Groups and the Buckyball

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1 Introduction

The purpose of this article is to collect a number of remarkable group theoretical facts having to do with icosahedral symmetry. Some of these have been already applied to the discovery and identification of the new C_{60} carbon molecule, called the Buckminsterfullerene, or buckyball, for short, and we hope that other results described here will find applications in physical properties of these molecules. We begin with a description of the molecule.

Take the regular icosahedron. It has twelve vertices with five edges emanating from each vertex, so thirty edges and twenty faces. If we truncate each vertex so as to get a pentagon, each of the (triangular) faces of the icosahedron becomes a hexagon. (They become regular hexagons if we truncate each vertex one third of the way along each edge.) Doing so, we obtain a figure with 60 vertices, each vertex has three emanating edges, two of which lie in pentagonal directions and the third is an edge of the hexagon. This is the buckyball. The icosahedral group, I , is the group of rotational symmetries of this figure which has 60 vertices, twelve pentagonal faces and twenty hexagonal faces so 32 faces. It has $5 \times 12 = 60$ pentagonal edges (the pentagons do not touch one another) and each hexagon has three edges which are not pentagonal, but shared with an adjacent hexagon so $20 \times 3/2 = 30$ such edges, so 90 edges in all. The Euler formula can be easily checked:

$$32 - 90 + 60 = 2.$$

The group I acts transitively on the space of vertices of the icosahedron, and the isotropy subgroup of each vertex consists of rotations through angles $\frac{2k\pi}{5}$. Thus on the buckyball this subgroup is the isotropy group of a pentagon, and acts transitively on the vertices of the pentagon. So I acts simply transitively on the vertices of the buckyball. It is this fact that accounts for its most remarkable properties from a mathematical point of view.

Although I acts transitively on the vertices, it does not act transitively on the edges. In fact, each vertex, v, lies on exactly one pentagon, and hence two of the edges emanating from v are pentagonal and one is hexagonal. In other words, every other edge of each hexagon is purely hexagonal in that it lies on two hexagons, while the other three edges lie on a hexagon and a pentagon. So I acts transitively on the set of hexagonal edges and on the set of pentagonal edges. In the a simplified chemical model for C_{60} it is assumed that a carbon atom is placed at each vertex of the buckyball and that the pentagonal edges are single bonds while the hexagonal edges are double bonds. We will adopt this chemical language: we will call the pentagonal edges single bonds and the hexagonal edges double bonds.

The rotation, t_a, which maps the vertex a into the vertex b connected to a by the double bond u emanating from a must map u into the unique double bond emanating from b, and this double bond is u. Hence $t_a u = u$ and therefore $t_a b = a$. Thus $t_a^2 a = a$ and since I acts simply transitively this implies that

$$t_a^2 = id.$$

Similarly, if s_a denotes the clockwise rotation which moves a to its nearest neighbor on the unique pentagon on which a lies, then

$$s_a^5 = id.$$

In other words, motion along a single bond is a rotation through angle $2\pi/5$.

We can ask, within the 60! element group of all permutations of the vertices (isomorphic to S_{60}), which transformations commute with the action of I ? This will be another sixty element group isomorphic with I. Indeed, once we fix some vertex, we can use the action to identify all the vertices with I, where I acts on itself by left multiplication. But the elements which commute with left multiplication on a group are right multiplication.

Call this commuting group R. Fix one vertex, say a, so we get an identification of C_{60} with I under which a corresponds to the identity element, e. Let $t \in R$ be the element which corresponds to right multiplication by t_a and similarly $s = s_a$. So t carries a into the unique vertex joined to a by a double bond. But then, by the transitivity of the action of I, t must carry every vertex into the neighbor connected to it by a double bond. Similarly, the single bonds emanating from every vertex will correspond to either s or s^{-1}. Now we can clearly walk from any vertex to any other by a succession of single or double bonds. This shows that s and t generate R and hence that s_a and t_a generate I.

If G is any group, and $\{g\}$ is a set of generators of G then the associated *Cayley graph* is defined to be the graph whose vertices are the elements of G, and two vertices a and b are joined by an edge if $a = gb$ or $a = g^{-1}b$ where g is one of the set of preferred generators. So what we have shown is that

Theorem 1 *C_{60} is a Cayley graph .*

Having fixed a vertex, the above construction associates the generator t to every double bond, while our construction associates either s or s^{-1} to each single bond. But we can make a global choice as follows: Think of the buckyball as a polyhedron, that is, put in the faces. Then a choice of orientation of $\mathbf{R}^3$ determines an orientation of the surface of the buckyball and hence of each pentagon. Since each pentagonal edge lies on a unique pentagon, the orientation of the pentagons induces an orientation of every pentagonal edge, so now every vertex has a unique pentagonal edge emanating from it. So if s is the group element which moves a into its nearest neighbor along the pentagonal edge emanating from a, we have labelled every pentagonal edge by s.

Notice that the buckyball is also invariant under the central inversion through the origin, call this transformation P for "parity". We will let

$$I_h = I \times \mathbf{Z}_2,$$

the direct product of I with the group of central inversion through the origin. So $I_h \subset O(3)$ is the full group of orthogonal symmetries of C_{60} while $I \subset SO(3)$ is the full group of rotational symmetries.

The group I_h is a trivial central extension of I, it is a direct product. From a mathematical point of view, there is a much more interesting central extension, which can be described as follows:

There is a homomorphism $\pi : SU(2) \to SO(3)$ which is a double cover, i.e. $\ker\pi = \{e, -e\}$. We can then consider the 120 element group $G = \pi^{-1}I$. This group will play the hero's role in what follows.

2 Group identifications

In this section we describe the group isomorphisms

$$I \sim A_5 \sim Pl(2,5)$$

and

$$G \sim Sl(2,5)$$

as well as the remarkable Galois embedding

$$Sl(2,5) \to Sl(2,11).$$

We begin with the isomorphism $I \sim A_5$. For this, it is enough to find a five element set on which I acts effectively, since A_5 is the only sixty element subgroup of S_5: Any double bond of the buckyball has a unique opposite double bond, and together they determine a plane. There will be exactly two pairs of of opposite bonds whose planes are orthogonal to these planes, and they will be orthogonal to each other. So the set of thirty double bonds decomposes into five classes of six elements each, i.e. five classes of mutually perpendicular "coordinate planes". This gives a homomorphism of I into the group of permutations of these five classes of coordinate systems, and it is easy to check that this is an isomorphism. We now turn to the relation with the general linear groups.

For any finite field $\mathbf{F}_q$ with q elements, the group $Gl(2,q)$ of all invertible two by two matrices with entries in $\mathbf{F}_q$ has $(q^2-1)(q^2-q)$ elements, because there are q^2-1 choices for the entries in the first column and for each first column, the second column must be linearly independent, so q^2-q choices for the second column. So the number of elements in $Sl(2,q)$ is given by $(q^2-1)(q^2-q)/(q-1) = q(q^2-1)$. For $q=5$ we see that

$$\mid Sl(2,5) \mid = 120.$$

The group $Sl(2,q)$ acts on the projective space, $\mathbf{P}^1_q$ of lines through the origin in the plane $\mathbf{F}^2_q$, and the kernel of this action consists of $\{id, -id\}$. If q is odd, this kernel contains two elements, if q is even, then $-id = id$. The corresponding quotient group, the group of projective transformations is known as $Pl(2,q)$. So if $q=5$ the group $Pl(2,5)$ has 60 elements and is isomorphic to A_5. This can be seen as follows. There are $(q^2-1)/(q-1) = q+1$ points on the projective line, $\mathbf{P}^1_q$. For our case, $q=5$, we will identify these six points with the six lines through the centers of opposite pentagonal faces of the buckyball. (Or, what amounts to the same thing, to the six lines through opposite vertices of the original icosahedron.) Let us call these six lines pentagonal axes. The subgroup of the icosahedral group, I, fixing a given pentagonal axis is the dihedral group, D_5, consisting of rotations through angles $2k\pi/5$ about the axis, together with five rotations through 180 degrees in the plane perpendicular to the axis, and which interchange the two opposite pentagons. On the other hand, the subgroup of $Sl(2,q)$ fixing a point in the projective line, say the point $[(1,0)]^\dagger$ is the Borel subgroup

$$B = \left\{ \begin{pmatrix} a & b \\ 0 & a^{-1} \end{pmatrix} \right\}, \ a \in \mathbf{F}^*_q, \ b \in \mathbf{F}_q,$$

of all upper triangular matrices in $Sl(2,q)$. This subgroup has $q(q-1)$ elements, so 20 for the case $q=5$. It is clear that $B/\{id,-id\} = D_5$. So we identify $\mathbf{P}^1_5 = Sl(2,5)/B$ with the set of pentagonal axes which is I/D_5, giving an action of $Pl(2,5)$ on the buckyball and hence a homomorphism of $Pl(2,5)$ into I which must be an isomorphism since $Pl(2,5)$ is simple.

