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Recognizing Patterns in Mathematical Physics

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...Not that I aspire to complete coherence. Our mistake is to confuse our limitations with the bounds of possibility and clap the universe into a rationalist hat or some other. But I may find the indications of a pattern that will include me, even if the outer edges tail off into ignorance.
— William Golding, *Free Fall (1959)*

Abstract

Many calculations in mathematical physics seem to become a jumble of seemingly unrelated numbers. However, one can often spot patterns that can lead to new conjectures and thence to hitherto unrecognised new theorems. A number of specific examples will be given.

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Balmer's Remarkable Discovery

In 1884 the Swiss school teacher, J. Balmer, learnt of the existence of three lines of the spectrum of hydrogen, H_α, H_β and H_δ and noted the ratios

$$\begin{aligned} H_\alpha/H_\beta &= \frac{656.2}{486.1} = 1.3499 \approx \frac{27}{20} = 1.35 \\ H_\alpha/H_\delta &= \frac{656.2}{410.1} = 1.600 \approx \frac{8}{5} = 1.6 \\ H_\beta/H_\delta &= \frac{486.1}{410.1} = 1.1853 \approx \frac{32}{27} = 1.1852 \end{aligned}$$

Balmer then conjectured that the wavelength of any member of the series would be given by

$$\lambda_n = \frac{n^2}{n^2 - 2^2}\lambda_0 \quad \text{where } n = 3, 4, 5 \ldots$$

with $\lambda_0 = 364.56nm$. Using Balmer's conjecture we find

n	λ_n			
3	$\frac{9}{9-4}\lambda_0$	$= \frac{9}{5}\lambda_0$	$= 656.2nm$	H_α
4	$\frac{16}{16-4}\lambda_0$	$= \frac{4}{3}$	$= 486.1nm$	H_β
5	$\frac{25}{25-4}\lambda_0$	$= \frac{25}{21}\lambda_0$	$= 434.0nm$	H_γ
6	$\frac{36}{36-4}\lambda_0$	$= \frac{9}{8}\lambda_0$	$= 410.1nm$	H_δ
∞	λ_0		$= 346.6nm$	H_∞

His conjecture readily reproduced the observed ratios and correctly gave the H_γ line. Balmer's result, having absolutely no theoretical foundation, was later to play a key role in Bohr's quantum model of the $H-$atom and in the subsequent development of Schrödinger's equation.

Spinors and the Rotation Groups

The rotation groups $SO(n)$ play an important role in many areas of chemistry and physics. The full rotation group $O(n)$ possess a basic spin representation Δ of degree $2^{[\frac{n}{2}]}$ which is irreducible under $O(n) \to SO(n)$ if n is *odd* or reducible into a pair of conjugate irreps $\Delta_{\pm}$. In 1935 Brauer and Weyl gave a complete resolution of the Kronecker square of the basic spinor irreps of $SO(n)$ into their symmetric and antisymmetric components. Further results were obtained by Littlewood by exploiting known automorphisms and isomorphisms for the $n = 3 \ldots 8$ cases but he noted "The construction of the concomitants of degree higher than 2 in 10 or more variables would appear to present a formidable problem". Nevertheless, in 1981 a complete solution for the resolution of the third powers was obtained by King, Luan Dehuai and Wybourne following upon an observation by the author. For the even rotation groups $SO(2\nu)$ one uses difference characters such that

$$\Delta'' = \Delta_{+} - \Delta_{-}$$

The problem was then to resolve the Kronecker cube of Δ''. One had the special cases for $\Delta'' \otimes \{21\}$

$$\begin{array}{rl}
SO(4) & -\Delta''([1]-[0]) \\
SO(6) & -\Delta''([1^2]-[1]) \\
SO(8) & -\Delta''([1^3]-[1^2]-[0]) \\
SO(10) & -\Delta''([1^4]-[1^3]-[1]+[0])
\end{array}$$

