2} (\cos\phi_{ij})^{2\nu + \lambda_1 + \lambda_2} (\sin\phi_{ij})^{2\mu + \lambda_3 + \lambda_4} \,, \end{aligned} \tag{18}$$

where the summation is restricted by the following conditions:

$$\begin{aligned} \vec{L} &= \vec{l}_{x_j} + \vec{l}_{y_j} && = \vec{l}_{x_i} + \vec{l}_{y_i} \,, \\ K &= 2n_j + l_{x_j} + l_{y_j} && = 2n_i + l_{x_i} + l_{y_i} \,, \\ &= 2\mu + 2\nu + \lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 \,. \end{aligned} \tag{19}$$

In Eq. (18), the quantities $C^{\alpha}_{\beta\gamma}$ and $f(a, b; c)$ are given by

$$\begin{aligned} C^{\alpha}_{\beta\gamma} &= \frac{\Gamma(2\alpha + \beta + \gamma + 2)}{\Gamma(\alpha + \beta + 3/2)\Gamma(\alpha + \gamma + 3/2)\Gamma(\alpha + 1)\Gamma(\alpha + \beta + \gamma + 2)} \\ f(a, b; c) &= \sqrt{(2a+1)(2b+1)} < a0b0|c0 > \,, \end{aligned} \tag{20}$$

where $< j_1 m_1 j_2 m_2 | jm >$ is a Clebsch-Gordan coefficient (CGC), and the quantity within the large brakets in Eq. (18) is a 9-j symbol.

3. Numerical computation of RRC

The Raynal-Revai coefficient $< l_{x_j} l_{y_j} | l_{x_i} l_{y_i} >_{KL}$ vanishes unless $\vec{l}_{x_j} + \vec{l}_{y_j} = \vec{L} = \vec{l}_{x_i} + \vec{l}_{y_i}$. Furthermore, since $K = 2n_i + l_{x_i} + l_{y_i} = 2n_j + l_{x_j} + l_{y_j}$, ($n_i$, n_j being non-negative integers), we have

$$\begin{array}{lcccccc} |l_{x_j} - l_{y_j}| & \leq & L & \leq & (l_{x_j} + l_{y_j}) & \leq & K\,, \\ |l_{x_i} - l_{y_i}| & \leq & L & \leq & (l_{x_i} + l_{y_i}) & \leq & K\,, \end{array} \tag{21}$$

$$(K - l_{x_i} - l_{y_i}) \quad \text{and} \quad (K - l_{x_j} - l_{y_j}) \quad \text{must be both even integers}\,. \tag{22}$$

Condition (22) further shows that

$$l_{x_i} + l_{y_i} + l_{x_j} + l_{y_j} \quad \text{must be an even integer}\,. \tag{23}$$

The RRC vanishes whenever any one of the conditions (21) and (23) is not satisfied.

Next we note from Eq. (20) (using the symmetry property of the Clebsch-Gordan coefficients) that $f(a, b; c)$ vanishes unless $(a + b - c)$ is an even integer. Hence, from Eq. (18) we must have

$$\begin{array}{lcl} \lambda_1 + \lambda_3 - l_{x_i} & = & 2n_1\,, \\ \lambda_4 + \lambda_2 - l_{y_i} & = & 2n_2\,, \\ \lambda_1 + \lambda_4 - l_{x_j} & = & 2n_3\,, \\ \lambda_3 + \lambda_2 - l_{y_j} & = & 2n_4\,, \end{array} \tag{24}$$

where n_1, n_2, n_3 and n_4 are integers. From the second and fourth relations of Eq. (24), we have

$$\lambda_4 + \lambda_3 + l_{y_j} - l_{y_i} = 2(n_2 - n_4) + 2\lambda_3\,. \tag{25}$$

Next, for the 9-j symbol in Eq. (18) to be nonvanishing, we must have the angular momenta additions:

$$\begin{array}{lcl} \vec{\lambda}_1 + \vec{\lambda}_3 & = & \vec{l}_{x_i}\,, \\ \vec{\lambda}_4 + \vec{\lambda}_2 & = & \vec{l}_{y_i}\,, \\ \vec{\lambda}_1 + \vec{\lambda}_4 & = & \vec{l}_{x_j}\,, \\ \vec{\lambda}_3 + \vec{\lambda}_2 & = & \vec{l}_{y_j}\,. \end{array} \tag{26}$$