If we identify the six axes of the icosahedron with the six points of the projective line $\mathbf{P}^1_5$, we are in the following situation: A_5 and $PSL(2,5)$ are both identified as simple subgroups of order 60 of the permutation group S_6. We must show that they are isomorphic. Since they are both simple subgroups, they are, in fact, subgroups of A_6. So, we can make use of the following assertion:

Let B and C be two subgroups of index 6 in A_6. Then there is a $\phi \in AuT(A_6)$ such that $\phi(A) = B$.

Proof. Consider the two six element sets A_6/A and A_6/B. The group A_6 acts as permutations of each of these six element sets. So let us choose an identification of A_6/A with the set $\{1, 2, 3, 4, 5, 6\}$ so that A is identified with 6. This gives a homomorphism of A_6 with a subgroup of S_6; call this homomorphism, ϕ_A. Since A_6 is simple, this is an injection; and since the only subgroup of index 2 in S_n is the alternating subgroup (for any $n > 1$),this is an isomorphism of A_6 onto the alternating subgroup of S_6. Similarly for A_6/B. Hence

$$\phi = \phi_B \circ \phi_A^{-1}$$

is an automorphism of A_6 with $\phi(A) = B$.

Every alternating group A_n has outer automorphisms coming from conjugation by odd elements of S_n. But notice that the automorphism, ϕ given above is not of this type. Indeed, $PSl(2, 5)$ acts transitively on $\mathbf{P}^1_5$ while A_5 fixes a point. Hence the isomorphism between $PSl(2, 5)$ and A_5 given above illustrates a remarkable (and unique) property of A_6 among all simple alternating groups:

$AuT(A_6)$ is bigger that S_6.

An extension of the above argument shows that

$$G \sim Sl(2, 5)$$

where, we recall, G is the double cover of I sitting as a subgroup of $SU(2)$.

We should also mention that if we take $q = 4$, then $Sl(2, 4) = Pl(2, 4)$ has 60 elements and is also isomorphic to A_5. Indeed, there are five points in $\mathbf{P}^1_4$ which are permuted by the action of $Sl(2, 4)$. This gives an isomorphism of $Sl(2, 4)$ onto a sixty element subgroup of S_5 and hence onto A_5. To visualize this isomorphism on C_{60}, each class of coordinate planes is identified with a point of $\mathbf{P}^1_4$. So

$$I \sim Sl(2, 4).$$

In our identification of I with $Pl(2, 5)$ we considered a pair of opposite pentagons as a point in $\mathbf{P}^1_5$. But we can consider the individual pentagons (i.e. the vertices of the original icosahedron) as points of $\mathbf{P}^1_{11}$. It was proved by Galois (in a letter to Chevalier written on the eve of his fatal duel) that $Pl(2, p)$ does not have a non-trivial permutation representation on fewer that $p + 1$ elements if $p > 11$. However for $p = 2, 3, 5, 7, 11$ there exist transitive permutation representations on p elements, and this p element set can be realized as a set of

p configurations of pairs of points in $\mathbf{P}^1_p$. Here is a sketch of the construction. We refer the reader to the book by Conway and Sloane, [4], p.268 for details. Let us label the twelve points of $\mathbf{P}^1_{11}$ as

$$0,\ 1,\ 2,\ 3,\ 4,\ 5,\ 6,\ 7,\ 8,\ 9,\ 10, \infty.$$

The group $Pl(2,11)$ acts on $\mathbf{P}^1_{11}$ by fractional linear transformations:

$$x \mapsto \frac{ax+b}{cx+d}.$$

Let C denote the set of partitions of the above letters into six pairs, so a point of C will be a partition of the form

$$\{a,b\}\{c,d\}\{e,f\}\{g,h\}\{i,j\}\{k,l\}$$

where $a \ldots l$ is a permutation of the above twelve letters representing points of $\mathbf{P}^1_{11}$. As the group $Pl(2,11)$ acts on $\mathbf{P}^1_{11}$, it acts on C. In general, the orbit of an element of C will be quite large. But, it turns out that there is an eleven element orbit! Consider the configuration,

$$c_0 = \{\infty, 0\}\{1,6\}\{3,7\}\{9,10\}, \{5,8\}, \{4,2\}.$$

Along with the pair $\{\infty, 0\}$, this configuration contains in each pair exactly one non-zero square in $\mathbf{F}^{11}$, namely $s = 1,4,9,5,3$ along with $6s$. In other words,

$$c_0 = \{\infty, 0\} \cup \bigcup_{s \in \mathbf{F}^{*2}_{11}} \{s, 6s\}.$$

Now the diagonal subgroup $\Delta \subset Sl(2,11)$ acts on $\mathbf{P}_{11}$ as fractional linear transformations by sending

$$x \mapsto k^2 x, \quad k \in \mathbf{F}^*_{11}$$

and so Δ preserves c_0. So if we let c_i denote the image of c_0 under the translation $x \mapsto x+i, \quad i \in \mathbf{F}_{11}$, then the eleven element set

$$C_{11} = \{c_0, c_1, c_2, \ldots, c_{10}\}$$

is preserved by the Borel subgroup, B. So much would be true for any odd prime, p, and 6 replaced by any non square in $\mathbf{F}_p$. However the following miracle occurs for the choice of $p = 11$ and c_0 as above: Let

$$w = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

be the Weyl group generator so

$$wx = -x^{-1}$$

as a fractional linear transformation. Then c_0, c_1 and c_8 are all preserved by w while

$$wc_2 = c_{10}, \quad wc_3 = c_4, \quad wc_5 = c_9, \quad wc_6 = c_7$$

which can be checked by direct computation. For $w^2 = id$ as a fractional linear transformation, this shows that C_{11} is preserved by w and hence by all of $Sl(2,11)$, since B and w generate all of $Sl(2,11)$. As the translations act transitively on C_{11}, we conclude that the 660 element group, $Pl(2,11)$ acts transitively on C_{11}, and hence the isotropy group of a point, say c_0, has sixty elements. One checks that this subgroup is isomorphic to I. For example, within this isotropy group the subgroup that fixes the pair $(\infty, 0)$ is the image in $Pl(2,11)$ of the group generated by the diagonal matrices and w, hence the subgroup is isomorphic to D_5. It is easy to find within the isotropy group an element of order three that does not centralize the D_5 and this shows that the subgroup is isomorphic to I. The fact that subgroup fixing the pair $(\infty, 0)$ is D_5, shows that we should think of the pairs entering into the definition of c_0 as pairs of opposite pentagons (opposite vertices of the original icosahedron). Thus the geometry of the icosahedron is determined group theoretically by the identifying its vertices with points of $\mathbf{P}^1_{11}$ and its pairs of opposite vertices as forming a configuration like c_0. The relation between the groups I and $Pl(2,11)$ is visible at the representation theoretical level when we compute the electronic spectra of the buckyball in the Hückel model as we let the strength of the double bond tend to zero. We will explain this in section 7. For this purpose we record the fact that under our embedding of $Pl(2,5) \to Pl(2,11)$ the subgroup of $Pl(2,5)$ fixing a pentagon (say the point ∞ of $\mathbf{P}^1_{11}$) which is a cyclic group of order five, goes group

$$x \mapsto k^2 x$$

of multiplication by squares (the action of diagonal matrices).

3 Icosahedral structures and $\mathbf{P}^1_{11}$.

The vertices and edges of an icosahedron define a graph with 12 vertices and 30 edges. A 12-element set Y will be said to have an *icosahedral structure* if 30 pairs of verticies are chosen so that, as edges, the resulting graph is isomorphic to the graph of an icosahedron.

Assume Y has an icosahedral structure S. If $y \in Y$ then there is a unique point y', referred to as the antipode of y, such that any edge path joining y and y' has at least 3 edges. Of course $y'' = y$. We refer to $\{y, y'\}$ as an *antipodal pair*. If $\{y, y'\} \subset Y$ is an antipodal pair and $x \in Y \setminus \{y, y'\}$ then either $\{x, y\}$ is an edge or $\{x, y'\}$ is an edge but both are not edges. If $\{x, y\}$ is an edge we refer to x as a neighbor of y. Every $y \in Y$ has 5 neighbors. The 5 neighbors of y'

are referred as to as coneighbors of y. Of course being a neighbor or coneighbor is a reflexive relation. Any $\sigma \in Perm\,Y$ defines another icosahedral structure σS on Y where $\{x, y\}$ is an edge for σS if and only if $\{\sigma^{-1}x, \sigma^{-1}y\}$ is an edge for S. The subgroup B of $Perm\,Y$ which preserves the icosahedral structure S operates transitively on Y and is isomorphic to the full icosahedral group I_h.

