Adventures with group theory:
counting and constructing polynomial invariants for applications in quantum entanglement and molecular phylogenetics

or: THE POWER OF PLETHYSM

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"Die Gruppenpest"

E Schrödinger

P Dirac
M Born

E Wigner

It has been rumoured that the group pest is gradually being cut out of quantum physics
−H. Weyl, *The Theory of Groups and Quantum Mechanics*, 1930

We wish finally to make a few remarks concerning the place of the theory of groups in the study of the quantum mechanics of atomic spectra. The reader will have heard that this mathematical discipline is of great importance for the subject. We manage to get along without it.

– E. U. Condon and G. H. Shortley, *Theory of Atomic Spectra*, 1935

$\cdots$ I dont think [Pauli] liked it particularly $\cdots$ there was a word, Die Gruppenpest, and you have to chase away the Gruppenpest. But Johnny Neumann, told me, "Oh these are old fogeys; in five years every student will learn group theory as a matter of course," and essentially he was right.

−Eugene P. Wigner, *Interview with T. S. Kuhn*, 1963; ©AIP.

This is the birthplace of
WIGNER JENÖ
1902-1995
Nobel Prize in Physics
Student of the Fasori Lutheran
Secondary School
Honorary Doctorate at the Eotvos
Lorand University
Honorary Member of the Eotvos Lorand
Physics Society
Proud Hungarian
With his involvement in the Manhattan Project and in the field of Nuclear Physics left a lasting impression on humankind.

The classical groups

$$
\begin{aligned}
GL(N,\mathbb{C}) &= \{m_{i,j}, 1 \leq i,j \leq N : \det(m) \neq 0\} \\
U(N) &= \{m_{i,j}, 1 \leq i,j \leq N : \det(m) \neq 0 \,\&\, m^*_{ij} = m^{-1}_{ji}\} \\
O(N,\mathbb{C}) &= \{m_{i,j}, 1 \leq i,j \leq N : m^T m = I\} \\
Sp(N,\mathbb{C}) &= \{m_{i,j}, 1 \leq i,j \leq N : m^T J m = J, J = -J^T\}
\end{aligned}
$$

Let $g \in G$ let have eigenvalues $x_1, x_2, \cdots, x_N$. Then the *character* of the *defining representation* is

$$Tr(g) = \sum\nolimits_i x_i$$

The classical groups (and a not-so-classical one)

$$GL(N,\mathbb{C}) = \{m_{i,j}, 1 \leq i,j \leq N : \det(m) \neq 0\}$$
$$U(N) = \{m_{i,j}, 1 \leq i,j \leq N : \det(m) \neq 0, \,\&\, m^*_{ij} = m^{-1}_{ji}\}$$
$$O(N,\mathbb{C}) = \{m_{i,j}, 1 \leq i,j \leq N : m^T m = I\}$$
$$Sp(N,\mathbb{C}) = \{m_{i,j}, 1 \leq i,j \leq N : m^T J m = J, J = -J^T\}$$

Let $g \in G$ let have eigenvalues $x_1, x_2, \cdots, x_N$. Then the *character* of the *defining representation* is

$$Tr(g) = \sum\nolimits_i x_i$$

$$GL_1(N,\mathbb{C}) = \{m_{i,j}, 1 \leq i,j \leq N : \det(m) \neq 0, \,\&\, \sum\nolimits_i m_{ij} = 1, \forall j\}$$

Group Characters 101

- For $g \otimes g$ acting on $V \otimes V$ we have

$$Tr(g \otimes g) = Tr(g)^2 = \sum_{i,j} x_i x_j$$

- Consider $W_\pm = V \otimes V / \langle (v \otimes w \pm w \otimes v) \rangle$. – taking a generating set $\{e_i \otimes e_j \pm e_j \otimes e_i\}$ and diagonal matrices,

$$Tr_+(g \otimes g) = \sum_{i<j} x_i x_j + \sum_i x_i^2 = \sum_{i \leq j} x_i x_j,$$

$$Tr_-(g \otimes g) = \sum_{i<j} x_i x_j$$

- **Theorems**
  (i)(Schur-Weyl) The characters of irreducible tensor representations of $GL(N)$ are certain symmetric polynomials $s_\lambda(x)$, where $\lambda = (\lambda_1, \lambda_2, \cdots, \lambda_N)$ is an integer partition.
  (ii)The character formula can be written combinatorially via tableaux as