Since each of l_{x_i}, l_{y_i}, l_{x_j} and l_{y_j} are integers (being orbital angular momenta associated with the corresponding variables), Eq. (26) shows that either all λ_i's must be integral or all λ_i's must be half integral. In the latter case, Eq. (25) shows that $(\lambda_4 + \lambda_3 + l_{y_j} - l_{y_i})$ is an odd integer and hence from Eq. (18) we see that all RRC must be imaginary. This corresponds to an overall phase factor $e^{i\pi/2}$ in $\mathcal{Y}_{K\alpha_i}(\Omega_i)$ (see Eq. (16)). On the other hand, if all λ_i's are integers, Eq. (25) shows that $(\lambda_4 + \lambda_3 + l_{y_j} - l_{y_i})$ is an even integer and hence Eq. (18) shows that each RRC is real. Since an overall phase is unimportant, we take all λ_i's to be integral and consequently all RRC become real. The last of the relations in Eq. (19) shows that the maximum value of $(\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4)$ is K. Hence, in the numerical algorithm, we select the values of $(\lambda_1, \lambda_2, \lambda_3, \lambda_4)$ and (μ, ν) for a given values of $(K, L, l_{x_i}, l_{y_i}, l_{x_j}, l_{y_j})$ in the following way :

(1) Take all integral values of λ_1 in the interval

$$0 \quad \leq \quad \lambda_1 \quad \leq K\,. \tag{27}$$

(2) For a chosen value of λ_1, integral values of λ_3 are chosen in the interval (using the first relation of Eq. (26))

$$|\lambda_1 - l_{x_i}| \quad \leq \quad \lambda_3 \quad \leq (\lambda_1 + l_{x_i})\,. \tag{28}$$

(3) Similarly for a chosen value of λ_1, integral values of λ_4 are obtained from (using the third relation of Eq. (26))

$$|\lambda_1 - l_{x_j}| \quad \leq \quad \lambda_4 \quad \leq \quad (\lambda_1 + l_{x_j})\,. \tag{29}$$

(4) Since λ_2 must be an integer satisfying <u>both</u> the second and fourth relations of Eq. (26), we have

$$(\lambda_2)_{\min} \quad \leq \quad \lambda_2 \quad \leq \quad (\lambda_2)_{\max}\,, \tag{30}$$

where

$$\begin{aligned} (\lambda_2)_{\min} &= \mathrm{Max}\{|\lambda_3 - l_{y_j}|,\ |\lambda_4 - l_{y_i}|\}\,, \\ (\lambda_2)_{\max} &= \mathrm{Min}\{|\lambda_3 + l_{y_j}|,\ |\lambda_4 + l_{y_i}|\}\,. \end{aligned} \tag{31}$$

(5) For such choices of $\{\lambda_1, \lambda_2, \lambda_3, \lambda_4\}$, we chose only those values which satisfy

$$(K - \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4) = \quad \text{even non} - \text{negative integer} \tag{32}$$

(see the last relation of Eqs. (19)). For one allowed set of values of λ_2, λ_3 and λ_4, we have from the last relation of Eq. (19)

$$\mu + \nu = (K - \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4)/2 = p \quad (\text{integer} \geq 0)\,. \tag{33}$$

(6) We chose integral μ in the interval

$$0 \quad \leq \quad \mu \quad \leq \quad p\,. \tag{34}$$

(7) For a given value of μ, the integral ν is given by

$$\nu = p - \mu \,. \tag{35}$$

With these choices, the indicated sums in Eq. (18) are carried out. Standard codes for Clebsch-Gordan coefficients and 9-j symbols have been used.

A simple check of the calculated RRC is provided by the fact that the RRC form a unitary matrix corresponding to the unitary transformation, Eq. (16), between the orthonormal bases in the partitions "j" and "i":

$$\sum_{l_{x_j} l_{y_j}} < l_{x_j} l_{y_j} \mid l'_{x_i} l'_{y_i} >_{KL} < l_{x_j} l_{y_j} \mid l_{x_i} l_{y_i} >_{KL} = \delta_{l_{x_i} l'_{x_i}} \delta_{l_{y_i} l'_{y_i}} \,. \tag{36}$$

This has been checked for calculated RRC's. In Table 1, we present a few typical (K, L) values with the corresponding sets of allowed (l_{x_i}, l_{y_i}) and (l'_{x_i}, l'_{y_i}) values.

Table 1. Check of the orthonormality relation of RRC for some representative values of the quantum numbers.