Now conversely assume that X is any 12-element set and $A \subset Perm\,X$ is a subgroup which is isomorphic to I and which operates transitively on X. Recall that there exists 2 conjugacy classes F, F' of elements of order 5 in A. One defines an A-invariant icosahedral structure S on X by declaring that $\{x, y\}$ is an edge, for distinct $x, y \in X$, if there exists $g \in F$ such that $g \cdot x = y$. Replacing F by F' defines a second A-invariant icosahedral structure S'. Then since any two transitive actions of I on a 12-element set are isomorphic and since an isotropy group of this action has index 2 in its normalizer one readily proves

Proposition 1 *There exists exactly 2 icosahedral structures S, S' on X which are invariant under A. Furthermore the centralizer $c = c(A)$ of A in $Perm\,X$ is a group of order 2 and the orbits of c are the sets of antipodal pairs for both S and S'. Also $x, y \in Y$ are neighbors for S if and only if they are coneighbors for S'.*

For any 12-element set, X, let $\mathcal{S}$ be the set of all icosahedral structures on X - so that $\mathcal{S}$ has the structure of a $Perm\,X$-set. For any $S \in \mathcal{S}$ let $A_S \subset Perm\,X$ be its (icosahedral) symmetry group. If $S \in \mathcal{S}$ then a distinct $S' \in \mathcal{S}$ is called its twin, and S, S' are referred to as a pair, in case $A_S = A_{S'}$.

We apply these considerations to the case where $X = P_{11}$, the projective line over a field F_{11} of 11 elements. We may regard $Pl(2, 11) \subset Perm\,X$ so that $Pl(2, 11)$ is a 660-element group of permutations of X.

An icosahedral structure S on X will be said to be $Pl(2, 11)$ compatible if $A_S \subset Pl(2, 11)$. We will be interested in such structures. The set C of 6-pair partitions of X, considered above, may clearly be identified with set of all subgroups $c \subset Perm\,X$ of order 2 such that c has no fixed points on X. As noted above there exists $c_0 \in C$ whose centralizer, A_0, in $Pl(2, 11)$ is isomorphic to I and which operates transitively on X. Obviously

$$c(A_0) = c_0$$

In particular $Pl(2, 11)$ contains a subgroup which is isomorphic to I. Let $\mathcal{A}$ be the $Pl(2, 11)$-set (under conjugation) of all subgroups of $Pl(2, 11)$ which are isomorphic to I. If $A \in \mathcal{A}$ and Z_{11} is any cyclic subgroup of order 11 in $Pl(2, 11)$ then since obviously $A \cap Z_{11} = \{e\}$ considerations of order immediately implies that

$$Pl(2, 11) = A\,Z_{11} \tag{1}$$

By the simplicity of $Pl(2,11)$ obviously then any $A \in \mathcal{A}$ is equal to its own normalizer in $Pl(2,11)$. Any element in $a \in Gl(2,11)$ whose determinant is not a square induces, by conjugation, an outer automophism α of $Pl(2,11)$ which interchanges the 2 conjugacy classes of elements of order 11 but does not interchange the 2 conjugacy classes of elements of order 5. This is clear by noting that this is obviously the case for diagonal elements in $GL(2,11)$. It follows that if $A \in \mathcal{A}$ then $\alpha(A)$ is not conjugate to A. Indeed otherwise there would exist a non-central element in $b \in GL(2,11)$ which commutes with A. This is clearly impossible since by conjugation (noting that any cyclic group of order 5 is a Sylow subgroup) we can assume $\Delta \subset A$, i.e. A contains all the image of the set of diagonal elements of determinant 1. But that forces b to be diagonal and non-central. Thus if $\mathcal{A}_I$ is the $Pl(2,11)$-orbit in $\mathcal{A}$ which contains A_0 and $\mathcal{A}_{II} = \alpha(\mathcal{A}_I)$ then $\mathcal{A}_I \neq \mathcal{A}_{II}$.

Proposition 2 *There are 22 elements in $\mathcal{A}$. Furthermore, under the action of $Pl(2,11)$, $\mathcal{A}$ decomposes into two 11-element orbits*

$$\mathcal{A} = \mathcal{A}_I \cup \mathcal{A}_{II}$$

Moreover there exists $\alpha' \in Perm\,X$, in the normalizer of $Pl(2,11)$, which induces an outer automorphism α of $Pl(2,11)$ interchanging $\mathcal{A}_I$ and $\mathcal{A}_{II}$. Correspondingly there exists there exists 22 pairs of $Pl(2,11)$ compatible iscoahedral structures on X. Again correspondly they fall into 2 $Pl(2,11)$-orbits.

Proof. We will show that if $A \in \mathcal{A}$ and $A \notin A_I$ then $A \in A_{II}$. Let $A \in \mathcal{A} \setminus \mathcal{A}_I$. Furthermore, as above, up to $Pl(2,11)$-conjugacy, we can assume that $\Delta \subset A$. Choose the element $a \in Gl(2,11)$ which induced α to be diagonal so that α fixes the elements of Δ. Consider the action of $Pl(2,11)$ on the 11-element set C_{11}. Since $A \notin \mathcal{A}_I$ it has no fixed point on C_{11}. Thus the only possible orbit structure it can have on C_{11} is two orbits O_5, O_6 with respectively 5 and 6 elements. On the other hand, as we have seen in the preceeding section, the subgroup $\Delta \subset A$, has exactly two 5-element orbits, $D = (F_{11}^*)^2$ and $D' = -(F_{11}^*)^2$on C_{11}. Thus one must have $O_5 = D$ or $O_5 = D'$.

As our subgroup A_0 also contains Δ and α preserves Δ the group $\alpha(A_0)$ will also have a five element orbit on C_{11} which will be either D or D'. Let us denote its five element orbit by O_5^α. Now suppose that $A' = \alpha(A) \notin \mathcal{A}_I$. Let O_5' and O_6' be the 5 and 6 element orbits of A' in C_{11}. Again $O_5' = D$ or D'. But since A' is not conjugate to A one cannot have $O_5 = O_5'$. Indeed, by (1), any two distinct elements of $\mathcal{A} \setminus \mathcal{A}_I$ generate $Pl(2,11)$ and hence cannot have the same 5-orbit in C_{11}. Thus $\{O_5, O_5'\} = \{D, D'\}$. But $O_5^\alpha \in \{D, D'\}$. Thus $\alpha(A_0)$ is equal to A or A'. This is a contradiction since α^2 is clearly an inner automorphism. Thus $\mathcal{A}_I$ and $\mathcal{A}_{II}$ exhaust $\mathcal{A}$. The group $Gl(2,11)$ operates on the projective line X. Clearly if one defines α' to be the permutation action of a then α' normalizes $Pl(2,11)$ and induces α on $Pl(2,11)$. QED

Let $\mathcal{A}_I$ be normalized as in the proof of the preceeding proposition so that $A_o \in \mathcal{A}_I$. We now observe that C_{11} is not the only 11-element $Pl(2,11)$-orbit in C.

Proposition 3. *Let*

$$C'_{11} = \{c(A) | A \in \mathcal{A}_{II}\}$$

Then C'_{11} is an 11-element orbit of $Pl(2,11)$ in C and C'_{11} is distinct from C_{11}.

Proof. Obviously $C'_{11} = \alpha' C_{11} {\alpha'}^{-1}$ so that C'_{11} is an 11-element $Pl(2,11)$-orbit. It is distinct from C_{11} since as noted in the proof of Proposition 2, no element $A \in \mathcal{A}_{II}$ has a fixed point on C_{11} whereas $c(A)$ is fixed by A. QED

Let $A \in \mathcal{A}_I$. Associated to A is a pair of A-invariant icosahedral structures S, S' on the projective line X. The 2-element permutation group $c(A)$ tells the pairs of antipodal points for S and S' but it does not tell us what the edges are. Remarkably the cross-ratio $[x_1, x_2, x_3, x_4]$ for $x_i \in X$ can be used to determine at least one of the two structures S, S'. Elsewhere we will prove

Theorem 2 *Let $\tau \in c(A)$ be the non-trivial element. Let $x, y \in X$ with $\{x, u, v, y\}$ stable under τ. Then $\{x, y\}$ is an edge for an A-invariant icosahedral structure on X if and only if*

$$[x, u, v, y] = -1.$$

4 Representations

The representations of all the alternating groups were determined by Frobenius: Regard A_n as a subgroup of S_n. The irreducibles of S_n are given by Young diagrams. If a Young diagram is not the same as its conjugate diagram, the representation remains irreducible when restricted to A_n and is equivalent to the restriction of the conjugate diagram. A self conjugate diagram splits into two irreducibles of half the dimension. For the case of S_5, the irreducibles can be labelled as 1,4,5,6,5',4',1 where the ' describes conjugate diagrams and the 6, corresponding to the partition [3,1,1], is self conjugate and so splits into two three dimensional representations, so we can list the representations of I as $\mathbf{1}, \mathbf{3}, \mathbf{4}, \mathbf{5}, \mathbf{3'}$. They can be described as follows:

The action of $Pl(2,p)$ on $\mathbf{P}^1_p$ is doubly transitive, and so the induced action on the $p-$dimensional space of functions, $\mathcal{F}(\mathbf{P}^1_p)$ splits into two pieces, the constants and an irreducible of dimension p, called the Steinberg representation. For the case $p = 5$ this gives the five dimensional representation. The four dimensional representation is restriction of the fundamental representation of S_5: the group A_5 acts doubly transitively on the set of five objects and so the permutation representation splits into the constants and a four dimensional irreducible. Equally well, we can regard **4** as the Steinberg representation of $Sl(2,4)$. We will have occasion to use the case $p = 11$ of the Steinberg representation in the section 7. The two three dimensional representations are two inequivalent ways of regarding A_5 as a subgroup of $SO(3)$ depending on whether the five cycle (12345) is sent into a rotation through angle $2\pi/5$ or $4\pi/5$.

