# Bell Polynomials

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Introduction. Recently I had occasion<sup>1</sup> to write

$$\det(\mathbb{I} - x\mathbb{A}) = \exp\left\{ \operatorname{tr} \log(\mathbb{I} - x\mathbb{A}) \right\}$$
$$= \exp\left\{ -T_1 x - \frac{1}{2}T_2 x^2 - \frac{1}{3}T_3 x^3 - \frac{1}{4}T_4 x^4 - \cdots \right\}$$
(1)

where  $T_k \equiv \operatorname{tr}(\mathbb{A}^k)$ ; *i.e.*, to display  $\det(\mathbb{I} - x \mathbb{A})$  as a composite function. I look here to general features of the class of formulae of which (1) provides a valuable instance. Setting aside all convergence considerations, let f(x) and g(x) be formal power series; we look to the formal expansion of F(x) = f(g(x)).

**Bare bones of the problem.** The terms in power series typically wear  $\frac{1}{n}$  or  $\frac{1}{n!}$  or other such decorations. Stripping those away, let

$$g(x) = a_1 x^1 + a_2 x^2 + a_3 x^3 + a_4 x^4 + a_5 x^5 + \cdots$$
(2.1)

$$f(x) = \frac{1}{1-x} = 1 + x^2 + x^3 + x^4 + x^5 + \dots$$
(2.2)

Then Mathematica supplies

$$F(x) = 1 + a_1 x^2 + (a_1^2 + a_2) x^2 + (a_1^3 + 2a_1a_2 + a_3) x^3 + (a_1^4 + 3a_1^2a_2 + a_2^2 + 2a_1a_2 + a_4) x^4 + (a_1^5 + 4a_1^3a_2 + 3a_1a_2^2 + 3a_1^2a_3 + 2a_2a_3 + 2a_1a_4 + a_5) x^5$$

$$\vdots \qquad (3.1)$$

$$\equiv D_0 + D_1 x^1 + D_2 x^2 + D_3 x^3 + D_4 x^3 4 + D_5 x^5 + \cdots$$
 (3.2)

 $^1\,$  "Newton and the characteristic polynomial of a matrix" (December 2019), page 4.

The terms that appear in the development of (say)  $D_5$  can be described

 $a_1^{j_1}a_2^{j_2}a_3^{j_3}a_4^{j_4}a_5^{j_5}$  subject to the constraint  $j_1 + 2j_2 + 3j_3 + 4j_4 + 5j_5 = 5$ 

while those that contribute to  $D_n$  are of the form

$$\prod_{i=1}^{n} a_i^{j_i} : j_1 + 2j_2 + 3j_3 + \dots + nj_n = n$$

But those expressions provide no indication of the numerical prefactors that appear in the description of  $D_5$  (and generally of  $D_n$ ). This problem is resolved when one recognizes that the terms in  $D_5$  arise from the *partitions* of 5. In the following table I have used Reverse[IntegerPartitions[5]] to list the partitions of 5, and Length[Permutations[•]] to count the number of distinct permutations of each partition:

That data serves to construct

$$D_5 = (a_1^5 + 4a_1^3a_2 + 3a_1a_2^2 + 3a_1^2a_3 + 2a_2a_3 + 2a_1a_4 + a_5)$$

Because p(n) (use PartitionsP[n]) is such a rapidly growing function of n the description of  $D_n$  becomes rapidly unmanageable; we find

$$D_{10} = \text{sum of } 42 \text{ terms}$$
$$D_{100} = \text{sum of } 190569292 \text{ terms}$$

I now pull from my hat (mystery to be removed in a moment) the Toeplitz matrix

$$\mathbb{T}_{5} = \begin{pmatrix}
a_{1} & a_{2} & a_{3} & a_{4} & a_{5} \\
-1 & a_{1} & a_{2} & a_{3} & a_{4} \\
0 & -1 & a_{1} & a_{2} & a_{3} \\
0 & 0 & -1 & a_{1} & a_{2} \\
0 & 0 & 0 & -1 & a_{1}
\end{pmatrix}$$
(4.5)

(the construction of  $\mathbb{T}_n$  is obvious) and observe (with *Mathematica*'s assistance) that

$$\det \mathbb{T}_5 = D_5$$

# Putting meat on the bare bones

Laplace expansion on the final column (bottom to top) gives

$$D_5 = a_1 D_4 + a_2 D_3 + a_3 D_2 + a_4 D_1 + a_5 D_0$$

were it is understood that  $D_0 = 1, D_1 = a_1$ . Generally, we have the recursion relation

$$D_n = \sum_{k=1}^n a_k D_{n-k} \tag{5}$$

which can be seen to follow from the assembly of the composite function F(x) = f(g(x)), and might be used to *motivate* the construction of the Toeplitz matrices  $\mathbb{T}_n$ .

**Putting meat on the bare bones.** The preceding discussion owes its bare bones simplicity to the circumstance that no non-trivial numerical coefficients entered at (2.2) into the construction of f(x); all of the numerics that appear in (3.1) derive from the procedure (counting distinct permutations of individual partitions) described on the preceding page. Look now to the most general case, in which arbitrary numerics  $\{k_1, k_2, \ldots\}$  enter into the construction of the monic series

$$f(x) = 1 + k_1 x^2 + k_2 x^2 + \dots + k_i x^i + \dots$$
(6)

Mathematica now supplies

$$F(x) = 1 + a_1k_1x^2 + (a_1^2k_2 + a_2k_1)x^2 + (a_1^3k_3 + 2a_1a_2k_2 + a_3k_1)x^3 + (a_1^4k_4 + 3a_1^2a_2k_3 + a_2^2k_2 + 2a_1a_2k_2 + a_4k_1)x^4 + (a_1^5k_5 + 4a_1^3a_2k_4 + 3a_1a_2^2k_3 + 3a_1^2a_3k_3 + 2a_2a_3k_2 + 2a_1a_4k_2 + a_5k_1)x^5 \\ \vdots \qquad (7.1)$$

$$\equiv \mathcal{D}_0 + \mathcal{D}_1(k_1)x^1 + \mathcal{D}_2(k_1, k_2)x^2 + \mathcal{D}_3(k_1, k_2, k_3)x^3 + \mathcal{D}_4(k_1, k_2, k_3, k_4)x^4 + \mathcal{D}_5(k_1, k_2, k_3, k_4, k_5)x^5 + \cdots$$
(7.2)

which give back (3) when  $k_1 = k_2 = \cdots = 1$ .

It is apparently not possible in the general case to construct determinental descriptions of the  $\mathcal{D}$ -coefficients, except by the following **formal device**: from Toeplitz matrices of the form

$$\mathbb{T}_{5}(k) = \begin{pmatrix} ka_{1} & ka_{2} & ka_{3} & ka_{4} & ka_{5} \\ -1 & ka_{1} & ka_{2} & ka_{3} & ka_{4} \\ 0 & -1 & ka_{1} & ka_{2} & ka_{3} \\ 0 & 0 & -1 & ka_{1} & ka_{2} \\ 0 & 0 & 0 & -1 & ka_{1} \end{pmatrix}$$
(8.5)

we obtain

$$\det \mathbb{T}_5(k) = (a_1^5 k^5 + 4a_1^3 a_2 k^4 + 3a_1 a_2^2 k^3 + 3a_1^2 a_3 k^3 + 2a_2 a_3 k^2 + 2a_1 a_4 k^2 + a_5 k^1)$$

which gives back  $\mathcal{D}_5(k_1, k_2, k_3, k_4, k_5)$  when each of the exponentiated k-factors is rewritten as a subscripted k-factor:  $k^p \to k_p$ . Generally

$$\mathcal{D}_5(k_1, k_2, \dots, k_n) = \det \mathbb{T}_n(k) \Big|_{k^p \to k_p : p = 1, 2, \dots, n}$$
 (9.5)

Computation establishes that

$$\det \mathbb{T}_5(k) = a_1 k \det \mathbb{T}_4(k) + a_2 k \det \mathbb{T}_3(k)$$
$$+ a_3 k \det \mathbb{T}_2(k) + a_4 k \det \mathbb{T}_1(k) + a_5 k$$

so in general we have the recursion relation (compare (5))

$$\det \mathbb{T}_n(k) = \sum_{m=1}^n a_m k \det \mathbb{T}_{n-m}(k) \tag{10}$$

But because (except in special cases)

$$k^{u}k^{v}\Big|_{k^{p}\to k_{p}}\neq k_{u}k_{v}$$

this does not translate into a recursion relation among the  $\mathcal{D}$ -coefficients.

In some special cases results sharper than those described above can be obtained. When we set  $k_n = 1$  (all n) we recover the simplest/sharpest of all cases: the bare bones case We turn now to the important case  $k_n = \frac{1}{n!}$ .

