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Spinor representation of the double group of Icosahedron and entangled states of fullerene C_{60} wave functions

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Symmetry of the icosahedron group is a basic principle producing the analytical description of the fullerene by means of the theory of molecular orbitals. Further development of the fullerene model requires consideration of the half-integer statistics of the electron states. Double group of the icosahedron describes both statistics cases, but we use only fermions case, in other words, the spinor representation of the icosahedron group. In this representation, it is possible to remove restriction defining the parity of the wave function coordinate part and to build a table of characters for arbitrary meaning of the total momentum. Symmetry of the icosahedron produces algebraic structure of the residue ring on the modulo 5, when using momentum projection on chosen axis. If the momentum projection equals both $\pm 5/2$ the states come into one representation. If the momentum projection by absolute value is higher 5/2, the wave function occupies state with several entangled spinor.

Keywords: Double group of the icosahedron, irreducible representations, spinors, spin-orbit interaction, entangled states

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1. Introduction

It will be demonstrated below that fullerene and graphene, its two-dimensional counterpart, both feature unusual topological properties. It is known that a one-sided surface [1] (Möbius strip) made of graphene turns a conductor into a topological insulator (current may flow only along the edge of the strip). Rolling a strip into a tube, one may switch the conducting properties between conductor, semi-conductor and insulator (depending on the way of splicing [2]).

Fullerene and its two-dimensional counterpart exhibited unusual properties. For example, Rb_3C_{60} becomes superconducting at 30 K [3]. The most intriguing property of a fullerene molecule is its icosahedral symmetry. This symmetry type has long existed only hypothetically. The discovery of molecule C_{60} [4] opened up the opportunity to examine experimentally the properties associated with this point symmetry. The symmetry properties allow one to characterize the structure of electron levels of π electrons for atoms positioned at the nodes of a truncated icosahedron. The vibrational structure of the molecule is also governed by the same symmetry. While the phonon subsystem may be considered in integer statistics, the wave properties of electrons follow half-integer statistics. Therefore, the icosahedral group was expanded to incorporate this type of statistics. The obtained object was called the double icosahedral group. If the influence of spins on the positioning of electron energy levels is neglected, the common icosahedral group yields ten symmetry representations. Sixty π electrons form 60 different level types. Thirty of them are occupied (two electrons per level with account for spin). The remaining ones are unoccupied. The representation theory provides an opportunity to predict the type of each level (i.e., its energy and to what representation does it correspond). The representation dimension specifies the degree of degeneracy of an energy level (number of sublevels with the same energy). The consideration of fermions in the double icosahedral group complicates the analysis. The number of levels increases twofold: there are now 120 of them. Sixty lower ones are occupied if the molecule is in the ground state. Wave functions are characterized by spinors; energy levels (with exchange forces being neglected) are conserved. However, the elements of representations are new. This leads to novel unexpected results of the topological nature. However, in order to reveal these features, we had to construct a complete table of wave functions (only the first 60 elements for occupied levels of the system are presented here) within the spinor representation of the double icosahedral group. The non-uniqueness of expansion in new group representations is lifted via the application of a weak spin–orbit interaction.

2. Problem formulation

The model of a molecule with an icosahedral symmetry (C_{12} and C_{60}) is considered. One carbon atom is located at each vertex; the lower index denotes the number of atoms. The first case is that of a regular icosahedron; the second one is a truncated icosahedron. The Hückel molecular orbital approach is applicable in both cases. In the fist case, the Hamiltonian for the molecular orbital method characterizes the interaction between nearest neighbors with the use of a single coupling constant. The tabular representation of the Hamiltonian features only the bond topology of a molecule. The matrix rank may be reduced to 6 by separating the solutions in symmetry with respect to the center of inversion. Molecule C_{12} features an icosahedral symmetry. The complete icosahedral group has 120 elements. Its subgroup covering all rotations about axes of the fifth, the third, and the second orders contains half as much elements (i.e., 60). Isomorphism between the subgroup of rotations and alternating group A_5 may be established. Therefore, the icosahedral group may be analyzed in algebraic and geometric terms. We chose the second option. The dimension of the group of vertices C_{12} is lower than the dimension of the icosahedral group itself. This provides an opportunity to examine how the irreducible representations are occupied. Interestingly, a dual regular dodecahedron has the same symmetry, but more (20) vertices. Since the icosahedral group has $5 \times 2 = 10$ classes of conjugate elements, ten irreducible representations are possible. The analysis of alternating group A_5 suggests a set of representations of dimension 1, 3, 3, 4, 5. Each representation in the set may be either even (index g) or odd (index u). In the geometric approach, the fifth-order axis gives rise to five types of circular symmetry of the form $e^{im\varphi}$, where integer $m = 0, \pm1, \pm2$. The representations differ in sets of numbers m. Representation A has only $m = 0$. Representation T_1 has a dimension of 3 and $m = 0, \pm1$, while T_2 has a dimension of 3 and $m = 0, \pm2$. Representation G has a dimension of 4 with $m = \pm1, \pm2$. Representation H covers the entire set of five numbers. In quantum mechanics, these numbers are projections of the orbital moment onto an axis. Solving the eigenproblem for a matrix of rank 6 in the molecular orbital model, one finds two representations (A_g and H_g) in the even case with $\lambda_{\text{even}} = 2 \pm 3$ and two representations (T_{1u} and T_{2u}) in the odd case with $\lambda_{\text{odd}} = \pm\sqrt{5}$. The total dimension of spaces in both cases is 6. Representation G is lacking. The analysis of molecule C_{60} within the molecular orbital model also leads to the solution of the eigenproblem for matrices of rank 6. The difference consists in the fact that two different coupling constants need to be introduced to characterize a truncated icosahedron, since the edge length of a pentagon differs from the length of a hexagon edge that connects the pentagons. The Hamiltonian matrix for a molecule of 60 vertices has rank 60, which is again reduced to 6 by choosing the symmetry via quantum number m and parity of the solution. Since the number of vertices corresponds to the order of group A_5, the total number of actualized representations matches, in accordance with the representation theory, the group order; i.e., $1^2 + 3^2 + 3^2 + 4^2 + 5^2 = 60$. Specifically, T_1 and T_2 appear three times: two times as an odd representation and one time as an even representation. The so-called spontaneous symmetry breaking occurs, since 3 may be represented as a sum of two integers only in this way: $3 = 2 + 1$. Likewise, $5 = 2 + 3$ and representation H appears five times (three times as an even one). Representation A_g appears once, and A_u is lacking. Representation G is present twice as an even one and twice as an odd one.

Thus, the transition from an icosahedron to a truncated icosahedron in the molecular orbital model allows one to fill nine out of ten lines of the character table of the icosahedral group along the dimension of irreducible representations. Only representation A_u is lacking in the group of 60 vertices arranged at the sites of carbon atoms of molecule C_{60} and, consequently, featuring icosahedral symmetry. The character table allows one to introduce the scalar multiplication operation. Different irreducible representations are orthogonal, and a square of the irreducible representation modulus is equal to the group order. Any object in the space of representations may also be expanded in irreducible representations.

The table of representations may be used to characterize both the vibrations of atoms in a fullerene molecule [5] and the electron states of the π-electron system for carbon atoms bound into a fullerene molecule. In the simplest version of the theory, two electrons with opposite spins are located at each level obtained within the model. As always, they are filled from the bottom of the well. Electron spins do not interact with each other.

The idea of a double group belongs to Bethe [6]. He introduced operation R that denotes rotation by 360°. While rotation by 2π is a unit operation for common point groups from I_h, this rotation in double symmetry group I_h^D produces a different result for new irreducible representations $\mathfrak{T}_\sigma(I_h^D) \subset \mathfrak{T}(I_h^D)$. Only transformation R repeated twice is a unit operation for them. It means that $R^2 = 1$ and $R = -1$ for new representations, which is indicative of half-integer statistics. Thus, the values in cells of the character table produced by new operation R that are generated by representations $A, T_1, T_2, G, H \subset \mathfrak{T}(I_h^D)$ are the same as the ones obtained without this operation. The characters of new representations change sign after operation R is performed. The dimensions of new irreducible representations are integer numbers: 2, 2, 4, 6. The sum of their squares again yields the number of vertices: $2^2 + 2^2 + 4^2 + 6^2 = 60$. We will call this part of irreducible representations of the double group a spinor one $\mathfrak{T}_\sigma(I_h^D)$, since the wave functions of free nonrelativistic particles with spin $\frac{1}{2}$ ($SU(2)$ symmetry) are represented via spinor spherical functions [7]. The following designations were chosen for representations from $\mathfrak{T}_\sigma(I_h^D)$: $\Gamma_6 \equiv \Gamma_{1/2}$, $\Gamma_7 \equiv \Gamma_{7/2}$ and $\Gamma_8 \equiv G_{3/2}$, $\Gamma_9 \equiv I_{5/2}$. Their orthogonality to irreducible representations of the icosahedral group $\mathfrak{T}(I_h)$ is ensured only over an extended set of classes of conjugate elements (operations). Owing to the parity of representations, the operation of rotation about second-order axes yields a zero value in the corresponding column of the character table. The total number of (even and odd) irreducible representations is as follows: 2 two-dimensional in each irreducible representation, 4 four-dimensional, and 6 six-dimensional. It is expected that the case with parity is symmetric.