The conjugacy classes of A_5 are easy to determine from those of S_5. If

$$\rho = (ab \cdot \cdot\cdot)(c \cdot \cdot) \cdot \cdot$$

is a permutation written in cycle form, and π is some other permutation, then

$$\pi\rho\pi^{-1} = (\pi(a)\pi(b) \cdot \cdot\cdot)(\pi(c) \cdot \cdot) \cdot \cdot.$$

So a conjugacy class in S_n is determined by its cycle structure. The conjugacy classes of even permutations in S_5 are

$$e \quad (ab)(cd) \quad (abc) \quad (abcde).$$

It is easy to check that any two $(ab)(cd)$ are conjugate to one another by an even permutation as are any two (abc). But the element $s = (12345)$ is not conjugate to its square $s^2 = (13524)$ by any even permutation, since any conjugating permutation is determined up to right multiplication by a power of s (which is even) and one such conjugating permutation is the four cycle (2354) which is odd. So the five cycles split into two conjugacy classes in A_5. Thus the table of conjugacy classes is as follows:

size	1	15	20	12	12
order	1	2	3	5	5
rep	e	(12)(34)	(123)	(12345)	(13524)

In a permutation representation, the character of any element is equal to the number, $fix(x)$, of fixed points. Hence, when we subtract off the constants, the character, $\chi(a)$, of the remaining representation for any element a is given by $fix(a) - 1$. For the Steinberg representation, the order two elements have two fixed points, the order three elements none, and the order five elements one fixed point. (These facts can be checked on the axes of the buckyball, but will become even more transparent in terms of the representatives in $Sl(2,5)$ that we will choose later on.) Thus, in terms of the order of conjugacy classes in the above table, the character of the five dimensional irreducible has values 5,1,-1,0,0. (Check: 25+15+20 =60.)

Acting as permutations on five letters,the order two elements have one fixed point, the order three elements have two, and the order five elements have none. So the character values for the four dimensional representation are 4,0,1,-1,-1. (Check 16+20+12+12 =60.)

The trace of any rotation through angle θ in three dimensional space is $1 + 2\cos\theta = 1 + e^{i\theta} + e^{-i\theta}$. In all that follows we will set

$$\epsilon = e^{2\pi i/5}.$$

So if we choose our identification of A_5 with the icosahedral group so that (12345) goes over into rotation through angle $2\pi/5$, the character values are 3, -1, 1, 1+$\epsilon + \epsilon^4$, $1 + \epsilon^2 + \epsilon^3$. The other three dimensional representation will then correspond the opposite choice, so that (12345) corresponds to rotation through $4\pi i/5$. This will have the effect of interchanging the last two values. So the character table for A_5 is given by

size	1	15	20	12	12
order	1	2	3	5	5
rep	e	(12)(34)	(123)	(12345)	(13524)
trivial	1	1	1	1	1
3	3	-1	0	$1+\epsilon+\epsilon^4$	$1+\epsilon^2+\epsilon^3$
5	5	1	-1	0	0
4	4	0	1	-1	-1
3′	3	-1	0	$1+\epsilon^2+\epsilon^3$	$1+\epsilon+\epsilon^4$

For the purposes of applying Frobenius reciprocity later on, it is important to record how each of these representations restricts to a two element subgroup of I consisting of the identity and an element of order two, that is, how many times the sign representation occurs and how many times the trivial representation occurs in the restriction. A rotation through 180° in three dimensional space has two eigenvalues -1 and one eigenvalue $+1$. So the restriction of each of the three to $\mathbf{Z}_2$ contains the sign representation twice and the trivial representation once. The restriction of the permutation representation of A_5 acting on five objects to $\mathbf{Z}_2$ is clearly the direct sum of the trivial representation and two copies of the two dimensional permutation representation. Hence the four dimensional representation restricted to $\mathbf{Z}_2$ contains two copies of the trivial representation and two copies of the sign representation. For the five dimensional representation we record the following fact which has applications to the Raman spectrum.

Proposition 3 *The representation of I on $S^2(\mathbf{R}^3)$ decomposes into* $\mathbf{1} \oplus \mathbf{5}$ *where* *the* **1** *corresponds to multiples of the Euclidean metric and the* **5** *consists of the traceless symmetric tensors.*

Proof. The decomposition into multiples of $x^2 + y^2 + z^2$ and traceless tensors is clearly invariant under I. On the other hand, there can not be any other invariant line in $S^2(\mathbf{R}^3)$ since this would contradict the irreducibility of the three dimensional representation. Since there is no two dimensional irreducible, we see that there is no way for the the traceless tensors to decompose. QED.

If we choose our rotation to be about the z-axis, the monomials z^2, x^2, y^2, xy are invariant while xz and yz are eigenvectors with eigenvalue -1. Hence the **5** when restricted contains three copies of the trivial representation and two copies of the sign representation. To summarize we have the table

rep	**1**	**3**	**4**	**5**	**3′**
tr	1	1	2	3	1
sgn	0	2	2	2	2

(2)

The group I_h is just the direct product of I with $\mathbf{Z}_2$, so the irreducibles of I_h are just the tensor product of those of I with those of $\mathbf{Z}_2$. In other words, they can be labeled by attaching a $+$ or $-$ sign to the label of the representation of I according to whether it is the trivial or sign representation of Z_2 which is tensored in. (In the chemical literature this $\pm$ labeling is given by a subscript g (for *gerade*) for the + and a subscript u (for *umgerade*) for the -.) The subgroup of I_h which fixes a point, call it H, is a two element group consisting of the identity and Pr where r is rotation through 180° and P is the parity operator. So the table corresponding to (2) where now we list the restrictions to H is

rep	$\mathbf{1}^+$	$\mathbf{3}^+$	$\mathbf{4}^+$	$\mathbf{5}^+$	$\mathbf{3}^{+\prime}$	$\mathbf{1}^-$	$\mathbf{3}^-$	$\mathbf{4}^-$	$\mathbf{5}^-$	$\mathbf{3}^{-\prime}$
tr	1	1	2	3	1	0	2	2	2	2
sgn	0	2	2	2	2	1	1	2	3	1

(3)

By Frobenius reciprocity we can read the entries of this table as giving the multiplicities of each irreducible of I_h in the representation induced from the trivial or the sign representation of H. In the electronic spectrum one is particularly interested in the representation induced from the sign representation, hence the second row of (3). In the vibrational spectrum one is interested in the representation induced from the restriction of $\mathbf{3}^-$ to H. From the above table the restriction of $\mathbf{3}^-$ is given by

$$\mathbf{3}^- \downarrow = 2 \cdot tr \oplus 1 \cdot sgn$$

and hence the corresponding induced representation, $(\mathbf{3}^- \downarrow) \uparrow$ is given by

$$2 \cdot \mathbf{1}^+ \oplus 4 \cdot \mathbf{3}^+ \oplus 6 \cdot \mathbf{4}^+ \oplus 8 \cdot \mathbf{5}^+ \oplus 4 \cdot \mathbf{3'}^+ \oplus \cdot \mathbf{1}^- \oplus 5 \cdot \mathbf{3}^- \oplus 6 \cdot \mathbf{4} \oplus 7 \cdot \mathbf{5}^- \oplus 5 \cdot \mathbf{3'}^-. \quad (4)$$

Thus finding the eigenvalues of any I_h invariant operator on this space involves dealing with at most an eight by eight matrix, as was pointed out in [6]. The vibrational spectrum under the assumption of bond stretching and angle bending forces was calculated in [6]. The space of vibrational states is the above induced representation with one $\mathbf{3}^-$ (overall translations) and one $\mathbf{3}^+$ (overall rotations) removed. The infrared lines corresponding to vacuum to one phonon (dipole) transitions correspond to these four representations, and hence, by (4) there are four lines in the infrared spectrum. The Raman spectrum corresponds to a quadrupole interaction, and hence to symmetric tensors of order two. By Proposition 1 and (4) we see that there should be ten Raman lines in all, two corresponding to $\mathbf{1}^+$ and eight corresponding to $\mathbf{5}^+$, and all ten lines have been observed. See [2] for a picture of these ten lines.

