Int J Theor Phys (2010) 49: 2230–2245
DOI 10.1007/s10773-010-0410-6

The Transformation of Irreducible Tensor Operators Under Spherical Functions

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Received: 7 April 2010 / Accepted: 14 June 2010 / Published online: 1 July 2010

Abstract The irreducible tensor operators and their tensor products employing Racah algebra are studied. Transformation procedure of the coordinate system operators act on are introduced. The rotation matrices and their parametrization by the spherical coordinates of vector in the fixed and rotated coordinate systems are determined. A new way of calculation of the irreducible coupled tensor product matrix elements is suggested. As an example, the proposed technique is applied for the matrix element construction for two electrons in a field of a fixed nucleus.

Keywords Irreducible tensor operator · Rotation matrix · Spherical function · Matrix element

1 Introduction

The main aim of present work is to parametrize irreducible matrix representation of either $SO(3)$ or $SU(2)$ group by the coordinates of $S^2 \times S^2$, where S^2 denotes the unit 2-dimension sphere. The motivation is grounded on the following occasions: (i) the difficulties in theoretical atomic spectroscopy arising through multiple integrals of N-electron angular parts; (ii) inconvenience of the application of Wigner-Eckart theorem for irreducible tensor operator matrix elements on the basis of functions, expressed in terms of Wigner D-function.

In theoretical atomic physics the algorithms of matrix element calculation for atomic quantities on the basis of many-electron wave functions are well known and widely used [1, 2]. The construction of matrix element is based on the structure of many-electron function which is represented by coupled tensor product of one-electron eigenstates. The latter formulation leads to the complicated N-electron angular parts and various techniques,

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in order to simplify the calculation of many-electron matrix element [3–5]. According to Racah [6, 7], the basis eigenstates ϕ_m^λ behave in the same way as the spherical tensor operators T_m^λ by means of the transformations under irreducible matrix representations. The eigenstates ϕ_m^λ of the central-field atomic Hamiltonian are usually enunciated by spherical functions on $SO(3)/SO(2)$ quotient group, multiplied by 2×1 spin matrices. However, in [8] it was showed that $\phi(\hat{x}_\xi)=\phi(\theta_\xi,\varphi_\xi)$ can be expressed by the Wigner $D(\bar{\Omega}_\xi)$ functions on $SU(2)$, where $\bar{\Omega}_\xi=(\Phi_\xi,\Theta_\xi,0)=(\varphi_\xi+\pi/2,\theta_\xi,0)$. Furthermore, Bhatia et al. [9] constructed two-electron wave function $\Phi(\hat{x}_1,\hat{x}_2)$ in terms of the spherical functions $D(\Omega)$, where Ω, as usually, denotes Euler angles (Φ,Θ,Ψ), i.e., the rotation on S^2 from $\hat{x}_1$ to $\hat{x}_2$ and vice versa. Unfortunately, it is evident that for this basis the Wigner-Eckart theorem can not be applied directly, what leads to a necessity to expand $D(\Omega)$ over $\hat{x}_1,\hat{x}_2$.

In this work, we start from notations in [1, 10]. We express rotation matrix by the spherical coordinates of vector in the fixed and rotated coordinate systems, rather than the rotation angles in an explicit form (Sects. 3 and 4). Following this route, we demonstrate the technique of matrix element construction, when $2N$-integral (over the spherical coordinates θ_ξ,φ_ξ with $\xi=1,2,\dots,N$) is reduced up to a double one (Sect. 6). The technique is based on studied properties of integrity for obtained spherical functions (Sect. 5) and proposed transformation coefficients, called the rotated Clebsch-Gordan coefficients (CGC) or simply RCGC (Sect. 6.1).

2 Preliminaries

The well known transformation formula for the k-rank spherical tensor operators T_q^k, $q\in[-k,+k]$, is given by

$$T_q^k(K_2)=\sum_{q'}D_{qq'}^k(\Omega)T_{q'}^k(K_1), \tag{1}$$

where the symbols K_1 and K_2 show that the corresponding tensor operator is defined in the fixed and rotated coordinate system, respectively. The generalized spherical function $D_{qq'}^k$ on $SO(3)$ or $SU(2)$ is of the form [10]

$$D_{qq'}^k(\Omega)=a(k,q,q')\mathrm{e}^{\mathrm{i}(q\Phi+q'\Psi)}\left\{\cos\left(\frac{1}{2}\Theta\right)\right\}^{2k}\sum_p b_p(k,q,q')\left\{\tan\left(\frac{1}{2}\Theta\right)\right\}^{2p-q+q'}, \tag{2}$$

$$a(k,q,q')=\mathrm{i}^{q'-q}\sqrt{(k+q)!(k-q)!(k+q')!(k-q')!}, \tag{3}$$

$$b_p(k,q,q')=\frac{(-1)^p}{p!(p+q'-q)!(k+q-p)!(k-q'-p)!}, \tag{4}$$

where $\Phi,\Psi\in[0,2\pi]$ and $\Theta\in[0,\pi]$. In this work, the standard phase system is used, where the complex and Hermitian conjugate operators accordingly denote $\overline{D_{qq'}^k}=(-1)^{q-q'}D_{-q-q'}^k$ and $T_q^{k\dagger}=(-1)^{k-q}T_{-q}^k$. It follows from (1), the rotated coordinate system K_2 depends on the fixed system K_1 and the rotation angles Ω. Such dependency can be reformulated in a different way: the rotation angles Ω depend on the coordinates of given (or known) point, located on S^2 in the fixed and rotated coordinate systems. These spherical coordinates will be denoted $\hat{x}_1$ (in K_1) and $\hat{x}_2$ (in K_2). On the other hand, the spherical function D that depends on Ω, can also be expressed as a function of the variables $\hat{x}_1,\hat{x}_2$. In the next section the latter dependency in an explicit form is presented.

3 The Geometry of Rotation Angles

In order to express the generalized spherical function D by the coordinates $\hat{x}_1$, $\hat{x}_2$ of vector in the fixed and rotated coordinate system, the following geometry is defined. Suppose we have a map $\Omega : S^2 \times S^2 \mapsto SO(3)$. Its representation onto the linear space of vectors $\hat{r}_i = \boldsymbol{r}_i/|\boldsymbol{r}_i| = (x_i \;\; y_i \;\; z_i)^{\mathrm{T}} \in \mathbf{R}^3$ ($|\boldsymbol{r}_i| = \text{const.}\ \forall i \in \mathbb{Z}^+$—positive integers) is associated in the following way

$$\begin{cases} \hat{r}_2 = R(\Omega)\hat{r}_1, \\ x_i = \sin\theta_i \cos\varphi_i, \qquad y_i = \sin\theta_i \sin\varphi_i, \qquad z_i = \cos\theta_i, \end{cases} \tag{5}$$

where the coordinate system K_1 is rotated (the ZXZ convention) by the rotation matrix R of $SO(3)$ [10, 11]. Then the system of three equations in (5) is rewritten in the form

$$\begin{cases} x_2 = -x_1' \sin\varphi - u' \cos\varphi, \\ y_2 = x_1' \cos\varphi - u' \sin\varphi, \\ z_2 = y_1' \sin\theta + z_1' \cos\theta, \end{cases} \tag{6}$$

where

$$u' = y_1' \cos\theta - z_1' \sin\theta, \tag{7}$$

$$\begin{cases} x_1' = x_1 \cos\Psi - y_1 \sin\Psi, \\ y_1' = x_1 \sin\Psi + y_1 \cos\Psi, \\ z_1' = z_1. \end{cases} \tag{8}$$

The parameter Ψ is chosen optionally in the range $[0, 2\pi]$. Partial solutions of the subsystems (x_2, z_2) and (y_2, z_2) for θ, φ are substituted then in (2). Optimal values of Ψ are found by solving the variational equation, varying obtained spherical function with respect to Ψ (for details see Appendix A). We attain, that solutions in $\mathbb{R}$ satisfy equation

$$\sin\theta_1 \cos(\varphi_1 + \Psi) = 0. \tag{9}$$

The solutions are:

1. $\cos(\varphi_1 + \Psi) = 0 \Rightarrow \Psi = -\varphi_1 + \sigma' \frac{\pi}{2} + \bar{\sigma}\pi + 2\pi n', n' \in \mathbb{Z}^+, \sigma' = \pm 1,\ \bar{\sigma} = 0, \pm 1.$
2. $\sin\theta_1 = 0,\ \forall \Psi \in [0, 2\pi].$