#### Exponentially composite functions. Set

$$f(x) = e^x = 1 + x + \frac{1}{2!}x^2 + \frac{1}{3!}x^3 + \frac{1}{4!}x^4 + \frac{1}{5!}x^5 + \cdots$$

and maintain the generic form of g(x). Then

$$F(x) = 1 + \frac{1}{1!}a_{1}x^{1} + \frac{1}{2!}(a_{1}^{2} + a_{2})x^{2} + \frac{1}{3!}(a_{1}^{3} + 6a_{1}a_{2} + 6a_{3})x^{2} + \frac{1}{4!}(a_{1}^{4} + 12a_{1}^{2}a_{2} + 12a_{2}^{2} + 24a_{1}a_{3} + 24a_{4})x^{2} + \frac{1}{5!}(a_{1}^{5} + 20a_{1}^{3}a_{2} + 60a_{1}a_{2}^{2} + 60a_{1}^{2}a_{3} + 120a_{2}a_{3} + 120a_{1}a_{4} + 120a_{5})$$

$$\vdots$$

$$\equiv 1 + \mathcal{E}_{1}x^{1} + \mathcal{E}_{2}x^{2} + \mathcal{E}_{3}x^{3} + \mathcal{E}_{4}x^{4} + \mathcal{E}_{5}x^{5} + \cdots$$
(11)

where we verify that (for example)  $\mathcal{E}_5 = \frac{1}{5!} \mathcal{D}_5(\frac{1}{1!}, \frac{1}{2!}, \frac{1}{3!}, \frac{1}{4!}, \frac{1}{5!}).$ 

A little experimentation motivates the introduction of matrices the non-Toplitz form (note the sub-diagonal) exemplified by

$$\mathbb{E}_{5} = \begin{pmatrix} a_{1} & 2a_{2} & 3a_{3} & 4a_{4} & 5a_{5} \\ -1 & a_{1} & 2a_{2} & 3a_{3} & 4a_{4} \\ 0 & -2 & a_{1} & 2a_{2} & 3a_{3} \\ 0 & 0 & -3 & a_{1} & 2a_{2} \\ 0 & 0 & 0 & -4 & a_{1} \end{pmatrix}$$
(12)

# Exponentially composite functions: Bell polynomials

because they permit us to write

$$\mathcal{E}_n = \frac{1}{n!} \det \mathbb{E}_n \tag{13}$$

Laplace expansion up the last column gives

$$\mathcal{E}_5 = 4! \Big\{ \frac{1}{4!} a_1 \mathcal{E}_4 + \frac{2}{3!} a_2 \mathcal{E}_3 + \frac{3}{2!} a_3 \mathcal{E}_2 + \frac{4}{1!} a_4 \mathcal{E}_1 + \frac{5}{0!} a_5 \mathcal{E}_0 \Big\}$$

where  $0! = \mathcal{E}_0 = 1$ ; in the general case

$$\mathcal{E}_{n} = (n-1)! \sum_{m=1}^{n} \frac{m}{(n-m)!} a_{m} \mathcal{E}_{n-m}$$
(14)

**Bell polynomials.** Set  $a_n = \frac{1}{n!}b_n$ , which is to say, let g(x) be defined

$$g(x) = b_1 x^1 + \frac{1}{2!} b_2 x^2 + \frac{1}{3!} b_3 x^3 + \frac{1}{4!} b_4 x^4 + \frac{1}{5!} b_5 x^5 + \dots$$
(15)

Retaining the assumption that  $f(x) = e^x$  we find that computation then gives

$$F(x) = 1 + \frac{1}{1!}b_1x^1 + \frac{1}{2!}(b_1^2 + b_2)x^2 + \frac{1}{3!}(b_1^3 + 3b_1b_2 + b_3)x^2 + \frac{1}{4!}(b_1^4 + 6b_1^2b_2 + 3b_2^2 + 4b_1b_3 + b_4)x^2 + \frac{1}{5!}(b_1^5 + 10b_1^3b_2 + 15b_1b_2^2 + 10b_1^2b_3 + 10b_2b_3 + 5b_1b_4 + b_5) \vdots \equiv 1 + \frac{1}{1!}B_1(b_1)x^1 + \frac{1}{2!}B_2(b_1, b_2)x^2 + \frac{1}{3!}B_3(b_1, b_2, b_3)x^3 + \frac{1}{4!}B_4(b_1, b_2, b_3, b_4)x^4 + \frac{1}{5!}B_5(b_1, b_2, b_3, b_4, b_5)x^5 + \cdots$$
 (16)

where the  $B_n(\bullet)$  are the "complete exponential Bell polynomials." Working from  $\mathbb{E}_5$  we are led to construct

$$\mathbb{B}_{5}(b_{1}, b_{2}, b_{3}, b_{4}, b_{5}) = \begin{pmatrix} b_{1} & b_{2} & \frac{1}{2!}b_{3} & \frac{1}{3!}b_{4} & \frac{1}{4!}b_{5} \\ -1 & b_{1} & b_{2} & \frac{1}{2!}b_{3} & \frac{1}{3!}b_{4} \\ 0 & -2 & b_{1} & b_{2} & \frac{1}{2!}b_{3} \\ 0 & 0 & -3 & b_{1} & b_{2} \\ 0 & 0 & 0 & -4 & b_{1} \end{pmatrix}$$
(17)

which gives

 $B_5(b_1, b_2, b_3, b_4, b_5) = \det \mathbb{B}_5(b_1, b_2, b_3, b_4, b_5)$ 

and (again by Laplace expansion up the last column) find

$$B_5 = b_1 B_4 + 4b_2 B_3 + 6b_3 B_2 + 4b_4 B_1 + b_5 B_0$$
$$= \sum_{m=0}^4 \binom{4}{m} b_{m+1} B_{4-m}$$

Generally,

$$B_n = \det \mathbb{B}_n$$
 : arguments surpressed (18)

where the nearly-Toplitzian structure of  $\mathbb{B}_n$  is made obvious by that of  $\mathbb{B}_5$ , and where the general recursion relation reads

$$B_{n+1}(b_1, b_2, \dots, b_{n+1}) = \sum_{m=0}^n \binom{n}{m} b_{m+1} B_{n-m}(b_1, b_2, \dots, b_{n-m})$$
(19)

A determinantal representation sometimes found in the literature<sup>2</sup>

	$b_1$	$\binom{5-1}{1}b_2$	$\binom{5-1}{2}b_3$	$\binom{5-1}{3}b_4$	$\binom{5-1}{4}b_5$
	-1	$b_1$	$\binom{5-2}{1}b_2$	$\binom{5-2}{2}b_3$	$\binom{5-2}{3}b_4$
$B_{5} =$	0	-1	$b_1$	$\binom{5-3}{1}b_2$	$\binom{5-3}{2}b_3$
	0	0	-1	$b_1$	$\binom{5-4}{1}b_2$
	0	0	0	-1	$b_1$

also works, but is above the diagonal profoundly non-Toplitzian, and does not share with (17) the property that advancing  $n \to n+1$  is accomplished simply by introducing an additional right column and bottom row of obvious design.

The complete Bell polynomials, of which the first few-generated by

$$\exp\left\{\sum_{k=1}^{\infty} \frac{1}{k!} a_k x^k\right\} = \sum_{n=0}^{\infty} \frac{1}{n!} B_n(a_1, a_2, \dots, a_n) x^n$$
(20)

—are, to recapitulate,

$$B_{0} = 1$$

$$B_{1}(a_{1}) = a_{1}$$

$$B_{2}(a_{1}, a_{2}) = a_{1}^{2} + a_{2}$$

$$B_{3}(a_{1}, a_{2}, a_{3}) = a_{1}^{3} + 3a_{1}a_{2} + a_{3}$$

$$B_{4}(a_{1}, a_{2}, a_{3}, a_{4}) = a_{1}^{4} + 6a_{1}^{2}a_{2} + 4a_{1}a_{3} + 3a_{2}^{2} + a_{4}$$

$$B_{5}(a_{1}, a_{2}, a_{3}, a_{4}, a_{5}) = a_{1}^{5} + 10a_{1}^{3}a_{2} + 15a_{1}a_{2}^{2} + 10a_{1}^{2}a_{3} + 10a_{2}a_{3} + 5a_{1}a_{4} + a_{5}$$

which are, of course, actually *multinomials*. Comparison with this result

$$D_5 = a_1^5 + 4a_1^3a_2 + 3a_1a_2^2 + 3a_1^2a_3 + 2a_2a_3 + 2a_1a_4 + a_5$$

 $<sup>^2</sup>$  See, for example, the Wikipedia article "Bell polynomials." One can use familiar procedures (for example: arbitrary similarity transformations) to produce infinitely many determinant-preserving modifications of any given matrix. And, indeed, to preserve *all* of the coefficients in the characteristic polynomial.

#### Bell polynomials, Bell numbers & number/set partitions

of the bare bones theory shows that the a-factors arise here as there from the partitions of 5, but that the numeric factors have been altered by the factorials in the generating function. Evidently

$$B_n(a_1, a_2, \ldots, a_n)$$
 is a sum of  $p(n)$  terms

**Set partitions.** What have come to be called "Bell polynomials" were, by Eric Temple Bell (1883–1960) himself, when he introduced them in the late 1920s, called "partition polynomials." We have already seen how integer partitions enter the picture. Bell was interested, however, in the ennumerative properties of *set* partitions.

The set containing a solitary element can be partitioned in **1** way: (1). A 2-element set can be partitioned in **2** ways: (1)(2), (1, 2). A 3-element set can be partitioned in **5** ways:

$$(1)(2)(3)(1,2)(3), (1,3)(2), (2,3)(1)(1,2,3)$$

A 4-element set can be partitioned in 15 ways:

 $\begin{array}{l} (1)(2)(3)(4) \\ (1,2)(3)(4), \ (1,3)(2)(4), \ (1,4)(2)(3), \ (2,3)(1)(4), \ (2,4)(1)(3), \ (3,4)(1)(2) \\ (1,2)(3,4), \ (1,3)(2,4), \ (1,4)(2,3) \\ (1,2,3)(4), \ (1,2,4)(3), \ (1,3,4)(2), \ (2,3,4)(1) \\ (1,2,3,4) \end{array}$ 

A 5-element set can be partitioned in **52** ways.<sup>3</sup> **Bell numbers**  $B_n$  arise from Bell polynomials be setting all *a*-variables to unity:

$$B_n = B_n(1, 1, \dots, 1)$$

Reading from (21) we find  $\{B_0, B_1, B_2, B_4, B_5, \ldots\} = \{1, 1, 2, 5, 15, 52, \ldots\}$ , which reproduces precise the sequence obtained above. We thank Bell for proof that the agreement continues: Bell numbers count set partitions.

Bell devised a Pascal-like algorithm for generating Bell numbers. Starting from  $\frac{1}{1}$ , add the stacked couplet and record the result, producing

$$\begin{array}{c} 1 \\ 1 \end{array}$$

<sup>&</sup>lt;sup>3</sup> See the figure in the Wikipedia article "Partition of a set." Authors seem unable to resist associating that 52 with the 54 chapters of the early  $11^{\text{th}}$  century Japanese classic, *The Tale of Genji*.

Use the last digit to begin a new row, keep adding couplets and recording the results, to produce

Again use the last digit to launch a new row and proceed as before:

Five iterations of that procedure produce

The Bell numbers appear on the edges of the triangle.