Let us now turn to the double cover, and begin by describing the conjugacy classes, which are best described in terms of familiar subgroups. We have already described the Borel subgroup B consisting of all upper triangular matrices. We can write $B = TU$ where T is the subgroup of diagonal matrices and U consists of upper triangular matrices with ones on the diagonal. (The subgroup T is called a split torus and the elements of U are unipotents.) In general, T will contain $q-1$ elements, in our case of $q=5$ this comes to 4. One of these elements is id, another is $-id$ and the remaining two elements are of order four. They are conjugate to one another, say by the matrix

$$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

So the fifteen order two elements in A_5 are each covered by two elements of order four in $Sl(2,5)$ giving thirty elements in all in this conjugacy class. The matrix $M = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$ is of order five and so must project onto one of the elements of order five in A_5. But $-M$ is of order ten and projects onto the same element. So we see that the inverse image of each of the two twelve element conjugacy classes in A_5 splits into two conjugacy classes, one consisting of elements of order 5 and the other of order ten. The matrix $N = \begin{pmatrix} 0 & 1 \\ -1 & -1 \end{pmatrix}$ is of order three, and hence maps onto an element of order three, and $-N$ is of order six and maps onto the same element. So the inverse image of the elements of order three in A_5 also splits into two conjugacy classes, one consisting of order three elements and the other of order six elements. So there are nine conjugacy classes in all, as listed in the following table:

size	1	1	30	20	20	12	12	12	12
order	1	1	4	6	3	10	10	5	5
rep	I	$-I$	$\begin{pmatrix} 2 & 0 \\ 0 & 3 \end{pmatrix}$	$\begin{pmatrix} 1 & 1 \\ -1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ -1 & -1 \end{pmatrix}$	$\begin{pmatrix} -1 & -1 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} -1 & -2 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 2 \\ 0 & 1 \end{pmatrix}$

A cyclic subgroup generated by an element of order six has the following interpretation in terms of the general theory of $Sl(2,q)$: The field $\mathbf{F}_q$ has a unique quadratic extension, $\mathbf{F}_{q^2}$ which we may regard as a two dimensional vector space over $\mathbf{F}_q$. The set of non-zero elements in $\mathbf{F}_{q^2}$ form a group under multiplication and multiplication by an element of $\mathbf{F}_{q^2}$ gives a linear transformation of $\mathbf{F}_q^2$. There are q^2-1 non-zero elements in $\mathbf{F}_{q^2}$ and $q-1$ values of the determinant, and so the elements whose multiplication have determinant 1 form a subgroup of order $q+1$. If we chose a basis of $\mathbf{F}_{q^2}$ we get subgroup, K of $Sl(2,q)$ of order $q+1$ called a 'non-split torus'. It is the finite field analogue of the unit circle in the extension of the real numbers by the complexes. In our case $q+1=6$ and each non-split torus covers a C_3 subgroup of A_5 generated by a three cycle.

In any event, since there are nine conjugacy classes, there are nine inequivalent irreducible representations, and we have found five of them, the representations coming from those of A_5. The general theory of the representations of $Sl(2,q)$ has been completely worked out, cf. for example [11]. Assuming the existence of a two dimensional representation, which we have already proved, we can work out the character table for our special case of $Sl(2,5)$ as follows. We identify our group with the inverse image of A_5 under the projection of $SU(2)$ onto $SO(3)$. Now the group $SU(2)$ has one irreducible representation of every dimension, the representation $\mathbf{k}$, of dimension k being on the space of homogeneous polynomials of degree $k-1$ in two variables. The value of the character of the representation $\mathbf{k}$ on a matrix whose eigenvalues are $e^{i\theta}, e^{-i\theta}$ is

$$\chi_k(\theta) = e^{-(k-1)i\theta} + e^{-(k-3)i\theta} + \cdots + e^{(k-1)i\theta}.$$

In particular, for $k=2$ we have

$$\chi_2(\theta) = e^{-i\theta} + e^{i\theta}.$$

So the character of the two dimensional representation is given by the second line in the table below. The first six lines of the table are just the evaluation of the characters χ_k on our 120 element subgroup of $SU(2)$ for $k=1,2,3,4,5,6$. A check shows that the sum of the absolute value squared of the elements multiplied by the number of elements in the conjugacy class adds up to 120 and shows that these characters are indeed irreducible. Thus $\mathbf{k}$ remains irreducible when restricted to our subgroup up until $k=7$, which splits into a 4 and a 3.

Here is the character table.

size	1	1	30	20	20	12	12	12	12
order	1	2	4	6	3	10	10	5	5
rep	I	$-I$	$\begin{pmatrix} 2 & 0 \\ 0 & 3 \end{pmatrix}$	$\begin{pmatrix} 1 & 1 \\ -1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ -1 & -1 \end{pmatrix}$	$\begin{pmatrix} -1 & -1 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} -1 & -2 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 2 \\ 0 & 1 \end{pmatrix}$
tr	1	1	1	1	1	1	1	1	1
2	2	-2	0	1	-1	$-(\epsilon^2+\epsilon^3)$	$-(\epsilon+\epsilon^4)$	$\epsilon^2+\epsilon^3$	$\epsilon+\epsilon^4$
3	3	3	-1	0	0	$\epsilon+\epsilon^4+1$	$\epsilon^2+\epsilon^3+1$	$\epsilon+\epsilon^4+1$	$\epsilon^2+\epsilon^3+1$
4	4	-4	0	-1	1	1	1	-1	-1
5	5	5	1	-1	-1	0	0	0	0
6	6	-6	0	0	0	-1	-1	1	1
4′	4	4	0	1	1	-1	-1	-1	-1
3′	3	3	-1	0	0	$\epsilon^2+\epsilon^3+1$	$\epsilon+\epsilon^4+1$	$\epsilon^2+\epsilon^3+1$	$\epsilon+\epsilon^4+1$
2′	2	-2	0	1	-1	$-(\epsilon+\epsilon^4)$	$-(\epsilon^2+\epsilon^3)$	$\epsilon+\epsilon^4$	$\epsilon^2+\epsilon^3$

5 The Clebsch Gordan decomposition for $Sl(2,5)$

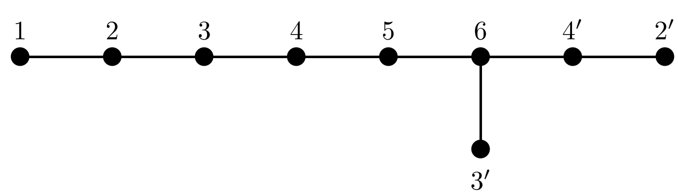
For many applications, it is important to know the decomposition of the tensor product of two irreducibles. For the case of $SU(2)$, the formula above for χ_k shows that

$$\chi_2 \cdot \chi_k = \chi_{k-1} + \chi_{k+1}$$

which is, of course a special case,

$$\mathbf{2} \otimes \mathbf{k} = (\mathbf{k-1}) \oplus (\mathbf{k+1}),$$

of the Clebsch Gordan decomposition. So we can apply this to each line in our table, multiplying by the second line and subtracting the preceding line to get the next line up until line 6. There, multiplying the 6th line by the 2nd and subtracting the fifth gives the sum of the next two lines. Also multiplying the **4** by the second line gives the sum of the 6 and the (other) 2 and multiplying the **3** by the second line gives the 6. We can summarize this discussion by saying that the effect of tensoring by **2** in the basis of irreducibles is given by the adjacency matrix of the graph



which is the extended Dynkin diagram of E_8. The integers 1,2,3 etc. placed near the nodes, i.e. the dimensions of the irreducible representations of G are the coefficients of the highest root of E_8! This is a case of the McKay correspondence which similarly associates a simple Lie algebra to every finite subgroup of $SU(2)$.

