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Algebraic Solution of Gaunt Coefficients via the Angular Momentum Ladder Operators

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Research Article

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Abstract

In this study, Gaunt coefficients, frequently encountered in quantum mechanical calculations of atomic and molecular structures, have been algebraically derived. Firstly, the Gaunt coefficient, equal to the integral over the solid angle of the product of three spherical harmonics, is written in terms of angular momentum ladder operators. Subsequently, raising or lowering operators are applied to spherical harmonics, and the obtained integrals are solved using the recurrence and orthogonality relations of spherical harmonics. As a result, algebraic expressions for Gaunt coefficients are obtained in terms of quantum numbers.

Keywords: Gaunt coefficients, ladder operators, spherical harmonics

Açısal Momentum Merdiven İşlemcileri ile Gaunt Katsayılarının Cebirsel Çözümü

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Öz

Bu çalışmada, atomik ve moleküler yapıların kuantum mekaniksel hesaplamalarında sıklıkla karşılaşılan Gaunt katsayıları cebirsel olarak türetilmiştir. İlk olarak, üç küresel harmoniğin çarpımının katı açı üzerinden integraline eşit olan Gaunt katsayısı, açısal momentum merdiven işlemcileri cinsinden yazılır. Daha sonra, yükseltme veya alçaltma işlemcileri küresel harmoniklere uygulanır ve elde edilen integralleri çözmek için küresel harmoniklerin tekrarlama ve diklik bağıntıları kullanılır. Sonuç olarak, Gaunt katsayıları için cebirsel ifadeler, kuantum sayıları cinsinden elde edilir.

Anahtar Kelimeler: Gaunt katsayıları, merdiven işlemcileri, küresel harmonikler

Introduction

In quantum mechanics, two formulations are used: matrix mechanics and wave mechanics. In matrix mechanics, developed by Heisenberg in 1925, dynamical quantities such as position, energy, momentum, and angular momentum are expressed in terms of matrices defined using algebraic equations and commutation relations. Well-known applications of matrix mechanics in quantum mechanics include the harmonic oscillator and angular momentum [1, 2]. Wave mechanics, which describes the dynamics of microscopic systems using the Schrödinger wave equation, was developed by Schrödinger in 1926. This method requires solving the Schrödinger wave equation, formulated as a second-order linear differential equation. For different potentials, power series, boundary conditions, and separation of variables methods are used for the analytical solution of the Schrödinger equation. Still, it cannot be solved exactly except for some simple systems, such as the hydrogen atom and the harmonic oscillator, and approximate methods are employed. The algebraic method, which depends on raising and lowering operators, is very useful for systems with a finite-dimensional matrix, such as angular momentum. This is because while the orbital angular momentum quantum number l has a certain value, the magnetic quantum number m takes a value of $2l+1$, and the angular momentum is represented by $2l+1$ dimensional matrices. In the case of a spherically symmetric potential, the Hamiltonian operator exhibits commutation with both the squared angular momentum operator and its z-component. As a consequence of this commutative behavior, these operators share identical eigenfunctions. These eigenfunctions are precisely the spherical harmonics derived as solutions to the angular part of the Laplace equation in spherical coordinates. The angular momentum operator algebra is one of the most commonly used methods for deriving spherical harmonics. In this method, raising and lowering operators of angular momentum, also known as ladder operators, are applied to a state of spherical harmonics to obtain spherical harmonics corresponding to different states. Many textbooks and articles in the literature use this method [3-7]. In atomic and molecular systems, particles have spin angular and orbital angular momentum. While the orbital and spin angular momentums are not conserved separately, the total angular momentum equal to their vector sum is conserved. In this case, the linear combination coefficients connecting the reducible and irreducible representations are called Clebsch-Gordan coefficients. According to this, Clebsch-Gordan coefficients are the most general coefficients related to angular momentum. Other coefficients related to angular momentum, such as Gaunt, Wigner 3*j*, and 6*j*, are written in terms of Clebsch-Gordan coefficients. Clebsch-Gordan coefficients can be calculated by different methods, either analytically or using recurrence relations [8-19]. Based on the variational principle, the Hartree Fock Roothaan (HFR) method is a widely used approximate technique for calculating atoms or molecules' physical and chemical properties in multi-electron systems. When employing this method to determine any physical property, we encounter Gaunt coefficients, which represent the integral of the product of three spherical harmonics over solid angles [20]. Due to the vast number of Gaunt coefficients that need to be computed (often in the hundreds of thousands), it is crucial to calculate these coefficients accurately and efficiently. In the literature, Gaunt coefficients are usually expressed as the product of two Clebsch-Gordan coefficients or 3*j* symbols. Calculations for Gaunt coefficients are performed using the explicit expressions of these coefficients in terms of different functions or recurrence relations [16, 21-25]. Other approaches used in calculating Gaunt coefficients can be found in Refs. [26-30]. First, this paper introduces the angular momentum ladder operators in the spherical coordinates and recurrence relations of spherical harmonics. Then, using these operators, the Gaunt coefficients, defined by integrating the tri-product of spherical harmonics, are calculated algebraically. Gaunt coefficients are given as master formulae based only on quantum numbers.