Less mysteriously, we learn from (20)—set all *a*-variables to unity—that the Bell numbers are generated by

$$\exp\left\{\sum_{k=1}^{\infty} \frac{1}{k!} x^k\right\} = \sum_{n=0}^{\infty} \frac{1}{n!} B_n x^n \tag{22}$$

and from (19) that they satisfy the recursion relation

$$B_{n+1} = \sum_{m=0}^{n} \binom{n}{m} B_{n-m} \tag{23}$$

Bell numbers arise also in other connections. Look, for example, to the Poisson distribution

$$P(k;\lambda) = \frac{\lambda^k e^{-\lambda}}{k!}$$

For the successive moments

$$m_n(\lambda) = \sum_{k=0}^{\infty} k^n P(k;\lambda)$$

Mathematica supplies

$$\begin{array}{cccccc} m_0(\lambda) & 1 & 1 \\ m_1(\lambda) & \lambda & 1 \\ m_2(\lambda) & \lambda + \lambda^2 & 2 \\ m_3(\lambda) & \lambda + 3\lambda^2 + \lambda^3 & 5 \\ m_4(\lambda) & \lambda + 7\lambda^2 + 6\lambda^3 + \lambda^4 & 15 \\ m_5(\lambda) & \lambda + 15\lambda^2 + 25\lambda^3 + 10\lambda^4 + \lambda^5 & 52 \end{array}$$

where in the final column we have set  $\lambda = 1$  and recovered the Bell numbers.

#### Bell polynomials, Bell numbers & number/set partitions

Concerning the Bell polynomials themselves, their maternal service (giving birth to Bell numbers) by no means exhausts their utility. A source cited above<sup>2</sup> mentions their relevance to, among other subjects,

• The formulation of Faà di Bruno's Formula ( $n^{\text{th}}$ -order differentiation composite functions), the context in which—60 years ago—I first acquired some familiarity with this subject.<sup>4</sup>

- The Lagrange inversion of series.
- The asymptotic expansion of Laplace-type integrals

$$I(\lambda) = \int_{a}^{b} e^{-\lambda f(x)} g(x) \, dx$$

which are central to the many physical/mathematical applications of the saddlepoint method and the method of steepest descent.

• Hermite polynomials: In (20) set  $x = t, a_1 = x, a_2 = -1, a_{k>2} = 0$ , get

$$\exp\left\{xt - \frac{1}{2}t^2\right\} = \sum_{n=0}^{\infty} \frac{1}{n!} B_n(x, -1, 0..., 0) t^n$$

But

$$\exp\left\{xt - \frac{1}{2}t^{2}\right\} = \sum_{n=0}^{\infty} \frac{1}{n!} He_{n}(x)t^{n}$$

so by (17)

$$He_5(x) = \det \begin{pmatrix} x & -1 & 0 & 0 & 0\\ -1 & x & -1 & 0 & 0\\ 0 & -2 & x & -1 & 0\\ 0 & 0 & -3 & x & -1\\ 0 & 0 & 0 & -4 & x \end{pmatrix} = x^5 - 10x^3 + 15x, \text{ etc.}$$

which (for what it's worth) appeared in my own work long ago.<sup>5</sup>

• Derivation of Newton's symmetric polynomial identities: The discussion in the Wikipedia article<sup>2</sup> is sketchy and opaque, but the argument follows clearly from results developed in the essay<sup>1</sup> that inspired the present effort. Taking A to be an  $n \times n$  matrix, it is shown there that

$$\det(\lambda \mathbb{I} - \mathbb{A}) = \lambda^n + \sum_{m=1}^n D_m \lambda^{n-m}$$

<sup>&</sup>lt;sup>4</sup> "Foundations and applications of the Schwinger action principle," doctoral dissertation, Brandeis University, 1960.

 $<sup>^5</sup>$  "Some applications of an elegant formula due to V. F. Ivanoff," Notes for a seminar presented on 28 May 1969 to the Applied Math Club at Porttland State University, page 10. Note that the determinant is unchanged if all the minus signs are omitted.

where

$$D_m = (-)^m \frac{1}{m!} \begin{vmatrix} T_1 & T_2 & T_3 & T_4 & \dots & T_m \\ 1 & T_1 & T_2 & T_3 & \dots & T_{m-1} \\ 0 & 2 & T_1 & T_2 & \dots & T_{m-2} \\ 0 & 0 & 3 & T_1 & \dots & T_{m-3} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \dots & T_1 \end{vmatrix} \qquad : \quad m = 1, 2, \dots, n$$
$$= 0 \qquad \qquad : \quad m > n$$

and  $T_k \equiv \text{tr}\mathbb{A}^k$ . That result—which lies at the heart of my derivation<sup>1</sup> of Newton's identities—can by (17) be formulated

$$\det(\lambda \mathbb{I} - \mathbb{A}) = \lambda^n + \sum_{m=1}^n \lambda^{n-m} \frac{1}{m!} B_m(t_1, t_2, \dots, t_m)$$
(24)

where

$$t_k \equiv -(k-1)! T_k$$

Setting  $\lambda = 0$  we obtain

$$\det \mathbb{A} = (-)^n \frac{1}{n!} B_n(t_1, t_2, \dots, t_n) \tag{25}$$

which is a trace-wise description of  $\det \mathbb{A}$ .

• Moments and cumulants of probability distributions: The generating function for the moments  $m_n$  of a given distribution—whether the random variable be continuous or discrete—is given<sup>6</sup> by

$$M(t) = 1 + \sum_{n=1}^{\infty} \frac{1}{n!} m_n t^n = \left\langle e^{xt} \right\rangle$$
 (26.1)

where  $\langle \bullet \rangle$  signifies "expectation value." The moments  $\{1, m_1, m_2, \ldots\}$  serve collectively to characterize the distribution. Alternatively/equivalently one has the "cumulants"  $\{0, c_1, c_2, \ldots\}$  which were introduced by the Danish astronomer/statistician Thorvald Thiele (1838–1910) in 1889, are useful in some contexts, and are generated by

$$K(t) = \sum_{n=1}^{\infty} \frac{1}{n!} c_n t^n = \log[M(t)]$$
(26.2)

$$P(x) = (\alpha/\pi) \frac{1}{\alpha^2 - (x - \beta)^2}$$
 :  $-\infty < x < \infty$ 

 $m_1$  and all higher moments are undefined.

<sup>&</sup>lt;sup>6</sup> When they exist. Recall that for the Cauchy-Lorenz distribution

# Bell polynomials, Bell numbers & number/set partitions

Inversely

$$M(t) = e^{K(t)}$$

so by (20) and (17) we have

$$m_n = B_n(c_1, c_2, \dots, c_n)$$

$$= \begin{pmatrix} c_1 & c_2 & \frac{1}{2!}c_3 & \frac{1}{3!}c_4 & \frac{1}{4!}c_5 & \dots & \frac{1}{n-1!}c_n \\ -1 & c_1 & c_2 & \frac{1}{2!}c_3 & \frac{1}{3!}c_4 & \dots & \frac{1}{n-2!}c_{n-1} \\ 0 & -2 & c_1 & c_2 & \frac{1}{2!}c_3 & \dots & \frac{1}{n-3!}c_{n-2} \\ 0 & 0 & -3 & c_1 & c_2 & \dots & \frac{1}{n-4!}c_{n-3} \\ 0 & 0 & 0 & -4 & c_1 & \dots & \frac{1}{n-5!}c_{n-4} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \dots & c_1 \end{pmatrix}$$

Explicitly—borrowing here from (21)—we have

$$m_{0} = 1$$

$$m_{1} = c_{1}$$

$$m_{2} = c_{1}^{2} + c_{2}$$

$$m_{3} = c_{1}^{3} + 3c_{1}c_{2} + c_{3}$$

$$m_{4} = c_{1}^{4} + 6c_{1}^{2}c_{2} + 4c_{1}c_{3} + 3c_{2}^{2} + c_{4}$$

$$m_{5} = c_{1}^{5} + 10c_{1}^{3}c_{2} + 15c_{1}c_{2}^{2} + 10c_{1}^{2}c_{3} + 10c_{2}c_{3} + 5c_{1}c_{4} + c_{5}$$
(27.1)

which on inversion<sup>7</sup> (accomplished in an instant by Mathematica's Solve command) become

$$c_{1} = m_{1}$$

$$c_{2} = m_{2} - m_{1}^{2} = \langle (x - m_{1})^{2} \rangle$$

$$c_{3} = m_{3} - 3m_{1}m_{2} + 2m_{1}^{2}$$

$$c_{4} = m_{4} - 4m_{1}m_{3} - 3m_{2}^{2} + 12m_{1}^{2}m_{2} - 6m_{1}^{4}$$

$$c_{5} = m_{5} - 5m_{1}m_{4} - 10m_{2}m_{3} + 20m_{1}^{2}m_{3} + 30m_{1}m_{2}^{2} - 60m_{1}^{3}m_{2} + 24m_{1}^{5}$$
(27.2)

Equations (27) assume a somewhat simpler appearance when expressed in terms of the central moments  $\mu_n = \langle (x - m_1)^n \rangle$ .<sup>8</sup> Equations (27.2) do not appear to admit of determinental formulation, but can be displayed as weighted sums

$$c_n = \sum_{k=1}^{n} (-)^{k-1} (k-1)! B_{n,k}(m_1, m_2, \dots, m_{n-k-1})$$
(28)

<sup>&</sup>lt;sup>7</sup> Alternatively, use  $K(t) = \log[1 + \Sigma(t)] = \Sigma - \frac{1}{2}\Sigma^2 + \frac{1}{3}\Sigma^3 - \frac{1}{4}\Sigma^4 + \cdots$ <sup>8</sup> See STATISTICAL PHYSICS & THERMODYNAMICS (1969–1970, 1971–1972), Chapter 1, pages 39–40 or the Wikipedia article "Cumulant."

of "incomplete Bell polynomials," an intricate  $subject^2$  that I had hoped to avoid, though it is central to Bell's theory and many of its diverse applications.