First of all let us analyze item (1)—the situation when $\sin\theta_1 \neq 0$. Then $y_1' = \sigma' \sin\theta_1$, if $\bar{\sigma} = 0$ and $y_1' = -\sigma' \sin\theta_1$ if $\bar{\sigma} = \pm 1$ (see (8)). Secondly, when item (2) is valid, we obtain that $\theta_1 = 0$ or $\theta_1 = \pi$. The parameter Ψ then could be of any value in $[0, 2\pi]$. It is clear that the solution $\sin\theta_1 = 0$ (item (2)) is a particular case of item (1) if the angle Ψ is chosen to be equal to $\Psi = -\varphi_1 + \sigma' \frac{\pi}{2} + \bar{\sigma}\pi + 2\pi n'$. Since in item (2) the solution Ψ can have arbitrary values in $[0, 2\pi]$, we choose it to be equal to the solution given by item (1). Consequently, the solutions of the system in (6) are

$$\Phi = \varphi_2 + \alpha \frac{\pi}{2}, \qquad \Theta = \beta(\theta_1 - \gamma\theta_2) + 2\pi n, \qquad \Psi = -\varphi_1 + \delta \frac{\pi}{2} + 2\pi n', \tag{10}$$

where $n' \in \mathbb{Z}^+$ and the values for α, β, γ, δ, n are presented in Table 1. The function $\Omega(\hat{x}_1, \hat{x}_2)$ may be expanded into several different geometries, representing miscellaneous rotations.

Table 1 The values for the parameters $\alpha, \beta, \gamma, \delta, n$

The maps			α	β	γ	δ	n	The maps		α	β	γ	δ	n
$\Omega_1^{\pm}$	Ω_1^+	Ω_{11}^+	+	+	+	−	0	$\Omega_2^{\pm}$	Ω_2^+	+	+	−	+	0
		Ω_{12}^+	−	+	+	+								
	Ω_1^-	Ω_{11}^-	+	−	+	−			$\Omega_2^{\pm}$	−	−	−	−	1
		Ω_{12}^-	−	−	+	+								

(a) $\theta_1 - \theta_2 \in [0, \pi]$.

$$\varphi_2 \in [0,\pi]: \quad \Omega_{11}^+ = \begin{cases} \Phi = \varphi_2 + \frac{\pi}{2}, \\ \Theta = \theta_1 - \theta_2, \\ \Psi = -\varphi_1 - \frac{\pi}{2}(2\pi); \end{cases} \qquad \varphi_2 \in (\pi, 2\pi]: \quad \Omega_{12}^+ = \begin{cases} \Phi = \varphi_2 - \frac{\pi}{2}, \\ \Theta = \theta_1 - \theta_2, \\ \Psi = -\varphi_1 + \frac{\pi}{2}(2\pi). \end{cases} \tag{11}$$

(b) $\theta_2 - \theta_1 \in [0, \pi]$.

$$\varphi_2 \in [0,\pi]: \quad \Omega_{11}^- = \begin{cases} \Phi = \varphi_2 + \frac{\pi}{2}, \\ \Theta = \theta_2 - \theta_1, \\ \Psi = -\varphi_1 - \frac{\pi}{2}(2\pi); \end{cases} \qquad \varphi_2 \in (\pi, 2\pi]: \quad \Omega_{12}^- = \begin{cases} \Phi = \varphi_2 - \frac{\pi}{2}, \\ \Theta = \theta_2 - \theta_1, \\ \Psi = -\varphi_1 + \frac{\pi}{2}(2\pi). \end{cases} \tag{12}$$

(c) $\theta_1 + \theta_2 \in (0, \pi]$.

$$\Omega_2^+ = \begin{cases} \Phi = \varphi_2 + \frac{\pi}{2}, \\ \Theta = \theta_1 + \theta_2, \\ \Psi = -\varphi_1 + \frac{\pi}{2}(2\pi). \end{cases} \tag{13}$$

(d) $\theta_1 + \theta_2 \in [\pi, 2\pi]$.

$$\Omega_2^- = \begin{cases} \Phi = \varphi_2 - \frac{\pi}{2}, \\ \Theta = 2\pi - \theta_1 - \theta_2, \\ \Psi = -\varphi_1 - \frac{\pi}{2}(2\pi). \end{cases} \tag{14}$$

The function $\Omega_1^+ = \{\Omega_{11}^+, \Omega_{12}^+\}$ is matched for the case when $\theta_1 \geq \theta_2$, while the function $\Omega_1^- = \{\Omega_{11}^-, \Omega_{12}^-\}$ is matched for the case when $\theta_2 \geq \theta_1$. The functions $\Omega_{11}^{\pm}$ describe the rotations for given $\varphi_2 \in [0, \pi]$; according to $\Omega_{12}^{\pm}$, rotations are realized for $\varphi_2 \in (\pi, 2\pi]$. The function $\Omega_2^{\pm} = \{\Omega_2^+, \Omega_2^-\}$ defines another possible rotation for the given angles $\theta_1 + \theta_2 \in (0, \pi]$ or $\theta_1 + \theta_2 \in [\pi, 2\pi]$. Note, if $\varphi_2 \in [\frac{3\pi}{2}, 2\pi]$, then for the rotation Ω_2^+, the angle $\Phi > 2\pi$. On the other hand, rotation over the angle 2π geometrically is equivalent to the initial state. Thus, one can choose whether $\Phi > 2\pi$ or $0 < \Phi - 2\pi < 2\pi$. This holds for the rotation Ω_2^-. Finally, when $\theta_1 = \theta_2 = 0$, the angle $\Theta = 0$ and the angles Φ, Ψ acquire any values in $[0, 2\pi]$. Then the rotation matrix $R(\Omega) = R_z(\Phi + \Psi)$. Hence, in this case the full rotation is made by the angle $\Phi + \Psi$ around the z-axis. In other words, if $\theta_1 = \theta_2 = 0$, the rotation by the Euler angles Ω is not singularly defined. Further it will be assumed that θ_1 and θ_2 are not equal to zero at the same time (that is why the range of $\theta_1 + \theta_2$ for Ω_2^+ is open from the left).

4 Spherical Functions

In the previous section, the mapping from $S^2 \times S^2$ to $SO(3)$ has been defined. It was demonstrated that possible rotations in $\mathbf{R}^3$ from K_1 to K_2 could be realized by the rotation angles $\Omega_1^{\pm} = \{\Omega_1^+, \Omega_1^-\} = \{\Omega_{11}^+, \Omega_{12}^+, \Omega_{11}^-, \Omega_{12}^-\}$ and $\Omega_2^{\pm} = \{\Omega_2^+, \Omega_2^-\}$. If substituting these functions in (2), we would obtain the following spherical function (for alternative expressions, see Appendix B)

$$\begin{aligned}
&\big(n, n'; \alpha, \beta, \gamma, \delta | \hat{x}_1, \hat{x}_2\big)^k_{qq'} \\
&\quad = \mathrm{i}^{\alpha q + \delta q'} (-1)^{2(nk+n'q')} \beta^{q'-q} a\big(k, q, q'\big) \mathrm{e}^{\mathrm{i}(q\varphi_2 - q'\varphi_1)} \\
&\qquad \times \left\{\cos\left[\frac{1}{2}(\theta_1 - \gamma\theta_2)\right]\right\}^{2k} \sum_p b_p(k, q, q') \left\{\tan\left[\frac{1}{2}(\theta_1 - \gamma\theta_2)\right]\right\}^{2p+q'-q}, \qquad (15)
\end{aligned}$$

where $k \in \mathbb{Z}^+, \mathbb{Q}^+$ and $\mathbb{Q}^+ = \{m + 1/2; m \in \mathbb{Z}^+\}$; the indices $q, q' \in [-k, +k]$. Let us define particular cases of (15) in the following way

$$\big(0, n'; +, \pm, +, - | \hat{x}_1, \hat{x}_2\big)^k_{qq'} = {}^{\pm}\xi^k_{qq'}\big(\hat{x}_1, \hat{x}_2\big), \qquad (16)$$

$$\big(0, n'; -, \pm, +, + | \hat{x}_1, \hat{x}_2\big)^k_{qq'} = {}^{\pm}\vartheta^k_{qq'}\big(\hat{x}_1, \hat{x}_2\big) = (-1)^{q'-q}\, {}^{\pm}\xi^k_{qq'}\big(\hat{x}_1, \hat{x}_2\big), \qquad (17)$$

$$\big(0, n'; +, +, -, + | \hat{x}_1, \hat{x}_2\big)^k_{qq'} = {}^{+}\zeta^k_{qq'}\big(\hat{x}_1, \hat{x}_2\big), \qquad (18)$$

$$\big(1, n'; -, -, -, - | \hat{x}_1, \hat{x}_2\big)^k_{qq'} = {}^{-}\zeta^k_{qq'}\big(\hat{x}_1, \hat{x}_2\big) = (-1)^{2q'}\, {}^{+}\zeta^k_{qq'}\big(\hat{x}_1, \hat{x}_2\big), \qquad (19)$$

and the matrices

$$\Omega_1^{\pm} :\ {}^{\pm}\eta^k\big(\hat{x}_1, \hat{x}_2\big) \in \big\{ {}^{\pm}\xi^k\big(\hat{x}_1, \hat{x}_2\big),\ {}^{\pm}\vartheta^k\big(\hat{x}_1, \hat{x}_2\big)\big\}. \qquad (20)$$