Angular Momentum Ladder Operators in the Spherical Coordinates

Since angular momentum has rotational symmetry, it is convenient to express the angular momentum operator $\hat{\mathbf{L}}$**,** which is defined by its three components $\hat{L}_x$, $\hat{L}_y$, and $\hat{L}_z$, in terms of spherical coordinates. In this case, the components of the angular momentum operator are expressed as [8-10].

$$\hat{L}_x = i\hbar\left(sin\phi\frac{\partial}{\partial\theta} + cot\theta cos\phi\frac{\partial}{\partial\phi}\right) \quad (1)$$

$$\hat{L}_y = i\hbar\left(-cos\phi\frac{\partial}{\partial\theta} + cot\theta sin\phi\frac{\partial}{\partial\phi}\right) \quad (2)$$

$$\hat{L}_z = -i\hbar\frac{\partial}{\partial\phi} \quad (3)$$

Using these equations, the operator $\hat{L}^2$, which consists of the sum of the squares of its components, is obtained as follows.

$$\hat{L}^2 = -\hbar^2\left[\frac{1}{sin\theta}\frac{\partial}{\partial\theta}\left(sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] \quad (4)$$

Since the differential form of angular momentum operators depends only on the θ and ϕ angles, their eigenfunctions are the spherical harmonics $Y_l^m(\theta,\phi)$. Accordingly, well-known eigenvalue equations of $\hat{L}^2$ and $\hat{L}_z$ operators are given below.

$$\hat{L}^2\, Y_l^m(\theta,\phi) = l\,(l+1)\,\hbar^2 Y_l^m(\theta,\phi)$$

$$\hat{L}_z Y_l^m(\theta,\phi) = m\hbar\, Y_l^m(\theta,\phi) \quad (5)$$

When performing analytical operations on angular momentum, it is necessary to solve the differential equation of the associated Legendre functions $P_l^m(cos\theta)$ given below.

$$\frac{1}{sin\theta}\frac{d}{d\theta}\left(sin\theta\,\frac{dP_l^m(cos\theta)}{d\theta}\right) + \left\{l(l+1) - \frac{m^2}{sin^2\theta}\right\}P_l^m(cos\theta) = 0 \quad (6)$$

For algebraic operations involving angular momentum, ladder operators need to be used. The angular momentum ladder operators, $\hat{L}_+$ and $\hat{L}_-$, are introduced as follows.

$$\hat{L}_\pm = \hat{L}_x \pm i\hat{L}_y = \pm\hbar e^{\pm i\phi}\left[\frac{\partial}{\partial\theta} \pm i cot\theta\frac{\partial}{\partial\phi}\right] \quad (7)$$

Here $\hat{L}_+$ and $\hat{L}_-$ are called raising (or creation) and lowering (or annihilation) operator, respectively. The following equation gives the action of angular momentum ladder operators on spherical harmonics:

$$\hat{L}_\pm Y_l^m(\theta,\phi) = \hbar[l(l+1) - m(m\pm 1)]^{1/2} Y_l^{m\pm 1}(\theta,\phi) \quad (8)$$

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According to this equation, while the angular momentum quantum number l remains unchanged, the magnetic quantum number m increases or decreases by one.

Recurrence Relations for Spherical Harmonics

In quantum mechanics, the spherical harmonics, $Y_l^m(\theta,\phi)$, that constitute the angular part of the wave function are also eigenfunctions of the orbital angular momentum operators $\hat{L}^2$, $\hat{L}_z$ and $\hat{L}_\pm$. $Y_l^m(\theta,\phi)$ is defined as below for non-negative values of *m* magnetic quantum number [31].

$$Y_l^m(\theta,\phi) = (-1)^m \sqrt{\frac{2\,l+1}{4\pi}\,\frac{(l-m)\,!}{(l+m)\,!}}\; P_l^m(cos\theta)\; e^{i\,m\,\phi} \tag{9}$$

Where $P_l^m(cos\theta)$ is represented as the associated Legendre polynomial. Also, for negative values of *m* we have

$$Y_l^{-m}(\theta,\phi) = (-1)^m Y_l^{m*}(\theta,\phi) \tag{10}$$

Spherical harmonics are orthogonal functions and orthogonality relation is given by

$$\int_{\phi=0}^{2\pi}\int_{\theta=0}^{\pi} Y_{l_1}^{m_1\,*}(\theta,\phi)\, Y_{l_2}^{m_2}(\theta,\phi) sin\theta\; d\theta\; d\phi \; = \delta_{l_1,l_2}\delta_{m_1,m_2} \tag{11}$$

Using the recurrence relations of the associated Legendre polynomials, recurrence relations can be written for spherical harmonics. Some of these relations, which are very useful in solving integrals consisting of the product of trigonometric functions and spherical harmonics, are given below [11, 31].