Using the above diagram recursively, or by examining the character table and seeing that the character of $\mathbf{2}$ separates all conjugacy classes, we conclude that every representation can be written as a polynomial in the basic two dimensional representation, $\mathbf{2}$. Explicitly the representation $\mathbf{k} = f_k(\mathbf{2})$ where the polynomials f_k are given by

$$\begin{aligned}
f_1(x) &= 1 \\
f_2(x) &= x \\
f_3(x) &= x^2 - 1 \\
f_4(x) &= x^3 - 2x \\
f_5(x) &= x^4 - 3x^2 + 1 \\
f_6(x) &= x^5 - 4x^3 + 3x \\
f_{4'}(x) &= x^8 - 7x^6 + 14x^4 - 7x^2 \\
f_{3'}(x) &= -x^8 + 8x^6 - 19x^4 + 13x^2 - 1 \\
f_{2'}(x) &= x^7 - 7x^5 + 14x^3 - 7x.
\end{aligned}$$

Thus the Grothendieck ring of G is given by $Z[x]/p(x)$ where $p(x)$ is the characteristic polynomial of A, where A is the adjacency matrix of the extended Dynkin diagram. This can be verifed directly, or, from the fact that

$$\mathbf{2} \otimes \mathbf{4}' = \mathbf{6} \oplus \mathbf{2}'$$

(which can be verified from the character table). If we substitute the polynomial expressions given in the preceding table for both sides of the above equation, the difference between both sides will give the characteristic polyno mial of A.

$$x^9 - 8x^7 + 20x^5 - 17x^3 + 4x$$

By using a general theorem of Kostant [7], tensoring by any representation is given by multiplication by the corresponding polynomial listed above, with the understanding that two polynomials are to be identified if they differ by a multiple of the characteristic polynomial.

In the study of the electronic properties of C_{60} one also needs to know the decomposition of the exterior powers of various representations, as these contain the Fermi allowed states. We discuss this problem in the next two sections. In the next section we discuss the general method, and in the following section we use some tricks special to the group, G.

6 Decomposing exterior powers

There is a general method which always works. In any given case, it might be simpler to use some special tricks. The general method is as follows: For any character, χ, let $P_k(\chi)$ denote the function on conjugacy classes,

$$P_k(\chi)(a) = \chi(a^k).$$

If ρ denotes the representation and the eigenvalues of $\rho(a)$ are $x_1, \ldots, x_n$ then

$$\chi(a) = \sum x_i$$

while

$$P_k(\chi)(a) = \sum x_i^k.$$

On the the other hand, the eigenvalues of the $k-$th exterior power of $\rho(a)$ are

$$x_{i_1} x_{i_2} \cdots x_{i_k}, \quad i_1 < i_2 < \ldots < i_k$$

so the character of the exterior power is

$$E_k(\chi)(a) = \sum_{i_1 < i_2 < \ldots < i_k} x_{i_1} x_{i_2} \cdots x_{i_k}.$$

So the problem is how to express the E's in terms of the P's. For example,

$$E_1 = P_1$$

and

$$E_2 = \frac{1}{2}[P_1^2 - P_2] = \frac{1}{2} \det \begin{pmatrix} P_1 & P_2 \\ 1 & P_1 \end{pmatrix}.$$

So the character on the second exterior power is

$$E_2(\chi)(a) = \frac{1}{2}[(\chi(a))^2 - \chi(a^2)].$$

Similarly,

$$E_3 = \frac{1}{3!}[P_1^3 - 3P_1P_2 + 2P_3] = \frac{1}{3!} \det \begin{pmatrix} P_1 & P_2 & P_3 \\ 1 & P_1 & P_2 \\ 0 & 2 & P_1 \end{pmatrix}.$$

So

$$E_3(\chi)(a) = \frac{1}{3!}[\chi(a)^3 - 3\chi(a)\chi(a^2) + 2\chi(a^3)].$$

The general formula expressing the E's in terms of the P's is

$$E_k = \frac{1}{k!} \det \begin{pmatrix} P_1 & P_2 & P_3 & \cdots & P_{k-1} & P_k \\ 1 & P_1 & P_2 & \cdots & P_{k-2} & P_{k-1} \\ 0 & 2 & P_1 & P_2 \cdots & P_{k-2} & \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & \cdots & k-1 & P_1 \end{pmatrix}.$$

In principle one can use this formula to compute the characters of the exterior power from the character table. In practice, this computation might get complicated.

7 Special tricks

Let U and V be vector spaces. Then

$$\wedge^k(U \oplus V) = \bigoplus_{i+j=k} \wedge^i(U) \otimes \wedge^j(V). \tag{5}$$

A similar formula works for the exterior power of the direct sum of any number of vector spaces. In particular, the calculation of the exterior power of any representation is reduced to the calculation for irreducibles.

If a representation is self contragredient (as is the case for all the irreducible representations of $G = Sl(2,5)$) then $\wedge^{n-k} \simeq \wedge^k$. So we need only compute the $\wedge^2$ of all the irreducible representations and also the $\wedge^3$ of the six dimensional representation. For the computation of the $\wedge^2$ we will use (5) and the well known fact

$$\wedge^2(X \otimes Y) = \wedge^2 X \otimes S^2 Y \oplus S^2 X \otimes \wedge^2 Y. \tag{6}$$

We can use (5) and (6) to recursively determine all the $\wedge^2$'s, starting with

$$\wedge^2 \mathbf{2} = tr = \mathbf{1}$$

and

$$\wedge^2 \mathbf{3} = \mathbf{3}.$$

From the multiplication table we get

$$S^2 \mathbf{2} = \mathbf{3}, \quad S^2(\mathbf{3}) = \mathbf{1} \oplus \mathbf{5}.$$

Then using (6)

$$\wedge^2(\mathbf{2} \otimes \mathbf{3}) = \mathbf{1} \oplus \mathbf{5} \oplus \mathbf{3} \otimes \mathbf{3} = \mathbf{1} \oplus \mathbf{5} \oplus \mathbf{1} \oplus \mathbf{3} \oplus \mathbf{5}.$$

But $\mathbf{2}\otimes\mathbf{3}=\mathbf{4}\oplus\mathbf{2}$ and from (5)

$$\wedge^2(\mathbf{4}\oplus\mathbf{2})=\wedge^2(\mathbf{4})\oplus\mathbf{4}\otimes\mathbf{2}\oplus\wedge^2(\mathbf{2})=\wedge^2\mathbf{4}\oplus\mathbf{3}\oplus\mathbf{5}\oplus\mathbf{1}.$$

From these two equations and the formula for $\mathbf{4}\otimes\mathbf{4}$ from the multiplication table we conclude that

$$\wedge^2\mathbf{4}=\mathbf{1}\oplus\mathbf{5},\quad S^2(\mathbf{4})=\mathbf{3}\oplus\mathbf{4}'\oplus\mathbf{3}'.$$

Proceeding in this way we find

$$\begin{aligned}\wedge^2\mathbf{2}&=\mathbf{1}\\ \wedge^2\mathbf{3}&=\mathbf{3}\\ \wedge^2\mathbf{4}&=\mathbf{1}\oplus\mathbf{5}\\ \wedge^2\mathbf{5}&=\mathbf{3}\oplus\mathbf{3}'\oplus\mathbf{4}'\\ \wedge^2\mathbf{6}&=\mathbf{1}\oplus 2\times\mathbf{5}\oplus\mathbf{4}'\\ \wedge^2\mathbf{3}'&=\mathbf{3}'\\ \wedge^2\mathbf{4}'&=\mathbf{3}\oplus\mathbf{3}'\\ \wedge^2\mathbf{2}'&=\mathbf{1}\end{aligned}$$

To compute $\wedge^3(\mathbf{6})$ we use a theorem of Kostant which generalizes (6). It says that the decomposition of $\wedge^k(X\otimes Y)$ into irreducibles under $Gl(X)\times Gl(Y)$ is given as follows, when $\dim X=m,\ \dim Y=n$: Construct all Young diagrams with k boxes which fit into a rectangle of size $m\times n$. Any such diagram (with at most m rows and n columns) corresponds an irreducible representation of $Gl(X)$. The same diagram flipped over (so it now has at most n rows and m columns) corresponds to an irreducible representation of $Gl(Y)$. So if we take the tensor product of these two representations we get an irreducible representation of $Gl(X)\times Gl(Y)$. Kostant's theorem says that $\wedge^k(X\otimes Y)$ decomposes into the direct sum of the representations associated as above with all possible diagrams with k boxes which fit into the rectangle of size $m\times n$. In case $m=2,n=3$ the only possible diagrams are [3] and [2,1]. The corresponding representations are $S^3(X)\otimes\wedge^3(Y)$ and $X\otimes U$ where U is an eight dimensional representation of $Gl(Y)$. This eight dimensional representation occurs twice in the decomposition of $Y\otimes Y\otimes Y$. Explicitly

$$Y\otimes Y\otimes Y=S^3Y\oplus 2\times U\oplus\wedge^3Y.$$

We wish to apply this to the case $X=\mathbf{2},\quad Y=\mathbf{3}'$and write $\mathbf{6}=\mathbf{2}\otimes\mathbf{3}'$. We must now decompose these representations when restricted to the double cover of I. Now $\wedge^3\mathbf{3}'=\mathbf{1},S^3\mathbf{2}=\mathbf{4}$ so the representation corresponding to [3] remains irreducible and becomes $\mathbf{4}$. To compute the term corresponding to [2,1] we must know how U decomposes. For this we check from the multiplication table that the only irreducibles which occur with multiplicity ≥ 2 in $\mathbf{3'} \otimes \mathbf{3'} \otimes \mathbf{3'}$ are $\mathbf{3'}$ and $\mathbf{5}$. so

$$U = \mathbf{5} \oplus \mathbf{3'}.$$

From the multiplication table,

$$\mathbf{2} \otimes [\mathbf{5} \oplus \mathbf{3'}] = \mathbf{4} + 2 \times \mathbf{6}.$$