K	L	l_{x_i}	l_{y_i}	l'_{x_i}	l'_{y_i}	Left side of Eq. (36)
2	0	0	0	1	1	2.5668486433594317E-17
2	0	0	1	0	1	1.0000000000000001E-00
4	0	2	2	1	1	1.2123413167461349E-16
4	0	2	2	2	2	0.9999999999999966E-00
6	0	2	2	3	3	2.2726910414369584E-16
6	0	3	3	3	3	0.9999999999999989E-00
8	0	0	0	4	4	9.2981178312356860E-16
8	0	4	4	4	4	1.0000000000000002E-00
10	0	5	5	4	4	-6.7465327215857769E-17
10	0	5	5	5	5	1.00000000000 0014E-00
12	0	3	3	6	6	1.3232560460243494E-16
12	0	5	5	5	5	1.0000000000000020E-00
14	0	5	5	2	2	-1.8127860232957633E-16
14	0	7	7	7	7	1.0000000000000045E-00
16	0	3	3	8	8	3.1556424208195771E-16
16	0	4	4	4	4	1.0000000000000026E-00
18	0	3	3	9	9	-1.2449605554415005E-15
18	0	8	8	8	8	1.0000000000000047E-00
20	0	10	10	10	10	1.0000000000000068E-00
20	0	10	10	8	8	3.6284689174711367E-15

The computed left side of Eq. (36), using double precision calculation on a Desktop 486 EISA machine, is shown in the last column.

4. Application to two-electron atoms

As a simple example, we apply the idea of the Raynal-Revai coefficients to the calculation of the ground state energy of two-electron atoms. We take the $i^{\rm th}$ particle as the nucleus of mass m_N and charge $+Ze$ and $j^{\rm th}$ and $k^{\rm th}$ particles as the two electrons of mass $m_j = m_k = m$ and charge $-e$. We have for the Jacobi coordinates describing the relative motion in the partition "i" (from Eq. (1))

$$\begin{aligned} \vec{x}_i &= \beta_i(\vec{r}_j - \vec{r}_k)\,, \\ \vec{y}_i &= (1/\beta_i)(r_i - (\vec{r}_j + \vec{r}_k)/2)) \end{aligned} \quad , \tag{37}$$

where the dimensionless parameter β_i is given by $\beta_i = [(m_N + 2m)/4m_N]^{1/4}$. The Hamiltonian in the partition "i" is [3]

$$H \;=\; -\,\frac{\hbar^2}{m}\beta_i^2(\nabla^2_{x_i} + \nabla^2_{y_i}) + \frac{e^2}{x_i}\beta_i - \frac{Ze^2}{\mid \beta_i\vec{y}_i - (1/(2\beta_i))\,\vec{x}_i \mid} - \frac{Ze^2}{\mid \beta_i\vec{y}_i + (1/(2\beta_i))\,\vec{x}_i \mid}\,. \tag{38}$$

In Eq. (38), the effective mass μ is given by

$$\mu \;=\; m\sqrt{m_N/(m_N + 2m)} \;=\; m/(2\beta_i^2)\,. \tag{39}$$

In atomic units we take $\hbar^2$=m=e^2=1.

Introducing hyperspherical variables as in Eqs. (3) and (4), the Hamiltonian in the partition "i" becomes (in atomic units) [3]

$$\begin{aligned} H \;&=\; -\beta_i^2\left[\frac{1}{\rho^5}\frac{\partial}{\partial\rho}\left(\rho^5\frac{\partial}{\partial\rho}\right) - \frac{\hat{\mathcal{K}}^2(\Omega_i)}{\rho^2}\right] + \frac{\beta_i}{\rho\,\cos\phi_i} \\ &- \frac{Z}{\rho\mid\beta_i\,\sin\phi_i\,\hat{y}_i \,-\, (1/(2\beta_i))\cos\phi_i\,\hat{x}_i\mid} \\ &- \frac{Z}{\rho\mid\beta_i\,\sin\phi_i\,\hat{y}_i \,+\, (1/(2\beta_i))\cos\phi_i\,\hat{x}_i\mid}\,. \end{aligned} \tag{40}$$

A straightforward calculation of the matrix elements of the last two terms in Eq. (40) would be prohibitively involved, both for analytical reduction to a computationally feasible form, as well as for the numerical calculation. Furthermore, the numerical calculation would be both time consuming and inaccurate. The use of the RRC simplifies the calculation to a considerable extent. In the partitions "k" and "j", the third and fourth terms of H become simply $Z\beta_k/(\rho\cos\phi_k)$ and $Z\beta_j/(\rho\cos\phi_j)$, respectively. In the case of a two-electron atom,

$$\beta_j = \beta_k = \left[1 - \frac{m^2}{(m_N + m)^2}\right]^{1/4}\,. \tag{41}$$

For a heavy nucleus, $m_N \gg m$ and $\beta_i \approx 1/\sqrt{2}$, $\beta_j = \beta_k \simeq 1$.