From this limited data could one guess the general result? The first clue was my observation that the dimensions of the terms enclosed in curved brackets was in each case $3^{\nu-1}$. The second guess was to note the combinatorial identity

$$3^{\nu-1} = \sum_x \left\{ \binom{2\nu}{\nu-1-6x} - \binom{2\nu}{\nu-2-6x} - \binom{2\nu}{\nu-4-6x} + \binom{2\nu}{\nu-5-6x} \right\}$$

which is consistent with the general result

$$\Delta'' \otimes \{21\} = \Delta'' \sum_x (-[1^{\nu-1-6x}] + [1^{\nu-2-6x}] + [1^{\nu-4-6x}] - [1^{\nu-5-6x}])$$

This result together with some similar results yielded the final solution.

Reduced notation and the Symmetric Group

The symmetric group $S(n)$ is of fundamental importance in quantum chemistry as well in nuclear models and symplectic models of mesoscopic systems. One wishes to discuss the properties of the symmetric group for general n and concentrate on stable results that are essentially $n-$independent. Here the reduced notation proves to be very useful. The tensor irreps $\{\lambda\}$ of $S(n)$ are labelled by ordered partitions(λ) of integers where $\lambda \vdash n$. In reduced notation the label $\{\lambda_1, \lambda_2, \ldots, \lambda_p\}$ for $S(n)$ is replaced by $\langle\lambda_2, \ldots, \lambda_p\rangle$. Kronecker products can then be fully developed in a $n-$independent manner and readily programmed. Thus one finds, for example, the terms arising in the reduced Kronecker product $\langle 21\rangle * \langle 2^2\rangle$ are

$$
\begin{array}{l}
<51> + <5> + <43> + <421> + 3<42> \\
+ 3<41^2> + 5<41> + 3<4> + <3^21> + 2<3^2> \\
+ <32^2> + <321^2> + 6<321> + 7<32> + 3<31^3> \\
+ 8<31^2> + 8<31> + 3<3> + <2^31> + 2<2^3> \\
+ 3<2^21^2> + 7<2^21> + 5<2^2> + <21^4> + 5<21^3> \\
+ 8<21^2> + 6<21> + 2<2> + <1^5> + 3<1^4> \\
+ 3<1^3> + 2<1^2> + <1>
\end{array}
$$

Looking at the above list one is immediately struck by the observation that the list is self-associated. That is every partition (λ) in the list either has a conjugate partner $(\tilde{\lambda})$ where the rows and columns of the Young frame of the partition (λ) have been interchanged or the partition (λ) is self-conjugate.

Some Kronecker products are self-associated while others are not. Is there a general theorem that would tell us immediately which products are self-associated? We note that the partition (21) is an example of a *staircase partition* (staircase partitions have the general form $(a, a-1, a-2, \ldots, 1)$) while the partition (2^2) is self-conjugate.

These observations led to the general theorem

Theorem *For H defined by $\langle\lambda\rangle * \langle\nu\rangle = \langle H\rangle$ to be self-associated, it is necessary and sufficient that one of the partitions be a staircase partition and the other be at least self-conjugate.*

One may also resolve symmetrised powers of irreps of $S(n)$ in reduced notaion. For example, one finds that the terms in $\langle 21\rangle \otimes \{21\}$ are

