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The Baker–Campbell–Hausdorff formula and nested commutator identities

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Neil Some sequences!

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The coefficients of the Baker–Campbell–Hausdorff expansion are calculated by using various methods. Comparison of the results yields several remarkable identities satisfied by multiple commutators, which, in turn, allow us to greatly simplify the form of the expansion up to order eight.

I. INTRODUCTION

The Baker–Campbell–Hausdorff (BCH) formula for Z in $\exp X \exp Y = \exp Z$, where X and Y are noncommuting operators, is of great interest for many problems of quantum and statistical mechanics. When X and Y commute with $[X,Y]$, we have the well-known result $Z = X + Y + \frac{1}{2}[X,Y]$. The generalization of this formula has been extensively discussed in the mathematical literature[1] since Campbell, Baker, and Hausdorff[2] considered, a long time ago, the problem of finding an explicit expression for Z. The solution is given as an infinite series of nested commutators of X and Y.

Several methods have been proposed to compute the terms in the BCH expansion. Thus Weiss and Maradudin,[3] and Magnus[4] have calculated Z up to the fifth order by hand while Richtmyer and Greenspan carried the expansion out to the tenth order by computer.[5] They reported however just a few terms because they are not all linearly independent (due to the Jacobi identity) and therefore the coefficients are not of much direct significance. Recently, Maltay[6] has reported the BCH series up to seventh order. The linear independence is guaranteed for he uses the so-called Lyndon's basis[7] of this algebra. Some different bases have also been proposed in the literature.[8] However, if we do not insist in using the concept of basis then it is possible to put the expansion in a shorter form. This is just our goal. We treat the question of writing the higher orders in the BCH expansion in a shortened form.

We have investigated the series expansion of Z with a number of different algorithms. Comparison of the results furnishes some higher-order identities between multiple commutators that induce many cancellations among the terms initially obtained. This leads to a much more compact expression of Z up to the eighth order. In Sec. II and III we shortly introduce the methods used for determining the successive terms in the BCH expansion. Section IV contains some new identities involving higher-order nested commutators and a reduced BCH formula up to order eight. A comparison with the method of polar derivatives is given in Sec. V. Finally, Sec. VI contains some comments and the conclusions.

II. BCH COEFFICIENTS ACCORDING TO GOLDBERG AND DYNKIN

The major result of Goldberg's work[9] is a formula for the coefficients in the formal power series for $\log(e^X e^Y)$. Following his notation we write the general term beginning with a power of X in a formal series expansion as

$$W_X = W_X(s_1,\dots,s_m) = X^{s_1} Y^{s_2} X^{s_3} \cdots, \tag{2.1}$$

and we denote the coefficient of the word W_X by $C_X(s_1,\dots,s_m)$. Here, we assume $s_1,\dots,s_m \neq 0$. Here, W_Y and C_Y are similarly defined.

Goldberg succeeded in obtaining a general integral representation for the coefficients C_X and C_Y:

$$C_X(s_1,\dots,s_m) = (-1)^{n-1} C_Y = \int_0^1 dt\, t^{m'} (t-1)^{m''} \prod_{i=1}^{m} G_{s_i}(t), \tag{2.2}$$

where

$$n = \sum_{i=1}^{m} s_i, \quad m' = \frac{m}{2}, \quad m'' = \frac{m-1}{2},$$

and the polynomials $G_k(t)$ are defined recursively by $G_1(t) = 1$ and $kG_k(t) = (d/dt)[t(t-1)G_{k-1}(t)]$ for $k \geqslant 2$. A method to compute easily these coefficients is developed in Appendix A, whereas a large table of numerical values has been built up by Newman and Thompson.[10]

Thus the Goldberg's commutator-free series reads

$$Z = \sum [C_X(s_1,\dots,s_m) W_X(s_1,\dots,s_m) + C_Y(s_1,\dots,s_m) W_Y(s_1,\dots,s_m)]. \tag{2.3}$$

On another side, a powerful algorithm due to Dynkin[11] allows us to provide Eq. (2.3) with a commutator structure. To this end we define an iterated commutator denoted by a curly bracket:

$$\{X^k, Y\} = \underbrace{[X,[\cdots[X}_{k},Y]\cdots]], \quad \{X^0, Y\} = Y. \tag{2.4}$$

Dynkin's theorem states that a general word, say $W_X(s_1,\dots,s_m)$, may be replaced by

$$[(-1)^{n-1}/n]\{\cdots\{X^{s_3},\{Y^{s_2},X^{s_1}\}\}\},$$

where $n = \Sigma_{i=1}^{m} s_i$ and $s_1 = 1$. The same is valid for W_Y. This important result allows us to write

$$Z = \sum \frac{(-1)^{n-1}}{n} C_X(1,s_2,\dots,s_m)\{\cdots\{X^{s_3},\{Y^{s_2},X\}\}\} + \sum \frac{(-1)^{n-1}}{n} C_Y(1,s_2,\dots,s_m)\{\cdots\{Y^{s_3},\{X^{s_2},Y\}\}\}. \tag{2.5}$$

Here, $n = 1 + \Sigma_{i=2}^{m} s_i$. Equation (2.5) has been used to compute numerically the coefficients in the BCH expansion.