$$s_\lambda(x) = \sum_{T \in SST_\lambda} x^T$$

Symmetric functions 102

- Extend $\mathbb{C}[x_1, x_2, \cdots, x_N]$ to the ring $\Lambda(X)$ in an infinite alphabet $X = (x_1, x_2, x_3, \cdots)$, with the Schur *functions* as natural basis.
- We need various binary operations (products):

$$\text{outer product:} \qquad s_\lambda \cdot s_\mu(X) = \sum c^{\nu}_{\lambda,\mu} s_\nu(X), \quad |\nu| = |\lambda| + |\nu|;$$

$$\text{inner product:} \qquad s_\lambda * s_\mu(X) = \sum g^{\nu}_{\lambda,\mu} s_\nu(X), \quad |\nu| = |\lambda| = |\mu|;$$

- $\cdots$ and their duals, expressing the expansion in composite alphabets $X+Y = (x_1, x_2, x_3, \cdots, y_1, y_2, \cdots), XY = (x_1y_1, x_2y_1, x_3y_1, \cdots; x_1y_1, x_2y_1, \cdots)$:

$$\text{outer coproduct:} \qquad s_\nu(X+Y) = \sum c^{\nu}_{\lambda,\mu} s_\lambda(X) s_\mu(Y);$$

$$\text{inner coproduct:} \qquad s_\nu(XY) = \sum g^{\nu}_{\lambda,\mu} s_\lambda(X) s_\mu(Y);$$

(– generically, we write these as
$f(X+Y) = \sum f_{(1)}(X) f_{(2)}(Y)$, $f(XY) = \sum f_{[1]}(X) f_{[2]}(Y)$.)

The power of plethysm

One further binary operation is *plethysm*, named by D E Littlewood for the operation of composition of symmetric function maps.

Definition:

let $s_\mu = \sum_{T \in SST_\mu} x^T$. Then $s_\lambda[s_\mu](X) := s_\lambda(Y)$, where Y is the alphabet $\{x^T\}_{T \in SST_\mu}$, and we have

$$\text{plethysm:} \qquad s_\lambda[s_\mu](X) = \sum p^\nu_{\lambda,\mu} s_\nu(X), \quad |\nu| = |\lambda||\mu|.$$

Often denoted multiplicatively, $\lambda[\mu] \equiv \mu \underline{\otimes} \lambda$ (because the underlying module is a projection of the tensor power $\otimes^{|\lambda|} V_\mu$).

(We could also have a plethysm *coproduct* with a compound alphabet say $X^Y = (x_1^{y_1}, x_2^{y_1}, x_3^{y_1}, \cdots ; x_1^{y_2}, x_2^{y_2}, x_3^{y_2}, \cdots ; \cdots)$, so $f(X^Y) = \sum f_{<1>}(X) f_{<2>}(Y)$).

Example: $s_{(1^2)}[s_{(2)}]$ in $GL(3)$

- The semi-standard tableaux T (and monomials x^T) for $\square\square$ are

$$SST_{\square\square} = \left\{ \boxed{1\,|\,1},\ \boxed{1\,|\,2},\ \boxed{1\,|\,3},\ \boxed{2\,|\,2},\ \boxed{2\,|\,3},\ \boxed{3\,|\,3} \right\},$$

$$\therefore\ s_{(2)} = x_1^2 + x_1x_2 + x_1x_3 + x_2^2 + x_2x_3 + x_3^2$$

  – that is, the alphabet $Y = \{x^T\} \equiv (x_1^2, x_1x_2, x_1x_3, x_2^2, x_2x_3, x_3^2)$.