$< 71 >$	$+\ 2 < 7 >$	$+\ < 621 >$	$+\ 5 < 62 >$
$+\ 5 < 61^2 >$	$+\ 17 < 61 >$	$+\ 14 < 6 >$	$+\ < 54 >$
$+\ 2 < 531 >$	$+\ 9 < 53 >$	$+\ < 52^2 >$	$+\ 2 < 521^2 >$
$+\ 20 < 521 >$	$+\ 45 < 52 >$	$+\ < 51^4 >$	$+\ 10 < 51^3 >$
$+\ 47 < 51^2 >$	$+\ 81 < 51 >$	$+\ 45 < 5 >$	$+\ < 4^21 >$
$+\ 5 < 4^2 >$	$+\ 3 < 432 >$	$+\ 3 < 431^2 >$	$+\ 25 < 431 >$
$+\ 47 < 43 >$	$+\ 3 < 42^21 >$	$+\ 20 < 42^2 >$	$+\ 2 < 421^3 >$
$+\ 30 < 421^2 >$	$+\ 118 < 421 >$	$+\ 149 < 42 >$	$+\ 10 < 41^4 >$
$+\ 64 < 41^3 >$	$+\ 163 < 41^2 >$	$+\ 185 < 41 >$	$+\ 78 < 4 >$
$+\ 3 < 3^221 >$	$+\ 16 < 3^22 >$	$+\ < 3^21^3 >$	$+\ 20 < 3^21^2 >$
$+\ 73 < 3^21 >$	$+\ 82 < 3^2 >$	$+\ < 32^3 >$	$+\ 2 < 32^21^2 >$
$+\ 25 < 32^21 >$	$+\ 73 < 32^2 >$	$+\ < 321^4 >$	$+\ 20 < 321^3 >$
$+\ 118 < 321^2 >$	$+\ 270 < 321 >$	$+\ 235 < 32 >$	$+\ 5 < 31^5 >$
$+\ 47 < 31^4 >$	$+\ 163 < 31^3 >$	$+\ 280 < 31^2 >$	$+\ 240 < 31 >$
$+\ 83 < 3 >$	$+\ < 2^41 >$	$+\ 5 < 2^4 >$	$+\ 9 < 2^31^2 >$
$+\ 47 < 2^31 >$	$+\ 82 < 2^3 >$	$+\ 5 < 2^21^4 >$	$+\ 45 < 2^21^3 >$
$+\ 149 < 2^21^2 >$	$+\ 235 < 2^21 >$	$+\ 162 < 2^2 >$	$+\ < 21^6 >$
$+\ 17 < 21^5 >$	$+\ 81 < 21^4 >$	$+\ 185 < 21^3 >$	$+\ 240 < 21^2 >$
$+\ 173 < 21 >$	$+\ 55 < 2 >$	$+\ 2 < 1^7 >$	$+\ 14 < 1^6 >$
$+\ 45 < 1^5 >$	$+\ 78 < 1^4 >$	$+\ 83 < 1^3 >$	$+\ 55 < 1^2 >$
$+\ 19 < 1 >$	$+\ 2 < 0 >$		

Theorem *If $\langle\lambda\rangle \otimes \{\mu\} = \langle H\rangle$, where (λ) and (μ) are staircase partitions, then H is self-associated.*

Kronecker Products for Two-Row Shapes in $S(n)$

The Pauli exclusion principle limits interest in quantum chemistry to just those irreps of $S(n)$ involving partitions whose Young frames having at most two rows. Thus in forming Kronecker products only irreps having at most two rows can yield physical states. In the case of reduced Kronecker products interest is restricted to one-part partitions. Consider the case of $\langle 5\rangle * \langle 4\rangle$ whose one-part content is

$$<9> + <8> + 2<7> + 2<6> + 3<5> + 2<4>$$
$$+ 2<3> + <2> + <1>$$

The first thing one notices is that the multiplicity distribution is unimodal. Is this a general feature? Indeed one finds that if we write

$$\langle k\rangle * \langle \ell\rangle = \sum_{\lambda} c^{\langle m\rangle}_{\langle k\rangle\langle \ell\rangle}\langle\lambda\rangle$$

then the coefficients $c^{\langle m\rangle}_{\langle k\rangle\langle \ell\rangle}$ are given by

$$c^{\langle m\rangle}_{\langle k\rangle\langle \ell\rangle} = \frac{1}{2}(\ell - k + m + 2) \quad \text{for} \quad k > m$$
$$c^{\langle m\rangle}_{\langle k\rangle\langle \ell\rangle} = \frac{1}{2}(k + \ell - m + 2) \quad \text{for} \quad m \geq k$$

and the coefficients exhibit the symmetry

$$c^{\langle m\rangle}_{\langle k\rangle\langle \ell\rangle} = c^{\langle 2k-m\rangle}_{\langle k\rangle\langle \ell\rangle}$$