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TABLE II. Total number n_t of nontrivial commutators for successive orders n in the BCH expansion. The corresponding number n_G of nonvanishing Goldberg coefficients (C_X or C_Y) is also given.

n	1	2	3	4	5	6	7	8	9	10
n_t	2	1	2	4	8	16	32	64	128	256
n_G	1	1	2	1	8	7	32	31	96	97

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Eqs. (3.7) and (3.8), can be expressed in terms of those defined by Goldberg. Thus Eqs. (3.7) and (3.8) are equivalent to

$$Z=\sum \frac{(-1)^{n-1}}{n_Y} C_Y(1,s_2,\ldots,s_m)\{\cdots\{Y^{s_3},\{X^{s_2},Y\}\}\} \tag{4.1}$$

and

$$Z=\sum \frac{(-1)^{n-1}}{n_X} C_X(1,s_2,\ldots,s_m)\{\cdots\{X^{s_3},\{Y^{s_2},X\}\}\}, \tag{4.2}$$

respectively. Here, $n=n_X+n_Y$. Equations (4.1) and (4.2) are true at least up to tenth order. Notice that Eq. (2.5) has a symmetric structure with respect to X and Y, unlike Eqs. (4.1) and (4.2). It is just this fact that can be used to simplify the BCH series. Since X and Y are two generic operators the average of terms containing a certain number, say n_X and n_Y, of operators X and Y, respectively, must be right the same in both Eqs. (4.1) and (4.2). One can, therefore, choose the simplest one of them in order to build up a shorter formula. This is the first simplifier ingredient. A second one results from comparison between the solutions furnished by Eqs. (2.5), (4.1), and (4.2). It provides some interesting identities satisfied by higher-order multiple commutators. The simplest one is

$$\{X,\{Y,\{X,Y\}\}\}=\{Y,\{X^2,Y\}\}=-\{X,\{Y^2,X\}\}. \tag{4.3}$$

Another identity, already found by Baker,[2] reads

$$\{X,\{Y^4,X\}\}-2\{Y,\{X,\{Y^3,X\}\}\}$$
$$+\{Y^2,\{X,\{Y^2,X\}\}\}=0. \tag{4.4}$$

We have been able to derive the following generalization of Eqs. (4.3) and (4.4) for the case of multiple commutators of even order $2n$ ($n>0$):

$$\sum_{k=0}^{n}\binom{n}{k}(-1)^k\{Y^k,\{X,\{Y^{2n-k-2},X\}\}\}=0. \tag{4.5}$$

Here, $\binom{n}{k}$ are the usual binomial coefficients. A short proof of Eq. (4.5) is given in Appendix B. Another useful identity with six operators reads:

$$\{X^2,\{Y^3,X\}\}-3\{X,\{Y,\{X,\{Y^2,X\}\}\}\}$$
$$+3\{Y,\{X^2,\{Y^2,X\}\}\}-\{Y^2,\{X^2,\{Y,X\}\}\}=0. \tag{4.6}$$

Reduction in the number of nonvanishing terms appearing in Table II has been carried out by using the above identities. Table III contains the coefficients of the BCH formula, after reduction, up to the eighth order. The central column stands for the powers involved in each commutator, with the convention that the rightmost operator is always Y. For instance, the term "2131" represents $\{X^2,\{Y,\{X^3,Y\}\}\}$. An asterisk indicates that the symmetric term (i.e., with all the X and Y interchanged) has to be added with the same coefficient. Thus in the above example we eventually get $(\{Y^2,\{X,\{Y^3,X\}\}\}+\{X^2,\{Y,\{X^3,Y\}\}\})/2520$. The final coefficients are all inverse integers and Table III gives just the denominators. The first four orders coincide with those of Weiss and Maradudin,[3] and Magnus.[4] The fifth-order contribution agrees with that of Magnus' paper, while Eq. (3.15) in Ref. 3 is incomplete (one easily checks that the term $\{X^4,Y\}$ is needed in order to restore symmetry).

The procedure followed in reducing the number of

TABLE III. Final structure of the BCH expansion up to order eight. All the coefficients C are inverse integers. Hence, the third column of the table stands for the inverses C^{-1}. The structure of the nested commutators is given by the central column. The rightmost operator is always a single Y. This is labeled "1" and the following numbers indicate how many (alternating) X and Y operators appear in each nested commutator. An asterisk means that for each term the symmetric one (i.e., with all X and Y's interchanged) has to be added with the same coefficient.

n	$\cdots XY$	C^{-1}
1*	1	1
2	11	2
3*	21	12
4	1111	−24
5*	1121	−120
	131	360
	41	−720
6	1311	1440
	2211	−720
	1221	240
	141	1440
7*	61	30240
	151	−10080
	2131	2520
	421	10080
	11221	−1680
	21121	−3360
	331	7560
	11131	−1260
	241	3360
8	1511	−60480
	2411	20160
	121211	−5040
	1421	20160
	161	−60480
	251	−20160
	12131	5040
	13121	−20160
	1331	15120
	121121	−6720
	111221	−3360
	3311	120960
	2321	−5040