We conclude

$$\wedge^3 \mathbf{6} = 2 \times [\mathbf{4} \oplus \mathbf{6}].$$

8 The electronic spectrum and the Galois embedding

In the Hückel model, the electronic energy levels are determined by the spectrum of the adjacency matrix of the graph of the buckyball. The adjacency matrix acts on the space of functions on the vertices, and depends (up to scale) on one real parameter, t, the relative strength of the double bonds to the single bonds. According to (3), finding the spectrum of any invariant operator on the space of functions involves diagonalizing at most a three by three matrix, and hence can be solved in closed form. In general, the eigenvalues for the adjacency matrix of a homogeneous graph can be treated by the method of Frobenius, cf. [2] for a modern exposition and [3] where this is worked out for the Buckyball and the characteristic polynomials as a function of t were determined to be

(a) $(x^2 + x - t^2 + t - 1)(x^3 - tx^2 - x^2 - t^2x + 2tx - 3x + t^3 - t^2 + t + 2) = 0$ with multiplicity 5;

(b) $(x^2 + x - t^2 - 1)(x^2 + x - (t + 1)^2) = 0$ with multiplicity 4;

(c) $(x^2 + (2t + 1)x + t^2 + t - 1)(x^4 - 3x^3 + (-2t^2 + t - 1)x^2 + (3t^2 - 4t + 8)x + t^4 - t^3 + t^2 + 4t - 4) = 0$ with multiplicity 3;

(d) $x - t - 2 = 0$ with multiplicity 1.

If we draw the eigenvalues as functions of t, we obtain

confirming by closed analytic expression the computational results of [5]. The fact that at the limit $t = 0$ we get the eigenvalues $2, 2\cos 2\pi/5 = \epsilon + \epsilon^4$, $2\cos 4\pi/5 = \epsilon^2 + \epsilon^3$ is not surprising, because at $t = 0$ all the pentagons disengage, and these are the eigenvalues of the cyclic pentagonal graph. What is more interesting is the decomposition into irreducibles of I or I_h when t is perturbed away from 0.

To understand this, recall that the eigenfunctions on the cyclic graph are exactly the characters of the cyclic group, the character taking the value ω on the cyclic generator having eigenvalue $2\cos\omega$. Thus the space of functions on the buckyball with eigenvalue 2 can be identified with the space of functions on the set of pentagons, i.e. on $\mathbf{P}^1_{11}$, the eigenfunctions with eigenvalue $2\cos 2\pi/5$ correspond to sections of the line bundle on $\mathbf{P}^1_{11}$ induced from the characters which take the values ϵ and ϵ^4 on the generator, and the eigenfunctions with eigenvalue $2\cos 4\pi/5$ correspond to sections of the line bundle on $\mathbf{P}^1_{11}$ induced from the characters ϵ^2 and ϵ^3. If we examine the restriction for the various representations of I to $\mathbf{Z}_5$ we have the following table:

rep	$\mathbf{1}$	$\mathbf{3}$	$\mathbf{4}$	$\mathbf{5}$	$\mathbf{3'}$
rep $\downarrow$	1	$1, \epsilon, \epsilon^4$	$\epsilon, \epsilon^2, \epsilon^3, \epsilon^4$	$1, \epsilon, \epsilon^2, \epsilon^3, \epsilon^4$	$1, \epsilon^2, \epsilon^3$.

So the break up into irreducibles when t is perturbed away from 0 is just Frobenius reciprocity. Recall the embedding of $Sl(2, 5)$ into $Sl(2, 11)$ which embeds the subgroup fixing a point as the diagonal matrices. From the point of view of $Sl(2,11)$, the space of functions on $\mathbf{P}^1_{11}$ is just the direct sum of the trivial representation and the Steinberg, while the representations induced from ϵ (isomorphic to that induced from ϵ^4) is a principal series representation as is the representation induced from ϵ^2 which is isomorphic to that induced from ϵ^3. So the above graph sees the restriction of these representations to I.

There is an interesting remark about the restriction of the Steinberg: The restriction of the irreducible representations of $SU(2)$ to a finite subgroup were all worked out in[8]. We will summarize the result for the case of $Sl(2,5)$ in the next section. In particular, the spin 5 eleven dimensional representation breaks up upon restriction to G as $\mathbf{5}\oplus\mathbf{3}\oplus\mathbf{3}'$, the same as the restriction of the eleven dimensional Steinberg. When we pointed this out to Dick Gross, he observed that the same is true for all the exceptional $Pl(2,p)$ which have a transitive permutation action on p letters. In fact, following a letter from Prof. Gross, let G be one of these exceptional $Pl(2,p)$ acting on p letters, and let K be the stabilizer of a letter so $(G:K)=p$. We have the table

p	G	K
2	$Pl(2,2)=S_3$	$\mathbf{Z}_3$
3	$Pl(2,3)=A_4$	$C_2\times C_2$
5	$Pl(2,5)=A_5$	A_4
7	$Pl(2,7)=Sl(2,3)$	S_4
11	$Pl(2,11)$	A_5

Note that K can always be realized as a subgroup of $SO(3)$, and when $p=2$, K lifts to a subgroup of $SU(2)$. Let V be the Steinberg representation of G, so dim $V=p$, and let W be the unique irreducible representation of $SU(2)$ of dimension p. When $p>2$ is odd, W descends to a representation of $SO(3)$. The observation is that in all these cases, the restrictions $W_{|K}$ and $V_{|K}$ are isomorphic as K modules and are multiplicity free. In fact we have the following table of decomposition:

p	$V_{\|K}\sim W_{\|K}$
2	$\mathbf{1}\oplus\mathbf{1}'$
3	$\mathbf{1}\oplus\mathbf{1}'\oplus\mathbf{1}''$
5	$\mathbf{1}\oplus\mathbf{1}'\oplus\mathbf{3}$
7	$\mathbf{1}\oplus\mathbf{3}\oplus\mathbf{3}'$
11	$\mathbf{3}\oplus\mathbf{3}'\oplus\mathbf{5}$.

9 Homogeneous magnetic energy.

In a fundamental paper of 1937 [10], London gave a generalization of the Hückel model to account for the presence of a magnetic field. It involves generalizing the notion of the adjecency matrix of a graph: Let $\mathcal{F}$ denote the space of functions on the set of vertices of our graph. If we have assigned real numbers (called bond strengths) to each of the edges of a graph, then the adjacency matrix A is the operator

$$A : \mathcal{F} \to \mathcal{F}, \quad (Af)(u) = \sum_{v \sim u} a_e f(v)$$

where the sum is over all vertices v adjacent to u, where e denotes the edge joining u to v, and where a_e is the weight attached to the edge e. Suppose we consider a (Hermitian) line bundle, L over the vertices of the vertices of the graph, and replace $\mathcal{F}$ by the space $\Gamma(L)$ of sections of L. Then the above definition does not make sense, since we have no way of comparing L_v with L_u. To get an adjacency matrix, we must also specify a *connection*, Θ. This means that for every vertex, x, and every edge, e emanating from x we must be given a unitary map

$$T_{x,e} : L_y \to L_x$$

where y is the other end of the edge e. The sole condition is that

$$T_{x,e} \circ T_{y,e} = id$$

for all edges e where x and y denote its end points. There is no hypothesis about the composition of the T's along edges of a path. In particular, the composition of the T's along the edges of a closed pathe starting and ending at x will be given by multiplication by a complex number of absolute value 1, known as the *holonomy* or the *flux* of the connection, Θ around the path.