It is seen, the spherical functions ${}^{\pm}\eta^k_{qq'}(\hat{x}_1, \hat{x}_2)$ and ${}^{\pm}\zeta^k_{qq'}(\hat{x}_1, \hat{x}_2)$ are the generalized spherical functions $D^k_{qq'}(\Omega_1^{\pm})$ and $D^k_{qq'}(\Omega_2^{\pm})$ parametrized by the coordinates of $S^2 \times S^2$, respectively. Particularly, the matrix ${}^{+}\eta^k(\hat{x}_1, \hat{x}_2)$ represents the rotation in $\mathbf{R}^3$ from K_1 to K_2, when $\theta_1 \geq \theta_2$ and it is associated to the map Ω_1^+, while the matrix ${}^{-}\eta^k(\hat{x}_1, \hat{x}_2)$ describes the rotation from K_1 to K_2 when $\theta_2 \geq \theta_1$ and it is associated to the map Ω_1^-. The matrices ${}^{+}\zeta^k(\hat{x}_1, \hat{x}_2)$ and ${}^{-}\zeta^k(\hat{x}_1, \hat{x}_2)$ are related to the maps Ω_2^+ and Ω_2^-.

In accordance with (16)–(19), the spherical functions ${}^{\pm}\xi$, ${}^{\pm}\vartheta$ and ${}^{\pm}\zeta$ are connected to each other as follows

$$\begin{aligned}
&{}^{-}\xi^k_{qq'} = (-1)^{q'-q}\, {}^{+}\xi^k_{qq'}, \qquad {}^{-}\vartheta^k_{qq'} = (-1)^{q'-q}\, {}^{+}\vartheta^k_{qq'}, \\
&{}^{+}\vartheta^k_{qq'} = {}^{-}\xi^k_{qq'}, \qquad {}^{-}\zeta^k_{qq'} = (-1)^{2q'}\, {}^{+}\zeta^k_{qq'}.
\end{aligned} \qquad (21)$$

It directly follows from (21) that

$${}^{+}\eta^k_{qq'} = {}^{-}\eta^k_{qq'} = \eta^k_{qq'} \in \big\{ {}^{+}\xi^k_{qq'},\ {}^{-}\xi^k_{qq'}\big\}, \qquad {}^{-}\xi^k_{qq'} = \overline{{}^{+}\xi^k_{-q-q'}}, \qquad (22)$$

where the column vectors of ${}^{\pm}\xi^k$ are orthonormal, i.e.,

$$\sum_q {}^{+}\xi^k_{qq'}\ {}^{-}\xi^k_{-q-q''} = \delta_{q'q''}. \qquad (23)$$

The latter condition holds for the rest of spherical functions.

It is noticeable, the matrices η^k and ${}^{\pm}\zeta^k$ are the unitary irreducible matrix representations of $SO(3)$ (for $k \in \mathbb{Z}^+$) or of $SU(2)$ (for $k \in \mathbb{Q}^+$), parametrized by the coordinates of $S^2 \times S^2$. Hence, the irreducible tensor operators T^k_q transform among themselves as follows (to compare, see (1))

$$\begin{aligned} \Omega_1^{\pm} &: T^k_q(K_2) = \sum_{q'} \eta^k_{qq'}(\hat{x}_1, \hat{x}_2) T^k_{q'}(K_1), \\ \Omega_2^{\pm} &: T^k_q(K_2) = \sum_{q'} {}^{\pm}\zeta^k_{qq'}(\hat{x}_1, \hat{x}_2) T^k_{q'}(K_1). \end{aligned} \tag{24}$$

The transformation formula for the maps $\Omega_1^{\pm}$ is restricted by the condition $\theta_1 \neq \theta_2$. In a contrary case, only the maps $\Omega_2^{\pm}$ are valid. Consequently, the reduction formulas for the spherical functions

$${}^{\pm}\tau^k_{qq'}(.,.) \in \left\{\eta^k_{qq'}(.,.),\ {}^{\pm}\zeta^k_{qq'}(.,.)\right\} \tag{25}$$

are these

$${}^{\pm}\tau^{k_1}_{q_1q_1'}(.,.)\,{}^{\pm}\tau^{k_2}_{q_2q_2'}(.,.) = \sum_k {}^{\pm}\tau^k_{qq'}(.,.) \begin{bmatrix} k_1 & k_2 & k \\ q_1 & q_2 & q \end{bmatrix} \begin{bmatrix} k_1 & k_2 & k \\ q_1' & q_2' & q' \end{bmatrix}, \tag{26}$$

where in the brackets $(.,.)$ the spherical coordinates of $S^2 \times S^2$ are given. The Clebsch-Gordan coefficients of $SU(2)$ are none zero only when $q = q_1 + q_2$ and $q' = q_1' + q_2'$. The summation is performed over $k = |k_1 - k_2|, |k_1 - k_2| + 1, \ldots, k_1 + k_2$.

Example Suppose, $\hat{x}_1 = (\frac{\pi}{6}, \frac{\pi}{4})$ and $\hat{x}_2 = (\frac{\pi}{3}, \pi)$. Possible rotations are realized then in accordance with $\Omega_{11}^{-} = (\frac{3\pi}{2}, \frac{\pi}{6}, \frac{5\pi}{4})$, $\Omega_2^{+} = (\frac{3\pi}{2}, \frac{\pi}{2}, \frac{\pi}{4})$. Transformation formulas in (24) are valid for the spherical functions ${}^{-}\xi^k_{qq'}(\frac{\pi}{6}, \frac{\pi}{4}, \frac{\pi}{3}, \pi)$ that are related to and ${}^{+}\zeta^k_{qq'}(\frac{\pi}{6}, \frac{\pi}{4}, \frac{\pi}{3}, \pi)$ which coequal to $D^k_{qq'}(\frac{3\pi}{2}, \frac{\pi}{6}, \frac{5\pi}{4})$ and $D^k_{qq'}(\frac{3\pi}{2}, \frac{\pi}{2}, \frac{\pi}{4})$. Suppose $k = \frac{5}{2}$ and $q = -\frac{1}{2}$, $q' = \frac{3}{2}$. Then

$$\begin{aligned} {}^{-}\xi^{\frac{5}{2}}_{-\frac{1}{2}\frac{3}{2}}\left(\frac{\pi}{6}, \frac{\pi}{4}, \frac{\pi}{3}, \pi\right) &= D^{\frac{5}{2}}_{-\frac{1}{2}\frac{3}{2}}\left(\frac{3\pi}{2}, \frac{\pi}{6}, \frac{5\pi}{4}\right) = \frac{(-1)^{\frac{1}{8}}}{32}(13 - 3\sqrt{3}), \\ {}^{+}\zeta^{\frac{5}{2}}_{-\frac{1}{2}\frac{3}{2}}\left(\frac{\pi}{6}, \frac{\pi}{4}, \frac{\pi}{3}, \pi\right) &= D^{\frac{5}{2}}_{-\frac{1}{2}\frac{3}{2}}\left(\frac{3\pi}{2}, \frac{\pi}{2}, \frac{\pi}{4}\right) = \frac{(-1)^{\frac{5}{8}}}{4}. \end{aligned}$$

In accordance with (21), it is possible to find out how all other spherical functions are related to the calculated functions above.