$$cos\theta\, Y_l^m(\theta,\phi) = \sqrt{\frac{(l-m+1)(l+m+1)}{(2l+1)(2l+3)}}\; Y_{l+1}^m(\theta,\phi) + \sqrt{\frac{(l-m)(l+m)}{(2l-1)(2l+1)}}\; Y_{l-1}^m(\theta,\phi) \tag{12}$$

$$e^{i\phi} sin\theta\, Y_l^m(\theta,\phi) = -\sqrt{\frac{(l+m+1)(l+m+2)}{(2l+1)(2l+3)}}\; Y_{l+1}^{m+1}(\theta,\phi) + \sqrt{\frac{(l-m-1)(l-m)}{(2l-1)(2l+1)}}\; Y_{l-1}^{m+1}(\theta,\phi) \tag{13}$$

$$e^{-i\phi} sin\theta\, Y_l^m(\theta,\phi) = \sqrt{\frac{(l-m+1)(l-m+2)}{(2l+1)(2l+3)}}\; Y_{l+1}^{m-1}(\theta,\phi) - \sqrt{\frac{(l+m-1)(l+m)}{(2l-1)(2l+1)}}\; Y_{l-1}^{m-1}(\theta,\phi) \tag{14}$$

$$(2l-1)(2l+3)\cos^2\theta\, Y_l^m(\theta,\phi) = (2l-1)\sqrt{\frac{((l+1)^2-m^2)((l+2)^2-m^2)}{(2l+1)(2l+5)}}\; Y_{l+2}^m(\theta,\phi)$$

$$+(2l(l+1)-2m^2-1)\,Y_l^m(\theta,\phi)$$

$$+(2l+3)\sqrt{\frac{(l^2-m^2)((l-1)^2-m^2)}{(2l+1)(2l-3)}}\,Y_{l-2}^m(\theta,\phi) \tag{15}$$

$$(2l-1)(2l+3)sin\theta\cos\theta\, e^{i\phi}Y_l^m(\theta,\phi)=$$

$$-(2l-1)\sqrt{\frac{((l+1)^2-m^2)(l+m+2)(l+m+3)}{(2l+1)(2l+5)}}\,Y_{l+2}^{m+1}(\theta,\phi)$$

$$-(2m+1)\sqrt{(l-m)(l+m+1)}\,Y_l^{m+1}(\theta,\phi)$$

$$+(2l+3)\sqrt{\frac{(l^2-m^2)(l-m-1)(l-m-2)}{(2l+1)(2l-3)}}\,Y_{l-2}^{m+1}(\theta,\phi) \tag{16}$$

$$(2l-1)(2l+3)sin\theta\cos\theta\, e^{-i\phi}Y_l^m(\theta,\phi)=$$

$$(2l-1)\sqrt{\frac{((l+1)^2-m^2)(l-m+2)(l-m+3)}{(2l+1)(2l+5)}}\,Y_{l+2}^{m-1}(\theta,\phi)$$

$$-(2m-1)\sqrt{(l+m)(l-m+1)}\,Y_l^{m-1}(\theta,\phi)$$

$$-(2l+3)\sqrt{\frac{(l^2-m^2)(l+m-1)(l+m-2)}{(2l+1)(2l-3)}}\,Y_{l-2}^{m-1}(\theta,\phi) \tag{17}$$

$$(2l-1)(2l+3)\ \sin^2\theta\ \ e^{2i\phi}\,Y_l^m(\theta,\phi)\ =\frac{(2l-1)}{\sqrt{(2l+1)(2l+5)}}\sqrt{\frac{(l+m+4)!}{(l+m)!}}\,Y_{l+2}^{m+2}(\theta,\phi)$$

$$-2\sqrt{\frac{(l+m+2)!\,(l-m)!}{(l-m-2)!\,(l+m)!}}\,Y_l^{m+2}(\theta,\phi)$$

$$+\frac{(2l+3)}{\sqrt{(2l+1)(2l-3)}}\sqrt{\frac{(l-m)!}{(l-m-4)!}}\,Y_{l-2}^{m+2}(\theta,\phi) \tag{18}$$

$$(2l-1)(2l+3)\ \sin^2\theta\ e^{-2i\phi}\, Y_l^m(\theta,\phi) = \frac{(2l-1)}{\sqrt{(2l+1)(2l+5)}}\sqrt{\frac{(l-m+4)!}{(l-m)!}}\, Y_{l+2}^{m-2}(\theta,\phi)$$

$$-2\sqrt{\frac{(l-m+2)!\,(l+m)!}{(l+m-2)!\,(l-m)!}}\, Y_l^{m-2}(\theta,\phi)$$

$$+\frac{(2l+3)}{\sqrt{(2l+1)(2l-3)}}\sqrt{\frac{(l+m)!}{(l+m-4)!}}\, Y_{l-2}^{m-2}(\theta,\phi) \qquad (19)$$

Algebraic Derivation of Gaunt Coefficients

The Gaunt coefficients are defined by the integral of the product of three spherical harmonics, $Y_l^m(\theta,\phi)$, or associated Legendre functions over solid angles by Gaunt [20].

$$Y_{l_1m_1,l_2m_2}^{l\,m} = \int_0^{2\pi}\int_0^{\pi} Y_{l_1}^{m_1\,*}(\theta,\phi)\, Y_{l_2}^{m_2}(\theta,\phi)\, Y_l^m(\theta,\phi) sin\theta d\theta d\phi \qquad (20)$$

Where selection rules are $m = m_1 - m_2$ and $|l_1 - l_2| \le l \le l_1 + l_2$.