3. Irreducible representations of the icosahedral group

A truncated icosahedron has $B = 12 \times 5 = 60$ vertices, $P = 30 + 12 \times 5 = 90$ edges, and $\Gamma = 20 + 12 = 32$ faces. Placing a carbon atom at each vertex of a truncated icosahedron, one obtains a model of fullerene C_{60}. To monitor the wave function state at 60 vertices within the Hückel molecular orbital theory, we may limit ourselves to the same number of interacting and the least tightly bound π electrons and assume that one π electron is located at each node. Since the icosahedral group contains 120 elements (60 of which correspond to rotations), the number of vertices of a truncated icosahedron is insufficient to implement a complete 10×10 character system (Table 1). The number of representations and classes of conjugate transformations is 10 (with P inversion taken into account). Classes are formed from a unit transformation, rotations about the fifth-order axis $12C_5$, $12C_5^2$ (here, 12 is the number of elements in a class), and rotations about the third- and second-order axes C_3, C_2. The other classes include inversion alongside with rotation [8]. The space dimension of each irreducible representation is listed in the column for unit transformation E. The total number of wave functions (electron states) matches the rank of the Hamiltonian matrix (i.e., the number of vertices). The dimension of space of representations $\mathfrak{T}(I_h)$ is specified by this number. The repetition factors in the decomposition into irreducible representations denote the number of times a given representation appears in $\mathfrak{T}(I_h)$. If we use the notation where the repetition factor precedes a representation, the following composition of irreducible representations corresponds to fullerene: $1A_g$, $2T_{1u}$, $2T_{2u}$, $1T_{1g}$, $1T_{2g}$, $2G_u$, $2G_g$, $2H_u$, $3H_g$. If parity is neglected, we obtain $1A$, $3T_1$, $3T_2$, $4G$, $5H$; the repetition factor of an irreducible representation is equal to its dimension (the number of vertices matches the order of alternating group A_5), and the total dimension of representations matches the order of the group. Irreducible representation A_u is also lacking.

Let us direct axis z so that it passes through the center of a truncated icosahedron and the center of a pentagon face (see the figure). The Cartesian set of axes is defined so that the symmetry axis of the template figure (highlighted) of six points is projected to axis x. Rotated about axis z by an angle divisible by $2\pi/5$, this figure covers all points of the body in the upper half-space. Specifying just six vertices at the indicated fragment of a truncated icosahedron, one may characterize all states of the system with the use of two quantum numbers setting the properties of symmetry with respect to the fifth-order axis and inversion with respect to the icosahedron center.

Table 1. Character table of irreducible representations of the icosahedral group $\mathfrak{T}(I_h)$, $r = (1+\sqrt{5})/2$ is the root of equation $r^2 = r + 1$. Indices g and u denote even and odd representations with respect to central inversion P

$\mathfrak{T}(I_h)$	E	$12C_5$	$12C_5^2$	$20C_3$	$15C_2$	P	$12S_{10}^3$	$12S_{10}$	$20S_3$	$15\sigma_v$
A_g	$+1$	$+1$	$+1$	$+1$	$+1$	$+1$	$+1$	$+1$	$+1$	$+1$
T_{1g}	$+3$	$+r$	$1-r$	0	-1	$+3$	r	$1-r$	0	-1
T_{2g}	$+3$	$1-r$	r	0	-1	$+3$	$1-r$	r	0	-1
G_g	$+4$	-1	-1	$+1$	0	$+4$	-1	-1	$+1$	0
H_g	$+5$	0	0	-1	$+1$	$+5$	0	0	-1	$+1$
A_u	$+1$	$+1$	$+1$	$+1$	$+1$	-1	-1	-1	-1	-1
T_{1u}	$+3$	$+r$	$1-r$	0	-1	-3	$-r$	$r-1$	0	$+1$
T_{2u}	$+3$	$1-r$	r	0	-1	-3	$r-1$	$-r$	0	$+1$
G_u	$+4$	-1	-1	$+1$	0	-4	$+1$	$+1$	-1	0
H_u	$+5$	0	0	-1	$+1$	-5	0	0	$+1$	-1

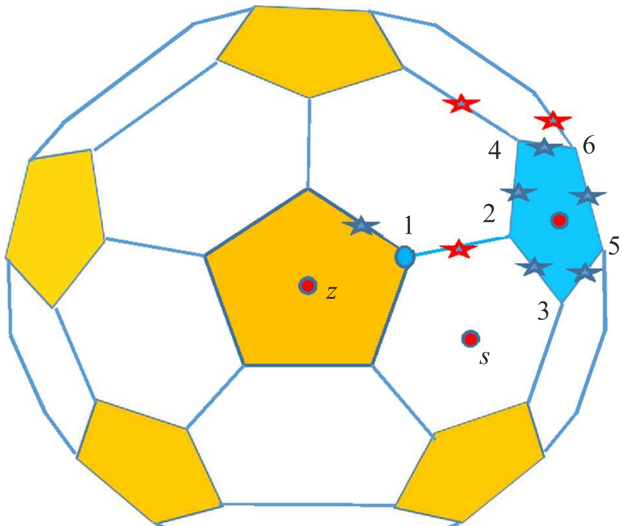

Diagram of fullerene and the template for the group of rotations from I_h.

We denote the first and the second quantum numbers as m and p. Representations $A_g, T_{1g}, T_{2g} \dots$ are symmetric with respect to inversion, and quantum number p assumes the value of 1. An antisymmetric combination of wave function values with respect to inversion corresponds to representations T_{1u}, T_{2u}, G_u, H_u, and quantum number p assumes the value of -1. Quantum number m specifies the factor outside a wave function $\eta^m = \exp(i\,\frac{2\pi}{5}m)$, which characterizes oscillations of this wave function at each rotation of the template. There are a total of five nontrivial variants or states (with $m = 0, \pm 1, \pm 2$). Irreducible representations differ in the set of combinations of the state

Table 2. Formulae for characters of irreducible representations of the icosahedral group

I_h representation	Formula for character $\chi(\varphi)$
A	1
T_1	$1 + 2\cos\varphi$
T_2	$1 + 2\cos 7\varphi$
G	$2\cos 3\varphi + 2\cos 4\varphi$
H	$1 + 2\cos\varphi + 2\cos 2\varphi$

Table 3. Character χ table for irreducible representations of the double icosahedral group, C_i are five different classes of conjugate rotations from the icosahedral group

$\mathfrak{T}(I_h^D)$	C_i	$P \times C_i$	$R \times C_i$	$R \times P \times C_i$
$\mathfrak{T}(I_h)$	$\chi(\mathfrak{T}(I_h))$		$\chi(\mathfrak{T}(I_h))$	
$\mathfrak{T}_\sigma(I_h^D)$	$\chi(\mathfrak{T}_\sigma(I_h^D))$		$-\chi(\mathfrak{T}_\sigma(I_h^D))$	

of number m. Representation A_g contains only the state with $m = 0$. Representation H includes all the possible states. Representation G is set by four projections with $m = \pm 1, \pm 2$, and representation T_1 is specified by three projections with $m = 0, \pm 1$. Representation T_2 is the most unusual one: it has no ± 1 projections (i.e., $m = 0, \pm 2$). Thus, number m corresponds to the projection of orbital moment $L = 2$ onto axis z for the irreducible representation of the group of rotations $SO(3)$ [9]. Note that this projection is specified by a set of integer numbers that do not exceed 2 in modulus (icosahedral group). A character table for orbital moment l may be obtained for a given set of rotations that preserves the positioning of a truncated icosahedron. A representation from $SO(3)$ with a given orbital moment is a direct sum of a series of irreducible representations of an icosahedron (the representations are equivalent only at $L \leq 2$).

Their values for characters at the left-hand side of Table 1 (without inversion operation P) may be represented by the formulae from Table 2 as functions of angle, where $\varphi = 0, \frac{2\pi}{5}, \frac{4\pi}{5}, \frac{2\pi}{3}, \pi$.

4. Irreducible representations of the double icosahedral group

The idea of a double symmetry group has been put forward long ago [6]. In the present study, we follow the approach from [10], which applies these ideas to the icosahedral group. Bethe introduced operation R to denote rotation by 2π. In the context of elements of integer statistics, it matches the common rotation and thus does not alter the character; in half-integer statistics, the sign changes relative to an element of the table without this operation (Table 3). In the first case, these are the representations listed earlier in Table 1 (irreducible representations A, T_1, T_2, G, H). If we could use the notation of continuous Lie groups, the second part of representations would feature symmetry $SU(2)$; however, we examine finite point groups. Elements of irreducible representations in the second case are denoted as $\Gamma_6 \equiv E_{1/2}, \Gamma_7 \equiv E_{7/2}$ and $\Gamma_8 \equiv G_{3/2}, \Gamma_9 \equiv I_{5/2}$. The author of [10] proposed to consider operation R for $\mathfrak{T}(I_h)$ representations as the motion along a normally spliced strip without a twist. In the second case for elements of irreducible representations from $\mathfrak{T}_\sigma(I_h^D)$, the strip is twisted into a one-sided surface (Möbius strip). A point returns to its initial position only after two turns.

The potential of the initial set of classes of conjugate elements (without operation R) was demonstrated in [11,12]. A truncated character table of the double icosahedral group is constructed by splitting elements of different statistics with respect to parity. Specifically, only even representations A_g, T_{1g}, T_{2g}, G_g, and H_g are taken from Table 1, and odd irreducible representations are taken from Table 4. These are two two-dimensional ($E_{u1/2}$ and $E_{u7/2}$), one four-dimensional ($G_{u3/2}$), and one six-dimensional ($I_{u5/2}$) representations. Representations of different parity are orthogonal in the truncated character table constructed over ten classes of conjugate elements only. The orthogonality of representations of the same parity is lost in it; this helps relate these representations to each other. Table 4 is the character table of irreducible representations from the set with half-integer statistics $\mathfrak{T}_\sigma(I_h^D)$ over the initial set of ten classes of conjugate elements. The remaining part of the character table of this representation is determined based on Table 3.