The above results give a complete description of the symmetric group Kronecker products needed in quantum chemistry. Results for specific values of n are found from the reduced results by simply prefixing the reduced labels $\langle k\rangle$, $\langle \ell\rangle$, $\langle m\rangle$ to give $\{n-k,k\}$, $\{n-\ell,\ell\}$ and $\{n-m,m\}$ respectively and remembering that for an irrep $\{p,q\}$ is non-standard if $p<q$ and must be made standard by use of the modification rule

$$\{p,q\} \equiv -\{q-1,p+1\} \qquad \text{if} \quad q>p$$

Thus for $S(18)$ we obtain for $\{13\ ,5\} * \{14\ ,4\}$

$$\{17\ 1\} + \ \{16\ 2\} + \ 2\{15\ 3\} + \ 2\{14\ 4\} + \ 3\{13\ 5\}$$
$$+ \ 2\{12\ 6\} + \ 2\{11\ 7\} + \ \{10\ 8\} + \ \{9^2\}$$

whereas for $S(12)$ we obtain for $\{7,5\} * \{8,4\}$ just

$$\{11\ 1\} + \{10\ 2\} + 2\{93\} + \{84\} + 2\{75\}$$

$n-$NonInteracting Particles in a Harmonic Oscillator Potential

I would like to briefly consider some problems that arise when one wishes to describe the states of $n-$noninteracting spin $\frac{1}{2}$ particles in an isotropic $d-$dimensional harmonic oscillator potential, a common starting point in a variety of nuclear and mesoscopic models. For a single particle there are two infinite sets of states, those of even parity and those of odd parity. These two sets of states span a single infinite dimensional irrep Δ of the metapletic group $Mp(2d)$ which is the covering group of the non-compact symplectic group $Sp(2d,R)$. Under $Mp(2n) \to Sp(2d,R)$ one has

$$\Delta \to \langle\frac{1}{2}(0)\rangle + \langle\frac{1}{2}(1)\rangle$$

The group $Sp(2d,R)$ has a maximal compact subgroup $U(d)$ such that under $Sp(2d,R) \to U(d)$ we have

$$\langle\frac{1}{2}(0)\rangle \to \varepsilon^{\frac{1}{2}} \cdot M_+$$
$$\langle\frac{1}{2}(1)\rangle \to \varepsilon^{\frac{1}{2}} \cdot M_-$$

where M_+ and M_- are effectively the even and odd terms in the infinite $S-$function series

$$M = \sum_{m=0}^{\infty} \{m\}$$

A number of problems arise in studying the properties of infinite dimensional irreps of $Sp(2d,R)$ in order to make practical applications. These include evaluating Kronecker products and resolving symmetrised powers of the basic irreps $\langle\frac{1}{2}(0)\rangle$ and $\langle\frac{1}{2}(1)\rangle$. The Kronecker products have been discussed elsewhere. The resolution of the symmetrised powers of the basic irreps is a particularly difficult problem and until now no general results have been known. The symmetrised squares of the basic irreps of $Sp(2d,R)$ have recently been studied in some detail for various values of d and up to terms of weight 20. This led me to guess that in general

$$< \frac{1}{2};(0) > \otimes\{2\} = \sum_{i=0}^{\infty} < 1;(0+4i) >$$

$$< \frac{1}{2};(0) > \otimes\{1^2\} = \sum_{i=0}^{\infty} < 1;(2+4i) >$$

$$< \frac{1}{2};(1) > \otimes\{2\} = \sum_{i=0}^{\infty} < 1;(2+4i) >$$

$$< \frac{1}{2};(1) > \otimes\{1^2\} =< 1;(1^2) > + \sum_{i=0}^{\infty} < 1;(4+4i) >$$

holds for all $Sp(2d,R)$ with $d \geq 2$. For $d=1$ the irrep $< 1;(1^2) >$ in the last equation must be deleted. But this would imply a hitherto unknown identity for symmetrised powers of the infinite $S-$function series, namely,

$$M_+ \otimes \{1^2\} = M_- \otimes \{2\}$$

which was readily proved.