The Gaunt coefficients can be expressed using the lowering and raising operators given in Eq. (8).

$$Y_{l_1m_1,l_2m_2}^{l\,m} = \frac{1}{\hbar\sqrt{l_2(l_2+1)-m_2(m_2-1)}}$$

$$\int_0^{2\pi}\int_0^{\pi} Y_{l_1}^{m_1\,*}(\theta,\phi)\left(\hat{L}_+ Y_{l_2}^{m_2-1}(\theta,\phi)\right) Y_l^m(\theta,\phi) sin\theta d\theta d\phi \qquad (21)$$

$$= \frac{1}{\hbar\sqrt{l_2(l_2+1)-m_2(m_2+1)}}$$

$$\int_0^{2\pi}\int_0^{\pi} Y_{l_1}^{m_1\,*}(\theta,\phi)\left(\hat{L}_- Y_{l_2}^{m_2+1}(\theta,\phi)\right) Y_l^m(\theta,\phi) sin\theta d\theta d\phi \qquad (22)$$

In Eq. (20), if we use $Y_{l_2}^{m_2}(\theta,\phi) = Y_0^0(\theta,\phi) = 1/\sqrt{4\pi}$ and the orthogonality relation of spherical harmonics for $l_2 = 0$ and $m_2 = 0$ the Gaunt coefficient is obtained easily as:

$$Y_{l_1m_1,00}^{l\,m} = \frac{1}{\sqrt{4\pi}}\delta_{l_1,l}\delta_{m_1,m} \qquad (23)$$

For $l_2 = 1$, m_2 takes the values $-1, 0$ and 1. To find the algebraic expressions of $Y_{l_1m_1,1m_2}^{l\,m}$ Gaunt coefficients we start $m_2 = 0$ value. For these values inserting $Y_{l_2}^{m_2}(\theta,\phi) = Y_1^0(\theta,\phi) = \sqrt{3/4\pi}cos\theta$ relation into Eq. (20) the Gaunt coefficient can be written as below

$$Y_{l_1 m_1,10}^{l\,m} = \sqrt{\frac{3}{4\pi}} \int_0^{2\pi} \int_0^{\pi} Y_{l_1}^{m_1\,*}(\theta,\phi) \left(cos\theta \, Y_l^m(\theta,\phi)\right) sin\theta d\theta d\phi \tag{24}$$

For the product of trigonometric function and spherical harmonic, we insert the recurrence relation of spherical harmonics given by Eq. (12) into Eq. (24). Then, using the orthogonality relation of spherical harmonics, for the values of $l_2 = 1$ and $m_2 = 0$ we obtain the Gaunt coefficient algebraically.

$$Y_{l_1 m_1,10}^{l\,m} = \sqrt{\frac{3}{4\pi}} \left\{ \left\{ \frac{(l-m+1)(l+m+1)}{(2l+1)(2l+3)} \right\}^{1/2} \delta_{l_1,l+1} \delta_{m_1,m} + \left\{ \frac{(l-m)(l+m)}{(2l-1)(2l+1)} \right\}^{1/2} \delta_{l_1,l-1} \delta_{m_1,m} \right\} \tag{25}$$

To obtain the expression of $Y_{l_1 m_1,11}^{l\,m}$ Gaunt coefficient from the $Y_{l_1 m_1,10}^{l\,m}$, we use the definition of Gaunt coefficients given by the Eq. (21). Therefore, we apply the raising operator of angular momentum $\hat{L}_+$ to $Y_1^0(\theta,\phi)$ substituted in Eq. (21).

$$Y_{l_1 m_1,11}^{l\,m} = \frac{1}{\sqrt{2}} \int_0^{2\pi} \int_0^{\pi} Y_{l_1}^{m_1\,*}(\theta,\phi) \left(\hat{L}_+ \left(\sqrt{3/4\pi} cos\theta \right) \right) Y_l^m(\theta,\phi) sin\theta d\theta d\phi \tag{26}$$

Using the differential form of $\hat{L}_+$ operator given by Eq. (7) we have

$$Y_{l_1 m_1,11}^{l\,m} = -\sqrt{\frac{3}{8\pi}} \int_0^{2\pi} \int_0^{\pi} Y_{l_1}^{m_1\,*}(\theta,\phi) \, (e^{i\phi} sin\theta \, Y_l^m(\theta,\phi)) sin\theta d\theta d\phi \tag{27}$$

Finally, when the recurrence relation given by Eq. (13) and orthogonality relation of spherical harmonics are used respectively in Eq. (27), for $l_2 = 1$ and $m_2 = 1$, the Gaunt coefficient $Y_{l_1 m_1,11}^{l\,m}$ is algebraically obtained as follows.

$$Y_{l_1 m_1,11}^{LM} = \sqrt{\frac{3}{8\pi}} \left\{ \left\{ \frac{(l+m+1)(l+m+2)}{(2l+1)(2l+3)} \right\}^{1/2} \delta_{l_1,l+1} \, \delta_{m_1,m+1} - \left\{ \frac{(l-m)(l-m-1)}{(2l-1)(2l+1)} \right\}^{1/2} \delta_{l_1,l-1} \, \delta_{m_1,m+1} \right\} \tag{28}$$

Since atomic units are used in these calculations, the Planck's constant $\hbar$ is taken as 1.