We expand the three-body relative wave function in the complete set of HH appropriate to partition "i" as in Eq. (10). For the ground state of a two-electron atom, the spin wave function of the two electrons is singlet (antisymmetric) and the total orbital angular momentum $L = 0$. Consequently, $l_{x_i} = l_{y_i}$. Hence, the set of quantum numbers represented by α_i is $\{l_{x_i}, l_{x_i}, 0, 0\}$ and the quantum numbers $\{K\alpha_i\}$ can be represented by $\{Kl_{x_i}\}$ only. Furthermore, since the space part of the wave function must be symmetric under exchange of the two electrons, only even values of l_{x_i} ($\leq K/2$) are needed. Corresponding HH is given by [2, 3]

$$\begin{aligned}\mathcal{Y}_{K\alpha_i}(\Omega_i) &\equiv \mathcal{Y}_{Kl_{x_i}l_{x_i}00}(\Omega_i) \\ &= {}^{(2)}P_K^{l_{x_i}l_{x_i}}(\phi_i)\left[Y_{l_{x_i}m_{x_i}}(\theta_{x_i}\phi_{x_i})Y_{l_{x_i}-m_{x_i}}(\theta_{x_i}\phi_{x_i})\right]_{00} \\ &\quad (K \text{ even and } l_{x_i} = 0, 2, 4, \ldots, K/2)\ .\end{aligned} \tag{42}$$

The matrix element of the two-electron repulsion in our chosen partition "i", is

$$\begin{aligned}&< K'l'_{x_i}|\frac{\beta_i}{\rho\cos\phi_i}|Kl_{x_i} > \\ &= \frac{\beta_i}{\rho}\delta_{l'_{x_i},l_{x_i}}\int\limits_0^{\pi/2} {}^{(2)}P_{K'}^{l_{x_i}l_{x_i}}(\phi)\,{}^{(2)}P_K^{l_{x_i}l_{x_i}}(\phi)\sin^2\phi\ \cos\ \phi\,\mathrm{d}\phi\,,\end{aligned} \tag{43}$$

in which we have dropped the suffix i on ϕ, as it is only a variable of integration. Similarly, the matrix element of the third term in the partition "k" is [2, 3]

$$\begin{aligned}&< K'l'_{x_k} \mid \frac{\beta_k}{\rho\cos\phi_k} \mid Kl_{x_k} > \\ &= \frac{\beta_k}{\rho}\delta_{l'_{x_k},l_{x_k}}\int\limits_0^{\pi/2} {}^{(2)}P_{K'}^{l_{x_k}l_{x_k}}(\phi)\,{}^{(2)}P_K^{l_{x_k}l_{x_k}}(\phi)\sin^2\phi\cos\ \phi\,\mathrm{d}\phi\,.\end{aligned} \tag{44}$$

A similar relation holds for the matrix element of the last term of H in the partition "j". Eqs. (43) and (44) show that the matrix elements are essentially the same in the respective partitions, although l_{x_k} and l_{x_j} are not restricted to only even integer values. Each involves only a single, one-dimensional integral to be performed numerically. Using Eq. (17), the matrix elements of the third and fourth terms of H in our chosen partition (i.e., partition "i") become

$$\begin{aligned}< K'l'_{x_i} \mid \frac{Z}{r_{ij}} \mid Kl_{x_i} >= \textstyle\sum_{l_{x_k}} &< l_{x_k}l_{x_k} \mid l'_{x_i}l'_{x_i} >^*_{K'0} \\ &< l_{x_k}l_{x_k} \mid l_{x_i}l_{x_i} >_{K0} < K'l_{x_k} \mid \tfrac{Z\beta_k}{\rho\ \cos\phi_k} \mid Kl_{x_k} >\ .\end{aligned} \tag{45}$$

and

$$\begin{aligned}< K'l'_{x_i} \mid \frac{Z}{r_{ik}} \mid Kl_{x_i} >= \textstyle\sum_{l_{x_j}} &< l_{x_j}l_{x_j} \mid l'_{x_i}l'_{x_i} >^*_{K'0} \\ &< l_{x_j}l_{x_j} \mid l_{x_i}l_{x_i} >_{K0} < K'l_{x_j} \mid \frac{Z\beta_j}{\rho\ \cos\phi_j} \mid Kl_{x_j} >\ .\end{aligned} \tag{46}$$

In Eqs. (45) and (46), the sums over $l_{x'_k}$ and $l_{x'_j}$, respectively, have been performed using the Kronecker δ's in Eq. (44), and a similar one with suffix k replaced by suffix j. Thus, the calculation of the matrix elements of all interactions become very simple and easy to handle numerically.