The values for characters at the left-hand side of Table 4 (without inversion operation P) may be represented by the formulae from Table 5. Formulae may now be used to perform operations on characters. The character of a direct product of groups is specified at each group element as a product of characters. It follows from Table 5 that factor $2\cos(\varphi/2)$ is present in all representations and may be factorized. The factor in curly brackets is associated with representations from the icosahedral group $\mathfrak{T}(I_h)$ with integer statistics; i.e., $E_{1/2} = A \otimes E_{1/2}$. Representations T_{1u} and H_g correspond to states with integer orbital moments $L = 1, 2$. The direct product of representation $E_{1/2}$ with them is a sum of the following representations: $E_{1/2} \otimes T_1 = E_{1/2} \oplus G_{3/2}$ and $E_{1/2} \otimes H = G_{3/2} \oplus I_{5/2}$. Since two trigonometric expressions match ($\cos 4\varphi + \cos 7\varphi = \cos\varphi + \cos 2\varphi$) over the family of icosahedron rotations, $I_{5/2} \oplus (E_{7/2} \oplus I_{5/2}) = E_{1/2} \otimes \{G \oplus T_2\}$. These examples demonstrate that representation $G \oplus T_2$ with orbital moment $L = 3$ multiplied by a representation with

Table 4. Character table for $\mathfrak{T}_\sigma(I_h^D)$ irreducible representations from the double icosahedral group with half-integer statistics

$\mathfrak{T}_\sigma(I_h^D)$	E	$12C_5$	$12C_5^2$	$20C_3$	$15C_2$	P	$12S_{10}^3$	$12S_{10}$	$20S_3$	$15\sigma_v$
$E_{g1/2}$	$+2$	$+r$	$r-1$	$+1$	0	$+2$	$+r$	$r-1$	$+1$	0
$E_{g7/2}$	$+2$	$1-r$	$-r$	$+1$	0	$+2$	$1-r$	$-r$	$+1$	0
$G_{g3/2}$	$+4$	$+1$	-1	-1	0	$+4$	$+1$	-1	-1	0
$I_{g5/2}$	$+6$	-1	$+1$	0	0	$+6$	-1	$+1$	0	0
$E_{u1/2}$	$+2$	$+r$	$r-1$	$+1$	0	-2	$-r$	$1-r$	-1	0
$E_{u7/2}$	$+2$	$1-r$	$-r$	$+1$	0	-2	$r-1$	r	-1	0
$G_{u3/2}$	$+4$	$+1$	-1	-1	0	-4	-1	$+1$	$+1$	0
$I_{u5/2}$	$+6$	-1	$+1$	0	0	-6	$+1$	-1	0	0

Table 5. Character formulae for irreducible representations $\mathfrak{T}_\sigma$ of group I_h^D and expansion of certain tensor products of representations

$\mathfrak{T}_\sigma(I_h^D)$	Formula for character $\chi(\varphi)$
$E_{1/2}$	$2\cos(\varphi/2) = 2\cos(\varphi/2)\{1\}$
$E_{7/2}$	$2\cos(7\varphi/2) = 2\cos(\varphi/2)\{2\cos 3\varphi - 2\cos 2\varphi + 2\cos\varphi - 1\}$
$G_{3/2}$	$2\cos(\varphi/2) + 2\cos(3\varphi/2) = 2\cos(\varphi/2)\{2\cos\varphi\}$
$I_{5/2}$	$2\cos(\varphi/2) + 2\cos(3\varphi/2) + 2\cos(5\varphi/2) = 2\cos(\varphi/2)\{2\cos(2\varphi) + 1\}$
$E_{1/2} \otimes T_2 = I_{5/2}$ $E_{1/2} \otimes G = I_{5/2} \oplus E_{7/2}$ $E_{1/2} \otimes T_1 = E_{1/2} \oplus G_{3/2}$ $E_{1/2} \otimes H = G_{3/2} \oplus I_{5/2}$	$2\cos(\varphi/2)(1 + 2\cos 7\varphi) = 2\cos(\varphi/2)(1 + 2\cos 2\varphi)$ $4\cos(\frac{\varphi}{2})(\cos 3\varphi + \cos 4\varphi) = 4\cos(\frac{\varphi}{2})(\cos 3\varphi + \cos\varphi)$ $2\cos(\varphi/2)(1 + 2\cos\varphi)$ $2\cos(\varphi/2)\{2\cos 2\varphi + 2\cos\varphi + 1\}$

Table 6. Expansion of a representation with a given half-integer moment J into a direct sum of irreducible representations from the double icosahedral group

Modulus of total moment $\mathbf{J} = \mathbf{L} + \mathbf{S}$	Sum of representations in $\mathfrak{T}_\sigma(I_h^D)$	Sum of dimensions in $\mathfrak{T}_\sigma(I_h^D)$
$J = 1/2$	$E_{1/2}$	2
$J = 3/2$	$G_{3/2}$	4
$J = 5/2$	$I_{5/2}$	6
$J = 7/2$	$E_{7/2} \oplus I_{5/2}$	$2 + 6$
$J = 9/2$	$G_{3/2} \oplus I_{5/2}$	$4 + 6$
$J = 11/2$	$E_{1/2} \oplus G_{3/2} \oplus I_{5/2}$	$2 + 4 + 6$
$J = 13/2$	$E_{1/2} \oplus E_{7/2} \oplus G_{3/2} \oplus I_{5/2}$	$2 + 2 + 4 + 6$
$J = 15/2$	$G_{3/2} \oplus 2I_{5/2}$	$4 + 2 \times 6$

spin $\frac{1}{2}$ is split into two representations with half-integer moment $L \pm \frac{1}{2} \to J_{L\pm\frac{1}{2}}$. These representations are entangled with each other. Irreducible representations in the $SO(3)$ rotation group differ in moment J, and their characters are specified [13] by formula $\chi_J(C_\varphi) = \sin[(2J+1)\varphi/2] / \sin(\varphi/2)$, where φ is the angle of rotation of operator C_φ. Expansions in irreducible representations are listed in Table 6. The parity of the coordinate part of the representation matches the parity of number L.

The characterization of properties of electron states of fullerene with a half-integer moment may now be performed using the data from [8], where the closest approximation of representations from $\mathfrak{T}(I_h)$ with spherical functions was obtained. These data may now be applied in expanding the representations from $\mathfrak{T}(I_h^D)$ in spinors.

5. Spinor representation

A free nonrelativistic electron with total moment $\mathbf{J} = \mathbf{L} + \mathbf{S}$ may be characterized by spinors using the $3j$ Wigner symbol method. Since spin assumes values $\sigma = \pm 1/2$, the wave function of an electron is defined by a set of quantum numbers $j, l = j \mp 1/2, m$. Here, l is the orbital moment and j, m are the half-integer total moment and its projection onto axis z. Thus, the wave function is a sum of two components [14]:

$$\psi_{jl}^{m} = (-1)^{l-j+1/2} c_{jl,+m} \varphi_{l,m-1/2}(\mathbf{r}) \chi(\uparrow) + c_{jl,-m} \varphi_{l,m+1/2}(\mathbf{r}) \chi(\downarrow).$$

When $l = j - 1/2$, $c_{jl,+m} = \sqrt{\frac{j+m}{2j}}$ and $\varphi_{l,m\mp 1/2} = Y_{l,m\mp 1/2}$ are spherical functions. If $l = j + 1/2$, $c_{jlm} = \sqrt{\frac{j-m+1}{2j+2}}$, the coordinate function retains its form, but a minus sign emerges at the first term. We express spinor $\psi_{jl}^{m} \equiv |{}^{m}_{jl}\rangle$ in the two-component form as

$$\begin{pmatrix} (-1)^{l-j+1/2} c_{jl,m} Y_{l,m-1/2} \\ c_{jl,-m} Y_{l,m+1/2} \end{pmatrix}.$$

As was already noted, the Hamiltonian for a π electron in the state with symmetry characterized by the icosahedral group may be characterized by a 6×6 matrix. The dimension of this matrix for the double icosahedral group increases by a factor of 2, since two spinor components are present. It can be seen in the figure that vertex 6 of the template has a bond with a vertex in the lower hemisphere (denoted with a red star). In order to calculate the interaction of vertex 6 along a bond with the vertex in the lower hemisphere, one needs to derive the wave function value from the initial template using the operations of rotation about axis z and inversion. Note that spin is an axial vector. In the case of inversion, such vectors do not change their sign and preserve the value of projection onto axis z. Therefore, under inversion, each spinor component may transform only via itself:

$$P \begin{pmatrix} \psi_\uparrow \\ \psi_\downarrow \end{pmatrix} \to \pm i \begin{pmatrix} \psi_\uparrow \\ \psi_\downarrow \end{pmatrix}. \tag{1}$$

The constant for a fermion after two applications of inversion is -1. In the case of rotation about axis z, each spinor component also transforms only via itself:

$$U_z(\varphi) = \begin{pmatrix} e^{i\varphi/2} & 0 \\ 0 & e^{-i\varphi/2} \end{pmatrix}.$$

Only the rotation about axes x or y flips the spin. Therefore, the Hamiltonian with symmetry of the double icosahedral group may be presented in the block-diagonal form:

$$\hat{H}^D \begin{pmatrix} \psi_\uparrow \\ \psi_\downarrow \end{pmatrix} = \begin{pmatrix} \hat{H} & 0 \\ 0 & \hat{H} \end{pmatrix} \begin{pmatrix} \psi_\uparrow \\ \psi_\downarrow \end{pmatrix}. \tag{2}$$

Since the spectrum of eigenvalues of diagonal blocks of the Hamiltonian is defined by a set of irreducible representations from $\mathfrak{T}(I_h)$, the solution in $\mathfrak{T}(I_h^D)$ may be constructed with the same eigenvalue when one and the same irreducible representation is taken for the upper and lower parts of the spinor (if the dimension of irreducible representations is higher than 1, the wave functions themselves differ). All that is lacking is to find normalizing factors.

Thus, as in the case of icosahedral group I_h, the eigenproblem is a problem with a 6×6 matrix. The matrix Hamiltonian contains only real numbers. Unit transformation U may be used to transform Hamiltonian $\hat{H} = U^{+} H U$ to form (3) [8,9] (see below).