For the values $l_2 = 1$ and $m_2 = -1$, when obtaining the expression of $Y_{l_1 m_1,1-1}^{l\,m}$ Gaunt coefficient from $Y_{l_1 m_1,10}^{l\,m}$, we use the definition of Gaunt coefficients given by the Eq. (22). To do this, we must apply the lowering operator of angular momentum $\hat{L}_-$ to $Y_1^0(\theta,\phi)$ substituted in Eq. (22)

$$Y_{l_1 m_1,1-1}^{l\,m} = \frac{1}{\sqrt{2}} \int_0^{2\pi} \int_0^{\pi} Y_{l_1}^{m_1\,*}(\theta,\phi) \left(\hat{L}_- \left(\sqrt{3/4\pi} cos\theta \right) \right) Y_l^m(\theta,\phi) sin\theta d\theta d\phi \tag{29}$$

and then we use the differential form of $\hat{L}_-$ operator given by Eq. (7) in Eq. (29):

$$Y_{l_1 m_1,1-1}^{l\,m} = -\sqrt{\frac{3}{8\pi}} \int_0^{2\pi} \int_0^{\pi} Y_{l_1}^{m_1\,*}(\theta,\phi) (e^{-i\phi} sin\theta Y_l^m(\theta,\phi)) sin\theta d\theta d\phi \tag{30}$$

Substitution of Eq. (14) into Eq. (30) and using orthogonality relation of spherical harmonics gives the algebraical expression of Gaunt coefficient for $l_2 = 1$ and $m_2 = -1$ as follows.

$$Y_{l_1 m_1, 1-1}^{l\,m} = \sqrt{\frac{3}{8\pi}}\left\{\left\{\frac{(l-m+1)(l-m+2)}{(2l+1)(2l+3)}\right\}^{1/2} \delta_{l_1,l+1}\,\delta_{m_1,m-1} - \left\{\frac{(l+m)(l+m-1)}{(2l-1)(2l+1)}\right\}^{1/2} \delta_{l_1,l-1}\,\delta_{m_1,m-1}\right\} \quad (31)$$

In order to get algebraically the Gaunt coefficients with the value $l_2 = 2$ we start the value of $m_2 = 0$. To do this, $Y_{l_2}^{m_2}(\theta,\phi) = Y_2^0(\theta,\phi) = \sqrt{(5/16\pi)}(3cos^2\theta - 1)$ is written in definition of the Gaunt coefficient $Y_{l_1 m_1, 2\,0}^{LM}$ in Eq. (20).

$$Y_{l_1 m_1, 20}^{l\,m} = \sqrt{\frac{5}{16\pi}} \int_0^{2\pi}\int_0^{\pi} Y_{l_1}^{m_1 *}(\theta,\phi)\big((3cos^2\theta - 1)\, Y_l^m(\theta,\phi)\big) sin\theta d\theta d\phi \quad (32)$$

If we use Eq. (15) and the orthogonality relation of spherical harmonics, the algebraical expression of the $Y_{l_1 m_1, 20}^{LM}$ Gaunt coefficients is obtained easily in terms of Kronecker delta functions as follows.

$$Y_{l_1 m_1, 20}^{l\,m} = \sqrt{\frac{5}{16\pi}}\left\{\frac{3}{(2l+3)}\left\{\frac{((l+1)^2 - m^2)((l+2)^2 - m^2)}{(2l+1)(2l+5)}\right\}^{1/2} \delta_{l_1,l+2}\delta_{m_1,m} + \frac{(2l(l+1) - 6m^2)}{(2l-1)(2l+3)} \delta_{l_1,l}\,\delta_{m_1,m} + \frac{3}{(2l-1)}\left\{\frac{(l^2 - m^2)((l-1)^2 - m^2)}{(2l+1)(2l-3)}\right\}^{1/2} \delta_{l_1,l-2}\delta_{m_1,m}\right\} \quad (33)$$

According to the Eq. (21), if the raising operator of angular momentum $\hat{L}_+$ is applied one time on $Y_{l_1 m_1, 20}^{lm}$, we obtain $Y_{l_1 m_1, 21}^{lm}$, if it is applied two times we obtain $Y_{l_1 m_1, 22}^{lm}$.

$$Y_{l_1 m_1, 21}^{l\,m} = \frac{3}{2}\sqrt{\frac{5}{6\pi}}\left\{\frac{1}{(2l+3)}\left\{\frac{((l+1)^2 - m^2)(l+m+2)(l+m+3)}{(2l+1)(2l+5)}\right\}^{1/2} \delta_{l_1,l+2}\delta_{m_1,m+1} + \frac{(2m+1)\sqrt{(l-m)(l+m+1)}}{(2l-1)(2l+3)} \delta_{l_1,l}\delta_{m_1,m+1}\right.$$