Briefly, the polynomials  $B_{n,k}(a_1, a_2, \ldots, a_{n-k+1})$  :  $k = 0, 1, 2, \ldots, n$  are generated by

$$\sum_{n=k}^{\infty} \frac{1}{n!} B_{n,k}(a_1, a_2, \dots, a_{n-k+1}) x^n = \frac{1}{k!} \left( \sum_{j=1}^{\infty} \frac{1}{j!} a_j x^j \right)^k$$
(29)

which (as does the command  $BellY[n, k, \{a_1, a_2, ..., a_{n-k+1}\}]$ ) gives rise to the following list:

$$\begin{array}{l} B_{0,0}(a_1)=1\\ B_{1,0}(a_1,a_2)=0\\ B_{1,1}(a_1)=a_1\\ B_{2,0}(a_1,a_2,a_3)=0\\ B_{2,1}(a_1,a_2)=a_2\\ B_{2,2}(a_1)=a_1^2\\ B_{3,0}(a_1,a_2,a_3,a_4)=0\\ B_{3,1}(a_1,a_2,a_3)=a_3\\ B_{3,2}(a_1,a_2)=3a_1a_2\\ B_{3,3}(a_1)=a_1^3\\ B_{4,0}(a_1,a_2,a_3,a_4,a_5)=0\\ B_{4,1}(a_1,a_2,a_3,a_4)=a_4\\ B_{4,2}(a_1,a_2,a_3)=3a_2^2+4a_1a_3\\ B_{4,3}(a_1,a_2)=6a_1^2a_2\\ B_{4,4}(a_1)=a_1^4\\ B_{5,0}(a_1,a_2,a_3,a_4,a_5)=a_5\\ B_{5,2}(a_1,a_2,a_3,a_4,a_5)=a_5\\ B_{5,2}(a_1,a_2,a_3,a_4)=10a_2a_3+5a_1a_4\\ B_{5,3}(a_1,a_2,a_3,a_4)=15a_1a_2^2+10a_1^2a_3\\ B_{5,4}(a_1,a_2=10a_1^3a_2\\ B_{5,5}(a_1)=a_1^5\\ B_{6,0}(a_1,a_2,a_3,a_4,a_5,a_6)=a_6\\ B_{6,2}(a_1,a_2,a_3,a_4,a_5)=10a_3^2+15a_2a_4+6a_1a_5\\ B_{6,3}(a_1,a_2,a_3,a_4)=15a_2^3+60a_1a_2a_3+15a_1^2a_4\\ B_{6,4}(a_1,a_2,a_3)=45a_1^2a_2^2+20a_1^3a_3\\ B_{6,5}(a_1,a_2)=15a_4a_2\\ B_{6,6}(a_1)=a_1^6\end{array}$$

# Bell polynomials, Bell numbers & number/set partitions

Bell's interest in "partition polynomials" sprang from the circumstance that they are replete with allusions to the ennumerative properties of the partitions of integers and sets. For example, let

$$N_{n,k}$$
 = number of k-part partitions of  $n$ :  $\sum_{k=1}^{n} N_{n,k} = p(n)$ 

In the case n = 5 we have

and in the case n = 6 have

$$\begin{array}{cccc} (6) & N_{6,1} = 1 \\ (1,5), (2,4), (3,3) & N_{6,2} = 3 \\ (1,1,4), (1,2,3), (2,2,2) & N_{6,3} = 3 \\ (1,1,1,3), (1,1,2,2) & N_{6,4} = 2 \\ (1,1,1,1,2) & N_{6,5} = 1 \\ (1,1,1,1,1,1) & N_{6,6} = 1 \end{array} p(6) = 11$$

Looking to the  $B_{n,k}$ -table, we see that

$$B_{n,k}$$
 = weighted sum of  $N_{n,k}$  monomials

Look in particular to the incomplete Bell polynomial

$$B_{6,2}(a_1, a_2, a_3, a_4, a_5) = 10a_3^2 + 15a_2a_4 + 6a_1a_5$$

The subscript tells Bell "Think of a set of 6 elements partitioned into 2 blocks." The  $6a_1a_5$  term says there are 6 such partitions with blocks of sizes 1 and 5; the  $15a_2a_4$  says there are 15 such partitions of sizes 2 and 4; the  $10a_3^2$  term says there are 10 such partitions with 3 blocks of size 2.9

The  $B_{n,k}$ -table supplies

$$\sum_{k=1}^{5} B_{5,k} = a_5 + (10a_2a_3 + 5a_1a_4) + (15a_1a_2^2 + 10a_2^2a_3) + 10a_1^3a_2 + a_1^5$$
$$= B_5(a_1, a_2, a_3, a_4, a_5)$$

which illustrates the general proposition that

$$B_n(a_1, a_2, \dots, a_n) = \sum_{k=1}^n B_{n,k}(a_1, a_2, \dots, a_{n-k+1})$$
(30)  
=  $\sum$  terms sorted by degreee k of homogeneity

 $<sup>^9\,</sup>$  The command SetPartitions on my computer in inoperative; I have here quoted directly from the Wikipedia article.^2

Thus do incomplete Bell polynomials sum to completion. We observe finally that

$$\sum_{k=1}^{5} (-)^{k-1} (k-1)! B_{5,k}(m_1, m_2, \dots, m_{n-k+1}) = m_5 - 1! (10m_2m_3 + 5m_1m_4) + 2! (15m_1m_2^2 + 10m_2^2m_3) - 3! (10m_1^3m_2) + 4! (m_1^5) = c_5 \text{ of } (27.2)$$

It was to achieve this illustration of (28) that I undertook this  $B_{n,k}$  digression, of which now I can't let go.

**Taylor expansion of arbitrary composite functions.** We look to the expansion (about the origin) of F(x) = f(g(x)), subject to the simplifying assumption that g(0) = 0:

$$f(x) = \sum_{n=0}^{\infty} \frac{1}{n!} b_n x^n, \qquad g(x) = \sum_{m=1}^{\infty} \frac{1}{m!} a_m x^m$$

We might on the one hand proceed from

$$F(x) = \sum_{n=0}^{\infty} \frac{1}{n!} \left[ \left( \frac{d}{dx} \right)^n f(g(x)) \right]_0 x^n \equiv \sum_{n=0}^{\infty} \frac{1}{n!} F_n x^n$$

by means of (V. F. Ivanoff's formulation of) Faà di Bruno's formula

$$\left(\frac{d}{dx}\right)^n f(g(x)) = \begin{vmatrix} g'D & g''D & g'''D & g'''D & \dots & g^{(n)}D \\ -1 & g'D & 2g''D & 3g'''D & \dots & \binom{n-1}{1}g^{(n-1)}D \\ 0 & -1 & g'D & 3g''D & \dots & \binom{n-1}{2}g^{(n-2)}D \\ 0 & 0 & -1 & g'D & \dots & \binom{n-1}{3}g^{(n-3)}D \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \dots & g'D \end{vmatrix} f(x)\Big|_{x=0}$$

where  $D^k f(x) \equiv f^{(k)}(x)$ . This gives

$$\left[ \left(\frac{d}{dx}\right)^n f(g(x)) \right]_0 = \begin{vmatrix} a_1 D & a_2 D & a_3 D & a_4 D & \dots & a_n D \\ -1 & a_1 D & 2a_2 D & 3a_3 D & \dots & \binom{n-1}{2} a_{(n-1)} D \\ 0 & -1 & a_1 D & 3a_2 D & \dots & \binom{n-1}{2} a_{(n-2)} D \\ 0 & 0 & -1 & a_1 D & \dots & \binom{n-1}{3} a_{(n-3)} D \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \dots & a_1 D \end{vmatrix} f(x) \Big|_{x=0}$$

Thus

$$F_4 = \left\{ a_4 D + (3a_2^2 + 4a_1a_3)D^2 + 6a_1^2a_2D^3 + a_1^4D^4 \right\} f(x) \Big|_{x=0}$$
  
=  $a_4 b_1 + (3a_2^2 + 4a_1a_3)b_2 + 6a_1^2a_2b_3 + a_1^4b_4$ 

14

F

# Taylor expansion of composite functions

Similarly

$$F_{3} = a_{3}b_{1} + 3a_{1}^{2}a_{2}b_{2} + a_{1}^{3}b_{3}$$

$$F_{2} = a_{2}b_{1} + a_{1}^{2}b_{2}$$

$$F_{1} = a_{1}b_{1}$$

$$F_{0} = b_{0}$$

so in  $4^{\text{th}}$  order

$$f(g(x)) = b_0 + a_1 b_1 x + \frac{1}{2!} [a_2 b_1 + a_1^2 b_2] x^2 + \frac{1}{3!} [a_3 b_1 + 3a_1^2 a_2 b_2 + a_1^3 b_3] x^3 + \frac{1}{4!} [a_4 b_1 + (3a_2^2 + 4a_1 a_3) b_2 + 6a_1^2 a_2 b_3 + a_1^4 b_4] x^4 + \cdots$$
(31)

This is precisely the result produced by the command  $Series[f(g(x)), \{x, 0, 4\}]$ .

But we might, on the other hand, proceed from

$$F(x) = \sum_{k=0}^{\infty} \frac{1}{k!} b_k [g(x)]^k$$

$$\frac{1}{k!} [g(x)]^k = \sum_{n=k}^{\infty} \frac{1}{n!} \Big[ \frac{1}{k!} \Big( \frac{d}{dx} \Big)^n [g(x)]^k \Big]_0 x^n$$

$$= \sum_{n=k}^{\infty} \frac{1}{n!} B_{n,k} (a_1, a_2, \dots, a_{n-k+1}) x^n$$

$$= \sum_{n=0}^{\infty} \frac{1}{n!} \Big\{ \sum_{k=0}^n b_k B_{n,k} (a_1, a_2, \dots, a_{n-k+1}) \Big\} x^n$$

$$= \sum_{n=0}^{\infty} \frac{1}{n!} F_n x^n$$
(32)

Taking  $B_{n,k}$  values from page 12, we again recover (31).