5 The Integral of Spherical Functions

The choice of geometries $\Omega_1^{\pm}$, $\Omega_2^{\pm}$ is convenient for other applications of obtained spherical functions ${}^{\pm}\tau^k_{qq'}$. This is because the parameters θ_1, θ_2 and φ_1, φ_2 are separated. Consequently, the functions which depend on these parameters can be integrated separately, i.e., the integral on S^2 is naturally separated into the integrals over φ_i and over θ_i. By definition, the functions

${}^{\pm}\tau^k_{qq'}(\hat{x}_1,\hat{x}_2)$ are determined in different areas $L^2(\Omega)\subset S^2$, which restrict the existence of integrity. Therefore, we construct the integral

$$\mathcal{S}^k_{qq'}(\hat{x}_1;\gamma)=\int_{S^2}\mathrm{d}\hat{x}_2\big(n,n';\alpha,\beta,\gamma,\delta|\hat{x}_1,\hat{x}_2\big)^k_{qq'}. \tag{27}$$

Suppose, $\gamma=+1$, i.e., the map $\Omega_1^{\pm}$ is realized. Let the areas (or paths of integration) on S^2 be

$$\begin{aligned} L^2\big(\Omega^+_{11}\big)&=\big\{\varphi_2\in[0,\pi];\theta_2\in[0,\theta_1]\big\},\\ L^2\big(\Omega^+_{12}\big)&=\big\{\varphi_2\in[\pi,2\pi];\theta_2\in[0,\theta_1]\big\},\\ L^2\big(\Omega^-_{11}\big)&=\big\{\varphi_2\in[0,\pi];\theta_2\in[\theta_1,\pi]\big\},\\ L^2\big(\Omega^-_{12}\big)&=\big\{\varphi_2\in[\pi,2\pi];\theta_2\in[\theta_1,\pi]\big\}.\end{aligned} \tag{28}$$

Here $\Omega^{\pm}_{11}$ and $\Omega^{\pm}_{12}$ mark the existence of integrable spherical functions ${}^{\pm}\xi^k_{qq'}(\hat{x}_1,\hat{x}_2)$ in the corresponding areas $L^2(\Omega^{\pm}_{11})$ and $L^2(\Omega^{\pm}_{12})$. The parameters $\alpha,\beta,\gamma,\delta,n$ are determined then according to the values presented in Table 1 and the equations in (10). It is clear, the spherical function ${}^{+}\xi$ is integrable in $L^2(\Omega^+_{11})$ with $n'\in\{1,2\}$ and in $L^2(\Omega^-_{12})$ with $n'\in\{0,1\}$; the function ${}^{-}\xi$ is integrable in $L^2(\Omega^-_{11})$ with $n'\in\{1,2\}$ and in $L^2(\Omega^+_{12})$ with $n'\in\{0,1\}$. But ${}^{-}\xi^k_{qq'}=(-1)^{q'-q}\,{}^{+}\xi^k_{qq'}$ (see (21)). This implies

$$\begin{aligned}\mathcal{S}^k_{qq'}\big(\hat{x}_1;+\big)&=\int_{L^2(\Omega^+_{11})}\mathrm{d}\hat{x}_2\,{}^{+}\xi^k_{qq'}\big(\hat{x}_1,\hat{x}_2\big)+\int_{L^2(\Omega^-_{11})}\mathrm{d}\hat{x}_2\,{}^{-}\xi^k_{qq'}\big(\hat{x}_1,\hat{x}_2\big)\\ &\quad+\int_{L^2(\Omega^+_{12})}\mathrm{d}\hat{x}_2\,{}^{-}\xi^k_{qq'}\big(\hat{x}_1,\hat{x}_2\big)+\int_{L^2(\Omega^-_{12})}\mathrm{d}\hat{x}_2\,{}^{+}\xi^k_{qq'}\big(\hat{x}_1,\hat{x}_2\big)\\ &=\lambda_{q'}(\varphi_1)\mathrm{i}^{q-q'-1}\frac{(-1)^q-1}{q}\big((-1)^{q'}+1\big)a(k,q,q')\mathrm{e}^{-\mathrm{i}q'\varphi_1}\\ &\quad\times\sum_p b_p(k,q,q')\big({}_pI^k_{qq'}(\theta_1;+;0,\theta_1)+(-1)^{q-q'}\,{}_pI^k_{qq'}(\theta_1;+;\theta_1,\pi)\big),\end{aligned} \tag{29}$$

$$\lambda_{q'}(\varphi_1)=\begin{cases}(-1)^{q'}, & \varphi_1\in[0,\frac{\pi}{2}],\\ (-1)^{2q'}, & \varphi_1\in(\frac{\pi}{2},\frac{3\pi}{2}],\\ (-1)^{3q'}, & \varphi_1\in(\frac{3\pi}{2},2\pi].\end{cases} \tag{30}$$

The definition of ${}_pI^k_{qq'}$ is given by the formula

$${}_pI^k_{qq'}(\theta_1;\gamma;a,b)=\int_a^b\mathrm{d}\theta_2\sin\theta_2\left\{\cos\left[\frac{1}{2}(\theta_1-\gamma\theta_2)\right]\right\}^{2k}\left\{\tan\left[\frac{1}{2}(\theta_1-\gamma\theta_2)\right]\right\}^{2p+q'-q}. \tag{31}$$

For $\gamma=+1$, the integration is performed making the change of integrand $z=\tan[(\theta_1-\theta_2)/2]$. After some ordinary trigonometric manipulations it acquires the form

$${}_pI^k_{qq'}(\theta_1;+;a,b)=2\big\{2I_1^{p+}(a,b)\cos\theta_1+(I_2^{p+}(a,b)-I_0^{p+}(a,b))\sin\theta_1\big\}, \tag{32}$$

$$I_s^{p+}(a,b)=I_s^{p+}\left(\tan\frac{\theta_1-b}{2}\right)-I_s^{p+}\left(\tan\frac{\theta_1-a}{2}\right) \tag{33}$$

with $s = 0, 1, 2$ and $I_s^{p+}(z)$ defined by

$$I_s^{p+}(z) = \int_{\mathbb{R}} \mathrm{d}z \frac{z^{2p+q'-q+s}}{(1+z^2)^{k+2}} = \frac{z^{2p+q'-q+s+1}}{2p+q'-q+s+1} \times {}_2F_1\left(\frac{2p+q'-q+s+1}{2}, k+2; \frac{2p+q'-q+s+3}{2}; -z^2\right) + \text{const.}, \quad (34)$$

where ${}_2F_1$ denotes Gauss hypergeometric function.

When $\theta_1 = 0$ or $\theta_1 = \pi$, the function $I_s^{p+}(0, \pi)$ depends on infinite variables ($z = \pm\infty$). For this reason bellow the boundary values of ${}_pI_{qq'}^k(\theta; +; 0, \pi)$ are presented.

1. $\theta = 0$. Then ${}_pI_{qq'}^k(0; +; 0, \pi) = 4I_1^{p+}(-\infty)$ (since $I_1^{p+}(0) = 0$), where

$$I_1^{p+}(-\infty) = \frac{(-1)^{q'-q}}{2} B\left(k+1-p+\frac{q-q'}{2}, 1+p+\frac{q'-q}{2}\right) \quad (35)$$

   with B being Beta function.
2. $\theta = \pi$. Then

$${}_pI_{qq'}^k(\pi; +; 0, \pi) = (-1)^{q-q'}\, {}_pI_{qq'}^k(0; +; 0, \pi). \quad (36)$$

For example, it directly follows from (31), (36) that

$$I_2 = \int_0^\pi \mathrm{d}\theta \sin^{2k+1}\theta \cos^\gamma\theta = [1+(-1)^\gamma] I_1^p(\infty), \quad (37)$$

$$I_1^p(\infty) = \frac{1}{2} B\left(k+1, \frac{\gamma+1}{2}\right), \quad (38)$$

where the left hand side of I_2 is the same integral discussed by Pinchon et al. [12] ((19)–(20)), when developing rotation matrices for real spherical harmonics.

When $k \in \mathbb{Z}^+$, the integral of the spherical function η acquires the form

$$\mathcal{S}_{qq'}^k(\hat{x}_1; +) = \delta_{q0}\pi \mathrm{i}^{-q'}((-1)^{q'}+1) a(k, 0, q') \mathrm{e}^{-\mathrm{i}q'\varphi_1} \times \sum_p b_p(k, 0, q')_p I_{0q'}^k(\theta_1; +; 0, \pi). \quad (39)$$

Hence, for integer k, the integral of $(0, n'; \alpha, \beta, +, \delta|\hat{x}_1, \hat{x}_2)_{qq'}^k$ is non-zero only if $q = 0$ and q' is even. Particularly, $\mathcal{S}_{00}^0(\hat{x}_1; +) = 4\pi$.