The spectrum of eigenvalues follows from the equation in which determinant $\det(\hat{H} - \lambda E)$ is equated to zero. Here, $c_m = \cos(\frac{2\pi m}{5})$, $s_m = \sin(\frac{2\pi m}{5})$ and $\eta^m = \exp(i\frac{2\pi}{5}m)$, and $\eta^m + \eta^{-m} = 2c_m$. The matrix of the unitary transformation is

$$U = \begin{pmatrix} E & 0 & 0 \\ 0 & T & 0 \\ 0 & 0 & T \end{pmatrix}, \; E = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \; T = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ 1 & -i \end{pmatrix}.$$

The first 18 irreducible representations in the spinor representation of the icosahedral group are listed in Table 7.

The solution is easy to find at $L \leq 2$, since the representation has a solution in the form of a single spinor. Projections $\pm\frac{5}{2}$ are present only in representation $I_{g5/2}$! Nontrivialities emerge already in the examination of an orbital moment equal to 3. The representation with orbital moment $L = 3$ expands into a sum of two irreducible representations $G_u \oplus T_{2u}$, which differ in the set of available projections. Representation G_u has no zero projection, and T_{2u} has no projections with $m = \pm 1$. In addition, it was already demonstrated that $E_{1/2} \otimes T_2 = I_{5/2}$ and $E_{1/2} \otimes G = I_{5/2} \oplus E_{7/2}$.

$$\hat{H} = \begin{pmatrix} -\alpha 2c_m & -(2-\alpha) & 0 & 0 & 0 & 0 \\ -(2-\alpha) & 0 & -\alpha\sqrt{2} & 0 & 0 & 0 \\ 0 & -\alpha\sqrt{2} & -(2-\alpha)c_m & (2-\alpha)s_m & -\alpha & 0 \\ 0 & 0 & (2-\alpha)s_m & (2-\alpha)c_m & 0 & -\alpha \\ 0 & 0 & -\alpha & 0 & -\alpha-(2-\alpha)pc_{3m} & (2-\alpha)ps_{3m} \\ 0 & 0 & 0 & -\alpha & (2-\alpha)ps_{3m} & \alpha+(2-\alpha)pc_{3m} \end{pmatrix}. \quad (3)$$

Let us consider the case of $L = 3$. The projection of orbital moment $m = 2$ onto axis z is indistinguishable over the set of rotations of the icosahedral group from the projection of moment $m = -3$. This is the property that underlies the algebra of the residue ring modulo a prime number (5). Therefore, when the total moment emerges based on the orbital moment equal to (or higher than) 3, the representation is formed by at least two spinors with different projections of the total moment. Let us consider a combination of spinors of the form

$$\left(-\sqrt{\frac{3}{5}}\Big|^{5/2}_{5/2,3}\Big\rangle + \sqrt{\frac{2}{5}}\Big|^{-5/2}_{7/2,3}\Big\rangle\right)$$

$$= \begin{pmatrix} \sqrt{\frac{1}{7}}\left(\sqrt{\frac{3}{5}}Y_{3,2} + \sqrt{\frac{2}{5}}Y_{3,-3}\right)_{T_u} \\ \sqrt{\frac{6}{7}}\left(-\sqrt{\frac{3}{5}}Y_{3,3} + \sqrt{\frac{2}{5}}Y_{3,-2}\right)_{\bar{G}_u} \end{pmatrix}. \quad (4)$$

The upper spinor component takes the form of representation T_u; the lower one, of $\bar{G}_u$, where the bar indicates inversion of coordinate z. The combination of spinors

$$\left(\sqrt{\frac{6}{7}}\Big|^{5/2}_{5/2,3}\Big\rangle + \sqrt{\frac{1}{7}}\Big|^{5/2}_{7/2,3}\Big\rangle\right) = \begin{pmatrix} 0 \\ Y_{3,3} \end{pmatrix}$$

allows one to transform the lower spinor component to representation T_u ($\sqrt{5}$ is the normalization factor):

$$\frac{1}{\sqrt{5}} \begin{pmatrix} \left(\sqrt{\frac{3}{5}}Y_{3,2} + \sqrt{\frac{2}{5}}Y_{3,-3}\right)_{T_u} \\ 2\left(-\sqrt{\frac{2}{5}}Y_{3,3} + \sqrt{\frac{3}{5}}Y_{3,-2}\right)_{T_u} \end{pmatrix}$$

$$= \sqrt{\frac{7}{5}} \times \left\{ \left(-\sqrt{\frac{3}{5}}\Big|^{5/2}_{5/2,3}\Big\rangle + \sqrt{\frac{2}{5}}\Big|^{-5/2}_{7/2,3}\Big\rangle\right) + \sqrt{\frac{2}{35}}\left(\sqrt{\frac{6}{7}}\Big|^{5/2}_{5/2,3}\Big\rangle + \sqrt{\frac{1}{7}}\Big|^{5/2}_{7/2,3}\Big\rangle\right)\right\}.$$

If we use the combination of spinors

$$\left(\sqrt{\frac{1}{7}}\Big|^{-5/2}_{5/2,3}\Big\rangle + \sqrt{\frac{6}{7}}\Big|^{-5/2}_{7/2,3}\Big\rangle\right) = \begin{pmatrix} 0 \\ Y_{3,-2} \end{pmatrix},$$

the spinor representation has a different coefficient in the lower spinor part:

$$\sqrt{\frac{7}{10}}\left(-\sqrt{\frac{3}{5}}\Big|^{5/2}_{5/2,3}\Big\rangle + \sqrt{\frac{2}{5}}\Big|^{-5/2}_{7/2,3}\Big\rangle\right) + \sqrt{\frac{1}{10}}\left(\sqrt{\frac{1}{7}}\Big|^{-5/2}_{5/2,3}\Big\rangle + \sqrt{\frac{6}{7}}\Big|^{-5/2}_{7/2,3}\Big\rangle\right) = \sqrt{\frac{1}{10}} \begin{pmatrix} \left(\sqrt{\frac{3}{5}}Y_{3,2} + \sqrt{\frac{2}{5}}Y_{3,-3}\right)_{T_u} \\ 3\left(-\sqrt{\frac{2}{5}}Y_{3,3} + \sqrt{\frac{3}{5}}Y_{3,-2}\right)_{T_u} \end{pmatrix}.$$

This ambiguity demonstrates that two orthogonal vectors may be chosen based on these two combinations. The results for these and other versions of spinors are listed in Tables 7–10.

Since $E_{1/2} \otimes G = I_{5/2} \oplus E_{7/2}$, the initial representation $5G_u(3)$ decomposes into two representations: two-dimensional $E_{7/2}$ and six-dimensional $I_{5/2}$. The projections of total moment $m_j = \pm 3/2$ are duplicated in both representations. This refers to representations 25–26 and 29–30. The selection of split is rather tentative in this case, since the representations have equal level energies. This indeterminacy will be lifted below. The orthogonality of a set of elements of representations is ensured by construction. Note that complexities in the representation arise primarily due to the omission of certain axial projections of the moment in the base representation. For example, representation 19 constructed based on $4T_{2u}(3)$ has no projections of the orbital moment equal to ± 1. Therefore, the coefficient of the lower component of the wave function at $Y_{3,1}$ should be zero. This is achieved using a superposition of the form $\sqrt{3/7}|^{1/2}_{5/2,3}\rangle - \sqrt{4/7}|^{1/2}_{7/2,3}\rangle$. The other cases are similar. Thus, this example (Table 8) tells us that the representations for $L = 3$ are superpositions of spinors with $J = 5/2$ and $J = 7/2$. They are entangled to establish group properties of the system. Note that both components (upper and lower) of the coordinate part of the wave function should be solutions of the Hamiltonian with one and the same energy. This translates into a requirement that they belong to one and the same representation. Certain topological restrictions are applied as a result: pure jj representations are lacking. An additional electron–atom interaction is produced due to the fact that an electron has a spin and the associated magnetic moment. The motion of an electron in the electrostatic field of an atomic nucleus induces a magnetic field in the coordinate system of this electron. The magnetic field is a vector product of the electron velocity and the electric field of the nucleus. The field is directed along the radius vector, and vector product $[\mathbf{r} \times \mathbf{v}]$ yields the orbital moment of the electron. This is the reason why this interaction is called the spin–orbit one. The following estimate is obtained for the spin–orbit interaction with account for screening of the nucleus by other electrons in molecule C_{60} [15]:

$$V = \frac{\hbar^2}{m^2c^2}\left(\frac{dU}{dr}\right)\Big|_{r=1.4a_B}\frac{\mathbf{ls}}{R_f} = R_y\,\frac{a_B}{R_f}\,\frac{\alpha^2}{2}\,(\mathbf{j}^2 - \mathbf{l}^2 - \mathbf{s}^2).$$

Table 7. Irreducible representations of the double icosahedral group I_h^D, $L \le 2$