The incomplete Bell polynomials are doubly-indexed objects, so invite interpretaton/display as elements of an infinite-dimensional square **Bell matrix** 

$$\mathbb{B}[g] = \begin{pmatrix} 1 & 0 & 0 & 0 & \dots & 0 & \dots \\ 0 & B_{1,1} & 0 & 0 & \dots & 0 & \dots \\ 0 & B_{2,1} & B_{2,2} & 0 & \dots & 0 & \dots \\ 0 & B_{3,1} & B_{3,2} & B_{3,3} & \dots & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & B_{n,1} & B_{n,2} & B_{n,3} & \dots & B_{n,n} & \dots \\ \vdots & \vdots & \vdots & \vdots & \dots & \vdots & \ddots \end{pmatrix}$$

where the 0's (except for those in the leading column) are artifacts of the condition g(0) = 0. By (30), the elements on the  $n^{\text{th}}$  row sum to  $B_n(a_1, \ldots, a_n)$ .

Standad notational conventions make it more convenient/natural to in place of (32) write

$$F(x) = \sum_{n=0}^{\infty} \left\{ \sum_{k=0}^{n} b_k C_{k,n}(a_1, a_2, \dots, a_{n-k+1}) \right\} x^n$$
$$C_{k,n} = B_{n,k}$$

and in place of the Bell matrix to introduce the Carleman matrix  $^{10}$ 

$$\mathbb{M}[g] = \begin{pmatrix} 1 & 0 & 0 & 0 & \dots & 0 & \dots \\ 0 & C_{1,1} & C_{1,2} & C_{1,3} & \dots & C_{1,n} & \dots \\ 0 & 0 & C_{2,2} & C_{2,3} & \dots & C_{2,n} & \dots \\ 0 & 0 & 0 & C_{3,3} & \dots & C_{3,n} & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \dots & C_{n,n} & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \end{pmatrix}$$

Writing

$$oldsymbol{x} = egin{pmatrix} 1 \ x \ x^2 \ x^3 \ dots \end{pmatrix}$$

we in this notation have

$$\mathbb{M}[g]\boldsymbol{x} = \text{ Taylor expansion of } \boldsymbol{g}(x) \equiv \begin{pmatrix} 1 \\ [g(x)]^1 \\ [g(x)]^2 \\ [g(x)]^3 \\ \vdots \end{pmatrix}$$

and so have—again in agreement with (31)—

Expansion of 
$$F(x) \equiv f(g(x)) = \boldsymbol{b}^{\mathsf{T}} \boldsymbol{g}(x) = \boldsymbol{b}^{\mathsf{T}} \mathbb{M}[g] \boldsymbol{x}$$

where  $\boldsymbol{b}^{\mathsf{T}} = \left(\frac{1}{0!}b_0, \frac{1}{1!}b_1\frac{1}{2!}b_2, \frac{1}{3!}b_3, \dots\right)$ . If

$$e(x) = \sum_{n=0}^{\infty} \frac{1}{n!} c_n x^n, \qquad f(x) = \sum_{m=1}^{\infty} \frac{1}{m!} b_m x^m, \qquad g(x) = \sum_{m=1}^{\infty} \frac{1}{m!} a_m x^m$$

then that same line of argument gives

$$e(f(g(x))) = \boldsymbol{e}^{\mathsf{T}} \mathbb{M}[f] \mathbb{M}[g] \boldsymbol{x}$$

 $<sup>^{10}</sup>$  Torsten Carlman (1892–1949) was a Swedish mathematician who made important contributions also to fundamental physics (ergodic theory, kinetic theory of gases).

#### Application to quantum perturbation theory

**Perturbed energy spectra of simple quantum systems.** Nearly twenty years ago I described in a series of three papers<sup>10</sup> how formulae of the type

$$E_n(\lambda) = E_{n,0} + \lambda E_{n,1} + \lambda^2 E_{n,2} + \cdots$$

could be constructed (and carried to high order) without the usual reference<sup>11</sup> to perturbed eigenfunctions  $|n\rangle_{\lambda} = |n,0\rangle + \lambda |n,1\rangle + \lambda^2 |n,2\rangle + \cdots$ , which are tedious to develop, and usually of no physical interest. Earlier experience<sup>4</sup> made me aware as I wrote that Bell polynomials lurked in the wings, but did not pursue that connection. Which is what I propose to do here.

We study systems of the form  $\mathbf{H} = \mathbf{H}_0 + \lambda \mathbf{V}$ , which in finite-dimensional cases are described by hermitian matrices  $\mathbb{H} = \mathbb{H}_0 + \lambda \mathbb{V}$ , where in the unperturbed basis  $\mathbb{H}_0$  is diagonal. We will assume the unperturbed spectrum to be nondegenerate.

# SIMPLE DETERMINENTAL APPROACHES

In the 2-dimensional case we seek the solutions  $\{E_1,E_2\}$  of the quadratic chacteristic polynomial

$$\det\left[\begin{pmatrix} e_1 & 0\\ 0 & e_2 \end{pmatrix} + \lambda \begin{pmatrix} v_{11} & v_{12}\\ v_{21} & v_{22} \end{pmatrix} - w \begin{pmatrix} 1 & 0\\ 0 & 1 \end{pmatrix}\right] = 0$$
(33)

which are

$$w = \frac{1}{2} \left\{ \begin{bmatrix} e_1 + e_2 + \lambda(v_{11} + v_{22}) \end{bmatrix} \\ \pm \begin{bmatrix} [e_1 + e_2 + \lambda(v_{11} + v_{22})]^2 \\ -4[e_1e_2 + \lambda(e_1v_{22} + e_2v_{11}) + \lambda^2(v_{11}v_{22} - v_{12}v_{21})] \end{bmatrix}^{\frac{1}{2}} \right\}$$

Expansion in powers of  $\lambda$  gives

$$w = \begin{cases} e_1 + \lambda v_{11} + \lambda^2 \frac{v_{12}v_{21}}{e_1 - e_2} - \lambda^3 \frac{v_{12}v_{21}(v_{11} - v_{22})}{(e_1 - e_2)^2} + \cdots \\ e_2 + \lambda v_{22} - \lambda^2 \frac{v_{12}v_{21}}{e_1 - e_2} + \lambda^3 \frac{v_{12}v_{21}(v_{11} - v_{22})}{(e_1 - e_2)^2} + \cdots \end{cases}$$
(34)

This simple argument has led to results that already capture characteristic

 $<sup>^{10}</sup>$   $[\mathbf{1}]$  "Perturbed spectra without (it says here) pain," (April, 2000);

<sup>[2] &</sup>quot;Higher-order spectral perturbation by a new determinental method," (September, 2000);

<sup>[3] &</sup>quot;Stark essentials of the determinental approach to time-independent spectral perturbation theory," (October, 2000).

<sup>&</sup>lt;sup>11</sup> See, for example, David Griffith & Darrell Schroeter, Introduction to Quantum Mechanics (3<sup>rd</sup> edition, 2018), pages 279–285.

features of the general case, but suffers from the defect that it is inapplicable to higher-dimensional systems, for it requires one to construct symbolic descriptions of the roots of polynomials of ascending degree, which is awkward for cubics and quartics, and impossible for degree (dimension)  $n \ge 5$ .

To circumvent this difficulty we at (33) write  $w_0 + \lambda w_1 + \lambda^2 w_2 + \lambda^3 w_3 + \cdots$ in place of w and by expansion obtain an equation of the form

$$W(w_0) + \lambda W(w_0, w_1) + \lambda^2 W(w_0, w_1, w_2) + \lambda^3 W(w_0, w_1, w_2, w_3) + \lambda^4 W(w_0, w_1, w_2, w_3, w_4) + \cdots 0$$
(35)

with

$$\begin{split} W(w_0) &= e_1 e_2 - (e_1 + e_2) w_0 + w_0^2 = (w_0 - e_1)(w_0 - e_2) \\ W(w_0, w_1) &= e_1 v_{22} + e_2 v_{11} - (v_{11} + v_{22}) w_0 - (e_1 + e_2) w_1 + 2 w_0 w_1 \\ W(w_0, w_1, w_2) &= (v_{11} v_{22} - v_{12} v_{21}) - (v_{11} + v_{22}) w_1 + w_1^2 \\ &- (e_1 + e_2) w_2 + 2 w_0 w_2 \\ W(w_0, w_1, w_2, w_3) &= -(v_{11} + v_{22}) w_2 + 2 w_1 w_2 - (e_1 + e_2) w_3 + 2 w_0 w_3 \\ &\vdots \end{split}$$

From

$$W(w_0) = 0 \implies w_0 = e_1 \text{ else } w_0 = e_2$$

the argument is seen to have bifurcated. Pick a branch by (say) setting  $w_0 = e_1$ . Then, proceeding recursively,

$$W(w_0, w_1) = 0 \implies w_1 = v_{11}$$

$$W(w_0, w_1, w_2) = 0 \implies w_2 = \frac{v_{12}v_{21}}{e_1 - e_2}$$

$$W(w_0, w_1, w_2, w_3) = 0 \implies w_3 = -\frac{v_{12}v_{21}(v_{11} - v_{22})}{(e_1 - e_2)^2}$$

—in precise agreement with (34). Simple *Mathematica* commands permit the argument very easily to be carried to much higher order. No polynomials of high degree are encountered, except trivially in 0<sup>th</sup> order; at each iteration the unknown enters linearly. And the argument works in any dimension. The method is susceptible only to the criticism that it leads to results in which the components of  $\mathbb{V}$  are not packaged in natural (unitarily invariant) ways.