The equality

$$< \frac{1}{2}; (0) > \otimes \{1^2\} \equiv < \frac{1}{2}; (1) > \otimes \{2\}$$

has a surprising, and seemingly unnoticed, feature. The left-hand-side describes the $S = 1$ states formed by placing two of the fermions in even parity orbitals while the right-hand-side describes the $S = 0$ states formed by placing two particles in odd parity orbitals. This implies there is a one-to-one mapping between the orbital states for these two sets of states. Indeed, if one enumerates the two-particle $LS-$states for an isotropic three-dimensional isotropic harmonic oscillator potential formed by having one particle in the $n = 0$ $s-$orbital and a second in the $n = 2$ $s-$ or $d-$orbital one finds the spectroscopic terms $^{3.1}SD$ while placing both particles in the $n = 1$ $p-$orbital yields the spectroscopic terms ^3P and ^1SD. Clearly the map $^3(SD) \rightarrow ^1(SD)$ exists as predicted.

The Quantum Hall Effect and the Dangers of Extrapolation

I end with a cautionary example from the quantum Hall effect. Laughlin describes the fractional quantum Hall effect in terms of a (unnormalized) wavefunction

$$\Psi^m_{Laughlin}(z_1, \ldots, z_N) = \prod_{i \leq j}^{N} (z_i - z_j)^{2m+1} exp(-\frac{1}{2}\sum_{i=1}^{N}|z_i|^2)$$

where $z = x + iy$ and m is an integer corresponding to states of a fractional filling $1/(2m+1)$ of the lowest Landau level. The Laughlin wavefunction may be expanded as a linear combination of Slater determinantal wavefunctions for states of a given angular momentum

$$J_{Laughlin} = (2m+1)\frac{1}{2}N(N-1)$$

The Vandermonde alternating function in N variables is defined as

$$V(z_1, \ldots, z_N) = \prod_{i<j}^{N}(z_i - z_j)$$

While V is an alternating function even powers of V, say V^{2m}, is necessarily a *symmetric* function and hence must be expandable in any suitable linear integral basis of symmetric functions, such as the Schur functions

$$s_\lambda(z_i - z_j) = \{\lambda\} = \{\lambda_1, \ldots, \lambda_p\}$$

which are indexed by partitions of the integer

$$n = mN(N-1)$$

Dropping questions of normalization, we may write

$$\frac{\Psi_{Laughlin}}{V} = V^{2m} = \sum_{\lambda \vdash n} c^{\lambda}\{\lambda\}$$

The coefficients c^{λ} are signed integers and are precisely the same integers that arise in the expansion of the Laughlin wavefunction as a linear combination of Slater determinants. Of particular interest is the determination of the expansion coefficients as the number N increases. The problem is combinatorially explosive.

The late Claude Itzykson and colleagues made a careful study of the problem and calculated the coefficients for up to $N = 5$ where there are 59 distinct partitions involved which they termed the number of *admissible tableaux* and endeavoured to give a general result to predict the number of admissible tableaux as a function of N. They presented a table of the number of admissible tableaux for $N = 2, \ldots, 29$ based upon a conjecture and remarked "*The above reasoning does not however insure that this is exactly the total number of terms, ... as some coefficients might still vanish. However experience up to $N = 5$ seems to indicate that such accidents do not happen.*"

I was developing, along with Thibon and Scharf, some new algorithms for expanding powers of the Vandermonde determinant and computed results for $N = 6$ and $N = 7$ with complete agreement with the Itzykson conjecture - at $N = 8$ the conjecture failed!

Concluding Remarks

I have tried in the preceding remarks to show that sometimes guesses and hunches can sometimes lead to unexpected discoveries. Patterns can sometimes be discerned if we exercise our human imagination. Of course ultimately we must move to demonstrate the validity of our guesses and hunches.