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$$-\frac{1}{(2l-1)}\left\{\frac{(l^2-m^2)(l-m-1)(l-m-2)}{(2l+1)(2l-3)}\right\}^{1/2}\delta_{l_1,l-2}\delta_{m_1,m+1}\Bigg\} \quad (34)$$

$$Y_{l_1m_1,22}^{l\,m}=\frac{3}{4}\sqrt{\frac{5}{6\pi}}\Bigg\{\frac{1}{(2l+3)\sqrt{(2l+1)(2l+5)}}\sqrt{\frac{(l+m+4)!}{(l+m)!}}\delta_{l_1,l+2}\delta_{m_1,m+2}$$

$$+\frac{1}{(2l-1)\sqrt{(2l+1)(2l-3)}}\sqrt{\frac{(l-m)!}{(l-m-4)!}}\delta_{l_1,l-2}\delta_{m_1,m+2}$$

$$-\frac{2}{(2l-1)(2l+3)}\sqrt{\frac{(l+m+2)!\,(l-m)!}{(l-m-2)!\,(l+m)!}}\delta_{l_1,l}\delta_{m_1,m+2}\Bigg\} \quad (35)$$

Similarly, to calculate $Y_{l_1m_1,2-1}^{lm}$ we must apply one time the lowering operator of angular momentum $\hat{L}_-$ on $Y_{l_1m_1,20}^{lm}$.

$$Y_{l_1m_1,2-1}^{l\,m}=\frac{3}{2}\sqrt{\frac{5}{6\pi}}\Bigg\{\frac{1}{(2l+3)}\left\{\frac{((l+1)^2-m^2)(l-m+2)(l-m+3)}{(2l+1)(2l+5)}\right\}^{1/2}\delta_{l_1,l+2}\delta_{m_1,m-1}$$

$$-\frac{(2m-1)\sqrt{(l+m)(l-m+1)}}{(2l-1)(2l+3)}\delta_{l_1,l}\delta_{m_1,m-1}$$

$$-\frac{1}{(2l-1)}\left\{\frac{(l^2-m^2)(l+m-1)(l+m-2)}{(2l+1)(2l-3)}\right\}^{1/2}\delta_{l_1,l-2}\delta_{m_1,m-1}\Bigg\} \quad (36)$$

If we apply two time the lowering operator of angular momentum $\hat{L}_-$ on $Y_{l_1m_1,20}^{lm}$, we find that

$$Y_{l_1m_1,2-2}^{l\,m}=\frac{3}{4}\sqrt{\frac{5}{6\pi}}\Bigg\{\frac{1}{(2l+3)\sqrt{(2l+1)(2l+5)}}\sqrt{\frac{(l-m+4)!}{(l-m)!}}\delta_{l_1,l+2}\delta_{m_1,m-2}$$

$$+\frac{1}{(2l-1)\sqrt{(2l+1)(2l-3)}}\sqrt{\frac{(l+m)!}{(l+m-4)!}}\delta_{l_1,l-2}\delta_{m_1,m-2}$$

$$-\frac{2}{(2l-1)(2l+3)}\sqrt{\frac{(l-m+2)!\,(l+m)!}{(l+m-2)!\,(l-m)!}}\delta_{l_1,l}\delta_{m_1,m-2}\Bigg\} \quad (37)$$

Results

Spherical harmonics are orthogonal functions that depend on polar (θ) and azimuth (ϕ) angles. Using ladder operators when numerically calculating the Gaunt coefficients obtained from the integral of the product of three spherical harmonics as given Eq. (20), since the integral over azimuth angles have the following value.

$$\int_0^{2\pi} e^{i(-m_1+m_2+m)\phi} d\phi = 2\pi\delta_{-m_1+m_2+m,0} \quad (38)$$

According to this result, the selection rule based on magnetic quantum numbers must satisfy the $-m_1 + m_2 + m = 0$ condition for the Gaunt coefficients to be different from zero. The remaining integral over polar angles consists of the product of three associated Legendre polynomials. In some special cases, this integral takes the following form.

$$\int_0^{\pi} P_{l_1}^{m_1}(cos\theta)\big(f(\theta)P_l^m(cos\theta)\big)\, sin\theta d\theta \quad (39)$$

Here, $f(\theta)$ is a function depending on trigonometric functions. Using the recurrence relation of associated Legendre polynomials, the product $f(\theta)P_l^m(cos\theta)$ is written as the sum of associated Legendre polynomials of different degrees. After this process is performed, the integral over polar angles becomes the integral of the product of two associated Legendre polynomials. This gives the orthogonality relation for associated Legendre polynomials given below.

$$\int_0^{\pi} P_{l_1}^{m}(cos\theta)P_l^m(cos\theta)\, sin\theta d\theta = \frac{2}{2l+1}\frac{(l+m)!}{(l-m)!}\delta_{l_1,l} \quad (40)$$