#### BELLY DETERMINENTAL METHODS

We look first to how Bell polynomials enter into the discussion. We have interest in the (perturbed) roots of the the polynomial  $det(w\mathbb{I} - \mathbb{H}) : \mathbb{H} = \mathbb{H}_0 + \lambda \mathbb{V}$ . In the *n*-dimensional case we have

$$\det(w\mathbb{I} - \mathbb{H}) = w^n \det(\mathbb{I} - x\mathbb{H}) \quad : \quad x \equiv w^{-1}$$

# Application to quantum perturbation theory

and—as was remarked already at (1)—

$$det(\mathbb{I} - x\mathbb{H}) = \exp\left\{ tr \log(\mathbb{I} - x\mathbb{H}) \right\}$$
  
= exp \{ - T\_1 x - \frac{1}{2}T\_2 x^2 - \frac{1}{3}T\_3 x^3 - \frac{1}{4}T\_4 x^4 - \cdots \}

where again,  $T_k = \operatorname{tr} \mathbb{H}^k$ . But it was seen at (15) that

$$\exp\left\{b_1x + \frac{1}{2!}b_2x^2 + \frac{1}{3!}b_3x^3 + \frac{1}{4!}b_4x^4 + \cdots\right\} = 1 + \frac{1}{1!}B_1(b_1)x^1 \\ + \frac{1}{2!}B_2(b_1, b_2)x^2 \\ + \frac{1}{3!}B_3(b_1, b_2, b_3)x^3 \\ + \frac{1}{4!}B_4(b_1, b_2, b_3, b_4)x^4$$

so setting

$$b_1 = -T_1, b_2 = -T_2, b_3 = -2!T_3, \dots, b_k = -(k-1)!T_k, \dots$$

we have

$$det(\mathbb{I} - x \mathbb{H}) = 1 + \frac{1}{1!} B_1(-T_1) x^1 + \frac{1}{2!} B_2(-T_1, -T_2) x^2 + \frac{1}{3!} B_3(-T_1, -T_2, -2T_3) x^3 + \frac{1}{4!} B_4(-T_1, -T_2, -2T_3, -3T_4) x^4$$

which (by the Cayley-Hamilton theorem) terminates at order=dimension n, giving

$$det(w\mathbb{I} - \mathbb{H}) = w^{n} + \frac{1}{1!}B_{1}(-T_{1})w^{n-1} + \frac{1}{2!}B_{2}(-T_{1}, -T_{2})w^{n-2} + \frac{1}{3!}B_{3}(-T_{1}, -T_{2}, -2T_{3})w^{n-3} + \frac{1}{4!}B_{4}(-T_{1}, -T_{2}, -2T_{3}, -3T_{4})w^{n-4} \vdots + \frac{1}{n!}B_{n}(-T_{1}, -T_{2}, -2T_{3}, \dots, -(n-1)T_{n})w^{0} = 0$$
(36)

In the 2-dimensional case this—by (16)—gives

$$\det(w\mathbb{I} - \mathbb{H}) = w^2 - T_1 w + \frac{1}{2!}(T_1^2 - T_2)$$
(37.2)

When we make the replacement  $w \to w_0 + \lambda w_1 + \lambda^2 w_2 + \lambda^3 w_3 + \cdots$  and expand in powers of  $\lambda$  we recover (34), and so are led recursively back again to the familiar results.

It is important to note that (37.2) pertains only to 2-state systems. For 3-state systems, bring  $B_3(a_1, a_2, a_3) = a_1^3 + 3a_1a_2 + a_3$  to (35) and obtain

$$\det(w\mathbb{I} - \mathbb{H}) = w^3 - T_1 w^2 + \frac{1}{2!} (T_1^2 - T_2) w + \frac{1}{3!} (-T_1^3 + 3T_1 T_2 - 2T_3)$$
(37.3)

Such expressions are assembled from powers of traces of powers of  $\mathbb{H} = \mathbb{H}_0 + \lambda \mathbb{V}$ . From fundamental properties if the trace

$$\operatorname{tr}(\mathbb{X} + \mathbb{Y}) = \operatorname{tr}\mathbb{X} + \operatorname{tr}\mathbb{Y}, \qquad \operatorname{tr}\mathbb{X}\mathbb{Y} = \operatorname{tr}\mathbb{Y}\mathbb{X}$$

one has

$$\mathrm{tr}(\mathbb{X}+\mathbb{Y})^2 = \mathrm{tr}(\mathbb{X}\mathbb{X}+\mathbb{X}\mathbb{Y}+\mathbb{Y}\mathbb{X}+\mathbb{Y}\mathbb{Y}) = \mathrm{tr}\mathbb{X}^2 + 2\mathrm{tr}\mathbb{X}\mathbb{Y} + \mathrm{tr}\mathbb{Y}^2$$

and more generally

$$\operatorname{tr}(\mathbb{X} + \mathbb{Y})^n = \sum_{k=0}^n \binom{n}{k} \operatorname{tr}(\mathbb{X}^{n-k} \mathbb{Y}^k)$$

even when X and Y fail to commute. In particular, we have

$$\operatorname{tr} \mathbb{H}^{n} = \operatorname{tr}(\mathbb{H}_{0} + \lambda \mathbb{V})^{n} = \sum_{k=0}^{n} \binom{n}{k} \operatorname{tr}(\mathbb{H}_{0}^{n-k} \mathbb{V}^{k}) \lambda^{k}$$

which could be used to develop the explicit  $\lambda$ -dependence of the expressions that appear on the right side of (37). But the result after the replacement  $w \rightarrow w_0 + \lambda w_1 + \lambda^2 w_2 + \lambda^3 w_3 + \cdots$  is an ugly (unitarily invariant) mess. And ultimately useless, since our objective is to construct a description of the perturbed roots of det $(w\mathbb{I} - \mathbb{H}) = 0$ , and to that end must sooner or later (better sooner than later) abandon trace-wise formalism in favor of the element-wise formalism encountered already on page 18, allowing all of the complicated details to remain hidden in the mind of *Mathematica*.

In short: the Bell-based equations (36) have led efficiently to construction of equations of the form (37), but are otherwise of no practical utility.

**Integer/set partitions, multinomial coefficients & Bell.** All of the ingredients in that cocktail have played roles in the preceding discussion. I undertake here to make explicit, by means of examples, their interconnections.

In the expanded product

$$(a+b+c)^4 = (a^4+b^4+c^4) + 4(a^3b+a^3c+ab^3+b^3c+ac^3+bc^3) + 6(a^2b^2+a^2b^2+b^2c^2) + 12(a^2bc+ab^2c+abc^2)$$
(38)

we encounter 4<sup>th</sup>-order terms of four types:  $\{x^4, x^3y, x^2y^2, x^2yz\}$ . Multinomial coefficients are defined

$$\begin{aligned} \text{Multinomial} [n_1, n_2, \cdots, n_k] &= \frac{(n_1 + n_2 + \cdots + n_k)!}{n_1! n_2! \cdots n_k!} \\ &= \# \text{Permutations} [\underbrace{a, a, \dots, a}_{n_1}, \underbrace{b, b, \dots, b}_{n_2}, \cdots, \underbrace{s, s, \dots, s}_{n_k}] \end{aligned}$$

where **#Permutations** refers to the number of *distinct* permutations of the

# Integer/set partitions, multinomial coefficients & Bell

symbols in question. The coefficients in (38) are multinomial coefficients. Specifically,

```
terms of type x^4 have coefficient

Multinomial[1] = #Permutations[x, x, x, x] = 1

terms of type x^3y have coefficient

Multinomial[3,1] = #Permutations[x, x, x, y] = 4

terms of type x^2y^2 have coefficient

Multinomial[2,2] = #Permutations[x, x, y, y] = 6

terms of type x^2yz have coefficient

Multinomial[2,1,1] = #Permutations[x, x, y, z] = 12
```

So much for the coefficients that appear in  $(a_1 + a_2 + \cdots + a_m)^N$ . How many terms appear in the expansion of such a product? Classify the terms

 $a_1^{n_1}a_2^{n_2}\cdots a_m^{n_m}$  :  $n_1+n_2+\cdots+n_m=N$ 

by the number of 0's that appear among the exponents, a number which ranges on  $\{0, 1, 2, \ldots, m-1\}$ . The exponents  $\{n_1, n_2, \ldots, n_m\}$  refer to a partition of N. A list of the partitions of N into p parts  $(p = 1, 2, \ldots, m)$  is produced by the command IntegerPartitions  $[m, \{p\}]$ . Pad each such partition with enough 0's to produce m-element sets, and count the number of distinct permutations of each such set. I illustrate the procedure as it pertains to our example (38), where m = 3, N = 4:

```
# terms of type x^4:

IntegerPartitions [4, \{1\}] \rightarrow \{4\}

#Permutations [\{4, 0, 0\}] = 3

# terms of types x^3y and x^2y^2:

IntegerPartitions [4, \{2\}] \rightarrow \{3, 1\}, \{2, 2\}

#Permutations [\{3, 1, 0\}] = 6

#Permutations [\{2, 2, 0\}] = 3

# terms of type x^2yz:

IntegerPartitions [4, \{3\}] \rightarrow \{2, 1, 1\}

#Permutations [\{2, 1, 1\}] = 3
```

We note that 3 + 6 + 3 + 3 = 15 is indeed the number of terms in (38).

Return  $\mathrm{now}^{12}$  to the ennumerative properties of Bell polynomials, looking specifically to the case

$$B_{6,2}(a_1, a_2, a_3, a_4, a_5) = 6a_1a_5 + 15a_2a_4 + 10a_3^2$$
(39)

<sup>&</sup>lt;sup>12</sup> See again page 13.

that is produced by the command BellY[6, 2,  $\{a_1, a_2, a_3, a_4, a_5\}$ ]. From (39) we see that  $B_{6,2}$  is a multinomial of degree 6 in 5 variables. We are informed by *Mathematica* that Multinomial  $[n_1, n_2, \ldots, n_m]$  gives "the number of ways of partitioning  $N = n_1 + n_2 + \cdots + n_m$  into blocks of sizes  $\{n_1, n_2, \ldots, n_m\}$ ," in short: that multinomial coefficients ennumerate set partitions. Looking in this light to the  $B_{6,2}$  of (39), we find that

Multinomial 
$$[1,5] = 6$$
  
Multinomial  $[2,4] = 15$ 

as anticipated, but

$$Multinomial[3,3] = 20$$

which is twice the anticipated 10. To see how that comes about (what went wrong) we list the set partitions in question:

SetPartitions[1,5] = 
$$\begin{cases} (a)(bbbbb) & \# = 1 \times 1\\ (b)\langle abbbb \rangle & \# = 1 \times 5 \end{cases}$$
 Total = 6

where  $\langle \bullet \rangle \equiv$  "all permutations of  $\bullet$ ". Similarly

$$\texttt{SetPartitions[2,4]} = \begin{cases} (aa)(bbbb) & \# = 1 \times 1 \\ \langle ab \rangle \langle abbb \rangle & \# = 2 \times 4 \\ (bb) \langle aabb \rangle & \# = 1 \times 6 \end{cases} \text{Total} = 15$$

and

$$\texttt{SetPartitions[3,3]} = \begin{cases} (aaa)(bbb) & \# = 1 \times 1 \\ \langle aab \rangle \langle abb \rangle & \# = 3 \times 3 \\ \langle abb \rangle \langle aab \rangle & \# = 3 \times 3 \\ (bbb)(aaa) & \# = 1 \times 1 \end{cases} \quad \text{Total} = 20$$

But here the last pair of set partitions is redundant with (a mere reordering of) the first pair, so the 20 reduces to 10 when we speak of *distinct* set partitions.