Finally, the integration of $(n, n'; \alpha, \beta, -, \delta|\hat{x}_1, \hat{x}_2)_{qq'}^k$ must be proceeded. For the maps $\Omega_2^\pm$ there is no difference which value of θ_1 and θ_2 is greater or less (or equal). It has been demonstrated earlier, that for Ω_2^+ the condition $0 \le \theta_1 + \theta_2 \le \pi$ ($\alpha = \beta = \delta = +$, $n = 0$) must be satisfied, while for Ω_2^- the restriction is: $\pi \le \theta_1 + \theta_2 \le 2\pi$ ($\alpha = \beta = \delta = -$, $n = 1$). But when integrating ${}^\pm\zeta_{qq'}^k(\hat{x}_1, \hat{x}_2)$ over θ_2, the angle θ_2 acquires all values in $[0, \pi]$. This means the map Ω_2^+ is valid only if $\theta_1 = 0$ and the map Ω_2^- is realized only for $\theta_1 = \pi$. Hence, the integration of ${}^\pm\zeta_{qq'}^k(\hat{x}_1, \hat{x}_2)$ can not be correctly performed for any values of θ_1, except for $\theta_1 = 0$ or $\theta_1 = \pi$. In other words, the spherical functions ${}^\pm\zeta_{qq'}^k(\hat{x}_1, \hat{x}_2)$, representing the rotations $\Omega_2^\pm$, are not integrable on S^2, in general. For this reason, we conclude, that the most preferable spherical functions (at least for integration) are $\eta_{qq'}^k(\hat{x}_1, \hat{x}_2)$, i.e., those which represent the geometries $\Omega_1^{\pm}$. Note, the angles (θ_1, φ_1) and (θ_2, φ_2) are fully determined on S^2 for the maps $\Omega_1^{\pm}$. This implies that for any values of θ_1, φ_1, θ_2, φ_2 there will always exist at least one rotation from the set $\Omega_1^{\pm} = \{\Omega_{11}^{\pm}, \Omega_{12}^{\pm}\}$. Consequently, the loss of geometry $\Omega_2^{\pm}$ does not imply the loss of generality by means of the existence of at least one spherical function from the set $\{^+\xi, {}^-\xi\}$.

6 RCGC Technique

Since the irreducible matrix representations $\eta^{\lambda}(\hat{x}_1, \hat{x}_2)$ depend on known coordinates $\hat{x}_1$ and $\hat{x}_2$, it is worth to exploit them in the study of tensor products of irreducible tensor operators T (or basis functions ϕ) directly, but not formally, as in most cases, when tensor operators are transformed under representations $D^{\lambda}(\Omega)$. Moreover, most of the physical operators T_q^k, basically studied in atomic spectroscopy, are expressed in terms of D and their various combinations. These are, for example, the spherical operators $C_q^k(\hat{x}) = \mathrm{i}^k D_{q0}^k(\bar{\Omega})$, the spherical harmonics $Y_q^k(\hat{x}) = \sqrt{(2k+1)/4\pi}\, C_q^k(\hat{x})$. The expressions over D of other operators, such as spin operator S^1, the angular momentum operator L^1, can be found, for instance, in [8]. All these mentioned operators also transform among themselves according to (24). Hence, it is natural for such operators to write $T(\hat{x})$ instead of $T(K)$, which is a general case. We say the operator $T(\hat{x})$ acts on $\hat{x}$ coordinate. Below the latter notation will be used.

6.1 Transformation Coefficients

The reduction formula for tensor product reads (see (24))

$$T_{m_1}^{\lambda_1}(\hat{x}_1) T_{m_2}^{\lambda_2}(\hat{x}_2) = \sum_{\lambda} \bar{T}_m^{\lambda}(\hat{x}_1) c_{m_1 m_2 m}^{\lambda_1 \lambda_2 \lambda}(\hat{x}_1, \hat{x}_2). \tag{40}$$

In this paper, the so-called for simplicity rotated Clebsch-Gordan coefficient of the first type or simply RCGC I is defined by

$$c_{m_1 m_2 m}^{\lambda_1 \lambda_2 \lambda}(\hat{x}_1, \hat{x}_2) = \sum_{m_2'} \eta_{m_2 m_2'}^{\lambda_2}(\hat{x}_1, \hat{x}_2) \begin{bmatrix} \lambda_1 & \lambda_2 & \lambda \\ m_1 & m_2' & m \end{bmatrix}. \tag{41}$$

From (40) we obtain the next expression

$$\bar{\bar{T}}_m^{\lambda}(\hat{x}_1, \hat{x}_2) = \sum_{\lambda' m'} C_{m' m}^{\lambda_1 \lambda_2 \lambda' \lambda}(\hat{x}_1, \hat{x}_2) \bar{T}_{m'}^{\lambda'}(\hat{x}_1), \tag{42}$$

where rotated Clebsch-Gordan coefficient of the second type or simply RCGC II is

$$C_{m' m}^{\lambda_1 \lambda_2 \lambda' \lambda}(\hat{x}_1, \hat{x}_2) = \sum_{m_1 m_2} c_{m_1 m_2 m'}^{\lambda_1 \lambda_2 \lambda'}(\hat{x}_1, \hat{x}_2) \begin{bmatrix} \lambda_1 & \lambda_2 & \lambda \\ m_1 & m_2 & m \end{bmatrix}. \tag{43}$$

Irreducible tensor operators $\bar{T}_m^{\lambda}(\hat{x}_1)$ and $\bar{\bar{T}}_m^{\lambda}(\hat{x}_1, \hat{x}_2)$ are derived by applying reduction rules for the Kronecker product $\lambda_1 \times \lambda_2 \to \lambda$. However, $\bar{T}_m^{\lambda}$ acts on $\hat{x}_1$, while $\bar{\bar{T}}_m^{\lambda}$ acts on $\hat{x}_1$, $\hat{x}_2$. For example, if T represents the normalized spherical harmonic C, then the coupled tensor product $\bar{T}^{\lambda}_{m}(\hat{x}_1) = \mathrm{i}^{\lambda_1+\lambda_2-\lambda} C^{\lambda}_{m}(\hat{x}_1)\left[\begin{smallmatrix}\lambda_1 & \lambda_2 & \lambda\\ 0 & 0 & 0\end{smallmatrix}\right]$. Contrarily, the tensor operator $\bar{\bar{T}}^{\lambda}_{m}(\hat{x}_1, \hat{x}_2)$ can not be reduced into one C^{λ}_{m} due to the different spaces, in which $T^{\lambda_i}_{m_i}(\hat{x}_i)$ $(i = 1, 2)$ act on.

Another useful circumstance for RCGC application is based on a possibility to reduce these coefficients. In accordance with (26), we directly attain

$$c^{\lambda_1\lambda_2\lambda}_{m_1m_2m}(.,.)c^{\bar{\lambda}_1\bar{\lambda}_2\bar{\lambda}}_{\bar{m}_1\bar{m}_2\bar{m}}(.,.) = \sum_{\Lambda_2} \eta^{\Lambda_2}_{M_2M'_2}(.,.) \sum_{m'_2\bar{m}'_2} \begin{bmatrix}\lambda_1 & \lambda_2 & \lambda\\ m_1 & m'_2 & m\end{bmatrix}\begin{bmatrix}\bar{\lambda}_1 & \bar{\lambda}_2 & \bar{\lambda}\\ \bar{m}_1 & \bar{m}'_2 & \bar{m}\end{bmatrix}$$
$$\times \begin{bmatrix}\lambda_2 & \bar{\lambda}_2 & \Lambda_2\\ m_2 & \bar{m}_2 & M_2\end{bmatrix}\begin{bmatrix}\lambda_2 & \bar{\lambda}_2 & \Lambda_2\\ m'_2 & \bar{m}'_2 & M'_2\end{bmatrix}. \quad (44)$$

Combining (43)–(44), we may also derive reduction formula for RCGC II. It is obvious, demonstrated reduction procedure (see (42)) can be extended and for many-electron wave functions.