- Forming $\sum_{T<T'} x^T x^{T'}$ gives 15 monomials,

$$x_1^3x_2 + x_1^3x_3 + x_1^2x_2^2 + x_1^2x_2x_3 + x_1^2x_3^2 +$$
$$x_1^2x_2x_3 + x_1x_2^3 + x_1x_2^2x_3 + x_1x_2x_3^2 + x_1x_2^2x_3 +$$
$$x_1x_2x_3^2 + x_1x_3^3 + x_2^3x_3 + x_2^2x_3^2 + x_2x_3^3$$

$$\therefore\ s_{(1^2)}[s_{(2)}] = s_{(3,1)} \leftrightarrow \left\{ \begin{matrix} \begin{smallmatrix}1&1&1\\2\end{smallmatrix}, & \begin{smallmatrix}1&1&1\\3\end{smallmatrix}, & \begin{smallmatrix}1&1&2\\2\end{smallmatrix}, & \begin{smallmatrix}1&1&2\\3\end{smallmatrix}, & \begin{smallmatrix}1&1&3\\3\end{smallmatrix}, \\ \begin{smallmatrix}1&1&3\\2\end{smallmatrix}, & \begin{smallmatrix}1&2&2\\2\end{smallmatrix}, & \begin{smallmatrix}1&2&2\\3\end{smallmatrix}, & \begin{smallmatrix}1&2&3\\3\end{smallmatrix}, & \begin{smallmatrix}1&2&3\\2\end{smallmatrix}, \\ \begin{smallmatrix}1&3&3\\2\end{smallmatrix}, & \begin{smallmatrix}1&3&3\\3\end{smallmatrix}, & \begin{smallmatrix}2&2&2\\3\end{smallmatrix}, & \begin{smallmatrix}2&2&3\\3\end{smallmatrix}, & \begin{smallmatrix}2&3&3\\3\end{smallmatrix}. \end{matrix} \right\}.$$

Invariants of group representations

- Standard problem of invariant theory is, given a space W carrying a representation of some group, construct tensor products W, $W \otimes W$, $W \otimes W \otimes W, \cdots, \otimes^n W$, and study group-invariant elements.
- The space of 'polynomials in the components of W' is in fact $\mathbb{C}[W^*]$, so the relevant tensor spaces are the symmetric powers W, $W \vee W$, $W \vee W \vee W, \cdots, \vee^n W$.
- **Theorem (Molien)**:
  Let $h_n = \dim \mathbb{C}[W^*]_n^G$ and define the Hilbert series $h(z) = \sum_0^\infty h_n z^n$. For G semisimple and compact,

$$h(z) = \int d\mu \frac{1}{\det(I - z\rho(g))}$$

  where $d\mu$ is the Haar measure, and $\rho(g)$ is the group representation.

Molien's theorem via plethysms

- Suppose the representation ρ is some irreducible with character $s_\lambda(x)$. Then the diagonal elements of $\rho(g)$ are $\{x^T\}_{T \in SST_\lambda}$, and

$$\frac{1}{\det(I - z\rho(g))} = 1 + z\sum x^T + z^2 \sum_{T \leq T'} x^T x^{T'} + z^3 \sum_{T \leq T' \leq T''} x^T x^{T'} x^{T''} + \cdots$$

$$\therefore \qquad h_n = \int d\mu \, s_{(n)}[s_\lambda](x) \equiv p^{(0)}_{(n),\lambda}.$$

- We enumerate the Hilbert series term-by-term by computing the appropriate plethysm of group characters. All evaluations are done with the software package ©`Schur`.
- Consider a model space V (of dimension N) carrying the defining representation of a matrix group G, and the tensor product W of K isomorphic copies $W = V \otimes V \otimes \cdots \otimes V = \otimes^K V$, with group $G \times G \times \cdots \times G = \times^K G$.

Counting entanglement invariants

(a) Quantum pure states: $V \cong \mathbb{C}^N$, $G = GL(N)$:

Let $N \vdash n$, $n = rN$, and let τ be the partition (r^N) (that is, with Ferrers diagram a rectangular array of r columns of length N). Then

$$h_n = g^{(n)}_{\tau,\tau,\cdots,\tau} \quad (K\text{-fold inner product}).$$

If $N \not\vdash n$, then $h_n = 0$.