Representation		Wave function (and expansion in spinors)
$\mathfrak{T}(I_h)(L)$	$\mathfrak{T}_\sigma(I_h^D)$	$\Psi_{jl}^m \equiv \|{}^m_{j,l}\rangle$
$1A_g(0)$	$E_{g1/2}$	1. $\begin{pmatrix} Y_{00} \\ 0 \end{pmatrix} = \|{}^{1/2}_{1/2,0}\rangle$ 2. $\begin{pmatrix} 0 \\ Y_{00} \end{pmatrix} = \|{}^{-1/2}_{1/2,0}\rangle$
$2T_{1u}(1)$	$E_{u1/2}$	3. $\begin{pmatrix} -\sqrt{1/3}Y_{1,0} \\ \sqrt{2/3}Y_{1,1} \end{pmatrix} = \|{}^{+1/2}_{1/2,1}\rangle$ 4. $\begin{pmatrix} -\sqrt{2/3}Y_{1,-1} \\ \sqrt{1/3}Y_{1,0} \end{pmatrix} = \|{}^{-1/2}_{1/2,1}\rangle$
$2T_{1u}(1)$	$G_{u3/2}$	5. $\begin{pmatrix} \sqrt{2/3}Y_{1,0} \\ \sqrt{1/3}Y_{1,1} \end{pmatrix} = \|{}^{+1/2}_{3/2,1}\rangle$ 6. $\begin{pmatrix} \sqrt{1/3}Y_{1,-1} \\ \sqrt{2/3}Y_{1,0} \end{pmatrix} = \|{}^{-1/2}_{3/2,1}\rangle$
		7. $\begin{pmatrix} Y_{1,1} \\ 0 \end{pmatrix} = \|{}^{+3/2}_{3/2,1}\rangle$ 8. $\begin{pmatrix} 0 \\ Y_{1,-1} \end{pmatrix} = \|{}^{-3/2}_{3/2,1}\rangle$
$3H_g(2)$	$G_{g3/2}$	9. $\begin{pmatrix} -\sqrt{2/5}Y_{2,0} \\ \sqrt{3/5}Y_{2,1} \end{pmatrix} = \|{}^{+1/2}_{3/2,2}\rangle$ 10. $\begin{pmatrix} -\sqrt{3/5}Y_{2,-1} \\ \sqrt{2/5}Y_{2,0} \end{pmatrix} = \|{}^{-1/2}_{3/2,2}\rangle$
		11. $\begin{pmatrix} -\sqrt{1/5}Y_{2,1} \\ \sqrt{4/5}Y_{2,2} \end{pmatrix} = \|{}^{+3/2}_{3/2,2}\rangle$ 12. $\begin{pmatrix} -\sqrt{4/5}Y_{2,-2} \\ \sqrt{1/5}Y_{2,-1} \end{pmatrix} = \|{}^{-3/2}_{3/2,2}\rangle$
$3H_g(2)$	$I_{g5/2}$	13. $\begin{pmatrix} \sqrt{3/5}Y_{2,0} \\ \sqrt{2/5}Y_{2,1} \end{pmatrix} = \|{}^{+1/2}_{5/2,2}\rangle$ 14. $\begin{pmatrix} \sqrt{2/5}Y_{2,-1} \\ \sqrt{3/5}Y_{2,0} \end{pmatrix} = \|{}^{-1/2}_{5/2,2}\rangle$
		15. $\begin{pmatrix} \sqrt{4/5}Y_{2,1} \\ \sqrt{1/5}Y_{2,2} \end{pmatrix} = \|{}^{+3/2}_{5/2,2}\rangle$ 16. $\begin{pmatrix} \sqrt{1/5}Y_{2,-2} \\ \sqrt{4/5}Y_{2,-1} \end{pmatrix} = \|{}^{-3/2}_{5/2,2}\rangle$
		17. $\begin{pmatrix} Y_{2,2} \\ 0 \end{pmatrix} = \|{}^{+5/2}_{5/2,2}\rangle$ 18. $\begin{pmatrix} 0 \\ Y_{2,-2} \end{pmatrix} = \|{}^{-5/2}_{5/2,2}\rangle$

Here, $a_B = \frac{\hbar^2}{me^2}$ is the Bohr radius, $R_y = \frac{e^2}{2a_B}$ is the energy unit (Rydberg), $\alpha = \frac{e^2}{\hbar c}$ is the fine-structure constant, and $R_f/a_B = 6.62$ is the radius of a fullerene molecule in atomic units. Since $\langle \mathbf{l}^2\rangle = L(L+1)$, $\langle \mathbf{s}^2\rangle = 3/4$, and the difference between the values of $\langle \mathbf{j}^2\rangle$ for states with total moments $J = 5/2$ and $J = 7/2$ $(L = 3)$ is 7, the maximum energy splitting of sublevels of different spinor representations does not exceed

$$\Delta V = R_y \frac{7a_B}{R_f}\frac{\alpha^2}{2} = 0.4\,\text{meV}. \tag{5}$$

Estimate (5) allows for the fact that different sublevels have different weight coefficients in spinor superpositions. The table reveals the set of eigenfunctions for occupied electron states in fullerene. Spinors with moments $J = L - 1/2 \oplus J = L + 1/2$ become entangled almost without exception. If we take the spin–orbit interaction into account, degeneracy may be lifted. The expansion of the initial representation (e.g., $E_{1/2} \otimes H = G_{3/2} \oplus I_{5/2}$) will proceed in this case in such a way that the energy of elements within new representations is kept equal. The arbitrariness of choice of subspaces $G_{3/2} \oplus I_{5/2}$ due to the matching of energies of levels persists until we introduce spin–orbit splitting. The inclusion of the spin–orbit interaction provides an opportunity to introduce an invariant that defines the energy level within new representations (this invariant is set by summing the squares of nonzero amplitudes of spinors in the considered representation with weights $\xi_{1,2}$ depending on moment J):

$$\xi_{1,2} = \frac{1}{2}\left(J(J+1) - L(L+1) - 3/4\right) = \frac{-L-1}{2},\ \frac{L}{2},$$

$$Inv = \xi_1 \sum_p |\alpha^p_{L-1/2,L}|^2 + \xi_2 \sum_r |\alpha^r_{L+1/2,L}|^2. \tag{6}$$

The $Inv = \text{const}$ condition needs to be satisfied for all wave functions from the same representation in order for Hamiltonian perturbation V to preserve the icosahedral symmetry and the energy degeneracy of levels within the representation. This problem turned out to be solvable. The results are presented in the tables. For example, the wave function for line number 41 (Table 9) is

$$\frac{1}{3}\sqrt{\frac{1}{15}}\Big(-(c\sqrt{60} - s\sqrt{40})\big|{}^{1/2}_{\frac{7}{2},4}\big\rangle + (\sqrt{32}s + \sqrt{75}c)\big|{}^{1/2}_{\frac{9}{2},4}\big\rangle + 3\sqrt{7}s\big|{}^{-9/2}_{\frac{9}{2},4}\big\rangle\Big). \tag{7}$$

Here, parameters $c = \cos\beta$ and $s = \sin\beta$

$$Inv = \frac{1}{135}\left(\left(-\frac{5}{2}\right)(60c^2 + 40s^2 - 40\sqrt{6}cs) + 2(32s^2 + 75c^2 + 40\sqrt{6}sc + 63s^2)\right) = \frac{1}{3}(2s^2 + 4\sqrt{6}sc)$$

$$= 2 = 2(c^2 + s^2) \Rightarrow 2s^2 - 2\sqrt{6}cs + 3c^2 = 0,$$

$$s/c = \sqrt{3/2}. \tag{8}$$

Table 8. Continuation of Table 7. Irreducible representations of the double icosahedral group I_h^D with $L = 3$ and expansion in spinors $\Psi_{jl}^m = \sum \alpha_{jlm}|^m_{j,l}\rangle$