Suppose, for instance, one needs to calculate the matrix element of $T^k_q(\hat{x})$ on the basis of eigenfunctions $Y^l_m(\hat{x})$, described on $SO(3)/SO(2)$. The application of RCGC technique directly indicates that in present case

$$[l\|T^k\|\bar{l}] = \mathrm{i}^{\bar{l}-l}[(2\bar{l}+1)/(2l+1)]^{1/2} T^k_0(\hat{0}) \begin{bmatrix}\bar{l} & k & l\\ 0 & 0 & 0\end{bmatrix}. \quad (45)$$

The proof is produced in Appendix C. Here it is assumed that $\hat{0} \equiv (0, 0)$. The reduced matrix element $[l\|T^k\|\bar{l}]$ is obtained from the Wigner-Eckart theorem $\langle lm|T^k_q|\bar{l}\bar{m}\rangle = (-1)^{2k}[l\|T^k\|\bar{l}]\left[\begin{smallmatrix}\bar{l} & k & l\\ \bar{m} & q & m\end{smallmatrix}\right]$. Particularly, if $T^k = C^k$, then operator $T^k_0(\hat{0}) = \mathrm{i}^k$, and obtained formula is in fully consistence with (2.52) in [2]. Thus, (45) is a generalization of this special case. Going on this route, one can derive matrix the expressions of matrix element on the basis of more complex eigenfunctions.

One can see from (42), the specific feature of technique, based on coordinate transformations (or simply RCGC technique), is that the tensor structure of operator and wave functions is preserved, and the resultant matrix element is calculated on the basis of transformed operators $\bar{T}(\hat{x})$, i.e., the calculation of multiple integrals transforms to the calculation of a single integral (over $\hat{x}$). This is because each N-electron matrix element

$$\int_{S^2} \mathrm{d}\hat{x}_1 \int_{S^2} \mathrm{d}\hat{x}_2 \ldots \int_{S^2} \mathrm{d}\hat{x}_N \Phi^{\Lambda^{bra}\dagger}_{M}(\hat{x}_1, \hat{x}_2, \ldots, \hat{x}_N)$$
$$\times T^K_Q(\hat{x}_1, \hat{x}_2, \ldots, \hat{x}_N)\Phi^{\Lambda^{ket}}_{M'}(\hat{x}_1, \hat{x}_2, \ldots, \hat{x}_N)$$

is transformed to

$$\int_{S^2} \mathrm{d}\hat{x}_1 \bar{\Phi}^{\lambda^{bra}\dagger}_{m}(\hat{x}_1)\bar{T}^k_q(\hat{x}_1)\bar{\Phi}^{\lambda^{ket}}_{m'}(\hat{x}_1)$$
$$\times \int_{S^2} \mathrm{d}\hat{x}_2 \int_{S^2} \mathrm{d}\hat{x}_3 \ldots \int_{S^2} \mathrm{d}\hat{x}_N \overline{\eta^{\lambda^{bra}_2}_{m_2\mu_2}(\hat{x}_1, \hat{x}_2)\eta^{\lambda^{bra}_3}_{m_3\mu_3}(\hat{x}_1, \hat{x}_3)} \ldots \overline{\eta^{\lambda^{bra}_N}_{m_N\mu_N}(\hat{x}_1, \hat{x}_N)}$$
$$\times \eta^{k_2}_{q_2\pi_2}(\hat{x}_1, \hat{x}_2)\eta^{k_3}_{q_3\pi_3}(\hat{x}_1, \hat{x}_3) \ldots \eta^{k_N}_{q_N\pi_N}(\hat{x}_1, \hat{x}_N)$$
$$\times \eta^{\lambda^{ket}_2}_{m'_2\mu'_2}(\hat{x}_1, \hat{x}_2)\eta^{\lambda^{ket}_3}_{m'_3\mu'_3}(\hat{x}_1, \hat{x}_3) \ldots \eta^{\lambda^{ket}_N}_{m'_N\mu'_N}(\hat{x}_1, \hat{x}_N),$$

where $\bar{\Phi}$ and $\bar{T}$ indicate coupled the tensor products of $\phi^{\lambda_i}(\hat{x}_1)$ and $T^{k_i}(\hat{x}_1)$, respectively. The application of (26) for all $\eta^{\lambda_\xi^{bra}}_{m_\xi\mu_\xi}(\hat{x}_1,\hat{x}_\xi)$, $\eta^{k_\xi}_{q_\xi\pi_\xi}(\hat{x}_1,\hat{x}_\xi)$, $\eta^{\lambda_\xi^{ket}}_{m'_\xi\mu'_\xi}(\hat{x}_1,\hat{x}_\xi)$, $\xi=2,3,\dots,N$ implies that initially determined $2N$-integral reduces to a double one

$$\int_{S^2}\mathrm{d}\hat{x}_1\bar{\Phi}^{\lambda^{bra}\dagger}_m(\hat{x}_1)\bar{T}^k_q(\hat{x}_1)\mathcal{S}^{\Lambda_2}_{M_2M'_2}(\hat{x}_1;+)\mathcal{S}^{\Lambda_3}_{M_3M'_3}(\hat{x}_1;+)\dots\mathcal{S}^{\Lambda_N}_{M_NM'_N}(\hat{x}_1;+)\bar{\Phi}^{\lambda^{ket}}_{m'}(\hat{x}_1).$$

Instead of that, for given N-electron wave functions we produce $N-1$ functions $\mathcal{S}$ (see (29)) and a product of momenta coupling coefficients (CGC) that can be decomposed into $3nj$-coefficients, if summing over projections.

6.2 Example

A simple application of RCGC technique can be demonstrated, for example, in a study of two electrons, located in some external field (of fixed nucleus, for instance). We refer to [9], where a two-electron wave function is presented by

$$\Psi^l_m(\boldsymbol{r}_1,\boldsymbol{r}_2)=\sum_\mu g^l_\mu(r_1,r_2,\theta_{12})D^l_{m\mu}(\Omega), \tag{46}$$

with $r_i=|\boldsymbol{r}_i|$; $l\in\mathbb{Z}^+$. In the same paper (Bhatia et al. [9]), it was determined that Laplacian, involving θ_{12} (the angle between vectors $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$), does not affect the orbital angular momentum $l>0$. Thus we may assume, that g is a radial function not going into a deeper analysis, since our aim is the angular part. Then Ψ^l_m may be rewritten as follows

$$\Psi^l_m(\boldsymbol{r}_1,\boldsymbol{r}_2)=\sum_\mu g^l_\mu(r_1,r_2,\theta_{12})\eta^l_{m\mu}(\hat{x}_1,\hat{x}_2). \tag{47}$$

Suppose we want to calculate the Coulomb $1/r_{12}$ matrix element. In this case, the interaction in a tensor form reads $T^0_0(\boldsymbol{r}_1,\boldsymbol{r}_2)=\sum_k(r^k_</r^{k+1}_>)(C^k(\hat{x}_1)\cdot C^k(\hat{x}_2))$, where $r_<=\min(r_1,r_2)$ and $r_>=\max(r_1,r_2)$. The scalar product $(C^k(\hat{x}_1)\cdot C^k(\hat{x}_2))$ is reduced in agreement with (42), what leads to the following construction of $\langle\Psi^l_m|r^{-1}_{12}|\Psi^{l'}_{m'}\rangle$ (taking into account only angular part)

$$\begin{aligned}
&\langle\Psi^l_m|r^{-1}_{12}|\Psi^{l'}_{m'}\rangle\\
&\quad=(-1)^{m-m'}\sum_\mu(-1)^\mu\overline{g^l_\mu(r_1,r_2,\theta_{12})}g^{l'}_{\mu+m-m'}(r_1,r_2,\theta_{12})\\
&\qquad\times\sum_k\frac{r^k_<}{r^{k+1}_>}\sum_K\sum_{Q=\text{even}}\mathrm{i}^{-K}\begin{bmatrix}k&k&K\\0&0&0\end{bmatrix}\sum_{\bar{L}}\int_{S^2}\mathrm{d}\hat{x}C^K_Q(\hat{x})\mathcal{S}^{\bar{L}}_{0Q}(\hat{x};+)\\
&\qquad\times\sum_L\begin{bmatrix}k&k&K\\m-m'&Q+m'-m&Q\end{bmatrix}\begin{bmatrix}l&k&L\\-m&m-m'&-m'\end{bmatrix}\begin{bmatrix}L&l'&\bar{L}\\-m'&m'&0\end{bmatrix}\\
&\qquad\times\begin{bmatrix}l&k&L\\-\mu&Q+m'-m&Q+m'-m-\mu\end{bmatrix}\\
&\qquad\times\begin{bmatrix}L&l'&\bar{L}\\Q+m'-m-\mu&m-m'+\mu&Q\end{bmatrix}.
\end{aligned}\tag{48}$$

It is evident, this way of calculation is more efficient in comparison with the direct integration of $\iint_{S^2} \mathrm{d}\hat{x}_1 \mathrm{d}\hat{x}_2 \overline{D^l_{m\mu}(\Omega)}(C^k(\hat{x}_1)\cdot C^k(\hat{x}_2))D^{l'}_{m'\mu'}(\Omega)$, because otherwise one should change integrands, when mapping from $\hat{x}$ to Ω. Consequently, that would lead to complex manipulations of trigonometric equations, given in (6).