(b) Quantum mixed states: $V \cong \mathbb{C}^N \otimes \mathbb{C}^{N*}$, $G = GL(N)$:

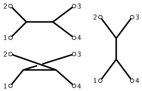
$$h_n = \sum_{|\tau|=n, \ell(\tau)\leq N^2} \left(\sum_{|\sigma|=n, \ell(\sigma)\leq N} g^{\tau}_{\sigma,\sigma} \right)^2$$

(c) Phylogenetic pattern frequencies, general Markov model: $G = GL_1(N)$:

Let $n = rN + s$, $s \geq 0$. Then

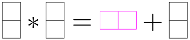
$$h_n = g^{(n)}_{\tau_1,\tau_2,\cdots,\tau_K} \quad (K\text{-fold inner product}),$$

for each τ_k of the form $(r_k + s_k, r_k^{(N-1)})$.

Example	model space V	tensor space W	state	
2 qubits	$\mathbb{C}^2$	$V \otimes V$	$\|00\rangle + \|11\rangle$	concurrence $(= \det) \neq 0$
3 qubits	$\mathbb{C}^2$	$V \otimes V \otimes V$	$\|000\rangle + \|111\rangle$ $\|001\rangle + \|010\rangle + \|001\rangle$	tangle $\neq 0$ tangle $= 0$
2 qubits (mixed)	$\mathbb{C}^2 \otimes \mathbb{C}^{*2}$	$V \otimes V$	$\sum \rho^{ia}_{bj} e_i \otimes f^j \otimes e_a \otimes f^b$	(20 invariants)
	$\mathbb{C}^4$	$V \otimes V \otimes V \otimes V$	$\sum P_{ijk\ell} e_i \otimes e_j \otimes e_k \otimes e_\ell$ $\sum P_{ijk\ell} = 1$	(squangles)

Warmups

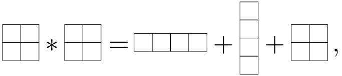
- $\mathfrak{S}_2$: $n = 2$, $(r^N) = (1^2)$:

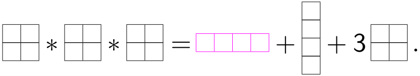


- Concurrence (determinant function):

$$\det(\psi) = \psi_{00}\psi_{11} - \psi_{01}\psi_{10}$$

- $\mathfrak{S}_4$: $n = 4$, $(r^N) = (2^2)$:





- Tangle (hyperdeterminant):

$$\begin{aligned}\mathrm{hdet}(\psi) = & -\psi_{011}^2\psi_{100}^2 + 2\psi_{010}\psi_{011}\psi_{100}\psi_{101} - \psi_{010}^2\psi_{101}^2 + 2\psi_{001}\psi_{011}\psi_{100}\psi_{110} \\ & + 2\psi_{001}\psi_{010}\psi_{101}\psi_{110} - 4\psi_{000}\psi_{011}\psi_{101}\psi_{110} - \psi_{001}^2\psi_{110}^2 \\ & - 4\psi_{001}\psi_{010}\psi_{100}\psi_{111} + 2\psi_{000}\psi_{011}\psi_{100}\psi_{111} + 2\psi_{000}\psi_{010}\psi_{101}\psi_{111} \\ & + 2\psi_{000}\psi_{001}\psi_{110}\psi_{111} - \psi_{000}^2\psi_{111}^2 .\end{aligned}$$

Molecular phylogenetics

- Taxa are represented by DNA sequences

$$\texttt{ACGTTGAACTGG}\cdots \quad (\text{or } \texttt{RYRYYRRRYYRR}\cdots)$$

- Genetic information content is sparse, so we can talk about *probabilities* (relative frequencies)

$$p_A, p_C, p_G, p_T \quad \text{with} \quad p_A + p_C + p_G + p_T = 1$$
$$(\text{or } p_0, p_1 \quad \text{with} \quad p_0 + p_1 = 1 \;)$$

- Mutations are mostly 'neutral', so these probabilities are subject to *random changes* under a Markov process – just given by matrix multiplication:

$$\begin{pmatrix} p_0 \\ p_1 \end{pmatrix} \to \begin{pmatrix} m_{00} & m_{01} \\ m_{10} & m_{11} \end{pmatrix} \begin{pmatrix} p_0 \\ p_1 \end{pmatrix} \quad \Leftrightarrow \quad p \to M\, p$$

- From the base sequences of an alignment of genes from different species, for example with two or three species

```
ACGTTGAACTGG···      ACGTTGAACTGG···
AAGTCGAACACG···      AAGTCGAACACG···
                     AATTCGATCAGG···
```

we form the two-way, three-way, $\cdots$, pattern arrays *(relative frequencies)*.