Representation		Wave function (and expansion in spinors)
$\mathfrak{T}(I_h)(L)$	$\mathfrak{T}_\sigma(I_h^D)$	$\Psi_{jl}^m = \sum \alpha_{jlm}|^m_{j,l}\rangle$
$4T_{2u}(3)$	$I_{u5/2}$	19. $\begin{pmatrix} -Y_{3,0} \\ 0 \end{pmatrix} = \sqrt{3/7}|^{1/2}_{5/2,3}\rangle - \sqrt{4/7}|^{1/2}_{7/2,3}\rangle$
	$Inv = 0$	20. $\begin{pmatrix} 0 \\ Y_{3,0} \end{pmatrix} = \sqrt{3/7}|^{-1/2}_{5/2,3}\rangle + \sqrt{4/7}|^{-1/2}_{7/2,3}\rangle$
		21. $\frac{1}{\sqrt{5}}\begin{pmatrix} 0 \\ \sqrt{3}Y_{3,2} + \sqrt{2}Y_{3,-3} \end{pmatrix} = \sqrt{\frac{3}{5}}(\sqrt{\frac{5}{7}}|^{3/2}_{5/2,3}\rangle + \sqrt{\frac{2}{7}}|^{3/2}_{7/2,3}\rangle) + \sqrt{\frac{2}{5}}|^{-7/2}_{7/2,3}\rangle$
		22. $\frac{1}{\sqrt{5}}\begin{pmatrix} \sqrt{2}Y_{3,3} - \sqrt{3}Y_{3,-2} \\ 0 \end{pmatrix} = \sqrt{\frac{3}{5}}(\sqrt{\frac{5}{7}}|^{-3/2}_{5/2,3}\rangle + \sqrt{\frac{2}{7}}|^{-3/2}_{7/2,3}\rangle) + \sqrt{\frac{2}{5}}|^{7/2}_{7/2,3}\rangle$
		23. $\frac{1}{\sqrt{10}}\begin{pmatrix} \sqrt{3}Y_{3,2} + \sqrt{2}Y_{3,-3} \\ \sqrt{3}Y_{3,-2} - \sqrt{2}Y_{3,3} \end{pmatrix} = \sqrt{\frac{1}{2}} \times \{(-\sqrt{\frac{27}{35}}|^{5/2}_{5/2,3}\rangle$ $\sqrt{\frac{8}{35}}|^{5/2}_{7/2,3}\rangle) + (-\sqrt{\frac{3}{35}}|^{-5/2}_{5/2,3}\rangle + \sqrt{\frac{32}{35}}|^{-5/2}_{7/2,3}\rangle)\}$
		24. $\frac{1}{\sqrt{10}}\begin{pmatrix} \sqrt{2}Y_{3,-3} + \sqrt{3}Y_{3,2} \\ \sqrt{2}Y_{3,3} - \sqrt{3}Y_{3,-2} \end{pmatrix} = \sqrt{\frac{1}{2}} \times \{(-\sqrt{\frac{27}{35}}|^{-5/2}_{5/2,3}\rangle$ $- \sqrt{\frac{8}{35}}|^{-5/2}_{7/2,3}\rangle) + (\sqrt{\frac{3}{35}}|^{5/2}_{5/2,3}\rangle + \sqrt{\frac{32}{35}}|^{-5/2}_{7/2,3}\rangle)\}$
$5G_u(3)$	$E_{u7/2}$	25. $\frac{1}{\sqrt{10}}\begin{pmatrix} -\sqrt{5}Y_{3,1} \\ -\sqrt{2}Y_{3,2} + \sqrt{3}Y_{3,-3} \end{pmatrix} = \frac{1}{\sqrt{10}}(-\sqrt{7}|^{3/2}_{7/2,3}\rangle + \sqrt{3}|^{-7/2}_{7/2,3}\rangle)$
	$Inv = \frac{3}{2}$	26. $\frac{1}{\sqrt{10}}\begin{pmatrix} -\sqrt{2}Y_{3,-2} - \sqrt{3}Y_{3,3} \\ -\sqrt{5}Y_{3,-1} \end{pmatrix} = \frac{1}{\sqrt{10}}(-\sqrt{7}|^{-3/2}_{7/2,3}\rangle - \sqrt{3}|^{7/2}_{7/2,3}\rangle)$
$5G_u(3)$	$I_{u5/2}$	27. $\begin{pmatrix} 0 \\ Y_{3,1} \end{pmatrix} = \frac{1}{\sqrt{7}}(\sqrt{4}|^{1/2}_{5/2,3}\rangle + \sqrt{3}|^{1/2}_{7/2,3}\rangle)$
	$Inv = -\frac{1}{2}$	28. $\begin{pmatrix} -Y_{3,-1} \\ 0 \end{pmatrix} = \frac{1}{\sqrt{7}}(\sqrt{4}|^{-1/2}_{5/2,3}\rangle - \sqrt{3}|^{-1/2}_{7/2,3}\rangle)$
		29. $\frac{1}{\sqrt{10}}\begin{pmatrix} \sqrt{5}Y_{3,1} \\ -\sqrt{2}Y_{3,2} + \sqrt{3}Y_{3,-3} \end{pmatrix} = \frac{1}{\sqrt{2}}$ $\times \{(-\sqrt{\frac{8}{7}}|^{3/2}_{5/2,3}\rangle + \sqrt{\frac{9}{35}}|^{3/2}_{7/2,3}\rangle) + \sqrt{\frac{3}{5}}|^{-7/2}_{7/2,3}\rangle\}$
		30. $\frac{1}{\sqrt{10}}\begin{pmatrix} -\sqrt{2}Y_{3,-2} - \sqrt{3}Y_{3,3} \\ \sqrt{5}Y_{3,-1} \end{pmatrix} = \frac{1}{\sqrt{2}}$ $\times \{(-\sqrt{\frac{8}{7}}|^{-3/2}_{5/2,3}\rangle + \sqrt{\frac{9}{35}}|^{-3/2}_{7/2,3}\rangle) - \sqrt{\frac{3}{5}}|^{7/2}_{7/2,3}\rangle\}$
		31. $\frac{1}{\sqrt{10}}\begin{pmatrix} \sqrt{3}Y_{3,-3} - \sqrt{2}Y_{3,2} \\ -\sqrt{2}Y_{3,-2} - \sqrt{3}Y_{3,3} \end{pmatrix} = \sqrt{\frac{1}{2}} \times \{(-\sqrt{\frac{32}{35}}|^{-5/2}_{5/2,3}\rangle$ $- \sqrt{\frac{3}{35}}|^{-5/2}_{7/2,3}\rangle) + (-\sqrt{\frac{8}{35}}|^{5/2}_{5/2,3}\rangle - \sqrt{\frac{27}{35}}|^{5/2}_{7/2,3}\rangle)\}$
		32. $\frac{1}{\sqrt{10}}\begin{pmatrix} -\sqrt{2}Y_{3,2} + \sqrt{3}Y_{3,-3} \\ \sqrt{3}Y_{3,3} + \sqrt{2}Y_{3,-2} \end{pmatrix} = \sqrt{\frac{1}{2}} \times \{(\sqrt{\frac{32}{35}}|^{5/2}_{5/2,3}\rangle$ $- \sqrt{\frac{3}{35}}|^{5/2}_{7/2,3}\rangle) + (-\sqrt{\frac{8}{35}}|^{-5/2}_{5/2,3}\rangle + \sqrt{\frac{27}{35}}|^{-5/2}_{7/2,3}\rangle)\}$

It follows from expression (7) that the root of equation s/c is multiple, $c = \sqrt{2/5}$, $s = \sqrt{3/5}$. We then insert the obtained root into (6). Following simplification, we find

$$\frac{1}{5}\left(\sqrt{18}|^{1/2}_{\frac{9}{2},4}\rangle + \sqrt{7}|^{-9/2}_{\frac{9}{2},4}\rangle\right).$$

Likewise, wave function 45 (Table 9) is defined as

$$\frac{1}{3\sqrt{15}}\Big\{(\sqrt{40}c + \sqrt{60}s)\big|^{1/2}_{\frac{7}{2},4}\rangle + (\sqrt{32}c - \sqrt{75}s)\big|^{1/2}_{\frac{9}{2},4}\rangle + 3c\sqrt{7}\big|^{-9/2}_{\frac{9}{2},4}\rangle\Big\}. \quad (9)$$

Table 9. Continuation of Table 7. Irreducible representations I_h^D for $L = 4$

Representation		Wave function (and expansion in spinors)
$\mathfrak{T}(I_h)(L)$	$\mathfrak{T}_\sigma(I_h^D)$	$\Psi_{jl}^m = \sum \alpha_{jlm} \vert^m_{j,l}\rangle$
$6G_g(4)$	$E_{g7/2}$	33. $\frac{1}{\sqrt{30}}\begin{pmatrix}\sqrt7Y_{4,1}-\sqrt8Y_{4,-4}\\ -\sqrt{14}Y_{4,2}+Y_{4,-3}\end{pmatrix} = (-\sqrt{\frac{7}{10}}\vert^{3/2}_{\frac72,4}\rangle+\sqrt{\frac{3}{10}}\vert^{-7/2}_{\frac72,4}\rangle)$
	$Inv = -\frac{5}{2}$	34. $\frac{1}{\sqrt{30}}\begin{pmatrix}\sqrt{14}Y_{4,-2}+Y_{4,3}\\ -(\sqrt7Y_{4,-1}+\sqrt8Y_{4,4})\end{pmatrix} = -\sqrt{\frac{7}{10}}\vert^{-3/2}_{\frac72,4}\rangle-\sqrt{\frac{3}{10}}\vert^{7/2}_{\frac72,4}\rangle$
	$I_{g5/2}$	35. $\sqrt{\frac{1}{15}}\begin{pmatrix}0\\ \sqrt7Y_{4,1}-\sqrt8Y_{4,-4}\end{pmatrix}$ $= \sqrt{\frac{7}{15}}(\sqrt{\frac59}\vert^{1/2}_{\frac72,4}\rangle+\sqrt{\frac49}\vert^{1/2}_{\frac92,4}\rangle)-\sqrt{\frac{8}{15}}\vert^{-9/2}_{\frac92,4}\rangle$
	$Inv = \frac{5}{6}$	36. $\sqrt{\frac{1}{15}}\begin{pmatrix}-\sqrt7Y_{4,-1}-\sqrt8Y_{4,4}\\ 0\end{pmatrix}$ $= \sqrt{\frac{7}{15}}(\sqrt{\frac59}\vert^{-1/2}_{\frac72,4}\rangle-\sqrt{\frac49}\vert^{-1/2}_{\frac92,4}\rangle)-\sqrt{\frac{8}{15}}\vert^{9/2}_{\frac92,4}\rangle$
		37. $\sqrt{\frac{1}{30}}\begin{pmatrix}\sqrt7Y_{4,1}-\sqrt8Y_{4,-4}\\ (\sqrt{14}Y_{4,2}-Y_{4,-3})\end{pmatrix}=\sqrt{\frac{1}{30}}$ $\times\{(\sqrt{\frac73}\vert^{3/2}_{\frac72,4}\rangle+2\sqrt{\frac{14}{3}}\vert^{3/2}_{\frac92,4}\rangle)+(\frac73\vert^{-7/2}_{\frac72,4}\rangle-\frac23\sqrt8\vert^{-7/2}_{\frac92,4}\rangle)\}$
		38. $\frac{1}{\sqrt{30}}\begin{pmatrix}\sqrt{14}Y_{4,-2}+Y_{4,3}\\ \sqrt7Y_{4,-1}+\sqrt8Y_{4,4}\end{pmatrix}=\sqrt{\frac{1}{30}}$ $\times\{(-\sqrt{\frac73}\vert^{-3/2}_{\frac72,4}\rangle+2\sqrt{\frac{14}{3}}\vert^{-3/2}_{\frac92,4}\rangle)+(\frac73\vert^{7/2}_{\frac72,4}\rangle+\frac23\sqrt8\vert^{7/2}_{\frac92,4}\rangle)\}$
		39. $\frac{1}{\sqrt{30}}\begin{pmatrix}\sqrt{14}Y_{4,2}-Y_{4,-3}\\ Y_{4,3}+\sqrt{14}Y_{4,-2}\end{pmatrix}=\frac{1}{\sqrt{30}}\times\{(-\sqrt{\frac79}\vert^{5/2}_{\frac72,4}\rangle$ $+8\sqrt{\frac29}\vert^{5/2}_{\frac92,4}\rangle)+(3\sqrt{\frac79}\vert^{-5/2}_{\frac72,4}\rangle+6\sqrt{\frac29}\vert^{-5/2}_{\frac92,4}\rangle)\}$
		40. $\frac{1}{\sqrt{30}}\begin{pmatrix}\sqrt{14}Y_{4,2}-Y_{4,-3}\\ -(Y_{4,3}+\sqrt{14}Y_{4,-2})\end{pmatrix}=\frac{1}{\sqrt{30}}\times\{(-3\sqrt{\frac79}\vert^{5/2}_{\frac72,4}\rangle$ $+6\sqrt{\frac29}\vert^{5/2}_{\frac92,4}\rangle)-(\sqrt{\frac79}\vert^{-5/2}_{\frac72,4}\rangle+8\sqrt{\frac29}\vert^{-5/2}_{\frac92,4}\rangle)\}$
$7H_g(4)$	$G_{g3/2}$	41. $\sqrt{\frac{1}{15}}\begin{pmatrix}c\sqrt{15}Y_{4,0}\\ s(\sqrt8Y_{4,1}+\sqrt7Y_{4,-4})\end{pmatrix}=\frac15\{\sqrt{18}\vert^{1/2}_{\frac92,4}\rangle+\sqrt7\vert^{-9/2}_{\frac92,4}\rangle\}$ $c=\sqrt{2/5},\ s=\sqrt{3/5}$
	$Inv = 2$	42. $\sqrt{\frac{1}{15}}\begin{pmatrix}s(\sqrt8Y_{4,-1}-\sqrt7Y_{4,4})\\ c\sqrt{15}Y_{4,0}\end{pmatrix}=\frac15\{\sqrt{18}\vert^{-1/2}_{\frac92,4}\rangle-\sqrt7\vert^{9/2}_{\frac92,4}\rangle\}$
	$s = 2c$	43. $\frac{1}{\sqrt{15}}\begin{pmatrix}c(\sqrt8Y_{4,1}+\sqrt7Y_{4,-4})\\ s(Y_{4,2}+\sqrt{14}Y_{4,-3})\end{pmatrix}=\frac15\{2\vert^{3/2}_{\frac92,4}\rangle+\sqrt{21}\vert^{-7/2}_{\frac92,4}\rangle\}$
	$s = 2c$	44. $\frac{1}{\sqrt{15}}\begin{pmatrix}s(Y_{4,-2}-\sqrt{14}Y_{4,3})\\ c(\sqrt8Y_{4,-1}-\sqrt7Y_{4,4})\end{pmatrix}=\frac15\{2\vert^{-3/2}_{\frac92,4}\rangle-\sqrt{21}\vert^{7/2}_{\frac92,4}\rangle\}$
	$I_{g5/2}$	45. $\frac{1}{\sqrt{15}}\begin{pmatrix}-s\sqrt{15}Y_{4,0}\\ c(\sqrt8Y_{4,1}+\sqrt7Y_{4,-4})\end{pmatrix}=\frac{1}{3\sqrt{15}}\times\{(\sqrt{40}c+\sqrt{60}s)\vert^{1/2}_{\frac72,4}\rangle$ $+(\sqrt{32}c-\sqrt{75}s)\vert^{1/2}_{\frac92,4}\rangle+3c\sqrt7\vert^{-9/2}_{\frac92,4}\rangle\}$, $\frac{s}{c}=\sqrt{\frac32}$
	$Inv = -\frac{4}{3}$	46. $\sqrt{\frac{1}{15}}\begin{pmatrix}c(\sqrt8Y_{4,-1}-\sqrt7Y_{4,4})\\ -s\sqrt{15}Y_{4,0}\end{pmatrix}=\frac{1}{3\sqrt{15}}\times(-(c\sqrt{40}+s\sqrt{60})\vert^{-1/2}_{\frac72,4}\rangle$ $+(c\sqrt{32}-s\sqrt{75})^{-1/2}_{\frac92,4}\rangle-3c\sqrt7\vert^{9/2}_{\frac92,4}\rangle)$
	$s = 2c$	47. $\frac{1}{\sqrt{15}}\begin{pmatrix}s(\sqrt8Y_{4,1}+\sqrt7Y_{4,-4})\\ -c(Y_{4,2}+\sqrt{14}Y_{4,-3})\end{pmatrix}=\frac{1}{3\sqrt{15}}\{(-\sqrt6(2s+c)\vert^{3/2}_{\frac72,4}\rangle$ $+\sqrt3(4s-c)\vert^{3/2}_{\frac92,4}\rangle)-(\sqrt{14}(2s+c)\vert^{-7/2}_{\frac72,4}\rangle+\sqrt7(4c-s)\vert^{-7/2}_{\frac92,4}\rangle)\}$