7 Summary

In present study, we produced a parametrization of the standard Wigner D-function on $SU(2)$ by the coordinates $(\hat{x}_1, \hat{x}_2)$ of vector in the fixed and rotated coordinate systems. As a result, we found the set of spherical functions, conformed to $D(\Omega)$ in miscellaneous areas $L^2(\Omega) \subset S^2$. We showed that offered parametrization of $D(\Omega)$ provides an opportunity to reduce the angular $2N$-integrals, which are of special interest in theoretical atomic spectroscopy, to a double one. Particularly, we demonstrated a new way of construction of irreducible tensor operator matrix element which plays the role of a generalization of previously obtained special cases (see, for example, (45)). Another convenient usage of suggested RCGC technique, based on coordinate transformation, is applied to the calculation of matrix elements on the basis of functions, expressed in terms of the standard $D(\Omega)$ functions (for two-electron case, see Sect. 6.2).

Acknowledgements The authors are grateful to R. Kisielius for attentive revision of this paper and for various useful remarks.

Appendix A: Optimal Values for Ψ

Here the solutions $\Omega = (\varphi + \pi/2, \theta, \Psi) \in \mathbb{R}\ \forall \hat{x}_i \in S^2$ of (6) will be studied in a more detail. Partial solutions of the systems (x_2, z_2) and (y_2, z_2) for θ, φ are

$$\theta_{\sigma_1\sigma_2} = \sigma_1 \arccos \frac{z_1 z_2 + \sigma_2 |y'_1| \sqrt{z_1^2 - z_2^2 + y'^2_1}}{z_1^2 + y'^2_1} + 2\pi n_1, \quad n_1 \in \mathbb{Z}^+, \tag{49}$$

$$\varphi^{(1)}_{\sigma_3\sigma_4} = \sigma_3 \arccos \frac{x'_1 y_2 + \sigma_4 |x_2| \sqrt{1 - x'^2_1 - z_2^2}}{1 - z_2^2} + 2\pi n_2, \quad n_2 \in \mathbb{Z}^+, \tag{50}$$

$$\varphi^{(2)}_{\sigma_3\sigma_4} = \sigma_3 \arccos \frac{x_2 \sqrt{1 - x'^2_1 - z_2^2} + \sigma_4 |x'_1 y_2|}{\mathrm{sgn}(y'_1)(1 - z_2^2)} + 2\pi n_2, \quad n_2 \in \mathbb{Z}^+, \tag{51}$$

where $\sigma_i \in \{-1, +1\}$; $\mathrm{sgn}(y'_1)$ denotes the sign of y'_1. Let us mark the common values of $\varphi^{(1)}_{\sigma_3\sigma_4}$ and $\varphi^{(2)}_{\sigma_3\sigma_4}$ by $\varphi_{\sigma_3\sigma_4} = {}_{n_2}\mathbf{w}_{\sigma_3\sigma_4}(\hat{x}_1, \hat{x}_2; \Psi)$. Let us also denote

$$\sin^2 \frac{\theta_{\sigma_1\sigma_2}}{2} = \mathbf{x}_{\sigma_2}(\hat{x}_1, \hat{x}_2; \Psi) = \frac{z_1^2 - z_1 z_2 + y'^2_1 + \sigma_2 y'_1 \sqrt{z_1^2 - z_2^2 + y'^2_1}}{2(z_1^2 + y'^2_1)}. \tag{52}$$

Obtained functions $\mathbf{x}$ and $\mathbf{w}$ are substituted in (2). The generalized spherical function D is rearranged to the following function

$$\{{}_{n_2}Z^k_{qq'}(\hat{x}_1,\hat{x}_2;\Psi)\}_{\sigma_2\sigma_3\sigma_4} = a(k,q,q')\mathrm{e}^{\mathrm{i}q(\frac{\pi}{2}+{}_{n_2}\mathbf{w}_{\sigma_3\sigma_4}(\hat{x}_1,\hat{x}_2;\Psi))+\mathrm{i}q'\Psi}\sum_p b_p(k,q,q')$$
$$\times\,\mathbf{x}_{\sigma_2}^{p-\frac{q-q'}{2}}(\hat{x}_1,\hat{x}_2;\Psi)(1-\mathbf{x}_{\sigma_2}(\hat{x}_1,\hat{x}_2;\Psi))^{-p+k+\frac{q-q'}{2}}. \quad (53)$$

In order to look for optimal Ψ values, we carry out variational procedure for the gauge Ψ, applying it for all possible distributions of $\sigma_2, \sigma_3, \sigma_4$, i.e., $(\delta/\delta\Psi)\,{}_{n_2}Z^k_{qq'} = 0$. This implies

$$\mathrm{i}\,{}_{n_2}Z^k_{qq'}\left(q' + q\frac{\delta\,{}_{n_2}\mathbf{w}_{\sigma_3\sigma_4}}{\delta\Psi}\right) + a\mathrm{e}^{\mathrm{i}q(\frac{\pi}{2}+{}_{n_2}\mathbf{w}_{\sigma_3\sigma_4})+\mathrm{i}q'\Psi}\sum_p b_p\frac{\delta\mathbf{x}_{\sigma_2}}{\delta\Psi}$$
$$\times\,\mathbf{x}_{\sigma_2}^{p-\frac{q-q'}{2}-1}(1-\mathbf{x}_{\sigma_2})^{-p+k+\frac{q-q'}{2}-1}\left(p-\frac{q-q'}{2}-k\mathbf{x}_{\sigma_2}\right) = 0. \quad (54)$$

Applying obvious fact, that $A = B = 0$ if $A, B \in \mathbb{R}$ in $A + \mathrm{i}B = 0$, we finally gain

$$\begin{cases} \frac{\delta\mathbf{x}_{\sigma_2}}{\delta\Psi} = 0, \\ \mathbf{x}_{\sigma_2} = \eta, \quad \eta \in \{0, 1, \frac{q'-q}{2k}\}, \\ q' + q\frac{\delta\,{}_{n_2}\mathbf{w}_{\sigma_3\sigma_4}}{\delta\Psi} = 0, \quad q \neq 0. \end{cases} \quad (55)$$

It follows from equation $\mathbf{x}_{\sigma_2} = \eta$, that $y'_1 \in \mathbb{C}$. Thus, Ψ does not belong to $\mathbb{R}$. Equation $\frac{\delta\mathbf{x}_{\sigma_2}}{\delta\Psi} = 0$ is rewritten in the form

$$\frac{\delta\mathbf{x}_{\sigma_2}}{\delta\Psi} = \frac{\delta\mathbf{x}_{\sigma_2}}{\delta y'_1}\frac{\delta y'_1}{\delta\Psi} = \frac{\delta\mathbf{x}_{\sigma_2}}{\delta y'_1}x'_1 = 0. \quad (56)$$

The solutions of $\frac{\delta\mathbf{x}_\pm}{\delta y'_1} = 0$ for y'_1 do not belong to $\mathbb{R}$. Thus, equation $x'_1 = 0$ has to be solved. The latter is equivalent to (9). Finally, when studying the third equation in (55), we would get some individual values of Ψ, which depend on q, q' (for $q = 0$, present equation vanishes). Thus, the set of solutions would be the subset of solutions given by the first equation, independent of q, q'.