This result demonstrates that the selection rules depending on the orbital angular momentum quantum number are $l_1 + l_2 + l = 2n$. Here n is an integer. In solutions using algebraic methods, the encountered integrals can be easily solved using the functions' orthogonality relations and recurrence relations without the need to solve integral and differential equations. Whichever method is used, analytic or algebraic, the physical results are the same, even if the obtained mathematical expressions differ. In this paper, the Gaunt coefficients are derived algebraically using the definition given in Eq. (20). To do this, angular momentum ladder operators, which are frequently used in the derivation of spherical harmonics in quantum mechanics, are applied to $Y_{l_2}^{m_2}(\theta,\phi)$ in Eq. (20). We start with the case $m_2 = 0$, which corresponds a given value of l_2. As given in Eq. (21) and Eq. (22), applying the raising operator $\hat{L}_+$ we get the cases $m_2 > 0$ and applying the lowering operator $\hat{L}_-$ we get the cases $m_2 < 0$. This algebraic operation is performed for all physical values of the m_2 magnetic quantum number, corresponding to the constant values $l_2 = 0, 1, 2$. As can be seen from the derived algebraic expressions in Eqs. (23, 25, 28, 31, 33, 34, 35, 36, 37), the values of the l_1 and m_1 are determined by the values of l and m quantum numbers. Accordingly, the algebraic formulae given for Gaunt coefficients in the 5th column of Table

1 are expressed solely in the l and m quantum numbers. Gaunt coefficients can be easily computed by substituting the desired physical values into the l and m quantum numbers, as indicated in Table 1.

Table 1. *Algebraic expressions of Gaunt coefficients for $l_2 = 0, 1, 2$ values*

l_1	m_1	l_2	m_2	$Y^{l\,m}_{l_1 m_1, l_2 m_2}$
l	m	0	0	$1/\sqrt{4\pi}$
$l+1$	m	1	0	$\sqrt{\frac{3}{4\pi}\frac{(l-m+1)(l+m+1)}{(2l+1)(2l+3)}}$
$l-1$	m	1	0	$\sqrt{\frac{3}{4\pi}\frac{(l-m)(l+m)}{(2l-1)(2l+1)}}$
$l+1$	$m+1$	1	1	$\sqrt{\frac{3}{8\pi}\frac{(l+m+1)(l+m+2)}{(2l+1)(2l+3)}}$
$l-1$	$m+1$	1	1	$-\sqrt{\frac{3}{8\pi}\frac{(l-m)(l-m-1)}{(2l-1)(2l+1)}}$
$l+1$	$m-1$	1	-1	$\sqrt{\frac{3}{8\pi}\frac{(l-m+1)(l-m+2)}{(2l+1)(2l+3)}}$
$l-1$	$m-1$	1	-1	$-\sqrt{\frac{3}{8\pi}\frac{(l+m)(l+m-1)}{(2l-1)(2l+1)}}$
$l+2$	m	2	0	$\frac{3}{(2l+3)}\sqrt{\frac{5}{16\pi}\frac{((l+1)^2-m^2)((l+2)^2-m^2)}{(2l+1)(2l+5)}}$
l	m	2	0	$\sqrt{\frac{5}{16\pi}\frac{(2l(l+1)-6m^2)}{(2l-1)(2l+3)}}$
$l-2$	m	2	0	$\frac{3}{(2l-1)}\sqrt{\frac{5}{16\pi}\frac{(l^2-m^2)((l-1)^2-m^2)}{(2l+1)(2l-3)}}$
$l+2$	$m+1$	2	1	$\frac{3}{(2l+3)}\sqrt{\frac{5}{24\pi}\frac{((l+1)^2-m^2)(l+m+2)(l+m+3)}{(2l+1)(2l+5)}}$
l	$m+1$	2	1	$\frac{3(2m+1)}{(2l-1)(2l+3)}\sqrt{\frac{5(l-m)(l+m+1)}{24\pi}}$
$l-2$	$m+1$	2	1	$-\frac{3}{(2l-1)}\sqrt{\frac{5}{24\pi}\frac{(l^2-m^2)(l-m-1)(l-m-2)}{(2l+1)(2l-3)}}$
$l+2$	$m+2$	2	2	$\frac{3}{(2l+3)\sqrt{(2l+1)(2l+5)}}\sqrt{\frac{5}{96\pi}\frac{(l+m+4)!}{(l+m)!}}$
l	$m+2$	2	2	$-\frac{6}{(2l-1)(2l+3)}\sqrt{\frac{5}{96\pi}\frac{(l+m+2)!\,(l-m)!}{(l-m-2)!\,(l+m)!}}$
$l-2$	$m+2$	2	2	$\frac{3}{(2l-1)\sqrt{(2l+1)(2l-3)}}\sqrt{\frac{5}{96\pi}\frac{(l-m)!}{(l-m-4)!}}$
$l+2$	$m-1$	2	-1	$\frac{3}{(2l+3)}\sqrt{\frac{5}{24\pi}\frac{((l+1)^2-m^2)(l-m+2)(l-m+3)}{(2l+1)(2l+5)}}$