Table 10. Continuation of Table 7. Irreducible representations I_h^D for $L = 4,\ 5$

Representation		Wave function (and expansion in spinors)
$\mathfrak{T}(I_h)(L)$	$\mathfrak{T}_\sigma(I_h^D)$	$\Psi^m_{jl} = \sum \alpha_{jlm}\vert^{m}_{j,l}\rangle$
$7H_g(4)$	$I_{g5/2}$	48. $\frac{1}{\sqrt{15}}\begin{pmatrix} c(Y_{4,-2}-\sqrt{14}Y_{4,3}) \\ -s(\sqrt{8}Y_{4,-1}-\sqrt{7}Y_{4,4}) \end{pmatrix} = \frac{1}{3\sqrt{15}}\{-(\sqrt{6}(c+2s)\vert^{-3/2}_{\frac{7}{2},4}\rangle + \sqrt{3}(4s-c)\vert^{-3/2}_{\frac{9}{2},4}\rangle) + \sqrt{14}(c+2s)\vert^{7/2}_{\frac{7}{2},4}\rangle - \sqrt{7}(4c-s)\vert^{7/2}_{\frac{9}{2},4}\rangle\},\ \frac{s}{c}=2$
	$Inv = -\frac{4}{3}$	49. $\frac{1}{\sqrt{30}}\begin{pmatrix} (\sqrt{14}Y_{4,-3}+Y_{4,2}) \\ (Y_{4,-2}-\sqrt{14}Y_{4,3}) \end{pmatrix} = \frac{1}{\sqrt{30}} \times \{(-\sqrt{8}\vert^{-5/2}_{\frac{7}{2},4}\rangle + \sqrt{7}\vert^{-5/2}_{\frac{9}{2},4}\rangle) - \frac{1}{3}(8\sqrt{2}\vert^{5/2}_{\frac{7}{2},4}\rangle + \sqrt{7}\vert^{5/2}_{\frac{9}{2},4}\rangle)\}$
		50. $\frac{1}{\sqrt{30}}\begin{pmatrix} (\sqrt{14}Y_{4,-3}+Y_{4,2}) \\ -(Y_{4,-2}-\sqrt{14}Y_{4,3}) \end{pmatrix} = \frac{1}{\sqrt{30}} \times \{\frac{1}{3}(-8\sqrt{2}\vert^{-5/2}_{\frac{7}{2},4}\rangle + \sqrt{7}\vert^{-5/2}_{\frac{9}{2},4}\rangle) + (\sqrt{8}\vert^{5/2}_{\frac{7}{2},4}\rangle + \sqrt{7}\vert^{5/2}_{\frac{9}{2},4}\rangle)\}$
$8H_u(5)$	$G_{u3/2}$	51. $\frac{1}{\sqrt{10}}\begin{pmatrix} c(\sqrt{5}Y_{5,-5}+\sqrt{5}Y_{5,5}) \\ s(\sqrt{3}Y_{5,-4}-\sqrt{7}Y_{5,1}) \end{pmatrix} = \frac{1}{\sqrt{10\times 11}}\{\frac{-7}{\sqrt{5}}\vert^{-9/2}_{\frac{9}{2},5}\rangle + \sqrt{32}\vert^{-9/2}_{\frac{11}{2},5}\rangle + \sqrt{22}\vert^{11/2}_{\frac{11}{2},5}\rangle - \sqrt{\frac{21}{5}}(\sqrt{6}\vert^{1/2}_{\frac{9}{2},5}\rangle + \sqrt{5}\vert^{1/2}_{\frac{11}{2},5}\rangle)\},\ \frac{s}{c} = \sqrt{\frac{3}{2}}$
	$Inv = \frac{3}{4}$	52. $\frac{1}{\sqrt{10}}\begin{pmatrix} s(\sqrt{7}Y_{5,-1}+\sqrt{3}Y_{5,4}) \\ c(\sqrt{5}Y_{5,-5}+\sqrt{5}Y_{5,5}) \end{pmatrix} = \frac{1}{\sqrt{10\times 11}}\{\frac{7}{\sqrt{5}}\vert^{9/2}_{\frac{9}{2},5}\rangle + \sqrt{32}\vert^{9/2}_{\frac{11}{2},5}\rangle + \sqrt{22}\vert^{-11/2}_{\frac{11}{2},5}\rangle - \sqrt{\frac{21}{5}}(\sqrt{6}\vert^{-1/2}_{\frac{9}{2},5}\rangle - \sqrt{5}\vert^{-1/2}_{\frac{11}{2},5}\rangle)\}$
		53. $\frac{1}{\sqrt{10}}\begin{pmatrix} c(\sqrt{3}Y_{5,-4}-\sqrt{7}Y_{5,1}) \\ s(-\sqrt{6}Y_{5,-3}-\sqrt{4}Y_{5,2}) \end{pmatrix} = \frac{c}{\sqrt{10\times 11}} \{-\sqrt{3}(7\vert^{-7/2}_{\frac{9}{2},5}\rangle + 5\sqrt{2}\vert^{-7/2}_{\frac{11}{2},5}\rangle) - 2\sqrt{7}\vert^{3/2}_{\frac{9}{2},5}\rangle - 15\vert^{3/2}_{\frac{11}{2},5}\rangle\},\ s = 2c$
		54. $\frac{1}{\sqrt{10}}\begin{pmatrix} -s(\sqrt{4}Y_{5,-2}-\sqrt{6}Y_{5,3}) \\ c(-\sqrt{7}Y_{5,-1}-\sqrt{3}Y_{5,4}) \end{pmatrix} = \frac{c}{\sqrt{10\times 11}} \{+\sqrt{3}(-7\vert^{7/2}_{\frac{9}{2},5}\rangle + 5\sqrt{2}\vert^{7/2}_{\frac{11}{2},5}\rangle) + 2\sqrt{7}\vert^{-3/2}_{\frac{9}{2},5}\rangle - 15\vert^{-3/2}_{\frac{11}{2},5}\rangle\}$
	$I_{u5/2}$	55. $\frac{1}{\sqrt{10}}\begin{pmatrix} -s(\sqrt{5}Y_{5,-5}+\sqrt{5}Y_{5,5}) \\ c(\sqrt{3}Y_{5,-4}-\sqrt{7}Y_{5,1}) \end{pmatrix} = \frac{1}{\sqrt{10\times 11}}\{-\sqrt{33}\vert^{11/2}_{\frac{11}{2},5}\rangle - \sqrt{\frac{14}{5}}(\sqrt{6}\vert^{1/2}_{\frac{9}{2},5}\rangle + \sqrt{5}\vert^{1/2}_{\frac{11}{2},5}\rangle) + (\frac{6\sqrt{6}}{\sqrt{5}}\vert^{-9/2}_{\frac{9}{2},5}\rangle + \sqrt{3}\vert^{-9/2}_{\frac{11}{2},5}\rangle)\},\ \frac{s}{c} = \sqrt{\frac{3}{2}}$
	$Inv = -\frac{1}{2}$	56. $\frac{1}{\sqrt{10}}\begin{pmatrix} -c(\sqrt{7}Y_{5,-1}+\sqrt{3}Y_{5,4}) \\ s(\sqrt{5}Y_{5,-5}+\sqrt{5}Y_{5,5}) \end{pmatrix} = \frac{1}{\sqrt{10\times 11}}\{\sqrt{33}\vert^{-11/2}_{\frac{11}{2},5}\rangle + \sqrt{\frac{14}{5}}(\sqrt{6}\vert^{-1/2}_{\frac{9}{2},5}\rangle - \sqrt{5}\vert^{-1/2}_{\frac{11}{2},5}\rangle) + (\frac{6\sqrt{6}}{\sqrt{5}}\vert^{9/2}_{\frac{9}{2},5}\rangle - \sqrt{3}\vert^{9/2}_{\frac{11}{2},5}\rangle)\},\ \frac{s}{c} = \sqrt{\frac{3}{2}}$
		57. $\frac{1}{\sqrt{10}}\begin{pmatrix} s(\sqrt{3}Y_{5,-4}-\sqrt{7}Y_{5,1}) \\ c(\sqrt{6}Y_{5,-3}+\sqrt{4}Y_{5,2}) \end{pmatrix} = \frac{c}{\sqrt{10\times 11}} \{\sqrt{3}(-4\vert^{-7/2}_{\frac{9}{2},5}\rangle + 5\sqrt{2}\vert^{-7/2}_{\frac{11}{2},5}\rangle) + (6\sqrt{7}\vert^{3/2}_{\frac{9}{2},5}\rangle - 10\vert^{3/2}_{\frac{11}{2},5}\rangle)\},\ \frac{s}{c} = 2$
		58. $\frac{1}{\sqrt{10}}\begin{pmatrix} -c(\sqrt{4}Y_{5,-2}-\sqrt{6}Y_{5,3}) \\ s(\sqrt{7}Y_{5,-1}+\sqrt{3}Y_{5,4}) \end{pmatrix} = \frac{c}{\sqrt{10\times 11}} \{+\sqrt{3}(4\vert^{7/2}_{\frac{9}{2},5}\rangle + 5\sqrt{2}\vert^{7/2}_{\frac{11}{2},5}\rangle) + (6\sqrt{7}\vert^{-3/2}_{\frac{9}{2},5}\rangle + 10\vert^{-3/2}_{\frac{11}{2},5}\rangle)\},\ \frac{s}{c} = 2$
		59. $\frac{1}{5}\begin{pmatrix} (-\sqrt{3}Y_{5,-3}-\sqrt{2}Y_{5,2}) \\ 2(-\sqrt{2}Y_{5,-2}+\sqrt{3}Y_{5,3}) \end{pmatrix} = -\frac{\sqrt{11}}{5}\vert^{-5/2}_{\frac{11}{2},5}\rangle + \frac{1}{\sqrt{11}}(\sqrt{6}\vert^{5/2}_{\frac{9}{2},5}\rangle + \frac{2}{5}\vert^{5/2}_{\frac{11}{2},5}\rangle)$
		60. $\frac{1}{5}\begin{pmatrix} 2(\sqrt{3}Y_{5,-3}+\sqrt{2}Y_{5,2}) \\ (-\sqrt{2}Y_{5,-2}+\sqrt{3}Y_{5,3}) \end{pmatrix} = \frac{\sqrt{11}}{5}\vert^{5/2}_{\frac{11}{2},5}\rangle + \frac{1}{\sqrt{11}}(-\sqrt{6}\vert^{-5/2}_{\frac{9}{2},5}\rangle + \frac{2}{5}\vert^{-5/2}_{\frac{11}{2},5}\rangle)$