General Markov model

- Thus the number of patterns is 16, or 64, or $4^{\#\text{ of leaves}}$:

$$(p_{AA}, p_{AC}, p_{AG}, p_{AT}; p_{CA}, \cdots; \cdots, p_{TG}, p_{TT})$$

$$(p_{AAA}, p_{AAC}, p_{AAG}, p_{AAT}; p_{ACA}, \cdots; \cdots, p_{TTG}, p_{TTT})$$

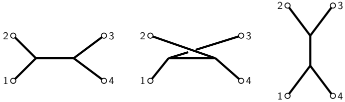
$$\text{or} \qquad (p_{00}, p_{01}, p_{10}, p_{11}), \quad (p_{000}, p_{001}, \cdots; \cdots p_{110}, p_{111}).$$

- If the two sequences derive from a common ancestor, then just after speciation, the lists are

$$(p_A, p_C, p_G, p_T) \rightarrow (p_{AA} = p_A, p_{AC} \equiv 0, \cdots; \cdots, p_{TG} \equiv 0, p_{TT} = p_T)$$

$$\text{or} \qquad (p_0, p_1) \rightarrow (p_{00} = p_0, p_{01} \equiv 0, p_{10} \equiv 0, p_{11} = p_1)$$

- Patterns on each edge evolve independently thereafter, according to the Markov process;
- For example for quartet trees, we can construct 3 *phylogenetic tensors* P_{abcd} by starting with any leaf as root, and decorating the pendant and internal edges with matrices M_1, M_2, M_3, M_4, and M_5:



Stochastic tangles and quartet trees:

- $N = 4$, $n = 5$, $(r+s, r^{N-1}) = (2, 1^3)$:

$$(2,1^3) * (2,1^3) * (2,1^3) * (2,1^3) = 5(5) + \cdots$$

- Under $\mathfrak{S}_4$ (leaf permutations), these 5 invariants give $3(4) + (2^2)$. Two of these are algebraically dependent, but the tree-informative ones are (2^2).
- Under each of the three equivalent quartet tree isotropy groups, $\mathfrak{S}_2 \wr \mathfrak{S}_2 < \mathfrak{S}_4$, we have the branching rule $(2^2) \rightarrow (\mathrm{id}) + (\mathrm{sgn})$. Define

$$q_1 = \mathrm{sgn}_{12|34}, \quad q_2 = \mathrm{sgn}_{13|24}, \quad q_3 = \mathrm{sgn}_{14|23}$$

- These are the *squangles* (stochastic quartet tangles) – degree 5 polynomials in 256 variables, with 66,744 terms.
- We have $q_1 + q_2 + q_3 = 0$ and

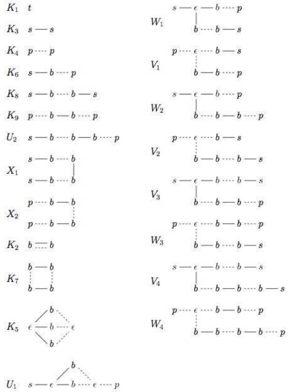
Hypothesis	Quartet	$E[q_1]$	$E[q_2]$	$E[q_3]$
$\mathcal{H}_1$	12|34	0	$-u$	u
$\mathcal{H}_2$	13|24	v	0	$-v$
$\mathcal{H}_3$	14|23	$-w$	w	0

Entanglement invariants for mixed 2 qubit states

- The Hilbert series can be evaluated via contour integration for $SU(2)$:

$$H(q) = \frac{1+q^4+q^5+3q^6+2q^7+2q^8+3q^9+q^{10}+q^{11}+q^{15}}{(1-q)(1-q^2)^3(1-q^3)^2(1-q^4)^3(1-q^6)}$$

- The task is to sort out algebraic dependencies amongst candidate invariants:



There is trouble finding the right set of fundamental invariants ...