In Table 2, we compare a few typical matrix elements of $V(\rho, \Omega_i)$ in partition "i" by using RRC (Eq. (45)) and by direct numerical integration. The latter involves expanding $1/r_{ij}$ and $1/r_{ik}$ as the generating function of Legendre polynomials, and then using the addition theorem of spherical harmonics [4]. It is seen that the use of RRC is both accurate and fast compared to the direct evaluation. Furthermore, one should note that although the direct calculation of the matrix element of $1/r_{ij}$ in the partition "i" is possible by the method of Ref. [4], it is not possible for an interaction other than Coulomb or harmonic oscillator. For an arbitrary interaction potential, a direct calculation of the matrix element will involve five-dimensional angular integrations. This becomes very time consuming and inaccuracies creep in easily. Thus, the use of RRC in such cases becomes essential.

Table 2. Comparision of the matrix element of the total interaction (V) evaluated at $\rho = 1$ by using RRC and by direct integration.

$< K, l_1 \vert V \vert K', l'_1 >$	By RRC	By direct integration
$< 0, 0 \vert V \vert 0, 0 >$	-5.589726896	-5.590107406
$< 10, 0 \vert V \vert 2, 0 >$	0.209860018	0.209874304
$< 10, 0 \vert V \vert 10, 0 >$	-4.327704613	-4.327999211
$< 12, 4 \vert V \vert 12, 2 >$	1.266261341	1.266347540
$< 14, 2 \vert V \vert 0, 0 >$	0.000189867	0.000189879
$< 14, 6 \vert V \vert 10, 0 >$	-0.195161836	-0.195175122
$< 16, 8 \vert V \vert 16, 8 >$	-9.600012346	-9.600665855
$< 18, 8 \vert V \vert 2, 0 >$	-0.063249646	-0.063253953
$< 20, 10 \vert V \vert 10, 4 >$	0.000574136	0.000574179
$< 20, 10 \vert V \vert 0, 0 >$	-0.333234831	-0.333257516
$< 20, 10 \vert V \vert 20, 10 >$	-9.857809299	-9.858480377

Table 3. Comparision of binding energies.

$K_{\max}$	BE using RRC	BE by direct calculation
4	2.783965	2.783883
8	2.849803	2.849720
12	2.875594	2.875508
16	2.887128	2.887043
20	2.893168	2.893083

For completeness, we compare in Table 3 the binding energies calculated by an exact numerical solution of the coupled differential equation by the renormalized Numerov method [21], by the present method and one in which matrix elements are calculated by direct numerical integration [2, 3]. We find, the results agree within computational errors.

5. Conclusion

We note that the use of RRC is essential in solving the three-body equation if the interparticle interaction is other than Coulomb or harmonic oscillator. We have proposed here an algorithm for the computation of the RRC which is fast and accurate. These coefficients may be calculated once only and stored, resulting in an efficient and highly economical numerical computation.

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RAČUN RAYNAL-REVAIJEVIH KOEFICIJENATA ZA HIPERSFERIČNI PRISTUP PROBLEMU TRI TIJELA

Račun matričnih elemenata dvočestičnih međudjelovanja, potreban za metodu hipersferičnih harmonika u sustavu tri tijela, bitno se pojednostavi razvojem bra i ket vektora u bazi hipersfreričnih harmonika koja je prikladna za razdjelu koja odgovara paru koji međudjeluje. To uključuje Raynal-Revaijeve koeficijente (RRC) koji su transformacijski koeficijenti između baza hipersferičnih harmonika koje odgovaraju dvjema razdjelama. U ovom se radu izlaže brz algoritam za točno računalno određivanje RRC. Primijenili smo tu tehniku za dvoelektronske atome sa čistim Coulombovim međudjelovanjem parova, te usporedili dobivene ishode s ishodima izravnih numeričkih integracija. Kako pojedini matrični elementi, tako i energije vezanja slažu se do na pogrešku računanja.