The calculation of the invariant yields

$$Inv = \frac{1}{135}\left(\left(-\frac{5}{2}\right)(40c^2 + 60s^2 + 40\sqrt{6}cs)\right.$$

$$\left. + 2(32c^2 + 75s^2 - 40\sqrt{6}sc + 63c^2)\right) = \frac{1}{3}(2c^2 - 4\sqrt{6}sc)$$

$$= -\frac{4}{3} = -\frac{4}{3}(c^2 + s^2) \Rightarrow 2s^2 - 2\sqrt{6}cs + 3c^2 = 0,$$

$$s/c = \sqrt{3/2}. \quad (10)$$

It is evident that the roots of equations derived from invariants in formulae (8) and (10) are compatible. Note that the invariants of representations with moment $L = 4$ (namely, $G_{g3/2}$, $(dim = 4)$ and $I_{g5/2}$, $(dim = 6)$) are interrelated by a formula with a zero right-hand side: $2 \times 4 + (-\frac{4}{3}) \times 6 = 0$. Therefore, the value of the invariant is determined unambiguously from the representation for wave function number 49 (or 50) where the wave function is represented by a superposition of spinors with projections $m = \pm\frac{5}{2}$ of moment J. The upper and the lower components of the wave function representation take the form (accurate to within the normalization factor) set by the corresponding representation of the icosahedral group obtained earlier in [8]. The designations of this initial representation are presented in the first column of the table. The second column lists the representations of the spinor icosahedral group and the invariant values (in certain lines, the ratios of values s and c for wave functions from the third column and the same line are also indicated here to reduce the size of the table). The expression for the wave function and its expansion in spinors are given in the third column. Thus, the inclusion of weak spin–orbit interaction provides an opportunity to decompose unambiguously two-dimensional spaces, which emerge in transition from the icosahedral group to the double icosahedral group, into one-dimensional ones, which lie in their irreducible representations. All the sublevels of these new representations are degenerate in energy. The energy splitting between adjacent representations obtained by performing an operation of the form $E_{1/2} \otimes H = G_{3/2} \oplus I_{5/2}$ is small, since fullerene has a large radius.

6. Conclusion

Thus, we examined the first 60 wave functions of (occupied) electron states of fullerene lying below the Fermi level. Each state with a projection of total moment of $\pm\frac{1}{2}, \pm\frac{3}{2}$ is represented by a two-dimensional space in the spinor representation. The inclusion of the spin–orbit interaction provides an opportunity to decompose such spaces into two one-dimensional ones by referring the corresponding subspaces to their representations (e.g., $G_{3/2}$ or $I_{5/2}$; see the example of wave functions 41 and 45 above). Note that the corresponding states for moments with a projection of $\pm\frac{5}{2}$ are indistinguishable in the icosahedral symmetry field. Therefore, the two-dimensional space corresponding to them falls completely within one representation (functions 49–50). Functions 41 and 45 do not only belong to different representations, but also have slightly different energy levels. The difference is 0.36 meV. It bears reminding that $kT = 25$ meV at room temperature. With the moment of inertia of a fullerene molecule C_{60} ($I = 10^{-43}\,\text{kg}\cdot\text{m}^2$, $\varepsilon = \hbar^2/2I = 3.3\cdot 10^{-4}\,\text{meV}$) taken into account, approximately 275 rotational states should be occupied at this temperature (i.e., $N(N+1)\varepsilon = 25$), and the rotational transition quantum is on the order of 0.2 meV ($2N\varepsilon = 0.2$). A molecule in the excited state with an electron from state 41 (or 45) migrating to a band above the Fermi level gains the capacity to oscillate between states 41 and 45 owing to the interaction via quantum exchange between spin-electron and rotational states (if the rotational temperature of the molecule is on the order of 100 meV, which is needed to establish resonance between them). A similar effect is observed for all electron states split due to the spin–orbit interaction. Since the characteristic energy of vibrational quanta falls within the 20–200 meV range, the influence of vibrational states of a molecule on spin–orbit processes is immaterial.

The wave function is decomposed into a sum of spinors. In the general case, this sum includes spinors having both values of total moment $J = L \mp 1/2$ (but the same projections of the moment onto axis z). Thus, owing to the molecule topology, wave functions contain spinors in entangled states. Note also that the sum includes sets of moment projections coinciding in a ring modulo 5. For example, projection $-\frac{9}{2}$ is included alongside with projection $\frac{1}{2}$ in the case of wave function 41. An attempt at classifying the wave functions of the icosahedral group (the double one included) has already been made in [16], but the influence of the spin–orbit interaction was neglected there, and certain functions in [16] are inconsistent with classical studies [3,17] (e.g., for $T_{2u}(L = 3)$). The notation adopted in the present study allows one to classify wave functions both by means of spherical harmonics and with the use of the classical spinor definition [14]. It is worth reminding that the form of representations of the icosahedral group was determined by solving exactly the Hamiltonian matrix and projecting the point solution to the space of spherical functions. The coefficients of expansion in spherical functions were determined using the pseudoinverse matrix method. This is the best approximation in the sense of the least squares technique. All coefficients turned out to be roots of ratios of integer numbers. The set of eigen wave functions of the Hamiltonian allows one to construct matrix elements for the excitation cross sections of electron states above the Fermi level.

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