The next task is to determine sets of primary and secondary invariants, and thereby express $\mathcal{R}^G$ in the Hironaka decomposition form (1.3). Comparison of the general form (1.4) of the Molien series with the explicit form (3.4) reveals that there are precisely ten algebraically independent invariants, with respect to which $\mathcal{R}^G$ is free. From (6.9), we have 11 candidates, namely $X_1, X_2, K_1, \ldots, K_9$. However, X_1 and X_2 are not algebraically independent of one another and $K_1, K_2, \ldots, K_9$. This is so because there exists a syzygy, still of the first kind, linking X_1, X_2 and all these K_i. It is obtained by finding an element $SX \in \mathcal{P}$ in the subideal $\langle SY[1], SY[2], SY[43]\rangle$ of $\mathcal{S}$, which is a polynomial in $X_1, X_2, K_1, \ldots, K_9$, and does not contain U_1 and U_2. This has been done using Maple. The polynomial SX is about ten pages long and is of degree 48. Its dependence on X_1 and X_2 is illustrated by setting $K_i = z^{\deg(K_i)}$ for $i = 1, 2, \ldots, 9$, which gives

$$
\begin{aligned}
SX|_{K_i=z^{\deg(K_i)}} = {} & 16X_1^4X_2^4 + 8832z^{36}X_1X \\
& - 2112z^{30}X_1^3 - 1088z^{42} \\
& + 144z^{24}X_2^4 + 896X_1^3z^{18}X \\
& - 64X_1^4z^6X_2^3 + 192z^{18}X_1^4 \\
& - 6512z^{48} + 192z^{18}X_2^4X_1
\end{aligned}
$$

Because $SX \in \mathcal{S}$, under the map ϕ we c
that X_1 and X_2 cannot both be primary i

A mixed two-qubit system and the structure of its ring of local invariants

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Abstract
The local invariants of a mixed two-qubit system are discussed. These invariants are polynomials in the elements of the corresponding density matrix. They are counted by means of group-theoretic branching rules which relate this problem to one arising in spin–isospin nuclear shell models. The corresponding Molien series and a refinement in the form of a four-parameter generating function are determined. A graphical approach is then used to construct explicitly a fundamental set of 21 invariants. Relations between them are found in the form of syzygies. By using these, the structure of the ring of local invariants is determined, and complete sets of primary and secondary invariants are identified: there are 10 of the former and 15 of the latter.

PACS numbers: 02.10.Hh, 02.20.Qs, 03.67.-a

Brian Garner Wybourne (1935–2003)

. . . Brian realized that this is an elementary example of what Littlewood has called a *plethysm*, which treats the symmetry of the products of objects that themselves possess symmetry. Elliott had used plethysms in his nuclear studies, but no one had noticed their relevance to atomic shell theory before. At a conference at the US National Bureau of Standards in 1967, Brian unflinchingly described the details of the mathematics. The audience was stunned. At the end of Brians presentation a despairing voice asked, 'What *is* a plethysm?' We were all surprised to hear Brian say that a full explanation would take too much time. . .
– B R Judd, **Interaction with Brian Wybourne**, 2004

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Stehen Low
Otto Campoamor-Stursberg
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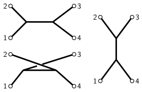
Example	model space V	tensor space W	state	
2 qubits	$\mathbb{C}^2$	$V \otimes V$	$\lvert 00\rangle + \lvert 11\rangle$	concurrence $(= \det) \neq 0$
3 qubits	$\mathbb{C}^2$	$V \otimes V \otimes V$	$\lvert 000\rangle + \lvert 111\rangle$ $\lvert 001\rangle + \lvert 010\rangle + \lvert 001\rangle$	tangle $\neq 0$ tangle $= 0$
2 qubits (mixed)	$\mathbb{C}^2 \otimes \mathbb{C}^{*2}$	$V \otimes V$	$\sum \rho^{ia}_{bj} e_i \otimes f^j \otimes e_a \otimes f^b$	(20 invariants)
	$\mathbb{C}^4$	$V \otimes V \otimes V \otimes V$	$\sum P_{ijk\ell} e_i \otimes e_j \otimes e_k \otimes e_\ell$ $\sum P_{ijk\ell} = 1$	(squangles)
matrix multiplic'n	$\mathbb{C}^2 \otimes \mathbb{C}^{*2}$	$V \otimes V^* \otimes V^*$	$\mu = \sum e_i{}^j \otimes f_j{}^k \otimes f_k{}^i$	(Strassen's algorithm)