Now, for each choice of connection (and bond strengths), define

$$A(\Theta) : \Gamma(L) \to \Gamma(L), \qquad A(\Theta)f(u) = \sum_{v \sim u} a_e T_{v,e} f(v).$$

In matrix terms, we might think of the original definition of the adjacency matrix as refering to a choice of trivialization of the line bundle, with corresponding trivial connection. Then a choice of Θ amounts to a choice of phase factor $e^{i\theta_{xy}}$ for each non-zero entry of A, with

$$\theta_{yx} = -\theta_{xy}$$

and replacing

$$A = (a_{xy}) \text{ by } A(\Theta) = (a_{xy} e^{i\theta_{xy}}).$$

The operator $A(\Theta)$ is self adjoint and has trace zero. It is easy to check that the spectrum of $A(\Theta)$ depends only on the holonomy of Θ. London's generalization of the Hückel model says that the presence of a magnetic field gives rise to a choice of connection. As $trA(\Theta) = 0$, an important invariant is

$$E_A(\Theta) = \sum_{\lambda > 0} \lambda(A(\Theta)) = \frac{1}{2} \sum |\lambda(A(\Theta))|,$$

the sum of the poisitive eigenvalues. As in the Hückel model, the larger $E_A(\Theta)$, the lower the ground state energy for the n-electron state (where n is the number of vertices, assumed even for simplicity). London uses this theory in [10] to discuss the diamagnetic properties of aromatic compounds.

In a recent paper,[9] Lieb and Loss discuss the following problem: For a given choice of bond strengths, A, find the connection (or rather the holonomy) which maximizes $E_A(\Theta)$. They show that for some special classes of planar graphs, such as cycles, necklaces, and some "tree-like" graphs, the maximum is achieved at the *canonical flux* one which associates flux $\pi/2$ to each oriented triangle in a triangulation of the graph. (One can show that if such a flux exists, it is independent of the triangulation; and that the canonical flux exists for the class of graphs they consider.) What is remarkable about their result is that the answer is independent of the choice of bond strengths. This is a property of the special class of graphs they consider.

For the case of the buckyball, a general magnetic field will destroy icosahedral symmetry. But we can ask the Lieb-Loss question for homogenous connections, i.e ones which are G- invariant: For a fixed value of the double bond strength, t, which G-invariant connections maximize $E_t(\Theta)$?

In order to deal with this question, we must first list the G-equivariant line bundles. Since the isotropy group of a vertex is $H = \mathbf{Z}_2$, the trivial bundle and the non-trivial bundle correponding to the sign representation of $\mathbf{Z}_2$. If we denote the non-trivial bundle by L, then Frobenius reciprocity says that $\Gamma(L)$ decomposes as

$$\Gamma(L) = 2 \times \mathbf{2} \oplus 4 \times \mathbf{4} \oplus 6 \times \mathbf{6} \oplus 2 \times \mathbf{2}',$$

i.e. as a direct sum of the representations of G which don't descend to I, each occurring with a multiplicity equal to its dimension.

For a general homogeneous graph, with H the isotropy group of a chosen, vertex, v, and $B \subset G$ the set group elements which move v to an adjacent vertex, specifying a G-invariant connection on a G-equivariant line bundle amounts to assigning a complex number z_b with $|z_b| = 1$ to each $b \in B$ subject to the conditions

$$z_{hb} = z_{bh} = \rho(h) z_b,\ h \in H, b \in B, \quad \text{and} \quad z_{b^{-1}} = z_b^{-1}$$

where ρ is the character determining the line bundle, cf. [1]. In the case at hand, this last condition implies that $z_w = \pm 1$ for the double bond generator in the case of the trivial bundle, and $z_w = \pm i$ for the double bond in the case of the non-trivial bundle, but there is an arbitrary choice of phase for a pentagonal generator. so in each case, the space of G-invariant connections consists of a circle. Here in the following figure , we illustrate the values of $E_1(\theta)$ where θ ranging from 0 to 2π for the case of $t = 1$. Notice that the absolute maximum is achieved for the non-trivial bundle and with canonical flux! In particular, this gives a minimum energy justification for passing to the double cover.

(Had we taken $t = 0$ and hence decoupled into twelve pentagons, the maximum would be achieved at phase 0, so the result does depend on the bond strengths.)

10 Restriction from $SU(2)$

For various reasons it is important to know how the irreducible representations of $SU(2)$ restrict to the subgroup $G = Sl(2,5)$. This problem was completely solved in [8] for all finite subgroups of $SU(2)$. We record the results for $Sl(2,5)$ here. If we let $a_{k,r}$ denote the multiplicity of the representation r in the restriction of the spin $k/2$ representation of $SU(2)$ to G, then we can form the generating series

$$Z_r(t) = \sum a_{k,r} t^k.$$

We list these series for each of the nine values of r. Each generating series is a rational function, and they all have the same denominator: we have

$$Z_r(t) = \frac{P_r(t)}{(1-t^{12})(1-t^{20})}$$

where only the numerator, the polynomial P_r depends on the representation, r. So we must list the polynomials P_r. They are given as

$$P_{\mathbf{1}} = 1 + t^{30}$$

$$
\begin{aligned}
P_{\mathbf{2}} &= t + t^{11} + t^{19} + t^{29} \\
P_{\mathbf{3}} &= t^2 + t^{10} + t^{12} + t^{18} + t^{20} + t^{28} \\
P_{\mathbf{4}} &= t^3 + t^9 + t^{11} + t^{13} + t^{17} + t^{19} + t^{21} + t^{27} \\
P_{\mathbf{5}} &= t^4 + t^8 + t^{10} + t^{12} + t^{14} + t^{16} + t^{18} + t^{20} + t^{26} \\
P_{\mathbf{6}} &= t^5 + t^7 + t^9 + t^{11} + t^{13} + 2t^{15} + t^{17} + t^{19} + t^{21} + t^{23} + t^{25} \\
P_{\mathbf{4}^\sim} &= t^6 + t^8 + t^{12} + t^{14} + t^{16} + t^{18} + t^{22} + t^{24} \\
P_{\mathbf{3'}} &= t^6 + t^{10} + t^{14} + t^{16} + t^{20} + t^{24} \\
P_{\mathbf{2'}} &= t^7 + t^{13} + t^{17} + t^{23}
\end{aligned}
$$

where $\mathbf{4}^\sim$ denotes the representation of G which descends to the four dimensional representation of I. In particular, note the highly suggestive form for the generating function of the invariants:

$$
Z_{\mathbf{1}}(t) = \frac{1 + t^{30}}{(1 - t^{12})(1 - t^{20})}
$$

where 30 is the number of edges, 12 the number of vertices, and 20 the number of faces of the icosahedron.

The integer spin (corresponding to even values of k) representations of $SU(2)$ descend to representations of $SO(3)$, and can be realized as the action of $SO(3)$ on harmonic polynomials on $\mathbf{R}^3$ of degree $\frac{1}{2}k$. The full group $O(3)$ acts on these spaces, with P acting as $+id$ if $\frac{1}{2}k$ is even and as $-id$ if $\frac{1}{2}k$ is odd. So for even values of k we can use the above series to determine the restriction of the harmonic polynomial representation to I_h. For example, from the above series for $Z_{\mathbf{1}}$ we see that the first few occurrences of the trivial representation are for the k values $k = 1, 12, 20, 30$ and of these $k = 30$ is the first case where $\frac{1}{2}k$ is odd. So the first occurrence of $\mathbf{1}^-$ is in spin fifteen.

11 The covers of $O(3)$

The connected group $SO(3)$ has the unique double cover, $SU(2)$ which is its universal cover. But this is not the case for the disconnected group $O(3)$. There are basically two natural choices: if Q denotes one of the two elements projecting onto the parity operator, P, we can have $Q^2 = id$ or $Q^2 = -id$. In other words Q can be either of order two or of order four. The "covering group" can be either $SU(2) \times \mathbf{Z}_2$ or $U(2)$. (In terms of Clifford algebras and Pin groups, the element in the Pin group covering P will be $Q = e_1e_2e_3$ where the e's form an orthonormal basis. So the question of whether Q is of order two or four hinges on whether the metric we are using is negative or positive definite. In terms of representation theory this difference expresses itself as follows: In both cases all representations of the double cover carry an additional label of $\pm$ along with the spin. For even spin, in both cases the $\pm$ means that Q is represented by $\pm Identity$. But for odd spin, if the group is $SU(2) \times \mathbf{Z}_2$ the $\pm$ means that Q is represented by $\pm Identity$, while if the group is $U(2)$, then the $\pm$ signifies that the chosen generator Q is represented by the scalar $\pm i$. Since $(\pm 1)^3 = \pm 1$ while $(\pm i)^3 = \mp i$ this makes a difference in terms of selection rules. Although these two possibilities were recognized as early as 1937 by Racah, they are not usually mentioned in the physics literature.

It is, of course, a matter of physics to determine which of the two choices describes the real world. From the point of view of the group G, the choice of $U(2)$ as covering group is more pleasant. Because for this choice, the 240 element group covering I_h becomes a complex reflection group. Indeed, the elements in G which project onto rotations through 180° are of order four - their square is $-id \in SU(2)$. If we multiply them by the scalar matrix i, we get elements of order two which generate the covering group. Thus the covering group is a complex reflection group.

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