 $B_{n,k}$  inherits its terms from IntegerPartitions  $[n, \{k\}]$ , the respective partitions of n into k parts, where k = 1, 2, ..., n. So

 $B_{n,k}$  is a sum of #IntegerPartitions[ $n, \{k\}$ ] many terms

It is instructive from several points of view to look to the case

$$B_{8,5}(a_1, a_2, a_3, a_4) = 70a_1^4a_4 + 560a_1^3a_2a_3 + 420a_1^2a_2^3 \tag{40}$$

which springs from

$$\texttt{IntegerPartitions[8, {5}]} = \begin{cases} \{1, 1, 1, 1, 4\} \\ \{1, 1, 1, 2, 3\} \\ \{1, 1, 2, 2, 2\} \end{cases}$$

# Some Bell-inspired quantum dynamical remarks

There are 3 such partitions, so  $B_{8,5}$  is a sum of 3 terms. We have

Multinomial[1,1,1,1,4] = 1680

and observe that

$$\frac{1680}{(\text{number of 1-repeats})!} = \frac{1680}{4!} = 70$$

Similarly

$$\frac{\text{Multinomial}[1,1,1,2,3] = 3360}{(\text{number of 1-repeats})!} = \frac{3360}{3!} = 560$$

and

$$\frac{\text{Multinomial}[1,1,2,2,2] = 5040}{5040}$$
  
(number of 1-repeats)!(number of 2-repeats)! =  $\frac{3360}{2!3!} = 420$ 

Thus have we recovered the coefficients that appear in (40) and—more generally —demonstrated how number of distinct set partitions can be extracted from multinomial coefficients. We have, moreover, shown how incomplete Bell polynomials  $B_{n,k}(\mathbf{a})$  can be constructed *ab initio*, without recourse to the **BellY** command. This construction shows why  $B_{n,k}(\mathbf{a})$  is homogenious of degree k and on which of the variables  $\mathbf{a} = \{a_1, a_2, \ldots, a_n\}$  each of its terms depends. From

$$IntegerPartitions[n] = \bigcup_{k=1}^{n} IntegerPartitions[n, \{k\}]$$

we recover (30), and see why  $B_n(\boldsymbol{a})$  is a sum of p(n) terms.

Some Bell-inspired quantum dynamical remarks. By way of orientation: Quantum kinematics springs (in the Schrödinger picture) from the assumption that the motion of states  $|\psi\rangle$  is linear and norm-preserving; in short, unitary:

$$\psi_{0} \longrightarrow |\psi_{t} = \mathbf{U}(t)|\psi_{0}$$
 :  $\mathbf{U}^{+}(t)\mathbf{U}(t) = \mathbf{I}$ 

Writing  $\partial \equiv \frac{d}{dt}$ , and **U** for  $\mathbf{U}(t)$ ,  $|\psi\rangle$  for  $|\psi\rangle_t$  when no confusion can result, we have

$$\partial |\psi\rangle_t = (\partial \mathbf{U}) \mathbf{U}^+ |\psi\rangle_t \tag{41.1}$$

From  $\partial(\mathbf{U}\mathbf{U}^+) = (\partial\mathbf{U})\mathbf{U}^+ + \mathbf{U}(\partial\mathbf{U}^+) = (\partial\mathbf{U})\mathbf{U}^+ + [(\partial\mathbf{U})\mathbf{U}^+]^+ = \partial\mathbf{I} = \mathbf{0}$  we see that  $(\partial\mathbf{U})\mathbf{U}^+$  is antiself-adjoint (the negative of its adjoint). Therefore

$$i(\partial \mathbf{U})\mathbf{U}^+ \equiv \mathbf{K}(t)$$
 is self-adjoint (41.2)

and (41.1) assumes the form

$$i\partial|\psi\rangle = \mathbf{K}(t)|\psi\rangle$$
 equivalently  $i\partial(\psi| = -(\psi|\mathbf{K}(t))$  (41.3)

Observables are represented by self-adjoint operators A, the construction of which typically isn't—but in the general case might be—time-dependent. Fundamental to the theory is the assumption that observables reveal themselves only *via* their statistical properties, principally their expectation values

$$\langle \mathbf{A} \rangle_{\psi} \equiv (\psi | \mathbf{A} | \psi) \tag{41.4}$$

To describe differentially the kinematic motion of expectation values, we have

$$\partial \langle \mathbf{A} \rangle_{\psi} = i(\psi | \mathbf{K} \mathbf{A} | \psi) - i(\psi | \mathbf{A} \mathbf{K} | \psi) + (\psi | \partial \mathbf{A} | \psi)$$
  
=  $(\psi | i[\mathbf{K}, \mathbf{A}] | \psi) + (\psi | \partial \mathbf{A} | \psi)$  (41.5)  
=  $(\psi | i[\mathbf{K}, \mathbf{A}] | \psi)$  for time-independent observables

where [K, A] denotes the commutator KA - AK. The integrated motion is described (her again  $U \equiv U(t)$  and we assume  $\partial A = 0$ )

$$\langle \mathbf{A} \rangle_{\psi}(t) = (\psi_0 | \mathbf{U}^+ \mathbf{A} \mathbf{U} | \psi_0)$$
(41.6)

which in the SCHRÖDINGER PICTURE we attribute to

$$\psi_{0} \longrightarrow |\psi_{t} = \mathbf{U}|\psi_{0}$$

$$\mathbf{A}_{0} \longrightarrow \mathbf{A}_{t} = \mathbf{A}_{0}$$
(41.71)

and in the HEISENBERG PICTURE to

$$\begin{aligned} |\psi\rangle_0 &\longrightarrow |\psi\rangle_t = |\psi\rangle_0 \\ \mathbf{A}_0 &\longrightarrow \mathbf{A}_t = \mathbf{U}^+ \mathbf{A}_0 \mathbf{U} \end{aligned}$$
(41.72)

In the former the burden of motion is born entirely by the state, in the latter entirely by the observable. There exist, however, an infinitude of intermediate pictures in which the burden is shared. Writing

$$\langle \mathbf{A} \rangle_{\psi}(t) = (\psi_0 | \mathbf{U}^+ \mathbf{W} \cdot \mathbf{W}^+ \mathbf{A} \mathbf{W} \cdot \mathbf{W}^+ \mathbf{U} | \psi_0)$$

where  $\mathbf{W}(t)$  is an arbitrarily time-dependent unitary operator, we have

$$\begin{aligned} |\psi\rangle_0 &\longrightarrow |\psi\rangle_t = \mathbf{W}^+ \mathbf{U} |\psi\rangle_0 \\ \mathbf{A}_0 &\longrightarrow \mathbf{A}_t = \mathbf{W}^+ \mathbf{A}_0 \mathbf{W} \end{aligned}$$
(41.73)

Quantum dynamics emerges from quantum kinematics when we associate  $\mathbf{K}(t)$  with the Hamiltonian  $\mathbf{H}$ —usually (as below) taken to be time-independent —of the mechanical system in question.<sup>13</sup> In that notation (41.2) reads

$$i\partial \mathbf{U} = (1/\hbar)\mathbf{H}\mathbf{U} \implies \mathbf{U}(t) = e^{-(i/\hbar)\mathbf{H}t}$$
 (42)

and the Schrödinger equation (41.3) becomes

$$i\hbar\partial|\psi\rangle = \mathbf{H}|\psi\rangle \tag{43}$$

Equivalently—and advantageously, since the initial condition is now explicit—

$$|\psi\rangle_t = e^{-(i/\hbar)\mathbf{H}t}|\psi\rangle_0 \tag{44}$$

$$= |\psi\rangle_0 - (i/\hbar) \int_0^t \mathbf{H} |\psi\rangle_\tau d\tau \tag{45}$$

<sup>&</sup>lt;sup>13</sup> For dimensional reasons the association actually reads  $\mathsf{K} \longleftrightarrow \frac{1}{\hbar}\mathsf{H}$ .

#### Some Bell-inspired quantum dynamical remarks

Equation (41.5) has become

$$\partial \langle \mathbf{H} \rangle_{\psi} = (\psi | i [\mathbf{H}, \mathbf{H}] | \psi) = 0 \quad : \quad \text{all } | \psi )$$

which announces energy conservation. We note in passing that

$$e^{-(i/\hbar)\mathbf{H}t} = \lim_{N \to \infty} \sum_{n=0}^{N} \frac{1}{n!} \left[ -(i/\hbar)\mathbf{H}t \right]^n$$

is unitary only in the limit.