Table 1. *...contiuned*

l	$m-1$	2	-1	$-\frac{3(2m-1)}{(2l-1)(2l+3)}\sqrt{\frac{5(l+m)(l-m+1)}{24\pi}}$
$l-2$	$m-1$	2	-1	$-\frac{3}{(2l-1)}\sqrt{\frac{5}{24\pi}\frac{(l^2-m^2)(l+m-1)(l+m-2)}{(2l+1)(2l-3)}}$
$l+2$	$m-2$	2	-2	$\frac{3}{(2l+3)\sqrt{(2l+1)(2l+5)}}\sqrt{\frac{5}{96\pi}\frac{(l-m+4)!}{(l-m)!}}$
l	$m-2$	2	-2	$-\frac{6}{(2l-1)(2l+3)}\sqrt{\frac{5}{96\pi}\frac{(l-m+2)!\,(l+m)!}{(l+m-2)!\,(l-m)!}}$
$l-2$	$m-2$	2	-2	$\frac{3}{(2l-1)\sqrt{(2l+1)(2l-3)}}\sqrt{\frac{5}{96\pi}\frac{(l+m)!}{(l+m-4)!}}$

In the Mathematica programming language, the Gaunt coefficients, defined by integral representation in Eq. (20), are calculated numerically using the integral command below.

```
Integrate [Conjugate [spherical [l1,m1,θ,ϕ]]*spherical[l2,m2,θ,ϕ]
*spherical [l,m,θ,ϕ]*Sin[θ],{ϕ,0,2*Pi},{θ,0,Pi}]
```
(41)

The spherical harmonics employed in Eq. (41) are derived using angular momentum lowering and raising operators, and the program utilized for this purpose is detailed in the appendix. The Gaunt coefficients are calculated numerically for the chosen quantum sets using the Mathematica program provided in the appendix for Eq. (41) and the algebraic expressions presented in Table 1. The numerical results obtained are in complete agreement and are shown in the 6th column of Table 2.

Table 2. *Numerical values and CPU times of Gaunt coefficients for some quantum sets*

l_1	m_1	l_2	m_2	l	$Y^{l\,m}_{l_1m_1,l_2m_2}$	CPU times (seconds)	
						Algebraic expressions in Table 1	Eq. (41)
1	0	1	0	2	0.252313252202016	0.	0.125000
3	0	1	1	4	-0.194663900273006	0.	0.421875
5	-2	1	-1	6	-0.129207486045503	0.	0.828125
8	3	2	1	8	0.110108998314263	0.	1.046875
10	4	2	-1	12	-0.247740673270131	0.	5.734375
12	-5	2	-2	14	0.047285232345527	0.	129.812500
20	5	2	2	18	0.140116470887863	0.	221.296875

Additionally, CPU times are computed and presented in the 7th and 8th columns of Table 2. When the obtained CPU times are compared, it is seen that the use of algebraic expressions in calculating the Gaunt coefficients is more efficient. The programs are executed on an Intel(R) Core (TM) i7-6500U CPU @ 2.50 GHz computer.

Appendix. Mathematica code

The Mathematica program presented in this section calculates the Gaunt coefficients and CPU times using the integral definition consisting of the product of three spherical harmonics shown in Eq. (41). The spherical harmonics employed within the program are derived using lowering and raising angular momentum operators.

Program:

```
In[1]:= ClearAll["Global`*"];
        carpp[pl_,pm_]:= Sqrt[pl*(pl+1)-pm*(pm+1)];
        carpm[ml_,mm_]:= Sqrt[ml*(ml+1)-mm*(mm-1)];
        plusop[pt_,pf_,khf_]:= Exp[I*pf]*(D[khf,pt]+I*Cot[pt]*D[khf,pf]);
        minop[mt_,mf_,khf_]:= -Exp[-I*mf]*(D[khf,mt]-I*Cot[mt]*D[khf,mf]);
          spherical[sl_,sm_,θ_,ϕ_]:= Block[{sphr=0},
            mek=0;
            fonkpl= SphericalHarmonicY[sl,mek,θ,ϕ];
            If[sm > 0,
              For[i=1,i<=sm,i++,
                  kat= carpp[sl,mek];
            fonkp= plusop[θ,ϕ,fonkpl];
            fonkpl= fonkp/kat;
            mek= mek+1],
       If[sm < 0,
          For[i=-1,i>=sm,i=i-1,
                kat= carpm[sl,mek];
          fonkm= minop[θ,ϕ,fonkpl];
          fonkpl= fonkm/kat;
```

```
mek= mek-1]]];
sphr= fonkpl];
l1=3; m1=0;
l2=1; m2=1;
l=4; m= m1-m2;
f1=spherical[l1,m1,θ,ϕ];
f2=spherical[l2,m2,θ,ϕ];
f3=spherical[l,m,θ,ϕ];
Timing[N[Integrate[Conjugate[f1]*f2*f3*Sin[θ],{ϕ,0,2*Pi},{θ,0,Pi}],15]]
```

Out[1]= {0.421875,-0.194663900273006}

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