GUESSES - HUNCHES - FORMULAE - DISCOVERIES

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Abstract

A number of examples of informed guesses and hunches leading to discoveries and unanticipated theorems are given.

1. Introduction

One of the most remarkable discoveries in all of atomic physics came as the result of a guess followed by a hunch that the guess was right and the formula highly suggestive but only much later was the discovery confirmed. I refer, of course, to Balmer's incredible guess that the wavelengths of the spectral lines of the hydrogen atom could be represented by simple formula in terms of integers. Balmer's guess was pure numerology based upon knowing the wavelengths of just three lines, his hunch was that his result would extend to other spectral lines of hydrogen. Balmer was unable to give any rational basis to his hunch but his discovery was to lead to a new age in atomic physics, in the hands of Neils Bohr. Few have made such momentous and far reaching discoveries and yet the process of discovery often involves guesses and hunches in a way inconsistent with most philosophical discussions of the so-called scientific method. Herein I propose to give a few examples of of guesses based upon very limited data that have led to unanticipated theorems of relevance to problems in chemistry and physics.

2. 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[1] 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[2]–[4] by exploiting known automorphisms and

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isomorphisms for the $n = 3 \ldots 8$ casaes but he noted[4] "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[12] 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.

3. 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[6]–[9] 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

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

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[10]

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

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

Again one observes that the list is self-associated and again one is led to a new and unanticipated theorem[10]

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

4. Kronecker products for two-row shapes

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

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

The first thing one notices is that the multiplicity distribution is unimodal. Is this a general feature? Indeed one finds[10] 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

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

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 $\langle k\rangle$, $\langle \ell\rangle$, $\langle m\rangle$ by $\{n-k, k\}$, $\{n-\ell, \ell\}$ 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[4]

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

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

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

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

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

5. $n-$NonInteracting Particles in a Harmonic Oscillator Potential

As a last topic 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 metaplectic 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

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

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[11]–[13]. 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

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

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.

6. 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.

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