Suppose the (time-independent) Hamiltonian to have the perturbed structure  $\mathbf{H} + \lambda \mathbf{V}$  with  $[\mathbf{H}, \mathbf{V}] \neq \mathbf{0}$ . Here we encounter an instance of

$$e^{\mathbf{A}+\mathbf{B}} = \mathbf{I} + (\mathbf{A} + \mathbf{B})$$
  
+  $\frac{1}{2!}(\mathbf{A}\mathbf{A} + \mathbf{A}\mathbf{B} + \mathbf{B}\mathbf{A} + \mathbf{B}\mathbf{B})$   
+  $\frac{1}{3!}(\mathbf{A}\mathbf{A}\mathbf{A} + \mathbf{A}\mathbf{A}\mathbf{B} + \mathbf{A}\mathbf{B}\mathbf{A} + \mathbf{B}\mathbf{A}\mathbf{A}$   
+  $\mathbf{B}\mathbf{B}\mathbf{A} + \mathbf{B}\mathbf{A}\mathbf{B} + \mathbf{A}\mathbf{B}\mathbf{B} + \mathbf{B}\mathbf{B}\mathbf{B}) + \cdots$ 

which is clearly unworkable. Campbell-Baker-Hausdorff theory  $^{14}$  supplies this unpublished result due to Hans Zassenhaus:

$$e^{\mathbf{A}+\mathbf{B}} = e^{\mathbf{A}}e^{\mathbf{B}}e^{\mathbf{C}_2}e^{\mathbf{C}_3}\cdots$$

where

$$C_{2} = -\frac{1}{2}[A, B]$$
  

$$C_{3} = \frac{1}{6}[A, [A, B]] + \frac{1}{3}[B, [A, B]]$$
  
:

 $\mathsf{C}_n = \operatorname{recursively}$  defined linear combination of nested commutators

This can be very useful when nested commutators of low order vanish (as do  $[\mathbf{x}, [\mathbf{x}, \mathbf{p}]]$  and  $[\mathbf{p}, [\mathbf{x}, \mathbf{p}]]$ ), but is again usually of little use. A more effective way to deal with this problem is to work in the INTERACTION PICTURE, which was devised by Dirac in 1926 and is the special instnce of (41.73) that results from setting  $\mathbf{W} = \exp\{-(i/\hbar)\mathbf{H}t\}$ . Then observables move as they would in the Heisenberg picture under the V-independent action of H; only the motion of states is V-dependent (and would cease in the case  $\mathbf{V} = \mathbf{0}$ ): working from

$$|\psi\rangle_0 \longrightarrow |\Psi\rangle_t = e^{(i/\hbar)\,\mathsf{H}\,t} e^{-(i/\hbar)(\mathsf{H}+\lambda\mathsf{V})t} |\psi\rangle_0 \tag{46}$$

where the  $|\Psi\rangle$ -notation reflects the fact that  $|\psi\rangle_t$  and  $|\Psi\rangle_t$  have evolved by

 $<sup>^{14}</sup>$  For a survey, see NEW Chapter 0, pages 30–34 of my Quantum Notes (2000).

distinct unitary transformations from the same initial state  $|\psi\rangle_0 = |\Psi\rangle_0$ , we have

$$i\hbar\partial|\Psi\rangle_{t} = e^{(i/\hbar)\mathsf{H}t} \{-\mathsf{H} + (\mathsf{H} + \lambda\mathsf{V})e^{-(i/\hbar)(\mathsf{H}+\mathsf{V})t}|\Psi\rangle_{0}$$
  
$$= \lambda e^{(i/\hbar)\mathsf{H}t} \mathsf{V}\mathsf{I} e^{-(i/\hbar)(\mathsf{H}+\mathsf{V})t}|\Psi\rangle_{0}$$
  
$$\mathsf{I} = e^{-(i/\hbar)\mathsf{H}t} \cdot e^{(i/\hbar)\mathsf{H}t}$$
  
$$= \lambda \mathsf{V}(t)|\Psi\rangle_{t}$$
(47.1)

with

$$\mathbf{V}(t) = e^{(i/\hbar)\,\mathbf{H}\,t}\,\mathbf{V}e^{-(i/\hbar)\,\mathbf{H}\,t} \tag{47.2}$$

According to (47.1),  $|\Psi\rangle_t$  moves as it would in the Schrödinger picture under action of the small time-dependent Hamiltonian  $\lambda \mathbf{V}(t)$ .

Equations (47) present two challenging problems: (i) effective construction of  $\mathbf{V}(t)$  and—once such a construction is in hand—(ii) solution of (47.1). A formal (meaning if we set aside convergence considerations) solution of (47.1) springs from the observation that when formulated as an integral equation

$$|\Psi)_t = |\Psi)_0 + \omega \int_0^t \mathbf{V}(t_1) |\Psi)_{t_1} dt_1 \quad : \quad \omega = \lambda/i\hbar$$
(48)

it invites solution by iteration:

$$\begin{split} |\Psi)_t &= |\Psi)_0 + \omega \int_0^t \mathbf{V}(t_1) |\Psi)_0 dt_1 \\ &+ \omega^2 \int_0^t \int_0^{t_1} \mathbf{V}(t_1) \mathbf{V}(t_2) |\Psi)_0 dt_1 dt_2 \\ &+ \omega^3 \int_0^t \int_0^{t_1} \int_0^{t_2} \mathbf{V}(t_1) \mathbf{V}(t_2) \mathbf{V}(t_3) |\Psi)_0 dt_1 dt_2 dt_3 + \cdots \end{split}$$

In the last integral we have  $t \ge t_1 \ge t_2 \ge t_3$ . Noting that  $t \ge \{t_1, t_2, t_3\} \ge 0$  can stand in 3! such relationships, and writing

$$\mathcal{P}[\mathbf{A}(t_1)\mathbf{B}(t_2)] = \begin{cases} \mathbf{A}(t_1)\mathbf{B}(t_2) & \text{if } t_1 > t_2 \\ \mathbf{B}(t_2)\mathbf{A}(t_1) & \text{if } t_1 < t_2 \end{cases}$$

to illustrate the action of the "chronological ordering operator"  $\mathcal{P}$ , we can write

$$|\Psi\rangle_{t} = \left\{ \mathbf{I} + \frac{1}{1!}\omega \int_{0}^{t} \mathcal{P}[\mathbf{V}(t_{1})] dt_{1} + \frac{1}{2!}\omega^{2} \int_{0}^{t} \int_{0}^{t} \mathcal{P}[\mathbf{V}(t_{1})\mathbf{V}(t_{2})] dt_{1} dt_{2} + \frac{1}{3!}\omega^{3} \int_{0}^{t} \int_{0}^{t} \int_{0}^{t} \mathcal{P}[\mathbf{V}(t_{1})\mathbf{V}(t_{2})\mathbf{V}(t_{3})] dt_{1} dt_{2} dt_{3} + \cdots \right\} |\Psi\rangle_{0}$$

$$(49.1)$$

#### Some Bell-inspired quantum dynamical remarks

of which "Dyson's formula"

$$|\Psi\rangle_t = \mathcal{P}\left[e^{\omega \int_0^t \mathbf{V}(\tau) d\tau}\right] |\Psi\rangle_0 \tag{49.2}$$

provides an elegant abbreviation.<sup>15</sup>

Let Dyson's (49.1) be written

$$\begin{split} |\Psi\rangle_t &= \big\{ \mathbf{I} + \frac{1}{1!} \omega \mathbf{a}_1 + \frac{1}{2!} \omega^2 \mathbf{a}_2 + \frac{1}{3!} \omega^3 \mathbf{a}_3 + \cdots \big\} |\Psi\rangle_0 \\ &= \big\{ \mathbf{I} + \mathbf{T}(t) \big\} |\Psi\rangle_0 \end{split}$$

where the **a**-notation is intended to emphasize that the objects in question are **operator-valued** and  $\{\mathbf{I} + \mathbf{T}(t)\}$  is a *t*-dependent unitary operator. With (20) in mind we are tempted to write

$$\mathbf{T} = \exp\left\{\sum_{k=1}^{\infty} \frac{1}{k!} \mathbf{a}_k \omega^k\right\} = \sum_{n=0}^{\infty} \frac{1}{n!} B_n(\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_n) \omega^n$$
(50.1)

To what practical purpose I do not know...except to say that in this analog

$$B_n(\mathbf{a}_1, \mathbf{a}_2, \dots \mathbf{a}_n) = \sum_{k=1}^n B_{n,k}(\mathbf{a}_1, \mathbf{a}_2, \dots \mathbf{a}_{n-k+1})$$
(50.2)

of (30) I smell classification of the Feynman diagrams of any given order. But the faciful equations (50) are nonsense as they stand: Bell polynomials spring

$$\frac{d}{dt}x(t) = V(t)x(t) \implies x(t) = e^{\int_0^t V(\tau) d\tau} x(0)$$

"Dyson's formula" acquired it's name from the prominent role it plays in his seminal "The radiation theories of Tomonga, Schwinger and Feynman," Phys. Rev. **75**, 486–502 (1949), reproduced in *Selected Papers of Freeman Dyson,* with Commentary (1996). The relevant commentary appears on pages 10–14. Working within the context provided by QED, Dyson shows (§V) how to extract from (49.2) Schwinger's "Green Functions" and Feynman's "Propagators," which latter can be formulated as "sums over paths." In his §VII he recovers Feynman's graphical representation of matrix elements (Feynman diagrams, but draws none of them). For carefully detailed discussion of (mainly) other approches to time-dependent quantum perturbation theory, see Chapter 11 in Griffiths & Schroeter.<sup>11</sup>

<sup>&</sup>lt;sup>15</sup> HISTORICAL NOTE: Finite-dimensional linear systems  $\dot{\boldsymbol{x}}(t) = \mathbb{V}(t)\boldsymbol{x}(t)$  have been studied for centuries (Joseph Lagrange(1736–1813), Józef Wronski (1776– 1853)) and occur in a great many pure/applied contexts. In one dimension

(*via* integer/set partitions) from the theory of multinomial coefficients, and in that the presumption is that all variables commute. Look again to the discussion of

$$B_{8,5}(a_1, a_2, a_3, a_4) = 70a_1^4a_4 + 560a_1^3a_2a_3 + 420a_1^2a_2^3 \tag{40}$$

that was presented on pages 22/23. To assign meaning to  $B_{8,5}(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3, \mathbf{a}_4)$  in cases where the **a**-variables fail to commute we might expect to

replace  $a_1^4 a_4$  with the sum of the 5 permuted products of  $\{a_1, a_1, a_1, a_1, a_4\}$ replace  $a_1^3 a_2 a_3$  with the sum of the 20 permuted products of  $\{a_1, a_1, a_1, a_2, a_3\}$ replace  $a_1^2 a_2^3$  with the sum of the 20 permuted products of  $\{a_1, a_1, a_2, a_2, a_2\}$ 

which would at the very least require sharp notational innovation. Whether a workable theory of "Bell polynomials with non-commutative arguments" can be devised, I do not know (seems likely). Whether such a tool would have useful quantum-theotetic applications I also do not know, but am reminded once again that it was from a quantum field-theoretic discussion<sup>4</sup> that I first became aware of Bell's invention.