Appendix B: The Alternative Expressions of Spherical Functions

In accordance with (3)–(4), the product of coefficients a and b_p can be rewritten as follows

$$a(k,q,q')b_p(k,q,q') = \mathrm{i}^{q'-q}(-1)^p\left[\frac{(k+q)!(k-q)!}{(k+q')!(k-q')!}\right]^{\frac{1}{2}}\binom{k-q'}{p}\binom{k+q'}{p+q'-q}, \quad (57)$$

where the last two quantities on the right hand side of (57) denote binomial coefficients. Further, let us mark the term

$$A^k_{qq'}(\gamma) = a(k,q,q')\left\{\cos\left[\frac{1}{2}(\theta_1-\gamma\theta_2)\right]\right\}^{2k}\sum_p b_p(k,q,q')\left\{\tan\left[\frac{1}{2}(\theta_1-\gamma\theta_2)\right]\right\}^{2p+q'-q}. \quad (58)$$

According to (57), $A^k_{qq'}(\gamma)$ may be revised by

$$A^k_{qq'}(\gamma)=\mathrm{i}^{q'-q}\left[\frac{(k+q)!(k-q)!}{(k+q')!(k-q')!}\right]^{\frac{1}{2}}\sum_p(-1)^p\binom{k-q'}{p}\binom{k+q'}{p+q'-q}\frac{z^{p+\frac{q'-q}{2}}}{(1+z)^k}, \quad (59)$$

where $z=\tan^2[\frac{1}{2}(\theta_1-\gamma\theta_2)]$. Performing the summation over p, we obtain

$$\begin{aligned}&\sum_p(-1)^p\binom{k-q'}{p}\binom{k+q'}{p+q'-q}\frac{z^{p+\frac{q'-q}{2}}}{(1+z)^k}\\&=(-1)^{q-q'}\binom{k-q'}{q-q'}z^{\frac{q-q'}{2}}(1+z)^{1+k}\,{}_2F_1(k+1+q,k+1-q';1+q-q';-z)\\&(q\geq q') \qquad (60a)\\&=\binom{k+q'}{q'-q}z^{\frac{q'-q}{2}}(1+z)^{1+k}\,{}_2F_1(k+1+q',k+1-q;1+q'-q;-z)\\&(q'\geq q). \qquad (60b)\end{aligned}$$

Thus if: (a) $A^{>k}_{qq'}=A^k_{qq'}$, for $q\geq q'$; (b) $A^{<k}_{qq'}=A^k_{qq'}$, for $q'\geq q$, then

$$\begin{aligned}&A^{>k}_{qq'}(\gamma)\\&=\frac{\mathrm{i}^{q-q'}}{(q-q')!}\left[\frac{(k+q)!(k-q')!}{(k+q')!(k-q)!}\right]^{\frac{1}{2}}\left\{\tan\left[\frac{1}{2}(\theta_1-\gamma\theta_2)\right]\right\}^{q-q'}\left\{\cos\left[\frac{1}{2}(\theta_1-\gamma\theta_2)\right]\right\}^{-2-2k}\\&\quad\times\,{}_2F_1\left(k+1+q,k+1-q';1+q-q';-\tan^2\left[\frac{1}{2}(\theta_1-\gamma\theta_2)\right]\right), \qquad (61)\\&A^{<k}_{qq'}(\gamma)=A^{>k}_{q'q}(\gamma). \qquad (62)\end{aligned}$$

Substituting A in (15) we gather

$$(n,n';\alpha,\beta,\gamma,\delta|\hat{x}_1,\hat{x}_2)^k_{qq'}=\begin{cases}(n,n';\alpha,\beta,\gamma,\delta|\hat{x}_1,\hat{x}_2)^{>k}_{qq'}, & q\geq q',\\(n,n';\alpha,\beta,\gamma,\delta|\hat{x}_1,\hat{x}_2)^{<k}_{qq'}, & q\leq q',\end{cases} \quad (63)$$

$$(n,n';\alpha,\beta,\gamma,\delta|\hat{x}_1,\hat{x}_2)^{>k}_{qq'}=\mathrm{i}^{\alpha q+\delta q'}(-1)^{2(nk+n'q')}\beta^{q'-q}\mathrm{e}^{\mathrm{i}(q\varphi_2-q'\varphi_1)}A^{>k}_{qq'}(\gamma), \quad (64)$$

$$(n,n';\alpha,\beta,\gamma,\delta|\hat{x}_1,\hat{x}_2)^{<k}_{qq'}=\mathrm{i}^{(\alpha-\delta)(q-q')}\mathrm{e}^{\mathrm{i}(\varphi_1+\varphi_2)(q-q')}(n,n';\alpha,\beta,\gamma,\delta|\hat{x}_1,\hat{x}_2)^{>k}_{q'q}. \quad (65)$$

Appendix C: Reduced Matrix Element on the Basis of Spherical Harmonics

Here a proof of (45), exploiting RCGC technique, will be offered. The matrix element of $T^k_q(\hat{x})$ on the basis of arbitrary functions $\psi^{l\dagger}_m(\hat{x})$ and $\psi^{\bar{l}}_{\bar{m}}(\hat{x})$ is written by

$$\langle lm|T^k_q|\bar{l}\bar{m}\rangle=[l\|T^k\|\bar{l}]\begin{bmatrix}\bar{l} & k & l\\ \bar{m} & q & m\end{bmatrix}=\int_{S^2}\mathrm{d}\hat{x}\,\psi^{l\dagger}_m(\hat{x})T^k_q(\hat{x})\psi^{\bar{l}}_{\bar{m}}(\hat{x}). \quad (66)$$

Direct adaptation of (24) points to

$$\langle lm|T_q^k|\bar{l}\bar{m}\rangle = \int_{S^2} \mathrm{d}\hat{x} \sum_{m'q'\bar{m}'} \psi_{m'}^{l\dagger}(\hat{x}')T_{q'}^k(\hat{x}')\psi_{\bar{m}'}^{\bar{l}}(\hat{x}')\overline{\eta_{mm'}^{l}(\hat{x}',\hat{x})}\eta_{qq'}^k(\hat{x}',\hat{x})\eta_{\bar{m}\bar{m}'}^{\bar{l}}(\hat{x}',\hat{x}). \quad (67)$$

Transformed functions ψ and operator T depend on the fixed coordinates $\hat{x}'$. Consequently, they can be located in front of the integral. Recalling that $\overline{\eta_{mm'}^l} = (-1)^{m-m'}\eta_{-m-m'}^l$, and exploiting the reduction rules for the Kronecker products $l \times k \to \bar{L}$, $\bar{L} \times \bar{l} \to L$ (see (26)), we attain $\eta_{MM'}^L(\hat{x}', \hat{x})$. The integral of present spherical function is defined in (29), and in this case it equals to $\mathcal{S}_{0M'}^L(\hat{x}'; +)$ (see (39)), since $L \in \mathbb{Z}^+$. Thus

$$\langle lm|T_q^k|\bar{l}\bar{m}\rangle = \sum_{m'q'\bar{m}'} (-1)^{m-m'}\psi_{m'}^{l\dagger}(\hat{x}')T_{q'}^k(\hat{x}')\mathcal{S}_{0M'}^L(\hat{x}'; +)\psi_{\bar{m}'}^{\bar{l}}(\hat{x}')$$
$$\times \begin{bmatrix} l & k & \bar{L} \\ -m & q & -\bar{m} \end{bmatrix}\begin{bmatrix} l & k & \bar{L} \\ -m' & q' & \bar{M}' \end{bmatrix}\begin{bmatrix} \bar{L} & \bar{l} & L \\ -\bar{m} & \bar{m} & 0 \end{bmatrix}\begin{bmatrix} \bar{L} & \bar{l} & L \\ \bar{M}' & \bar{m}' & M' \end{bmatrix}. \quad (68)$$

The matrix element does not depend on $\hat{x}'$, thus one can choose any value. We select the most simple case $\hat{x}' = \hat{0} \equiv (0, 0)$. The application of orthogonality condition for Clebsh-Gordan coefficients, combining (66), (68), leads to equalities $\bar{L} = \bar{l}$, $L = 0$; thus $\mathcal{S}_{00}^0(\hat{0}; +) = 4\pi$ and

$$[l\|T^k\|\bar{l}] = \frac{4\pi}{2l+1} \sum_{m'q'\bar{m}'} \psi_{m'}^{l\dagger}(\hat{0})T_{q'}^k(\hat{0})\psi_{\bar{m}'}^{\bar{l}}(\hat{0}) \begin{bmatrix} \bar{l} & k & l \\ \bar{m}' & q' & m' \end{bmatrix}. \quad (69)$$

It is noticeable, by applying the technique of coordinate transformations, the obtained expression coincides with (41) in [8], if reducing given Kronecker products $l \times k \to L'$, $L' \times \bar{l} \to L''$. This would signify $L' = \bar{l}$ and $L'' = 0$. At this step, we turn to a special case of eigenfunctions $\psi_m^l(\hat{x}) = Y_m^l(\hat{x})$, what implies the equality $Y_m^l(\hat{0}) = \delta_{m0}\mathrm{i}^l\sqrt{(2l+1)/4\pi}$. Hence, (69) becomes equal to the expression, presented in (45). One should also be reminded that in general, in (69) the arguments $\hat{0}$ can be replaced by any values $\hat{x}$.

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